Hrothgar

Parallel fitting and Markov Chain Monte Carlo of CPU-intensive functions
Version 2.3, updated 20 July 2014

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This manual is for Hrothgar (version 2.3, 20 July 2014), which provides parallel fitting and Markov Chain Monte Carlo of CPU-intensive functions.

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1 Invocation

```
#include <hrothgar.h>

void hrothgar_init_pars(struct hrothgar_setup *setup,
              int ntotparams, char **paramnames,
              double *pmin, double *pmax, double *initvals,
              int *dofit, char **pcomment);


void hrothgar_init_string_pars(struct hrothgar_setup *setup,
              int ntotstringparams, char **stringparamnames,
              char **stringparamvalues, char **pcomment);

int hrothgar_init(struct hrothgar_setup *setup, int argc,
              char **argv);

void hrothgar(unsigned long ndata, double *x,
              double *data, double *error,
              int (*get_model)(double *x,
                               double *params,
                               double *model,
                               double *errors,
                               double *logprior,
                               unsigned long *ndata,
                               void *dataptr),
              void *dataptr,
              struct hrothgar_setup *setup);

void hrothgar_statonly(double (*get_stat)(double *params,
                              int np, void *dataptr),
                              void *dataptr,
                   struct hrothgar_setup *setup)


<linked program> [OPTIONS] [[input-file] output-file]
```

2 Description

Hrothgar is a library that carries out nonlinear fitting of data to functions of arbitrarily many variables. The fitting can be carried out either on a single machine, or on a computer cluster using a Message Passing Interface (MPI) library. Multi-CPU and multicore machines can take advantage of OpenMP. There are two modes: Levenberg-Marquardt (LM) mode, or Markov-Chain-Montecarlo (MCMC) mode.

In LM Mode, which assumes uncorrelated errors, the calling program provides the data, model, errors and the fitting function `f(a,x)`, where `a` are the N free parameters and `x` are the M data points. Starting from an initial vector in the N dimensional minimization space, Hrothgar calculates the MxN Jacobian of `f(a,x)` numerically and proceeds downhill using a Levenberg-Marquardt alogrithm. Hrothgar can do this will conducting random walks uphill. The program concludes by saving the best-fit parameters, the associated errors, and graphical images of the N(N-1)/2 separate pairwise joint probability distributions of the best-fit parameters.

In MCMC mode, instead of `f(a,x)`, the calling program can simply provide -2 ln P (equal to the chi square for normally distributed variables), and Hrothgar will conduct an MCMC chain analysis with importance sampling and a robust exploration of the topology. The accompanying program `mcmcprob` allows for visualization of this topology and calculation of error parameters.

Any program which is usable in LM mode (i.e., contains uncorrelated errors AND is able to provide all data and errors to Hrothgar) can also be run in MCMC mode.

2.1 Installation and SCIUTILS package

In addition to a POSIX environment Hrothgar also requires the GNU Scientific Library (GSL), the compression library zlib, and the CFITSIO library to be installed. Plotting MCMC chains requires the pgplot library. These packages maybe installed through your system's package manager (Linux) or through macports (Mac OS X).

Included with Hrothgar is the SCIUTILS package also by A. Mahdavi. This package will compile along with Hrothgar; see the sciutils subdirectory and sciutils.pdf for details.

On a Linux system the full list of required packages is

```
openmpi-bin
texinfo
zlib1g-dev
libcfitsio3-dev
libfftw3-dev
libgsl0-dev
libopenmpi-dev
pgplot5
libreadline6-dev
pdfjam
```

these can all be installed via apt-get on a system like Ubuntu. For a Macintosh system, the required Macports packages are

```
openmpi
```

```
gsl
zlib
cfitsio
pgplot
ghostscript
pdfjam
```

For installation to /usr/local, installation proceeds via standard

```
./configure; make; sudo make install
```

Those without root access may install to another location via

```
./configure --prefix=/other/place; make; make install
```

2.2 Initialization

Hrothgar should be called from another program that provides the function to be minimized as well as its parameters. There are three steps involved in initialization.

First the program needs to register the default fit parameters via a call to `hrothgar_init_pars`, providing the total number of fit parameters `(ntotparams)`, the names of the parameters `(paramnames)`, the minimum and maximum allowed values of the parameters `(pmin,pmax)`, their default values `(initvals)`, their default fitting states `(dofit)`, and optionally a comment describing the variables `(pcomment)`. The `setup` variable needs to be declared, but can otherwise be safely ignored by the calling program. The development files for the readline utility are highly recommended.

Next, the program call `hrothgar_init` to parse the command line arguments. Upon success, `hrothgar_init` will return the rank of the node assigned to it by MPI (or 0 in a single CPU setting).

Finally, the main program makes one of two calls:

1. In case of diagonal (uncorrelated) errors, the full Hrothgar functionality, including both Levenberg-Marquardt involves a call outright call to `hrothgar` with the number of data points `ndata`, abscissae `x`, the actual `data` and `errors`, and fitting function `get_model`. An auxilliary pointer `dataptr` can be used to convey auxilliary information necessary for the fit; `dataptr` will be passed straight to `get_model` without modification.
2. The user may also choose to only supply only -2 ln P, in which case a call to `hrothgar_statonly` should be made instead. This only requires the fitting function `get_stat` to be supplied `dataptr` will be passed straight to `get_stat` without modification.

Following the call to Hrothgar, everything is handled automatically.

Optionally, non-fittable string parameters may be given to Hrothgar by calling the `hrothgar_init_stringpars()` function prior to calling `hrothgar_init`. The number of of string parameters is `nstringpars`, and the character matrices `stringparname`, `stringparval`, and `stringparcomment` are the names of the string parameter names, default values, and comments, respectively. String parameters may be altered via the command line and may be useful for the calling program's internal initialization.

2.3 Configuration files

When run with the `--defaults` argument, the main program will carry out a fit with the default input parameters discussed above. However, it is useful to store all the parameters in a configuration file. For this purpose, the `-d` command line parameter outputs the default configuration file (generated using the default variables passed to `hrothgar_init_pars` and `hrothgar_init_stringpars`) to standard output.

If `input-file`, is specified, its contents override the default settings, except for `pmin` and `pmax`, which may never be overridden. In addition, the `-p` command line parameter can override the default settings (see *Index* below).

If `output-file` is specified, the results of the minimization run are stored in a similar output configuration file, with the fittable parameters at the best-fit minimum. In addition, any changes in input parameters expressed via the `-p` command line parameter are reflected in `output-file`.

Any characters in a line following and including a pound sign ("#") are treated as comments . Information from the hrothgar run, including the random number seed, the date and time, the best-fit statistic, and 1D confidence intervals for the free parameters, are appended to `output-file` as comments.

The configuration file has two types of entries; normal, fittable parameter entries, and non-fittable, string parameter entries. A normal line has five whitespace-delimited elements. The first element contains the (unique) name of the fittable parameter; the second element contains the starting value of the parameter; the third element is either a zero or or one, indicating whether the parameter is to be fit (0) or frozen (1). The next two numbers are optional and specify the minimum and maximum allowed value for the parameter, e.g.:

```
slope     0.3 0 -5 5
intercept 7.9 1
```

In the above example, there are two parameters, "slope" and "intercept." Slope is a free parameter, and it will be constrained to lie between -5 and 5. Intercept is a frozen parameter, and it will not be varied during the fit. Suppose however we use the command line string `-p intercept~`; in that case, interecept will be thawed (i.e. fit), and the minimum and maximum allowed values will be the values set by `pmin` and `pmax`.

The second type of allowed parameter is a string parameter. These parameters have no influence on the fit, and their values will simply be copied from the input file to the output file, unless `-p` is used on the command line. Example:

```
logfile simpleline.log # File name to use for logging
```

After launch, operation is automatic and requires no user interaction. Three basic modes of operation are available.

2.4 Levenberg-Marquardt Minimization

This is the first possible mode of operation. The merit function is evaluated at the values specified in `input-file`, and the Levenberg-Marquardt steeping routine steps downhill until convergence. Optionally with the `-P` parameter, a powell-style minimization is also attempted (available only with multiple CPUs). Optionally with the `-f` parameter, a number of uphill steps are taken following each convergence. This to help increase the likelihood of convergence to a global minimum.

Hrothgar utilizes bounded Levenberg-Marquardt minimization. This means that each fit parameter is always bounded by a global upper and lower limit, specified by `pmin` and `pmax`. The limits specified in `input-file` may never exceed these limits.

The bounded minimization is achieved through the following transformation:

```
y = arcsin((2 x - xmax - xmin)/(xmax - xmin)).
```

With the above transformation, the Levenberg-Marquardt routine can operate in an unbounded and continuously differentiable space.

Levenberg-Marquardt errors are derived assuming that the minimum is well approximated by a suitably-dimensional paraboloid. This is frequently not the case, in which case MCMC chains are a better choice.

2.5 MCMC chain

Instead of minimization, the `-m <N>` command line parameter prompts Hrothgar to attempt a Markov Chain Monte Carlo procedure, generating one or more chains of total length at least `<N>` times the number of free parameters. For example, if there are 5 free parameters in the model, the total length of all chains will be at least 5`<N>`, if not more. Without MPI, only one chain is run.

With MPI, several chains (equal to the number of MPI nodes engaged) are run and checked for convergence. The convergence test is that the means of all the free parameters for each chain lie within one standard deviation of the means of all the other chains. Again, under the example of 5 free parameters, if the chains converge, Hrothgar will run to at least $5<N>$ total chain length; if they do not converge, Hrothgar will run to at most $50<N>$ total chain length, or until the chains converge.

See the example below for a description of how data in the chains is stored and see the visualization section for how display and use it.

3 Example

3.1 Fitting a Gaussian

I now present a worked example, which may also be used as a test suite for Hrothgar, or even a template using which users may build their own fitting routines. The following program generates a number of Gaussian deviates, bins them into a group size specified by the user, and fits a Gaussian to the result. It is in effect "testing" the accuracy of the GSL Gaussian distribution.

3.2 Annotated Code

The contents of hrothgar_test.c:

```
#include <gsl/gsl_rng.h>
#include <gsl/gsl_randist.h>
#include <gsl/gsl_sort.h>
#include <hrothgar.h>
#include <math.h>

// HAVE_MPI is automatically defined in the build process for Hrothgar.
#ifdef HAVE_MPI
#include <mpi.h>
#endif

// This function simply returns a Gaussian distribution for
// ndata values of x, storing them in model.  par[0] is the mean,
// par[1] is the sigma, and par[2] is the normalization of the
// gaussian.
// The user can use this function as a template for building fits.

int gaussian_model(double *x, double *pars, double *model,
                   double *error, double *logprior,
                   unsigned long ndata, void *extra){

  double diff;
  unsigned long i;

  for (i = 0; i < ndata; ++i) {
    diff = (x[i]-pars[0])/pars[1];
    model[i] = pars[2]*exp(-diff*diff/2.)/(pars[1]*2.5066283);
  }

  return 0;

}
```

```
/* double gaussian_model_stat(double *pars, int npar, void *extra) */
/* { */
/*   double diff; */
/*   diff = pow((1 - pars[0]),2.)+pow((2-pars[1]),2.)+pow((0.5-pars[2]),2.); */
/*   return diff; */
/*  } */

int main(int argc, char *argv[]) {

  unsigned long i,j;
  double tempmean;

  // This is a required declaration.
  struct hrothgar_setup setup;

  // There are 3 total fit parameters:  the mean, sigma, and
  // normalization of the Gaussian
  // Parameter names as they should appear in the default config file
  static char *paramnames[] = { "mean", "sigma", "norm" };

  // Which parameters should be frozen?  None, in our case, we are
  // fitting them all.  This is a default only, and can be overridden.
  static int frozen[] = { 0, 0, 0 };

  // Optional comments describing what each parameter means:
  static char *comments[] = { "Mean", "Sigma",
                              "Normalization" };

  // Use remote initial values for the minimization.
  static double initvalues[] = { -1, 3., 23.  };

  // Minimum and maximum values allowed for minimization
  static double parmin[] = { -10., 0.001, 0.0001 };
  static double parmax[] = { 10., 100., 10000.  };

  // String parameters.  These are parameters not used during
  // the fit.  In this case, we'll use string parameters to
  // generate our synthetic data.

  char *stringparname[] = { "simmean", "simsig", "nsims" };

  // By default, we'll simulate a centered Gaussian with unit sigma
  // Note that the parameters need to be string valued here.
  // By default we are doing 1000 simulations.  On a modern system,
  // you will need 30000000 (3e7) simulations or more before you will
  // see a big slowdown on the fit.
  char *stringparval[] = { "0.", "1.", "1000" };
```

```
char *stringparcomments[] = { "Simulated mean",
                              "Simulated sigma",
                              "Number of Simulations"};


/******************** Program starts here **********************/

// Initialize the string parameters.  Pointers to them are stored
// within the setup structure.
hrothgar_init_stringpars(&setup,3,stringparname,stringparval,
                         stringparcomments);

// Initialize the fit parameters
hrothgar_init_pars(&setup,3,paramnames,parmin,parmax,
                   initvalues,frozen,comments);

// Initialize the hrothgar core.
// Note that any command line modifications to the string
// parameters will be written to stringparval at this point
if (hrothgar_init(&setup,argc,argv) < 0) { return; }

// Get the mean and sigma of the Gaussian to simulate, as well
// as the total number of simulations to perform.
double simmean = atof(stringparval[0]);
double simsig = atof(stringparval[1]);
unsigned long nsim = atol(stringparval[2]);

// Use 30 data points per bin
if (nsim < 150) BYE("Too few simulations.");
unsigned long nbins = nsim/30;
printf("Init %d\n",setup.node);


// Allocate room for the binned data.
double *x = (double *)malloc(nbins*sizeof(double));
double *y = (double *)malloc(nbins*sizeof(double));
double *ye = (double *)malloc(nbins*sizeof(double));

// Now it is time to generate the data.  For simiplicity, we'll have
// only the master MPI node generate the data.  If we're not running
// MPI, the node number will be 0 by default anyway.

if (setup.node == 0) {

  // At this point, hrothgar_init has already conveniently
  // initialized and seeded a random number generator for us.
  gsl_rng *rng = setup.generator;
```

```
    double *data = (double *)malloc(nsim*sizeof(double));

    // Generate the Gaussians
    for (i = 0; i < nsim; ++i)
      data[i] = simmean+gsl_ran_gaussian(rng,simsig);

    // Sort them
    gsl_sort(data,1,nsim);

    // Bin them into a histogram of width 30
    j = 0;
    tempmean = 0.;

    for (i = 0; i < nsim; ++i) {
      tempmean += data[i];

      if (i % 30 == 29) {
        x[j] = tempmean/30.;
        tempmean = 0.;
        y[j] = 30./(nsim*(data[i]-data[i-29]));
        ye[j] = 5.5/(nsim*(data[i]-data[i-29]));
        ++j;
      }
    }
    free(data);
  }


    // Conditional MPI section
#ifdef HAVE_MPI
    // Send all the slaves the binned data.
  printf("Trying %d\n",setup.node);
    MPI_Bcast(x,nbins,MPI_DOUBLE,0,MPI_COMM_WORLD);
    MPI_Bcast(y,nbins,MPI_DOUBLE,0,MPI_COMM_WORLD);
    MPI_Bcast(ye,nbins,MPI_DOUBLE,0,MPI_COMM_WORLD);
#endif
    printf("OK %d\n",setup.node);
  // Run the fit
  hrothgar(nbins,x,y,ye,gaussian_model,NULL,&setup);
  //hrothgar_statonly(gaussian_model_stat,NULL,&setup);

}
```

3.3 Running the Test Suite

To run the test suite following installation, simply run

```
hrothgar_test -D
```

This should measure the mean of the Gaussian to be near 0; the sigma and the normalization should be near 1.

To examine the format of the default configuration file and save the results of the fit:

```
hrothgar_test -d > input.cfg
hrothgar_test -Xtf50 input.cfg output.cfg
```

In the above example, Hrothgar will perform an uphill step and reminimize the merit function, repeating the procedure 50 times and outputting timing statistics. The Gaussian-approximated errors are stored in the output configuration file.

3.4 Parallel Runs (MPI and OpenMP)

Hrothgar is capable of running in either or both of the MPI and OpenMP parallel environments.

Hrothgar does not require any special treatment when running in an MPI context. It will automatically realize that it is in a parallel environment and take advantage of its capability. If users wish to limit the number of CPUs that hrothgar uses, they can specify `-n` on the command line.

In minimization mode, Hrothgar uses MPI primarily for calculating the Jacobian of the merit function. For a fit with m parameters, this requires $2m$ calculations of the merit function. Thus, during minimization Hrothgar can take full advantage of at most $2m$+1 CPUs, hence its attractiveness for high-dimensional problems.

In MCMC mode, each MPI slave node runs a different MCMC chain, which are checked for convergence by the master mode.

To test the performance of your MPI setup relative to the single CPU setup:

```
mpirun -np 4 hrothgar_test -Xtm300000 input.cfg output.cfg
```

The output of this program is stored in binary files called output.cfg.??.mcmc, which can be viewed using the included mcmcprob utility. See the visualizations section below.

Users with capable compilers may use OpenMP within their merit functions; Hrothgar does not use OpenMP capabilities in a way that interferes with this. Thus OpenMP can be used together with MPI for even larger speed gains.

3.5 Visualizing MCMC chains

The included mcmcmprob utility can be used to extract statistics from the mcmc chains, as well as to plot them if the optional pgplot package is available. The syntax is

```
mcmcprob [FILE ... [+ FILE... ] [-i | -d | -p filename | -a ] BN cmds...
```

Here FILE indicates a *mcmc output by Hrothgar; all files mentioned together are plotted using the same symbols, but encountering a "+" in the file list causes the symbol to be switched, so that different data sets can be contrasted.

Burnin is the number of chain events to ignore at the begining of the chain prior to starting the statistic.

One of the four available commands can be selected. -i enters an interactive mode, which requires pgplot. In interactive mode, a simple command line interface is available. To plot

variable against variable, type "c1 c2" which will generate a plot of the chain points in the c1-c2 space. Typing "c1 c2 c3" will generate three separate plots of the chain points in c1-c2, c1-c3, and c2-c3 space; and so on. Typing "l" will list all fields available. Two special fields are also available: "ord," which retains memory of the order in which each chain point was selected, and "chisq," which retains - 2 ln P. These can also be plotted against any of the other fields. Preceding a series of fields with "c", as in "c col1 col2" will generate contours of 68% and 95% confidence instead of plotting the MCMC points. "q" quites. In the above example "cmds" can be any command that is valid in interactive mode.

The command -p tells pgplot to create a postscript file called filename, rather than printing the output to the screen.

The command -d simply prints out the marginalized 1D error bars in the listed quantities of c1 c2. Each of c1 and c2 is treated as a regular expression and any matching columns will be printed out. The command -a outputs more detailed statistics. The -d and -a commands are the only ones available if pgplot is not selected.

For example, following the above MCMC run, the following command

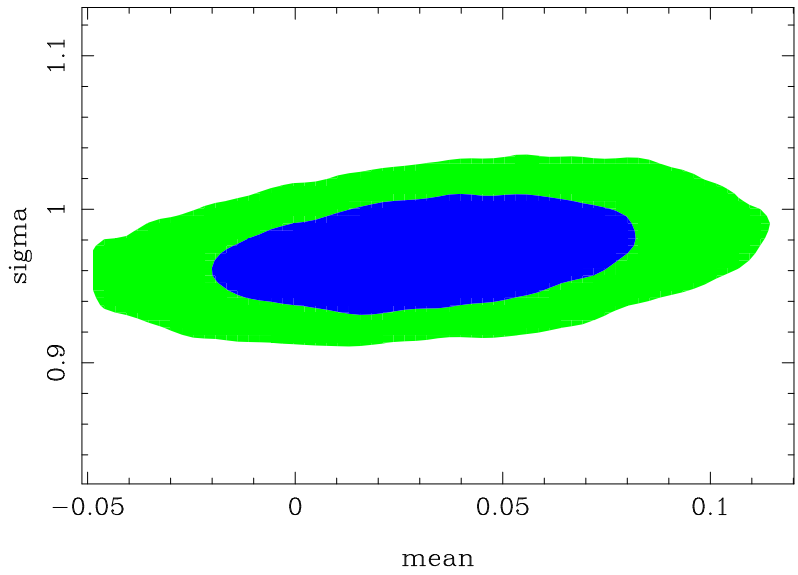
```
mcmcprob output.cfg.*mcmc -d 0 mean sigma
```

will yield an output similar to

```
mean                        -1.392447E-03         1.927497E-03
sigma                        9.982855E-01         1.351426E-03
```

```
mcmcprob output.cfg.*mcmc -p hrothgar-example.ps 0 c mean sigma
```

Will yield something like attached image (with 'c' meaning "contour").



4 Index of command line parameters

The default values of the command line parameters may be seen by specifying `--help [parameter]` on the command line.

`-C, --conf` *level*

Specify confidence level at which 1D errors are reported.

`-D, --defaults`

Run without any configuration files, using internal default parameters. If the configuration files are specified, -D does nothing.

`-E, --evalonly`

Evaluate the merit function at the initial vector and quit—do not carry out any fitting or error analysis.

`-H, --hardlimits`

Ignore the limits set in the input parameter file; use hard limits on the parameter values as specified by the calling program.

`-L, --license`

Display the terms for copying, modifying and redistributing this program.

`-R, --remember`

Normally, if the user modifies the fit/frozen state of parameters via the `--parameter` command line option, the new state is recorded in the output file. With `--remember`, the old state is recorded instead. This is useful in conjunction with the `%` modifier to `--parameter`.

`-S, --seed` *number*

The random number seed is normally read from /dev/random. This uses the user specified value instead. Random numbers are used in the Tree MCMC mode, as well as in the uphill steps taken using the `--floataround` option. Implies `--predictable` in Tree MCMC mode.

`-X, --overwrite`

Overwrite all existing files, rather than exiting with an error condition.

`-a, --inputaccuracy` *eps*

Specify the fractional accuracy of the fitting function provided by the calling program. This is used in estimating the error on the numerical derivatives.

`-c, --covaronly`

Do not conduct minimization. If the covariance matrix exists on the disk already, read it in and use it to output confidence contours. If not, or if `--ignorecovar` is specified, calculate the covariance matrix using the initial conditions.

`-d, --dumpconfig`

Write the default configuration file to standard output.

`-e, --eps` *eps*

Specify the fractional tolerance for convergence.

`-g, --gaussstep` *[sigma]*

For MCMC mode only. Initial sigma of Gaussian by which to step the parameters fractionally.

`-h, --help` *[parameters]*

Summarize the available options. If *parameters* are specified, show their default value.

`-m, --mcmc` *number*

Do not minimize. Instead, generate a Tree Markov Chain Monte Carlo Chain of length *number*.

`-p, --parameter` *name*[%=~@][*value*]

This powerful option allows manipulation of the fit or frozen parameters, and may be specified as many times as needed. The parameter *name* is selected. The operator '`@`' freezes it at *value*, or at its initial value if *value* is not specified. The operator '`~`' does the opposite: it causes *name* to be fit, starting with *value*, or with its initial value if *value* is not specified. The operators '`=`' respects the initial fit/frozen state of *name*, but sets its initial value to *value*. Finally, the '`%`' operator causes *name* to be fit, but freezes all other parameters not previously modified by '`%`'.

Examples:

`-p slope=2` sets *slope* to 2, but does not change its fit/frozen status

`-p slope~` causes *slope* to be fit starting at its initial value, even if it was frozen by default

`-p slope@3` freezes *slope* at the value 3.

`-p slope%2 -p intercept%` freezes all parameters except *slope* and *intercept*; *slope* is fit with an initial value of 2, while *intercept* is fit starting at its default initial value.

`-q, --quiet`

Try to output as little text as possible.

`-t, --timer`

Measure Hrothgar's performance (the time it takes for each Levenberg-Marquardt step). Works with the clustered as well as the single CPU modes.

`-v, --verbose`

Show lots of diagnostic output.

5 Acknowledgments

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