Stan: Probabilistic Modeling & Bayesian Inference

Development Team

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Stan 2.17 (November 2017)

http://mc-stan.org

Stan Language

Stan is a Programming Language

- Not a graphical specification language like BUGS or JAGS
- Stan is a Turing-complete imperative programming language for specifying differentiable log densities
 - reassignable local variables and scoping
 - full conditionals and loops
 - functions (including recursion)
- With automatic "black-box" inference on top (though even that is tunable)
- Programs computing same thing may have different efficiency

Basic Program Blocks

- · data (once)
 - content: declare data types, sizes, and constraints
 - execute: read from data source, validate constraints
- parameters (every log prob eval)
 - content: declare parameter types, sizes, and constraints
 - execute: transform to constrained, Jacobian
- **mode1** (every log prob eval)
 - content: statements defining posterior density
 - execute: execute statements

Derived Variable Blocks

transformed data (once after data)

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- content: declare and define transformed data variables
- execute: execute definition statements, validate constraints
- transformed parameters (every log prob eval)
 - content: declare and define transformed parameter vars
 - execute: execute definition statements, validate constraints
 - generated quantities (once per draw, double type)
 - content: declare and define generated quantity variables; includes pseudo-random number generators (for posterior predictions, event probabilities, decision making)
 - execute: execute definition statements, validate constraints

Model: Read and Transform Data

- · Only done once for optimization or sampling (per chain)
- Read data
 - read data variables from memory or file stream
 - validate data
- · Generate transformed data
 - execute transformed data statements
 - validate variable constraints when done

Model: Log Density

- · Given parameter values on unconstrained scale
- Builds expression graph for log density (start at 0)
- · Inverse transform parameters to constrained scale
 - constraints involve non-linear transforms
 - e.g., positive constrained x to unconstrained $y = \log x$
- account for curvature in change of variables
 - e.g., unconstrained y to positive $x = \log^{-1}(y) = \exp(y)$
 - e.g., add log Jacobian determinant, $\log |\frac{d}{dy} \exp(y)| = y$
- · Execute model block statements to increment log density

Model: Log Density Gradient

- · Log density evaluation builds up expression graph
 - templated overloads of functions and operators
 - efficient arena-based memory management
- · Compute gradient in backward pass on expression graph
 - propagate partial derivatives via chain rule
 - work backwards from final log density to parameters
 - dynamic programming for shared subexpressions
- · Linear multiple of time to evaluate log density

Model: Generated Quantities

- · Given parameter values
- · Once per iteration (not once per leapfrog step)
- · May involve (pseudo) random-number generation
 - Executed generated quantity statements
 - Validate values satisfy constraints
- $\cdot \,$ Typically used for
 - Event probability estimation
 - Predictive posterior estimation
- · Efficient because evaluated with double types (no autodiff)

Variable Transforms

- Code HMC and optimization with \mathbb{R}^n support
- Transform constrained parameters to unconstrained
 - lower (upper) bound: offset (negated) log transform
 - lower and upper bound: scaled, offset logit transform
 - simplex: centered, stick-breaking logit transform
 - ordered: free first element, log transform offsets
 - unit length: spherical coordinates
 - covariance matrix: Cholesky factor positive diagonal
 - correlation matrix: rows unit length via quadratic stickbreaking

Variable Transforms (cont.)

- Inverse transform from unconstrained \mathbb{R}^n
- · Evaluate log probability in model block on natural scale
- · Optionally adjust log probability for change of variables
 - adjustment for MCMC and variational, not MLE
 - add log determinant of inverse transform Jacobian
 - automatically differentiable

Variable and Expression Types

Variables and expressions are strongly, statically typed.

- · Primitive: int, real
- Matrix: matrix[M,N], vector[M], row_vector[N]
- Bounded: primitive or matrix, with
 <lower=L>, <upper=U>, <lower=L,upper=U>
- Constrained Vectors: simplex[K], ordered[N], positive_ordered[N], unit_length[N]
- Constrained Matrices: cov_matrix[K], corr_matrix[K], cholesky_factor_cov[M,N], cholesky_factor_corr[K]
- · Arrays: of any type (and dimensionality)

Integers vs. Reals

- · Different types (conflated in BUGS, JAGS, and R)
- Distributions and assignments care
- · Integers may be assigned to reals but not vice-versa
- Reals have not-a-number, and positive and negative infinity
- Integers single-precision up to +/- 2 billion
- · Integer division rounds (Stan provides warning)
- Real arithmetic is inexact and reals should not be (usually) compared with ==

Arrays vs. Vectors & Matrices

- · Stan separates arrays, matrices, vectors, row vectors
- Which to use?
- · Arrays allow most efficient access (no copying)
- · Arrays stored first-index major (i.e., 2D are row major)
- Vectors and matrices required for matrix and linear algebra functions
- · Matrices stored column-major (memory locality matters)
- Are not assignable to each other, but there are conversion functions

Logical Operators

Op.	Prec.	Assoc.	Placement	Description
	9	left	binary infix	logical or
&&	8	left	binary infix	logical and
==	7	left	binary infix	equality
! =	7	left	binary infix	inequality
<	6	left	binary infix	less than
<=	6	left	binary infix	less than or equal
>	6	left	binary infix	greater than
>=	6	left	binary infix	greater than or equal

Arithmetic and Matrix Operators

Op.	Prec.	Assoc.	Placement	Description
+	5	left	binary infix	addition
-	5	left	binary infix	subtraction
*	4	left	binary infix	multiplication
/	4	left	binary infix	(right) division
\	3	left	binary infix	left division
.*	2	left	binary infix	elementwise multiplication
./	2	left	binary infix	elementwise division
!	1	n/a	unary prefix	logical negation
-	1	n/a	unary prefix	negation
+	1	n/a	unary prefix	promotion (no-op in Stan)
^	2	right	binary infix	exponentiation
,	0	n/a	unary postfix	transposition
0	0	n/a	prefix, wrap	function application
[]	0	left	prefix, wrap	array, matrix indexing

Assignment Operators

Op.	Description			
=	assignment			
+=	compound add and assign			
-=	compound subtract and assign			
*=	compound multiply and assign			
/=	compound divide and assign			
.*=	compound elementwise multiply and assign			
./=	compound elementwise divide and assign			

· these work with all relevant matrix types

Built-in Math Functions

- All built-in C++ functions and operators
 C math, TR1, C++11, including all trig, pow, and special log1m, erf, erfc, fma, atan2, etc.
- Extensive library of statistical functions e.g., softmax, log gamma and digamma functions, beta functions, Bessel functions of first and second kind, etc.
- Efficient, arithmetically stable compound functions e.g., multiply log, log sum of exponentials, log inverse logit

Built-in Matrix Functions

- Basic arithmetic: all arithmetic operators
- · Elementwise arithmetic: vectorized operations
- · Solvers: matrix division, (log) determinant, inverse
- Decompositions: QR, Eigenvalues and Eigenvectors, Cholesky factorization, singular value decomposition
- · Compound Operations: quadratic forms, variance scaling, etc.
- · Ordering, Slicing, Broadcasting: sort, rank, block, rep
- Reductions: sum, product, norms
- · Specializations: triangular, positive-definite,

Atomic Statements

- Sampling: y ~ normal(mu,sigma) (increments log probability)
- Increment log density: target += lp;
- Assignment: y_hat = x * beta;

Block of Statements

• Block: { ...; ...; }

(allows initial local variables)

Control Statements

- For loop: for (n in 1:N) ...
- While loop: while (cond) ...
- Conditional: if (cond) ...; else if (cond) ...; else ...;
- Break: break
- · Continue: continue

Side-Effect Statements

- Print: print("theta=", theta);
- **Reject**: reject("arg to foo must be positive, found y=", y);

"Sampling" Increments Log Prob

- · A Stan program defines a log posterior
 - typically through log joint and Bayes's rule
- · Sampling statements are just "syntactic sugar"
- · A shorthand for incrementing the log posterior
- $\cdot~$ The following define the same* posterior

- y ~ poisson(lambda);

- increment_log_prob(poisson_log(y, lambda));
- * up to a constant
- Sampling statement drops constant terms

Local Variable Scope Blocks

y ~ bernoulli(theta);

٠

is more efficient with sufficient statistics

```
{
  real sum_y; // local variable
  sum_y = 0;
  for (n in 1:N)
    sum_y = sum_y + y[n]; // reassignment
  sum_y ~ binomial(N, theta);
}
```

· Simpler, but roughly same efficiency:

```
sum(y) ~ binomial(N, theta);
```

User-Defined Functions

- functions (compiled with model)
 - *content*: declare and define general (recursive) functions (use them elsewhere in program)
 - execute: compile with model
- Example

```
functions {
  real relative_difference(real u, real v) {
    return 2 * fabs(u - v) / (fabs(u) + fabs(v));
  }
}
```

Special User-Defined Functions

- When declared with appropriate naming, user-defined functions may
 - be used in sampling statements: real return and suffix _lpdf or _lpmf
 - use RNGs: suffix _rng
 - use target accumulator: suffix _1p

User-Defined PDFs and CDFs

- $\cdot\,$ May be used with sampling and PDF/PMF notation
 - density: suffix _1pdf if variate (first arg) is real
 - mass: Suffix _1pmf if variate (first arg) is integer

```
functions {
  real centered_normal_lpdf(real y, real sigma) {
    return -0.5 * (y / sigma)^2;
  }
model {
    y ~ centered_normal(2.5); // sampling
```

```
target += centered_normal_lpdf(y | 2.5); // pdf notation
```

Target Incrementing Functions

- · May access target or use sampling statements
- · Only usable in model block
 - must end in _1p

```
functions {
  vector non_center_lp(vector beta_std, real mu, real sigma) {
    beta_std ~ normal(0, 1);
    return mu + sigma * beta_raw;
  }
parameters {
  vector[K] beta_std;
model {
    vector[K] beta = non_center_lp(beta_std);
    y ~ normal(x * beta, sigma);
  }
}
```

RNG Functions

- · Only usable in generated quantities block
 - must end in _rng

```
functions {
   real centered_normal_rng(real sigma) {
     return normal_rng(0, sigma);
   }
```

```
generated quantities {
   real alpha = centered_normal_rng(2.7);
```

Differential Equation Solver

- System expressed as function
 - given state (y) time (t), parameters (θ), and data (x)
 - return derivatives $(\partial y / \partial t)$ of state w.r.t. time
- · Simple harmonic oscillator diff eq

Differential Equation Solver (cont.)

 Solution via functional, given initial state (y0), initial time (t0), desired solution times (ts)

mu_y = integrate_ode(sho, y0, t0, ts, theta, x_r, x_i);

- Use noisy measurements of y to estimate θ
 - y ~ normal(mu_y, sigma);
 - Pharmacokinetics/pharmacodynamics (PK/PD),
 - soil carbon respiration with biomass input and breakdown

Built-in Diff Eq Solvers

- Non-stiff solver: Runge-Kutta 4th/5th order (RK45)
- · Stiff solver: backward-differentiation formula (BDF)
 - slower
 - more robust for derivatives of different scales or high curvature
- specified by suffix _bdf or _rk45

Diff Eq Derivatives

- User defines system $\frac{\partial}{\partial t}y$
- Need derivatives of solution y w.r.t. parameters θ
- · Couple derivatives of system w.r.t. parameters

$$\left(\frac{\partial}{\partial t}\, y, \quad \frac{\partial}{\partial t}\, \frac{\partial}{\partial \theta}\, y\right)$$

Calculate coupled system via nested autodiff of second term

$$\frac{\partial}{\partial t} \frac{\partial}{\partial \theta} y = \frac{\partial}{\partial \theta} \frac{\partial}{\partial t} y.$$

Distribution Library

- Each distribution has
 - log density or mass function
 - cumulative distribution functions, plus complementary versions, plus log scale
 - Pseudo-random number generators
- Alternative parameterizations

(e.g., Cholesky-based multi-normal, log-scale Poisson, logit-scale Bernoulli)

New multivariate correlation matrix density: LKJ
 degrees of freedom controls shrinkage to (expansion from) unit matrix

Print and Reject

- Print statements are for debugging
 - printed every log prob evaluation
 - print values in the middle of programs
 - check when log density becomes undefined
 - can embed in conditionals
- Reject statements are for error checking
 - typically function argument checks
 - cause a rejection of current state (0 density)

Prob Function Vectorization

- · Stan's probability functions are vectorized for speed
 - removes repeated computations (e.g., $-\log\sigma$ in normal)
 - reduces size of expression graph for differentiation
- · Consider: y ~ normal(mu, sigma);
- $\cdot\,$ Each of y, mu, and sigma may be any of
 - scalars (integer or real)
 - vectors (row or column)
 - 1D arrays
- · All dimensions must be scalars or having matching sizes
- · Scalars are broadcast (repeated)

Parsing and Compilation

- Stan code parsed to abstract syntax tree (AST) (Boost Spirit Qi, recursive descent, lazy semantic actions)
- C++ model class code generation from AST (Boost Variant)
- · C++ code compilation
- Dynamic linking for RStan, PyStan

What Stan Does

Full Bayes: No-U-Turn Sampler

- · Adaptive Hamiltonian Monte Carlo (HMC)
 - Potential Energy: negative log posterior
 - Kinetic Energy: random standard normal per iteration
- Adaptation during warmup
 - step size adapted to target total acceptance rate
 - mass matrix (scale/rotation) estimated with regularization
- Adaptation during sampling
 - simulate forward and backward in time until U-turn
 - slice sample along path

(Hoffman and Gelman 2011, 2014)

Posterior Inference

- Generated quantities block for inference: predictions, decisions, and event probabilities
- · Extractors for samples in RStan and PyStan
- · Coda-like posterior summary
 - posterior mean w. MCMC std. error, std. dev., quantiles
 - split- \hat{R} multi-chain convergence diagnostic (Gelman/Rubin)
 - multi-chain effective sample size estimation (FFT algorithm)
- Model comparison with WAIC
 - in-sample approximation to cross-validation

MAP / Penalized MLE

- Posterior mode finding via L-BFGS optimization
 (uses model gradient, efficiently approximates Hessian)
- Disables Jacobians for parameter inverse transforms
- · Models, data, initialization as in MCMC
- Standard errors on unconstrained scale (estimated using curvature of penalized log likelihood function
- Very Near Future
 - Standard errors on constrained scale) (sample unconstrained approximation and inverse transform)

"Black Box" Variational Inference

- Black box so can fit any Stan model
- · Multivariate normal approx to unconstrained posterior
 - covariance: diagonal mean-field or full rank
 - not Laplace approx around posterior mean, not mode
 - transformed back to constrained space (built-in Jacobians)
- Stochastic gradient-descent optimization
 - ELBO gradient estimated via Monte Carlo + autodiff
- · Returns approximate posterior mean / covariance
- · Returns sample transformed to constrained space

Stan as a Research Tool

- Stan can be used to explore algorithms
- Models transformed to **unconstrained support** on \mathbb{R}^n
- · Once a model is compiled, have
 - log probability, gradient, and Hessian
 - data I/O and parameter initialization
 - model provides variable names and dimensionalities
 - transforms to and from constrained representation (with or without Jacobian)

Under Stan's Hood

Euclidean Hamiltonian Monte Carlo

- Phase space: q position (parameters); p momentum
- **Posterior density**: $\pi(q)$
- Mass matrix: M
- **Potential energy**: $V(q) = -\log \pi(q)$
- **Kinetic energy**: $T(p) = \frac{1}{2}p^{T}M^{-1}p$
- Hamiltonian: H(p,q) = V(q) + T(p)
- Diff eqs:

$$\frac{dq}{dt} = +\frac{\partial H}{\partial p} \qquad \qquad \frac{dp}{dt} = -\frac{\partial H}{\partial q}$$

Leapfrog Integrator Steps

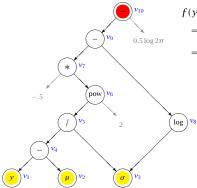
- Solves Hamilton's equations by simulating dynamics (symplectic [volume preserving]; ε³ error per step, ε² total error)
- Given: step size ϵ , mass matrix M, parameters q
- Initialize kinetic energy, $p \sim Normal(0, I)$
- **Repeat** for *L* leapfrog steps:

$$p \leftarrow p - \frac{\epsilon}{2} \frac{\partial V(q)}{\partial q}$$
 [half step in momentum]
 $q \leftarrow q + \epsilon M^{-1} p$ [full step in position]
 $p \leftarrow p - \frac{\epsilon}{2} \frac{\partial V(q)}{\partial q}$ [half step in momentum]

Reverse-Mode Auto Diff

- · Eval gradient in (usually small) multiple of function eval time
 - independent of dimensionality
 - time proportional to number of expressions evaluated
- · Result accurate to machine precision (cf. finite diffs)
- Function evaluation builds up expression tree
- · Dynamic program propagates chain rule in reverse pass
- Reverse mode computes ∇g in one pass for a function $f:\mathbb{R}^N \to \mathbb{R}$

Autodiff Expression Graph



 $f(y, \mu, \sigma)$

î

 $= \log(\text{Normal}(y|\mu,\sigma))$

$$= -\frac{1}{2} \left(\frac{\gamma - \mu}{\sigma}\right)^2 - \log \sigma - \frac{1}{2} \log(2\pi)$$

$$\frac{\partial}{\partial y} f(y, \mu, \sigma) = -(y - \mu) \sigma^{-2}$$

$$\begin{aligned} & \frac{\partial}{\partial \mu} f(y,\mu,\sigma) \\ & = (y-\mu)\sigma^{-2} \end{aligned}$$

$$\stackrel{\frac{\partial}{\partial \sigma}}{}_{\sigma} f(y, \mu, \sigma)$$

$$= (y - \mu)^2 \sigma^{-3} - \sigma^{-1}$$

Autodiff Partials

var	value	partials	
v_1	y y		
v_2	μ		
v_3	σ		
v_4	$v_1 - v_2$	$\partial v_4 / \partial v_1 = 1$	$\partial v_4 / \partial v_2 = -1$
v_5	v_4/v_3	$\partial v_5 / \partial v_4 = 1 / v_3$	$\partial v_5 / \partial v_3 = -v_4 v_3^{-2}$
v_6	$(v_5)^2$	$\partial v_6 / \partial v_5 = 2v_5$	
<i>v</i> ₇	$(-0.5)v_6$	$\partial v_7 / \partial v_6 = -0.5$	
v_8	$\log v_3$	$\partial v_8 / \partial v_3 = 1 / v_3$	
v_9	$v_7 - v_8$	$\partial v_9 / \partial v_7 = 1$	$\partial v_9 / \partial v_8 = -1$
v_{10}	$v_9 - (0.5 \log 2\pi)$	$\partial v_{10} / \partial v_9 = 1$	

Autodiff: Reverse Pass

var	operation	adjoint	result
$a_{1:9}$	=	0	$a_{1:9} = 0$
a_{10}	=	1	$a_{10} = 1$
a_9	+=	$a_{10} \times (1)$	$a_9 = 1$
a_7	+=	$a_9 \times (1)$	$a_7 = 1$
a_8	+=	$a_9 \times (-1)$	$a_8 = -1$
a_3	+=	$a_8 \times (1/v_3)$	$a_3 = -1/v_3$
a_6	+=	$a_7 \times (-0.5)$	$a_6 = -0.5$
a_5	+=	$a_6 \times (2v_5)$	$a_5 = -v_5$
a_4	+=	$a_5 \times (1/v_3)$	$a_4 = -v_5/v_3$
a_3	+=	$a_5 \times (-v_4 v_3^{-2})$	$a_3 = -1/v_3 + v_5 v_4 v_3^{-2}$
a_1	+=	$a_4 \times (1)$	$a_1 = -v_5/v_3$
a_2	+=	$a_4 \times (-1)$	$a_2 = v_5 / v_3$

Stan's Reverse-Mode

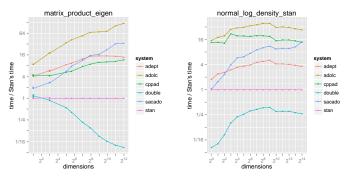
- Easily extensible object-oriented design
- · Code nodes in expression graph for primitive functions
 - requires partial derivatives
 - built-in flexible abstract base classes
 - lazy evaluation of chain rule saves memory
- · Autodiff through templated C++ functions
 - templating on each argument avoids excess promotion

Stan's Reverse-Mode (cont.)

- Arena-based memory management
 - specialized C++ operator new for reverse-mode variables
 - custom functions inherit memory management through base
- Nested application to support ODE solver

Stan's Autodiff vs. Alternatives

- · Stan is fastest (and uses least memory)
 - among open-source C++ alternatives



Forward-Mode Auto Diff

- Evaluates expression graph forward from one independent variable to any number of dependent variables
- · Function evaluation propagates chain rule forward
- · In one pass, computes $\frac{\partial}{\partial x} f(x)$ for a function $f : \mathbb{R} \to \mathbb{R}^N$

- derivative of N outputs with respect to a single input

Stan's Forward Mode

- · Templated scalar type for value and tangent
 - allows higher-order derivatives
- Primitive functions propagate derivatives
- No need to build expression graph in memory
 - much less memory intensive than reverse mode
- · Autodiff through templated functions (as reverse mode)

Second-Order Derivatives

· Compute Hessian (matrix of second-order partials)

$$H_{i,j} = \frac{\partial^2}{\partial x_i \partial x_j} f(x)$$

- · Required for Laplace covariance approximation (MLE)
- · Required for curvature (Riemannian HMC)
- · Nest reverse-mode in forward for second order
- \cdot N forward passes: takes gradient of derivative

Third-Order Derivatives

- Required for Riemannian HMC
- · Gradients of Hessians (tensor of third-order partials)

$$\frac{\partial^3}{\partial x_i \partial x_j \partial x_k} f(x)$$

- N^2 forward passes: gradient of derivative of derivative

Third-order Derivatives (cont.)

- · Gradient of trace of Hessian times matrix
 - $\nabla tr(HM)$, or
 - needed for Riemannian Hamiltonian Monte Carlo
 - computable in quadratic time for fixed M

Jacobians

- Assume function $f : \mathbb{R}^N \to \mathbb{R}^M$
- Partials for multivariate function (matrix of first-order partials)

$$J_{i,j} = \frac{\partial}{\partial x_i} f_j(x)$$

- · Required for stiff ordinary differential equations
 - differentiate is coupled sensitivity autodiff for ODE system
- Two execution strategies
 - 1. Multiple reverse passes for rows
 - 2. Forward pass per column (required for stiff ODE)

Autodiff Functionals

- · Functionals map templated functors to derivatives
 - fully encapsulates and hides all autodiff types
- · Autodiff functionals supported
 - gradients: $\mathcal{O}(1)$
 - Jacobians: $\mathcal{O}(N)$
 - gradient-vector product (i.e., directional derivative): $\mathcal{O}(1)$
 - Hessian-vector product: $\mathcal{O}(N)$
 - Hessian: $\mathcal{O}(N)$
 - gradient of trace of matrix-Hessian product: $\mathcal{O}(N^2)$ (for SoftAbs RHMC)

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 - lower and upper bound: scaled, offset logit transform
 - simplex: centered, stick-breaking logit transform
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Coding Probability Functions

- Vectorized to allow scalar or container arguments (containers all same shape; scalars broadcast as necessary)
- Avoid repeated computations, e.g. $\log\sigma$ in

log Normal $(y|\mu,\sigma) = \sum_{n=1}^{N} \log \text{Normal}(y_n|\mu,\sigma)$

$$= \sum_{n=1}^{N} -\log\sqrt{2\pi} - \log\sigma - \frac{y_n - \mu}{2\sigma^2}$$

- recursive expression templates to broadcast and cache scalars, generalize containers (arrays, matrices, vectors)
- traits metaprogram to drop constants (e.g., $-\log\sqrt{2\pi}$ or $\log\sigma$ if constant) and calculate intermediate and return types