Stan

Probabilistic Programming Language

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Stan 2.7.0 (July 2015) http://mc-stan.org

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 numerical stability
- *Solutions*: Taylor expansions, e.g., `log1p()`
  compound functions, e.g., `log_sum_exp()`, `BernoulliLogit()`
  limits at boundaries, e.g., `multiply_log()`

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
  - Black-Box VB for approximate Bayes
  - MLE for penalized maximum likelihood estimation

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?

- 1200 **users group** registrations; 10,000 manual **downloads** (2.5.0); 100+ published papers
- **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

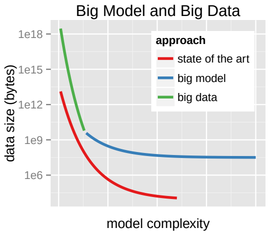
Documentation

- *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, StataStan
  - RStan vignette

Books and Model Sets

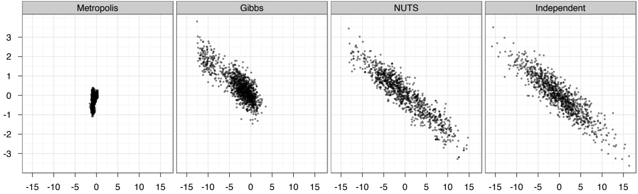
- **Model Sets** Translated to Stan
  - BUGS and JAGS examples (most of all 3 volumes)
  - Gelman and Hill (2009) *Data Analysis Using Regression and Multilevel/Hierarchical Models*
  - Wagenmakers and Lee (2014) *Bayesian Cognitive Modeling*
- **Books** with Sections on Stan
  - Gelman et al. (2013) *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: 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

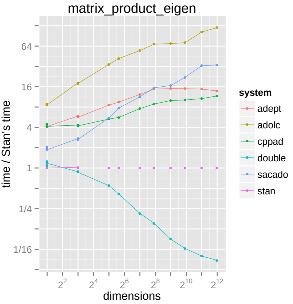
NUTS vs. Gibbs and Metropolis

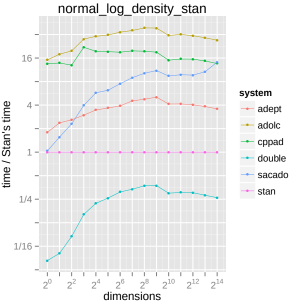


- Two dimensions of highly correlated 250-dim normal
- **1,000,000 draws** from Metropolis and Gibbs (thin to 1000)
- **1000 draws** from NUTS; 1000 independent draws

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)





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

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

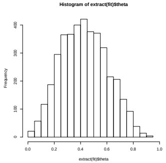
Bayesian Posterior

```
> 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
lp__   -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] ~ 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> y[N];
}
parameters {
  vector[K] beta;
}
model {
   beta ~ cauchy(0, 2.5);          // prior
   y ~ 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)
    ~ 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 θ, 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);
}
```

- 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 (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);
}
```

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

```
for (n in 1:N) {
  real lp1;  real lp2;

  lp1 <- bernoulli_log(0, lambda)
           + normal_log(y[n], mu[1], sigma[1]);

  lp2 <- bernoulli_log(1, lambda)
           + normal_log(y[n], mu[2], sigma[2]);

  increment_log_prob(log_sum_exp(lp1,lp2));
```

- local variables reassigned; direct increment of log posterior
- $\mathrm{log\_sum\_exp}(\alpha, \beta) = \log(\exp(\alpha) + \exp(\beta))$
- **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 Ω
- $\text{LKJCorr}(\Omega \mid \nu) \propto \det(\Omega)^{(\nu-1)}$
  - $\nu = 1$ uniform
  - $\nu > 1$ concentrates around unit matrix
- Work with Cholesky factor L_Ω s.t. $\Omega = L_\Omega L_\Omega^\top$
  - Density: $\text{LKJCorrCholesky}(L_\Omega \mid \nu) \propto |J| \det(L_\Omega L_\Omega^\top)^{(\nu-1)}$
  - Jacobian adjustment for Cholesky factorization

Lewandowski, Kurowicka, and Joe (2009)

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]]);
```

- 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

```
functions {
  real[] sho(real t, real[] y, real[] theta,
             real[] x_r, int[] x_i) {
    real dydt[2];
    dydt[1] <- y[2];
    dydt[2] <- -y[1] - theta[1] * y[2];
    return dydt;
  }
}
```

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);
  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
- **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)

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]`
- **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)

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
- **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 (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

Diff Eq Derivatives

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

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

- Calculate coupled system via nested autodiff of second term

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

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`;
- **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

- Forward-mode auto-diff for all 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 (*JRSS, 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” EP

- Fast, approximate inference (like VB)
  - VB and EP minimize divergence in opposite directions
  - especially useful for Gaussian processes
- Asynchronous, data-parallel **expectation propagation** (EP)
- Cavity distributions control subsample variance
- Prototypte stage
- collaborating with Seth Flaxman, Aki Vehtari, Pasi Jylänki, John Cunningham, Nicholas Chopin, Christian Robert

The End

Questions from Chad Scherer

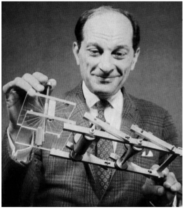
1. What were the **best design decisions** you made?
   - Anything you would do **differently**?
2. What new capability would most **change** the way probabilistic programming **is used**?
3. Any thoughts on characterizing some portion of the **design space** of probabilistic programming?
4. Any experience, ideas, or caveats on **“democratizing”** this kind of modeling?

Answers

- Best: define log density not graphical model, use C++
- Worst: use C++, define log density not graphical model
- Design: Stan programs use “random” variables, but only to define density and predictions imperatively (no metaprogramming, lacks modularity)
- Democratizing: remove the programming — scientists and statisticians want statistical/computational robustness, not a programming challenge
- New capabilities: Riemannian and adiabatic HMC for hard problems; VB, EP, and MML for fast approximation

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