The Stan Core Roadmap

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34 active devs, ≈ 10 *full-time equivalents*

Stan 2.18.0 (June 2018) http://mc-stan.org

Part I

Rear-View Mirror

Stan 2.18 Released

- Math, Stan, CmdStan 2.18 currently
- RStan and PyStan 2.18 out soon
- Stan 2.19 to follow soon after

Multi-core Processing has Landed!

- Not just parallel chains
- Distribute log density and gradient calculations over
  - multiple cores on a single machine using **C++11 threading**
  - multiple cores on a single machine or cluster using **MPI**
  - also runs sequentially with memory-locality savings
- Nearly **embarassingly parallel**
  - In representative experiments, 100 cores ran 80+ times faster than a single core with MPI on a standard cluser

Multi-Process Parallelism

- Implemented with the message passing interface (MPI)
- Runs cross-platform with standards-compliant MPI
  - tested on Linux and Mac OS X
  - based on a generalized higher-order map function, e.g.,

$$\mathrm{map}(f)(x_1, \ldots, x_N) = (f(x_1), \ldots, f(x_N))$$

  - applies f to each element of a sequence $(x_1, \ldots, x_N)$
- pushes data arguments to processors once
- pushes arguments to processors per eval (map)
- synchronizes reassembly in root expression graph (reduce)

Map Function

- The mapped function has signature

```
vector f(vector, vector, data real[], data int[])
```

- The higher-order map function has signature

```
vector map_rect(F f, vector phi, vector[] theta,
                data real[, ] x_r, data int[, ] x_i)
```

- The result is computed as follows

```
map_rect(f, phi, theta, x_r, x_i)

= append_col(f(phi, theta[1], x_r[1], x_i[1]),
             ...,
             f(phi, theta[N], x_r[N], x_i[N]))
```

New Built-in Functions

- multivariate normal RNG and Cholesky normal RNG
- many RNGs now vectorized (the rest to come soon)
- thin QR decomposition
- matrix-exponential multiply action plus scaled version
- Adams ODE integrator
- generalize log mixture function beyond two arguments
- standard normal distribution
- vectorized ordered probit and logistic

Manuals to HTML

- Breaking 2.17 manual into three parts:
  - *Stan Reference Manual*: specification of the language and algorithms
  - *Stan Functions Reference Manual*: specification of built-in functions
  - *Stan User's Guide*: programming techniques and example model
- Reference manual in bookdown for HTML and pdf
  - user's guide, function manual HTML soon
- Expand *User's Guide* to reproducible ***Stan Book***

Improved Effective Sample Size

- Aki Vehtari has been working on better calibration
- NUTS can produce anti-correlated draws
  - effective sample size may exceed number of iterations!
- pushed to CmdStan, RStan, and PyStan

Foreach Loops

- Loop over elements of container rather than numbers
- Works for any array type, looping over elements
- Also works for vector and matrix types

```
matrix[3, 4] ys[7];
for (matrix y : ys) {
  ... do something with y...
}
```

replaces

```
for (i in 1:7) {
  matrix[3, 4] y = ys[i];
  ... do something with y ...
}
```

Data-qualified Arguments

- Allow data qualifier on function arguments
- Requires argument to be data-only expression
- User-defined functions w. algebraic solver, ODEs, map-reduce, etc.
- For example, to parallelize logistic regression, define

```
real logistic_glm(vector beta, vector dummy,
                  data real[] x_r, data int[] y) {
  return bernoulli_logit_lpmf(y | to_matrix(x_r) * beta);
}
```

Bug Fixes and Enhancements

- Lots of little things in the parser
  - better parser error messages
  - fixed compound arithmetic/assignment and ternary operator syntax edge cases
- Allow initializatioin to continue through constraint violation in transformed parameters
- Exceptions/rejections in generated quantities produce all not-a-number values rather than failure

Math Library Enhancements

- In 2.18 math lib, scheduled for Stan 2.19
- Covariance functions
  - squared exponential
  - dot product
  - periodic
- Definite integrator (one dimensional)
- Add-diagonal and log-inverse-logit-difference functions
- GLM primitives for Bernoulli-logit and Poisson-log
- Vectorized ordered logit and probit

CmdStan Enhancements

- Allow Euclidean metric (inverse mass matrix) specification
- Precompiled header support for faster compilation
  - C++ compilers are getting slower with more optimizations

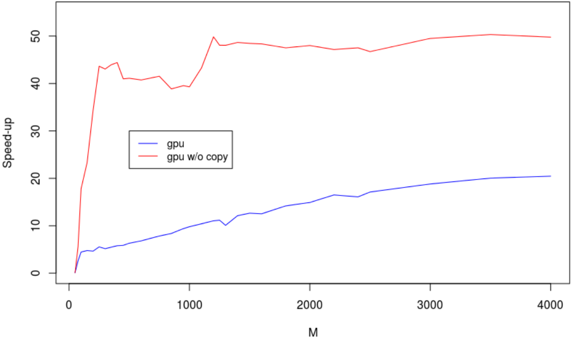
Part II
The Road in Front

GPU Support

- OpenCL for double-precision arithmetic & portability
  - may also eventually include a CUDA interface
- Initial rollout in Stan 2.19 for
  - matrix-matrix multiply (N^3 data, N^2 computation)
  - Cholesky factorization (N^3 data, N^2 computation)
  - matrix-vector multiply (N^2 data, N^2 computation)
- Order of magnitude speedup without loss of precision for large problems
  - Gaussian processes, factor models, etc.

GPU Speedup, Cholesky (40+ times)

- Time to solve for L for positive-definite $\Sigma = L L^\top$
- with an affordable GPU and Linux desktop



PDEs, DAEs & Definite Integrals

- Partial differential equation (PDE) solver framework
  - common framework for pluggable solvers
  - problem-specific solvers for PDEs
- Differential algebraic equation (DAE) solver
  - extends the existing algorithmic solver
  - differential implicit functions
- Definite integral solver
  - Density normalization inside language

Tuples (i.e., Product Types)

- Hold sequences of heterogeneous types
- Like typed, unnamed R lists or Python dictionaries

```
tuple<matrix, vector> eigen_decompose(matrix x);

matrix z;
tuple<matrix, vector> ed = eigen_decompose(z);

// accessors
matrix z_eigenvecs = ed.1;
vector z_eigenvals = ed.2;

// constructors
tuple<matrix, vector> ed2 = (ed.1, ed.2);
```

Ragged Arrays

- Arrays where
  - all elements are the same shape (e.g., ‘real[,]‘)
  - not all elements are the same size
- Critical for a range of applications
- Declared with array of sizes

```
int<lower = 0> M;     // rows
int<lower = 0> N[M];  // cols for row
real[N] y;  // y has M rows; row m has N[m] cols
```

Lambdas and Function Types

- Define anonymous inline functions (may be assigned, passed)
- Define higher-order functions
- Closures capture variables (static, lexical scope)
  - no more data arguments to ODE system functions
- Transpile directly to C++ closures
- Example uses manual function syntax

```
int n = 3;
(real):real cube = (real x).x^n;  // binds n
real x = 2.5;
real x_cubed = cube(x);  // x_cubed == 15.625
```

Independent Generated Quants

- Stored posterior sample with new generated quantities
  - parameter declarations must match
  - model block is ignored
  - generated quantities may vary
- Provides flexible posterior predictive inference
  - e.g., allows streaming posterior predictions for new items
  - e.g., decouples decision theory from posterior generation
  - e.g., allows exploratory posterior predicive checks
- Already built into C++ core; needs pull from interfaces

Adjoint-Jacobian Product Functor

- Efficient matrix autodiff without fiddling code/memory
  - supports direct matrix derivative code
  - reduces reverse pass to single virtual function call
  - lazy adjoint-Jacobian product avoids storing Jacobian
  - store state during functor `operator()` call
  - multiply-adjoint-Jacobian may be called multiple times

```
struct my_vector_fun {
  VectorXd operator()(const VectorXd& x) { ... }

  VectorXd multiply_adjoint_jacobian(const VectorXd& fx_adj)
    const { ... }
};
```

Mass Matrix/Step Size Init

- User may provide mass matrix (inverse Euclidean metric)
  - may already provide step size (temporal discretization)
- Allows metric initialization with known parameter scales
- Allows restart after adaptation or with more adaptation
  - requires save of RNG state for exact match
- Already built into C++ core; needs pull from interfaces

Variadic Functions, not Packing

- coded with parameter packs in C++11
- map won't need to pack shared parameters

```
map_rect(f, theta, phi1, ..., phiN, x1, ..., xM)

= append_col(f(theta[1], phi1, ..., phiN, x1, ..., xM)
             ...,
             f(theta[N], phi1, ..., phiN, x1, ..., xM)
```

- integrate ODE won't need to pack parameters or data

```
system:  f(t, y, theta1, ..., thetaN, x1, ..., xM)

ode_integrate(f, y0, t0, ts, theta1, ..., thetaN,
                             x1, ..., xM)
```

Part III

The Longer Road

Faster Compile Times

- **Key is** replacing model template with base class
  - Stan program translated to a specific C++ class
  - algorithms and service functions templated for class
  - math library primarily header only
  - so **everything recompiles for each Stan program**
  - model base class **eliminates most recompilation**
- **And precompiling** as much of math library as possible
  - vectorized operations combinatorially prohibitive

Blockless Stan Language

- No required block declarations
  - optional qualification for **backward compatibility**
  - infer block structure for rest
  - allow missing data a la BUGS (continuous only)
  - allow modules with parameters, e.g., non-centered prior
  - retain imperative execution order, functions, etc.
- Inspired by composability in language theory
- Inspired by & partially realized by transpilers
  - **StataStan**: CiBO Technologies, open source
  - **SlicStan**: Maria Gorinova's M.S. thesis

Blockless Linear Regression

```
real alpha ~ normal(0, 4);                       // param
real beta ~ normal(0, 4);                        // param
int<lower = 0> N;                                // data (unmodeled)
vector[N] x;                                     // data (unmodeled)
vector[N] mu_y = alpha + beta * x;               // trans param
real<lower = 0> sigma_y ~ normal(0, 2);          // param
vector[N] y ~ normal(mu_y, sigma_y);             // data (modeled)
```

- Allow model in generative order (parameters to data)
- Variable use moves closer to declarations

Non-Centered Normal Module

- Declare module for non-centered normal prior
- Parameters and transformed parameters in module

```
module non_ctr_normal(int N, real mu, real sigma) {
  vector[N] alpha_std ~ normal(0, 1);          // param
  vector[N] alpha = mu + sigma * alpha_std;    // trans param
}
real mu_alpha ~ normal(0, 5);                        // param
real<lower = 0> sigma_alpha ~ normal(0, 5);          // param
int <lower = 1> K;                                   // data
module ncn = non_ctr_normal(K, mu_alpha, sigma_alpha);
int<lower = 0> N;                                    // data
int<lower = 1, upper = K> ii[N];                     // data
vector[n] y ~ normal(ncn.alpha[ii] + beta * x, tau); // data
```

Protocol Buffer I/O

- Protobuf is a **standardized**, widely supported
- Efficient **binary representation**
- Originally developed by Google
- **Schema driven**
  - efficient binary output formats without extraneous meta-data
- Will replace the current hacked R dump format for input
- *Probably* replacing numerical outputs
- Auto-convertible to/from human-readable **JSON**

Logging Standards

- Add logger for console-type output
- Allow finer control of verbosity through interfaces
  - DEBUG (?): information to help developers
  - INFO: regular output reminders
  - WARN: warnings
  - ERROR: errors
  - FATAL: fatal errors
- Configurable **static logger** eases algorithm dev

Program Transformations

- For **optimization**
  - reducing common subexpressions
  - eliminate dead code
  - transform block location
  - auto-vectorize
- For **arithmetic stability**
  - log-scale and special functions
- Transform intermediate **abstract syntax tree**
  - refactor from C++ variant types to S-expressions

Questions?

Suggestions?