Stan:

a Probabilistic Programming Language

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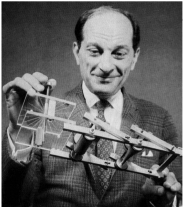
Stan’s Namesake

- 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

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 **explict use of probability for quantifying uncertainty** in inferences based on statistical analysis."

Gelman et al., *Bayesian Data Analysis*, 3rd edition, 2013

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 caclulate posterior probability of unobserved quantities (e.g., parameters, predictions, missing data)
- **Evaluate**
  - model fit and implications of posterior
- **Repeat** as necessary

Ibid.

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 reasoable 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[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
  - θ: 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 θ fixed (prob function)
  - Likelihood is function of θ 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

$$
\begin{aligned}
p(\theta|y) &= \frac{p(y,\theta)}{p(y)} && \text{[def of conditional]} \\
&= \frac{p(y|\theta)\,p(\theta)}{p(y)} && \text{[chain rule]} \\
&= \frac{p(y|\theta)\,p(\theta)}{\int_\Theta p(y,\theta')\,d\theta'} && \text{[law of total prob]} \\
&= \frac{p(y|\theta)\,p(\theta)}{\int_\Theta p(y|\theta')\,p(\theta')\,d\theta'} && \text{[chain rule]}
\end{aligned}
$$

- *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 θ out of posterior and likelihood

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

- 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.

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

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

- 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)

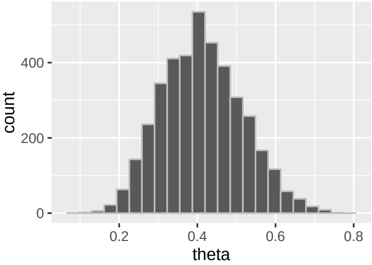
```
> mean(theta_draws);
[1] 0.4128373
```

- 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

	sinister	*dexter*	TOTAL
male	9 (y_1)	43	52 (N_1)
female	4 (y_2)	44	48 (N_2)

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

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

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];
}
```

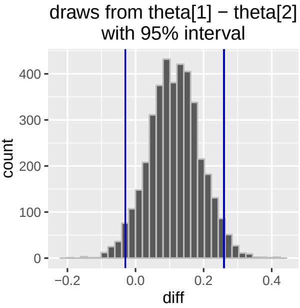
Results

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

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

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: $p(\tilde{y}|\theta)$

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

- 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, opthalmology, 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

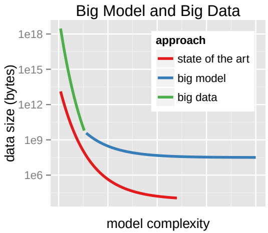
Model Sets Translated to Stan

- 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



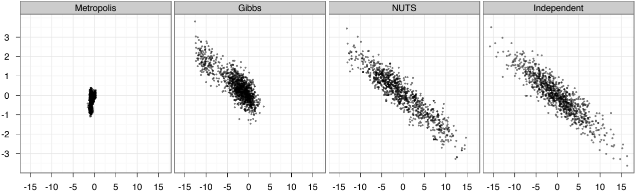
- Types of Scaling: data, parameters, **models**

- Time to converge and per effective sample size:

  0.5–∞ 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, $\log |\frac{d}{dy} \exp(y)| = y$
- 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 evalue 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

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	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 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, lamda));`
- * 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 (θ), 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 (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

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 differentation
- Consider: `y ~ 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?