

# CmdStan Interface

## User's Guide

Stan Development Team

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## **Part I**

# **Introduction**

# 1. Overview

This document is a user's guide for the CmdStan interface to the Stan probabilistic modeling language. CmdStan takes Stan programs and generates executables that can be run directly from the command line. CmdStan is one of several interfaces to Stan; there are also R, Python, and Matlab interfaces.

## 1.1. Stan Home Page

For links to up-to-date code, examples, manuals, bug reports, feature requests, and everything else Stan related, see the Stan home page:

<http://mc-stan.org/>

## 1.2. Licensing

CmdStan and Stan are both licensed under the new BSD license (3-clause). See Appendix A for details, including licensing terms for the dependent packages Boost and Eigen.

## 1.3. Modeling Language User's Guide and Reference

Stan's modeling language is shared across all of its interfaces. Stan's language, along with a programming guide and many example models, is detailed in the *Stan Modeling Language User's Guide and Reference Manual*, which is available from the Stan home page (see Section 1.1).

## 1.4. Example Models

There are many example models for Stan, in addition to those in the user's guide and reference. These are all linked from the Stan home page (see Section 1.1).

## 1.5. Benefits of CmdStan

Although CmdStan has the least amount of functionality among the Stan interfaces, the minimal nature of CmdStan makes it trivial to install and use the latest development version of the Stan library. It also has the fewest dependencies, which makes it easier to run in limited environments such as clusters. The output generated is in CSV format and can be post-processed using other Stan interfaces or general tools.

## 2. Getting Started

This chapter is designed to help users get acquainted with the CmdStan interface. Later chapters are devoted to expanding on the material in this chapter with full reference documentation. See the Stan user’s manual for details about the Stan language.

### 2.1. Installation

For information about supported versions of Windows, Mac, and Linux platforms see Appendix B. For step-by-step installation instructions, see

- Windows: Appendix B.3
- Mac: Appendix B.4
- Linux: Appendix B.5.

### 2.2. Building CmdStan

Building CmdStan involves generating the Stan compiler, `stanc`, and a basic posterior analysis tool, `print`. The build process utilizes the `make` command-line utility and works the same way across all supported platforms.

1. Open a command-line terminal window and change directories to the CmdStan directory.

```
> cd <cmdstan-home>
```

2. *Optional:* Set local `make` variables by editing the file `make/local`. For most installations, this step can be skipped. See Appendix B.6 for a list of available options.
3. Use `make` to build CmdStan. If multiple CPU cores are available, the call to `make` can be parallelized with the `-jN` option, where  $N$  is the number of CPU cores. The parallel option (`-jN`) can be safely omitted. For instance, to run on 2 cores, use

```
> make build -j2
```

**Warning:** The `make` program may take 10+ minutes and consume 2+ GB of memory to build CmdStan. Compiler warnings, such as `uname: not found` or `warning: unused variable`, may be safely ignored.

When CmdStan is successfully built, the `make` program will report

--- CmdStan built ---

and there will be two executables in the bin folder:

- `stanc`, the Stan compiler. The Stan compiler translates a Stan program into C++ code. See Chapter 4 for details.
- `print`, a posterior analysis tool. The `print` command summarizes the comma-separated values files that are generated from Stan program runs. For each parameter within the Stan program, `print` reports the mean, standard deviation, quantiles,  $\hat{R}$ , and other values. See Chapter 5 for details.

## 2.3. Compiling and Executing a Stan Program

The rest of this quick-start guide explains how to code and run a very simple Bayesian model.

### A Simple Bernoulli Model

The following is a simplet, complete Stan program for a Bernoulli model of binary data.<sup>1</sup>

```
data {  
  int<lower=0> N;  
  int<lower=0,upper=1> y[N];  
}  
parameters {  
  real<lower=0,upper=1> theta;  
}  
model {  
  theta ~ beta(1,1);  
  for (n in 1:N)  
    y[n] ~ bernoulli(theta);  
}
```

The model assumes the binary observed data  $y[1], \dots, y[N]$  are i.i.d. with Bernoulli chance-of-success  $\theta$ . The prior on  $\theta$  is  $\text{beta}(1, 1)$  (i.e., uniform).

---

<sup>1</sup>The model is distributed with Stan's example models repository, [https://github.com/stan-dev/example-models/blob/master/basic\\_estimators/bernoulli.stan](https://github.com/stan-dev/example-models/blob/master/basic_estimators/bernoulli.stan), and is also available with the CmdStan distribution at the path `examples/bernoulli/bernoulli.stan`.



## Data Set

A data set of  $N = 10$  observations is coded as follows.<sup>2</sup>

```
N <- 10
y <- c(0,1,0,0,0,0,0,0,0,1)
```

This defines the contents of two variables, `N` and `y`, using an R-like syntax (see Chapter C for more information).

## Compiling a Stan Program

A single call to `make` will translate a Stan program to C++, then compile the C++ code to an executable for the command line.

A Stan program must be in a file with the file extension `.stan`. To create an executable from a Stan program, `make` will be called with the name of the executable as its argument. For Mac and Linux, it is the name of the Stan program with the `.stan` omitted. For Windows, replace `.stan` with `.exe`.

To build the Bernoulli example, from `<cmdstan-home>` issue the following command for Mac and Linux:

```
> make stan/example-models/basic_estimators/bernoulli
```

For Windows, the command is the same with the addition of `.exe` at the end of the target:

```
> make stan/example-models/basic_estimators/bernoulli.exe
```

The generated C++ code and the compiled executable will be placed in the same directory as the Stan program.

## Sampling from the Stan Program

The program can be executed from the directory in which it resides.

```
> cd stan/example-models/basic_estimators
```

To execute sampling of the model under Linux or Mac, use

```
> ./bernoulli sample data file=bernoulli.data.R
```

---

<sup>2</sup> The data is also available from the `example-models` repository on GitHub, [https://github.com/stan-dev/example-models/blob/master/basic\\_estimators/bernoulli.data.R](https://github.com/stan-dev/example-models/blob/master/basic_estimators/bernoulli.data.R). It is also included with the CmdStan distribution and can be found at path `stan/example-models/basic_estimators/bernoulli.data.R`.

In Windows, the `./` prefix is not needed, resulting in the following command.

```
> bernoulli.exe sample data file=bernoulli.data.R
```

The output is the same across all supported platforms. First, the configuration of the program is echoed to the standard output:

```
method = sample (Default)
sample
  num_samples = 1000 (Default)
  num_warmup = 1000 (Default)
  save_warmup = 0 (Default)
  thin = 1 (Default)
adapt
  engaged = 1 (Default)
  gamma = 0.050000000000000003 (Default)
  delta = 0.80000000000000004 (Default)
  kappa = 0.75 (Default)
  t0 = 10 (Default)
  init_buffer = 75 (Default)
  term_buffer = 50 (Default)
  window = 25 (Default)
algorithm = hmc (Default)
hmc
  engine = nuts (Default)
  nuts
    max_depth = 10 (Default)
    metric = diag_e (Default)
    stepsize = 1 (Default)
    stepsize_jitter = 0 (Default)
id = 0 (Default)
data
  file = bernoulli.data.R
init = 2 (Default)
random
  seed = 4294967295 (Default)
output
  file = output.csv (Default)
  diagnostic_file = (Default)
  refresh = 100 (Default)
```

After the configuration has been displayed, a short timing message is given.

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

```
take 0.04 seconds.  
Adjust your expectations accordingly!
```

Next, the sampler reports the iteration number, reporting the percentage complete.

```
Iteration: 1 / 2000 [ 0%] (Warmup)  
Iteration: 100 / 2000 [ 5%] (Warmup)  
...  
Iteration: 2000 / 2000 [100%] (Sampling)
```

### *Sampler Output*

Each execution of the model results in draws from a single Markov chain being written to a file in comma-separated value (CSV) format. The default name of the output file is `output.csv`.

The first part of the output file records the version of the underlying Stan library and the configuration as comments (i.e., lines beginning with the pound sign (#)).

```
# stan_version_major = 2  
# stan_version_minor = 5  
# stan_version_patch = 0  
# model = bernoulli_model  
# method = sample (Default)  
#   sample  
#     num_samples = 1000 (Default)  
#     num_warmup = 1000 (Default)  
#     save_warmup = 0 (Default)  
#     thin = 1 (Default)  
...
```

This is followed by a CSV header indicating the names of the values sampled.

```
lp__,accept_stat__,stepsize__,treedepth__,n_leapfrog__,n_divergent__,theta
```

The first column reports the unnormalized log probability of the model. The next columns provide sampler-dependent information; here, it is columns two through five. For basic Hamiltonian Monte Carlo (HMC) and its adaptive variant, the No-U-Turn sampler (NUTS), the sampler-dependent parameters are described in the following table.

<i>Sampler</i>	<i>Parameter</i>	<i>Description</i>
NUTS	accept_stat__	Metropolis acceptance probability averaged over samples in the slice
NUTS	stepsize__	Integrator step size
NUTS	treedepth__	Tree depth
NUTS	n_leapfrog__	Number of leapfrog calculations
NUTS	n_divergent__	Number of divergent iterations
HMC	accept_stat__	Metropolis acceptance probability
HMC	stepsize__	Integrator step size
HMC	int_time__	Total integration time

The remaining columns correspond to model parameters. For the Bernoulli model, it is just the sixth column, `theta`. The header line is streamed to the output file before warmup begins.

The next section describes the results of adaptation taking place during the warmup phase.

```
# Adaptation terminated
# Step size = 1.81311
# Diagonal elements of inverse mass matrix:
# 0.415719
```

The default sampler is NUTS with an adapted step size and a diagonal inverse mass matrix. For this example, the step size is 1.81311, and the inverse mass contains the single entry 0.415719 corresponding to the parameter `theta`.

Draws from the posterior distribution are printed out next, each line containing a single draw with the columns corresponding to the header.<sup>3</sup>

```
-7.22574,1,1.09068,1,1,0.383089
-6.95293,0.945991,1.09068,2,3,0.335074
-6.92373,0.938744,1.09068,1,1,0.181194
-6.83655,0.934833,1.09068,2,3,0.304882
-7.01732,1,1.09068,1,1,0.348244
...
```

The output ends with timing details,

```
# Elapsed Time: 0.006811 seconds (Warm-up)
#               0.011645 seconds (Sampling)
#               0.018456 seconds (Total)
```

---

<sup>3</sup>There are repeated entries due to the Metropolis accept step in the No-U-Turn sampling algorithm.

## Summarizing Sampler Output

The command-line program `bin/print` will display summary information about the run (for more information, see Chapter 5). To run `print` on the output file generated for `bernoulli` on Linux or Mac, type

```
> <cmdstan-home>/bin/print output.csv
```

For Windows, use backslashes to call the `print.exe`.

```
> <cmdstan-home>\bin\print.exe output.csv
```

The output of the command will display information about the run followed by information for each parameter and generated quantity. For `bernoulli`, we ran 1 chain and saved 1000 iterations. The information is echoed to the standard output stream. The output is

```
Inference for Stan model: bernoulli_model
1 chains: each with iter=(1000); warmup=(0); thin=(1); 1000 iterations saved.
```

```
Warmup took (0.014) seconds, 0.014 seconds total
Sampling took (0.027) seconds, 0.027 seconds total
```

	Mean	MCSE	StdDev	5%	50%	95%	N_Eff	N_Eff/s	R_hat
lp__	-7.3	4.6e-02	7.4e-01	-8.7	-7.0	-6.8	255	9267	1.0e+00
accept_stat__	0.94	2.7e-03	8.5e-02	0.76	0.98	1.0	1000	36395	1.0e+00
stepsize__	0.79	1.1e-15	7.8e-16	0.79	0.79	0.79	0.50	18	1.0e+00
treedepth__	1.9	2.2e-02	6.5e-01	1.0	2.0	3.0	844	30733	1.0e+00
n_leapfrog__	3.1	6.4e-02	1.9e+00	1.0	3.0	7.0	897	32644	1.0e+00
n_divergent__	0.00	0.0e+00	0.0e+00	0.00	0.00	0.00	1000	36395	nan
theta	0.26	5.9e-03	1.2e-01	0.091	0.25	0.48	420	15292	1.0e+00

Samples were drawn using hmc with nuts.

For each parameter, `N_Eff` is a crude measure of effective sample size, and `R_hat` is the potential scale reduction factor on split chains (at convergence, `R_hat=1`).

In addition to the general information about the runs, `print` displays summary statistics for each parameter and generated quantity.

In the `bernoulli` model, there is a single parameter, `theta`. The mean, standard error of the mean, standard deviation, the 5%, 50%, and 95% quantiles, number of effective samples (total and per second), and  $\hat{R}$  value are displayed. These quantities and their uses are described in detail in the introductory Markov chain Monte Carlo (MCMC) chapter of the language user's guide and reference manual.

The command `bin/print` can be called with more than one csv file by separating filenames with spaces. It will also take wildcards in specifying filenames. A typical usage of Stan from the command line would first create one or more Markov chains

by calling the model executable, typically in parallel, writing the output CSV file for each into its own directory. After all of the processes are finished, the results would be analyzed using `print` to assess convergence and inspect the means and quantiles of the fitted variables. Additionally, downstream inferences may be performed using the draws (e.g., to make decisions or predictions for unseen data).

## Optimization

CmdStan can be used for finding posterior modes as well as sampling from the posterior distribution. The executable does not need to be recompiled in order to switch from optimization to sampling, and the data input format is the same. The following is a minimal call to Stan's optimizer using defaults for everything but the location of the data file. See Section 7.3 for more details.

```
> ./bernoulli optimize data file=bernoulli.data.R
```

Executing this command prints the following.

```
method = optimize
  optimize
    algorithm = lbfgs (Default)
      lbfgs
        init_alpha = 0.001 (Default)
        tol_obj = 9.999999999999998e-13 (Default)
        tol_rel_obj = 10000 (Default)
        tol_grad = 1e-08 (Default)
        tol_rel_grad = 10000000 (Default)
        tol_param = 1e-08 (Default)
        history_size = 5 (Default)
      iter = 2000 (Default)
      save_iterations = 0 (Default)
  id = 0 (Default)
  data
    file = bernoulli.data.R
  init = 2 (Default)
  random
    seed = 4294967295 (Default)
  output
    file = output.csv (Default)
    diagnostic_file = (Default)
    refresh = 100 (Default)

initial log joint probability = -5.18908
  Iter   log prob      ||dx||      ||grad||    alpha  alpha0  # evals  Notes
    4      -5.00402    0.00400907  7.80306e-05      1      1      7
Optimization terminated normally:
  Convergence detected: relative gradient magnitude is below tolerance
```

The first part of the output reports on the configuration used, here indicating the default L-BFGS optimizer, with default initial stepsize and tolerances for monitoring convergence. The second part of the output indicates how well the algorithm fared, here converging and terminating normally. The numbers reported indicate that it took 4 iterations and 7 gradient evaluations, resulting in a final state where the change in parameters was roughly 0.004 and the length of the gradient roughly  $8e-5$ . The alpha value is for step size used. This is, not surprisingly, far fewer iterations than required for sampling; even fewer iterations would be used with less stringent user-specified convergence tolerances.

### *Optimization Output*

The output from optimization is written into the file `output.csv` by default. The output follows the same pattern as the output for sampling, first dumping the entire set of parameters used.

```
# stan_version_major = 2
# stan_version_minor = 5
# stan_version_patch = 0
# model = bernoulli_model
# method = optimize
#   optimize
#     algorithm = lbfgs (Default)
#       lbfgs
#         init_alpha = 0.001 (Default)
#         tol_obj = 9.999999999999998e-13 (Default)
#         tol_rel_obj = 10000 (Default)
#         tol_grad = 1e-08 (Default)
#         tol_rel_grad = 10000000 (Default)
#         tol_param = 1e-08 (Default)
#         history_size = 5 (Default)
#       iter = 2000 (Default)
#       save_iterations = 0 (Default)
#   id = 0 (Default)
# data
#   file = bernoulli.data.R
#   init = 2 (Default)
#   random
#     seed = 458923754
#   output
#     file = output.csv (Default)
#     diagnostic_file = (Default)
#     refresh = 100 (Default)
```

```
lp__,theta  
-5.00402,0.200008
```

Note that everything is a comment other than a line for the header, and a line for the values. Here, the header indicates the unnormalized log probability with `lp__` and the model parameter `theta`. The maximum log probability is -5.0 and the posterior mode for `theta` is 0.20. The mode exactly matches what we would expect from the data.<sup>4</sup> Because the prior was uniform, the result 0.20 represents the maximum likelihood estimate (MLE) for the very simple Bernoulli model. Note that no uncertainty is reported.

## Configuring Command-Line Options

The command-line options for running a model are detailed in Chapter 7. They can also be printed on the command line using Linux or Mac OS with

```
> ./bernoulli help-all
```

and on Windows with

```
> bernoulli.exe help-all
```

---

<sup>4</sup>The Jacobian adjustment included for the sampler's log probability function is not applied during optimization, because it can change the shape of the posterior and hence the solution.



# **Part II**

## **CmdStan Tools**

## 3. Overview

CmdStan is the command-line interface for Stan. The next two chapters describes tools that are built as part of CmdStan installation: `stanc` and `print`. The process of building a CmdStan executable from a Stan program is as follows:

1. A Stan program is written to file with a `.stan` extension.
2. `stanc` is used to translate the Stan program into a C++ file. This C++ file is not a full program that can be compiled to executable directly, but a translation from the Stan language into a C++ concept. Each interface will generate identical C++ for the same Stan program.
3. A CmdStan executable is generated from the CmdStan source and the generated C++. Each Stan program will have its own CmdStan executable. The options to the CmdStan executable are described in Chapter 7.

### 3.1. Building the CmdStan Tools

The easy way to build CmdStan is through the use of `make`. From a command line window, type:

```
> cd <cmdstan-home>
> make build
```

This will build both `stanc` and `print`. If your computer has multiple cores and sufficient ram, the build process can be parallelized by providing the `-j` option. For example, to build on 2 cores, type:

```
> cd <cmdstan-home>
> make -j2 build
```

**Warning:** The `make` program may take 10+ minutes and consume 2+ GB of memory to build CmdStan. Compiler warnings, such as `uname: not found`, may be safely ignored.

## 4. **stanc**: Translating Stan to C++

### 4.1. Building the **stanc** Compiler

Before the **stanc** compiler can be used, it must be built. It can be compiled directly using the makefile as follows. For Mac and Linux:

```
> make bin/stanc
```

For Windows:

```
> make bin/stanc.exe
```

To change the default compiler or the optimization level, see [Appendix B.6](#).

### 4.2. The **stanc** Compiler

The **stanc** compiler converts Stan programs to C++ concepts. The first stage of compilation involves parsing the text of the Stan program. If the parser is successful, the second stage of compilation generates C++ code. If the parser fails, it will provide a diagnostic error message indicating the location in the input where the failure occurred and reason for the failure.

The following example illustrates a fully qualified call to **stanc** to build the simple Bernoulli model.

For Linux and Mac:

```
> cd <cmdstan-home>
> bin/stanc --name=bernoulli --o=bernoulli.hpp \
  stan/example-models/basic_estimators/bernoulli.stan
```

The backslash (\) indicates a continuation of the same line.

For Windows:

```
> cd <cmdstan-home>
> bin\stanc.exe --name=bernoulli --o=bernoulli.hpp ^
  stan/example-models/basic_estimators/bernoulli.stan
```

The caret (^) indicates continuation on Windows.

This call specifies the name of the model, here **bernoulli**. This will determine the name of the class implementing the model in the C++ code. Because this name is the name of a C++ class, it must start with an alphabetic character (a-z or A-Z) and contain only alphanumeric characters (a-z, A-Z, and 0-9) and underscores (\_) and should not conflict with any C++ reserved keyword.

The C++ code implementing the class is written to the file `bernoulli.hpp` in the current directory. The final argument, `bernoulli.stan`, is the file from which to read the Stan program.

### 4.3. Command-Line Options for `stanc`

The model translation program `stanc` is called as follows.

```
> stanc [options] model_file
```

The argument *model\_file* is a path to a Stan model file ending in suffix `.stan`. The options are as follows.

**--help**

Displays the manual page for `stanc`. If this option is selected, nothing else is done.

**--version**

Prints the version of `stanc`. This is useful for bug reporting and asking for help on the mailing lists.

**--name=*class\_name***

Specify the name of the class used for the implementation of the Stan model in the generated C++ code.

Default: *class\_name* = *model\_file\_model*

**--o=*cpp\_file\_name***

Specify the name of the file into which the generated C++ is written.

Default: *cpp\_file\_name* = *class\_name.hpp*

## 5. **print**: Output Analysis

CmdStan is distributed with a `print` command that is able to read in the output of one or more Markov chains and summarize the posterior fits. This operation mimics the `print(fit)` command in RStan, which itself was modeled on the `print` functions from R2WinBUGS and R2jags.

### 5.1. Building the Print Command

CmdStan's `print` command is built along with `stanc` into the `bin` directory. It can be compiled directly using the makefile as follows.

```
> cd <cmdstan-home>
> make bin/print
```

### 5.2. Running the Print Command

The `print` command is executed on one or more `output.csv` files. These files may be provided as command-line arguments separated by spaces. That means that wild-cards may be used, as they will be replaced by space-separated file names by the operating system's command-line interpreter.

Suppose there are three samples files in a directory generated by fitting a negative binomial model to a small data set.

```
> ls output*.csv

output1.csv      output2.csv      output3.csv

> bin/print output*.csv
```

The result of `bin/print` is displayed in Figure 5.1.<sup>1</sup> The posterior is skewed to the high side, resulting in posterior means ( $\alpha = 17$  and  $\beta = 10$ ) that are a long way away from the posterior medians ( $\alpha = 9.5$  and  $\beta = 6.2$ ); the posterior median is the value listed under 50%, which is the 50th percentile of the posterior values.

For Windows, the forward slash in paths need to be converted to backslashes.

---

<sup>1</sup>RStan's and PyStan's output analysis print may be different than that in the command-line version of Stan.

```

Inference for Stan model: negative_binomial_model
1 chains: each with iter=(1000); warmup=(0); thin=(1); 1000 iterations saved.

Warmup took (0.054) seconds, 0.054 seconds total
Sampling took (0.059) seconds, 0.059 seconds total

```

	Mean	MCSE	StdDev	5%	50%	95%	N_Eff	N_Eff/s	R_hat
lp__	-14	6.2e-02	1.0e+00	-16	-14	-13	283	4773	1.00
accept_stat__	0.88	5.6e-03	1.8e-01	0.51	0.95	1.0	1000	16881	1.00
stepsize__	0.30	1.3e-15	8.9e-16	0.30	0.30	0.30	0.50	8.5	1.00
treedepth__	1.4	2.6e-02	8.0e-01	0.00	1.0	2.0	946	15978	1.00
n_divergent__	1.4	0.0e+00	0.0e+00	0.00	0.0	0.0	1000	16949	1.00
alpha	17	1.8e+00	2.5e+01	1.9	9.5	50	181	3054	1.00
beta	10	1.1e+00	1.4e+01	1.2	6.2	31	181	3057	1.00

Samples were drawn using hmc with nuts.  
For each parameter, N\_Eff is a crude measure of effective sample size,  
and R\_hat is the potential scale reduction factor on split chains (at  
convergence, R\_hat=1).

Figure 5.1: Example output from bin/print. The model parameters are alpha and beta. The values for each quantity are the posterior means, standard deviations, and quantiles, along with Monte-Carlo standard error, effective sample size estimates (per second), and convergence diagnostic statistic. These values are all estimated from samples. In addition to the parameters, the value lp\_\_ is the total log probability computed by the model (up to an additive constant). The quantity accept\_stat\_\_ is the NUTS acceptance statistic used by NUTS for slice and Metropolis rejection, stepsize\_\_ the step size used by NUTS in its Hamiltonian simulation, and treedepth\_\_ is the depth of tree used by NUTS, which is the log (base 2) of the number of leapfrog steps taken during the Hamiltonian simulation. n\_divergent\_\_ gives the number of leapfrog iterations with diverging error; because NUTS terminates at the first divergent iteration this should always be either 0 or 1.

## Output of Print Command

### n\_divergent

CmdStan uses a symplectic integrator to approximate the exact solution of the Hamiltonian dynamics and when the step size is too large relative to the curvature of the log posterior this approximation can diverge and threaten the validity of the sampler. n\_divergent counts the number of iterations within a given sample that have diverged and any non-zero value suggests that the samples may be biased in which case the step size needs to be decreased. Note that, because sampling is immediately terminated once a divergence is encountered, n\_divergent should be only 0 or 1.

### 5.3. Command-line Options

In addition to the filenames, `print` includes three flags to customize the output.

`help`

Prints usage information

No help output by default

`sig_figs=<int>`

Sets the number of significant figures displayed in the output

Valid values: 0 <sig\_figs

(default = 2 )

`autocorr=<int>`

Calculates and then displays the autocorrelation of the specified chain

Valid values: Any integer matching a chain index

(No autocorrelation output by default)

## **Part III**

# **CmdStan Executables**



## 6. Compiling CmdStan Executables

Preparing a Stan program to be run involves two steps,

1. translating the Stan program to C++, and
2. compiling the resulting C++ to an executable.

This chapter discusses both steps, as well as their encapsulation into a single make target.

### 6.1. Translating and Compiling through make

The simplest way to compile a CmdStan program is through the make build tool, which encapsulates the translation and compilation step into a single command. The commands making up the make target for compiling a model are described in the following sections, and the following chapter describes how to run a compiled model.

#### Translating and Compiling Test Models

There are a number of example models distributed with CmdStan which unpack into the path `stan/example-models`. To build the simple example `stan/example-models/basic_estimators/bernoulli.stan`, the following call to make suffices. First the directory is changed to CmdStan's home directory by replacing `<cmdstan-home>` with the appropriate path.

```
> cd <cmdstan-home>
```

The following call will build an executable form of the Bernoulli estimator. On Windows, replace `bernoulli` with `bernoulli.exe`.

```
> make stan/example-models/basic_estimators/bernoulli
```

This will translate the model `bernoulli.stan` to a C++ file and compile a CmdStan program using the generated C++ file, putting the executable in `stan/example-models/basic_distributions/bernoulli(.exe)`.

#### Dependencies in make

When executing a make target, all its dependencies are checked to see if they are up to date, and if they are not, they are rebuilt. If the make target to build the Bernoulli estimator is invoked a second time, it will see that it is up to date, and will not recompile the program.

If the file containing the Stan program is updated, the next call to make will rebuild the CmdStan executable.

## Getting Help from the makefile

CmdStan's makefile, which contains the top-level instructions to make, provides extensive help in terms of targets and options. It is located at the top-level of the distribution, so first change directories to that location.

```
> cd <cmdstan-home>
```

and then invoke make with the target `help`,

```
> make help
```

## Options to make

CmdStan allows users to change compilers, library versions for Eigen and Boost, as well as compilation options such as optimization.

For a full list of options, see [Appendix B.6](#)

### *Clean Targets*

A very useful target is `clean-all`, invoked as

```
> make clean-all
```

This removes the CmdStan tools. This step is necessary when changing compilers or other make options.

## 7. Running a CmdStan Program

Once a CmdStan program is compiled, it can be run in many different ways. It can be used to sample or optimize parameters, or to diagnose a model. Before diving into the detailed configurations, the first section provides some simple examples.

### 7.1. Getting Started by Example

Once a CmdStan program has been converted to a C++ program for that model (see Chapter 4) and the resulting C++ program compiled to a platform-specific executable (see Chapter 6), the model is ready to be run.

All of the CmdStan functionality is highly configurable from the command line; the options are defined later in this chapter. Each command option also has defaults, which are used in this section.

#### Sampling

Suppose the executable is in file `my_model` and the data is in file `my_data`, both in the current working directory. To generate samples from a data set using the default settings, use one of the following, depending on platform.

##### *Mac OS and Linux*

```
> ./my_model sample data file=my_data
```

##### *Windows*

```
> my_model sample data file=my_data
```

On both platforms, this command reads the data from file `my_data`, runs warmup tuning for 1000 iterations (the values of which are discarded), and then runs the fully-adaptive NUTS sampler for 1000 iterations, writing the parameter (and other) values to the file `samples.csv` in the current working directory. When no random number seed is specified, a seed is generated from the system time.

#### Sampling in Parallel

The previous example executes one chain, which can be repeated to generate multiple chains. However, users may want to execute chains in parallel on a multicore machine.

## Mac OS and Linux

To sample four chains using a Bash shell on Mac OS or Linux, execute<sup>1</sup>

```
> for i in {1..4}
do
  ./my_model sample random seed=12345
  id=$i data file=my_data
  output file=samples$i.csv &
done
```

The ampersand (&) at the end of the nested command pushes each process into the background, so that the loop can continue without waiting for the current chain to finish. The `id` value makes sure that a non-overlapping set of random numbers are used for each chain. Also note that the output file is explicitly specified, with the variable `$i` being used to ensure the output file name for each chain is unique.

The terminal standard output will be interleaved for all chains running concurrently. To suppress all terminal output, direct the standard output to the “null” device. This is achieved by postfixing `> /dev/null` to a command, which in the above case, means changing the second-to-last line to

```
output file=samples$i.csv > /dev/null & \
```

## Windows

On Windows, the following is functionally equivalent to the Bash snippet above

```
> for /l %x in (1, 1, 4) do start /b model sample ^
random seed=12345 id=%x data file=my_data ^
output file=samples%x.csv
```

The caret (^) indicates a line continuation in DOS.

## Combining Parallel Chains

CmdStan has commands to analyze the output of multiple chains, each stored in their own file; see Chapter 5. RStan also has commands to read in multiple CSV files produced by CmdStan’s command-line sampler.

To compute posterior quantities, it is sometimes easier to have the chains merged into a single CSV file. If the `grep` and `sed` programs are installed, then the following will combine the four comma-separated values files into a single comma-separated values file. The command is the same on Windows, Mac OS and Linux.

---

<sup>1</sup>Complicated multiline commands such as this one are prime candidates for putting into a script file.

```
> grep lp__ samples1.csv > combined.csv  
> sed '/^[#]/d' samples*.csv >> combined.csv
```

### *Scripting and Batching*

The previous examples show how to sample in parallel from the command line. Operations like these can also be scripted, using shell scripts (.sh) on Mac OS and Linux and DOS batch (.bat) files on Windows. A sequence of several such commands can be executed from a single script file. Such scripts might contain `stanc` commands (see Chapter 4) and `print` commands (see Chapter 5) can be executed from a single script file. At some point, it is worthwhile to move to something with stronger dependency control such as `makefiles`.

### **Optimization**

CmdStan can find the posterior mode (assuming there is one). If the posterior is not convex, there is no guarantee Stan will be able to find the global mode as opposed to a local optimum of log probability.

For optimization, the mode is calculated without the Jacobian adjustment for constrained variables, which shifts the mode due to the change of variables. Thus modes correspond to modes of the model as written.

#### *Windows*

```
> my_model optimize data file=my_data
```

#### *Mac OS and Linux*

```
> ./my_model optimize data file=my_data
```

## **7.2. Diagnostics**

CmdStan has a basic diagnostic feature that will calculate gradients of the initial state and compare them with those calculated with finite differences. If there are discrepancies, there is a problem with the model or initial states (or a bug in Stan). To run on the different platforms, use one of the following.

#### *Windows*

```
> my_model diagnose data file=my_data
```

```
> ./my_model diagnose data file=my_data
```

### 7.3. Command-Line Options

CmdStan executables are highly configurable, allowing the user to specify and customize not only the calculation method but also the data, output, initialization, and random number generation. The arguments are defined hierarchically so that, for example, optimization settings are not necessary when sampling.

The atomic elements of the hierarchy (i.e., those without corresponding values) are *categorical arguments* (sometimes called “flags”) which define self-contained categories of arguments.

CmdStan’s commands have more hierarchical structure than is typical of command line executables, which usually have at most two subgroups of commands. Arguments grouped within a category are not ordered with respect to each other. The only ordering is that the global options come before the method argument and subcommand-specific options after the method argument. For example, the following four commands all define the same configuration:<sup>2</sup>

```
> ./model sample output file=samples.csv          \  
                      diagnostic_file=diagnostics.csv \  
                      random seed=1  
  
> ./model sample output diagnostic_file=diagnostics.csv \  
                      file=samples.csv              \  
                      random seed=1  
  
> ./model sample random seed=1                    \  
                      output file=samples.csv        \  
                      diagnostic_file=diagnostics.csv  
  
> ./model sample random seed=1                    \  
                      output diagnostic_file=diagnostics.csv \  
                      file=samples.csv
```

The categorical arguments `output` and `random` can be in any order provided that the subarguments follow their respective parent, here `diagnostic_file` and `file`

---

<sup>2</sup> The backslash (\) is used at the end of a line in a command to indicate that it continues on the next line. The indentation to indicate the structure of the command is for pedagogical purposes only; the same result would be obtained writing each command on one line with single spaces separating the elements.

following output and seed coming after random. These four configurations exhaust all valid combinations.

Categorical arguments may appear is isolation, for example when introducing `sample` or `random`, or they may appear as the values for other arguments, such as `hmc` which not only introduces a category of HMC related arguments but also defines the value of the argument `algorithm`. A visual diagram of the available categorical arguments is shown in Figure 7.1, with the mutual exclusivity of these arguments as values shown in Figure 7.2. Specifying conflicting arguments causes the execution to immediately terminate.

Note that any valid argument configuration must either specify a method or a help request.

## Method

All commands other than `help` must include at least one method, specified explicitly as `method=method_name` or implicitly with only `method_name`. Currently `CmdStan` supports the following methods:

<i>Method</i>	<i>Description</i>
<code>sample</code>	sample using MCMC
<code>optimize</code>	find posterior mode using optimization
<code>diagnose</code>	diagnose models

All remaining configurations are option, with default values provided for all arguments not explicitly specified.

## Help

Informative output can be retrieved either globally, by requesting help at the top-level, or locally, by requesting help deeper into the hierarchy. Note that after any help has been displayed the execution immediately terminates, even if a method has been specified.

### *Top-Level Help*

If `help` is specified as the only argument then a usage message is displayed. Similarly, specifying `help_all` by itself displays the entire argument hierarchy.

### *Context-Sensitive Help*

Specifying `help` after any argument displays a description and valid options for that argument. For example,

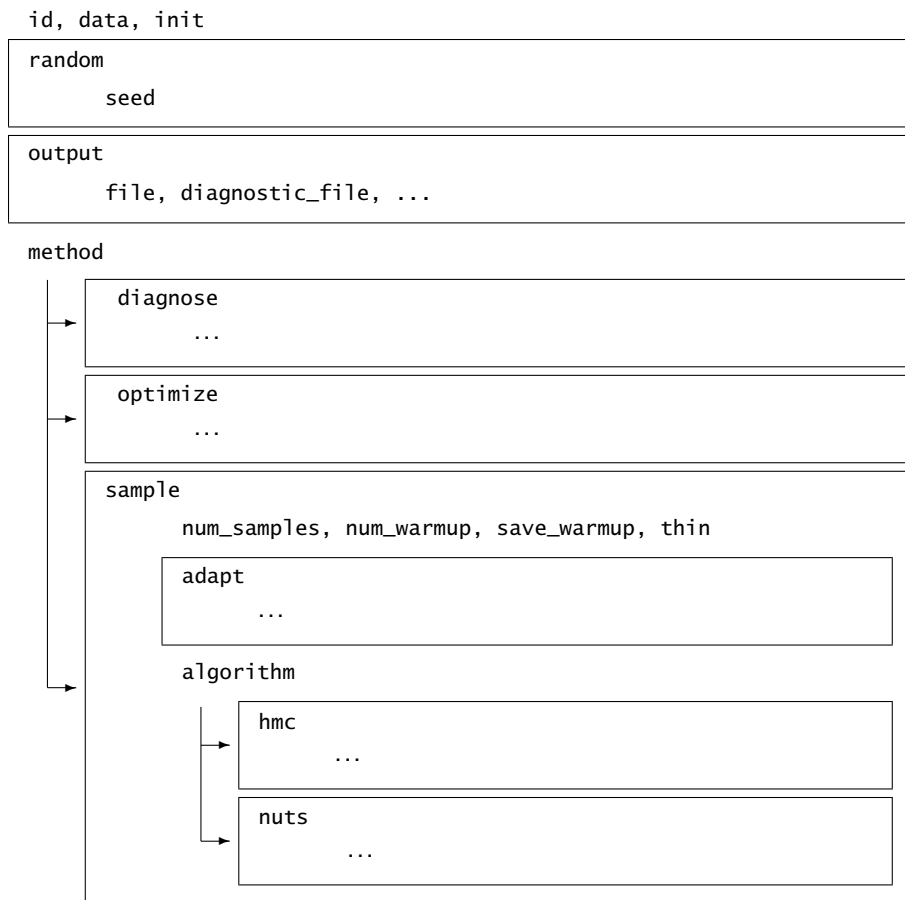


Figure 7.1: In the hierarchical argument structure, certain arguments, such as `random` and `output`, introduce new categories of arguments. Categorical arguments may also appear as values of other arguments, such as `diagnose`, `optimize`, and `sample`, which define the mutually exclusive values for the argument `method`.



id, data, init

random

seed

output

file, diagnostic\_file, ...

method

diagnose

...

optimize

...

sample

num\_samples, num\_warmup, save\_warmup, thin

adapt

...

algorithm

hmc

...

nuts

...

Figure 7.2: A valid argument configuration defines only one mutually exclusive argument. If conflicting arguments are specified, for example `method=optimize method=sample`, then execution immediately terminates with a warning message.

```
./my_model sample help
```

provides the top-level options for the `sample` method.

Detailed information on the argument, and all arguments deriving from it, can be accessed by specifying `help-all` instead,

```
./my_model sample help-all
```

## 7.4. Full Argument Hierarchy

Here we present the full argument hierarchy, along with relevant details. Some typical use-case examples are provided in the next section.

### Typographical Conventions

The following typographical conventions are obeyed in the hierarchy.

- **arg=<value-type>**  
Arguments with values; displays the value type, legal values, and default value
- **arg**  
Isolated categorical arguments; displays all valid subarguments
- *value*  
Values; describes effect of selecting the value
- **value**  
Categorical arguments that appear as values to other arguments; displays all valid subarguments

### Top-Level Method Argument

Every command must have exactly one method specified as the very first argument. The value type of `list element` means that the valid values are enumerated as a list.

**method=<list element>**

Analysis method (Note that `method=` is optional)

Valid values: `sample`, `optimize`, `diagnose`

(Defaults to `sample`)

## Sampling-Specific Arguments

The following arguments are specific to sampling. The method argument `sample` (or `method=sample`) must come first in order to enable the subsequent arguments. The other arguments are optional and may appear in any order.

### └ **sample**

Bayesian inference with Markov Chain Monte Carlo

Valid subarguments: `num_samples`, `num_warmup`, `save_warmup`,  
`thin`, `adapt`, `algorithm`

### └ └ `num_samples=<int>`

Number of sampling iterations

Valid values:  $0 \leq \text{num\_samples}$   
(Defaults to 1000)

### └ └ `num_warmup=<int>`

Number of warmup iterations

Valid values:  $0 \leq \text{warmup}$   
(Defaults to 1000)

### └ └ `save_warmup=<boolean>`

Stream warmup samples to output?

Valid values: 0, 1  
(Defaults to 0)

### └ └ `thin=<int>`

Period between saved samples

Valid values:  $0 < \text{thin}$   
(Defaults to 1)

## Sampling Adaptation-Specific Parameters

When adaptation is engaged the warmup period is split into three stages (Figure 7.3), with two *fast* intervals surrounding a series of growing *slow* intervals. Here fast and slow refer to parameters that adapt using local and global information, respectively; the Hamiltonian Monte Carlo samplers, for example, define the step size as a fast parameter and the (co)variance as a slow parameter. The size of the the initial and final fast intervals and the initial size of the slow interval are all customizable, although user-specified values may be modified slightly in order to ensure alignment with the warmup period.

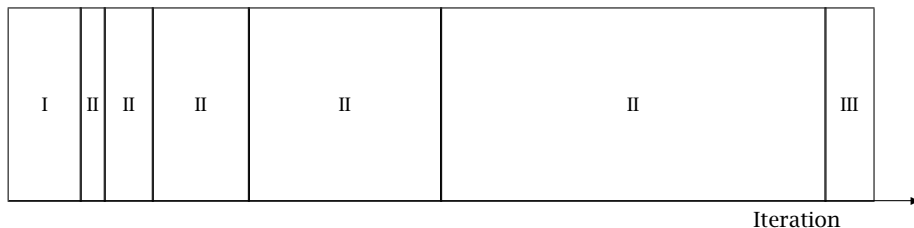


Figure 7.3: Adaptation during warmup occurs in three stages: an initial fast adaptation interval (I), a series of expanding slow adaptation intervals (II), and a final fast adaptation interval (III). For HMC, both the fast and slow intervals are used for adapting the step size, while the slow intervals are used for learning the (co)variance necessitated by the metric. Iteration numbering starts at 1 on the left side of the figure and increases to the right.

The motivation behind this partitioning of the warmup period is to allow for more robust adaptation. In the initial fast interval the chain is allowed to converge towards the typical set,<sup>3</sup> with only parameters that can learn from local information adapted. After this initial stage parameters that require global information, for example (co)variances, are estimated in a series of expanding, memoryless windows; often fast parameters will be adapted here as well. Lastly the fast parameters are allowed to adapt to the final update of the slow parameters.

Currently all Stan sampling algorithms utilize dual averaging to optimize the step size (this optimization during adaptation of the sampler should not be confused with running Stan’s optimization method). This optimization procedure is extremely flexible and for completeness we have exposed each option, using the notation of (Hoffman and Gelman, 2011, 2014). In practice the efficacy of the optimization is sensitive to the value of these parameters, and we do not recommend changing the defaults without experience with the dual averaging algorithm. For more information, see the discussion of dual averaging in (Hoffman and Gelman, 2011, 2014).

Variances or covariances are estimated using Welford accumulators to avoid a loss of precision over many floating point operations.

The following subarguments are introduced by the categorical argument `adapt`. Each subargument must contiguously follow `adapt`, though they may appear in any order.

## `adapt`

Warmup Adaptation

Valid subarguments: `engaged`, `gamma`, `delta`, `kappa`, `t0`

<sup>3</sup>The typical set is a concept borrowed from information theory and refers to the neighborhood (or neighborhoods in multimodal models) of significant posterior probability mass through which the Markov chain will travel in equilibrium.

- └─┬─┬─ `engaged=<boolean>`  
Adaptation engaged?  
Valid values: 0, 1  
(Defaults to 1)
- └─┬─┬─ `gamma=<double>`  
Adaptation regularization scale  
Valid values: 0 < gamma  
(Defaults to 0.05)
- └─┬─┬─ `delta=<double>`  
Adaptation target acceptance statistic  
Valid values: 0 < delta < 1  
(Defaults to 0.8)
- └─┬─┬─ `kappa=<double>`  
Adaptation relaxation exponent  
Valid values: 0 < kappa  
(Defaults to 0.75)
- └─┬─┬─ `t0=<double>`  
Adaptation iteration offset  
Valid values: 0 < t0  
(Defaults to 10)
- └─┬─┬─ `init_buffer=<unsigned int>`  
Width of initial fast adaptation interval  
Valid values: All  
(Defaults to 75)
- └─┬─┬─ `term_buffer=<unsigned int>`  
Width of final fast adaptation interval  
Valid values: All  
(Defaults to 50)
- └─┬─┬─ `window=<unsigned int>`  
Initial width of slow adaptation interval  
Valid values: All  
(Defaults to 25)

By setting the acceptance statistic `delta` to a value closer to 1 (its value must be strictly less than 1 and its default value is 0.8), adaptation will be forced to use smaller step sizes. This can improve sampling efficiency (effective samples per iteration)

at the cost of increased iteration times. Raising the value of `delta` will also allow some models that would otherwise get stuck overcome their blockages; see also the `stepsize_jitter` argument.

### *Sampling Algorithm- and Engine-Specific Arguments*

The following batch of arguments are used to control the sampler used for sampling. The top-level specification is for `engine`, the only valid value of which is `hmc` (this will change in the future as we add new samplers).

```
└─┬─ algorithm=<list element>
    Sampling algorithm
    Valid values: hmc, fixed_param
    (Defaults to hmc)
```

Hamiltonian Monte Carlo is a very general approach to sampling that utilizes techniques of differential geometry and mathematical physics to generate efficient MCMC transitions. This generality manifests in a wealth of implementation choices.

```
└─┬─┬─ hmc
    Hamiltonian Monte Carlo
    Valid subarguments: engine, metric, stepsize, stepsize_jitter
```

All HMC implementations require at least two parameters: an integration step size and a total integration time. We refer to different specifications of the latter as *engines*.

In the `static_hmc` implementation the total integration time must be specified by the user, where as the `nuts` implementation uses the No-U-Turn Sampler to determine an optimal integration time dynamically.

```
└─┬─┬─┬─ engine=<list element>
    Engine for Hamiltonian Monte Carlo
    Valid values: static, nuts
    (Defaults to nuts)
```

The following options are activated for static HMC.

```
└─┬─┬─┬─┬─ static
    Static integration time
    Valid subarguments: int_time
```

```
└─┬─┬─┬─┬─┬─ int_time=<double>
    Total integration time for Hamiltonian evolution
    Valid values: 0 < int_time
    (Defaults to 2 $\pi$ )
```

These options are for NUTS, an adaptive version of HMC.

└ └ └ └ └ **nuts**

The No-U-Turn Sampler

Valid subarguments: `max_depth`

### *Tree Depth*

NUTS generates a proposal by evolving the initial system both forwards and backwards in time to form a balanced binary tree. At each iteration of the NUTS algorithm the tree depth is increased by one, doubling the number of leapfrog steps and effectively doubles the computation time. The algorithm terminates in one of two ways: either the NUTS criterion is satisfied for a new subtree or the completed tree, or the depth of the completed tree hits `max_depth`.

Both the tree depth and the actual number of leapfrog steps computed are reported along with the parameters in the output as `treedepth__` and `n_leapfrog__`, respectively. Because the final subtree may only be partially constructed, these two will always satisfy

$$2^{\text{treedepth}-1} - 1 < N_{\text{leapfrog}} \leq 2^{\text{treedepth}} - 1.$$

`treedepth__` is an important diagnostic tool for NUTS. For example, `treedepth__ = 0` occurs when the first leapfrog step is immediately rejected and the initial state returned, indicating extreme curvature and poorly-chosen step size (at least relative to the current position). On the other hand, if `treedepth__ = max_depth` then NUTS is taking many leapfrog steps and being terminated prematurely to avoid excessively long execution time. For the most efficient sampling `max_depth` should be increased to ensure that the NUTS tree can grow as large as necessary.

For more information on the NUTS algorithm see (Hoffman and Gelman, 2011, 2014).

└ └ └ └ └ └ `max_depth=<int>`

Maximum tree depth

Valid values:  $0 < \text{max\_depth}$

(Defaults to 10)

### *Euclidean Metric*

All HMC implementations in Stan utilize quadratic kinetic energy functions which are specified up to the choice of a symmetric, positive-definite matrix known as a *mass matrix* or, more formally, a *metric* (Betancourt and Stein, 2011).

If the metric is constant then the resulting implementation is known as *Euclidean* HMC. Stan allows for three Euclidean HMC implementations: a unit metric, a diagonal metric, and a dense metric. These can be specified with the values `unit_e`, `diag_e`, and `dense_e`, respectively.

Future versions of Stan will also include dynamic metrics associated with *Riemannian* HMC (Girolami and Calderhead, 2011; Betancourt, 2012).

```
└─┬─┬─┬─┬─ metric=<list element>  
  Geometry of base manifold  
  Valid values: unit_e, diag_e, dense_e  
  (Defaults to diag_e)
```

```
└─┬─┬─┬─┬─┬─ unit_e  
  Euclidean manifold with unit metric
```

```
└─┬─┬─┬─┬─┬─ diag_e  
  Euclidean manifold with diag metric
```

```
└─┬─┬─┬─┬─┬─ dense_e  
  Euclidean manifold with dense metric
```

### *Step Size and Jitter*

All implementations of HMC also use numerical integrators requiring a step size. We also allow that step size to be “jittered” randomly during sampling to avoid any poor interactions with a fixed step size and regions of high curvature. The maximum amount of jitter is 1, which will cause step sizes to be selected in the range of 0 to twice the adapted step size. Low step sizes can get HMC samplers unstuck that would otherwise get stuck with higher step sizes. The downside is that jittering below the adapted value will increase the number of leapfrog steps required and thus slow down iterations, whereas jittering above the adapted value can cause premature rejection due to simulation error in the Hamiltonian dynamics calculation. See (Neal, 2011) for further discussion of step-size jittering.

```
└─┬─┬─┬─┬─┬─ stepsize=<double>  
  Step size for discrete evolution  
  Valid values:  $0 < \text{stepsize}$   
  (Defaults to 1)
```

```
└─┬─┬─┬─┬─┬─ stepsize_jitter=<double>  
  Uniformly random jitter of the stepsize, in percent  
  Valid values:  $0 \leq \text{stepsize\_jitter} \leq 1$   
  (Defaults to 0)
```



## Fixed Parameter Sampler

The fixed parameter sampler generates a new sample without changing the current state of the Markov chain; only generated quantities may change. This can be useful when, for example, trying to generate pseudo-data using the generated quantities block. If the parameters block is empty (no parameters) then using `algorithm=fixed_param` is mandatory.

└ └ └ **fixed\_param**  
Fixed Parameter Sampler

## Optimization-Specific Commands

The following arguments are for the top-level method `optimize`. They allow control of the optimization algorithm, and some of its configuration. The other arguments may appear in any order.

└ **optimize**  
Point estimation  
Valid subarguments: `algorithm`, `iter`, `save_iterations`

└ └ `algorithm=<list element>`  
Optimization algorithm  
Valid values: `bfgs`, `lbfgs`, `newton`  
(Defaults to `bfgs`)

The following options are for the (L-)BFGS optimizer. BFGS is the default optimizer and also much faster than the other optimizers.

Convergence monitoring in (L-)BFGS is controlled by a number of tolerance values, any one of which being satisfied causes the algorithm to terminate with a solution.

- The log probability is considered to have converged if

$$|\log p(\theta_i|y) - \log p(\theta_{i-1}|y)| < \text{tol\_obj}$$

or

$$\frac{|\log p(\theta_i|y) - \log p(\theta_{i-1}|y)|}{\max(|\log p(\theta_i|y)|, |\log p(\theta_{i-1}|y)|, 1.0)} < \text{tol\_rel\_obj} * \epsilon.$$

- The parameters are considered to have converged if

$$||\theta_i - \theta_{i-1}|| < \text{tol\_param}.$$

- The gradient is considered to have converged to 0 if

$$||g_i|| < \text{tol\_grad}$$

or

$$\frac{g_i^T \hat{H}_i^{-1} g_i}{\max(|\log p(\theta_i|y)|, 1.0)} < \text{tol\_rel\_grad} * \epsilon.$$

Here,  $i$  is the current iteration,  $\theta_i$  is the value of the parameters at iteration  $i$ ,  $y$  is the data,  $p(\theta_i|y)$  is the posterior probability of  $\theta_i$  up to a proportion,  $\nabla_\theta$  is the gradient operator with respect to  $\theta$ ,  $g_i = \nabla_\theta \log p(\theta_i|y)$  is the gradient at iteration  $i$ ,  $\hat{H}_i$  is the estimate of the Hessian at iteration  $i$ ,  $|u|$  is absolute value (L1 norm) of  $u$ ,  $||u||$  is vector length (L2 norm) of  $u$ , and  $\epsilon \approx 2e - 16$  is machine precision. Any of the convergence tests can be disabled by setting its corresponding tolerance parameter to zero.

The other command-line argument for BFGS is `init_alpha`, which is first step size to try on the initial iteration. If the first iteration takes a long time (and requires a lot of function evaluations) set `init_alpha` to be the roughly equal to the alpha used in that first iteration. `init_alpha` has a tiny default value, which is reasonable for many problems but might be too large or too small depending on the objective function and initialization. Being too big or too small just means that the first iteration will take longer (i.e., require more gradient evaluations) before the line search finds a good step length. It's not a critical parameter, but for optimizing the same model multiple times (as you tweak things or with different data) being able to change it can save some real time.

Finally, L-BFGS has a additional command-line argument, `history_size`, which controls how much memory is used maintaining the approximation of the Hessian. This should be less than the dimensionality of the parameter space and, in general, relatively small values (5 - 10) are sufficient. If L-BFGS performs badly but BFGS is performing well, then consider increasing this. Note that increasing this will increase the memory usage, although this is unlikely to be an issue for typical Stan models.

### └ └ └ (1)bfgs

(L-)BFGS with linesearch

Valid subarguments: `init_alpha`, `tol_obj`, `tol_rel_obj`, `tol_grad`, `tol_rel_grad`, `tol_param`, `history_size` (lbfgs only)

### └ └ └ └ init\_alpha=<double>

Line search step size for first iteration

Valid values:  $0 \leq \text{init\_alpha}$

(Defaults to 0.001)

- └ └ └ └ `tol_obj=<double>`  
 Convergence tolerance on changes in objective function value  
 Valid values:  $0 \leq \text{tol\_obj}$   
 (Defaults to  $1e-12$ )
- └ └ └ └ `tol_rel_obj=<double>`  
 Convergence tolerance on relative changes in objective function value  
 Valid values:  $0 \leq \text{tol\_rel\_obj}$   
 (Defaults to  $1e+4$ )
- └ └ └ └ `tol_grad=<double>`  
 Convergence tolerance on the norm of the gradient  
 Valid values:  $0 \leq \text{tol\_grad}$   
 (Defaults to  $1e-8$ )
- └ └ └ └ `tol_rel_grad=<double>`  
 Convergence tolerance on the relative norm of the gradient  
 Valid values:  $0 \leq \text{tol\_rel\_grad}$   
 (Defaults to  $1e+7$ )
- └ └ └ └ `tol_param=<double>`  
 Convergence tolerance on changes in parameter value  
 Valid values:  $0 \leq \text{tol\_param}$   
 (Defaults to  $1e-8$ )
- └ └ └ └ `history_size=<int>`  
 Number of update vectors to use in Hessian approximations (lbfgs only)  
 Valid values:  $0 < \text{history\_size}$   
 (Defaults to 5)

The following argument is for Newton's optimization method; there are currently no configuration parameters for Newton's method, and it is not recommended because of the slow Hessian calculation involving finite differences.

- └ └ └ **`newton`**  
 Newton's method

The remaining arguments apply to all optimizers.

- └ └ `iter=<int>`  
 Total number of iterations  
 Valid values:  $0 < \text{iter}$   
 (Defaults to 2000)

- └ └ `save_iterations=<boolean>`  
Stream optimization progress to output?  
Valid values: 0, 1  
(Defaults to 0)

## Diagnostic-Specific Arguments

The following arguments are specific to diagnostics. As of now, the only diagnostic is gradients of the log probability function.

- └ ***diagnose***  
Model diagnostics  
Valid subarguments: `test`
- └ └ `test=<list element>`  
Diagnostic test  
Valid values: `gradient`  
(Defaults to `gradient`)
- └ └ └ ***gradient***  
Check model gradient against finite differences Valid subarguments: `epsilon`,  
`error`
- └ └ └ └ `epsilon=<real>`  
Finite difference step size  
Valid values:  $0 < \text{epsilon}$   
(Defaults to  $1\text{e-}6$ )
- └ └ └ └ `error=<real>`  
Error threshold  
Valid values:  $0 < \text{error}$   
(Defaults to  $1\text{e-}6$ )

## General-Purpose Arguments

The following arguments may be used with any of the previous configurations. They may come either before or after the other subarguments of the top-level method.

### *Process Identifier Argument*

- `id=<int>`  
Unique process identifier, used to advance random number generator so that random numbers do not overlap across chains

Valid values:  $0 < id$   
(Defaults to 0)

### *Input Data Arguments*

#### **data**

Input data options  
Valid subarguments: **file**

↳ **file**=<*string*>

Input data file  
Valid values: Path to existing file  
(Defaults to empty path)

### *Initialization Arguments*

Initialization is only applied to parameters defined in the parameters block. Any initial values supplied for transformed parameters or generated quantities are ignored.

**init**=<*string*>

Initialization method:

- real number  $x > 0$  initializes randomly between  $[-x, x]$ ;
- 0 initializes to 0;
- non-number interpreted as a data file

Valid values: All  
(Defaults to 2)

### *Random Number Generator Arguments*

#### **random**

Random number configuration  
Valid subarguments: **seed**

↳ **seed**=<*unsigned int*>

Random number generator seed  
Valid values:

- **seed**  $\geq 0$  generates seed;
- **seed**  $< 0$  uses seed generated from time

(Defaults to -1)

## Output Arguments

### output

File output options

Valid subarguments: `file`, `diagnostic_file`,  
`refresh`

#### └ `file=<string>`

Output file

Valid values: Valid path

(Defaults to `output.csv`)

#### └ `diagnostic_file=<string>`

Auxiliary output file for diagnostic information

Valid values: Valid path

(Defaults to empty path)

#### └ `refresh=<int>`

Number of iterations between screen updates

Valid values:  $0 < \text{refresh}$

(Defaults to 100)

## 7.5. Command-Line Option Examples

The hierarchical structure of the command-line options can be intimidating, and here we provide an example workflow to help ease the introduction to new users, especially those used to Stan 1.3 or earlier releases. The examples in this section are for Mac OS and Linux; on Windows, just remove the `./` before the executable and change the line-continuation character from Unix's `\` to DOS's `^`. As in previous sections, the indentation on continued lines is for pedagogical purposes only and does not convey any content to the executable.

Let's say that we've just built our model, `model`, and are ready to run. We begin by specifying data and init files,

```
> ./model data file=model.data.R init=model.init.R
```

but our model doesn't run. Instead, the above command prints

```
A method must be specified!
```

```
Failed to parse arguments, terminating Stan
```

The problem is that we forgot to specify a method.

All Stan arguments have default values, except for the method. This is the only argument that must be specified by the user and a model will not run without it (not to say that the model will run without error, for example a model that requires data will eventually fail unless an input file is specified with `file` under `data`). Assuming that we want to draw MCMC samples from our model, we can either specify a method implicitly,

```
> ./model sample data file=model.data.R init=model.init.R
```

or explicitly,

```
> ./model method=sample data file=model.data.R \
    init=model.init.R
```

In either case our model now executes without any problem.

Now let's say that we want to customize our execution. In particular we want to set the seed for the random number generator, but we forgot the specific argument syntax. Information for each argument can displayed by calling `help`,

```
> ./model random help
```

which returns

```
random
Random number configuration
Valid subarguments: seed
...
```

before printing usage information. For information on the seed argument we just call `help` one level deeper,

```
> ./model random seed help
```

which returns

```
seed=<unsigned int>
Random number generator seed
Valid values: seed > 0, if negative seed is generated from time
Defaults to -1
...
```

Fully informed, we can now run with a given seed,

```
> ./model method=sample data file=model.data.R \
    init=model.init.R \
    random seed=5
```

The arguments `method`, `data`, `init`, and `random` are all top-level arguments. To really see the power of a hierarchical argument structure let's try to drill down and specify the metric we use for HMC: instead of the default diagonal Euclidean metric, we want to use a dense Euclidean metric. Attempting to specify the metric we try

```
> ./model method=sample data file=model.data.R \
      init=model.init.R \
      random seed=5 \
      metric=unit
```

only to have the execution fail with the message

```
metric=unit_e is either mistyped or misplaced.
Perhaps you meant one of the following valid configurations?
  method=sample algorithm=hmc metric=<list_element>
Failed to parse arguments, terminating Stan
```

The argument `metric` does exist, but not at the top-level. In order to specify it we have to drill down into `sample` by first specifying the sampling algorithm, as noted in the suggestion,

```
> ./model method=sample algorithm=hmc metric=unit \
      data file=model.data.R \
      init=model.init.R \
      random seed=5
```

Unfortunately we still messed up,

```
unit is not a valid value for "metric"
Valid values: unit_e, diag_e, dense_e
Failed to parse arguments, terminating Stan
```

Tweaking the metric name we make one last attempt,

```
> ./model method=sample algorithm=hmc metric=unit_e \
      data file=model.data.R \
      init=model.init.R \
      random seed=5
```

which successfully runs.

Finally, let's consider the circumstance where our model runs fine but the NUTS iterations keep saturating the default tree depth limit of 10. We need to change the limit, but how do we specify NUTS let alone the maximum tree depth? To see how



let's take advantage of the `help-all` option which prints all arguments that derive from the given argument. We know that NUTS is somehow related to sampling, so we try

```
> ./model method=sample help-all
```

which returns the verbose output,

`sample`

Bayesian inference with Markov Chain Monte Carlo

Valid subarguments: `num_samples`, `num_warmup`,  
`save_warmup`, `thin`, `adapt`, `algorithm`

`num_samples=<int>`

Number of sampling iterations

Valid values:  $0 \leq \text{num\_samples}$

Defaults to 1000

`num_warmup=<int>`

Number of warmup iterations

Valid values:  $0 \leq \text{warmup}$

Defaults to 1000

`save_warmup=<boolean>`

Stream warmup samples to output?

Valid values: [0, 1]

Defaults to 0

`thin=<int>`

Period between saved samples

Valid values:  $0 < \text{thin}$

Defaults to 1

`adapt`

Warmup Adaptation

Valid subarguments: `engaged`, `gamma`, `delta`, `kappa`, `t0`

`engaged=<boolean>`

Adaptation engaged?

Valid values: [0, 1]

Defaults to 1

`gamma=<double>`

Adaptation regularization scale

Valid values:  $0 < \text{gamma}$



```

max_depth=<int>
    Maximum tree depth
    Valid values: 0 < max_depth
    Defaults to 10

metric=<list element>
    Geometry of base manifold
    Valid values: unit_e, diag_e, dense_e
    Defaults to diag_e

unit_e
    Euclidean manifold with unit metric

diag_e
    Euclidean manifold with diag metric

dense_e
    Euclidean manifold with dense metric

stepsize=<double>
    Step size for discrete evolution
    Valid values: 0 < stepsize
    Defaults to 1

stepsize_jitter=<double>
    Uniformly random jitter of the stepsize, in percent
    Valid values: 0 <= stepsize_jitter <= 1
    Defaults to 0

...

```

Following the hierarchy, the maximum tree depth derives from `nuts`, which itself is a value for the argument `engine` which derives from `hmc`. Adding this to our previous call we attempt

```

> ./model method=sample \
    algorithm=hmc \
    metric=unit_e \
    engine=nuts max_depth=-15 \
    data file=model.data.R \
    init=model.init.R \
    random seed=5 \

```

which yields

```
-1 is not a valid value for "max_depth"
Valid values: 0 < max_depth
Failed to parse arguments, terminating Stan
```

Where did that negative sign come from? Clumsy fingers are nothing to be embarrassed about, especially with such complex argument configurations. Removing the guilty character, we try

```
> ./model method=sample \
      algorithm=hmc \
      metric=unit_e \
      engine=nuts max_depth=15 \
      data file=model.data.R \
      init=model.init.R \
      random seed=5
```

which finally runs without issue.

## 7.6. Command Templates

This section provides templates for all of the arguments deriving from each of the possible methods: `sample`, `optimize`, and `diagnose`. Arguments in square brackets are optional, those not in square brackets are required for the template.

### Sampling Templates

The No-U-Turn sampler (NUTS) is the default (and recommended) sampler for Stan. The full set of configuration options is in Figure 7.4.

A standard Hamiltonian Monte Carlo (HMC) sampler with user-specified integration time may also be used. Its set of configuration options are shown in Figure 7.5.

Both NUTS and HMC may be configured with either a unit, diagonal or dense Euclidean metric, with a diagonal metric the default.<sup>4</sup> A unit metric provides no parameter-by-parameter scaling, a diagonal metric scales each parameter independently, and a dense metric also rotates the parameters so that correlated parameters may move together. Although dense metrics offer the hope of superior simulation performance, they require more computation per iteration. Specifically for  $m$  samples of a model with  $n$  parameters, the dense metric requires  $\mathcal{O}(n^3 \log(m) + n^2 m)$  operations, whereas diagonal metrics require only  $\mathcal{O}(nm)$ . Furthermore, dense metrics are difficult to estimate, given the  $\mathcal{O}(n^2)$  components with complex interdependence.

---

<sup>4</sup>In Euclidean HMC, a diagonal metric emulates different step sizes for each parameter. Explicitly varying step sizes were used in Stan 1.3 and before; Neal (2011) discusses the equivalence.

```

> ./my_model sample \
    algorithm=hmc \
    engine=nuts \
    [max_depth=<int>] \
    [metric={unit_e,diag_e,dense_e}] \
    [stepsize=<double>] \
    [stepsize_jitter=<double>] \
    [num_samples=<int>] \
    [num_warmup=<int>] \
    [save_warmup=<boolean>] \
    [thin=<int>] \
    [adapt \
    [engaged=<boolean>] \
    [gamma=<double>] \
    [delta=<double>] \
    [kappa=<double>] \
    [t0=<double>] ] \
    [data file=<string>] \
    [init=<string>] \
    [random seed=<int>] \
    [output \
    [file=<string>] \
    [diagnostic_file=<string>] \
    [refresh=<int>] ]

```

Figure 7.4: Command skeleton for invoking the no-U-turn sampler (NUTS). This is the same skeleton as that for basic HMC in Figure 7.5. Elements in braces are optional. All arguments and their default values are described in detail in Section 7.4.

## Optimization Templates

CmdStan supports several optimizers. These share many of their configuration options with the samplers. The default optimizer is the the limited memory Broyden-Fletcher-Goldfarb-Shanno (L-BFGS) method; [Nocedal and Wright \(2006\)](#) contains an excellent overview of both the BFGS and L-BFGS algorithms. The command skeleton for L-BFGS is in Figure 7.6 and the one for BFGS is in Figure 7.7. Stan also supports Newton’s method; see [\(Nocedal and Wright, 2006\)](#) for more information. This method is the least efficient of the three, but has the advantage of setting its own step size. Other than not having a stepsize argument, the skeleton for Newton’s method shown in Figure 7.8 is identical to that for BFGS.

```

> ./my_model sample \
    algorithm=hmc \
    engine=static \
    [int_time=<double>] \
    [metric={unit_e,diag_e,dense_e}] \
    [stepsize=<double>] \
    [stepsize_jitter=<double>] \
    [num_samples=<int>] \
    [num_warmup=<int>] \
    [save_warmup=<boolean>] \
    [thin=<int>] \
    [adapt \
    [engaged=<boolean>] \
    [gamma=<double>] \
    [delta=<double>] \
    [kappa=<double>] \
    [t0=<double>] ] \
    [data_file=<string>] \
    [init=<string>] \
    [random_seed=<int>] \
    [output \
    [file=<string>] \
    [diagnostic_file=<string>] \
    [refresh=<int>] ]

```

Figure 7.5: Command skeleton for invoking the basic Hamiltonian Monte Carlo sampler (HMC). This is the same as the NUTS command skeleton shown in Figure 7.4 other than for the engine. Elements in braces are optional. All arguments and their default values are described in detail in Section 7.4.

## Diagnostic Command Skeleton

Stan reports on gradients for the model at a specified or randomly generated initial value. The command-skeleton in this case is very simple, and shown in Figure 7.9.

```

> ./my_model optimize                                     \
    algorithm=lbgfs                                       \
        [init_alpha=<double>]                             \
        [tol_obj=<double>]                                 \
        [tol_rel_obj=<double>]                             \
        [tol_grad=<double>]                               \
        [tol_rel_grad=<double>]                           \
        [tol_param=<double>]                             \
        [history_size=<int>]                               \
    [iter=<int>]                                           \
    [save_iterations=<boolean>]                           \
[data file=<string>]                                       \
[init=<string>]                                           \
[random seed=<int>]                                       \
[output                                                  \
    [file=<string>]                                       \
    [diagnostic_file=<string>]                           \
    [refresh=<int>] ]

```

Figure 7.6: Command skeleton for invoking the L-BFGS optimizer. All arguments and their default values are described in detail in Section 7.4.

```

> ./my_model optimize                                     \
    algorithm=bfgs                                       \
        [init_alpha=<double>]                             \
        [tol_obj=<double>]                                 \
        [tol_rel_obj=<double>]                             \
        [tol_grad=<double>]                               \
        [tol_rel_grad=<double>]                           \
        [tol_param=<double>]                             \
    [iter=<int>]                                           \
    [save_iterations=<boolean>]                           \
[data file=<string>]                                       \
[init=<string>]                                           \
[random seed=<int>]                                       \
[output                                                  \
    [file=<string>]                                       \
    [diagnostic_file=<string>]                           \
    [refresh=<int>] ]

```

Figure 7.7: Command skeleton for invoking the BFGS optimizer. All arguments and their default values are described in detail in Section 7.4.

```

> ./my_model optimize
    algorithm=newton
    [iter=<int>]
    [save_iterations=<boolean>]
[data file=<string>]
[init=<string>]
[random seed=<int>]
[output
    [file=<string>]
    [diagnostic_file=<string>]
    [refresh=<int>] ]

```

Figure 7.8: Command skeleton for invoking the Newton optimizer. All arguments and their default values are described in detail in Section 7.4.

```

> ./my_model diagnose
    [test=gradient]
    [epsilon=<real>]
    [error=<real>]
[data file=<string>]
[init=<string>]
[random seed=<int>]

```

Figure 7.9: Command skeleton for invoking model diagnostics. All arguments and their default values are described in detail in Section 7.4.



# Appendices

## A. Licensing

CmdStan, Stan, and Stan’s two dependent libraries, Boost and Eigen, are distributed under liberal freedom-respecting<sup>1</sup> licenses approved by the Open Source Initiative.<sup>2</sup>

In particular, the licenses for CmdStan and its dependent libraries have no “copy-left” provisions requiring applications of CmdStan or Stan to be open source if they are redistributed.

This chapter describes the licenses for the tools that are distributed with CmdStan. The next chapter explains some of the build tools that are not distributed with CmdStan, but are required to build and run Stan models.

### A.1. CmdStan’s License

CmdStan is distributed under the BSD 3-clause license (BSD New).

<http://www.opensource.org/licenses/BSD-3-Clause>

### A.2. Stan’s License

Stan is distributed under the BSD 3-clause license (BSD New).

<http://www.opensource.org/licenses/BSD-3-Clause>

### A.3. Boost License

Boost is distributed under the Boost Software License version 1.0.

<http://www.opensource.org/licenses/BSL-1.0>

### A.4. Eigen License

Eigen is distributed under the Mozilla Public License, version 2.

<http://http://opensource.org/licenses/mpl-2.0>

---

<sup>1</sup>The link <http://www.gnu.org/philosophy/open-source-misses-the-point.html> leads to a discussion about terms “open source” and “freedom respecting.”

<sup>2</sup>See <http://opensource.org>.

## A.5. Google Test License

CmdStan uses Google Test for unit testing; it is not required to compile or execute models. Google Test is distributed under the BSD 2-clause license.

<http://www.opensource.org/licenses/BSD-License>

## B. Installation and Compatibility

This appendix describes the hardware and software required to run CmdStan. The software required includes CmdStan and its libraries, as well as a contemporary C++ compiler. CmdStan requires hardware powerful enough to build and execute the models. Ideally, that will be a 64-bit computer with at least 4GB of memory and multiple processor cores.

### B.1. Operating System

CmdStan is written in portable C++ without C++11 features, as are the libraries on which it depends. Therefore, CmdStan should run on any machine for which a suitable C++ compiler is available. In practice, CmdStan, like the Boost and Eigen libraries on which it depends, is very hard on the compiler and linker.

CmdStan has been tested on the following operating systems.

- Linux (Debian, Ubuntu, Red Hat),
- Mac OS X (10.10 “Yosemite,” 10.9 “Mavericks,” 10.8 “Mountain Lion,” 10.7 “Lion,” and 10.6 “Snow Leopard”)
- Windows (XP, 7, 8).

CmdStan should work on other versions of these operating systems if compatible C++ compilers can be found. The plan is to keep up with new versions of these operating systems and gradually phase out testing on older versions.

### B.2. Required Software and Tools

The only two absolute requirements for running CmdStan are the CmdStan source code (and dependent libraries) and a C++ compiler.

#### CmdStan Source

In order to compile Stan program, the CmdStan source code is required. The CmdStan source code distribution includes CmdStan’s source code, Stan’s source code, documentation, build scripts, unit tests, example models, documentation and source for the required libraries Boost and Eigen, and the source for an optional testing library, Google Test.

### *CmdStan: Stable Releases*

The latest release version of CmdStan can be downloaded from the CmdStan home page:

<http://mc-stan.org/cmdstan.html>

### *CmdStan: Development Source Control*

The source code repository is hosted by GitHub, and contains the latest versions of CmdStan (and Stan) underdevelopment. See:

<http://mc-stan.org/source-repos.html>

### *Boost C++ Library Source*

Stan's parser and some of its mathematical functions and template metaprogramming facilities are implemented with the Boost C++ Library.

- Home: <http://www.boost.org/users/license.html>
- License: Boost Software License
- Tested Version: 1.54.0

The Boost source code is distributed with Stan.

### *Eigen Matrix and Linear Algebra Library Source*

Stan's matrix algebra depends on the Eigen C++ matrix and linear algebra library.

- Home: <http://eigen.tuxfamily.org>
- License: Mozilla Public License, version 2.0
- Tested Version: 3.2.0

The Eigen source code is distributed with Stan.

### **C++ Compiler**

Compiling CmdStan programs requires a C++ compiler. CmdStan has been primarily developed with `clang++` and `g++` and no promises are made for other compilers. The full set of compilers for which CmdStan has been tested is

- **g++**  
Tested Versions: Mac 4.2.1, 4.6, Linux 4.4-4.7 (plus trunk 4.8, 4.9), Windows 4.6.3  
Home: <http://gcc.gnu.org/>  
License: GPL3+
- **clang++**, Mac 2.9-3.1, Linux 2.9-3.1  
Home: <http://clang.llvm.org/>  
License: BSD
- **mingw-64**, version 2.0 (Windows 7, cross-compiled from Debian Linux)
- **Intel C++**, Linux version 12.1.3

### B.3. Step-by-Step Windows Install Instructions

CmdStan has been tested on Windows XP, Windows 7, and Windows 8.

CmdStan also runs under Cygwin, which provides a unix-like shell on top of Windows. Instructions for Cygwin installation are provided below in their own subsection.

#### Windows Tips

##### *Opening a Command Shell*

To open a Windows command shell, first open the **Start** Menu (usually in the lower left of the screen), select option **All Programs**, then option **Accessories**, then program **Command Prompt**.

Alternatively, enter [Windows+r] (both keys together on the keyboard), and enter **cmd** into the text field that pops up in the **Run** window, then press [Return] on the keyboard to run.

##### *32-bit Builds*

CmdStan defaults to a 64-bit build. On a 32-bit operating system, include **BIT=32** in **make/local**. See Appendix B.6 for more details.

#### Rtools C++ Development Environment

The simplest way to install a full C++ build environment that will work for CmdStan is to use the Rtools package designed for R developers on Windows (even if you don't plan to use R).

First, download the latest *frozen* (i.e., stable) version of Rtools from the Rtools home page, using

<http://cran.r-project.org/bin/windows/Rtools/>

Next, double click on the downloaded file to open the Rtools install wizard, then proceed through its options.

- *Language*: select language, click Next,
- *Welcome*: click Next,
- *Information*: click Next,
- *Setup Location*: accept default (c:\Rtools), click Next,
- *Select Components*: select default, Package Authoring, click Next,
- *Select Additional Tasks*: check Edit Path and Save Version in Registry, click Next,
- *System Path Report*: ensure that the paths to c:\Rtools\bin and c:\Rtools\gcc-4.6.3\bin are listed at the beginning of the path and click Next,
- *Ready to Install*: click Next, wait for the install to complete, then
- *Finish*: click Finish.
- *Confirm Path*: After the install has completed, open a command prompt and type PATH to ensure that the new path is activated and the Rtools folders are in the system path.

### *Checking the Path*

Make sure that c:\Rtools\bin has been added to your PATH environment variable, and then open another command window. You should be able to follow the last step, *Confirm Path*, above.

### **Verifying Tools**

To verify that g++ is installed, use the following command.

```
> g++ -v
```

This should report version information for g++. Next, verify that make is installed with the following command.

```
> make -v
```

This should print version information for make.

## Downloading and Unpacking CmdStan

The CmdStan source code distribution is named `cmdstan-2.6.2.tar.gz`; the versions here are major version 2, minor version 6, and patch level 0. Download the latest CmdStan source tarball from the CmdStan downloads page,

<https://github.com/stan-dev/cmdstan/releases>

to any non-temporary folder. (If in doubt, select **My Documents** on Windows XP or **Documents** on Windows 7.)

Change to the download directory (aka folder) using one of the following commands, replacing `<username>` with a Windows user name.

- *Windows XP*: From the default starting directory, use the following commands (quotes and all):

```
> cd "My Documents"
```

The full path (including quotes) will work from anywhere,

```
> cd "c:\Documents and Settings\<username>\My Documents"
```

- *Windows 7*: From the default starting directory, use

```
> cd Documents
```

or use the full path, including quotes, from anywhere,

```
> cd "c:\Users\<username>\Documents"
```

To verify that the downloaded `CmdStan.tar.gz` file is there, list the directory contents using:

```
> dir
```

Finally, unpack the distribution using the `tar` command (which is installed as part of Rtools).

```
> tar --no-same-owner -xzf cmdstan-cmdstanversion.tar.gz
```

The `-no-same-owner` flag is not strictly necessary, but it removes a bunch of irrelevant warnings.



## 64-bit Cygwin Install Instructions

CmdStan can be run under Cygwin, the Unix look-and-feel environment for Windows. Cygwin must have recent versions of `make` and `g++` (part of `gcc`) installed. Within a Cygwin shell, CmdStan will behave as under other Unixes. Follow the directions in Appendix B.5.

## B.4. Step-by-Step Mac Install Instructions

This section provides step-by-step install instructions for the Mac. CmdStan has been tested on Mac OS X versions Mavericks, Snow Leopard, Lion, and Mountain Lion.

### Install Xcode C++ Development Environment

The easiest (but not the only) way to install a C++ development environment on a Mac is to use Apple's Xcode development environment.

From the Xcode home page,

<https://developer.apple.com/xcode/>

click **View in Mac App Store**.

From the App Store, click **Install**, enter an Apple ID, and wait for Xcode to finish installing.

Open the Xcode application, click top-level menu **Preferences**, click top-row button **Downloads**, click button for **Components**, click on the **Install** button to the right of the **Command Line Tools** entry, then wait for it to finish installing.

Click the top-level menu item **Xcode**, then click item **Quit Xcode** to quit.

To test, open the Terminal application and enter

```
> make --version
> g++ --version
```

Verify that `make` is at version 3.81 or later and `g++` is at 4.2.1 or later.

### Download and Unpack CmdStan Source

Download the most recent version of `cmdstan-2.6.2.tar.gz` from the CmdStan downloads list,

<https://github.com/stan-dev/cmdstan/releases>

Open the folder containing the download in the Finder (typically, the user's top-level Downloads folder).

If the Mac OS has not automatically unpacked the `.tar.gz` file into file `cmdstan-2.6.2.tar`, double-click the `.tar.gz` file to unpack.

Double click on the `.tar` file to unarchive directory `cmdstan-2.6.2`.

Move the resulting directory to a location where it will not be deleted, henceforth called `<cmdstan-home>`.

## B.5. Step-by-Step Linux Install Instructions

CmdStan has been tested on various Linux installations, including Ubuntu, Debian, and Red Hat.

### Installing C++ Development Tools

On Linux, C++ compilers and `make` are often installed by default.

To see if the `g++` compiler and `make` build system are already installed, use the commands

```
> g++ --version
> make --version
```

If these are at least at `g++` version 4.2.1 or later and `make` version 3.81 or later, no additional installations are necessary. It may still be desirable to update the C++ compiler `g++`, because later versions are faster.

To install the latest version of these tools (or upgrade an older version), use the commands

```
> sudo apt-get install g++
> sudo apt-get install make
```

A password will likely be required by the superuser command `sudo`.

### Downloading and Unpacking CmdStan Source

Download the most recent stable version of CmdStan, `cmdstan-2.6.2.tar.gz`, from the CmdStan downloads page,

<https://github.com/stan-dev/cmdstan/releases>

to the directory where Stan will reside.

In a command shell, change directories to where the tarball was downloaded, say `<download-dir>`, with

```
> cd <download-dir>
```

where <download-dir> is replaced with the actual path to the directory.

Then, unpack the distribution into the subdirectory

```
<download-dir>/cmdstan-2.6.2
```

with

```
> tar -xzf cmdstan-\cmdstanversion.tar.gz
```

## B.6. make Options

### Setting a Variable

CmdStan uses make for building the CmdStan tools and compiling Stan programs as executables. Users can customize how the tools are built by editing `make/local` inside the `<cmdstan-home>` directory.

Customization is done by setting variables or appending to them. For each variable that needs to be set, write `<variable>=<value>` on its own line inside `make/local`. To append to existing variables, write `<variable>+=<value>`.

### Customizing make Options

#### *Compiler Settings*

The most common options to set are the compiler options:

- `CC`. The compiler used to build CmdStan and the Stan executables. The default is `CC=g++`.
- `O`. The optimization level for the compiler. The default is `O=3`. Both `g++` and `clang++` recognize `0`, `1`, `2`, `3`, and `s`.

#### *Changing Library Locations*

The next set of variables allow for easy replacement of dependent libraries. CmdStan depends on Stan, Boost, and Eigen. Although CmdStan is bundled with a particular version of Stan, other versions can be used. The same is true with Boost and Eigen.

The Stan developers typically replace the tagged version of Stan in `<cmdstan-home>/stan` with an updated version and do not set these variables. That said, it is easy to point CmdStan to other versions of these libraries in other directories.

- **STANAPI\_HOME.** The location of the Stan source directory. The default is `STANAPI_HOME=stan/`. Note: the trailing forward slash is necessary.
- **BOOST.** The location of the Boost library. The default is `BOOST=stan/lib/boost_1.54.0`. If `STANAPI_HOME` is set, the default will be the `lib/boost_1.54.0` folder within `STANAPI_HOME`.
- **EIGEN.** The location of the Eigen library. The default is `EIGEN=stan/lib/eigen_3.2.0`. If `STANAPI_HOME` is set, the default will be the `lib/eigen_3.2.0` folder within `STANAPI_HOME`.

### *Additional Options*

These are the additional options and typically do not need to be set.

- **O\_STANC.** The optimization level for building `stanc`. The default is `O_STANC=0`.
- **CFLAGS.** The compiler flags for building CmdStan programs. The default value is dependent on the operating system.
- **LDLIBS.** The libraries used for linking CmdStan programs. The default value is dependent on the operating system.
- **LDLIBS\_STANC.** The libraries used for linking the Stan compiler, `stanc`. The default is the value of `LDLIBS`.
- **BIT.** The bitness of the executable. This variable only applies to Windows. The default is `BIT=64`. If building on a 32-bit Windows machine, `BIT=32` must be set.
- **TEMPLATE\_DEPTH.** The maximum instantiation depth for template classes which is passed to `g++` or `clang++`. This variable only applies to Mac OS X due to the current compilers distributed through Xcode not specifying enough depth by default.
- **EXE.** The file extension for executables. The default is operating system dependent. On Windows, the default is `EXE=.exe`. On other operating systems, the default is empty, `EXE=`.

### **Rebuilding CmdStan**

When compiler flags are changed, CmdStan needs to be rebuilt in order for the changes to take place. The easiest way to do this is to type:

```
> make clean-all
```

Then rebuild CmdStan and the Stan programs of interest.

## B.7. MKL Compiler Instructions

### Getting the MKL

To purchase a license, see

<http://software.intel.com/en-us/intel-mkl>

For non-commercial development, see

<http://software.intel.com/non-commercial-software-development>

### Compiling with MKL

In order to use Intel's math kernel library (MKL) for C++, a few lines need to be added to `make/local`.

- `CC = icc`. Set the compiler to `icc`.
- `MKLROOT = /apps/intel/2013/mkl`. Create a new variable with the location of the MKL path.
- `CFLAGS += -I $(MKLROOT)/include -DEIGEN_USE_MKL_ALL`. This tells Eigen to use MKL and where to find the necessary header files.
- `LDLIBS += -L$(MKLROOT)/lib/intel64 -lmkl_intel_lp64` and `LDLIBS += -lmkl_core -lmkl_sequential -lpthread -lm`. This links in the MKL library for the CmdStan executables. The exact implementation will depend on the particular system. Use the MKL link line advisor for help.

*Note:* Make sure to do the above changes before compiling for the first time - otherwise Stan will be compiled with `g++` and you won't see any performance gains.

## B.8. Optional Components for Developers

CmdStan is developed using the following set of tools. The various command examples in this manual have assumed they can be found on the command path. The makefile allows precise locations to be plugged in.

### GNU Make Build Tool

CmdStan automates the build, test, documentation, and deployment tasks using scripts in the form of makefiles to run with GNU Make.

- Home: <http://www.gnu.org/software/make>

- License: GPLv3+
- Tested Versions: 3.81 (Mac OS X), 3.79 (Windows 7)

## **Doxygen Documentation Generator**

CmdStan's API documentation is generated using the Doxygen Tool.

- Home: <http://www.stack.nl/~dimitri/doxygen/index.html>
- License: GPL2
- Tested Version(s): Mac OS X 1.8.2, Windows 1.8.2

## **Git Version Control System**

CmdStan uses the Git version control system for its software, libraries, and documentations. Git is required to interact with the most recent versions of code in the version control repository.

- Home: <http://git-scm.com/>
- License: GPL2
- Tested Version(s): Mac versions 1.8.2.3 and 1.7.8.4; Windows version 1.7.9

## *Google Test C++ Testing Framework*

CmdStan's unit testing is based on the Google's googletest C++ testing framework.

- Home: <http://code.google.com/p/googletest/>
- License: BSD
- Tested Version(s): 1.7.0

The Google Test framework is distributed with Stan.

## **B.9. Tips for Mac OS X**

### *Finding and Opening Mac Applications and Files*

To open an application, use [Command-Space] (press both keys at once on the keyboard) to open Spotlight, enter the application's name in the text field, then click

on the application in the pop-up menu or [Return] if the right file or application is highlighted.

Spotlight can be used in the same way to find files or folders, such as the default Downloads folder for web downloads.

### *Open a Terminal for Shell Commands*

To run shell commands, open the built-in Terminal application (see the previous subsection for details on how to find and open applications).

## **Install Xcode**

Apple's Xcode contains both the `clang++` and `g++` compilers and make, all of the tools needed to work with CmdStan as a user. The version of Xcode to install depends on the version of Mac OS X.

### *Alternative, GCC-Only Installer*

A stripped down installer for just the GCC package, including the C++ compilers `g++` and `clang++`, available for Mac OS X 10.6 ("Snow Leopard") or later,

<https://github.com/kennethreitz/osx-gcc-installer/>

The full list of tools in this distribution is available at:

<http://www.opensource.apple.com/release/developer-tools-41/>

## **More Recent Compilers**

Alternative compilers to those distributed by Apple as part of Xcode are available at the following locations.

### *Homebrew*

One way to get pre-built binaries for Mac OS X is to use Homebrew, which is available from the following link.

<http://mxcl.github.com/homebrew/>

## MacPorts

MacPorts hosts recent versions of compilers for the Macintosh.

<https://distfiles.macports.org/MacPorts/>

After finding the appropriate `.dmg` file, clicking on it, then double clicking on the resulting `.pkg` file, and clicking through some more menus, the following will need to be entered from a terminal window to install it.

```
> sudo port install gccVersion
```

In this command, *gccVersion* is the name of a compiler version, such as `g++=mp-4.6`, for version 4.6. Errors may arise during the install such as the following.

```
Error: Target org.macports.activate returned: Image error:
/opt/local/include/gmp.h already exists and does not belong to
a registered port. Unable to activate port gmp. Use 'port -f
activate gmp' to force the activation.
```

This issue can be resolved by running the following command.

```
> sudo port -f activate gmp
```

## LaTeX Typesetting Package

CmdStan uses the LaTeX typesetting package for generating manuals, talks, and other materials (Doxygen is used for API documentation; see below). The first step is to download the MacTeX `.mpkg` file from the following URL [warning: the download is approximately 2GB and the installation approximately 3.5GB].

<http://www.tug.org/mactex/2011/>

Once it is downloaded, just click on the `.mpkg` file and then follow the installer instructions. The installer will add the command to the PATH environment variable so that the `pdflatex` used by Stan is available from the command line.

## Lucida Console Font

A free TrueType version of Lucida Console for the Mac is available at the following URL.

<http://www.fontpalace.com/font-details/Lucida+Console/>

Download the `.ttf` file, then click on it to install. It will then be available as a preference in the Mac terminal application.



## C. Dump Data Format

For representing structured data in files, CmdStan uses the dump format introduced in S and used in R and JAGS (and in BUGS, but with a different ordering). A dump file is structured as a sequence of variable definitions. Each variable is defined in terms of its dimensionality and its values. There are three kinds of variable declarations, one for scalars, one for sequences, and one for general arrays.

### C.1. Creating Dump Files

Dump files can be created from R using RStan. The function is `stan_rdump` in package `rstan`.

Using R's native `dump()` function can produce dump files which Stan cannot read in. The underlying cause is that R gets creative in the format it uses for output, only being constrained to something that can be executed in R. So it will write the array containing the values 1, 2, 3, 4 as `1:4` rather than as `c(1,2,3,4)`.

### C.2. Scalar Variables

A simple scalar value can be thought of as having an empty list of dimensions. Its declaration in the dump format follows the S assignment syntax. For example, the following would constitute a valid dump file defining a single scalar variable `y` with value 17.2.

```
y <-  
17.2
```

A scalar value is just a zero-dimensional array value.

### C.3. Sequence Variables

One-dimensional arrays may be specified directly using the S sequence notation. The following example defines an integer-value and a real-valued sequence.

```
n <- c(1,2,3)  
y <- c(2.0,3.0,9.7)
```

Arrays are provided without a declaration of dimensionality because the reader just counts the number of entries to determine the size of the array.

Sequence variables may alternatively be represented with R's colon-based notation. For instance, the first example above could equivalently be written as

```
n <- 1:3
```

The sequence denoted by `1:3` is of length 3, running from 1 to 3 inclusive. The colon notation allows sequences going from high to low, as in the first of the following examples, which is equivalent to the second.

```
n <- 2:-2
n <- c(2,1,0,-1,-2)
```

## C.4. Array Variables

For more than one dimension, the dump format uses a dimensionality specification. For example,

```
y <- structure(c(1,2,3,4,5,6), .Dim = c(2,3))
```

This defines a  $2 \times 3$  array. Data is stored in column-major order, meaning the values for `y` will be as follows.

```
y[1,1] = 1    y[1,2] = 3    y[1,3] = 5
y[2,1] = 2    y[2,2] = 4    y[2,3] = 6
```

The `structure` keyword just wraps a sequence of values and a dimensionality declaration, which is itself just a sequence of non-negative integer values. The product of the dimensions must equal the length of the array.

If the values happen to form a contiguous sequence of integers, they may be written with colon notation. Thus the example above is equivalent to the following.

```
y <- structure(1:6, .Dim = c(2,3))
```

The same applies to the specification of dimensions, though it is perhaps less likely to be used. In the above example, `c(2,3)` could be written as `2:3`.

Arrays of more than two dimensions are written in a last-index major form. For example,

```
z <- structure(1:24, .Dim = c(2,3,4))
```

produces a three-dimensional int (assignable to `real`) array `z` with values

```
z[1,1,1] = 1    z[1,2,1] = 3    z[1,3,1] = 5
z[2,1,1] = 2    z[2,2,1] = 4    z[2,3,1] = 6

z[1,1,2] = 7    z[1,2,2] = 9    z[1,3,2] = 11
z[2,1,2] = 8    z[2,2,2] = 10   z[2,3,2] = 12
```

$z[1,1,3] = 13$	$z[1,2,3] = 15$	$z[1,3,3] = 17$
$z[2,1,3] = 14$	$z[2,2,3] = 16$	$z[2,3,3] = 18$

$z[1,1,4] = 19$	$z[1,2,4] = 21$	$z[1,3,4] = 23$
$z[2,1,4] = 20$	$z[2,2,4] = 22$	$z[2,3,4] = 24$

## C.5. Matrix- and Vector-Valued Variables

The dump format for matrices and vectors, including arrays of matrices and vectors, is the same as that for arrays of the same shape.

### Vector Dump Format

The following three declarations have the same dump format for their data.

```
real a[K];
vector[K] b;
row_vector[K] c;
```

### Matrix Dump Format

The following declarations have the same dump format.

```
real a[M,N];
matrix[M,N] b;
```

### Arrays of Vectors and Matrices

The key to understanding arrays is that the array indexing comes before any of the container indexing. That is, an array of vectors is just that — provide an index and get a vector. See the chapter on array and matrix types in the user's guide section of the language manual for more information.

For the dump data format, the following declarations have the same arrangement.

```
real a[M,N];
matrix[M,N] b;
vector[N] c[M];
row_vector[N] d[M];
```

Similarly, the following also have the same dump format.

```

real a[P,M,N];
matrix[M,N] b[P];
vector[N] c[P,M];
row_vector[N] d[P,M];

```

## C.6. Integer- and Real-Valued Variables

There is no declaration in a dump file that distinguishes integer versus continuous values. If a value in a dump file's definition of a variable contains a decimal point (e.g., 132.3) or uses scientific notation (e.g., 1.323e2), Stan assumes that the values are real.

For a single value, if there is no decimal point, it may be assigned to an `int` or `real` variable in Stan. An array value may only be assigned to an `int` array if there is no decimal point or scientific notation in any of the values. This convention is compatible with the way R writes data.

The following dump file declares an integer value for `y`.

```

y <-
2

```

This definition can be used for a Stan variable `y` declared as `real` or as `int`. Assigning an integer value to a real variable automatically promotes the integer value to a real value.

Integer values may optionally be followed by `L` or `l`, denoting long integer values. The following example, where the type is explicit, is equivalent to the above.

```

y <-
2L

```

The following dump file provides a real value for `y`.

```

y <-
2.0

```

Even though this is a round value, the occurrence of the decimal point in the value, 2.0, causes Stan to infer that `y` is real valued. This dump file may only be used for variables `y` declared as `real` in Stan.

### Scientific Notation

Numbers written in scientific notation may only be used for real values in Stan. R will write out the integer one million as 1e+06.

## Infinite and Not-a-Number Values

Stan's reader supports infinite and not-a-number values for scalar quantities (see the section of the reference manual section of the language manual for more information on Stan's numerical data types). Both infinite and not-a-number values are supported by Stan's dump-format readers.

<i>Value</i>	<i>Preferred Form</i>	<i>Alternative Forms</i>
positive infinity	Inf	Infinity, infinity
negative infinity	-Inf	-Infinity, -infinity
not a number	NaN	

These strings are not case sensitive, so `inf` may also be used for positive infinity, or `NAN` for not-a-number.

## C.7. Quoted Variable Names

In order to support JAGS data files, variables may be double quoted. For instance, the following definition is legal in a dump file.

```
"y" <-  
c(1,2,3)
```

## C.8. Line Breaks

The line breaks in a dump file are required to be consistent with the way R reads in data. Both of the following declarations are legal.

```
y <- 2  
y <-  
3
```

Also following R, breaking before the assignment arrow are not allowed, so the following is invalid.

```
y  
<- 2 # Syntax Error
```

Lines may also be broken in the middle of sequences declared using the `c(...)` notation., as well as between the comma following a sequence definition and the dimensionality declaration. For example, the following declaration of a  $2 \times 2 \times 3$  array is valid.

```

y <-
  structure(c(1,2,3,
4,5,6,7,8,9,10,11,
12), .Dim = c(2,2,
3))

```

Because there are no decimal points in the values, the resulting dump file may be used for three-dimensional array variables declared as `int` or `real`.

## C.9. BNF Grammar for Dump Data

A more precise definition of the dump data format is provided by the following (mildly templated) Backus-Naur form grammar.

```

definitions ::= definition+

definition ::= name ("<-" | '=') value optional_semicolon

name ::= char*
      | ''' char* '''
      | """ char* """

value ::= value<int> | value<double>

value<T> ::= T
          | seq<T>
          | 'structure' '(' seq<T> ',' ".Dim" '=' seq<int> ')'

seq<int> ::= int ':' int
          | cseq<int>

seq<real> ::= cseq<real>

cseq<T> ::= 'c' '(' vseq<T> ')'

vseq<T> ::= T
          | T ',' vseq<T>

```

The template parameters `T` will be set to either `int` or `real`. Because Stan allows promotion of integer values to real values, an integer sequence specification in the dump data format may be assigned to either an integer- or real-based variable in Stan.

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