

# Stan:

## a Probabilistic Programming Language

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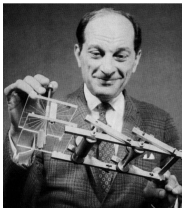
Stan 2.17.0 (October 2017)

<http://mc-stan.org>



# 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

**Prerequisite**

**Bayesian Inference**

# Bayesian Data Analysis

- “By Bayesian data analysis, we mean practical methods for making inferences from data using probability models for quantities we observe and about which we wish to learn.”
- “The essential characteristic of Bayesian methods is their **explicit use of probability for quantifying uncertainty** in inferences based on statistical analysis.”

# Bayesian Methodology

- Set up **full probability model**
  - for all observable & unobservable quantities
  - consistent w. problem knowledge & data collection
- **Condition** on observed data (where Stan comes in!)
  - to calculate posterior probability of unobserved quantities (e.g., parameters, predictions, missing data)
- **Evaluate**
  - model fit and implications of posterior
- **Repeat** as necessary

# Where do Models Come from?

- Sometimes model comes first, based on substantive considerations
  - toxicology, economics, ecology, physics, . . .
- Sometimes model chosen based on data collection
  - traditional statistics of surveys and experiments
- Other times the data comes first
  - observational studies, meta-analysis, . . .
- Usually its a mix

# Model Checking

- Do the inferences make sense?
  - are parameter values consistent with model's prior?
  - does simulating from parameter values produce reasonable fake data?
  - are marginal predictions consistent with the data?
- Do predictions and event probabilities for new data make sense?
- **Not:** Is the model true?
- **Not:** What is  $\Pr[\text{model is true}]$ ?
- **Not:** Can we “reject” the model?

# Model Improvement

- Expanding the model
  - hierarchical and multilevel structure ...
  - more flexible distributions (overdispersion, covariance)
  - more structure (geospatial, time series)
  - more modeling of measurement methods and errors
  - ...
- Including more data
  - breadth (more predictors or kinds of observations)
  - depth (more observations)



# Using Bayesian Inference

- Explores full range of parameters consistent with prior info and data\*
  - \* if such agreement is possible
  - Stan automates this procedure with diagnostics
- Inferences can be plugged in directly for
  - parameter estimates minimizing expected error
  - predictions for future outcomes with uncertainty
  - event probability updates conditioned on data
  - risk assesment / decision analysis conditioned on uncertainty

# Notation for Basic Quantities

- **Basic Quantities**

- $y$ : observed data
- $\theta$ : parameters (and other unobserved quantities)
- $x$ : constants, predictors for conditional (aka “discriminative”) models

- **Basic Predictive Quantities**

- $\tilde{y}$ : unknown, potentially observable quantities
- $\tilde{x}$ : constants, predictors for unknown quantities

# Naming Conventions

- **Joint:**  $p(y, \theta)$
- **Sampling / Likelihood:**  $p(y|\theta)$ 
  - Sampling is function of  $y$  with  $\theta$  fixed (prob function)
  - Likelihood is function of  $\theta$  with  $y$  fixed (*not* prob function)
- **Prior:**  $p(\theta)$
- **Posterior:**  $p(\theta|y)$
- **Data Marginal (Evidence):**  $p(y)$
- **Posterior Predictive:**  $p(\tilde{y}|y)$

# Bayes's Rule for Posterior

$$p(\theta|y) = \frac{p(y, \theta)}{p(y)} \quad \text{[def of conditional]}$$

$$= \frac{p(y|\theta) p(\theta)}{p(y)} \quad \text{[chain rule]}$$

$$= \frac{p(y|\theta) p(\theta)}{\int_{\Theta} p(y, \theta') d\theta'} \quad \text{[law of total prob]}$$

$$= \frac{p(y|\theta) p(\theta)}{\int_{\Theta} p(y|\theta') p(\theta') d\theta'} \quad \text{[chain rule]}$$

- *Inversion*: Final result depends only on sampling distribution (likelihood)  $p(y|\theta)$  and prior  $p(\theta)$

# Bayes's Rule up to Proportion

- If data  $y$  is fixed, then

$$\begin{aligned} p(\theta|y) &= \frac{p(y|\theta) p(\theta)}{p(y)} \\ &\propto p(y|\theta) p(\theta) \\ &= p(y, \theta) \end{aligned}$$

- Posterior proportional to likelihood times prior
- Equivalently, posterior proportional to joint
- The nasty integral for data marginal  $p(y)$  goes away

# Posterior Predictive Distribution

- Predict new data  $\tilde{y}$  based on observed data  $y$
- Marginalize parameters  $\theta$  out of posterior and likelihood

$$\begin{aligned} p(\tilde{y} | y) &= \mathbb{E}[p(\tilde{y}|\theta) | Y = y] \\ &= \int p(\tilde{y}|\theta) p(\theta|y) d\theta. \end{aligned}$$

- Weights predictions  $p(\tilde{y}|\theta)$ , by posterior  $p(\theta|y)$
- Integral notation shorthand for sums and/or integrals

# Event Probabilities

- Events are fundamental probability bearing units which
  - are defined by sets of outcomes
  - which occur or not with some probability
- Events typically defined as conditions on random variables, e.g.,
  - $\theta_b > \theta_g$  for more boy births than girl births
  - $z_k = 1$  for team A beating team B in game  $k$

## Event Probabilities, cont.

- $\theta = (\theta_1, \dots, \theta_N)$  is a sequence of random variables
- $c$  is a condition on  $\theta$ , so that  $c(\theta_1, \dots, \theta_N) \in \{0, 1\}$
- Suppose  $Y = y$  is some observed data
- The probability that the event holds conditioned on the data is given by

$$\begin{aligned}\Pr[c(\theta_1, \dots, \theta_N) | Y = y] &= \mathbb{E}[c(\theta_1, \dots, \theta_N) | Y] \\ &= \int c(\theta) p(\theta | y) d\theta\end{aligned}$$

- Not frequentist, because involves parameter probabilities



**Stan Example**

**Repeated Binary Trials**

# Stan Program

```
data {  
  int<lower=0> N;           // number of trials  
  int<lower=0, upper=1> y[N]; // success on trial n  
}  
parameters {  
  real<lower=0, upper=1> theta; // chance of success  
}  
model {  
  theta ~ uniform(0, 1); // prior  
  for (n in 1:N)  
    y[n] ~ bernoulli(theta); // likelihood  
}
```

# A Stan Program

- Defines log (posterior) density up to constant, so...
- Equivalent to define log density directly:

```
model {  
  increment_log_prob(0);  
  for (n in 1:N)  
    increment_log_prob(log(theta^y[n]  
                          * (1 - theta)^(1 - y[n])));  
}
```

- Also equivalent to (a) drop constant prior and (b) vectorize likelihood:

```
model {  
  y ~ bernoulli(theta);  
}
```

# R: Simulate Data

- Generate data

```
> theta <- 0.30;  
> N <- 20;  
> y <- rbinom(N, 1, 0.3);
```

```
> y
```

```
[1] 1 1 1 1 0 0 0 0 1 1 0 0 1 0 0 0 0 0 0 1
```

- Calculate MLE as sample mean from data

```
> sum(y) / N
```

```
[1] 0.4
```

# RStan: Fit

```
> library(rstan);  
  
> fit <- stan("bern.stan",  
             data = list(y = y, N = N));  
  
> print(fit, probs=c(0.1, 0.9));
```

*Inference for Stan model: bern.*

*4 chains, each with iter=2000; warmup=1000; thin=1;  
post-warmup draws per chain=1000,  
total post-warmup draws=4000.*

	mean	se_mean	sd	10%	90%	n_eff	Rhat
theta	0.41	0.00	0.10	0.28	0.55	1580	1

# Plug in Posterior Draws

- Extracting the posterior draws

```
> theta_draws <- extract(fit)$theta;
```

- Calculating posterior mean (estimator)

```
> mean(theta_draws);
```

```
[1] 0.4128373
```

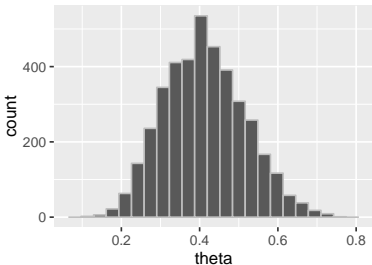
- Calculating posterior intervals

```
> quantile(theta_draws, probs=c(0.10, 0.90));
```

```
      10%      90%  
0.2830349 0.5496858
```

# ggplot2: Plotting

```
theta_draws_df <- data.frame(list(theta = theta_draws));  
plot <-  
  ggplot(theta_draws_df, aes(x = theta)) +  
  geom_histogram(bins=20, color = "gray");  
plot;
```



**Example**

**Fisher "Exact" Test**



# Bayesian “Fisher Exact Test”

- Suppose we observe the following data on handedness

	<i>sinister</i>	<i>dexter</i>	TOTAL
<i>male</i>	9 ( $y_1$ )	43	52 ( $N_1$ )
<i>female</i>	4 ( $y_2$ )	44	48 ( $N_2$ )

- Assume likelihoods  $\text{Binomial}(y_k | N_k, \theta_k)$ , uniform priors
- Are men more likely to be lefthanded?

$$\begin{aligned}\Pr[\theta_1 > \theta_2 | y, N] &= \int_{\Theta} \mathbb{I}[\theta_1 > \theta_2] p(\theta | y, N) d\theta \\ &\approx \frac{1}{M} \sum_{m=1}^M \mathbb{I}[\theta_1^{(m)} > \theta_2^{(m)}].\end{aligned}$$

# Stan Binomial Comparison

```
data {  
  int y[2];  
  int N[2];  
}  
parameters {  
  vector<lower=0,upper=1> theta[2];  
}  
model {  
  y ~ binomial(N, theta);  
}  
generated quantities {  
  real boys_minus_girls = theta[1] - theta[2];  
  int boys_gt_girls = theta[1] > theta[2];  
}
```

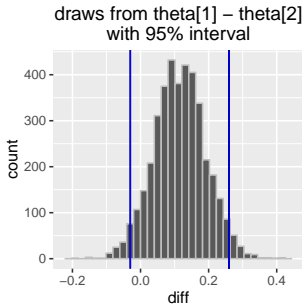
# Results

	<i>mean</i>	<i>2.5%</i>	<i>97.5%</i>
<i>theta[1]</i>	<i>0.22</i>	<i>0.12</i>	<i>0.35</i>
<i>theta[2]</i>	<i>0.11</i>	<i>0.04</i>	<i>0.21</i>
<i>boys_minus_girls</i>	<i>0.12</i>	<i>-0.03</i>	<i>0.26</i>
<i>boys_gt_girls</i>	<i>0.93</i>	<i>0.00</i>	<i>1.00</i>

- $\Pr[\theta_1 > \theta_2 \mid y] \approx 0.93$
- $\Pr[(\theta_1 - \theta_2) \in (-0.03, 0.26) \mid y] = 95\%$

# Visualizing Posterior Difference

- Plot of posterior difference,  $p(\theta_1 - \theta_2 \mid y, N)$  (men - women)



- Vertical bars: central 95% posterior interval  $(-0.03, 0.26)$

**Example**

**More Stan Models**

# Posterior Predictive Distribution

- Predict new data ( $\tilde{y}$ ) given observed data ( $y$ )
- Includes two kinds of uncertainty
  - parameter estimation uncertainty:  $p(\theta|y)$
  - sampling uncertainty:  $p(\tilde{y}|\theta)$

$$p(\tilde{y}|y) = \int p(\tilde{y}|\theta) p(\theta|y) d\theta$$
$$\approx \frac{1}{M} \sum_{m=1}^M p(\tilde{y}|\theta^{(m)})$$

- Can generate predictions as sample of draws  $\tilde{y}^{(m)}$  based on  $\theta^{(m)}$

# Linear Regression with Prediction

```
data {
  int<lower=0> N;                int<lower=0> K;
  matrix[N, K] x;              vector[N] y;
  matrix[N_tilde, K] x_tilde;
}
parameters {
  vector[K] beta;              real<lower=0> sigma;
}
model {
  y ~ normal(x * beta, sigma);
}
generated quantities {
  vector[N_tilde] y_tilde
    = normal_rng(x_tilde * beta, sigma);
}
```

# Transforming Precision

```
parameters {  
  real<lower=0> tau;      // precision  
  ...  
}  
transformed parameters {  
  real<lower=0> sigma;   // scale  
  sigma <- 1 / sqrt(tau);  
}
```



# Logistic Regression

```
data {  
  int<lower=1> K;  
  int<lower=0> N;  
  matrix[N,K] x;  
  int<lower=0,upper=1> y[N];  
}  
parameters {  
  vector[K] beta;  
}  
model {  
  beta ~ cauchy(0, 2.5);           // prior  
  y ~ bernoulli_logit(x * beta); // likelihood  
}
```

# Time Series Autoregressive: AR(1)

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

# Covariance Random-Effects Priors

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

## 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 (j in (i+1):N) {
      Sigma[i,j] <- eta_sq * exp(-rho_sq * square(x[i] - x[j]));
      Sigma[j,i] <- Sigma[i,j];
    }
  }
  for (k in 1:N) Sigma[k,k] <- eta_sq + sigma_sq;
  eta_sq, inv_rho_sq, sigma_sq ~ cauchy(0,5);
  y ~ multi_normal(rep_vector(0,N), Sigma);
}
```

# Non-Centered Parameterization

```
parameters {  
  vector[K] beta_raw; // non-centered  
  real mu;  
  real<lower=0> sigma;  
}  
transformed parameters {  
  vector[K] beta; // centered  
  beta <- mu + sigma * beta_raw;  
}  
model {  
  mu ~ cauchy(0, 2.5);  
  sigma ~ cauchy(0, 2.5);  
  beta_raw ~ normal(0, 1);  
}
```

**Overview**

**What is Stan?**

# 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
  - VB for approximate Bayesian inference
  - MLE for penalized maximum likelihood estimation

# Platforms and Interfaces

- **Platforms:** Linux, Mac OS X, Windows
- **C++ API:** portable, standards compliant (C++03; C++11 soon)
- **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)
- **Posterior Visualization & Exploration**
  - **ShinyStan:** Shiny (R) web-based



# Higher-Level Interfaces

- **R Interfaces**

- **RStanArm**: Regression modeling with R expressions
- **ShinyStan**: Web-based posterior visualization, exploration
- **Loo**: Approximate leave-one-out cross-validation

- **Containers**

- Dockerized Jupyter (iPython) Notebooks (R, Python, or Julia)

# Who's Using Stan?

- 1800+ **users group** registrations; 15,000+ **downloads** (per version just in Rstudio); 400+ Google scholar citations
- **Biological sciences**: clinical drug trials, entomology, ophthalmology, neurology, genomics, agriculture, botany, fisheries, cancer biology, epidemiology, population ecology, neurology
- **Physical sciences**: astrophysics, molecular biology, oceanography, climatology, biogeochemistry
- **Social sciences**: population dynamics, psycholinguistics, social networks, political science, surveys
- **Other**: materials engineering, finance, actuarial, sports, public health, recommender systems, educational testing, equipment maintenance

# Documentation

- *Stan User's Guide and Reference Manual*
  - 550+ (short) 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, StataStan
  - RStan vignette

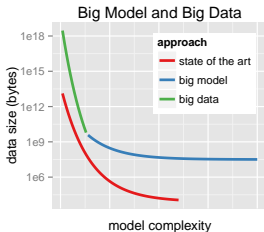
# Model Sets Translated to Stan

- BUGS 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*
- Kéry and Schaub (2014) *Bayesian Population Analysis Using WinBUGS*

# Books all or partly about Stan

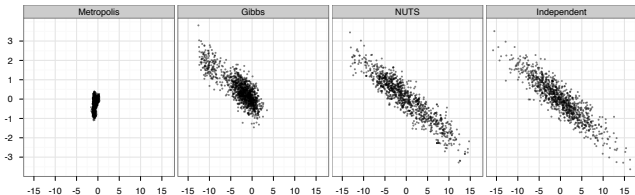
- McElreath (2016) *Statistical Rethinking: A Bayesian course with R and Stan*
- Korner-Nievergelt et al. (2015) *Bayesian Data Analysis in Ecology Using Linear Models with R, BUGS, and Stan*
- Kruschke (2014) *Doing Bayesian Data Analysis, Second Edition: A Tutorial with R, JAGS, and Stan*
- Gelman et al. (2013) *Bayesian Data Analysis*, 3rd Edition.
- More in prep (including two written by the Stan developers, one basic and one for econometrics)

# Scaling and Evaluation



- Types of Scaling: data, parameters, **models**
- Time to converge and per effective sample size:  
0.5- $\infty$  times faster than BUGS & JAGS
- Memory usage: 1-10% of BUGS & JAGS

# 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

**Overview**

**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

# 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

# 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,  $\log \left| \frac{d}{dy} \exp(y) \right| = y$
- 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
- 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 stick-breaking

## 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. 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
- Are not assignable to each other, but there are conversion functions

# Logical Operators

<i>Op.</i>	<i>Prec.</i>	<i>Assoc.</i>	<i>Placement</i>	<i>Description</i>
	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

<i>Op.</i>	<i>Prec.</i>	<i>Assoc.</i>	<i>Placement</i>	<i>Description</i>
+	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	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 log1 m, 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,

# Statements

- **Sampling:** `y ~ normal(mu, sigma)` (increments log probability)
- **Log probability:** `increment_log_prob(lp);`
- **Assignment:** `y_hat <- x * beta;`
- **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);`
- **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
- 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);`

is more efficient with sufficient statistics

```
{  
  real sum_y; // local variable  
  sum_y <- 0;  
  for (n in 1:N)  
    sum_y <- a + 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));  
    }  
  
}
```

# 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

```
real[] sho(real t,          // time
           real[] y,       // system state
           real[] theta,   // params
           real[] x_r,     // real data
           int[] x_i) {    // int data
  real dydt[2];
  dydt[1] <- y[2];
  dydt[2] <- -y[1] - theta[1] * y[2];
  return dydt;
}
```

# Differential Equation Solver

- Solution via functional, given initial state ( $y_0$ ), initial time ( $t_0$ ), desired solution times ( $t_s$ )

```
mu_y <- 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 with biomass input and breakdown

# 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:  $y \sim \text{normal}(\mu, \sigma)$ ;
- 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)



**Questions?**