# Stan

### **Probabilistic Programming Language**

#### Core Development Team:

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#### Stan's Namesake

- · Stanislaw Ulam (1909-1984)
- · Co-inventor of Monte Carlo method (and hydrogen bomb)



Ulam holding the Fermiac, Enrico Fermi's physical Monte Carlo simulator for random neutron diffusion

# Why Stan?

- · Application: Fit rich Bayesian statistical models
- · Problem: Gibbs and Metropolis too slow (diffusive)
- · Solution: Hamiltonian Monte Carlo (flow)
- · Problem: Interpreters slow and unscalable
- Solution: Compiled to C++
- · Problem: Need gradients of log posterior for HMC
- · Solution: Reverse-mode algorithmic differentation

# Why? (cont.)

- · Problem: Existing algo-diff slow, limited, unextensible
- · Solution: Our own algo-diff
- · Problem: Algo-diff requires functions templated on all args
- · Solution: Our own density library, Eigen linear algebra
- Problem: Need unconstrained parameters for HMC
- · Solution: Variable transforms w. Jacobian determinants

# Why? (cont.)

- · Problem: Need ease of use of BUGS
- · Solution: Compile a domain-specific language
- Problem: Pure directed graphical language inflexible
- · Solution: Imperative probabilistic programming language
- · Problem: Need to tune parameters for HMC
- Solution: Tune step size and estimate mass matrix during warmup; on-the-fly number of steps (NUTS)

### Why? (cont.)

- · Problem: Efficient up-to-proportion density calcs
- · Solution: Density template metaprogramming
- Problem: Limited error checking, recovery
- · Solution: Static model typing, informative exceptions
- · Problem: Poor boundary behavior
- · *Solution*: Calculate limits (e.g.  $\lim_{x\to 0} x \log x$ )

# Why? (continued)

- · Problem: Nobody knows everything
- · Solution: Expand project team with specialists
- · Problem: Expanding code and project team
- Solution: GitHub: branch, pull request, code review
- · Solution: Jenkins: continuous integration
- · Solution: ongoing refactoring and code simplification

# Why? (continued)

- · Problem: Heterogeneous user base
- · Solution: More interfaces (R, Python, MATLAB, Julia)
- · Solution: domain-specific examples, tutorials
- Problem: Restrictive licensing limits use
- · Solution: Code and doc open source (BSD, CC-BY)

#### What is Stan?

- · Stan is an imperative probabilistic programming language
  - cf., BUGS: declarative; Church: functional; Figaro: object-oriented

#### · Stan program

- declares data and (constrained) parameter variables
- defines log posterior (or penalized likelihood)

#### Stan inference

- MCMC for full Bayesian inference
- MLE for penalized maximum likelihood estimation
- Stan is open source (BSD core, some GPLv3 interfaces)
   hosted on GitHub; uses Eigen matrix lib, Boost C++ lib, googletest

#### **Platforms and Interfaces**

- · Platforms: Linux, Mac OS X, Windows
- C++ API: portable, standards compliant (C++03)
- Interfaces
  - CmdStan: Command-line or shell interface (direct executable)
  - RStan: R interface (Rcpp in memory)
  - **PyStan**: Python interface (Cython in memory)
  - MatlabStan: MATLAB interface (external process)
  - Stan.jl: Julia interface (external process)
  - StataStan: Stata interface (external process) [under testing]
- Posterior Visualization & Exploration
  - ShinyStan: Shiny (R) web-based

# Who's Using Stan?

- 1000+ users group registrations; 10,000 manual downloads (2.5.0)
- Biological sciences: clinical drug trials, entomology, opthalmology, neurology, genomics, agriculture, botany, fisheries, cancer biology, epidemiology, population ecology, neurology
- Physical sciences: astrophysics, molecular biology, oceanography, climatology
- Social sciences: population dynamics, psycholinguistics, social networks, political science
- Other: materials engineering, finance, actuarial, sports, public health, recommender systems, educational testing

#### **Documentation**

- · Stan User's Guide and Reference Manual
  - 500+ pages
  - Example models, modeling and programming advice
  - Introduction to Bayesian and frequentist statistics
  - Complete language specification and execution guide
  - Descriptions of algorithms (NUTS, R-hat, n\_eff)
  - Guide to built-in distributions and functions
  - Installation and getting started manuals by interface
    - RStan, PyStan, CmdStan, MatlabStan, Stan.jl
    - RStan vignette

#### **Books and Model Sets**

- Model Sets Translated to Stan
  - BUGS and JAGS examples (most of all 3 volumes)
  - Gelman and Hill (2009) Data Analysis Using Regression and Multilevel/Hierarchical Models
  - Wagenmakers and Lee (2014) Bayesian Cognitive Modeling
- Books with Sections on Stan
  - Gelman et al. (2013) Bayesian Data Analysis, 3rd Edition.
  - Kruschke (2014) Doing Bayesian Data Analysis, Second Edition: A Tutorial with R, JAGS, and Stan
  - Korner-Nievergelt et al. (2015) Bayesian Data Analysis in Ecology Using Linear Models with R, BUGS, and Stan

# **Scaling and Evaluation**

- Types of scaling
  - more data
  - more parameters
  - more complex models

(why we built Stan)

· for MCMC, measure

(vs. BUGS / JAGS)

time to convergence

(0.5-∞ faster)

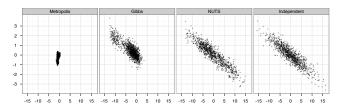
- time per effective sample after convergence

(ditto)

- memory usage

(90-99% less, linear scaling)

# **NUTS vs. Gibbs and Metropolis**



- · Two dimensions of highly correlated 250-dim normal
- · 1,000,000 draws from Metropolis and Gibbs (thin to 1000)
- 1000 draws from NUTS; 1000 independent draws

Part I

**Stan Front End** 

### **Estimate Proportion**

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

# Maximum (Penalized) Likelihood

```
> library(rstan);
> N <- 5:
> y <- c(0,1,1,0,0);
> model <- stan_model("bernoulli.stan");</pre>
> mle <- optimizing(model, data=c("N", "y"));</pre>
> print(mle, digits=2)
$par
                   $value (log density)
theta
                   [1] - 3.4
  0.4
```

- Posterior: Beta(1 + 2, 1 + 3); max 0.40; mean 0.43
- · Density: MLE w/o Jacobian; MCMC with Jacobian

# **Bayesian Posterior**

```
> N <- 5;  y <- c(0,1,1,0,0);
> fit <- stan("bernoulli.stan", data = c("N", "y"));
> print(fit, digits=2)
```

Inference for Stan model: bernoulli.
4 chains, each with iter=2000; warmup=1000; thin=1;

```
        mean
        se
        sd
        2.5%
        50%
        97.5%
        n_eff
        Rhat

        theta
        0.43
        0.01
        0.18
        0.11
        0.42
        0.78
        1229
        1

        7p__
        -5.33
        0.02
        0.80
        -7.46
        -5.04
        -4.78
        1201
        1
```

> hist( extract(fit)\$theta )



#### **Default Priors and Vectorization**

- · All parameters are uniform by default
- · Probability functions can be vectorized (more efficient)
- · Thus

```
theta ~ uniform(0,1);
for (n in 1:N)
  y[n] ~ bernoulli(theta);
```

reduces to

```
y ~ bernoulli(theta);
```

# **Linear Regression**

```
data {
  int<lower=0> N:
  vector[N] x:
  vector[N] y;
parameters {
  real alpha;
  real beta;
  real<lower=0> sigma;
model {
   y ~ normal(alpha + beta * x, sigma);
// for (n in 1:N)
       y[n] \sim normal(alpha + beta * x[n], sigma);
```

# Logistic Regression (w. Matrices)

```
data {
  int<lower=1> K:
  int<lower=0> N;
 matrix[N,K] x;
  int<lower=0.upper=1> v[N]:
parameters {
  vector[K] beta;
model {
   beta \sim cauchy(0, 2.5); // prior
   v ~ bernoulli logit(x * beta): // likelihood
```

- vectorized default prior for regression coefficients
- vectorized, logit-scale; y ~ bernoulli(inv\_logit(x \* beta))

# Time Series Autoregressive: AR(1)

```
data {
  int<lower=0> N;  vector[N] y;
}
parameters {
  real alpha;  real beta;  real sigma;
}
model {
  for (n in 2:N)
     y[n] ~ normal(alpha + beta * y[n-1], sigma);
}
```

· Likelihood more efficiently coded with vectorization as

```
tail(y, N - 1) \sim normal(alpha + beta * head(y, N - 1), sigma);
```

#### **Generalized Linear Models**

- · Direct parameterizations more efficient and stable
- Logistic regression (boolean/binary data)
  - y ~ bernoulli(inv\_logit(eta));
  - y ~ bernoulli\_logit(eta);
  - Probit via Phi (normal cdf)
  - Robit (robust) via Student-t cdf
- · Poisson regression (count data)
  - y ~ poisson(exp(eta));
  - y ~ poisson\_log(eta);
  - Overdispersion with negative binomial

### **GLMS**, continued

- Multi-logit regression (categorical data)
  - y ~ categorical(softmax(eta));
  - y ~ categorical\_logit(eta);
- Ordinal logistic regression (ordered data)
  - Add cutpoints c
  - y ~ ordered\_logistic(eta, c);
- Robust linear regression (overdispersed noise)
  - y ~ student\_t(nu, eta, sigma);

#### **Posterior Predictive Inference**

· Parameters  $\theta$ , observed data y and data to predict  $\tilde{y}$ 

$$p(\tilde{y}|y) = \int_{\Theta} p(\tilde{y}|\theta) \ p(\theta|y) \ d\theta$$

```
data {
   int<lower=0> N_tilde;
   matrix[N_tilde,K] x_tilde;
   ...
parameters {
   vector[N_tilde] y_tilde;
   ...
model {
   y_tilde ~ normal(x_tilde * beta, sigma);
```

### **Predict w. Generated Quantities**

· Replace sampling with pseudo-random number generation

```
generated quantities {
  vector[N_tilde] y_tilde;

for (n in 1:N_tilde)
   y_tilde[n] <- normal_rng(x_tilde[n] * beta, sigma);
}</pre>
```

- Must include noise for predictive uncertainty
- · PRNGs only allowed in generated quantities block
  - more computationally efficient per iteration
  - more statistically efficient with i.i.d. samples (i.e., MC, not MCMC)

#### **Example: Gaussian Process Estimation**

```
data {
 int<lower=1> N; vector[N] x; vector[N] y;
} parameters {
  real<lower=0> eta_sq, inv_rho_sq, sigma_sq;
} transformed parameters {
  real<lower=0> rho_sq; rho_sq <- inv(inv_rho_sq);
} model {
 matrix[N,N] Sigma;
 for (i in 1:(N-1)) {
    for (i in (i+1):N) {
      Sigma[i,j] \leftarrow eta_sq * exp(-rho_sq * square(x[i] - x[j]));
      Sigma[i,i] <- Sigma[i,i];
 }}
 for (k in 1:N) Sigma[k,k] <- eta_sq + sigma_sq;</pre>
 eta_sq, inv_rho_sq, sigma_sq ~ cauchy(0,5);
  y ~ multi_normal(rep_vector(0,N), Sigma);
```

#### **Gaussian Process Predictions**

- · Add predictors x\_tilde[M] for points to predict
- Declare predicted values y\_tilde[M] as unconstrained parameters
- Define Sigma[M+N,M+N] in terms of full append\_row(x, x\_tilde)
- · Model remains the same

```
append_row(y,y_tilde)
  ~ multi_normal(rep(0,N+M),Sigma);
```

### **Mixture of Two Normals**

- · local variables reassigned; direct increment of log posterior
- ·  $\log_{\text{sum}} \exp(\alpha, \beta) = \log(\exp(\alpha) + \exp(\beta))$
- · Much more efficient than sampling (Rao-Blackwell Theorem)

# **Other Mixture Applications**

- · Other multimodal data
- · Zero-inflated Poisson or hurdle models
- Model comparison or mixture
- · Discrete change-point model
- · Hidden Markov model, Kalman filter
- · Almost anything with latent discrete parameters
- · Other than variable choice, e.g., regression predictors
  - marginalization is exponential in number of vars

# LKJ Density and Cholesky Factors

- · Density on correlation matrices  $\Omega$
- · LKJCorr( $\Omega \mid v$ )  $\propto \det(\Omega)^{(v-1)}$ 
  - v = 1 uniform
  - v > 1 concentrates around unit matrix
- · Work with Cholesky factor  $L_{\Omega}$  s.t.  $\Omega = L_{\Omega} L_{\Omega}^{\mathsf{T}}$ 
  - Density: LKJCorrCholesky $(L_{\Omega} \mid v) \propto |J| \det(L_{\Omega} L_{\Omega}^{\mathsf{T}})^{(v-1)}$
  - Jacobian adjustment for Cholesky factorization

### **Covariance Random-Effects Priors**

```
parameters {
  vector[2] beta[G];
  cholesky_factor_corr[2] L_0mega;
  vector<lower=0>[2] sigma:
model {
  sigma \sim cauchy(0, 2.5);
  L_Omega ~ lkj_cholesky(4);
  beta ~ multi_normal_cholesky(rep_vector(0, 2),
                          diag post multiply(L Omega, sigma)):
  for (n in 1:N)
    y[n] ~ bernoulli_logit(... + x[n] * beta[gg[n]]);
```

· G groups with varying slope and intercept; gg indicates group

# **Dynamic Systems with Diff Eqs**

· Simple harmonic oscillator

$$\frac{d}{dt}y_1 = -y_2 \qquad \qquad \frac{d}{dt}y_2 = -y_1 - \theta y_2$$

· Code as a function in Stan

# **Fit Noisy State Measurements**

```
data {
  int<lower=1> T; real y[T,2];
  real t0:
                       real ts[T];
parameters {
  real y0[2];
                              // unknown initial state
  real theta[1];
                             // rates for equation
  vector<lower=0>[2] sigma; // measurement error
model {
  real y_hat[T,2];
  ...priors...
  y_hat <- integrate_ode(sho, y0, t0, ts, theta, x_r, x_i);</pre>
  for (t in 1:T)
   y[t] ~ normal(y_hat[t], sigma);
```

Part II

**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

#### 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
- Very Near Future
  - Standard errors on unconstrained scale (estimated using curvature of penalized log likelihood function
  - Standard errors on constrained scale)
     (sample unconstrained approximation and inverse transform)
  - L-BFGS optimizer

### 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)

Part IV

**Stan Language** 



# **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
- model (every log prob eval)
  - content: statements definining posterior density
  - execute: execute statements

### **Derived Variable Blocks**

- transformed data (once after data)
  - 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

# Variable and Expression Types

Variables and expressions are strongly, statically typed.

- · Primitive: int, real
- Matrix: matrix[M,N], vector[M], row\_vector[N]
- 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)

# **Logical Operators**

Ор.	Prec.	Assoc.	Placement	Description
П	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**

Ор.	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)
٨	2	right	binary infix	exponentiation
,	0	n/a	unary postfix	transposition
()	0	n/a	prefix, wrap	function application
[]	0	left	prefix, wrap	array, matrix indexing

#### **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 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
- · Ordering, Slicing, Broadcasting: sort, rank, block, rep
- · Reductions: sum, product, norms
- · Specializations: triangular, positive-definite, etc.

## **User-Defined Functions (Stan 2.3)**

- 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));
  }
}
```

# **Differential Equation Solver**

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

# **Differential Equation Solver**

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

```
mu_y \leftarrow integrate_ode(sho, y0, t0, ts, theta, x_r, x_i);
```

· Use noisy measurements of y to estimate  $\theta$ 

```
y ~ normal(mu_y, sigma);
```

- Pharmacokinetics/pharmacodynamics (PK/PD),
- soil carbon respiration

# **Diff Eq Derivatives**

- · Need derivatives of solution w.r.t. parameters
- · Couple derivatives of system w.r.t. parameters

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

Calculate coupled system via nested autodiff of second term

$$\frac{\partial}{\partial \theta} \frac{\partial}{\partial \theta}$$

# **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

#### **Statements**

- Sampling: y ~ normal(mu, sigma) (increments log probability)
- Log probability: increment\_log\_prob(lp);
- Assignment: y\_hat <- x \* beta;</li>
- For loop: for (n in 1:N) ...
- · While loop: while (cond) ...
- Conditional: if (cond) ...; else if (cond) ...; else ...;
- · Block: { ... } (allows local variables)
- Print: print("theta=",theta);

# Part V

# **Challenges for Stan**

### **Models with Discrete Parameters**

- e.g., simple mixture models, survival models, HMMs, discrete measurement error models, missing data
- Marginalize out discrete parameters
- Efficient sampling due to Rao-Blackwellization
- · Inference straightforward with expectations

 Too difficult for many of our users (exploring encapsulation options)

# **Models with Missing Data**

- In principle, missing data just additional parameters
- In practice, how to declare?
  - observed data as data variables
  - missing data as parameters
  - combine into single vector
     (in transformed parameters or local in model)

## **Position-Dependent Curvature**

- · Mass matrix does **global** adaptation for
  - parameter scale (diagonal) and rotation (dense)
- · Dense mass matrices hard to estimate ( $\mathcal{O}(N^2)$  estimands)
- Problem: Position-dependent curvature
  - Example: banana-shaped densities
    - \* arise when parameter is product of other parameters
  - Example: hierarchical models
    - \* hierarhcical variance controls lower-level parameters
- · Mitigate by reducing stepsize
  - initial (stepsize) and target acceptance (adapt\_delta)

Part VI

# **Next for Stan**

# **Higher-Order Auto-diff**

- · Finish higher-order auto-diff for probability functions
- May punt some cumulative distribution functions
   (Black art iterative algorithms required)

Code complete; under testing

#### Riemannian Manifold HMC

- Best mixing MCMC method (fixed # of continuous params)
- Moves on Riemannian manifold rather than Euclidean
  - adapts to position-dependent curvature
- geoNUTS generalizes NUTS to RHMC (Betancourt arXiv)
- SoftAbs metric (Betancourt arXiv)
  - eigendecompose Hessian and condition
  - computationally feasible alternative to original Fisher info metric of Girolami and Calderhead (IRSS, Series B)
  - requires third-order derivatives and implicit integrator
- · Code complete; awaiting higher-order auto-diff

# **Adiabatic Sampling**

- Physically motivated alternative to "simulated" annealing and tempering (not really simulated!)
- · Supplies external heat bath
- Operates through contact manifold
- · System relaxes more naturally between energy levels
- · Betancourt paper on arXiv

Prototype complete

# **Maximum Marginal Likelihood**

- · Fast, Approximate Inference
- · Marginalize out lower-level parameters
- Optimize higher-level parameters and fix
- · Optimize lower-level parameters given higher-level
- · Errors estimated as in MLE

Design complete; awaiting parameter tagging

### "Black Box" VB

- · Fast, Approximate Inference
- Black box so can run any model (Laplace or other approximations)
- · Stochastic, data-streaming variational Bayes (VB)
- Optimize parameteric approximation to posterior to minimize KL divergence
- · Code complete [integration testing]
- · collaboration with Dave Blei, Rajesh Ranganath

#### "Black Box" EP

- · Fast, Approximate Inference
- Data-parallel expectation propagation (EP) (cavity distributions provide general shard combination)
- Optimize parameteric approximation to posterior to minimize KL divergence (VB, EP measure divergence in opposite directions)
- · Prototypte stage
- collaborating with Nicolas Chopin, Christian Robert, John Cunningham, Aki Vehtari, Pasi Jylänki

# The End