
CmdStanPy Documentation

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Stan Development Team

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CmdStanPy is a lightweight interface to Stan for Python users which provides the necessary objects and functions to do Bayesian inference given a probability model and data. It wraps the [CmdStan](#) command line interface in a small set of Python classes which provide methods to do analysis and manage the resulting set of model, data, and posterior estimates.

INSTALLATION

CmdStanPy is a pure-Python3 package which wraps CmdStan, the command-line interface to Stan which is written in C++. Therefore, in addition to Python3, CmdStanPy requires a modern C++ toolchain in order to build and run Stan models. There are several ways to install CmdStanPy and the underlying CmdStan components.

- You can download CmdStanPy, CmdStan, and the C++ toolchain from conda-forge.
- You can download the CmdStanPy package from PyPI using `pip`.
- If you want the current development version, you can clone the GitHub [CmdStanPy](#) repository.

If you install CmdStanPy from PyPI or GitHub you will need to install CmdStan as well, see section [CmdStan Installation](#) below.

1.1 Conda: install CmdStanPy, CmdStan, C++ toolchain

If you use [conda](#), you can install CmdStanPy and the underlying CmdStan components from the [conda-forge](#) repository via the following command:

```
conda create -n stan -c conda-forge cmdstanpy
```

This command creates a new conda environment named `stan` and downloads and installs the `cmdstanpy` package as well as CmdStan and the required C++ toolchain.

To install into an existing environment, use the `conda install` command instead of `create`:

```
conda install -c conda-forge cmdstanpy
```

Whichever installation method you use, afterwards you must activate the new environment or deactivate/activate the existing one. For example, if you installed `cmdstanpy` into a new environment `stan`, run the command

```
conda activate stan
```

By default, the latest release of CmdStan is installed. If you require a specific release of CmdStan, CmdStan versions 2.26.1 and *newer* can be installed by specifying `cmdstan==VERSION` in the install command. Versions before 2.26.1 are not available from conda but can be downloaded from the CmdStan [releases](#) page.

A Conda environment is a directory that contains a specific collection of Conda packages. To see the locations of your conda environments, use the command

```
conda info -e
```

The shell environment variable `CONDA_PREFIX` points to the active conda environment (if any). Both CmdStan and the C++ toolchain are installed into the `bin` subdirectory of the conda environment directory, i.e., `$CONDA_PREFIX/bin/cmdstan` (Linux, MacOS), `%CONDA_PREFIX%\bin\cmdstan` (Windows).

1.2 PyPI: install package CmdStanPy

CmdStan can also be installed from PyPI via URL: <https://pypi.org/project/cmdstanpy/> or from the command line using `pip`:

```
pip install --upgrade cmdstanpy
```

The optional packages are

- `xarray`, an n-dimension labeled dataset package which can be used for outputs

To install CmdStanPy with all the optional packages:

```
pip install --upgrade cmdstanpy[all]
```

1.3 GitHub: install from the CmdStanPy repository

To install the current develop branch from GitHub:

```
pip install -e git+https://github.com/stan-dev/cmdstanpy@develop#egg=cmdstanpy
```

Note: Note for PyStan & RTools users: PyStan and CmdStanPy should be installed in separate environments if you are using the RTools toolchain (primarily Windows users). If you already have PyStan installed, you should take care to install CmdStanPy in its own virtual environment.

Jupyter notebook users: If you intend to run CmdStanPy from within a Jupyter notebook, you may need to install the `ipywidgets`. This will allow for progress bars implemented using the `tqdm` to display properly in the browser. For further help on Jupyter notebook installation and configuration, see [ipywidgets installation instructions](#) and [this tqdm GitHub issue](#).

1.4 CmdStan Installation

If you have installed CmdStanPy from PyPI or Github, **you must install CmdStan**. The recommended way to do so is via the `install_cmdstan` function *described below*.

If you installed CmdStanPy with conda, CmdStan and the C++ toolchain, both CmdStan and the C++ toolchain are installed into directory `$CONDA_PREFIX/bin` and you don't need to do any further installs.

1.4.1 C++ Toolchain Requirements

To compile a Stan program requires a modern C++ compiler and the GNU-Make build utility. These vary by operating system.

Linux The required C++ compiler is `g++ 4.9.3`. On most systems the GNU-Make utility is pre-installed and is the default make utility. There is usually a pre-installed C++ compiler as well, but not necessarily new enough.

MacOS The Xcode and Xcode command line tools must be installed. Xcode is available for free from the Mac App Store. To install the Xcode command line tools, run the shell command: `xcode-select --install`.

Windows We recommend using the [RTools 4.0](#) toolchain which contains a `g++ 8` compiler and `Mingw`, the native Windows equivalent of the GNU-Make utility. This can be installed along with CmdStan when you invoke the function `cmdstanpy.install_cmdstan()` with argument `compiler=True`.

1.4.2 Function `install_cmdstan`

CmdStanPy provides the function `cmdstanpy.install_cmdstan()` which downloads CmdStan from GitHub and builds the CmdStan utilities. It can be called from within Python or from the command line. The default install location is a hidden directory in the user `$HOME` directory named `.cmdstan`. This directory will be created by the install script. On Windows, the `compiler` option will install the C++ toolchain.

- From Python

```
import cmdstanpy
cmdstanpy.install_cmdstan()
cmdstanpy.install_cmdstan(compiler=True)  # only valid on Windows
```

- From the command line on Linux or MacOSX

```
install_cmdstan
ls -F ~/.cmdstan
```

- On Windows

```
install_cmdstan --compiler
dir "%HOME%/.cmdstan"
```

The argument `--interactive` (or `-i`) can be used to run the installation script in an interactive prompt. This will ask you about the various options to the installation script, with reasonable defaults set for all questions.

The named arguments: `-d <directory>` and `-v <version>` can be used to override these defaults:

```
install_cmdstan -d my_local_cmdstan -v 2.33.0
ls -F my_local_cmdstan
```

1.4.2.1 Alternate Linux Architectures

CmdStan can be installed on Linux for the following non-x86 architectures: arm64, armel, armhf, mips64el, ppc64el and s390x.

CmdStanPy will do its best to determine which of these is applicable for your machine when running `install_cmdstan`. If the wrong choice is made, or if you need to manually override this, you can set the `CMDSTAN_ARCH` environment variable to one of the above options, or to “false” to use the standard x86 download.

1.4.3 DIY Installation

If you wish to install CmdStan yourself, follow the instructions in the [CmdStan User’s Guide](#).

1.5 Locating the CmdStan installation directory

CmdStanPy uses the environment variable `CMDSTAN` to register the CmdStan installation location.

- If you use conda to install CmdStanPy, CmdStan is installed into location `$CONDA_PREFIX/bin/cmdstan` (Linux, MacOS), `%CONDA_PREFIX%\bin\cmdstan` (Windows) and the environment variable `CMDSTAN` is set accordingly.
- If no environment variable `CMDSTAN` is set, CmdStanPy will try to locate a CmdStan installation in the default install location, which is a directory named `.cmdstan` in your `$HOME` directory.

If you have installed CmdStan from a GitHub release or by cloning the CmdStan repository, you will need to set this location, either via the `CMDSTAN` environment variable, or via the CmdStanPy command `set_cmdstan_path`

```
from cmdstanpy import cmdstan_path, set_cmdstan_path

set_cmdstan_path(os.path.join('path', 'to', 'cmdstan'))
cmdstan_path()
```

USER'S GUIDE

This section provides examples and some narrative description about the usage of CmdStanPy.

2.1 Overview

CmdStanPy is a lightweight interface to [Stan](#) for Python. It provides a small set of classes and methods for doing Bayesian inference given a probability model and data. With CmdStanPy, you can:

- Compile a Stan model.
- Do inference on the model conditioned on the data, using one of Stan inference algorithms
 - Exact Bayesian estimation using the [NUTS-HMC sampler](#).
 - Approximate Bayesian estimation algorithms [Pathfinder](#) and [ADVI](#).
 - MAP estimation by [optimization](#).
- Generate new quantities of interest from a model given an existing sample.
- Manage the resulting inference engine outputs: extract information, summarize results, and save the outputs.

CmdStanPy wraps the [CmdStan](#) file-based command line interface. It is lightweight in that it uses minimal memory beyond the memory used by CmdStan, thus CmdStanPy has the potential to fit more complex models to larger datasets than might be possible in PyStan or RStan.

CmdStanPy is designed to support the development, testing, and deployment of a Stan model. CmdStanPy manages the Stan program files, data files, and CmdStan output files. By default, output files are written to a temporary filesystem which persists throughout the session. This is appropriate behavior during model development because it allows the user to test many models without filesystem clutter or worse. Once deployed into production, the user can specify the output directory for the CmdStan outputs.

2.2 “Hello, World!”

2.2.1 Fitting a Stan model using the NUTS-HMC sampler

In order to verify the installation and also to demonstrate the CmdStanPy workflow, we use CmdStanPy to fit the example Stan model `bernoulli.stan` to the dataset `bernoulli.data.json`. The `bernoulli.stan` is a [Hello, World!](#) program which illustrates the basic syntax of the Stan language. It allows the user to verify that CmdStanPy, CmdStan, the StanC compiler, and the C++ toolchain have all been properly installed.

For substantive example models and guidance on coding statistical models in Stan, see the [Stan User's Guide](#).

2.2.1.1 The Stan model

The model `bernoulli.stan` is a trivial model: given a set of N observations of i.i.d. binary data $y[1] \dots y[N]$, it calculates the Bernoulli chance-of-success θ .

```
data {  
  int<lower=0> N;  
  array[N] int<lower=0,upper=1> y;  
}  
parameters {  
  real<lower=0,upper=1> theta;  
}  
model {  
  theta ~ beta(1,1); // uniform prior on interval 0,1  
  y ~ bernoulli(theta);  
}
```

The `CmdStanModel` class manages the Stan program and its corresponding compiled executable. It provides properties and functions to inspect the model code and filepaths. A `CmdStanModel` can be instantiated from a Stan file or its corresponding compiled executable file.

```
# import packages  
In [1]: import os  
  
In [2]: from cmdstanpy import CmdStanModel  
  
# specify Stan program file  
In [3]: stan_file = os.path.join('users-guide', 'examples', 'bernoulli.stan')  
  
# instantiate the model object  
In [4]: model = CmdStanModel(stan_file=stan_file)  
  
# inspect model object  
In [5]: print(model)  
CmdStanModel: name=bernoulli  
    stan_file=/home/docs/checkouts/readthedocs.org/user_builds/cmdstanpy/checkouts/  
↳ v1.2.2/docsrc/users-guide/examples/bernoulli.stan  
    exe_file=/home/docs/checkouts/readthedocs.org/user_builds/cmdstanpy/checkouts/  
↳ v1.2.2/docsrc/users-guide/examples/bernoulli  
    compiler_options=stanc_options={}, cpp_options={}  
  
# inspect compiled model  
In [6]: print(model.exe_info())  
{'stan_version_major': '2', 'stan_version_minor': '34', 'stan_version_patch': '1', 'STAN_  
↳ THREADS': 'false', 'STAN_MPI': 'false', 'STAN_OPENCL': 'false', 'STAN_NO_RANGE_CHECKS':  
↳ 'false', 'STAN_CPP_OPTIMS': 'false'}
```

2.2.1.2 Data inputs

CmdStanPy accepts input data either as a Python dictionary which maps data variable names to values, or as the corresponding JSON file.

The bernoulli model requires two inputs: the number of observations N , and an N -length vector y of binary outcomes. The data file *bernoulli.data.json* contains the following inputs:

```
{
  "N" : 10,
  "y" : [0,1,0,0,0,0,0,0,0,1]
}
```

2.2.1.3 Fitting the model

The `sample()` method is used to do Bayesian inference over the model conditioned on data using using Hamiltonian Monte Carlo (HMC) sampling. It runs Stan’s HMC-NUTS sampler on the model and data and returns a `CmdStanMCMC` object. The data can be specified either as a filepath or a Python dictionary; in this example, we use the example datafile *bernoulli.data.json*: By default, the `sample` method runs 4 sampler chains.

```
# specify data file
In [7]: data_file = os.path.join('users-guide', 'examples', 'bernoulli.data.json')

# fit the model
In [8]: fit = model.sample(data=data_file)
INFO:cmdstanpy:CmdStan start processing

↳
↳
↳
INFO:cmdstanpy:CmdStan done processing.
```

Note this model can be fit using other methods

- the `pathfinder()` method does approximate Bayesian inference and returns a `CmdStanPathfinder` object
- the `variational()` method does approximate Bayesian inference and returns a `CmdStanVB` object
- the `optimize()` method does maximum likelihood estimation and returns a `CmdStanMLE` object

2.2.1.4 Accessing the results

The sampler outputs are the set of per-chain [Stan CSV files](#), a non-standard CSV file format. Each data row of the Stan CSV file contains the per-iteration estimate of the Stan model parameters, transformed parameters, and generated quantities variables. Container variables, i.e., vector, row-vector, matrix, and array variables are necessarily serialized into a single row’s worth of data. The output objects parse the set of Stan CSV files into a set of in-memory data structures and provide accessor functions for the all estimates and metadata. CmdStanPy makes a distinction between the per-iteration model outputs and the per-iteration algorithm outputs: the former are ‘stan_variables’ and the latter are ‘method_variables’.

The `CmdStanMCMC` object provides the following accessor methods:

- `stan_variable()`: returns an `numpy.ndarray` whose structure corresponds to the Stan program variable structure

- `stan_variables()`: returns a Python dictionary mapping the Stan program variable names to the corresponding numpy.ndarray.
- `draws()`: returns a numpy.ndarray which is either a 3-D array draws X chains X CSV columns, or a 2-D array draws X columns, where the chains are concatenated into a single column. The argument `vars` can be used to restrict this to just the columns for one or more variables.
- `draws_pd()`: returns a pandas.DataFrame over all columns in the Stan CSV file. The argument `vars` can be used to restrict this to one or more variables.
- `draws_xr()`: returns an xarray.Dataset which maps model variable names to their respective values. The argument `vars` can be used to restrict this to one or more variables.
- `method_variables()`: returns a Python dictionary over the sampler diagnostic/information output columns which by convention end in `__`, e.g., `lp__`.

```
# access model variable by name
In [9]: print(fit.stan_variable('theta'))
[0.253209 0.298111 0.306112 ... 0.402509 0.282059 0.120912]

In [10]: print(fit.draws_pd('theta')[:3])
      theta
0  0.253209
1  0.298111
2  0.306112

In [11]: print(fit.draws_xr('theta'))
<xarray.Dataset> Size: 40kB
Dimensions: (draw: 1000, chain: 4)
Coordinates:
  * chain    (chain) int64 32B 1 2 3 4
  * draw     (draw) int64 8kB 0 1 2 3 4 5 6 7 ... 993 994 995 996 997 998 999
Data variables:
  theta      (chain, draw) float64 32kB 0.2532 0.2981 0.3061 ... 0.2821 0.1209
Attributes:
  stan_version:      2.34.1
  model:             bernoulli_model
  num_draws_sampling: 1000

# access all model variables
In [12]: for k, v in fit.stan_variables().items():
...:     print(f'{k}\t{v.shape}')
...:
theta      (4000,)
```

```
# access the sampler method variables
In [13]: for k, v in fit.method_variables().items():
...:     print(f'{k}\t{v.shape}')
...:
lp__       (1000, 4)
accept_stat__ (1000, 4)
stepsize__  (1000, 4)
treedepth__ (1000, 4)
n_leapfrog__ (1000, 4)
divergent__ (1000, 4)
```

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```
energy__          (1000, 4)

# access all Stan CSV file columns
In [14]: print(f'numpy.ndarray of draws: {fit.draws().shape}')
numpy.ndarray of draws: (1000, 4, 8)

In [15]: fit.draws_pd()
Out[15]:
```

	chain__	iter__	draw__	...	divergent__	energy__	theta
0	1.0	1.0	1.0	...	0.0	6.75309	0.253209
1	1.0	2.0	2.0	...	0.0	7.08622	0.298111
2	1.0	3.0	3.0	...	0.0	6.86392	0.306112
3	1.0	4.0	4.0	...	0.0	7.02012	0.343846
4	1.0	5.0	5.0	...	0.0	7.52434	0.412824
...
3995	4.0	996.0	3996.0	...	0.0	7.42391	0.371617
3996	4.0	997.0	3997.0	...	0.0	7.97460	0.467119
3997	4.0	998.0	3998.0	...	0.0	7.86343	0.402509
3998	4.0	999.0	3999.0	...	0.0	7.24115	0.282059
3999	4.0	1000.0	4000.0	...	0.0	8.13725	0.120912

```
[4000 rows x 11 columns]
```

In addition to the MCMC sample itself, the CmdStanMCMC object provides access to the the per-chain HMC tuning parameters from the NUTS-HMC adaptive sampler, (if present).

```
In [16]: print(fit.metric_type)
diag_e

In [17]: print(fit.metric)
[[0.480061]
 [0.437506]
 [0.455099]
 [0.546715]]

In [18]: print(fit.step_size)
[1.13609  1.17629  0.811687 0.871036]
```

The CmdStanMCMC object also provides access to metadata about the model and the sampler run.

```
In [19]: print(fit.metadata.cmdstan_config['model'])
bernoulli_model

In [20]: print(fit.metadata.cmdstan_config['seed'])
24464
```

2.2.1.5 CmdStan utilities: `stansummary`, `diagnose`

CmdStan is distributed with a posterior analysis utility `stansummary` that reads the outputs of all chains and computes summary statistics for all sampler and model parameters and quantities of interest. The `CmdStanMCMC.summary()` runs this utility and returns summaries of the total joint log-probability density `lp__` plus all model parameters and quantities of interest in a `pandas.DataFrame`:

```
In [21]: fit.summary()
Out[21]:
```

	Mean	MCSE	StdDev	...	N_Eff	N_Eff/s	R_hat
lp__	-7.268160	0.019029	0.738517	...	1506.17	22480.2	1.00105
theta	0.250803	0.002983	0.119304	...	1599.35	23870.8	1.00090

[2 rows x 9 columns]

CmdStan is distributed with a second posterior analysis utility `diagnose` which analyzes the per-draw sampler parameters across all chains looking for potential problems which indicate that the sample isn't a representative sample from the posterior. The `diagnose()` method runs this utility and prints the output to the console.

```
In [22]: print(fit.diagnose())
Processing csv files: /tmp/tmpndo2bp00/bernoullijalxxvtf/bernoulli-20240326163641_1.csv, ↵
↵ /tmp/tmpndo2bp00/bernoullijalxxvtf/bernoulli-20240326163641_2.csv, /tmp/tmpndo2bp00/
↵ bernoullijalxxvtf/bernoulli-20240326163641_3.csv, /tmp/tmpndo2bp00/bernoullijalxxvtf/
↵ bernoulli-20240326163641_4.csv

Checking sampler transitions treedepth.
Treedepth satisfactory for all transitions.

Checking sampler transitions for divergences.
No divergent transitions found.

Checking E-BFMI - sampler transitions HMC potential energy.
E-BFMI satisfactory.

Effective sample size satisfactory.

Split R-hat values satisfactory all parameters.

Processing complete, no problems detected.
```

2.3 CmdStanPy Workflow

The statistical modeling enterprise has two principal modalities: development and production. The focus of development is model building, comparison, and validation. Many models are written and fitted to many kinds of data. The focus of production is using a trusted model on real-world data to obtain estimates for decision-making. In both modalities, the essential workflow remains the same: compile a Stan model, assemble input data, do inference on the model conditioned on the data, and validate, access, and export the results.

Model development and testing is an open-ended process, usually requiring many iterations of developing a model, fitting the data, and evaluating the results. Since more user time is spent in model development, CmdStanPy defaults favor development mode. CmdStan is file-based interface. On the assumption that model development will require many successive runs of a model, by default, outputs are written to a temporary directory to avoid filling up the filesystem.

tem with unneeded CmdStan output files. Non-default options allow all filepaths to be fully specified so that scripts can be used to distribute analysis jobs across nodes and machines.

The Bayesian workflow for model comparison and model expansion provides a framework for model development, much of which also applies to monitoring model performance in production. The following sections describe the process of building, running, and managing the resulting inference for a single model and set of inputs.

2.3.1 Compile the Stan model

The `CmdStanModel` class provides methods to compile and run the Stan program. A `CmdStanModel` object can be instantiated by specifying either a Stan file or the executable file, or both. If only the Stan file path is specified, the constructor will check for the existence of a correspondingly named exe file in the same directory. If found, it will use this as the exe file path.

By default, when a `CmdStanModel` object is instantiated from a Stan file, the constructor will compile the model as needed. The constructor argument `compile` controls this behavior.

- `compile=False`: never compile the Stan file.
- `compile="Force"`: always compile the Stan file.
- `compile=True`: (default) compile the Stan file as needed, i.e., if no exe file exists or if the Stan file is newer than the exe file.

```
import os
from cmdstanpy import CmdStanModel

my_stanfile = os.path.join('.', 'my_model.stan')
my_model = CmdStanModel(stan_file=my_stanfile)
my_model.name
my_model.stan_file
my_model.exe_file
my_model.code()
```

The `CmdStanModel` class also provides the `compile()` method, which can be called at any point to (re)compile the model as needed.

Model compilation is carried out via the GNU Make build tool. The CmdStan `makefile` contains a set of general rules which specify the dependencies between the Stan program and the Stan platform components and low-level libraries. Optional behaviors can be specified by use of variables which are passed in to the make command as name, value pairs.

Model compilation is done in two steps:

- The `stanc` compiler translates the Stan program to C++.
- The C++ compiler compiles the generated code and links in the necessary supporting libraries.

Therefore, both the constructor and the `compile` method allow optional arguments `stanc_options` and `cpp_options` which specify options for each compilation step. Options are specified as a Python dictionary mapping compiler option names to appropriate values.

In order parallelize within-chain computations using the Stan language `reduce_sum` function, or to parallelize running the NUTS-HMC sampler across chains, the Stan model must be compiled with C++ compiler flag `STAN_THREADS`. While any value can be used, we recommend the value `True`, e.g.:

```
import os
from cmdstanpy import CmdStanModel
```

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```
my_stanfile = os.path.join('.', 'my_model.stan')
my_model = CmdStanModel(stan_file=my_stanfile, cpp_options={'STAN_THREADS': 'true'})
```

2.3.2 Assemble input and initialization data

CmdStan is file-based interface, therefore all model input and initialization data must be supplied as JSON files, as described in the [CmdStan User's Guide](#).

CmdStanPy inference methods allow inputs and initializations to be specified as in-memory Python dictionary objects which are then converted to JSON via the utility function `cmdstanpy.write_stan_json()`. This method should be used to create JSON input files whenever these inputs contain either a collection compatible with numpy arrays or pandas.Series.

2.3.3 Run the CmdStan inference engine

For each CmdStan inference method, there is a corresponding method on the `CmdStanModel` class. An example of each is provided in the [next section](#).

- The `sample()` method runs Stan's [HMC-NUTS sampler](#).
It returns a `CmdStanMCMC` object which contains a sample from the posterior distribution of the model conditioned on the data.
- The `pathfinder()` method runs Stan's [Pathfinder Variational Inference algorithm](#).
It returns a `CmdStanPathfinder` object which contains a sample from a Gaussian approximation the posterior distribution.
- The `variational()` method runs Stan's [Automatic Differentiation Variational Inference \(ADVI\) algorithm](#).
It returns a `CmdStanVB` object which contains an approximation the posterior distribution.
- The `optimize()` runs one of Stan's [optimization algorithms](#) to find a mode of the density specified by the Stan program.
It returns a `CmdStanMLE` object.
- The `generate_quantities()` method runs Stan's [generate_quantities method](#), which generates additional quantities of interest from a mode. Its take an existing fit as input and uses the parameter estimates in the fit to run the Stan program's [generated quantities block](#).
It returns a `CmdStanGQ` object.

2.3.4 Validate, view, export the inference engine outputs

The inference method-specific results objects `CmdStanMCMC`, `CmdStanPathfinder`, `CmdStanVB`, `CmdStanMLE`, and `CmdStanGQ` contain the CmdStan method configuration information and the location of all output files produced. The provide a common set methods for accessing the inference results and metadata, as well as method-specific informational properties and methods.objects

2.3.4.1 Output data

The resulting Stan CSV file or set of files are assembled into an inference result object.

- `CmdStanMCMC` object contains the `sample()` outputs
- `CmdStanPathfinder` object contains the `pathfinder()` outputs
- `CmdStanVB` object contains the `variational()` outputs
- `CmdStanMLE` object contains the `optimize()` outputs
- `CmdStanGQ` object contains the `generate_quantities()` outputs

The objects provide accessor methods which return this information either as tabular data (i.e., in terms of the per-chain CSV file rows and columns), or as structured objects which correspond to the variables in the Stan model and the individual diagnostics produced by the inference method.

The `stan_variables` method returns a Python dict over all Stan model variables, see `stan_variables()`.

The `stan_variable` method returns a single model variable as a `numpy.ndarray` object with the same structure (per draw) as the Stan program variable, see `stan_variable()`.

The `method_variables` method returns a Python dict over all inference method variables, cf `method_variables()`

The output from the methods `CmdStanMCMC` and `CmdStanGQ` return the sample contents in tabular form, see `draws()` and `draws_pd()`. Similarly, the `draws_xr()` method returns the sample contents as an `xarray.Dataset` which is a mapping from variable names to their respective values.

2.4 Controlling Outputs

2.4.1 CSV File Outputs

Underlyingly, the CmdStan outputs are a set of per-chain Stan CSV files. The filenames follow the template ‘<model_name>-<YYYYMMDDHHMMSS>-<chain_id>’ plus the file suffix ‘.csv’. CmdStanPy also captures the per-chain console and error messages.

```
In [1]: import os

In [2]: from cmdstanpy import CmdStanModel

In [3]: stan_file = os.path.join('users-guide', 'examples', 'bernoulli.stan')

In [4]: model = CmdStanModel(stan_file=stan_file)

In [5]: data_file = os.path.join('users-guide', 'examples', 'bernoulli.data.json')

In [6]: fit = model.sample(data=data_file)
INFO:cmdstanpy:CmdStan start processing

↳
↳
↳
INFO:cmdstanpy:CmdStan done processing.

# printing the object reports sampler commands, output files
```

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```
In [7]: print(fit)
CmdStanMCMC: model=bernoulli chains=4['method=sample', 'algorithm=hmc', 'adapt',
↳ 'engaged=1']
csv_files:
    /tmp/tmpndo2bp00/bernoullix2ehgmcu/bernoulli-20240326163642_1.csv
    /tmp/tmpndo2bp00/bernoullix2ehgmcu/bernoulli-20240326163642_2.csv
    /tmp/tmpndo2bp00/bernoullix2ehgmcu/bernoulli-20240326163642_3.csv
    /tmp/tmpndo2bp00/bernoullix2ehgmcu/bernoulli-20240326163642_4.csv
output_files:
    /tmp/tmpndo2bp00/bernoullix2ehgmcu/bernoulli-20240326163642_0-stdout.txt
    /tmp/tmpndo2bp00/bernoullix2ehgmcu/bernoulli-20240326163642_1-stdout.txt
    /tmp/tmpndo2bp00/bernoullix2ehgmcu/bernoulli-20240326163642_2-stdout.txt
    /tmp/tmpndo2bp00/bernoullix2ehgmcu/bernoulli-20240326163642_3-stdout.txt
```

The `output_dir` argument is an optional argument which specifies the path to the output directory used by CmdStan. If this argument is omitted, the output files are written to a temporary directory which is deleted when the current Python session is terminated.

```
In [8]: fit = model.sample(data=data_file, output_dir="./outputs/")
INFO:cmdstanpy:created output directory: /home/docs/checkouts/readthedocs.org/user_
↳ builds/cmdstanpy/checkouts/v1.2.2/docsrsrc/outputs
INFO:cmdstanpy:CmdStan start processing
```

```
↳
↳
↳
INFO:cmdstanpy:CmdStan done processing.
```

```
In [9]: !ls outputs/
bernoulli-20240326163642_0-stdout.txt  bernoulli-20240326163642_2.csv
bernoulli-20240326163642_1-stdout.txt  bernoulli-20240326163642_3-stdout.txt
bernoulli-20240326163642_1.csv          bernoulli-20240326163642_3.csv
bernoulli-20240326163642_2-stdout.txt  bernoulli-20240326163642_4.csv
```

Alternatively, the `save_csvfiles()` function moves the CSV files to a specified directory.

```
In [10]: fit = model.sample(data=data_file)
INFO:cmdstanpy:CmdStan start processing
```

```
↳
↳
↳
INFO:cmdstanpy:CmdStan done processing.
```

```
In [11]: fit.save_csvfiles(dir='some/path')
```

```
In [12]: !ls some/path
bernoulli-20240326163642_1.csv          bernoulli-20240326163642_3.csv
bernoulli-20240326163642_2.csv          bernoulli-20240326163642_4.csv
```

2.4.2 Logging

You may notice CmdStanPy can produce a lot of output when it is running:

```
In [13]: fit = model.sample(data=data_file, show_progress=False)
INFO:cmdstanpy:CmdStan start processing
INFO:cmdstanpy:Chain [1] start processing
INFO:cmdstanpy:Chain [2] start processing
INFO:cmdstanpy:Chain [1] done processing
INFO:cmdstanpy:Chain [3] start processing
INFO:cmdstanpy:Chain [2] done processing
INFO:cmdstanpy:Chain [4] start processing
INFO:cmdstanpy:Chain [3] done processing
INFO:cmdstanpy:Chain [4] done processing
```

This output is managed through the built-in `logging` module. For example, it can be disabled entirely:

```
In [14]: import logging

In [15]: cmdstanpy_logger = logging.getLogger("cmdstanpy")

In [16]: cmdstanpy_logger.disabled = True

# look, no output!
In [17]: fit = model.sample(data=data_file, show_progress=False)
```

Or one can remove the logging handler that CmdStanPy installs by default and install their own for more fine-grained control. For example, the following code sends all logs (including the DEBUG logs, which are hidden by default), to a file.

DEBUG logging is useful primarily to developers or when trying to hunt down an issue.

```
In [18]: cmdstanpy_logger.disabled = False

# remove all existing handlers
In [19]: cmdstanpy_logger.handlers = []

In [20]: cmdstanpy_logger.setLevel(logging.DEBUG)

In [21]: handler = logging.FileHandler('all.log')

In [22]: handler.setLevel(logging.DEBUG)

In [23]: handler.setFormatter(
....:     logging.Formatter(
....:         '%(asctime)s - %(name)s - %(levelname)s - %(message)s',
....:         "%H:%M:%S",
....:     )
....: )
....:

In [24]: cmdstanpy_logger.addHandler(handler)
```

Now, if we run the model and check the contents of the file, we will see all the possible logging.

```

In [25]: fit = model.sample(data=data_file, show_progress=False)

In [26]: with open('all.log','r') as logs:
.....:     for line in logs.readlines():
.....:         print(line.strip())
.....:
16:36:44 - cmdstanpy - DEBUG - cmd: /home/docs/checkouts/readthedocs.org/user_builds/
↳cmdstanpy/checkouts/v1.2.2/docsrc/users-guide/examples/bernoulli info
cwd: None
16:36:44 - cmdstanpy - INFO - CmdStan start processing
16:36:44 - cmdstanpy - DEBUG - idx 0
16:36:44 - cmdstanpy - DEBUG - idx 1
16:36:44 - cmdstanpy - DEBUG - running CmdStan, num_threads: 1
16:36:44 - cmdstanpy - DEBUG - running CmdStan, num_threads: 1
16:36:44 - cmdstanpy - DEBUG - CmdStan args: ['/home/docs/checkouts/readthedocs.org/user_
↳builds/cmdstanpy/checkouts/v1.2.2/docsrc/users-guide/examples/bernoulli', 'id=1',
↳'random', 'seed=79006', 'data', 'file=users-guide/examples/bernoulli.data.json',
↳'output', 'file=/tmp/tmpndo2bp00/bernoullit__gejhg/bernoulli-20240326163644_1.csv',
↳'method=sample', 'algorithm=hmc', 'adapt', 'engaged=1']
16:36:44 - cmdstanpy - DEBUG - CmdStan args: ['/home/docs/checkouts/readthedocs.org/user_
↳builds/cmdstanpy/checkouts/v1.2.2/docsrc/users-guide/examples/bernoulli', 'id=2',
↳'random', 'seed=79006', 'data', 'file=users-guide/examples/bernoulli.data.json',
↳'output', 'file=/tmp/tmpndo2bp00/bernoullit__gejhg/bernoulli-20240326163644_2.csv',
↳'method=sample', 'algorithm=hmc', 'adapt', 'engaged=1']
16:36:44 - cmdstanpy - INFO - Chain [1] start processing
16:36:44 - cmdstanpy - INFO - Chain [2] start processing
16:36:44 - cmdstanpy - INFO - Chain [1] done processing
16:36:44 - cmdstanpy - DEBUG - idx 2
16:36:44 - cmdstanpy - DEBUG - running CmdStan, num_threads: 1
16:36:44 - cmdstanpy - DEBUG - CmdStan args: ['/home/docs/checkouts/readthedocs.org/user_
↳builds/cmdstanpy/checkouts/v1.2.2/docsrc/users-guide/examples/bernoulli', 'id=3',
↳'random', 'seed=79006', 'data', 'file=users-guide/examples/bernoulli.data.json',
↳'output', 'file=/tmp/tmpndo2bp00/bernoullit__gejhg/bernoulli-20240326163644_3.csv',
↳'method=sample', 'algorithm=hmc', 'adapt', 'engaged=1']
16:36:44 - cmdstanpy - INFO - Chain [3] start processing
16:36:44 - cmdstanpy - INFO - Chain [2] done processing
16:36:44 - cmdstanpy - DEBUG - idx 3
16:36:44 - cmdstanpy - DEBUG - running CmdStan, num_threads: 1
16:36:44 - cmdstanpy - DEBUG - CmdStan args: ['/home/docs/checkouts/readthedocs.org/user_
↳builds/cmdstanpy/checkouts/v1.2.2/docsrc/users-guide/examples/bernoulli', 'id=4',
↳'random', 'seed=79006', 'data', 'file=users-guide/examples/bernoulli.data.json',
↳'output', 'file=/tmp/tmpndo2bp00/bernoullit__gejhg/bernoulli-20240326163644_4.csv',
↳'method=sample', 'algorithm=hmc', 'adapt', 'engaged=1']
16:36:44 - cmdstanpy - INFO - Chain [4] start processing
16:36:44 - cmdstanpy - INFO - Chain [3] done processing
16:36:44 - cmdstanpy - INFO - Chain [4] done processing
16:36:44 - cmdstanpy - DEBUG - runset
RunSet: chains=4, chain_ids=[1, 2, 3, 4], num_processes=4
cmd (chain 1):
['/home/docs/checkouts/readthedocs.org/user_builds/cmdstanpy/checkouts/v1.2.2/docsrc/
↳users-guide/examples/bernoulli', 'id=1', 'random', 'seed=79006', 'data', 'file=users-
↳guide/examples/bernoulli.data.json', 'output', 'file=/tmp/tmpndo2bp00/bernoullit__
↳gejhg/bernoulli-20240326163644_1.csv', 'method=sample', 'algorithm=hmc', 'adapt',

```

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```

→ 'engaged=1']
retcodes=[0, 0, 0, 0]
per-chain output files (showing chain 1 only):
csv_file:
/tmp/tmpndo2bp00/bernoullit__gejhg/bernoulli-20240326163644_1.csv
console_msgs (if any):
/tmp/tmpndo2bp00/bernoullit__gejhg/bernoulli-20240326163644_0-stdout.txt
16:36:44 - cmdstanpy - DEBUG - Chain 1 console:
method = sample (Default)
sample
num_samples = 1000 (Default)
num_warmup = 1000 (Default)
save_warmup = 0 (Default)
thin = 1 (Default)
adapt
engaged = 1 (Default)
gamma = 0.05 (Default)
delta = 0.8 (Default)
kappa = 0.75 (Default)
t0 = 10 (Default)
init_buffer = 75 (Default)
term_buffer = 50 (Default)
window = 25 (Default)
save_metric = 0 (Default)
algorithm = hmc (Default)
hmc
engine = nuts (Default)
nuts
max_depth = 10 (Default)
metric = diag_e (Default)
metric_file = (Default)
stepsize = 1 (Default)
stepsize_jitter = 0 (Default)
num_chains = 1 (Default)
id = 1 (Default)
data
file = users-guide/examples/bernoulli.data.json
init = 2 (Default)
random
seed = 79006
output
file = /tmp/tmpndo2bp00/bernoullit__gejhg/bernoulli-20240326163644_1.csv
diagnostic_file = (Default)
refresh = 100 (Default)
sig_figs = -1 (Default)
profile_file = profile.csv (Default)
save_cmdstan_config = 0 (Default)
num_threads = 1 (Default)

```

Gradient evaluation took 4e-06 seconds
 1000 transitions using 10 leapfrog steps per transition would take 0.04 seconds.

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Adjust your expectations accordingly!

```

Iteration:    1 / 2000 [ 0%] (Warmup)
Iteration:   100 / 2000 [ 5%] (Warmup)
Iteration:   200 / 2000 [10%] (Warmup)
Iteration:   300 / 2000 [15%] (Warmup)
Iteration:   400 / 2000 [20%] (Warmup)
Iteration:   500 / 2000 [25%] (Warmup)
Iteration:   600 / 2000 [30%] (Warmup)
Iteration:   700 / 2000 [35%] (Warmup)
Iteration:   800 / 2000 [40%] (Warmup)
Iteration:   900 / 2000 [45%] (Warmup)
Iteration:  1000 / 2000 [50%] (Warmup)
Iteration:  1001 / 2000 [50%] (Sampling)
Iteration:  1100 / 2000 [55%] (Sampling)
Iteration:  1200 / 2000 [60%] (Sampling)
Iteration:  1300 / 2000 [65%] (Sampling)
Iteration:  1400 / 2000 [70%] (Sampling)
Iteration:  1500 / 2000 [75%] (Sampling)
Iteration:  1600 / 2000 [80%] (Sampling)
Iteration:  1700 / 2000 [85%] (Sampling)
Iteration:  1800 / 2000 [90%] (Sampling)
Iteration:  1900 / 2000 [95%] (Sampling)
Iteration:  2000 / 2000 [100%] (Sampling)

```

```

Elapsed Time: 0.006 seconds (Warm-up)
0.016 seconds (Sampling)
0.022 seconds (Total)

```

2.5 CmdStanPy Examples

2.5.1 MCMC Sampling

2.5.1.1 Overview

Stan's MCMC sampler implements the Hamiltonian Monte Carlo (HMC) algorithm and its adaptive variant the no-U-turn sampler (NUTS). It creates a set of draws from the posterior distribution of the model conditioned on the data, allowing for exact Bayesian inference of the model parameters. Each draw consists of the values for all parameter, transformed parameter, and generated quantities variables, reported on the constrained scale.

The `CmdStanModel.sample` method wraps the `CmdStan.sample` method. Underlyingly, the `CmdStan` outputs are a set of per-chain Stan CSV files. In addition to the resulting sample, reported as one row per draw, the Stan CSV files encode information about the inference engine configuration and the sampler state. The NUTS-HMC adaptive sampler algorithm also outputs the per-chain HMC tuning parameters `step_size` and `metric`.

The `sample` method returns a `CmdStanMCMC` object, which provides access to the disparate information from the Stan CSV files. Accessor functions allow the user to access the sample in whatever data format is needed for further analysis, either as tabular data (i.e., in terms of the per-chain CSV file rows and columns), or as structured objects which correspond to the variables in the Stan model and the individual diagnostics produced by the inference method.

- The `stan_variable` and `stan_variables` methods return a Python `numpy.ndarray` containing all draws from the sample where the structure of each draw corresponds to the structure of the Stan variable.
- The `draws` method returns the sample as either a 2-D or 3-D `numpy.ndarray`.
- The `draws_pd` method returns the entire sample or selected variables as a `pandas.DataFrame`.
- The `draws_xr` method returns a structured Xarray dataset over the Stan model variables.
- The `method_variables` returns a Python dict over all sampler method variables.

In addition, the `CmdStanMCMC` object has accessor methods for

- The per-chain HMC tuning parameters `step_size` and `metric`
- The CmdStan run configuration and console outputs
- The mapping between the Stan model variables and the corresponding CSV file columns.

Notebook prerequisites

CmdStanPy displays progress bars during sampling via use of package `tqdm`. In order for these to display properly in a Jupyter notebook, you must have the `ipywidgets` package installed. For more information, see the [installation instructions](#), also [this tqdm GitHub issue](#).

2.5.1.2 Fitting the model and data

In this example we use the CmdStan example model `bernoulli.stan` and data file `bernoulli.data.json`.

We instantiate a `CmdStanModel` from the Stan program file

```
[5]: import os
      from cmdstanpy import CmdStanModel

      # instantiate, compile bernoulli model
      model = CmdStanModel(stan_file='bernoulli.stan')
```

By default, the model is compiled during instantiation. The compiled executable is created in the same directory as the program file. If the directory already contains an executable file with a newer timestamp, the model is not recompiled.

We run the sampler on the data using all default settings: 4 chains, each of which runs 1000 warmup and sampling iterations.

```
[6]: # run CmdStan's sample method, returns object `CmdStanMCMC`
      fit = model.sample(data='bernoulli.data.json')
```

```
16:17:55 - cmdstanpy - INFO - CmdStan start processing
```

```
chain 1 |           | 00:00 Status
```

```
chain 2 |           | 00:00 Status
```

```
chain 3 |           | 00:00 Status
```

```
chain 4 |           | 00:00 Status
```

```
16:17:56 - cmdstanpy - INFO - CmdStan done processing.
```

The CmdStanMCMC object records the command, the return code, and the paths to the sampler output csv and console files. The sample is lazily instantiated on first access of either the draws or the HMC tuning parameters, i.e., the step size and metric.

The string representation of this object displays the CmdStan commands and the location of the output files. Output filenames are composed of the model name, a timestamp in the form YYYYMMDDhhmmss and the chain id, plus the corresponding filetype suffix, either '.csv' for the CmdStan output or '.txt' for the console messages, e.g. bernoulli-20220617170100_1.csv.

```
[7]: fit
```

```
[7]: CmdStanMCMC: model=bernoulli chains=4[method=sample, 'algorithm=hmc', 'adapt',
↪ 'engaged=1']
  csv_files:
    /var/folders/db/4jnggnf549s42z50bd61jskm0000gq/T/tmp0w4tqjfy/bernoulli1_4b9oav/
↪ bernoulli-20230925161756_1.csv
    /var/folders/db/4jnggnf549s42z50bd61jskm0000gq/T/tmp0w4tqjfy/bernoulli1_4b9oav/
↪ bernoulli-20230925161756_2.csv
    /var/folders/db/4jnggnf549s42z50bd61jskm0000gq/T/tmp0w4tqjfy/bernoulli1_4b9oav/
↪ bernoulli-20230925161756_3.csv
    /var/folders/db/4jnggnf549s42z50bd61jskm0000gq/T/tmp0w4tqjfy/bernoulli1_4b9oav/
↪ bernoulli-20230925161756_4.csv
  output_files:
    /var/folders/db/4jnggnf549s42z50bd61jskm0000gq/T/tmp0w4tqjfy/bernoulli1_4b9oav/
↪ bernoulli-20230925161756_0-stdout.txt
    /var/folders/db/4jnggnf549s42z50bd61jskm0000gq/T/tmp0w4tqjfy/bernoulli1_4b9oav/
↪ bernoulli-20230925161756_1-stdout.txt
    /var/folders/db/4jnggnf549s42z50bd61jskm0000gq/T/tmp0w4tqjfy/bernoulli1_4b9oav/
↪ bernoulli-20230925161756_2-stdout.txt
    /var/folders/db/4jnggnf549s42z50bd61jskm0000gq/T/tmp0w4tqjfy/bernoulli1_4b9oav/
↪ bernoulli-20230925161756_3-stdout.txt
```

```
[8]: print(f'draws as array: {fit.draws().shape}')
print(f'draws as structured object:\n\t{fit.stan_variables().keys()}')
print(f'sampler diagnostics:\n\t{fit.method_variables().keys()}')
```

```
draws as array: (1000, 4, 8)
draws as structured object:
  dict_keys(['theta'])
sampler diagnostics:
  dict_keys(['lp__', 'accept_stat__', 'stepsize__', 'treedepth__', 'n_leapfrog__',
↪ 'divergent__', 'energy__'])
```

Sampler Progress

Your model may take a long time to fit. The `sample` method provides two arguments:

- visual progress bar: `show_progress=True`
- stream CmdStan output to the console - `show_console=True`

By default, CmdStanPy displays a progress bar during sampling, as seen above. Since the progress bars are only visible while the sampler is running and the bernoulli example model takes no time at all to fit, we run this model for 200K iterations, in order to see the progress bars in action.

```
[9]: fit = model.sample(data='bernoulli.data.json', iter_warmup=100000, iter_sampling=100000,
↳ show_progress=True)
```

```
16:17:57 - cmdstanpy - INFO - CmdStan start processing
```

```
chain 1 |          | 00:00 Status
```

```
chain 2 |          | 00:00 Status
```

```
chain 3 |          | 00:00 Status
```

```
chain 4 |          | 00:00 Status
```

```
16:17:59 - cmdstanpy - INFO - CmdStan done processing.
```

To see the CmdStan console outputs instead of progress bars, specify `show_console=True`. This will stream all CmdStan messages to the terminal while the sampler is running. This option will allow you to debug a Stan program using the Stan language `print` statement.

```
[10]: fit = model.sample(data='bernoulli.data.json', chains=2, parallel_chains=1, show_
↳ console=True)
```

```
16:18:00 - cmdstanpy - INFO - Chain [1] start processing
```

```
16:18:00 - cmdstanpy - INFO - Chain [1] done processing
```

```
16:18:00 - cmdstanpy - INFO - Chain [2] start processing
```

```
16:18:00 - cmdstanpy - INFO - Chain [2] done processing
```

```
Chain [1] method = sample (Default)
```

```
Chain [1] sample
```

```
Chain [1] num_samples = 1000 (Default)
```

```
Chain [1] num_warmup = 1000 (Default)
```

```
Chain [1] save_warmup = 0 (Default)
```

```
Chain [1] thin = 1 (Default)
```

```
Chain [1] adapt
```

```
Chain [1] engaged = 1 (Default)
```

```
Chain [1] gamma = 0.050000000000000003 (Default)
```

```
Chain [1] delta = 0.80000000000000004 (Default)
```

```
Chain [1] kappa = 0.75 (Default)
```

```
Chain [1] t0 = 10 (Default)
```

```
Chain [1] init_buffer = 75 (Default)
```

```
Chain [1] term_buffer = 50 (Default)
```

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```

Chain [1] window = 25 (Default)
Chain [1] algorithm = hmc (Default)
Chain [1] hmc
Chain [1] engine = nuts (Default)
Chain [1] nuts
Chain [1] max_depth = 10 (Default)
Chain [1] metric = diag_e (Default)
Chain [1] metric_file = (Default)
Chain [1] stepsize = 1 (Default)
Chain [1] stepsize_jitter = 0 (Default)
Chain [1] num_chains = 1 (Default)
Chain [1] id = 1 (Default)
Chain [1] data
Chain [1] file = bernoulli.data.json
Chain [1] init = 2 (Default)
Chain [1] random
Chain [1] seed = 42783
Chain [1] output
Chain [1] file = /var/folders/db/4jnggnf549s42z50bd61jskm0000gq/T/tmp0w4tqjfy/
↳ bernoullibjig91zd/bernoulli-20230925161800_1.csv
Chain [1] diagnostic_file = (Default)
Chain [1] refresh = 100 (Default)
Chain [1] sig_figs = -1 (Default)
Chain [1] profile_file = profile.csv (Default)
Chain [1] num_threads = 1 (Default)
Chain [1]
Chain [1]
Chain [1] Gradient evaluation took 6e-06 seconds
Chain [1] 1000 transitions using 10 leapfrog steps per transition would take 0.06_
↳ seconds.
Chain [1] Adjust your expectations accordingly!
Chain [1]
Chain [1]
Chain [1] Iteration:    1 / 2000 [  0%] (Warmup)
Chain [1] Iteration:   100 / 2000 [  5%] (Warmup)
Chain [1] Iteration:   200 / 2000 [ 10%] (Warmup)
Chain [1] Iteration:   300 / 2000 [ 15%] (Warmup)
Chain [1] Iteration:   400 / 2000 [ 20%] (Warmup)
Chain [1] Iteration:   500 / 2000 [ 25%] (Warmup)
Chain [1] Iteration:   600 / 2000 [ 30%] (Warmup)
Chain [1] Iteration:   700 / 2000 [ 35%] (Warmup)
Chain [1] Iteration:   800 / 2000 [ 40%] (Warmup)
Chain [1] Iteration:   900 / 2000 [ 45%] (Warmup)
Chain [1] Iteration:  1000 / 2000 [ 50%] (Warmup)
Chain [1] Iteration:  1001 / 2000 [ 50%] (Sampling)
Chain [1] Iteration:  1100 / 2000 [ 55%] (Sampling)
Chain [1] Iteration:  1200 / 2000 [ 60%] (Sampling)
Chain [1] Iteration:  1300 / 2000 [ 65%] (Sampling)
Chain [1] Iteration:  1400 / 2000 [ 70%] (Sampling)
Chain [1] Iteration:  1500 / 2000 [ 75%] (Sampling)
Chain [1] Iteration:  1600 / 2000 [ 80%] (Sampling)
Chain [1] Iteration:  1700 / 2000 [ 85%] (Sampling)

```

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```

Chain [1] Iteration: 1800 / 2000 [ 90%] (Sampling)
Chain [1] Iteration: 1900 / 2000 [ 95%] (Sampling)
Chain [1] Iteration: 2000 / 2000 [100%] (Sampling)
Chain [1]
Chain [1] Elapsed Time: 0.004 seconds (Warm-up)
Chain [1] 0.012 seconds (Sampling)
Chain [1] 0.016 seconds (Total)
Chain [1]
Chain [1]
Chain [2] method = sample (Default)
Chain [2] sample
Chain [2] num_samples = 1000 (Default)
Chain [2] num_warmup = 1000 (Default)
Chain [2] save_warmup = 0 (Default)
Chain [2] thin = 1 (Default)
Chain [2] adapt
Chain [2] engaged = 1 (Default)
Chain [2] gamma = 0.050000000000000003 (Default)
Chain [2] delta = 0.80000000000000004 (Default)
Chain [2] kappa = 0.75 (Default)
Chain [2] t0 = 10 (Default)
Chain [2] init_buffer = 75 (Default)
Chain [2] term_buffer = 50 (Default)
Chain [2] window = 25 (Default)
Chain [2] algorithm = hmc (Default)
Chain [2] hmc
Chain [2] engine = nuts (Default)
Chain [2] nuts
Chain [2] max_depth = 10 (Default)
Chain [2] metric = diag_e (Default)
Chain [2] metric_file = (Default)
Chain [2] stepsize = 1 (Default)
Chain [2] stepsize_jitter = 0 (Default)
Chain [2] num_chains = 1 (Default)
Chain [2] id = 2
Chain [2] data
Chain [2] file = bernoulli.data.json
Chain [2] init = 2 (Default)
Chain [2] random
Chain [2] seed = 42783
Chain [2] output
Chain [2] file = /var/folders/db/4jnggnf549s42z50bd61jskm0000gq/T/tmp0w4tqjfy/
↳ bernoullibjig91zd/bernoulli-20230925161800_2.csv
Chain [2] diagnostic_file = (Default)
Chain [2] refresh = 100 (Default)
Chain [2] sig_figs = -1 (Default)
Chain [2] profile_file = profile.csv (Default)
Chain [2] num_threads = 1 (Default)
Chain [2]
Chain [2]
Chain [2] Gradient evaluation took 6e-06 seconds
Chain [2] 1000 transitions using 10 leapfrog steps per transition would take 0.06_

```

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```

↪seconds.
Chain [2] Adjust your expectations accordingly!
Chain [2]
Chain [2]
Chain [2] Iteration:    1 / 2000 [  0%] (Warmup)
Chain [2] Iteration:   100 / 2000 [  5%] (Warmup)
Chain [2] Iteration:   200 / 2000 [ 10%] (Warmup)
Chain [2] Iteration:   300 / 2000 [ 15%] (Warmup)
Chain [2] Iteration:   400 / 2000 [ 20%] (Warmup)
Chain [2] Iteration:   500 / 2000 [ 25%] (Warmup)
Chain [2] Iteration:   600 / 2000 [ 30%] (Warmup)
Chain [2] Iteration:   700 / 2000 [ 35%] (Warmup)
Chain [2] Iteration:   800 / 2000 [ 40%] (Warmup)
Chain [2] Iteration:   900 / 2000 [ 45%] (Warmup)
Chain [2] Iteration:  1000 / 2000 [ 50%] (Warmup)
Chain [2] Iteration:  1001 / 2000 [ 50%] (Sampling)
Chain [2] Iteration:  1100 / 2000 [ 55%] (Sampling)
Chain [2] Iteration:  1200 / 2000 [ 60%] (Sampling)
Chain [2] Iteration:  1300 / 2000 [ 65%] (Sampling)
Chain [2] Iteration:  1400 / 2000 [ 70%] (Sampling)
Chain [2] Iteration:  1500 / 2000 [ 75%] (Sampling)
Chain [2] Iteration:  1600 / 2000 [ 80%] (Sampling)
Chain [2] Iteration:  1700 / 2000 [ 85%] (Sampling)
Chain [2] Iteration:  1800 / 2000 [ 90%] (Sampling)
Chain [2] Iteration:  1900 / 2000 [ 95%] (Sampling)
Chain [2] Iteration:  2000 / 2000 [100%] (Sampling)
Chain [2]
Chain [2] Elapsed Time: 0.004 seconds (Warm-up)
Chain [2] 0.012 seconds (Sampling)
Chain [2] 0.016 seconds (Total)
Chain [2]
Chain [2]

```

2.5.1.3 Checking the fit

The first question to ask of the `CmdStanMCMC` object is: *is this a valid sample from the posterior?*

It is important to check whether or not the sampler was able to fit the model given the data. Often, this is not possible, for any number of reasons. To appreciate the sampler diagnostics, we use a hierarchical model which, given a small amount of data, encounters difficulty: the centered parameterization of the “8-schools” model (Rubin, 1981). The “8-schools” model is a simple hierarchical model, first developed on a dataset taken from an experiment was conducted in 8 schools, with only treatment effects and their standard errors reported.

The Stan model and the original dataset are in files `eight_schools.stan` and `eight_schools.data.json`.

`eight_schools.stan`

```

[11]: with open('eight_schools.stan', 'r') as fd:
      print(fd.read())

data {
  int<lower=0> J; // number of schools
  array[J] real y; // estimated treatment effect (school j)

```

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```

    array[J] real<lower=0> sigma; // std err of effect estimate (school j)
}
parameters {
    real mu;
    array[J] real theta;
    real<lower=0> tau;
}
model {
    theta ~ normal(mu, tau);
    y ~ normal(theta, sigma);
}

```

eight_schools.data.json

```
[12]: with open('eight_schools.data.json', 'r') as fd:
      print(fd.read())
```

```

{
  "J" : 8,
  "y" : [28,8,-3,7,-1,1,18,12],
  "sigma" : [15,10,16,11,9,11,10,18],
  "tau" : 25
}

```

Because there is not much data, the geometry of posterior distribution is highly curved, thus the sampler may encounter difficulty in fitting the model. By specifying the initial seed for the pseudo-random number generator, we insure that the sampler will have difficulty in fitting this model. In particular, some post-warmup iterations diverge, resulting in a biased sample. In addition, some post-warmup iterations hit the maximum allowed treedepth before the trajectory hits the “U-turn” condition of the NUTS algorithm, in which case the sampler may fail to properly explore the entire posterior.

These diagnostics are checked for automatically at the end of each run; if problems are detected, a WARNING message is logged.

```
[13]: eight_schools_model = CmdStanModel(stan_file='eight_schools.stan')
      eight_schools_fit = eight_schools_model.sample(data='eight_schools.data.json',
      ↪seed=55157)
```

```
16:18:01 - cmdstanpy - INFO - CmdStan start processing
```

```
chain 1 |          | 00:00 Status
```

```
chain 2 |          | 00:00 Status
```

```
chain 3 |          | 00:00 Status
```

```
chain 4 |          | 00:00 Status
```

```
16:18:01 - cmdstanpy - INFO - CmdStan done processing.
```

```
16:18:01 - cmdstanpy - WARNING - Some chains may have failed to converge.
```

```
    Chain 1 had 10 divergent transitions (1.0%)
```

```
    Chain 2 had 143 divergent transitions (14.3%)
```

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```
Chain 3 had 5 divergent transitions (0.5%)
Chain 4 had 4 divergent transitions (0.4%)
Chain 4 had 6 iterations at max treedepth (0.6%)
Use the "diagnose()" method on the CmdStanMCMC object to see further information.
```

More information on how to address convergence problems can be found at <https://mc-stan.org/misc/warnings>

The number of post-warmup divergences and iterations which hit the maximum treedepth can be inspected directly via properties `divergences` and `max_treedepths`.

```
[14]: print(f'divergences:\n{eight_schools_fit.divergences}\niterations at max_treedepth:\n
      ↪{eight_schools_fit.max_treedepths}')
```

```
divergences:
[ 10 143   5   4]
iterations at max_treedepth:
[0 0 0 6]
```

Summarizing the sample

The `summary` method reports the R-hat statistic, a measure of how well the sampler chains have converged.

```
[15]: eight_schools_fit.summary()
```

```
[15]:
```

	Mean	MCSE	StdDev	5%	50%	95%	\
lp__	-16.47510	1.393830	7.33884	-26.342300	-17.71920	-5.82214	
mu	7.36580	0.358441	5.36980	-0.090157	6.98708	16.39460	
theta[1]	11.02040	0.693969	8.59668	0.398902	9.67094	27.12670	
theta[2]	7.44547	0.222970	6.32424	-2.193170	6.77458	18.33640	
theta[3]	5.46814	0.230146	7.65499	-7.436710	5.20094	17.52600	
theta[4]	7.07208	0.257662	6.80149	-3.296620	6.58401	18.50130	
theta[5]	4.59664	0.193292	6.13195	-6.067650	4.04537	14.53360	
theta[6]	5.69326	0.199079	6.77053	-5.402900	5.30265	16.48680	
theta[7]	10.04950	0.628118	7.10079	0.675246	9.17402	23.36110	
theta[8]	7.84009	0.291526	8.04207	-4.016420	7.00731	21.58680	
tau	6.60333	0.557360	5.77492	1.019850	5.21419	17.68580	

	N_Eff	N_Eff/s	R_hat
lp__	27.72280	37.87270	1.12057
mu	224.43000	306.59800	1.03328
theta[1]	153.45500	209.63800	1.03967
theta[2]	804.49900	1099.04000	1.01501
theta[3]	1106.33000	1511.38000	1.00842
theta[4]	696.79800	951.91000	1.01756
theta[5]	1006.39000	1374.85000	1.00407
theta[6]	1156.63000	1580.09000	1.00729
theta[7]	127.80000	174.59100	1.03588
theta[8]	760.99400	1039.61000	1.01463
tau	107.35287	146.65692	1.04858

Sampler Diagnostics

The `diagnose()` method provides more information about the sample.

```
[16]: print(eight_schools_fit.diagnose())
```

```
Processing csv files: /var/folders/db/4jnggnf549s42z50bd61jskm0000gq/T/tmp0w4tqjfy/eight_
↳ schoolsz56j88wq/eight_schools-20230925161801_1.csv, /var/folders/db/
↳ 4jnggnf549s42z50bd61jskm0000gq/T/tmp0w4tqjfy/eight_schoolsz56j88wq/eight_schools-
↳ 20230925161801_2.csv, /var/folders/db/4jnggnf549s42z50bd61jskm0000gq/T/tmp0w4tqjfy/
↳ eight_schoolsz56j88wq/eight_schools-20230925161801_3.csv, /var/folders/db/
↳ 4jnggnf549s42z50bd61jskm0000gq/T/tmp0w4tqjfy/eight_schoolsz56j88wq/eight_schools-
↳ 20230925161801_4.csv

Checking sampler transitions treedepth.
6 of 4000 (0.15%) transitions hit the maximum treedepth limit of 10, or 2^10 leapfrog
↳ steps.
Trajectories that are prematurely terminated due to this limit will result in slow
↳ exploration.
For optimal performance, increase this limit.

Checking sampler transitions for divergences.
162 of 4000 (4.05%) transitions ended with a divergence.
These divergent transitions indicate that HMC is not fully able to explore the posterior
↳ distribution.
Try increasing adapt delta closer to 1.
If this doesn't remove all divergences, try to reparameterize the model.

Checking E-BFMI - sampler transitions HMC potential energy.
The E-BFMI, 0.18, is below the nominal threshold of 0.30 which suggests that HMC may
↳ have trouble exploring the target distribution.
If possible, try to reparameterize the model.

Effective sample size satisfactory.

Split R-hat values satisfactory all parameters.

Processing complete.
```

2.5.1.4 Accessing the sampler outputs

```
[17]: fit = model.sample(data='bernoulli.data.json')
```

```
16:18:09 - cmdstanpy - INFO - CmdStan start processing
```

```
chain 1 |          | 00:00 Status
```

```
chain 2 |          | 00:00 Status
```

```
chain 3 |          | 00:00 Status
```

```
chain 4 |          | 00:00 Status
```

```
16:18:09 - cmdstanpy - INFO - CmdStan done processing.
```

Extracting the draws as structured Stan program variables

Per-variable draws can be accessed as either a `numpy.ndarray` object via method `stan_variable` or as an `xarray.Dataset` object via `draws_xr`.

```
[18]: print(fit.stan_variable('theta'))  
[0.187637 0.167524 0.454131 ... 0.506709 0.14154 0.333167]
```

The `stan_variables` method returns a Python dict over all Stan variables in the output.

```
[19]: for k, v in fit.stan_variables().items():  
      print(f'name: {k}, shape: {v.shape}')  
name: theta, shape: (4000,)
```

```
[20]: print(fit.draws_xr('theta'))  
  
<xarray.Dataset>  
Dimensions: (draw: 1000, chain: 4)  
Coordinates:  
  * chain    (chain) int64 1 2 3 4  
  * draw     (draw) int64 0 1 2 3 4 5 6 7 8 ... 992 993 994 995 996 997 998 999  
Data variables:  
  theta     (chain, draw) float64 0.1876 0.1675 0.4541 ... 0.5067 0.1415 0.3332  
Attributes:  
  stan_version:      2.33.0  
  model:             bernoulli_model  
  num_draws_sampling: 1000
```

Extracting the draws in tabular format

The sample can be accessed either as a `numpy` array or a `pandas DataFrame`:

```
[21]: import xarray as x  
  
[22]: print(f'sample as ndarray: {fit.draws().shape}\nfirst 2 draws, chain 1:\n{fit.draws()[0, :2, :]}')  
sample as ndarray: (1000, 4, 8)  
first 2 draws, chain 1:  
[[-6.89001  0.981831 0.870591 1.          1.          0.          6.89017  
  0.187637]  
 [-7.01004  0.849367 0.870591 2.          3.          0.          8.19459  
  0.167524]]  
  
[23]: fit.draws_pd().head()
```

```
[23]:
```

	chain__	iter__	draw__	lp__	accept_stat__	stepsize__	treedepth__	\
0	1.0	1.0	1.0	-6.89001	0.981831	0.870591	1.0	
1	1.0	2.0	2.0	-7.01004	0.849367	0.870591	2.0	
2	1.0	3.0	3.0	-7.81650	0.825109	0.870591	1.0	
3	1.0	4.0	4.0	-6.78960	1.000000	0.870591	2.0	
4	1.0	5.0	5.0	-7.21778	0.940115	0.870591	2.0	

	n_leapfrog__	divergent__	energy__	theta
0	1.0	0.0	6.89017	0.187637
1	3.0	0.0	8.19459	0.167524
2	3.0	0.0	8.77706	0.454131
3	3.0	0.0	7.79596	0.215159
4	3.0	0.0	7.32770	0.143557

Extracting sampler method diagnostics

```
[24]: for k, v in fit.method_variables().items():
       print(f'name: {k}, shape: {v.shape}')
```

```
name: lp__, shape: (1000, 4)
name: accept_stat__, shape: (1000, 4)
name: stepsize__, shape: (1000, 4)
name: treedepth__, shape: (1000, 4)
name: n_leapfrog__, shape: (1000, 4)
name: divergent__, shape: (1000, 4)
name: energy__, shape: (1000, 4)
```

Extracting the per-chain HMC tuning parameters

```
[25]: print(f'adapted step_size per chain\n{fit.step_size}\nmetric_type: {fit.metric_type}\n
       ↪metric:\n{fit.metric}')
```

```
adapted step_size per chain
[0.870591 0.97456 1.00695 0.975628]
metric_type: diag_e
metric:
[[0.557946]
 [0.469587]
 [0.567582]
 [0.467572]]
```

Extracting the sample meta-data

```
[26]: print('sample method variables:\n{}\n'.format(fit.metadata.method_vars.keys()))
print('stan model variables:\n{}\n'.format(fit.metadata.stan_vars.keys()))
```

```
sample method variables:
dict_keys(['lp__', 'accept_stat__', 'stepsize__', 'treedepth__', 'n_leapfrog__',
↳ 'divergent__', 'energy__'])

stan model variables:
dict_keys(['theta'])
```

2.5.1.5 Saving the sampler output files

The sampler output files are written to a temporary directory which is deleted upon session exit unless the `output_dir` argument is specified. The `save_csvfiles` function moves the CmdStan CSV output files to a specified directory without having to re-run the sampler. The console output files are not saved. These files are treated as ephemeral; if the sample is valid, all relevant information is recorded in the CSV files.

2.5.1.6 Parallelization via multi-threaded processing

Stan's multi-threaded processing is based on the Intel Threading Building Blocks (TBB) library, which must be linked to by the C++ compiler. To take advantage of this option, you must compile (or recompile) the program with the the C++ compiler option `STAN_THREADS`. The `CmdStanModel` object constructor and its `compile` method both have argument `cpp_options` which takes as its value a dictionary of compiler flags.

We compile the example model `bernoulli.stan`, this time with arguments `cpp_options` and `compile`, and use the function `exe_info()` to check that the model has been compiled for multi-threading.

```
[27]: model = CmdStanModel(stan_file='bernoulli.stan',
                           cpp_options={'STAN_THREADS': 'TRUE'},
                           compile='force')
model.exe_info()
```

```
16:18:21 - cmdstanpy - WARNING - CmdStanModel(compile=...) is deprecated and will be
↳ removed in the next major version. The constructor will always ensure a model has a
↳ compiled executable.
If you wish to force recompilation, use force_compile=True instead.
16:18:21 - cmdstanpy - INFO - compiling stan file /Users/mitzi/github/stan-dev/cmdstanpy/
↳ docsrc/users-guide/examples/bernoulli.stan to exe file /Users/mitzi/github/stan-dev/
↳ cmdstanpy/docsrc/users-guide/examples/bernoulli
16:18:30 - cmdstanpy - INFO - compiled model executable: /Users/mitzi/github/stan-dev/
↳ cmdstanpy/docsrc/users-guide/examples/bernoulli
```

```
[27]: {'stan_version_major': '2',
      'stan_version_minor': '33',
      'stan_version_patch': '0',
      'STAN_THREADS': 'true',
      'STAN_MPI': 'false',
      'STAN_OPENCL': 'false',
      'STAN_NO_RANGE_CHECKS': 'false',
      'STAN_CPP_OPTIMS': 'false'}
```

Cross-chain multi-threading

As of version CmdStan 2.28, it is possible to run the NUTS-HMC sampler on multiple chains from within a single executable using threads. This has the potential to speed up sampling. It also reduces the overall memory footprint required for sampling as all chains share the same copy of data. When using within-chain parallelization all chains started within a single executable can share all the available threads and once a chain finishes the threads will be reused.

The sample program argument `parallel_chains` takes an integer value which specifies how many chains to run in parallel. For models which have been compiled with option `STAN_THREADS` set, all chains are run from within a single process and the value of the `parallel_chains` argument specifies the total number of threads.

```
[28]: fit = model.sample(data='bernoulli.data.json', parallel_chains=4)
```

```
16:18:30 - cmdstanpy - INFO - CmdStan start processing
```

```
chain 1 |          | 00:00 Status
```

```
chain 2 |          | 00:00 Status
```

```
chain 3 |          | 00:00 Status
```

```
chain 4 |          | 00:00 Status
```

```
16:18:30 - cmdstanpy - INFO - CmdStan done processing.
```

Within-chain multi-threading

The Stan language `reduce_sum` function provides within-chain parallelization. For models which require computing the sum of a number of independent function evaluations, e.g., when evaluating a number of conditionally independent terms in a log-likelihood, the `reduce_sum` function is used to parallelize this computation.

To see how this works, we run the “reflag” model, used in the `reduce_sum minimal example` case study. The Stan model and the original dataset are in files “redcard_reduce_sum.stan” and “redcard.json”.

```
[29]: with open('redcard_reduce_sum.stan', 'r') as fd:
      print(fd.read())
```

```
functions {
  real partial_sum(array[] int slice_n_redcards, int start, int end,
                  array[] int n_games, vector rating, vector beta) {
    return binomial_logit_lpmf(slice_n_redcards | n_games[start : end], beta[1]
                                + beta[2]
                                * rating[start :
→end]);
  }
}
data {
  int<lower=0> N;
  array[N] int<lower=0> n_redcards;
  array[N] int<lower=0> n_games;
  vector[N] rating;
  int<lower=1> grainsize;
```

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```

}
parameters {
  vector[2] beta;
}
model {
  beta[1] ~ normal(0, 10);
  beta[2] ~ normal(0, 1);

  target += reduce_sum(partial_sum, n_redcards, grainsize, n_games, rating,
                       beta);
}

```

As before, we compile the model specifying argument `cpp_options`.

```

[30]: redcard_model = CmdStanModel(stan_file='redcard_reduce_sum.stan',
                                   cpp_options={'STAN_THREADS': 'TRUE'},
                                   compile='force')
redcard_model.exe_info()

```

```

16:18:30 - cmdstanpy - WARNING - CmdStanModel(compile=...) is deprecated and will be
→ removed in the next major version. The constructor will always ensure a model has a
→ compiled executable.
If you wish to force recompilation, use force_compile=True instead.
16:18:30 - cmdstanpy - INFO - compiling stan file /Users/mitzi/github/stan-dev/cmdstanpy/
→ docsrc/users-guide/examples/redcard_reduce_sum.stan to exe file /Users/mitzi/github/
→ stan-dev/cmdstanpy/docsrc/users-guide/examples/redcard_reduce_sum
16:18:38 - cmdstanpy - INFO - compiled model executable: /Users/mitzi/github/stan-dev/
→ cmdstanpy/docsrc/users-guide/examples/redcard_reduce_sum

```

```

[30]: {'stan_version_major': '2',
      'stan_version_minor': '33',
      'stan_version_patch': '0',
      'STAN_THREADS': 'true',
      'STAN_MPI': 'false',
      'STAN_OPENCL': 'false',
      'STAN_NO_RANGE_CHECKS': 'false',
      'STAN_CPP_OPTIMS': 'false'}

```

The sample method argument `threads_per_chain` specifies the number of threads allotted to each chain; this corresponds to CmdStan’s `num_threads` argument.

```

[31]: redcard_fit = redcard_model.sample(data='redcard.json', threads_per_chain=4)

```

```

16:18:38 - cmdstanpy - INFO - CmdStan start processing

```

chain 1	00:00 Status
chain 2	00:00 Status
chain 3	00:00 Status
chain 4	00:00 Status


```
16:19:23 - cmdstanpy - INFO - CmdStan done processing.
```

The number of threads to use is passed to the model exe file by means of the shell environment variable `STAN_NUM_THREADS`.

On my machine, which has 4 cores, all 4 chains are run in parallel from within a single process. Therefore, the total number of threads used by this process will be `threads_per_chain * chains`. To check this, we examine the shell environment variable `STAN_NUM_THREADS`.

```
[32]: os.environ['STAN_NUM_THREADS']
```

```
[32]: '16'
```

2.5.2 Maximum Likelihood Estimation

Stan provides optimization algorithms which find modes of the density specified by a Stan program. Three different algorithms are available: a Newton optimizer, and two related quasi-Newton algorithms, BFGS and L-BFGS. The L-BFGS algorithm is the default optimizer. Newton's method is the least efficient of the three, but has the advantage of setting its own stepsize.

In this example we use the CmdStan example model `bernoulli.stan` and data file `bernoulli.data.json`

The `CmdStanModel` class method `optimize` returns a `CmdStanMLE` object which provides properties to retrieve the estimate of the penalized maximum likelihood estimate of all model parameters:

- `column_names`
- `optimized_params_dict`
- `optimized_params_np`
- `optimized_params_pd`

In the following example, we instantiate a model and do optimization using the default CmdStan settings:

```
[1]: import os
from cmdstanpy import CmdStanModel, cmdstan_path

bernoulli_dir = os.path.join(cmdstan_path(), 'examples', 'bernoulli')
stan_file = os.path.join(bernoulli_dir, 'bernoulli.stan')
data_file = os.path.join(bernoulli_dir, 'bernoulli.data.json')

# instantiate, compile bernoulli model
model = CmdStanModel(stan_file=stan_file)

# run CmdStan's optimize method, returns object `CmdStanMLE`
mle = model.optimize(data=data_file)
print(mle.column_names)
print(mle.optimized_params_dict)
mle.optimized_params_pd

16:36:30 - cmdstanpy - INFO - Chain [1] start processing
16:36:30 - cmdstanpy - INFO - Chain [1] done processing

('lp__', 'theta')
OrderedDict([('lp__', -5.00402), ('theta', 0.200004)])
```

```
[1]:      lp__      theta
0 -5.00402  0.200004
```

2.5.3 Variational Inference using Pathfinder

Stan supports the Pathfinder algorithm (Zhang, 2022). Pathfinder is a variational method for approximately sampling from differentiable log densities. Starting from a random initialization, Pathfinder locates normal approximations to the target density along a quasi-Newton optimization path, with local covariance estimated using the negative inverse Hessian estimates produced by the LBFGS optimizer. Pathfinder returns draws from the Gaussian approximation with the lowest estimated Kullback-Leibler (KL) divergence to the true posterior.

There are two Stan implementations of the Pathfinder algorithm: single-path Pathfinder and multi-path Pathfinder. Single-path Pathfinder generates a set of approximate draws from one run of the basic Pathfinder algorithm. Multi-path Pathfinder uses importance resampling over the draws from multiple runs of Pathfinder. This better matches non-normal target densities and also mitigates the problem of L-BFGS getting stuck at local optima or in saddle points on plateaus.

2.5.3.1 Example: variational inference with Pathfinder for model `bernoulli.stan`

The `CmdStanModel` `pathfinder` method wraps the `CmdStan` `pathfinder` method.

By default, CmdStanPy runs multi-path Pathfinder which returns an importance-resampled set of draws over the outputs of 4 independent single-path Pathfinders.

```
[1]: import os
from cmdstanpy.model import CmdStanModel, cmdstan_path
```

```
[2]: bernoulli_dir = os.path.join(cmdstan_path(), 'examples', 'bernoulli')
stan_file = os.path.join(bernoulli_dir, 'bernoulli.stan')
data_file = os.path.join(bernoulli_dir, 'bernoulli.data.json')
# instantiate, compile bernoulli model
model = CmdStanModel(stan_file=stan_file)
# run CmdStan's pathfinder method, returns object `CmdStanPathfinder`
pathfinder = model.pathfinder(data=data_file)
```

```
16:36:32 - cmdstanpy - INFO - Chain [1] start processing
```

```
16:36:32 - cmdstanpy - INFO - Chain [1] done processing
```

```
[3]: print(pathfinder)
print(pathfinder.metadata)
```

```
CmdStanPathfinder: model=bernoulli['method=pathfinder']
csv_files:
  /tmp/tmpvpctn2w2/bernoullieg4eq5bn/bernoulli-20240326163632.csv
output_files:
  /tmp/tmpvpctn2w2/bernoullieg4eq5bn/bernoulli-20240326163632_0-stdout.txt
Metadata:
{'stan_version_major': 2, 'stan_version_minor': 34, 'stan_version_patch': 1, 'model':
  ↳ 'bernoulli_model', 'start_datetime': '2024-03-26 16:36:32 UTC', 'method': 'pathfinder',
  ↳ 'init_alpha': 0.001, 'tol_obj': 1e-12, 'tol_rel_obj': 10000, 'tol_grad': 1e-08, 'tol_
  ↳ rel_grad': 10000000.0, 'tol_param': 1e-08, 'history_size': 5, 'num_psis_draws': 1000,
  ↳ 'num_paths': 4, 'save_single_paths': 0, 'psis_resample': 1, 'calculate_lp': 1, 'max_
  ↳ lbfgs_iters': 1000, 'num_draws': 1000, 'num_elbo_draws': 25, 'id': 1, 'data_file': '/'
```

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```

↪home/docs/checkouts/readthedocs.org/user_builds/cmdstanpy/conda/v1.2.2/bin/cmdstan/
↪examples/bernoulli/bernoulli.data.json', 'init': 2, 'seed': 87080, 'diagnostic_file': '
↪', 'refresh': 100, 'sig_figs': -1, 'profile_file': 'profile.csv', 'save_cmdstan_config
↪': 0, 'num_threads': 1, 'stanc_version': 'stanc3 v2.34.0', 'raw_header': 'lp_approx__
↪lp__,theta', 'column_names': ('lp_approx__', 'lp__', 'theta'))}

```

The pathfinder method returns a `CmdStanPathfinder` object, which provides access to the disparate information from the Stan CSV files.

- The `stan_variable` and `stan_variables` methods return a Python `numpy.ndarray` containing all draws from the sample where the structure of each draw corresponds to the structure of the Stan variable.
- The `draws` method returns the sample as a `numpy.ndarray`.

```
[4]: pathfinder.stan_variable("theta").shape
```

```
[4]: (1000,)
```

```
[5]: pathfinder.column_names
```

```
[5]: ('lp_approx__', 'lp__', 'theta')
```

```
[6]: pathfinder.draws().shape
```

```
[6]: (1000, 3)
```

2.5.3.2 Pathfinders as initialization for the MCMC sampler

The method `create_inits` returns a Python Dict containing a set of per-chain initializations for the model parameters. Each set of initializations is a random draw from the Pathfinder sample. These initializations can be used as the initial parameter values for Stan's NUTS-HMC sampler, which will reduce the number of warmup iterations needed.

```

[7]: inits = pathfinder.create_inits()
      print(inits)

[{'theta': array(0.295191)}, {'theta': array(0.197931)}, {'theta': array(0.351117)}, {
↪ 'theta': array(0.340779)}]

```

The `create_inits` takes two arguments:

- `seed` - used for random selection.
- `chains` - the number of draws to return, default is 4. This should match the number of sampler chains to run.

```

[8]: inits = pathfinder.create_inits(chains=3)
      print(inits)

[{'theta': array(0.235002)}, {'theta': array(0.314922)}, {'theta': array(0.188325)}]

```

2.5.4 Variational Inference using ADVI

Variational inference is a method for approximating complex Bayesian posterior distributions using simpler, parameterized distributions. The Automatic Differentiation Variational Inference (ADVI) algorithm searches over a family of simple densities to find the best approximate posterior density. ADVI produces an estimate of the parameter means together with a sample from the approximate posterior density.

ADVI uses stochastic gradient ascent to approximate the variational objective function, the evidence lower bound or ELBO. The algorithm ascends these gradients using an adaptive stepsize sequence that has one parameter `eta` which is adjusted during warmup. The number of draws used to approximate the ELBO is denoted by `elbo_samples`. ADVI heuristically determines a rolling window over which it computes the average and the median change of the ELBO. When this change falls below a threshold, denoted by `tol_rel_obj`, the algorithm is considered to have converged.

2.5.4.1 Example: variational inference for model `bernoulli.stan`

The `CmdStanModel` `variational` method wraps the `CmdStan` `variational` method.

```
[1]: import os
      from cmdstanpy.model import CmdStanModel
      from cmdstanpy.utils import cmdstan_path

      bernoulli_dir = os.path.join(cmdstan_path(), 'examples', 'bernoulli')
      stan_file = os.path.join(bernoulli_dir, 'bernoulli.stan')
      data_file = os.path.join(bernoulli_dir, 'bernoulli.data.json')
      # instantiate, compile bernoulli model
      model = CmdStanModel(stan_file=stan_file)
      # run CmdStan's variational inference method, returns object `CmdStanVB`
      vi = model.variational(data=data_file)
```

```
16:36:39 - cmdstanpy - INFO - Chain [1] start processing
```

```
16:36:39 - cmdstanpy - INFO - Chain [1] done processing
```

The class `CmdStanVB` <<https://mc-stan.org/cmdstanpy/api.html#cmdstanvb>> provides the following properties to access information about the parameter names, estimated means, and the sample:

- `column_names` - list of column names
- `columns` - number of columns
- `eta` - step size scaling parameter
- `variational_params_dict` - inferred parameter means as a Dict.
- `variational_params_np` - inferred parameter means as a `numpy.ndarray`.
- `variational_params_pd` - inferred parameter means as a `pandas.DataFrame`.
- `variational_sample` - the set of approximate posterior output draws as a `numpy.ndarray`.
- `variational_sample_pd` - the set of approximate posterior output draws as a `pandas.DataFrame`.

```
[2]: print(vi.column_names)

('lp__', 'log_p__', 'log_g__', 'theta')
```

```
[3]: print(vi.variational_params_dict['theta'])

0.223801
```

```
[4]: print(vi.variational_sample.shape)

(1000, 4)
```

These estimates are only valid if the algorithm has converged to a good approximation. When the algorithm fails to do so, the variational method will throw a `RuntimeError`.

```
[5]: model_fail = CmdStanModel(stan_file='eta_should_fail.stan')
vi_fail = model_fail.variational()

16:36:39 - cmdstanpy - INFO - Chain [1] start processing
16:36:39 - cmdstanpy - INFO - Chain [1] done processing

-----
RuntimeError                                Traceback (most recent call last)
Cell In[5], line 2
      1 model_fail = CmdStanModel(stan_file='eta_should_fail.stan')
----> 2 vi_fail = model_fail.variational()

File ~/checkouts/readthedocs.org/user_builds/cmdstanpy/checkouts/v1.2.2/cmdstanpy/model.py:1527, in CmdStanModel.variational(self, data, seed, inits, output_dir, sig_figs, save_latent_dynamics, save_profile, algorithm, iter, grad_samples, elbo_samples, eta, adapt_engaged, adapt_iter, tol_rel_obj, eval_elbo, draws, require_converged, show_console, refresh, time_fmt, timeout, output_samples)
    1525 if len(re.findall(pat, contents)) > 0:
    1526     if require_converged:
-> 1527         raise RuntimeError(
    1528             'The algorithm may not have converged.\n'
    1529             'If you would like to inspect the output, '
    1530             're-call with require_converged=False'
    1531         )
    1532     # else:
    1533     get_logger().warning(
    1534         '%s\n%s',
    1535         'The algorithm may not have converged.',
    1536         'Proceeding because require_converged is set to False',
    1537     )

RuntimeError: The algorithm may not have converged.
If you would like to inspect the output, re-call with require_converged=False
```

Unless you set `require_converged=False`:

```
[6]: vi_fail = model_fail.variational(require_converged=False)

16:36:40 - cmdstanpy - INFO - Chain [1] start processing
16:36:40 - cmdstanpy - INFO - Chain [1] done processing
16:36:40 - cmdstanpy - WARNING - The algorithm may not have converged.
Proceeding because require_converged is set to False
```

This lets you inspect the output to try to diagnose the issue with the model

```
[7]: vi_fail.variational_params_dict
```

```
[7]: OrderedDict([('lp__', 0.0),
                  ('log_p__', 0.0),
                  ('log_g__', 0.0),
                  ('mu[1]', 0.107986),
                  ('mu[2]', 0.0873905)])
```

See the [API documentation](#) for a full description of all arguments.

2.5.5 Using Variational Estimates to Initialize the NUTS-HMC Sampler

In this example we show how to use the parameter estimates return by Stan’s variational inference algorithms [pathfinder](#) and [ADVI](#) as the initial parameter values for Stan’s NUTS-HMC sampler. By default, the sampler algorithm randomly initializes all model parameters in the range `uniform[-2, 2]`. When the true parameter value is outside of this range, starting from the estimates from Pathfinder and ADVI will speed up and improve adaptation.

2.5.5.1 Model and data

The Stan model and data are taken from the [posteriorioRdb](#) package.

We use the [blr model](#), a Bayesian standard linear regression model with noninformative priors, and its corresponding simulated dataset [sblri.json](#), which was simulated via script [sblr.R](#). For convince, we have copied the posteriorioRdb model and data to this directory, in files `blr.stan` and `sblri.json`.

```
[1]: import os
from cmdstanpy import CmdStanModel

stan_file = 'blr.stan' # basic linear regression
data_file = 'sblri.json' # simulated data

model = CmdStanModel(stan_file=stan_file)

print(model.code())

data {
  int<lower=0> N;
  int<lower=0> D;
  matrix[N, D] X;
  vector[N] y;
}
parameters {
  vector[D] beta;
  real<lower=0> sigma;
}
model {
  // prior
  target += normal_lpdf(beta | 0, 10);
  target += normal_lpdf(sigma | 0, 10);
  // likelihood
  target += normal_lpdf(y | X * beta, sigma);
}
```

2.5.5.2 Run Stan's pathfinder or variational algorithm, obtain fitted estimates

The `CmdStanModel` `pathfinder` method wraps the `CmdStan` `pathfinder` method.

Pathfinder locates normal approximations to the target density along a quasi-Newton optimization path, with local covariance estimated using the negative inverse Hessian estimates produced by the LBFGS optimizer. Pathfinder returns draws from the Gaussian approximation with the lowest estimated Kullback-Leibler (KL) divergence to the true posterior. By default, CmdStanPy runs multi-path Pathfinder which returns an importance-resampled set of draws over the outputs of 4 independent single-path Pathfinders. This better matches non-normal target densities and also mitigates the problem of L-BFGS getting stuck at local optima or in saddle points on plateaus.

The method `create_inits` returns a Python Dict containing a set of per-chain initializations for the model parameters. Each set of initializations is a random draw from the Pathfinder sample.

```
[2]: pathfinder_fit = model.pathfinder(data=data_file, seed=123)
```

```
17:01:02 - cmdstanpy - INFO - Chain [1] start processing
17:01:02 - cmdstanpy - INFO - Chain [1] done processing
```

PosteriorioDb provides reference posteriors for all models. For the `blr` model, conditioned on the dataset `sblri.json`, the reference posteriors are in file `sblri-blr.json`

The reference posteriors for all elements of `beta` and `sigma` are all very close to 1.0.

The experiments reported in Figure 3 of the paper [Pathfinder: Parallel quasi-Newton variational inference](#) by Zhang et al. show that Pathfinder provides a better estimate of the posterior, as measured by the 1-Wasserstein distance to the reference posterior, than 75 iterations of the warmup Phase I algorithm used by the NUTS-HMC sampler. Furthermore, Pathfinder is more computationally efficient, requiring fewer evaluations of the log density and gradient functions. Therefore, using the estimates from Pathfinder to initialize the parameter values for the NUTS-HMC sampler will allow the sampler to do a better job of adapting the stepsize and metric during warmup, resulting in better performance and estimation.

```
[3]: pathfinder_inits = pathfinder_fit.create_inits()
print(pathfinder_inits)
```

```
{'beta': array([0.996649, 0.999455, 1.00093 , 0.99873 , 1.00207 ]), 'sigma': array(0.
→ 934232)}, {'beta': array([1.00016 , 0.998764, 1.00055 , 1.00212 , 1.00047 ]), 'sigma':
→ array(1.04441)}, {'beta': array([1.00139 , 0.997917, 1.00134 , 1.00123 , 1.00116 ]),
→ 'sigma': array(0.946814)}, {'beta': array([0.999491, 0.999225, 1.00114 , 0.999147, 0.
→ 998943]), 'sigma': array(0.977812)}
```

```
[4]: mcmc_pathfinder_inits_fit = model.sample(
    data=data_file, inits=pathfinder_inits, iter_warmup=75, seed=12345
)
```

```
17:01:05 - cmdstanpy - INFO - CmdStan start processing
```

```
chain 1 |          | 00:00 Status
```

```
chain 2 |          | 00:00 Status
```

```
chain 3 |          | 00:00 Status
```

```
chain 4 |          | 00:00 Status
```

```
17:01:05 - cmdstanpy - INFO - CmdStan done processing.
```

```
17:01:05 - cmdstanpy - WARNING - Non-fatal error during sampling:
```

```
Exception: normal_lpdf: Scale parameter is 0, but must be positive! (in '/Users/mitzi/
```

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```

↳github/stan-dev/cmdstanpy/docsrc/users-guide/examples/blr.stan', line 16, column 2 to_
↳column 45)
Exception: normal_lpdf: Scale parameter is 0, but must be positive! (in '/Users/mitzi/
↳github/stan-dev/cmdstanpy/docsrc/users-guide/examples/blr.stan', line 16, column 2 to_
↳column 45)
Exception: normal_lpdf: Scale parameter is 0, but must be positive! (in '/Users/mitzi/
↳github/stan-dev/cmdstanpy/docsrc/users-guide/examples/blr.stan', line 16, column 2 to_
↳column 45)
Consider re-running with show_console=True if the above output is unclear!

```

```
[ ]: mcmc_pathfinder_inits_fit.summary()
```

Using the default random parameter initializations, we need to run more warmup iterations. If we only run 75 warmup iterations with random inits, the result fails to estimate sigma correctly. It is necessary to run the model with at least 150 warmup iterations to produce a good set of estimates.

```
[ ]: mcmc_random_inits_fit = model.sample(data=data_file, iter_warmup=75, seed=12345)
```

```
[ ]: mcmc_random_inits_fit.summary()
```

```
[ ]: print(mcmc_random_inits_fit.diagnose())
```

The CmdStanModel method `variational` runs CmdStan's ADVI algorithm. Because this algorithm is unstable and may fail to converge, we run it with argument `require_converged` set to `False`. We also specify a seed, to avoid instabilities as well as for reproducibility.

```
[ ]: vb_fit = model.variational(data=data_file, require_converged=False, seed=123)
```

The ADVI algorithm provides estimates of all model parameters.

The `variational` method returns a CmdStanVB object, with method `stan_variables`, which returns the approximate posterior samples of all model parameters as a Python dictionary. Here, we report the approximate posterior mean.

```
[ ]: vb_mean = {var: samples.mean(axis=0) for var, samples in vb_fit.stan_
↳variables(mean=False).items()}
print(vb_mean)
```

```
[ ]: mcmc_vb_inits_fit = model.sample(
    data=data_file, inits=vb_mean, iter_warmup=75, seed=12345
)
```

```
[ ]: mcmc_vb_inits_fit.summary()
```

The sampler estimates match the reference posterior.

```
[ ]: print(mcmc_vb_inits_fit.diagnose())
```


2.5.6 Generating new quantities of interest.

The `generated quantities` block computes quantities of interest based on the data, transformed data, parameters, and transformed parameters. It can be used to:

- generate simulated data for model testing by forward sampling
- generate predictions for new data
- calculate posterior event probabilities, including multiple comparisons, sign tests, etc.
- calculating posterior expectations
- transform parameters for reporting
- apply full Bayesian decision theory
- calculate log likelihoods, deviances, etc. for model comparison

2.5.6.1 Example: add posterior predictive checks to `bernoulli.stan`

In this example we use the CmdStan example model `bernoulli.stan` and data file `bernoulli.data.json` as our existing model and data.

We instantiate the model `bernoulli`, as in the “Hello World” section of the CmdStanPy [tutorial](#) notebook.

```
[1]: import os
from cmdstanpy import cmdstan_path, CmdStanModel, CmdStanMCMC, CmdStanGQ

bernoulli_dir = os.path.join(cmdstan_path(), 'examples', 'bernoulli')
stan_file = os.path.join(bernoulli_dir, 'bernoulli.stan')
data_file = os.path.join(bernoulli_dir, 'bernoulli.data.json')

# instantiate, compile bernoulli model
model = CmdStanModel(stan_file=stan_file)
print(model.code())

data {
  int<lower=0> N;
  array[N] int<lower=0,upper=1> y;
}
parameters {
  real<lower=0,upper=1> theta;
}
model {
  theta ~ beta(1,1); // uniform prior on interval 0,1
  y ~ bernoulli(theta);
}
```

The input data consists of `N` - the number of bernoulli trials and `y` - the list of observed outcomes. Inspection of the data shows that on average, there is a 20% chance of success for any given Bernoulli trial.

```
[2]: # examine bernoulli data
import json
import statistics
with open(data_file, 'r') as fp:
```

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```
data_dict = json.load(fp)
print(data_dict)
print('mean of y: {}'.format(statistics.mean(data_dict['y'])))

{'N': 10, 'y': [0, 1, 0, 0, 0, 0, 0, 0, 0, 1]}
mean of y: 0.2
```

As in the “Hello World” tutorial, we produce a sample from the posterior of the model conditioned on the data:

```
[3]: # fit the model to the data
fit = model.sample(data=data_file)

16:36:34 - cmdstanpy - INFO - CmdStan start processing

chain 1 |          | 00:00 Status
chain 2 |          | 00:00 Status
chain 3 |          | 00:00 Status
chain 4 |          | 00:00 Status

16:36:35 - cmdstanpy - INFO - CmdStan done processing.
```

The fitted model produces an estimate of θ - the chance of success

```
[4]: fit.summary()

[4]:
```

	Mean	MCSE	StdDev	5%	50%	95%	N_Eff	\
lp__	-7.25218	0.017411	0.725342	-8.704980	-6.973450	-6.749910	1735.58	
theta	0.25184	0.003040	0.119423	0.086955	0.236589	0.476592	1542.74	

	N_Eff/s	R_hat
lp__	21969.3	1.00125
theta	19528.4	1.00119

To run a prior predictive check, we add a `generated quantities` block to the model, in which we generate a new data vector `y_rep` using the current estimate of θ . The resulting model is in file `bernoulli_ppc.stan`

```
[5]: model_ppc = CmdStanModel(stan_file='bernoulli_ppc.stan')
print(model_ppc.code())

data {
  int<lower=0> N;
  array[N] int<lower=0, upper=1> y;
}
parameters {
  real<lower=0, upper=1> theta;
}
```

(continues on next page)

(continued from previous page)

```

model {
  theta ~ beta(1, 1);
  y ~ bernoulli(theta);
}
generated quantities {
  array[N] int y_rep;
  for (n in 1 : N) {
    y_rep[n] = bernoulli_rng(theta);
  }
}

```

We run the `generate_quantities` method on `bernoulli_ppc` using existing sample fit as input. The `generate_quantities` method takes the values of `theta` in the fit sample as the set of draws from the posterior used to generate the corresponding `y_rep` quantities of interest.

The arguments to the `generate_quantities` method are: `+ data` - the data used to fit the model + `previous_fit` - either a `CmdStanMCMC`, `CmdStanVB`, or `CmdStanMLE` object or a list of stan-csv files

```
[6]: new_quantities = model_ppc.generate_quantities(data=data_file, previous_fit=fit)
```

```

16:36:35 - cmdstanpy - INFO - Chain [1] start processing
16:36:35 - cmdstanpy - INFO - Chain [1] done processing
16:36:35 - cmdstanpy - INFO - Chain [2] start processing
16:36:35 - cmdstanpy - INFO - Chain [2] done processing
16:36:35 - cmdstanpy - INFO - Chain [3] start processing
16:36:35 - cmdstanpy - INFO - Chain [3] done processing
16:36:35 - cmdstanpy - INFO - Chain [4] start processing
16:36:35 - cmdstanpy - INFO - Chain [4] done processing

```

The `generate_quantities` method returns a `CmdStanGQ` object which contains the values for all variables in the generated quantities block of the program `bernoulli_ppc.stan`. Unlike the output from the `sample` method, it doesn't contain any information on the joint log probability density, sampler state, or parameters or transformed parameter values.

In this example, each draw consists of the N-length array of replicate of the `bernoulli` model's input variable `y`, which is an N-length array of Bernoulli outcomes.

```
[7]: print(new_quantities.draws().shape, new_quantities.column_names)
for i in range(3):
    print (new_quantities.draws()[i,:])
```

```

16:36:35 - cmdstanpy - WARNING - Sample doesn't contain draws from warmup iterations,
↳rerun sampler with "save_warmup=True".
16:36:35 - cmdstanpy - WARNING - Sample doesn't contain draws from warmup iterations,
↳rerun sampler with "save_warmup=True".
16:36:35 - cmdstanpy - WARNING - Sample doesn't contain draws from warmup iterations,
↳rerun sampler with "save_warmup=True".

```

```
16:36:35 - cmdstanpy - WARNING - Sample doesn't contain draws from warmup iterations,
↳ rerun sampler with "save_warmup=True".
```

```
(1000, 4, 10) ('y_rep[1]', 'y_rep[2]', 'y_rep[3]', 'y_rep[4]', 'y_rep[5]', 'y_rep[6]',
↳ 'y_rep[7]', 'y_rep[8]', 'y_rep[9]', 'y_rep[10]')
[[0. 0. 0. 1. 0. 0. 0. 0. 0. 0.]
 [0. 0. 0. 1. 0. 0. 0. 0. 0. 0.]
 [1. 0. 1. 1. 0. 0. 1. 0. 1. 1.]
 [1. 0. 1. 1. 0. 0. 0. 0. 0. 1.]]
[[0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 1.]
 [1. 0. 1. 0. 1. 0. 0. 0. 0. 1.]
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 1.]]
[[0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 [0. 0. 0. 0. 0. 0. 0. 0. 1. 0.]
 [0. 1. 0. 1. 1. 1. 0. 0. 1. 0.]
 [0. 0. 0. 0. 0. 0. 0. 0. 1. 0.]]
```

We can also use `draws_pd(inc_sample=True)` to get a pandas DataFrame which combines the input drawset with the generated quantities.

```
[8]: sample_plus = new_quantities.draws_pd(inc_sample=True)
print(type(sample_plus), sample_plus.shape)
names = list(sample_plus.columns.values[7:18])
sample_plus.iloc[0:3, :]
```

```
16:36:35 - cmdstanpy - WARNING - Sample doesn't contain draws from warmup iterations,
↳ rerun sampler with "save_warmup=True".
```

```
<class 'pandas.core.frame.DataFrame'> (4000, 21)
```

```
[8]:
```

	lp__	accept_stat__	stepsize__	treedepth__	n_leapfrog__	divergent__	\
0	-7.65140	0.699827	0.817574	1.0	3.0	0.0	
1	-7.30336	1.000000	0.817574	1.0	1.0	0.0	
2	-6.99939	1.000000	0.817574	1.0	1.0	0.0	

	energy__	theta	chain__	iter__	...	y_rep[1]	y_rep[2]	y_rep[3]	\
0	8.57853	0.111130	1.0	1.0	...	0.0	0.0	0.0	
1	7.62178	0.135793	1.0	2.0	...	0.0	0.0	0.0	
2	7.25306	0.169045	1.0	3.0	...	0.0	0.0	0.0	

	y_rep[4]	y_rep[5]	y_rep[6]	y_rep[7]	y_rep[8]	y_rep[9]	y_rep[10]
0	1.0	0.0	0.0	0.0	0.0	0.0	0.0
1	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2	0.0	0.0	0.0	0.0	0.0	0.0	0.0

[3 rows x 21 columns]

For models as simple as the bernoulli models here, it would be trivial to re-run the sampler and generate a new sample which contains both the estimate of the parameters `theta` as well as `y_rep` values. For models which are difficult to fit, i.e., when producing a sample is computationally expensive, the `generate_quantities` method is preferred.

2.5.7 Advanced Topic: Using External C++ Functions

This is based on the relevant portion of the CmdStan documentation [here](#)

Consider the following Stan model, based on the bernoulli example.

```
[2]: from cmdstanpy import CmdStanModel
model_external = CmdStanModel(stan_file='bernoulli_external.stan', compile=False)
print(model_external.code())

functions {
  real make_odds(real theta);
}
data {
  int<lower=0> N;
  array[N] int<lower=0, upper=1> y;
}
parameters {
  real<lower=0, upper=1> theta;
}
model {
  theta ~ beta(1, 1); // uniform prior on interval 0, 1
  y ~ bernoulli(theta);
}
generated quantities {
  real odds;
  odds = make_odds(theta);
}
```

As you can see, it features a function declaration for `make_odds`, but no definition. If we try to compile this, we will get an error.

```
[3]: model_external.compile()

16:02:06 - cmdstanpy - INFO - compiling stan file /home/brian/Dev/py/cmdstanpy/docsrc/
↳ users-guide/examples/bernoulli_external.stan to exe file /home/brian/Dev/py/cmdstanpy/
↳ docsrc/users-guide/examples/bernoulli_external

-----
ValueError                                Traceback (most recent call last)
<ipython-input-3-ca7a518eb77d> in <module>
----> 1 model_external.compile()

~/Dev/py/cmdstanpy/cmdstanpy/model.py in compile(self, force, stanc_options, cpp_options,
↳ user_header, override_options)
    561             "If the issue persists please open a bug report"
--> 563         raise ValueError(
    562             )
    564         f"Failed to compile Stan model '{self._stan_file}'. "
    565         f"Console:\n{console}"

ValueError: Failed to compile Stan model '/home/brian/Dev/py/cmdstanpy/docsrc/users-
↳ guide/examples/bernoulli_external.stan'. Console:

--- Translating Stan model to C++ code ---
```

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```
bin/stanc --o=/home/brian/Dev/py/cmdstanpy/docsrc/users-guide/examples/bernoulli_
↳external.hpp /home/brian/Dev/py/cmdstanpy/docsrc/users-guide/examples/bernoulli_
↳external.stan
Semantic error in '/home/brian/Dev/py/cmdstanpy/docsrc/users-guide/examples/bernoulli_
↳external.stan', line 2, column 7 to column 16:
```

```
-----
1:  functions {
2:    real make_odds(real theta);
      ^
3:  }
4:  data {
-----
```

Function 'make_odds' is declared without specifying a definition.

```
make: *** [make/program:50: /home/brian/Dev/py/cmdstanpy/docsrc/users-guide/examples/
↳bernoulli_external.hpp] Error 1
```

```
Command ['make', '/home/brian/Dev/py/cmdstanpy/docsrc/users-guide/examples/bernoulli_
↳external']
error during processing No such file or directory
```

Even enabling the `--allow-undefined` flag to `stanc3` will not allow this model to be compiled quite yet.

```
[4]: model_external.compile(stanc_options={'allow-undefined':True})
```

```
16:02:10 - cmdstanpy - INFO - compiling stan file /home/brian/Dev/py/cmdstanpy/docsrc/
↳users-guide/examples/bernoulli_external.stan to exe file /home/brian/Dev/py/cmdstanpy/
↳docsrc/users-guide/examples/bernoulli_external
```

```
-----
ValueError                                Traceback (most recent call last)
<ipython-input-4-604c5622a59a> in <module>
----> 1 model_external.compile(stanc_options={'allow-undefined':True})

~/Dev/py/cmdstanpy/cmdstanpy/model.py in compile(self, force, stanc_options, cpp_options,
↳ user_header, override_options)
   561         "If the issue persists please open a bug report"
--> 563         raise ValueError(
   562             )
   564         f"Failed to compile Stan model '{self._stan_file}'. "
   565         f"Console:\n{console}"
```

```
ValueError: Failed to compile Stan model '/home/brian/Dev/py/cmdstanpy/docsrc/users-
↳guide/examples/bernoulli_external.stan'. Console:
```

```
--- Translating Stan model to C++ code ---
```

```
bin/stanc --allow-undefined --o=/home/brian/Dev/py/cmdstanpy/docsrc/users-guide/examples/
↳bernoulli_external.hpp /home/brian/Dev/py/cmdstanpy/docsrc/users-guide/examples/
↳bernoulli_external.stan
```

```
--- Compiling, linking C++ code ---
```

```
g++ -std=c++1y -pthread -D_REENTRANT -Wno-sign-compare -Wno-ignored-attributes -I_
```

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```

→stan/lib/stan_math/lib/tbb_2020.3/include      -O3 -I src -I stan/src -I stan/lib/
→rapidjson_1.1.0/ -I lib/CLI11-1.9.1/ -I stan/lib/stan_math/ -I stan/lib/stan_math/lib/
→eigen_3.4.0 -I stan/lib/stan_math/lib/boost_1.78.0 -I stan/lib/stan_math/lib/sundials_
→6.1.1/include -I stan/lib/stan_math/lib/sundials_6.1.1/src/sundials      -DBOOST_DISABLE_
→ASSERTS      -c -Wno-ignored-attributes      -include /home/brian/Dev/py/cmdstanpy/
→docsrc/users-guide/examples/user_header.hpp -x c++ -o /home/brian/Dev/py/cmdstanpy/
→docsrc/users-guide/examples/bernoulli_external.o /home/brian/Dev/py/cmdstanpy/docsrc/
→users-guide/examples/bernoulli_external.hpp
/home/brian/Dev/py/cmdstanpy/docsrc/users-guide/examples/bernoulli_external.hpp: In
→member function 'void bernoulli_external_model_namespace::bernoulli_external_model::
→write_array_impl(RNG&, VecR&, VecI&, VecVar&, bool, bool, std::ostream*) const':
/home/brian/Dev/py/cmdstanpy/docsrc/users-guide/examples/bernoulli_external.hpp:156:14:
→error: there are no arguments to 'make_odds' that depend on a template parameter, so a
→declaration of 'make_odds' must be available [-fpermissive]
    156 |         odds = make_odds(theta, pstream__);
        |         ^~~~~~
/home/brian/Dev/py/cmdstanpy/docsrc/users-guide/examples/bernoulli_external.hpp:156:14:
→note: (if you use '-fpermissive', G++ will accept your code, but allowing the use of
→an undeclared name is deprecated)
/home/brian/Dev/py/cmdstanpy/docsrc/users-guide/examples/bernoulli_external.hpp: In
→instantiation of 'void bernoulli_external_model_namespace::bernoulli_external_model::
→write_array_impl(RNG&, VecR&, VecI&, VecVar&, bool, bool, std::ostream*) const [with
→RNG = boost::random::additive_combine_engine<boost::random::linear_congruential_engine
→<unsigned int, 40014, 0, 2147483563>, boost::random::linear_congruential_engine
→<unsigned int, 40692, 0, 2147483399> >; VecR = Eigen::Matrix<double, -1, 1>; VecI =
→std::vector<int>; VecVar = Eigen::Matrix<double, -1, 1>; stan::require_vector_like_vt
→<std::is_floating_point, VecR>* <anonymous> = 0; stan::require_vector_like_vt<std::is_
→integral, VecI>* <anonymous> = 0; stan::require_vector_vt<std::is_floating_point,
→VecVar>* <anonymous> = 0; std::ostream = std::basic_ostream<char>]':
/home/brian/Dev/py/cmdstanpy/docsrc/users-guide/examples/bernoulli_external.hpp:275:21:
→required from 'void bernoulli_external_model_namespace::bernoulli_external_model::
→write_array(RNG&, Eigen::Matrix<double, -1, 1>&, Eigen::Matrix<double, -1, 1>&, bool,
→bool, std::ostream*) const [with RNG = boost::random::additive_combine_engine<boost::
→random::linear_congruential_engine<unsigned int, 40014, 0, 2147483563>, boost::random::
→linear_congruential_engine<unsigned int, 40692, 0, 2147483399> >; std::ostream = std::
→basic_ostream<char>]':
stan/src/stan/model/model_base_crtp.hpp:140:61:   required from 'void stan::model::model_
→base_crtp<M>::write_array(boost::random::ecuyer1988&, Eigen::VectorXd&, Eigen::
→VectorXd&, bool, bool, std::ostream*) const [with M = bernoulli_external_model_
→namespace::bernoulli_external_model; boost::random::ecuyer1988 = boost::random::
→additive_combine_engine<boost::random::linear_congruential_engine<unsigned int, 40014,
→0, 2147483563>, boost::random::linear_congruential_engine<unsigned int, 40692, 0,
→2147483399> >; Eigen::VectorXd = Eigen::Matrix<double, -1, 1>; std::ostream = std::
→basic_ostream<char>]':
stan/src/stan/model/model_base_crtp.hpp:136:8:   required from here
/home/brian/Dev/py/cmdstanpy/docsrc/users-guide/examples/bernoulli_external.hpp:156:23:
→error: 'make_odds' was not declared in this scope
    156 |         odds = make_odds(theta, pstream__);
        |         ~~~~~~^~~~~~
/home/brian/Dev/py/cmdstanpy/docsrc/users-guide/examples/bernoulli_external.hpp: In
→instantiation of 'void bernoulli_external_model_namespace::bernoulli_external_model::
→write_array_impl(RNG&, VecR&, VecI&, VecVar&, bool, bool, std::ostream*) const [with

```

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```

↳ RNG = boost::random::additive_combine_engine<boost::random::linear_congruential_engine
↳ <unsigned int, 40014, 0, 2147483563>, boost::random::linear_congruential_engine
↳ <unsigned int, 40692, 0, 2147483399> >; VecR = std::vector<double, std::allocator
↳ <double> >; VecI = std::vector<int>; VecVar = std::vector<double, std::allocator
↳ <double> >; stan::require_vector_like_vt<std::is_floating_point, VecR>* <anonymous> =
↳ 0; stan::require_vector_like_vt<std::is_integral, VecI>* <anonymous> = 0; stan::
↳ require_vector_vt<std::is_floating_point, VecVar>* <anonymous> = 0; std::ostream = std:
↳ :basic_ostream<char>]':
/home/brian/Dev/py/cmdstanpy/docsrc/users-guide/examples/bernoulli_external.hpp:291:21:
↳ required from 'void bernoulli_external_model_namespace::bernoulli_external_model::
↳ write_array(RNG&, std::vector<double, std::allocator<double> >&, std::vector<int>&,
↳ std::vector<double, std::allocator<double> >&, bool, bool, std::ostream*) const [with
↳ RNG = boost::random::additive_combine_engine<boost::random::linear_congruential_engine
↳ <unsigned int, 40014, 0, 2147483563>, boost::random::linear_congruential_engine
↳ <unsigned int, 40692, 0, 2147483399> >; std::ostream = std::basic_ostream<char>]
stan/src/stan/model/model_base_crtp.hpp:202:61: required from 'void stan::model::model_
↳ base_crtp<M>::write_array(boost::random::ecuyer1988&, std::vector<double, std::
↳ allocator<double> >&, std::vector<int>&, std::vector<double, std::allocator<double> >&,
↳ bool, bool, std::ostream*) const [with M = bernoulli_external_model_namespace::
↳ bernoulli_external_model; boost::random::ecuyer1988 = boost::random::additive_combine_
↳ engine<boost::random::linear_congruential_engine<unsigned int, 40014, 0, 2147483563>,
↳ boost::random::linear_congruential_engine<unsigned int, 40692, 0, 2147483399> >; std::
↳ ostream = std::basic_ostream<char>]
stan/src/stan/model/model_base_crtp.hpp:198:8: required from here
/home/brian/Dev/py/cmdstanpy/docsrc/users-guide/examples/bernoulli_external.hpp:156:23:
↳ error: 'make_odds' was not declared in this scope
make: *** [make/program:58: /home/brian/Dev/py/cmdstanpy/docsrc/users-guide/examples/
↳ bernoulli_external] Error 1

Command ['make', 'STANFLAGS+=--allow-undefined', '/home/brian/Dev/py/cmdstanpy/docsrc/
↳ users-guide/examples/bernoulli_external']
error during processing No such file or directory

```

To resolve this, we need to both tell the Stan compiler an undefined function is okay **and** let C++ know what it should be.

We can provide a definition in a C++ header file by using the `user_header` argument to either the `CmdStanModel` constructor or the `compile` method.

This will enable the `allow-undefined` flag automatically.

```

[5]: model_external.compile(user_header='make_odds.hpp')
assert model_external.exe_file is not None

```

```

16:03:06 - cmdstanpy - INFO - compiling stan file /home/brian/Dev/py/cmdstanpy/docsrc/
↳ users-guide/examples/bernoulli_external.stan to exe file /home/brian/Dev/py/cmdstanpy/
↳ docsrc/users-guide/examples/bernoulli_external
16:03:25 - cmdstanpy - INFO - compiled model executable: /home/brian/Dev/py/cmdstanpy/
↳ docsrc/users-guide/examples/bernoulli_external

```

We can then run this model and inspect the output


```
[6]: fit = model_external.sample(data={'N':10, 'y':[0,1,0,0,0,0,0,0,0,1]})
fit.stan_variable('odds')
```

```
16:03:31 - cmdstanpy - INFO - CmdStan start processing
chain 1 |          | 00:00 Status
```

```
chain 1 || 00:00 Sampling completed
chain 2 || 00:00 Sampling completed
chain 3 || 00:00 Sampling completed
chain 4 || 00:00 Sampling completed
```

```
16:03:31 - cmdstanpy - INFO - CmdStan done processing.
```

```
[6]: array([0.28554 , 0.395692, 0.38404 , ..., 0.581201, 0.406603, 0.244602])
```

The contents of this header file are presented without comment:

```
#include <ostream>

double make_odds(const double& theta, std::ostream *pstream__) {
    return theta / (1 - theta);
}
```

Additional guidance, including on writing functions with known derivatives, can be found in the [CmdStan documentation](#).

API REFERENCE

The following documents the public API of CmdStanPy. It is expected to be stable between versions, with backwards compatibility between minor versions and deprecation warnings preceding breaking changes. The documentation for the *internal API* is also provided, but the internal API does not guarantee either stability and backwards compatibility.

3.1 Internal API Reference

The following documents the internal API of CmdStanPy. No guarantees are made about backwards compatibility between minor versions and refactors are expected. If you find yourself needing something exposed here, please [open an issue](#) requesting it be added to the public *API*.

3.1.1 Classes

3.1.1.1 InferenceMetadata

class cmdstanpy.stanfit.InferenceMetadata(*config*)

CmdStan configuration and contents of output file parsed out of the Stan CSV file header comments and column headers. Assumes valid CSV files.

Parameters

config (*Dict[str, Any]*) –

property cmdstan_config: *Dict[str, Any]*

Returns a dictionary containing a set of name, value pairs parsed out of the Stan CSV file header. These include the command configuration and the CSV file header row information. Uses deepcopy for immutability.

property method_vars: *Dict[str, Variable]*

Method variable names always end in __, e.g. *lp__*.

property stan_vars: *Dict[str, Variable]*

These are the user-defined variables in the Stan program.

3.1.1.2 RunSet

```
class cmdstanpy.stanfit.RunSet(args, chains=1, *, chain_ids=None, time_fmt='%Y%m%d%H%M%S',  
                             one_process_per_chain=True)
```

Encapsulates the configuration and results of a call to any CmdStan inference method. Records the method return code and locations of all console, error, and output files.

RunSet objects are instantiated by the CmdStanModel class inference methods which validate all inputs, therefore “__init__” method skips input checks.

Parameters

- **args** (CmdStanArgs) –
- **chains** (*int*) –
- **chain_ids** (*Optional*[*List*[*int*]]) –
- **time_fmt** (*str*) –
- **one_process_per_chain** (*bool*) –

cmd(*idx*)

Assemble CmdStan invocation. When running parallel chains from single process (2.28 and up), specify CmdStan arg *num_chains* and leave chain idx off CSV files.

Parameters

- **idx** (*int*) –

Return type

List[*str*]

get_err_msgs()

Checks console messages for each CmdStan run.

Return type

str

save_csvfiles(*dir=None*)

Moves CSV files to specified directory.

Parameters

- **dir** (*Optional*[*str*]) – directory path

Return type

None

See also:

[*cmdstanpy.from_csv*](#)

property chain_ids: *List*[*int*]

Chain ids.

property chains: *int*

Number of chains.

property csv_files: *List*[*str*]

List of paths to CmdStan output files.

property diagnostic_files: *List*[*str*]

List of paths to CmdStan hamiltonian diagnostic files.

property method: Method

CmdStan method used to generate this fit.

property model: str

Stan model name.

property num_procs: int

Number of processes run.

property one_process_per_chain: bool

When True, for each chain, call CmdStan in its own subprocess. When False, use CmdStan's *num_chains* arg to run parallel chains. Always True if CmdStan < 2.28. For CmdStan 2.28 and up, *sample* method determines value.

property profile_files: List[str]

List of paths to CmdStan profiler files.

property stdout_files: List[str]

List of paths to transcript of CmdStan messages sent to the console. Transcripts include config information, progress, and error messages.

3.1.1.3 CompilerOptions

```
class cmdstanpy.compilation.CompilerOptions(*, stanc_options=None, cpp_options=None,
                                           user_header=None)
```

User-specified flags for stanc and C++ compiler.

Parameters

- **stanc_options** (*Optional[Dict[str, Any]]*) –
- **cpp_options** (*Optional[Dict[str, Any]]*) –
- **user_header** (*Optional[Union[str, PathLike]]*) –

stanc_options - stanc compiler flags, options

cpp_options - makefile options

Type

NAME=value

user_header - path to a user .hpp file to include during compilation

add(new_opts)

Adds options to existing set of compiler options.

Parameters

new_opts (*CompilerOptions*) –

Return type

None

add_include_path(path)

Adds include path to existing set of compiler options.

Parameters

path (*str*) –

Return type

None

compose(*filename_in_msg=None*)

Format makefile options as list of strings.

Parameters

filename_in_msg (*str*, *optional*) – filename to be displayed in stanc3 error messages (if different from actual filename on disk), by default None

Return type

List[*str*]

is_empty()

True if no options specified.

Return type

bool

validate()

Check compiler args. Raise ValueError if invalid options are found.

Return type

None

validate_cpp_opts()

Check cpp compiler args. Raise ValueError if bad config is found.

Return type

None

validate_stanc_opts()

Check stanc compiler args and consistency between stanc and C++ options. Raise ValueError if bad config is found.

Return type

None

validate_user_header()

User header exists. Raise ValueError if bad config is found.

Return type

None

property *cpp_options*: *Dict*[*str*, *Union*[*bool*, *int*]]

C++ compiler options.

property *stanc_options*: *Dict*[*str*, *Union*[*bool*, *int*, *str*, *Iterable*[*str*]]]

Stanc compiler options.

property *user_header*: *str*

user header.

3.1.1.4 CmdStanArgs

```
class cmdstanpy.cmdstan_args.CmdStanArgs(model_name, model_exe, chain_ids, method_args, data=None,
                                         seed=None, inits=None, output_dir=None, sig_figs=None,
                                         save_latent_dynamics=False, save_profile=False,
                                         refresh=None)
```

Container for CmdStan command line arguments. Consists of arguments common to all methods and an object which contains the method-specific arguments.

Parameters

- **model_name** (*str*) –
- **model_exe** (*Optional[Union[str, PathLike]]*) –
- **chain_ids** (*Optional[List[int]]*) –
- **method_args** (*Union[SamplerArgs, OptimizeArgs, GenerateQuantitiesArgs, VariationalArgs, LaplaceArgs, PathfinderArgs]*) –
- **data** (*Optional[Union[Mapping[str, Any], str]]*) –
- **seed** (*Optional[Union[int, List[int]]]*) –
- **inits** (*Optional[Union[int, float, str, List[str]]]*) –
- **output_dir** (*Optional[Union[str, PathLike]]*) –
- **sig_figs** (*Optional[int]*) –
- **save_latent_dynamics** (*bool*) –
- **save_profile** (*bool*) –
- **refresh** (*Optional[int]*) –

```
compose_command(idx, csv_file, *, diagnostic_file=None, profile_file=None)
```

Compose CmdStan command for non-default arguments.

Parameters

- **idx** (*int*) –
- **csv_file** (*str*) –
- **diagnostic_file** (*Optional[str]*) –
- **profile_file** (*Optional[str]*) –

Return type

List[str]

```
validate()
```

Check arguments correctness and consistency.

- input files must exist
- output files must be in a writeable directory
- if no seed specified, set random seed.
- length of per-chain lists equals specified # of chains

Return type

None

3.1.1.5 SamplerArgs

```
class cmdstanpy.cmdstan_args.SamplerArgs(iter_warmup=None, iter_sampling=None,
                                         save_warmup=False, thin=None, max_treedepth=None,
                                         metric=None, step_size=None, adapt_engaged=True,
                                         adapt_delta=None, adapt_init_phase=None,
                                         adapt_metric_window=None, adapt_step_size=None,
                                         fixed_param=False, num_chains=1)
```

Arguments for the NUTS adaptive sampler.

Parameters

- **iter_warmup** (*Optional[int]*) –
- **iter_sampling** (*Optional[int]*) –
- **save_warmup** (*bool*) –
- **thin** (*Optional[int]*) –
- **max_treedepth** (*Optional[int]*) –
- **metric** (*Optional[Union[str, Dict[str, Any], List[str], List[Dict[str, Any]]]]*) –
- **step_size** (*Optional[Union[float, List[float]]]*) –
- **adapt_engaged** (*bool*) –
- **adapt_delta** (*Optional[float]*) –
- **adapt_init_phase** (*Optional[int]*) –
- **adapt_metric_window** (*Optional[int]*) –
- **adapt_step_size** (*Optional[int]*) –
- **fixed_param** (*bool*) –
- **num_chains** (*int*) –

compose(*idx, cmd*)

Compose CmdStan command for method-specific non-default arguments.

Parameters

- **idx** (*int*) –
- **cmd** (*List[str]*) –

Return type

List[str]

validate(*chains*)

Check arguments correctness and consistency.

- adaptation and warmup args are consistent
- if file(s) for metric are supplied, check contents.
- length of per-chain lists equals specified # of chains

Parameters

- **chains** (*Optional[int]*) –

Return type

None

3.1.1.6 OptimizeArgs

```
class cmdstanpy.cmdstan_args.OptimizeArgs(algorithm=None, init_alpha=None, iter=None,
                                          save_iterations=False, tol_obj=None, tol_rel_obj=None,
                                          tol_grad=None, tol_rel_grad=None, tol_param=None,
                                          history_size=None, jacobian=False)
```

Container for arguments for the optimizer.

Parameters

- **algorithm** (*Optional[str]*) –
- **init_alpha** (*Optional[float]*) –
- **iter** (*Optional[int]*) –
- **save_iterations** (*bool*) –
- **tol_obj** (*Optional[float]*) –
- **tol_rel_obj** (*Optional[float]*) –
- **tol_grad** (*Optional[float]*) –
- **tol_rel_grad** (*Optional[float]*) –
- **tol_param** (*Optional[float]*) –
- **history_size** (*Optional[int]*) –
- **jacobian** (*bool*) –

```
compose(_idx, cmd)
```

compose command string for CmdStan for non-default arg values.

Parameters

- **_idx** (*int*) –
- **cmd** (*List[str]*) –

Return type*List[str]*

```
validate(_chains=None)
```

Check arguments correctness and consistency.

Parameters

- **_chains** (*Optional[int]*) –

Return type

None

3.1.1.7 LaplaceArgs

class cmdstanpy.cmdstan_args.LaplaceArgs(mode, draws=None, jacobian=True)

Arguments needed for laplace method.

Parameters

- **mode** (*str*) –
- **draws** (*Optional[int]*) –
- **jacobian** (*bool*) –

compose(_idx, cmd)

compose command string for CmdStan for non-default arg values.

Parameters

- **_idx** (*int*) –
- **cmd** (*List[str]*) –

Return type

List[str]

validate(_chains=None)

Check arguments correctness and consistency.

Parameters

- **_chains** (*Optional[int]*) –

Return type

None

3.1.1.8 PathfinderArgs

class cmdstanpy.cmdstan_args.PathfinderArgs(init_alpha=None, tol_obj=None, tol_rel_obj=None, tol_grad=None, tol_rel_grad=None, tol_param=None, history_size=None, num_psis_draws=None, num_paths=None, max_lbfgs_iters=None, num_draws=None, num_elbo_draws=None, save_single_paths=False, psis_resample=True, calculate_lp=True)

Container for arguments for Pathfinder.

Parameters

- **init_alpha** (*Optional[float]*) –
- **tol_obj** (*Optional[float]*) –
- **tol_rel_obj** (*Optional[float]*) –
- **tol_grad** (*Optional[float]*) –
- **tol_rel_grad** (*Optional[float]*) –
- **tol_param** (*Optional[float]*) –
- **history_size** (*Optional[int]*) –
- **num_psis_draws** (*Optional[int]*) –

- `num_paths` (*Optional*[*int*]) –
- `max_lbfgs_iters` (*Optional*[*int*]) –
- `num_draws` (*Optional*[*int*]) –
- `num_elbo_draws` (*Optional*[*int*]) –
- `save_single_paths` (*bool*) –
- `psis_resample` (*bool*) –
- `calculate_lp` (*bool*) –

`compose(_idx, cmd)`

compose command string for CmdStan for non-default arg values.

Parameters

- `_idx` (*int*) –
- `cmd` (*List*[*str*]) –

Return type

List[*str*]

`validate(_chains=None)`

Check arguments correctness and consistency.

Parameters

- `_chains` (*Optional*[*int*]) –

Return type

None

3.1.1.9 VariationalArgs

```
class cmdstanpy.cmdstan_args.VariationalArgs(algorithm=None, iter=None, grad_samples=None,
                                             elbo_samples=None, eta=None, adapt_iter=None,
                                             adapt_engaged=True, tol_rel_obj=None,
                                             eval_elbo=None, output_samples=None)
```

Arguments needed for variational method.

Parameters

- `algorithm` (*Optional*[*str*]) –
- `iter` (*Optional*[*int*]) –
- `grad_samples` (*Optional*[*int*]) –
- `elbo_samples` (*Optional*[*int*]) –
- `eta` (*Optional*[*float*]) –
- `adapt_iter` (*Optional*[*int*]) –
- `adapt_engaged` (*bool*) –
- `tol_rel_obj` (*Optional*[*float*]) –
- `eval_elbo` (*Optional*[*int*]) –
- `output_samples` (*Optional*[*int*]) –

compose(*idx*, *cmd*)

Compose CmdStan command for method-specific non-default arguments.

Parameters

- **idx** (*int*) –
- **cmd** (*List[str]*) –

Return type

List[str]

validate(*chains=None*)

Check arguments correctness and consistency.

Parameters

chains (*Optional[int]*) –

Return type

None

3.2 Classes

3.2.1 CmdStanModel

A CmdStanModel object encapsulates the Stan program. It manages program compilation and provides the following inference methods:

sample()

runs the HMC-NUTS sampler to produce a set of draws from the posterior distribution.

optimize()

produce a penalized maximum likelihood estimate or maximum a posteriori estimate (point estimate) of the model parameters.

laplace_sample()

draw from a Laplace approximation centered at the posterior mode found by **optimize**.

pathfinder()

runs the Pathfinder variational inference parameters to receive approximate draws from the posterior.

variational()

run CmdStan's automatic differentiation variational inference (ADVI) algorithm to approximate the posterior distribution.

generate_quantities()

runs CmdStan's generate_quantities method to produce additional quantities of interest based on draws from an existing sample.

class cmdstanpy.**CmdStanModel**(*model_name=None*, *stan_file=None*, *exe_file=None*, *force_compile=False*,
 stanc_options=None, *cpp_options=None*, *user_header=None*, *,
 compile=None)

The constructor method allows model instantiation given either the Stan program source file or the compiled executable, or both. This will compile the model if provided a Stan file and no executable,

Parameters

- **model_name** (*Optional*[*str*]) – Model name, used for output file names. Optional, default is the base filename of the Stan program file. Deprecated: In version 2.0.0, model name cannot be specified and will always be taken from executable.
- **stan_file** (*Optional*[*Union*[*str*, *PathLike*]]) – Path to Stan program file.
- **exe_file** (*Optional*[*Union*[*str*, *PathLike*]]) – Path to compiled executable file. Optional, unless no Stan program file is specified. If both the program file and the compiled executable file are specified, the base filenames must match, (but different directory locations are allowed).
- **force_compile** (*bool*) – If True, always compile, even if there is an existing executable file for this model.
- **stanc_options** (*Optional*[*Dict*[*str*, *Any*]]) – Options for stanc compiler, specified as a Python dictionary containing Stanc3 compiler option name, value pairs. Optional.
- **cpp_options** (*Optional*[*Dict*[*str*, *Any*]]) – Options for C++ compiler, specified as a Python dictionary containing C++ compiler option name, value pairs. Optional.
- **user_header** (*Optional*[*Union*[*str*, *PathLike*]]) – A path to a header file to include during C++ compilation. Optional.
- **compile** (*Optional*[*Union*[*bool*, *Literal*['force']]]) – Whether or not to compile the model. Default is True. If set to the string "force", it will always compile even if an existing executable is found. Deprecated: Use `force_compile` instead. The ability to instantiate a `CmdStanModel` without an executable will be removed in version 2.0.0.

code()

Return Stan program as a string.

Return type

Optional[*str*]

compile(*force=False*, *stanc_options=None*, *cpp_options=None*, *user_header=None*, *override_options=False*, *, *_internal=False*)

Deprecated: To compile a model, use the `CmdStanModel` constructor or `cmdstanpy.compile_stan_file()`.

Compile the given Stan program file. Translates the Stan code to C++, then calls the C++ compiler.

By default, this function compares the timestamps on the source and executable files; if the executable is newer than the source file, it will not recompile the file, unless argument `force` is True or unless the compiler options have been changed.

Parameters

- **force** (*bool*) – When True, always compile, even if the executable file is newer than the source file. Used for Stan models which have `#include` directives in order to force recompilation when changes are made to the included files.
- **stanc_options** (*Optional*[*Dict*[*str*, *Any*]]) – Options for stanc compiler.
- **cpp_options** (*Optional*[*Dict*[*str*, *Any*]]) – Options for C++ compiler.
- **user_header** (*Optional*[*Union*[*str*, *PathLike*]]) – A path to a header file to include during C++ compilation.
- **override_options** (*bool*) – When True, override existing option. When False, add/replace existing options. Default is False.
- **_internal** (*bool*) –

Return type

None

exe_info()

Run model with option ‘info’. Parse output statements, which all have form ‘key = value’ into a Dict. If exe file compiled with CmdStan < 2.27, option ‘info’ isn’t available and the method returns an empty dictionary.

Return type*Dict[str, str]***format**(*overwrite_file=False, canonicalize=False, max_line_length=78, *, backup=True*)

Deprecated: Use `cmdstanpy.format_stan_file()` instead.

Run stanc’s auto-formatter on the model code. Either saves directly back to the file or prints for inspection

Parameters

- **overwrite_file** (*bool*) – If True, save the updated code to disk, rather than printing it. By default False
- **canonicalize** (*Union[bool, str, Iterable[str]]*) – Whether or not the compiler should ‘canonicalize’ the Stan model, removing things like deprecated syntax. Default is False. If True, all canonicalizations are run. If it is a list of strings, those options are passed to stanc (new in Stan 2.29)
- **max_line_length** (*int*) – Set the wrapping point for the formatter. The default value is 78, which wraps most lines by the 80th character.
- **backup** (*bool*) – If True, create a stanfile.bak backup before writing to the file. Only disable this if you’re sure you have other copies of the file or are using a version control system like Git.

Return type

None

generate_quantities(*data=None, previous_fit=None, seed=None, gq_output_dir=None, sig_figs=None, show_console=False, refresh=None, time_fmt='%Y%m%d%H%M%S', timeout=None, *, mcmc_sample=None*)

Run CmdStan’s generate_quantities method which runs the generated quantities block of a model given an existing sample.

This function takes one of the Stan fit objects `CmdStanMCMC`, `CmdStanMLE`, or `CmdStanVB` and the data required for the model and calls to the CmdStan generate_quantities method to generate additional quantities of interest.

The `CmdStanGQ` object records the command, the return code, and the paths to the generate method output CSV and console files. The output files are written either to a specified output directory or to a temporary directory which is deleted upon session exit.

Output files are either written to a temporary directory or to the specified output directory. Output file-names correspond to the template ‘<model_name>-<YYYYMMDDHHMM>-<chain_id>’ plus the file suffix which is either ‘.csv’ for the CmdStan output or ‘.txt’ for the console messages, e.g. ‘bernoulli-201912081451-1.csv’. Output files written to the temporary directory contain an additional 8-character random string, e.g. ‘bernoulli-201912081451-1-5nm6as7u.csv’.

Parameters

- **data** (*Optional[Union[Mapping[str, Any], str, PathLike]]*) – Values for all data variables in the model, specified either as a dictionary with entries matching the data variables, or as the path of a data file in JSON or Rdump format.

- **previous_fit** (*Optional[Union[Fit, List[str]]]*) – Can be either a `CmdStanMCMC`, `CmdStanMLE`, or `CmdStanVB` or a list of stan-csv files generated by fitting the model to the data using any Stan interface.
- **seed** (*Optional[int]*) – The seed for random number generator. Must be an integer between 0 and $2^{32} - 1$. If unspecified, `numpy.random.default_rng()` is used to generate a seed which will be used for all chains. *NOTE: Specifying the seed will guarantee the same result for multiple invocations of this method with the same inputs. However this will not reproduce results from the sample method given the same inputs because the RNG will be in a different state.*
- **gq_output_dir** (*Optional[Union[str, PathLike]]*) – Name of the directory in which the CmdStan output files are saved. If unspecified, files will be written to a temporary directory which is deleted upon session exit.
- **sig_figs** (*Optional[int]*) – Numerical precision used for output CSV and text files. Must be an integer between 1 and 18. If unspecified, the default precision for the system file I/O is used; the usual value is 6. Introduced in CmdStan-2.25.
- **show_console** (*bool*) – If True, stream CmdStan messages sent to stdout and stderr to the console. Default is False.
- **refresh** (*Optional[int]*) – Specify the number of iterations CmdStan will take between progress messages. Default value is 100.
- **time_fmt** (*str*) – A format string passed to `strftime()` to decide the file names for output CSVs. Defaults to “%Y%m%d%H%M%S”
- **timeout** (*Optional[float]*) – Duration at which generation times out in seconds.
- **mcmc_sample** (*Optional[Union[CmdStanMCMC, List[str]]]*) –

Returns

CmdStanGQ object

Return type`CmdStanGQ[Fit]`

```
laplace_sample(data=None, mode=None, draws=None, *, jacobian=True, seed=None, output_dir=None,
               sig_figs=None, save_profile=False, show_console=False, refresh=None,
               time_fmt='%Y%m%d%H%M%S', timeout=None, opt_args=None)
```

Run a Laplace approximation around the posterior mode.

Parameters

- **data** (*Optional[Union[Mapping[str, Any], str, PathLike]]*) – Values for all data variables in the model, specified either as a dictionary with entries matching the data variables, or as the path of a data file in JSON or Rdump format.
- **mode** (*Optional[Union[CmdStanMLE, str, PathLike]]*) – The mode around which to place the approximation, either
 - A `CmdStanMLE` object
 - A path to a CSV file containing the output of an optimization run.
 - None - use default optimizer settings and/or any `opt_args`.
- **draws** (*Optional[int]*) – Number of approximate draws to return. Defaults to 1000
- **jacobian** (*bool*) – Whether or not to enable the Jacobian adjustment for constrained parameters. Defaults to True. Note: This must match the argument used in the creation of mode, if supplied.

- **output_dir** (*Optional* [*Union* [*str*, *PathLike*]]) – Name of the directory to which CmdStan output files are written. If unspecified, output files will be written to a temporary directory which is deleted upon session exit.
- **sig_figs** (*Optional* [*int*]) – Numerical precision used for output CSV and text files. Must be an integer between 1 and 18. If unspecified, the default precision for the system file I/O is used; the usual value is 6. Introduced in CmdStan-2.25.
- **save_profile** (*bool*) – Whether or not to profile auto-diff operations in labelled blocks of code. If *True*, CSV outputs are written to file ‘<model_name>-<YYYYMMDDHHMM>-profile-<path_id>’. Introduced in CmdStan-2.26, see https://mc-stan.org/docs/cmdstan-guide/stan_csv.html, section “Profiling CSV output file” for details.
- **show_console** (*bool*) – If *True*, stream CmdStan messages sent to stdout and stderr to the console. Default is *False*.
- **refresh** (*Optional* [*int*]) – Specify the number of iterations CmdStan will take between progress messages. Default value is 100.
- **time_fmt** (*str*) – A format string passed to `strftime()` to decide the file names for output CSVs. Defaults to “%Y%m%d%H%M%S”
- **timeout** (*Optional* [*float*]) – Duration at which Pathfinder times out in seconds. Defaults to *None*.
- **opt_args** (*Optional* [*Dict* [*str*, *Any*]]) – Dictionary of additional arguments which will be passed to `optimize()`
- **seed** (*Optional* [*int*]) –

Returns

A *CmdStanLaplace* object.

Return type

CmdStanLaplace

log_prob(*params*, *data=None*, *, *jacobian=True*, *sig_figs=None*)

Calculate the log probability and gradient at the given parameter values.

Note: This function is **NOT** an efficient way to evaluate the log density of the model. It should be used for diagnostics ONLY. Please, do not use this for other purposes such as testing new sampling algorithms!

Parameters

- **params** (*Union* [*Dict* [*str*, *Any*], *str*, *PathLike*]) – Values for all parameters in the model, specified either as a dictionary with entries matching the parameter variables, or as the path of a data file in JSON or Rdump format.
These should be given on the constrained (natural) scale.
- **data** (*Optional* [*Union* [*Mapping* [*str*, *Any*], *str*, *PathLike*]]) – Values for all data variables in the model, specified either as a dictionary with entries matching the data variables, or as the path of a data file in JSON or Rdump format.
- **jacobian** (*bool*) – Whether or not to enable the Jacobian adjustment for constrained parameters. Defaults to *True*.

- **sig_figs** (*Optional[int]*) – Numerical precision used for output CSV and text files. Must be an integer between 1 and 18. If unspecified, the default precision for the system file I/O is used; the usual value is 6.

Returns

A `pandas.DataFrame` containing columns “**lp__**” and additional columns for the gradient values. These gradients will be for the unconstrained parameters of the model.

Return type

DataFrame

optimize(*data=None, seed=None, inits=None, output_dir=None, sig_figs=None, save_profile=False, algorithm=None, init_alpha=None, tol_obj=None, tol_rel_obj=None, tol_grad=None, tol_rel_grad=None, tol_param=None, history_size=None, iter=None, save_iterations=False, require_converged=True, show_console=False, refresh=None, time_fmt='%Y%m%d%H%M%S', timeout=None, jacobian=False*)

Run the specified CmdStan optimize algorithm to produce a penalized maximum likelihood estimate of the model parameters.

This function validates the specified configuration, composes a call to the CmdStan `optimize` method and spawns one subprocess to run the optimizer and waits for it to run to completion. Unspecified arguments are not included in the call to CmdStan, i.e., those arguments will have CmdStan default values.

The `CmdStanMLE` object records the command, the return code, and the paths to the optimize method output CSV and console files. The output files are written either to a specified output directory or to a temporary directory which is deleted upon session exit.

Output files are either written to a temporary directory or to the specified output directory. Output file-names correspond to the template ‘<model_name>-<YYYYMMDDHHMM>-<chain_id>’ plus the file suffix which is either ‘.csv’ for the CmdStan output or ‘.txt’ for the console messages, e.g. ‘bernoulli-201912081451-1.csv’. Output files written to the temporary directory contain an additional 8-character random string, e.g. ‘bernoulli-201912081451-1-5nm6as7u.csv’.

Parameters

- **data** (*Optional[Union[Mapping[str, Any], str, PathLike]]*) – Values for all data variables in the model, specified either as a dictionary with entries matching the data variables, or as the path of a data file in JSON or Rdump format.
- **seed** (*Optional[int]*) – The seed for random number generator. Must be an integer between 0 and $2^{32} - 1$. If unspecified, `numpy.random.default_rng()` is used to generate a seed.
- **inits** (*Optional[Union[Mapping[str, Any], float, str, PathLike]]*) – Specifies how the sampler initializes parameter values. Initialization is either uniform random on a range centered on 0, exactly 0, or a dictionary or file of initial values for some or all parameters in the model. The default initialization behavior will initialize all parameter values on range $[-2, 2]$ on the *unconstrained* support. If the expected parameter values are too far from this range, this option may improve estimation. The following value types are allowed:
 - Single number, $n > 0$ - initialization range is $[-n, n]$.
 - 0 - all parameters are initialized to 0.
 - dictionary - pairs parameter name : initial value.
 - string - pathname to a JSON or Rdump data file.

- **output_dir** (*Optional* [*Union* [*str*, *PathLike*]]) – Name of the directory to which CmdStan output files are written. If unspecified, output files will be written to a temporary directory which is deleted upon session exit.
- **sig_figs** (*Optional* [*int*]) – Numerical precision used for output CSV and text files. Must be an integer between 1 and 18. If unspecified, the default precision for the system file I/O is used; the usual value is 6. Introduced in CmdStan-2.25.
- **save_profile** (*bool*) – Whether or not to profile auto-diff operations in labelled blocks of code. If True, CSV outputs are written to file ‘<model_name>-<YYYYMMDDHHMM>-profile-<chain_id>’. Introduced in CmdStan-2.26.
- **algorithm** (*Optional* [*str*]) – Algorithm to use. One of: ‘BFGS’, ‘LBFGS’, ‘Newton’
- **init_alpha** (*Optional* [*float*]) – Line search step size for first iteration
- **tol_obj** (*Optional* [*float*]) – Convergence tolerance on changes in objective function value
- **tol_rel_obj** (*Optional* [*float*]) – Convergence tolerance on relative changes in objective function value
- **tol_grad** (*Optional* [*float*]) – Convergence tolerance on the norm of the gradient
- **tol_rel_grad** (*Optional* [*float*]) – Convergence tolerance on the relative norm of the gradient
- **tol_param** (*Optional* [*float*]) – Convergence tolerance on changes in parameter value
- **history_size** (*Optional* [*int*]) – Size of the history for LBFGS Hessian approximation. The value should be less than the dimensionality of the parameter space. 5-10 usually sufficient
- **iter** (*Optional* [*int*]) – Total number of iterations
- **save_iterations** (*bool*) – When True, save intermediate approximations to the output CSV file. Default is False.
- **require_converged** (*bool*) – Whether or not to raise an error if Stan reports that “The algorithm may not have converged”.
- **show_console** (*bool*) – If True, stream CmdStan messages sent to stdout and stderr to the console. Default is False.
- **refresh** (*Optional* [*int*]) – Specify the number of iterations cmdstan will take between progress messages. Default value is 100.
- **time_fmt** (*str*) – A format string passed to `strftime()` to decide the file names for output CSVs. Defaults to “%Y%m%d%H%M%S”
- **timeout** (*Optional* [*float*]) – Duration at which optimization times out in seconds.
- **jacobian** (*bool*) – Whether or not to use the Jacobian adjustment for constrained variables in optimization. By default this is false, meaning optimization yields the Maximum Likelihood Estimate (MLE). Setting it to true yields the Maximum A Posteriori Estimate (MAP).

Returns

CmdStanMLE object

Return type

`CmdStanMLE`

```
pathfinder(data=None, *, init_alpha=None, tol_obj=None, tol_rel_obj=None, tol_grad=None,
            tol_rel_grad=None, tol_param=None, history_size=None, num_paths=None,
            max_lbfgs_iters=None, draws=None, num_single_draws=None, num_elbo_draws=None,
            psis_resample=True, calculate_lp=True, seed=None, inits=None, output_dir=None,
            sig_figs=None, save_profile=False, show_console=False, refresh=None,
            time_fmt='%Y%m%d%H%M%S', timeout=None, num_threads=None)
```

Run CmdStan's Pathfinder variational inference algorithm.

Parameters

- **data** (*Optional*[*Union*[*Mapping*[*str*, *Any*], *str*, *PathLike*]]) – Values for all data variables in the model, specified either as a dictionary with entries matching the data variables, or as the path of a data file in JSON or Rdump format.
- **num_paths** (*Optional*[*int*]) – Number of single-path Pathfinders to run. Default is 4, when the number of paths is 1 then no importance sampling is done.
- **draws** (*Optional*[*int*]) – Number of approximate draws to return.
- **num_single_draws** (*Optional*[*int*]) – Number of draws each single-pathfinder will draw. If `num_paths` is 1, only one of this and `draws` should be used.
- **max_lbfgs_iters** (*Optional*[*int*]) – Maximum number of L-BFGS iterations.
- **num_elbo_draws** (*Optional*[*int*]) – Number of Monte Carlo draws to evaluate ELBO.
- **psis_resample** (*bool*) – Whether or not to use Pareto Smoothed Importance Sampling on the result of the individual Pathfinders. If False, the result contains the draws from each path.
- **calculate_lp** (*bool*) – Whether or not to calculate the log probability for approximate draws. If False, this also implies that `psis_resample` will be set to False.
- **seed** (*Optional*[*int*]) – The seed for random number generator. Must be an integer between 0 and $2^{32} - 1$. If unspecified, `numpy.random.default_rng()` is used to generate a seed.
- **inits** (*Optional*[*Union*[*Dict*[*str*, *float*], *float*, *str*, *PathLike*]]) – Specifies how the algorithm initializes parameter values. Initialization is either uniform random on a range centered on 0, exactly 0, or a dictionary or file of initial values for some or all parameters in the model. The default initialization behavior will initialize all parameter values on range $[-2, 2]$ on the *unconstrained* support. If the expected parameter values are too far from this range, this option may improve adaptation. The following value types are allowed:
 - Single number $n > 0$ - initialization range is $[-n, n]$.
 - 0 - all parameters are initialized to 0.
 - dictionary - pairs parameter name : initial value.
 - string - pathname to a JSON or Rdump data file.
 - list of strings - per-path pathname to data file.
 - list of dictionaries - per-path initial values.
- **init_alpha** (*Optional*[*float*]) – For internal L-BFGS: Line search step size for first iteration
- **tol_obj** (*Optional*[*float*]) – For internal L-BFGS: Convergence tolerance on changes in objective function value

- **tol_rel_obj** (*Optional[float]*) – For internal L-BFGS: Convergence tolerance on relative changes in objective function value
- **tol_grad** (*Optional[float]*) – For internal L-BFGS: Convergence tolerance on the norm of the gradient
- **tol_rel_grad** (*Optional[float]*) – For internal L-BFGS: Convergence tolerance on the relative norm of the gradient
- **tol_param** (*Optional[float]*) – For internal L-BFGS: Convergence tolerance on changes in parameter value
- **history_size** (*Optional[int]*) – For internal L-BFGS: Size of the history for LBFGS Hessian approximation. The value should be less than the dimensionality of the parameter space. 5-10 is usually sufficient
- **output_dir** (*Optional[Union[str, PathLike]]*) – Name of the directory to which CmdStan output files are written. If unspecified, output files will be written to a temporary directory which is deleted upon session exit.
- **sig_figs** (*Optional[int]*) – Numerical precision used for output CSV and text files. Must be an integer between 1 and 18. If unspecified, the default precision for the system file I/O is used; the usual value is 6. Introduced in CmdStan-2.25.
- **save_profile** (*bool*) – Whether or not to profile auto-diff operations in labelled blocks of code. If True, CSV outputs are written to file ‘<model_name>-<YYYYMMDDHHMM>-profile-<path_id>’. Introduced in CmdStan-2.26, see https://mc-stan.org/docs/cmdstan-guide/stan_csv.html, section “Profiling CSV output file” for details.
- **show_console** (*bool*) – If True, stream CmdStan messages sent to stdout and stderr to the console. Default is False.
- **refresh** (*Optional[int]*) – Specify the number of iterations CmdStan will take between progress messages. Default value is 100.
- **time_fmt** (*str*) – A format string passed to `strftime()` to decide the file names for output CSVs. Defaults to “%Y%m%d%H%M%S”
- **timeout** (*Optional[float]*) – Duration at which Pathfinder times out in seconds. Defaults to None.
- **num_threads** (*Optional[int]*) – Number of threads to request for parallel execution. A number other than 1 requires the model to have been compiled with STAN_THREADS=True.

Returns

A `CmdStanPathfinder` object

Return type

`CmdStanPathfinder`

References

Zhang, L., Carpenter, B., Gelman, A., & Vehtari, A. (2022). Pathfinder: Parallel quasi-Newton variational inference. *Journal of Machine Learning Research*, 23(306), 1–49. Retrieved from <http://jmlr.org/papers/v23/21-0889.html>

```
sample(data=None, chains=None, parallel_chains=None, threads_per_chain=None, seed=None,
        chain_ids=None, inits=None, iter_warmup=None, iter_sampling=None, save_warmup=False,
        thin=None, max_treedepth=None, metric=None, step_size=None, adapt_engaged=True,
        adapt_delta=None, adapt_init_phase=None, adapt_metric_window=None, adapt_step_size=None,
        fixed_param=False, output_dir=None, sig_figs=None, save_latent_dynamics=False,
        save_profile=False, show_progress=True, show_console=False, refresh=None,
        time_fmt='%Y%m%d%H%M%S', timeout=None, *, force_one_process_per_chain=None)
```

Run or more chains of the NUTS-HMC sampler to produce a set of draws from the posterior distribution of a model conditioned on some data.

This function validates the specified configuration, composes a call to the CmdStan `sample` method and spawns one subprocess per chain to run the sampler and waits for all chains to run to completion. Unspecified arguments are not included in the call to CmdStan, i.e., those arguments will have CmdStan default values.

For each chain, the `CmdStanMCMC` object records the command, the return code, the sampler output file paths, and the corresponding console outputs, if any. The output files are written either to a specified output directory or to a temporary directory which is deleted upon session exit.

Output files are either written to a temporary directory or to the specified output directory. Output file-names correspond to the template ‘<model_name>-<YYYYMMDDHHMM>-<chain_id>’ plus the file suffix which is either ‘.csv’ for the CmdStan output or ‘.txt’ for the console messages, e.g. ‘bernoulli-201912081451-1.csv’. Output files written to the temporary directory contain an additional 8-character random string, e.g. ‘bernoulli-201912081451-1-5nm6as7u.csv’.

Parameters

- **data** (*Optional*[*Union*[*Mapping*[*str*, *Any*], *str*, *PathLike*]]) – Values for all data variables in the model, specified either as a dictionary with entries matching the data variables, or as the path of a data file in JSON or Rdump format.
- **chains** (*Optional*[*int*]) – Number of sampler chains, must be a positive integer.
- **parallel_chains** (*Optional*[*int*]) – Number of processes to run in parallel. Must be a positive integer. Defaults to `multiprocessing.cpu_count()`, i.e., it will only run as many chains in parallel as there are cores on the machine. Note that CmdStan 2.28 and higher can run all chains in parallel providing that the model was compiled with threading support.
- **threads_per_chain** (*Optional*[*int*]) – The number of threads to use in parallelized sections within an MCMC chain (e.g., when using the Stan functions `reduce_sum()` or `map_rect()`). This will only have an effect if the model was compiled with threading support. For such models, CmdStan version 2.28 and higher will run all chains in parallel from within a single process. The total number of threads used will be `parallel_chains * threads_per_chain`, where the default value for `parallel_chains` is the number of cpus, not chains.
- **seed** (*Optional*[*Union*[*int*, *List*[*int*]]]) – The seed for random number generator. Must be an integer between 0 and $2^{32} - 1$. If unspecified, `numpy.random.default_rng()` is used to generate a seed which will be used for all chains. When the same seed is used across all chains, the chain-id is used to advance the RNG to avoid dependent samples.

- **chain_ids** (*Optional*[*Union*[*int*, *List*[*int*]]]) – The offset for the random number generator, either an integer or a list of unique per-chain offsets. If unspecified, chain ids are numbered sequentially starting from 1.
- **inits** (*Optional*[*Union*[*Mapping*[*str*, *Any*], *float*, *str*, *List*[*str*], *List*[*Mapping*[*str*, *Any*]]]]) – Specifies how the sampler initializes parameter values. Initialization is either uniform random on a range centered on 0, exactly 0, or a dictionary or file of initial values for some or all parameters in the model. The default initialization behavior will initialize all parameter values on range [-2, 2] on the *unconstrained* support. If the expected parameter values are too far from this range, this option may improve adaptation. The following value types are allowed:
 - Single number $n > 0$ - initialization range is $[-n, n]$.
 - 0 - all parameters are initialized to 0.
 - dictionary - pairs parameter name : initial value.
 - string - pathname to a JSON or Rdump data file.
 - list of strings - per-chain pathname to data file.
 - list of dictionaries - per-chain initial values.
- **iter_warmup** (*Optional*[*int*]) – Number of warmup iterations for each chain.
- **iter_sampling** (*Optional*[*int*]) – Number of draws from the posterior for each chain.
- **save_warmup** (*bool*) – When True, sampler saves warmup draws as part of the Stan CSV output file.
- **thin** (*Optional*[*int*]) – Period between recorded iterations. Default is 1, i.e., all iterations are recorded.
- **max_treedepth** (*Optional*[*int*]) – Maximum depth of trees evaluated by NUTS sampler per iteration.
- **metric** (*Optional*[*Union*[*str*, *Dict*[*str*, *Any*], *List*[*str*], *List*[*Dict*[*str*, *Any*]]]]) – Specification of the mass matrix, either as a vector consisting of the diagonal elements of the covariance matrix ('diag' or 'diag_e') or the full covariance matrix ('dense' or 'dense_e').

If the value of the metric argument is a string other than 'diag', 'diag_e', 'dense', or 'dense_e', it must be a valid filepath to a JSON or Rdump file which contains an entry 'inv_metric' whose value is either the diagonal vector or the full covariance matrix.

If the value of the metric argument is a list of paths, its length must match the number of chains and all paths must be unique.

If the value of the metric argument is a Python dict object, it must contain an entry 'inv_metric' which specifies either the diagonal or dense matrix.

If the value of the metric argument is a list of Python dicts, its length must match the number of chains and all dicts must contain an entry 'inv_metric' and all 'inv_metric' entries must have the same shape.
- **step_size** (*Optional*[*Union*[*float*, *List*[*float*]]]) – Initial step size for HMC sampler. The value is either a single number or a list of numbers which will be used as the global or per-chain initial step size, respectively. The length of the list of step sizes must match the number of chains.
- **adapt_engaged** (*bool*) – When True, adapt step size and metric.

- **adapt_delta** (*Optional*[*float*]) – Adaptation target Metropolis acceptance rate. The default value is 0.8. Increasing this value, which must be strictly less than 1, causes adaptation to use smaller step sizes which improves the effective sample size, but may increase the time per iteration.
- **adapt_init_phase** (*Optional*[*int*]) – Iterations for initial phase of adaptation during which step size is adjusted so that the chain converges towards the typical set.
- **adapt_metric_window** (*Optional*[*int*]) – The second phase of adaptation tunes the metric and step size in a series of intervals. This parameter specifies the number of iterations used for the first tuning interval; window size increases for each subsequent interval.
- **adapt_step_size** (*Optional*[*int*]) – Number of iterations given over to adjusting the step size given the tuned metric during the final phase of adaptation.
- **fixed_param** (*bool*) – When True, call CmdStan with argument `algorithm=fixed_param` which runs the sampler without updating the Markov Chain, thus the values of all parameters and transformed parameters are constant across all draws and only those values in the generated quantities block that are produced by RNG functions may change. This provides a way to use Stan programs to generate simulated data via the generated quantities block. Default value is False.
- **output_dir** (*Optional*[*Union*[*str*, *PathLike*]]) – Name of the directory to which CmdStan output files are written. If unspecified, output files will be written to a temporary directory which is deleted upon session exit.
- **sig_figs** (*Optional*[*int*]) – Numerical precision used for output CSV and text files. Must be an integer between 1 and 18. If unspecified, the default precision for the system file I/O is used; the usual value is 6. Introduced in CmdStan-2.25.
- **save_latent_dynamics** (*bool*) – Whether or not to output the position and momentum information for the model parameters (unconstrained). If True, CSV outputs are written to an output file ‘<model_name>-<YYYYMMDDHHMM>-diagnostic-<chain_id>’, e.g. ‘bernoulli-201912081451-diagnostic-1.csv’, see https://mc-stan.org/docs/cmdstan-guide/stan_csv.html, section “Diagnostic CSV output file” for details.
- **save_profile** (*bool*) – Whether or not to profile auto-diff operations in labelled blocks of code. If True, CSV outputs are written to file ‘<model_name>-<YYYYMMDDHHMM>-profile-<chain_id>’. Introduced in CmdStan-2.26, see https://mc-stan.org/docs/cmdstan-guide/stan_csv.html, section “Profiling CSV output file” for details.
- **show_progress** (*bool*) – If True, display progress bar to track progress for warmup and sampling iterations. Default is True, unless package tqdm progress bar encounter errors.
- **show_console** (*bool*) – If True, stream CmdStan messages sent to stdout and stderr to the console. Default is False.
- **refresh** (*Optional*[*int*]) – Specify the number of iterations CmdStan will take between progress messages. Default value is 100.
- **time_fmt** (*str*) – A format string passed to `strftime()` to decide the file names for output CSVs. Defaults to “%Y%m%d%H%M%S”
- **force_one_process_per_chain** (*Optional*[*bool*]) – If True, run multiple chains in distinct processes regardless of model ability to run parallel chains (CmdStan 2.28+ feature). If False, always run multiple chains in one process (does not check that this is valid).

If None (Default): Check that CmdStan version is ≥ 2.28 , and that model was compiled

with `STAN_THREADS=True`, and utilize the parallel chain functionality if those conditions are met.

- **timeout** (*Optional*[*float*]) – Duration at which sampling times out in seconds.

Returns

CmdStanMCMC object

Return type

CmdStanMCMC

src_info()

Run stanc with option ‘-info’.

If stanc is older than 2.27 or if the stan file cannot be found, returns an empty dictionary.

Return type

Dict[*str*, *Any*]

variational(*data=None*, *seed=None*, *inits=None*, *output_dir=None*, *sig_figs=None*, *save_latent_dynamics=False*, *save_profile=False*, *algorithm=None*, *iter=None*, *grad_samples=None*, *elbo_samples=None*, *eta=None*, *adapt_engaged=True*, *adapt_iter=None*, *tol_rel_obj=None*, *eval_elbo=None*, *draws=None*, *require_converged=True*, *show_console=False*, *refresh=None*, *time_fmt='%Y%m%d%H%M%S'*, *timeout=None*, *, *output_samples=None*)

Run CmdStan’s variational inference algorithm to approximate the posterior distribution of the model conditioned on the data.

This function validates the specified configuration, composes a call to the CmdStan `variational` method and spawns one subprocess to run the optimizer and waits for it to run to completion. Unspecified arguments are not included in the call to CmdStan, i.e., those arguments will have CmdStan default values.

The `CmdStanVB` object records the command, the return code, and the paths to the variational method output CSV and console files. The output files are written either to a specified output directory or to a temporary directory which is deleted upon session exit.

Output files are either written to a temporary directory or to the specified output directory. Output file-names correspond to the template ‘<model_name>-<YYYYMMDDHHMM>-<chain_id>’ plus the file suffix which is either ‘.csv’ for the CmdStan output or ‘.txt’ for the console messages, e.g. ‘bernoulli-201912081451-1.csv’. Output files written to the temporary directory contain an additional 8-character random string, e.g. ‘bernoulli-201912081451-1-5nm6as7u.csv’.

Parameters

- **data** (*Optional*[*Union*[*Mapping*[*str*, *Any*], *str*, *PathLike*]]) – Values for all data variables in the model, specified either as a dictionary with entries matching the data variables, or as the path of a data file in JSON or Rdump format.
- **seed** (*Optional*[*int*]) – The seed for random number generator. Must be an integer between 0 and $2^{32} - 1$. If unspecified, `numpy.random.default_rng()` is used to generate a seed which will be used for all chains.
- **inits** (*Optional*[*float*]) – Specifies how the sampler initializes parameter values. Initialization is uniform random on a range centered on 0 with default range of 2. Specifying a single number $n > 0$ changes the initialization range to $[-n, n]$.
- **output_dir** (*Optional*[*Union*[*str*, *PathLike*]]) – Name of the directory to which CmdStan output files are written. If unspecified, output files will be written to a temporary directory which is deleted upon session exit.

- **sig_figs** (*Optional[int]*) – Numerical precision used for output CSV and text files. Must be an integer between 1 and 18. If unspecified, the default precision for the system file I/O is used; the usual value is 6. Introduced in CmdStan-2.25.
- **save_latent_dynamics** (*bool*) – Whether or not to save diagnostics. If True, CSV outputs are written to output file ‘<model_name>-<YYYYMMDDHHMM>-diagnostic-<chain_id>’, e.g. ‘bernoulli-201912081451-diagnostic-1.csv’.
- **save_profile** (*bool*) – Whether or not to profile auto-diff operations in labelled blocks of code. If True, CSV outputs are written to file ‘<model_name>-<YYYYMMDDHHMM>-profile-<chain_id>’. Introduced in CmdStan-2.26.
- **algorithm** (*Optional[str]*) – Algorithm to use. One of: ‘meanfield’, ‘fullrank’.
- **iter** (*Optional[int]*) – Maximum number of ADVI iterations.
- **grad_samples** (*Optional[int]*) – Number of MC draws for computing the gradient. Default is 10. If problems arise, try doubling current value.
- **elbo_samples** (*Optional[int]*) – Number of MC draws for estimate of ELBO.
- **eta** (*Optional[float]*) – Step size scaling parameter.
- **adapt_engaged** (*bool*) – Whether eta adaptation is engaged.
- **adapt_iter** (*Optional[int]*) – Number of iterations for eta adaptation.
- **tol_rel_obj** (*Optional[float]*) – Relative tolerance parameter for convergence.
- **eval_elbo** (*Optional[int]*) – Number of iterations between ELBO evaluations.
- **draws** (*Optional[int]*) – Number of approximate posterior output draws to save.
- **require_converged** (*bool*) – Whether or not to raise an error if Stan reports that “The algorithm may not have converged”.
- **show_console** (*bool*) – If True, stream CmdStan messages sent to stdout and stderr to the console. Default is False.
- **refresh** (*Optional[int]*) – Specify the number of iterations CmdStan will take between progress messages. Default value is 100.
- **time_fmt** (*str*) – A format string passed to `strftime()` to decide the file names for output CSVs. Defaults to “%Y%m%d%H%M%S”
- **timeout** (*Optional[float]*) – Duration at which variational Bayesian inference times out in seconds.
- **output_samples** (*Optional[int]*) –

Returns

CmdStanVB object

Return type

CmdStanVB

property `cpp_options`: `Dict[str, Union[bool, int]]`

Options to C++ compilers.

property `exe_file`: `Optional[Union[str, PathLike]]`

Full path to Stan exe file.

property `name`: `str`Model name used in output filename templates. Default is basename of Stan program or exe file, unless specified in call to constructor via argument `model_name`.

property stan_file: `Optional[Union[str, PathLike]]`

Full path to Stan program file.

property stanc_options: `Dict[str, Union[bool, int, str]]`

Options to stanc compilers.

property user_header: `str`

The user header file if it exists, otherwise empty

3.2.2 CmdStanMCMC

class `cmdstanpy.CmdStanMCMC(runset)`

Container for outputs from CmdStan sampler run. Provides methods to summarize and diagnose the model fit and accessor methods to access the entire sample or individual items. Created by `CmdStanModel.sample()`

The sample is lazily instantiated on first access of either the resulting sample or the HMC tuning parameters, i.e., the step size and metric.

Parameters

runset (`RunSet`) –

diagnose()

Run `cmdstan/bin/diagnose` over all output CSV files, return console output.

The diagnose utility reads the outputs of all chains and checks for the following potential problems:

- Transitions that hit the maximum treedepth
- Divergent transitions
- Low E-BFMI values (sampler transitions HMC potential energy)
- Low effective sample sizes
- High R-hat values

Return type

`Optional[str]`

draws(`*`, `inc_warmup=False`, `concat_chains=False`)

Returns a `numpy.ndarray` over all draws from all chains which is stored column major so that the values for a parameter are contiguous in memory, likewise all draws from a chain are contiguous. By default, returns a 3D array arranged (draws, chains, columns); parameter `concat_chains=True` will return a 2D array where all chains are flattened into a single column, preserving chain order, so that given `M` chains of `N` draws, the first `N` draws are from chain 1, up through the last `N` draws from chain `M`.

Parameters

- **inc_warmup** (`bool`) – When `True` and the warmup draws are present in the output, i.e., the sampler was run with `save_warmup=True`, then the warmup draws are included. Default value is `False`.
- **concat_chains** (`bool`) – When `True` return a 2D array flattening all all draws from all chains. Default value is `False`.

Return type

`ndarray`

See also:

[`CmdStanMCMC.draws_pd`](#), [`CmdStanMCMC.draws_xr`](#), [`CmdStanGQ.draws`](#)

draws_pd(*vars=None, inc_warmup=False*)

Returns the sample draws as a pandas DataFrame. Flattens all chains into single column. Container variables (array, vector, matrix) will span multiple columns, one column per element. E.g. variable 'matrix[2,2] foo' spans 4 columns: 'foo[1,1], ... foo[2,2]'.

Parameters

- **vars** (*Optional[Union[List[str], str]]*) – optional list of variable names.
- **inc_warmup** (*bool*) – When True and the warmup draws are present in the output, i.e., the sampler was run with `save_warmup=True`, then the warmup draws are included. Default value is False.

Return type

DataFrame

See also:

[`CmdStanMCMC.draws`](#), [`CmdStanMCMC.draws_xr`](#), [`CmdStanGQ.draws_pd`](#)

draws_xr(*vars=None, inc_warmup=False*)

Returns the sampler draws as a xarray Dataset.

Parameters

- **vars** (*Optional[Union[List[str], str]]*) – optional list of variable names.
- **inc_warmup** (*bool*) – When True and the warmup draws are present in the output, i.e., the sampler was run with `save_warmup=True`, then the warmup draws are included. Default value is False.

Return type

Dataset

See also:

[`CmdStanMCMC.draws`](#), [`CmdStanMCMC.draws_pd`](#), [`CmdStanGQ.draws_xr`](#)

method_variables()

Returns a dictionary of all sampler variables, i.e., all output column names ending in `_`. Assumes that all variables are scalar variables where column name is variable name. Maps each column name to a numpy.ndarray (draws x chains x 1) containing per-draw diagnostic values.

Return type

Dict[str, ndarray]

save_csvfiles(*dir=None*)

Move output CSV files to specified directory. If files were written to the temporary session directory, clean filename. E.g., save 'bernoulli-201912081451-1-5nm6as7u.csv' as 'bernoulli-201912081451-1.csv'.

Parameters

dir (*Optional[str]*) – directory path

Return type

None

See also:

[`stanfit.RunSet.save_csvfiles`](#), [`cmdstanpy.from_csv`](#)

stan_variable(var, inc_warmup=False)

Return a numpy.ndarray which contains the set of draws for the named Stan program variable. Flattens the chains, leaving the draws in chain order. The first array dimension, corresponds to number of draws or post-warmup draws in the sample, per argument `inc_warmup`. The remaining dimensions correspond to the shape of the Stan program variable.

Underlyingly draws are in chain order, i.e., for a sample with N chains of M draws each, the first M array elements are from chain 1, the next M are from chain 2, and the last M elements are from chain N.

- If the variable is a scalar variable, the return array has shape (draws * chains, 1).
- If the variable is a vector, the return array has shape (draws * chains, len(vector))
- If the variable is a matrix, the return array has shape (draws * chains, size(dim 1), size(dim 2))
- If the variable is an array with N dimensions, the return array has shape (draws * chains, size(dim 1), ..., size(dim N))

For example, if the Stan program variable `theta` is a 3x3 matrix, and the sample consists of 4 chains with 1000 post-warmup draws, this function will return a numpy.ndarray with shape (4000,3,3).

This functionality is also available via a shortcut using `.` - writing `fit.a` is a synonym for `fit.stan_variable("a")`

Parameters

- **var** (*str*) – variable name
- **inc_warmup** (*bool*) – When True and the warmup draws are present in the output, i.e., the sampler was run with `save_warmup=True`, then the warmup draws are included. Default value is False.

Return type

ndarray

See also:

`CmdStanMCMC.stan_variables`, `CmdStanMLE.stan_variable`, `CmdStanPathfinder.stan_variable`, `CmdStanVB.stan_variable`, `CmdStanGQ.stan_variable`, `CmdStanLaplace.stan_variable`

stan_variables()

Return a dictionary mapping Stan program variables names to the corresponding numpy.ndarray containing the inferred values.

See also:

`CmdStanMCMC.stan_variable`, `CmdStanMLE.stan_variables`, `CmdStanPathfinder.stan_variables`, `CmdStanVB.stan_variables`, `CmdStanGQ.stan_variables`, `CmdStanLaplace.stan_variables`

Return type

Dict[str, ndarray]

summary(percentiles=(5, 50, 95), sig_figs=6)

Run `cmdstan/bin/stansummary` over all output CSV files, assemble summary into DataFrame object. The first row contains statistics for the total joint log probability `lp__`, but is omitted when the Stan model has no parameters. The remaining rows contain summary statistics for all parameters, transformed parameters, and generated quantities variables, in program declaration order.

Parameters

- **percentiles** (*Sequence[int]*) – Ordered non-empty sequence of percentiles to report. Must be integers from (1, 99), inclusive. Defaults to (5, 50, 95)
- **sig_figs** (*int*) – Number of significant figures to report. Must be an integer between 1 and 18. If unspecified, the default precision for the system file I/O is used; the usual value is 6. If precision above 6 is requested, sample must have been produced by CmdStan version 2.25 or later and sampler output precision must equal to or greater than the requested summary precision.

Returns

pandas.DataFrame

Return type*DataFrame***property chain_ids:** *List[int]*

Chain ids.

property chains: *int*

Number of chains.

property column_names: *Tuple[str, ...]*

Names of all outputs from the sampler, comprising sampler parameters and all components of all model parameters, transformed parameters, and quantities of interest. Corresponds to Stan CSV file header row, with names munged to array notation, e.g. *beta[1]* not *beta.1*.

property divergences: *Optional[ndarray]*

Per-chain total number of post-warmup divergent iterations. When sampler algorithm ‘fixed_param’ is specified, returns None.

property max_treedepths: *Optional[ndarray]*

Per-chain total number of post-warmup iterations where the NUTS sampler reached the maximum allowed treedepth. When sampler algorithm ‘fixed_param’ is specified, returns None.

property metadata: *InferenceMetadata*

Returns object which contains CmdStan configuration as well as information about the names and structure of the inference method and model output variables.

property metric: *Optional[ndarray]*

Metric used by sampler for each chain. When sampler algorithm ‘fixed_param’ is specified, metric is None.

property metric_type: *Optional[str]*

Metric type used for adaptation, either ‘diag_e’ or ‘dense_e’, according to CmdStan arg ‘metric’. When sampler algorithm ‘fixed_param’ is specified, metric_type is None.

property num_draws_sampling: *int*

Number of sampling (post-warmup) draws per chain, i.e., thinned sampling iterations.

property num_draws_warmup: *int*

Number of warmup draws per chain, i.e., thinned warmup iterations.

property step_size: *Optional[ndarray]*

Step size used by sampler for each chain. When sampler algorithm ‘fixed_param’ is specified, step size is None.

property thin: *int*

Period between recorded iterations. (Default is 1).

3.2.3 CmdStanMLE

class cmdstanpy.CmdStanMLE(*runset*)

Container for outputs from CmdStan optimization. Created by [CmdStanModel.optimize\(\)](#).

Parameters

runset ([RunSet](#)) –

save_csvfiles(*dir=None*)

Move output CSV files to specified directory. If files were written to the temporary session directory, clean filename. E.g., save ‘bernoulli-201912081451-1-5nm6as7u.csv’ as ‘bernoulli-201912081451-1.csv’.

Parameters

dir ([Optional](#) [*str*]) – directory path

Return type

None

See also:

[stanfit.RunSet.save_csvfiles](#), [cmdstanpy.from_csv](#)

stan_variable(*var*, *, *inc_iterations=False*, *warn=True*)

Return a numpy.ndarray which contains the estimates for the for the named Stan program variable where the dimensions of the numpy.ndarray match the shape of the Stan program variable.

This functionality is also available via a shortcut using `.` - writing `fit.a` is a synonym for `fit.stan_variable("a")`

Parameters

- **var** (*str*) – variable name
- **inc_iterations** (*bool*) – When True and the intermediate estimates are included in the output, i.e., the optimizer was run with `save_iterations=True`, then intermediate estimates are included. Default value is False.
- **warn** (*bool*) –

Return type

[Union](#)[[ndarray](#), float]

See also:

[CmdStanMLE.stan_variables](#), [CmdStanMCMC.stan_variable](#), [CmdStanPathfinder.stan_variable](#), [CmdStanVB.stan_variable](#), [CmdStanGQ.stan_variable](#), [CmdStanLaplace.stan_variable](#)

stan_variables(*inc_iterations=False*)

Return a dictionary mapping Stan program variables names to the corresponding numpy.ndarray containing the inferred values.

Parameters

inc_iterations (*bool*) – When True and the intermediate estimates are included in the output, i.e., the optimizer was run with `save_iterations=True`, then intermediate estimates are included. Default value is False.

Return type

[Dict](#)[*str*, [Union](#)[[ndarray](#), float]]

See also:

`CmdStanMLE.stan_variable`, `CmdStanMCMC.stan_variables`, `CmdStanPathfinder.stan_variables`, `CmdStanVB.stan_variables`, `CmdStanGQ.stan_variables`, `CmdStanLaplace.stan_variables`

property column_names: `Tuple[str, ...]`

Names of estimated quantities, includes joint log probability, and all parameters, transformed parameters, and generated quantities.

property metadata: `InferenceMetadata`

Returns object which contains CmdStan configuration as well as information about the names and structure of the inference method and model output variables.

property optimized_iterations_np: `Optional[ndarray]`

Returns all saved iterations from the optimizer and final estimate as a `numpy.ndarray` which contains all optimizer outputs, i.e., the value for `lp__` as well as all Stan program variables.

property optimized_iterations_pd: `Optional[DataFrame]`

Returns all saved iterations from the optimizer and final estimate as a `pandas.DataFrame` which contains all optimizer outputs, i.e., the value for `lp__` as well as all Stan program variables.

property optimized_params_dict: `Dict[str, float64]`

Returns all estimates from the optimizer, including `lp__` as a Python Dict. Only returns estimate from final iteration.

property optimized_params_np: `ndarray`

Returns all final estimates from the optimizer as a `numpy.ndarray` which contains all optimizer outputs, i.e., the value for `lp__` as well as all Stan program variables.

property optimized_params_pd: `DataFrame`

Returns all final estimates from the optimizer as a `pandas.DataFrame` which contains all optimizer outputs, i.e., the value for `lp__` as well as all Stan program variables.

3.2.4 CmdStanLaplace

class `cmdstanpy.CmdStanLaplace(runset, mode)`

Parameters

- **runset** (`RunSet`) –
- **mode** (`CmdStanMLE`) –

draws()

Return a `numpy.ndarray` containing the draws from the approximate posterior distribution. This is a 2-D array of shape (draws, parameters).

Return type

`ndarray`

draws_xr (`vars=None`)

Returns the sampler draws as a xarray Dataset.

Parameters

vars (`Optional[Union[List[str], str]]`) – optional list of variable names.

Return type

`Dataset`

See also:

CmdStanMCMC.draws_xr, *CmdStanGQ.draws_xr*

method_variables()

Returns a dictionary of all sampler variables, i.e., all output column names ending in `__`. Assumes that all variables are scalar variables where column name is variable name. Maps each column name to a `numpy.ndarray` (draws x chains x 1) containing per-draw diagnostic values.

Return type

Dict[str, ndarray]

save_csvfiles(dir=None)

Move output CSV files to specified directory. If files were written to the temporary session directory, clean filename. E.g., save 'bernoulli-201912081451-1-5nm6as7u.csv' as 'bernoulli-201912081451-1.csv'.

Parameters

dir (*Optional[str]*) – directory path

Return type

None

See also:

stanfit.RunSet.save_csvfiles, *cmdstanpy.from_csv*

stan_variable(var)

Return a `numpy.ndarray` which contains the estimates for the for the named Stan program variable where the dimensions of the `numpy.ndarray` match the shape of the Stan program variable.

This functionality is also available via a shortcut using `.` - writing `fit.a` is a synonym for `fit.stan_variable("a")`

Parameters

var (*str*) – variable name

Return type

ndarray

See also:

CmdStanMLE.stan_variables, *CmdStanMCMC.stan_variable*, *CmdStanPathfinder.stan_variable*, *CmdStanVB.stan_variable*, *CmdStanGQ.stan_variable*

stan_variables()

Return a dictionary mapping Stan program variables names to the corresponding `numpy.ndarray` containing the inferred values.

Parameters

inc_warmup – When True and the warmup draws are present in the MCMC sample, then the warmup draws are included. Default value is False

Return type

Dict[str, ndarray]

See also:

CmdStanGQ.stan_variable, *CmdStanMCMC.stan_variables*, *CmdStanMLE.stan_variables*, *CmdStanPathfinder.stan_variables*, *CmdStanVB.stan_variables*

property column_names: `Tuple[str, ...]`

Names of all outputs from the sampler, comprising sampler parameters and all components of all model parameters, transformed parameters, and quantities of interest. Corresponds to Stan CSV file header row, with names munged to array notation, e.g. `beta[1]` not `beta.1`.

property metadata: `InferenceMetadata`

Returns object which contains CmdStan configuration as well as information about the names and structure of the inference method and model output variables.

property mode: `CmdStanMLE`

Return the maximum a posteriori estimate (mode) as a `CmdStanMLE` object.

3.2.5 CmdStanPathfinder

class `cmdstanpy.CmdStanPathfinder(runset)`

Container for outputs from the Pathfinder algorithm. Created by `CmdStanModel.pathfinder()`.

Parameters

runset (`RunSet`) –

create_inits(`seed=None, chains=4`)

Create initial values for the parameters of the model by randomly selecting draws from the Pathfinder approximation.

Parameters

- **seed** (`Optional[int]`) – Used for random selection, defaults to None
- **chains** (`int`) – Number of initial values to return, defaults to 4

Returns

The initial values for the parameters of the model.

Return type

`Union[List[Dict[str, ndarray]], Dict[str, ndarray]]`

If chains is 1, a dictionary is returned, otherwise a list of dictionaries is returned, in the format expected for the `inits` argument. of `CmdStanModel.sample()`.

draws()

Return a `numpy.ndarray` containing the draws from the approximate posterior distribution. This is a 2-D array of shape (draws, parameters).

Return type

`ndarray`

method_variables()

Returns a dictionary of all sampler variables, i.e., all output column names ending in `_`. Assumes that all variables are scalar variables where column name is variable name. Maps each column name to a `numpy.ndarray` (draws x chains x 1) containing per-draw diagnostic values.

Return type

`Dict[str, ndarray]`

save_csvfiles(`dir=None`)

Move output CSV files to specified directory. If files were written to the temporary session directory, clean filename. E.g., save 'bernoulli-201912081451-1-5nm6as7u.csv' as 'bernoulli-201912081451-1.csv'.

Parameters

dir (*Optional* [*str*]) – directory path

Return type

None

See also:

stanfit.RunSet.save_csvfiles, *cmdstanpy.from_csv*

stan_variable(var)

Return a numpy.ndarray which contains the estimates for the for the named Stan program variable where the dimensions of the numpy.ndarray match the shape of the Stan program variable.

This functionality is also available via a shortcut using `.` - writing `fit.a` is a synonym for `fit.stan_variable("a")`

Parameters

var (*str*) – variable name

Return type

ndarray

See also:

CmdStanPathfinder.stan_variables, *CmdStanMLE.stan_variable*, *CmdStanMCMC.stan_variable*, *CmdStanVB.stan_variable*, *CmdStanGQ.stan_variable*, *CmdStanLaplace.stan_variable*

stan_variables()

Return a dictionary mapping Stan program variables names to the corresponding numpy.ndarray containing the inferred values.

See also:

CmdStanPathfinder.stan_variable, *CmdStanMCMC.stan_variables*, *CmdStanMLE.stan_variables*, *CmdStanVB.stan_variables*, *CmdStanGQ.stan_variables*, *CmdStanLaplace.stan_variables*

Return type

Dict[*str*, *ndarray*]

property column_names: Tuple[str, ...]

Names of all outputs from the sampler, comprising sampler parameters and all components of all model parameters, transformed parameters, and quantities of interest. Corresponds to Stan CSV file header row, with names munged to array notation, e.g. *beta[1]* not *beta.1*.

property is_resampled: bool

Returns True if the draws were resampled from several Pathfinder approximations, False otherwise.

property metadata: InferenceMetadata

Returns object which contains CmdStan configuration as well as information about the names and structure of the inference method and model output variables.

3.2.6 CmdStanVB

class cmdstanpy.CmdStanVB(*runset*)

Container for outputs from CmdStan variational run. Created by `CmdStanModel.variational()`.

Parameters

runset (*RunSet*) –

save_csvfiles(*dir=None*)

Move output CSV files to specified directory. If files were written to the temporary session directory, clean filename. E.g., save ‘bernoulli-201912081451-1-5nm6as7u.csv’ as ‘bernoulli-201912081451-1.csv’.

Parameters

dir (*Optional[str]*) – directory path

Return type

None

See also:

`stanfit.RunSet.save_csvfiles`, `cmdstanpy.from_csv`

stan_variable(*var, *, mean=None*)

Return a numpy.ndarray which contains the estimates for the for the named Stan program variable where the dimensions of the numpy.ndarray match the shape of the Stan program variable, with a leading axis added for the number of draws from the variational approximation.

- If the variable is a scalar variable, the return array has shape (draws,).
- If the variable is a vector, the return array has shape (draws, len(vector))
- If the variable is a matrix, the return array has shape (draws, size(dim 1), size(dim 2))
- If the variable is an array with N dimensions, the return array has shape (draws, size(dim 1), ..., size(dim N))

This functionality is also available via a shortcut using `.` - writing `fit.a` is a synonym for `fit.stan_variable("a")`

Parameters

- **var** (*str*) – variable name
- **mean** (*Optional[bool]*) – if True, return the variational mean. Otherwise, return the variational sample. The default behavior will change in a future release to return the variational sample.

Return type

Union[ndarray, float]

See also:

`CmdStanVB.stan_variables`, `CmdStanMCMC.stan_variable`, `CmdStanMLE.stan_variable`, `CmdStanPathfinder.stan_variable`, `CmdStanGQ.stan_variable`, `CmdStanLaplace.stan_variable`

stan_variables(**, mean=None*)

Return a dictionary mapping Stan program variables names to the corresponding numpy.ndarray containing the inferred values.

See also:

`CmdStanVB.stan_variable`, `CmdStanMCMC.stan_variables`, `CmdStanMLE.stan_variables`,
`CmdStanGQ.stan_variables`, `CmdStanPathfinder.stan_variables`, `CmdStanLaplace.stan_variables`

Parameters

`mean` (*Optional*[*bool*]) –

Return type

Dict[*str*, *Union*[*ndarray*, *float*]]

property column_names: *Tuple*[*str*, ...]

Names of information items returned by sampler for each draw. Includes approximation information and names of model parameters and computed quantities.

property columns: *int*

Total number of information items returned by sampler. Includes approximation information and names of model parameters and computed quantities.

property eta: *float*

Step size scaling parameter ‘eta’

property metadata: *InferenceMetadata*

Returns object which contains CmdStan configuration as well as information about the names and structure of the inference method and model output variables.

property variational_params_dict: *Dict*[*str*, *ndarray*]

Returns inferred parameter means as Dict.

property variational_params_np: *ndarray*

Returns inferred parameter means as numpy array.

property variational_params_pd: *DataFrame*

Returns inferred parameter means as pandas DataFrame.

property variational_sample: *ndarray*

Returns the set of approximate posterior output draws.

property variational_sample_pd: *DataFrame*

Returns the set of approximate posterior output draws as a pandas DataFrame.

3.2.7 CmdStanGQ

class `cmdstanpy.CmdStanGQ`(*runset*, *previous_fit*)

Container for outputs from CmdStan `generate_quantities` run. Created by `CmdStanModel.generate_quantities()`.

Parameters

- `runset` (*RunSet*) –
- `previous_fit` (*Fit*) –

draws(*, *inc_warmup=False*, *inc_iterations=False*, *concat_chains=False*, *inc_sample=False*)

Returns a numpy.ndarray over the generated quantities draws from all chains which is stored column major so that the values for a parameter are contiguous in memory, likewise all draws from a chain are contiguous. By default, returns a 3D array arranged (draws, chains, columns); parameter *concat_chains=True* will return a 2D array where all chains are flattened into a single column, preserving chain order, so that given M chains of N draws, the first N draws are from chain 1, ..., and the the last N draws are from chain M.

Parameters

- **inc_warmup** (*bool*) – When True and the warmup draws are present in the output, i.e., the sampler was run with *save_warmup=True*, then the warmup draws are included. Default value is False.
- **concat_chains** (*bool*) – When True return a 2D array flattening all all draws from all chains. Default value is False.
- **inc_sample** (*bool*) – When True include all columns in the previous_fit draws array as well, excepting columns for variables already present in the generated quantities drawset. Default value is False.
- **inc_iterations** (*bool*) –

Return type

ndarray

See also:

[*CmdStanGQ.draws_pd*](#), [*CmdStanGQ.draws_xr*](#), [*CmdStanMCMC.draws*](#)

draws_pd(*vars=None*, *inc_warmup=False*, *inc_sample=False*)

Returns the generated quantities draws as a pandas DataFrame. Flattens all chains into single column. Container variables (array, vector, matrix) will span multiple columns, one column per element. E.g. variable 'matrix[2,2] foo' spans 4 columns: 'foo[1,1], ... foo[2,2]'.

Parameters

- **vars** (*Optional[Union[List[str], str]]*) – optional list of variable names.
- **inc_warmup** (*bool*) – When True and the warmup draws are present in the output, i.e., the sampler was run with *save_warmup=True*, then the warmup draws are included. Default value is False.
- **inc_sample** (*bool*) –

Return type

DataFrame

See also:

[*CmdStanGQ.draws*](#), [*CmdStanGQ.draws_xr*](#), [*CmdStanMCMC.draws_pd*](#)

draws_xr(*vars: Optional[Union[str, List[str]]] = None*, *inc_warmup: bool = False*, *inc_sample: bool = False*) → NoReturn

draws_xr(*vars: Optional[Union[str, List[str]]] = None*, *inc_warmup: bool = False*, *inc_sample: bool = False*) → Dataset

Returns the generated quantities draws as a xarray Dataset.

This method can only be called when the underlying fit was made through sampling, it cannot be used on MLE or VB outputs.

Parameters

- **vars** – optional list of variable names.

- **inc_warmup** – When True and the warmup draws are present in the MCMC sample, then the warmup draws are included. Default value is False.

See also:

CmdStanGQ.draws, *CmdStanGQ.draws_pd*, *CmdStanMCMC.draws_xr*

save_csvfiles(*dir=None*)

Move output CSV files to specified directory. If files were written to the temporary session directory, clean filename. E.g., save ‘bernoulli-201912081451-1-5nm6as7u.csv’ as ‘bernoulli-201912081451-1.csv’.

Parameters

dir (*Optional*[*str*]) – directory path

Return type

None

See also:

stanfit.RunSet.save_csvfiles, *cmdstanpy.from_csv*

stan_variable(*var, **kwargs*)

Return a numpy.ndarray which contains the set of draws for the named Stan program variable. Flattens the chains, leaving the draws in chain order. The first array dimension, corresponds to number of draws in the sample. The remaining dimensions correspond to the shape of the Stan program variable.

Underlyingly draws are in chain order, i.e., for a sample with N chains of M draws each, the first M array elements are from chain 1, the next M are from chain 2, and the last M elements are from chain N.

- If the variable is a scalar variable, the return array has shape (draws * chains, 1).
- If the variable is a vector, the return array has shape (draws * chains, len(vector))
- If the variable is a matrix, the return array has shape (draws * chains, size(dim 1), size(dim 2))
- If the variable is an array with N dimensions, the return array has shape (draws * chains, size(dim 1), ..., size(dim N))

For example, if the Stan program variable `theta` is a 3x3 matrix, and the sample consists of 4 chains with 1000 post-warmup draws, this function will return a numpy.ndarray with shape (4000,3,3).

This functionality is also available via a shortcut using `.` - writing `fit.a` is a synonym for `fit.stan_variable("a")`

Parameters

- **var** (*str*) – variable name
- **kwargs** (*bool*) – Additional keyword arguments are passed to the underlying `fit.stan_variable` method if the variable is not a generated quantity.

Return type

ndarray

See also:

CmdStanGQ.stan_variables, *CmdStanMCMC.stan_variable*, *CmdStanMLE.stan_variable*, *CmdStanPathfinder.stan_variable*, *CmdStanVB.stan_variable*, *CmdStanLaplace.stan_variable*

stan_variables(***kwargs*)

Return a dictionary mapping Stan program variables names to the corresponding numpy.ndarray containing the inferred values.

Parameters

kwargs (*bool*) – Additional keyword arguments are passed to the underlying fit's `stan_variable` method if the variable is not a generated quantity.

Return type

Dict[str, ndarray]

See also:

`CmdStanGQ.stan_variable`, `CmdStanMCMC.stan_variables`, `CmdStanMLE.stan_variables`,
`CmdStanPathfinder.stan_variables`, `CmdStanVB.stan_variables`, `CmdStanLaplace.stan_variables`

property chain_ids: `List[int]`

Chain ids.

property chains: `int`

Number of chains.

property column_names: `Tuple[str, ...]`

Names of generated quantities of interest.

property metadata: `InferenceMetadata`

Returns object which contains CmdStan configuration as well as information about the names and structure of the inference method and model output variables.

3.3 Functions

3.3.1 compile_stan_file

`cmdstanpy.compile_stan_file(src, force=False, stanc_options=None, cpp_options=None, user_header=None)`

Compile the given Stan program file. Translates the Stan code to C++, then calls the C++ compiler.

By default, this function compares the timestamps on the source and executable files; if the executable is newer than the source file, it will not recompile the file, unless argument `force` is `True` or unless the compiler options have been changed.

Parameters

- **src** (*Union[str, Path]*) – Path to Stan program file.
- **force** (*bool*) – When `True`, always compile, even if the executable file is newer than the source file. Used for Stan models which have `#include` directives in order to force recompilation when changes are made to the included files.
- **stanc_options** (*Optional[Dict[str, Any]]*) – Options for stanc compiler.
- **cpp_options** (*Optional[Dict[str, Any]]*) – Options for C++ compiler.
- **user_header** (*Optional[Union[str, PathLike]]*) – A path to a header file to include during C++ compilation.

Return type

`str`

3.3.2 format_stan_file

`cmdstanpy.format_stan_file(stan_file, *, overwrite_file=False, canonicalize=False, max_line_length=78, backup=True, stanc_options=None)`

Run stanc's auto-formatter on the model code. Either saves directly back to the file or prints for inspection

Parameters

- **stan_file** (*Union*[*str*, *PathLike*]) – Path to Stan program file.
- **overwrite_file** (*bool*) – If True, save the updated code to disk, rather than printing it. By default False
- **canonicalize** (*Union*[*bool*, *str*, *Iterable*[*str*]]) – Whether or not the compiler should 'canonicalize' the Stan model, removing things like deprecated syntax. Default is False. If True, all canonicalizations are run. If it is a list of strings, those options are passed to stanc (new in Stan 2.29)
- **max_line_length** (*int*) – Set the wrapping point for the formatter. The default value is 78, which wraps most lines by the 80th character.
- **backup** (*bool*) – If True, create a stanfile.bak backup before writing to the file. Only disable this if you're sure you have other copies of the file or are using a version control system like Git.
- **stanc_options** (*Optional*[*Dict*[*str*, *Any*]]) – Additional options to pass to the stanc compiler.

Return type

None

3.3.3 show_versions

`cmdstanpy.show_versions(output=True)`

Prints out system and dependency information for debugging

Parameters

output (*bool*) –

Return type

str

3.3.4 cmdstan_path

`cmdstanpy.cmdstan_path()`

Validate, then return CmdStan directory path.

Return type

str

3.3.5 install_cmdstan

```
cmdstanpy.install_cmdstan(version=None, dir=None, overwrite=False, compiler=False, progress=False,
                           verbose=False, cores=1, *, interactive=False)
```

Download and install a CmdStan release from GitHub. Downloads the release tar.gz file to temporary storage. Retries GitHub requests in order to allow for transient network outages. Builds CmdStan executables and tests the compiler by building example model `bernoulli.stan`.

Parameters

- **version** (*Optional[str]*) – CmdStan version string, e.g. “2.29.2”. Defaults to latest CmdStan release. If `git` is installed, a git tag or branch of `stan-dev/cmdstan` can be specified, e.g. “git:develop”.
- **dir** (*Optional[str]*) – Path to install directory. Defaults to hidden directory `$HOME/.cmdstan`. If no directory is specified and the above directory does not exist, directory `$HOME/.cmdstan` will be created and populated.
- **overwrite** (*bool*) – Boolean value; when `True`, will overwrite and rebuild an existing CmdStan installation. Default is `False`.
- **compiler** (*bool*) – Boolean value; when `True` on WINDOWS ONLY, use the C++ compiler from the `install_cxx_toolchain` command or install one if none is found.
- **progress** (*bool*) – Boolean value; when `True`, show a progress bar for downloading and unpacking CmdStan. Default is `False`.
- **verbose** (*bool*) – Boolean value; when `True`, show console output from all intallation steps, i.e., download, build, and test CmdStan release. Default is `False`.
- **cores** (*int*) – Integer, number of cores to use in the `make` command. Default is 1 core.
- **interactive** (*bool*) – Boolean value; if `true`, ignore all other arguments to this function and run in an interactive mode, prompting the user to provide the other information manually through the standard input.

This flag should only be used in interactive environments, e.g. on the command line.

Returns

Boolean value; `True` for success.

Return type

`bool`

3.3.6 set_cmdstan_path

```
cmdstanpy.set_cmdstan_path(path)
```

Validate, then set CmdStan directory path.

Parameters

path (*str*) –

Return type

`None`

3.3.7 cmdstan_version

`cmdstanpy.cmdstan_version()`

Parses version string out of CmdStan makefile variable `CMDSTAN_VERSION`, returns `Tuple(Major, minor)`.

If CmdStan installation is not found or cannot parse version from makefile logs warning and returns `None`. Lenient behaviour required for CI tests, per comment: <https://github.com/stan-dev/cmdstanpy/pull/321#issuecomment-733817554>

Return type

Optional[Tuple[int, ...]]

3.3.8 set_make_env

`cmdstanpy.set_make_env(make)`

set MAKE environmental variable.

Parameters

make (*str*) –

Return type

`None`

3.3.9 from_csv

`cmdstanpy.from_csv(path=None, method=None)`

Instantiate a CmdStan object from a the Stan CSV files from a CmdStan run. CSV files are specified from either a list of Stan CSV files or a single filepath which can be either a directory name, a Stan CSV filename, or a pathname pattern (i.e., a Python glob). The optional argument ‘method’ checks that the CSV files were produced by that method. Stan CSV files from CmdStan methods ‘sample’, ‘optimize’, and ‘variational’ result in objects of class `CmdStanMCMC`, `CmdStanMLE`, and `CmdStanVB`, respectively.

Parameters

- **path** (*Optional[Union[str, List[str], PathLike]]*) – directory path
- **method** (*Optional[str]*) – method name (optional)

Returns

either a `CmdStanMCMC`, `CmdStanMLE`, or `CmdStanVB` object

Return type

Optional[Union[CmdStanMCMC, CmdStanMLE, CmdStanVB, CmdStanPathfinder, CmdStan-Laplace]]

3.3.10 write_stan_json

`cmdstanpy.write_stan_json(path, data)`

Dump a mapping of strings to data to a JSON file.

Values can be any numeric type, a boolean (converted to int), or any collection compatible with `numpy.asarray()`, e.g a `pandas.Series`.

Produces a file compatible with the `Json Format for Cmdstan`

Parameters

- **path** (*str*) – File path for the created json. Will be overwritten if already in existence.
- **data** (*Mapping[str, Any]*) – A mapping from strings to values. This can be a dictionary or something more exotic like an `xarray.Dataset`. This will be copied before type conversion, not modified

Return type

None

WHAT'S NEW

For full changes, see the [Releases page](#) on GitHub.

4.1 CmdStanPy 1.2.2

- Updated Community page to link to the `bibat` package.
- Moved CmdStanPy's metadata to exclusively use the `pyproject.toml` file.
- Fixed an issue where the deprecation of the `compile=False` argument to `CmdStanModel` would make it impossible to use the canonicalizer to update old models. The new function `cmdstanpy.format_stan_file()` supports this use case.
- Fixed a bug preventing multiple inits from being used with `CmdStanModel.pathfinder()`.
- Added a helper argument `num_threads` to `CmdStanModel.pathfinder()`.

Reminder: The next non-bugfix release of CmdStanPy will be version 2.0, which will remove all existing deprecations.

4.2 CmdStanPy 1.2.1

- Switched from `numpy.random.RandomState` to `default_rng()`.
- Fixed minor doc typos.
- Stan 2.34: Fixed parsing of `unit_e` output files.
- Stan 2.34: Exposed new Pathfinder arguments.
- Allow the `vars` argument to `CmdStanMCMC.draws_pd()` to filter the `chain__`, `iter__`, and `draws__` columns.
- Fixed a bug involving the interaction of the `adapt_engaged` and `iter_warmup` arguments to `CmdStanMCMC.sample()`.

Reminder: The next non-bugfix release of CmdStanPy will be version 2.0, which will remove all existing deprecations.

4.3 CmdStanPy 1.2.0

- **New functionality**

- The Pathfinder algorithm (available in CmdStan 2.33+) is now available as `CmdStanModel.pathfinder()`.
- Laplace approximations (available in CmdStan 2.32+) are now available as `CmdStanModel.laplace_sample()`.
- The `CmdStanModel.optimize()` method now supports the `jacobian` boolean argument to enable change-of-variables adjustments. When enabled, the Maximum a posteriori estimate (MAP) is returned, rather than the MLE.
- The `cmdstanpy.install_cmdstan()` function and script can install development versions of CmdStan using the `git:` prefix in the version.

- **Deprecations** The next non-bugfix release of CmdStanPy will be version 2.0, which will remove all existing deprecations. Additional deprecations in this version:

- `CmdStanModel` will *require* that it has a compiled executable after construction. The `compile` argument is deprecated, (the ability to force recompilation is available under the argument `force_compile`), and the `compile()` method is deprecated. If you wish to compile Stan files independent of constructing a model, use `cmdstanpy.compile_stan_file()`.
- `CmdStanMLE.stan_variable()` will begin returning a `np.ndarray` in all cases, as opposed to the current behavior where sometimes a float is returned.
- `CmdStanVB.stan_variables()` will return the `_draws_` from the approximate posterior, rather than the optimized mean. A new argument, `mean`, can be set to `True` to return the mean instead. Additionally, a `np.ndarray` will be returned in all cases starting in the next version.
- `CmdStanModel.variational()` argument `output_samples` will have been renamed to `draws`.

- **Other changes**

- A list of dictionaries is now allowed as the `inits` argument to `CmdStanModel.sample()`.
- `cmdstanpy.install_cmdstan()` correctly fetches the CmdStan version for ppc64el machines.
- The documentation on how to use external C++ code was updated.
- Various other bug fixes.

Note: The minimum supported version for CmdStanPy is now Python 3.8.

4.4 CmdStanPy 1.1.0

- **New functionality**

- `CmdStanModel.generate_quantities()` can now accept samples from optimization and variational inference. The argument `mcmc_sample` has been renamed `previous_fit` to reflect this; the former name is still accepted but deprecated.
- `CmdStanModel.log_prob()` is able to return the log probability and its gradient with respect to a set of parameters. **Note** that this is *not* an efficient way of calculating this in general and should be reserved for debugging and model development.

- **Other changes**

- Improved some of the type hints in the package.
- Ensure draws are serialized if a fit object is pickled.
- `src_info()` now raises an error if the command fails, rather than returning {}.
- CmdStanPy has transitioned all unit tests from the `unittest` library to use `pytest`.

4.5 CmdStanPy 1.0.8

- `install_cmdstan` now downloads the correct CmdStan for non-x86 Linux machines.
- Improved reporting of errors during `compile()`.
- Fixed some edge cases in mixing arguments of the `optimize()` function.
- Fixed how NaN and infinite numbers were serialized to JSON.
- Removed dependency on `ujson`. For now, all JSON serialization is done with the Python standard library.
- Added a `timeout` parameter to all model methods which can be used to terminate the CmdStan process after the specified time.
- A model will now properly recompile if one of the `#include`-d files changed since it was last built.

4.6 CmdStanPy 1.0.7

- Fixed an issue where complex number containers in Stan program outputs were not being read in properly by CmdStanPy. The output would have the correct shape, but the values would be mixed up.

4.7 CmdStanPy 1.0.6

- Fixed a build error in the documentation
- Improved messages when model fails to compile due to C++ errors.

4.8 CmdStanPy 1.0.5

- Fixed a typo in `cmdstanpy.show_versions()`
- Reorganized and updated the documentation
- Reorganized a lot of internal code
- Cleaned up the output of `CmdStanMCMC.draws_pd()`
- Cleaned up the output of `CmdStanMCMC.summary()`
- Removed the logging which occurred when Python exited with `cmdstanpy` imported.

4.9 CmdStanPy 1.0.4

- Fix an issue with `cmdstanpy.install_cmdstan()` where the installation would report that it had failed even when it had not.

4.10 CmdStanPy 1.0.3

- Fix an issue where Stan fit objects were not pickle-able when they previously were.

<p>Warning: We still do not recommend pickling cmdstanpy objects, but rather using functions <code>save_csvfiles()</code> and <code>from_csv()</code>.</p>

4.11 CmdStanPy 1.0.2

- CmdStanPy can now format (and canonicalize) your Stan files with `CmdStanModel.format()`
- Stan variables can now be accessed from fit objects using the `.` syntax when no naming conflicts occur. For example, previous code `fit.stan_variable("my_cool_variable")` can now be written `fit.my_cool_variable`
- CmdStanPy is more robust to running in threaded environments and tries harder to not overwrite its own output files
- The `install_cmdstan` script can now be run in interactive mode using `--interactive/-i`
- CmdStanPy now computes some diagnostics after running HMC and will warn you about post-warmup divergences and treedepth exceptions
- Runtime exceptions in the `generated quantities` block should be recognized better now.
- The default level of precision used by `CmdStanMCMC.summary()` is now 6, as it is when `stansummary` is used from the command line.
- Various documentation improvements

4.12 CmdStanPy 1.0.1

- Support new optimizations in CmdStan 2.29
- Support complex numbers as both inputs and outputs of Stan programs
- Sped up assembling output by only reading draws at most once
- Fixed an issue where a command failing could change your working directory
- Improve error messages in some cases
- CmdStanPy no longer changes the global root logging level

Note: The minimum supported version for CmdStanPy is now Python 3.7.

4.13 CmdStanPy 1.0.0

- Initial release

COMMUNITY

This page highlights community projects that involve CmdStanPy. Check them out!

5.1 Project templates

Templates are a great way to piggy back on other users' work, saving you time when you start a new project.

- [bibat](#) A batteries-included template for Bayesian statistical analysis projects.
- [cookiecutter-cmdstanpy-wrapper](#) A cookiecutter template using Stan models in Python packages, including the ability to pre-compile the model as part of the package distribution.

5.2 Software

- [Prophet](#) A procedure for forecasting time series data based on an additive model where non-linear trends are fit with yearly, weekly, and daily seasonality, plus holiday effects.
- [ArviZ](#) A Python package (with a [Julia interface](#)) for exploratory analysis of Bayesian models. Includes functions for posterior analysis, data storage, model checking, comparison and diagnostics.
- [BridgeStan](#) A project which provides efficient in-memory access through Python, Julia, and R to the methods of a Stan model, including log densities, gradients, Hessians, and constraining and unconstraining transforms.

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