# Stan:
## Probabilistic Modeling & Bayesian Inference


### Development Team

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Stan 2.17 (November 2017) `http://mc-stan.org`

# StanCon 2018

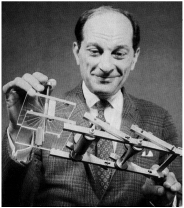
- 10–12 January 2018
- Asilomar (Pacific Grove, CA — 2 hrs south of SFO)
- Early registration still available
- Tutorials by Stan developers at all levels
- 6 keynotes from science and business
- Breakout “unconference” sessions

- http://mc-stan.org/events/stancon2018/

# What is Stan?

# Who is Stan?

- Named in honor of **Stanislaw Ulam** (1909–1984)
- Co-inventor of the **Monte Carlo method**



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

image from G. C. Geisler (2000) Los Alamos report LA-UR-2532

# 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

# Why Choose Stan?

- **Expressive**
  - Stan is a full imperative programming language
  - continuously differentiable log densities
- **Robust**
  - usually works; signals when it doesn't
- **Efficient**
  - effective sample size / time (i.e., information)
  - multi-core and GPU code complete on branches
- **Ongoing open source development**
- **Community support!**

# Intro
# Probability

# Probability is Epistemic

- **John Stuart Mill** (*Logic* 1882, Part III, Ch. 2):
  - ... the probability of an event is not a quality of the event itself, but a mere name for the degree of ground which we, or some one else, have for expecting it.
  - Every event is **in itself certain**, not probable; if we knew all, we should either know positively that it will happen, or positively that it will not.
  - ... its probability to us means the **degree of expectation of its occurrence**, which we are warranted in entertaining by our present evidence.
- Probabilities **quantify uncertainty**
- Statistical reasoning is **counterfactual**

# Random Variables

- Random variables are the currency of probability theory
- Random variables typically take numbers as values
- Imagine a bin filled with balls represneting the way the world might be
- A ball records the value of every random variable
- Examples
  - the sum of the three best among a roll of four dice (d6)
  - time before the next traffic accident on a given highway
  - prevalence of a disease in a population

# 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.*

# Properties of 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

# 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)

# 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

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

- *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 $\theta$ 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

# Posterior Event Probabilities

- Recall that an event $A$ is a collection of outcomes
- So $A$ may be defined by an indicator $f$ on parameters

$$f(\theta) = \begin{cases} 1 & \text{if } \theta \in A \\ 0 & \text{if } \theta \notin A \end{cases}$$

  - $f(\theta) = \mathrm{I}(\theta_1 > \theta_2)$ for $\Pr[\theta_1 > \theta_2 \mid y]$,
  - $f(\theta) = \mathrm{I}(\theta \in (0.50, 0.52)$ for $\Pr[\theta \in (0.50, 0.52) \mid y]$

- Defined by posterior expectation of indicator $f(\theta)$

$$\Pr[A \mid y] \;=\; \mathbb{E}[f(\theta) \mid y] \;=\; \int_{\Theta} f(\theta)\, p(\theta|y)\, d\theta.$$

# Repeated Binary Trials

# Repeated Binary Trial Model

- **Data**
  - $N \in \{0, 1, \ldots\}$: number of trials (constant)
  - $y_n \in \{0, 1\}$: trial $n$ success (known, modeled data)
- **Parameter**
  - $\theta \in [0, 1]$ : chance of success (unknown)
- **Prior**
  - $p(\theta) \;=\; \text{Uniform}(\theta \mid 0, 1) = 1$
- **Likelihood**
  - $p(y \mid \theta) \;=\; \prod_{n=1}^{N} \text{Bernoulli}(y_n \mid \theta) \;=\; \prod_{n=1}^{N} \theta^{y_n} \, (1 - \theta)^{1-y_n}$
- **Posterior**
  - $p(\theta \mid y) \propto p(\theta) \, p(y \mid \theta)$

# 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
  y ~ bernoulli(theta);               // likelihood
}
```

# A Stan Program...

- defines log (posterior) density up to constant, so...
- equivalent to define log density directly:

```
model {
  target += 0;
  for (n in 1:N)
    target += log(y[n] ? theta : (1 - theta));
}
```

- equivalent to drop constant prior and 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: Bayesian Posterior

```
> 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
```

# RStan: Posterior Sample

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

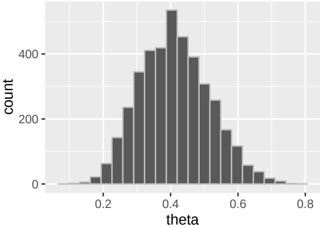
[1] 0.4128373

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

      10%       90%
0.2830349 0.5496858
```

# Marginal Posterior Histograms

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




- Displays the full posterior *marginal* distribution $p(\theta \mid y)$

# RStan: MAP, penalized MLE

- Stan's optimization for estimation; two views:
  - max posterior mode, aka max a posteriori (MAP)
  - max penalized likelihood (MLE)

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

# Plug in Posterior Draws

- Extracting the posterior draws

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

- Calculating posterior mean (estimator)

```
> mean(theta_draws);

[1] 0.4128373
```

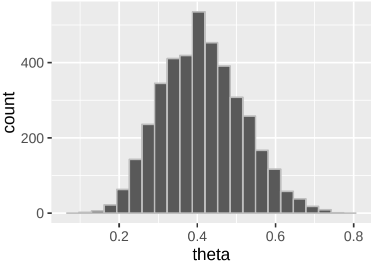
- Calculating posterior intervals

```
> 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;
```



# 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);
```

## Real Example

# Male Birth Ratio

# Birth Rate by Sex

- **Laplace**'s data on live births in Paris from 1745–1770:

| *sex* | *live births* |
|---|---|
| female | 241 945 |
| male | 251 527 |

- **Question 1** (Estimation)
  What is the birth rate of boys vs. girls?
- **Question 2** (Event Probability)
  Is a boy more likely to be born than a girl?
- Bayes (1763) set up the "Bayesian" model
- Laplace (1781, 1786) solved for the posterior

# Bayes's Binomial Model

- Data
  - $y$: total number of male live births (251,527)
  - $N$ : total number of live births (493,472)
- Parameter
  - $\theta \in (0,1)$: proportion of male live births
- Likelihood

$$p(y|N,\theta) \;=\; \text{Binomial}(y|N,\theta) \;=\; \binom{N}{y}\theta^{y}(1-\theta)^{N-y}$$

- Prior

$$p(\theta) \;=\; \text{Uniform}(\theta \mid 0,1) \;=\; 1$$

# Calculating Laplace's Answers

```
transformed data {
  int male = 251527;
  int female = 241945;
}
parameters {
  real<lower=0, upper=1> theta;
}
model {
  male ~ binomial(male + female, theta);
}
generated quantities {
  int<lower=0, upper=1> theta_gt_half = (theta > 0.5);
}
```

# And the Answer is...

```
> fit <- stan("laplace.stan", iter=100000);
> print(fit, probs=c(0.005, 0.995), digits=3)

                    mean    0.5%   99.5%
theta               0.51   0.508   0.512
theta_gt_half       1.00   1.000   1.000
```

- Q1: $\theta$ is 99% certain to lie in $(0.508, 0.512)$
- Q2: Laplace "morally certain" boys more prevalent

## Example 2

# A-B Testing

# 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];
}
```

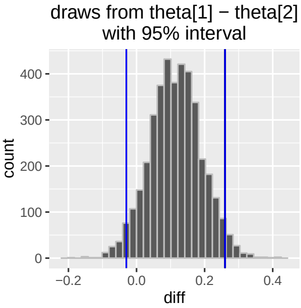
# Binomial Comparison Results

| | 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 |

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

# Visualizing Posterior Difference

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




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

# 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
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- 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++11)
- **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)
  - **MathematicaStan**: Stata interface (external process)

# Higher-Level Interfaces

- **R Interfaces**
  - **RStanArm**: regression modeling with R expressions
  - **ShinyStan**: web-based posterior visualization, exploration
  - **Loo**: approximate leave-one-out cross-validation
- **Jupyter Containers**
  - **Docker** versions for R, Python, Julia
  - **SageMath**: free online server (R)
- From others
  - **Prohet** (Facebook): time-series analysis (R and Python)
  - **brms** (Bürkner): regression modeling with R expressions

- **rethinking** (McElreath): simplified Stan embedded in R

# Who's Using Stan?

- 2500+ **users group** registrations; 20,000+ **downloads** (per version just in Rstudio); 1000+ Google scholar citations
- **Biological sciences**: clinical drug trials, entomology, pharmacology, toxicology, botany, neurology, genomics, agriculture, botany, fisheries, genomics, cellular biology, epidemiology, population ecology, neurology
- **Physical sciences**: astrophysics, particle physics, molecular biology, oceanography, climatology, biogeochemistry, materials science
- **Social sciences**: econometrics (macro and micro), population dynamics, cognitive science, psycholinguistics, social networks, political science, survey sampling

- **Other**: materials engineering, finance, actuarial science, sports, public health, recommender systems, educational testing, fleet maintenance, sports

# Documentation

- *Stan User's Guide and Reference Manual*
  - 600+ 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, MathematicaStan
- Many written and video tutorials by users and developers

# 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*.
- Kruschke (2014) *Doing Bayesian Data Analysis*.

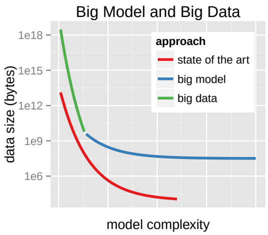
# Books about Stan

- Gelman and Hill (2018) *Regression and Other Stories*. Cambridge.
- Hilbe, de Souza, and Ishida (2017) *Bayesian Models for Astrophysical Data Using R, JAGS, Python, and Stan*. Cambridge.
- Matsuura (2016) *Bayesian Statistical Modeling Using Stan and R*. Kyoritsu. (Japanese)
- Faraway (2016) *Extending the Linear Model with R: Generalized Linear, Mixed Effects and Nonparametric Regression Models*, 2nd Edition. CRC.
- McElreath (2016) *Statistical Rethinking: A Bayesian course with R and Stan*. CRC.
- Korner-Nievergelt et al. (2015) *Bayesian Data Analysis in Ecology Using Linear Models with R, BUGS, and Stan*. Academic Press.

- Kruschke (2014) *Doing Bayesian Data Analysis, Second Edition: A Tutorial with R, JAGS, and Stan*. Academic Press.

- Gelman et al. (2013) *Bayesian Data Analysis*, 3rd Edition. CRC.

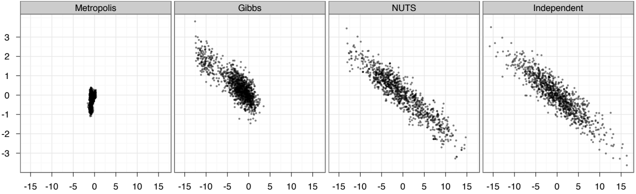
# Scaling and Evaluation




- 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

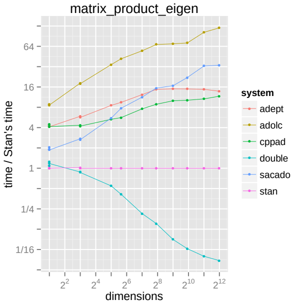
# NUTS vs. Gibbs and Metropolis

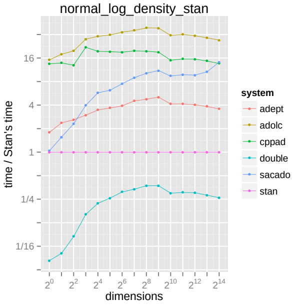



- Two dimensions of highly correlated 250-dim normal
- **1,000,000 draws** from Metropolis and Gibbs (thin to 1000)
- **1000 draws** from NUTS; 1000 independent draws

# Stan's Autodiff vs. Alternatives

- Among **C++ open-source** offerings: Stan is **fastest** (for gradients), **most general** (functions supported), and **most easily extensible** (simple OO)



# 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
- **`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

# 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. 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
- 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 |

# Assignment Operators

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

- these work with all relevant matrix types
  - e.g., `matrix *= matrix;`

# 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);`
- **Break, Continue**: `break`, `continue`

# "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));
  }

}
```

# 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 `_lp`

# 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 (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 $\theta$

```
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 $\theta$
- Couple derivatives of system w.r.t. parameters

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

- 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 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)

# 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
  - **Multinomial**: draw along trajectory
- 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)

# Animation

- animated GIFs (easy to produce!)

# Why HMC?

- Gibbs and Metropolis are both random walk **diffusions**
  - $\mathcal{O}(N^2)$ in $N$ dimensions to move across posterior
  - constant factor increases with correlation
- HMC uses gradient information of log posterior
  - gradient defines vector field along which trajectory **flows**
- Eliminates random walk behavior
  - $\mathcal{O}(N^{5/4})$
  - **lower constant factor** because less sensitive to correlation

# 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 + autdiff
- 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)

# What's Next

- Distributed likelihoods: **multi-core** (MPI)
- Big matrix operations: **GPU** (OpenCL)
- Streaming data:  myemphstochastic variational inference
- Distributed data: "black box" **expectation propagation**
- Approximations, visualizations, posterior analysis tools
- **Coursera** specialization (Bob Carpenter & Andrew Gelman) mid-2018

# StanCon 2018

- 10–12 January 2018
- Asilomar (Pacific Grove, CA — 2 hrs south of SFO)
- Early registration still available
- Tutorials by Stan developers at all levels
- 6 keynotes from science and business
- Breakout “unconference” sessions

- http://mc-stan.org/events/stancon2018/