Stan

a Probabilistic Programming Language

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Stan

Get the Slides

`http://mc-stan.org/workshops/ness2016`

Example I

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

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**
  - $p(y \mid \theta) \; = \; \prod_{n=1}^{N} \text{Bernoulli}(y_n \mid \theta) \; = \; \prod_{n=1}^{N} \theta^{y_n} \, (1 - \theta)^{1 - y_n}$

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])));
}
```

- Equivalent to (a) drop constant prior, (b) vectorize likelihood:

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

Simulating Repeated Binary Trials

- R Code: `rbinom(10, N, 0.3)`
  - **N = 10** trials (10% to 50% success rate)

    2 2 1 3 3 2 3 2 2 5
  - **N = 100** trials (27% to 34% success rate)

    29 34 27 31 25 31 27 29 32 26
  - **N = 1000** trials (29% to 32% success rate)

    291 297 289 322 305 296 294 297 314 292
  - **N = 10,000** trials (29.5% to 30.7% success rate)

    3014 3031 3017 2886 2995 2944 3067 3069 3051 3068
- Deviation goes down at rate: $\mathcal{O}(1/\sqrt{N})$

R: Simulate 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

> 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));
```

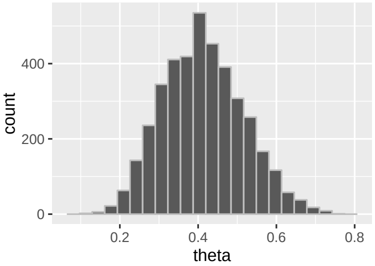
```
Inference for Stan model: bern.
4 chains, each with iter=2000; warmup=1000; thin=1;
post-warmup draws per chain=1000,
total post-warmup draws=4000.

        mean se_mean   sd    10%    90% n_eff Rhat
theta   0.41    0.00 0.10   0.28   0.55  1580    1
lp__  -15.40    0.02 0.71 -16.26 -14.89  1557    1

Samples drawn using NUTS(diag_e) at Thu Apr 21 19:38:16 2016.
```

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
```

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;
```



Binomial Distribution

- Don't know order of births, only total.
- If $y_1, \ldots, y_N \sim \text{Bernoulli}(\theta)$,

  then $(y_1 + \cdots + y_N) \sim \text{Binomial}(N, \theta)$
- The analytic form is

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

  where the binomial coefficient normalizes for permutations (i.e., which subset of n has $y_n = 1$),

$$\binom{N}{y} = \frac{N!}{y!\,(N-y)!}$$

Calculating Laplace’s Answers

```
transformed data {
  int male;
  int female;
  male <- 251527;
  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_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: θ is 99% certain to lie in $(0.508, 0.512)$
- Q2: Laplace "morally certain" boys more prevalent

Parameter Estimates

- Estimate **probability** that a parameter value in interval, e.g.,

$$\Pr[\theta \in (0.508, 0.512) \mid y]$$

- Conditions on observed data y

- **Bayesian parameter estimates are probabilistic**

Event Probabilities

- Random variable defined by **indicator** function

```
theta_gt_half <- (theta > 0.5);
```

- Indicators are random variables
  - with boolean (0 or 1) values
  - defined in terms of parameters (and data)
- For Laplace’s problem, calculus shows

$$\Pr[\theta \leq 0.5 \mid y] \approx 10^{-42}$$

- **Event probabilities are expectations of indicators**

Part I
Bayesian Inference

Observations, Counterfactuals, and Random Variables

- Assume we observe data $y = y_1, \ldots, y_N$
- Statistical modeling assumes even though y is observed, the values could have been different
- John Stuart Mill first characterized this **counterfactual** nature of statistical modeling in:

  A System of Logic, Ratiocinative and Inductive (1843)
- In measure-theoretic language, y modeled as a **random variable**

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
  - 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, . . .
- 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

(Donald) Rubin’s Philosophy

- All statistics is inference about missing data
- Question 1: What would you do if you had all the data?
- Question 2: What were you doing before you had any data?

(as relayed in course notes by Andrew Gelman)

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

- Finds parameters consistent with prior info and data*
    - * if such agreement is possible
- Automatically includes uncertainty and variability
- Inferences can be plugged in directly
    - risk assesment
    - decision analysis

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 out parameters from posterior

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

- Averages predictions $p(\tilde{y}|\theta)$, weight by posterior $p(\theta|y)$
  - $\Theta = \{\theta \mid p(\theta|y) > 0\}$ is support of $p(\theta|y)$
- Allows continuous, discrete, or mixed parameters
  - integral notation shorthand for sums and/or integrals

Event Probabilities

- Recall that an event A is a collection of outcomes
- Suppose event A is determined by indicator on parameters

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

- e.g., $f(\theta) = \mathrm{I}(\theta_1 > \theta_2)$ for $\Pr[\theta_1 > \theta_2 \mid y]$
- Bayesian event probabilities calculate posterior mass

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

- Not frequentist, because involves parameter probabilities

Detour: Beta Distribution

- For parameters $\alpha, \beta > 0$ and $\theta \in (0, 1)$,

$$\text{Beta}(\theta|\alpha, \beta) \;\propto\; \theta^{\alpha-1}\,(1-\theta)^{\beta-1}$$

- Euler's Beta function is used to normalize,

$$\text{B}(\alpha, \beta) \;=\; \int_0^1 u^{\alpha-1}(1-u)^{\beta-1}du \;=\; \frac{\Gamma(\alpha)\,\Gamma(\beta)}{\Gamma(\alpha+\beta)}$$

  so that

$$\text{Beta}(\theta|\alpha, \beta) \;=\; \frac{1}{\text{B}(\alpha, \beta)}\,\theta^{\alpha-1}\,(1-\theta)^{\beta-1}$$

- Note: $\text{Beta}(\theta|1, 1) = \text{Uniform}(\theta|0, 1)$

- Note: $\Gamma()$ is continuous generalization of factorial

Laplace Turns the Crank

- From Bayes's rule, the posterior is

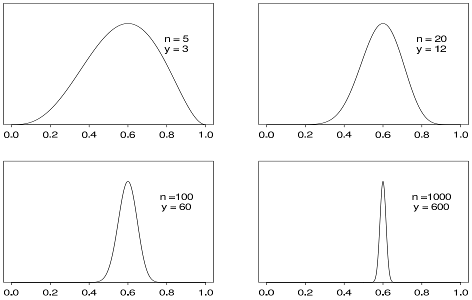
$$p(\theta|y, N) \;=\; \frac{\textsf{Binomial}(y|N, \theta)\,\textsf{Uniform}(\theta|0, 1)}{\int_{\Theta} \textsf{Binomial}(y|N, \theta')\, p(\theta')\; d\theta'}$$

- Laplace calculated the posterior analytically

$$p(\theta|y, N) \;=\; \textsf{Beta}(\theta \mid y + 1,\; N - y + 1).$$

Beta Distribution — Examples

- Unnormalized posterior density assuming uniform prior and y successes out of n trials (all with mean 0.6).



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

Estimation

- Posterior is Beta$(\theta \mid 1 + 241\,945,\ 1 + 251\,527)$
- Posterior mean:

$$\frac{1 + 241\,945}{1 + 241\,945 + 1 + 251\,527} \approx 0.490291\mathbf{3}$$

- Maximum likelihood estimate same as posterior mode (because of uniform prior)

$$\frac{241\,945}{241\,945 + 251\,527} \approx 0.490291\mathbf{2}$$

- As number of observations approaches ∞,
  MLE approaches posterior mean

Event Probability Inference

- What is probability that a male live birth is more likely than a female live birth?

$$\begin{aligned}
\Pr[\theta > 0.5] &= \int_{\Theta} \mathrm{I}[\theta > 0.5]\, p(\theta|y,N) d\theta \\
&= \int_{0.5}^{1} p(\theta|y,N) d\theta \\
&= 1 - F_{\theta|y,N}(0.5) \\
&\approx 10^{-42}
\end{aligned}$$

- $\mathrm{I}[\phi] = 1$ if condition ϕ is true and 0 otherwise.
- $F_{\theta|y,N}$ is posterior cumulative distribution function (cdf).

Mathematics vs. Simulation

- Luckily, we don't have to be as good at math as Laplace
- Nowadays, we calculate all these integrals by computer using tools like Stan

> If you wanted to do foundational research in statistics in the mid-twentieth century, you had to be bit of a mathematician, whether you wanted to or not. . . . if you want to do statistical research at the turn of the twenty-first century, you have to be a computer programmer.
>
> —from Andrew's blog

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?

$$\begin{aligned}\Pr[\theta_1 > \theta_2 \mid y, N] &= \int_{\Theta} \mathrm{I}[\theta_1 > \theta_2]\, p(\theta|y, N)\, d\theta \\ &\approx 0.91\end{aligned}$$

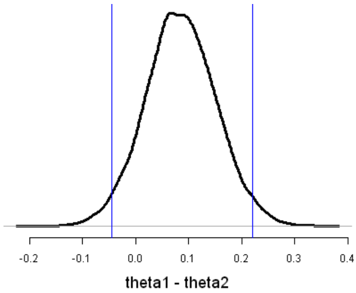
- Directly interpretable result; *not* a frequentist procedure

Stan Binomial Comparison

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

Visualizing Posterior Difference

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



- Vertical bars: central 95% posterior interval $(-0.05, 0.22)$

Technical Interlude
Conjugate Priors

Conjugate Priors

- Family $\mathcal{F}$ is a conjugate prior for family $\mathcal{G}$ if
  - prior in $\mathcal{F}$ and
  - likelihood in $\mathcal{G}$,
  - entails posterior in $\mathcal{F}$
- Before MCMC techniques became practical, Bayesian analysis mostly involved conjugate priors
- Still widely used because analytic solutions are more efficient than MCMC

Beta is Conjugate to Binomial

- Prior: $p(\theta|\alpha,\beta) = \text{Beta}(\theta|\alpha,\beta)$
- Likelihood: $p(y|N,\theta) = \text{Binomial}(y|N,\theta)$
- Posterior:

$$
\begin{aligned}
p(\theta|y,N,\alpha,\beta) &\propto p(\theta|\alpha,\beta)\, p(y|N,\theta) \\
&= \text{Beta}(\theta|\alpha,\beta)\, \text{Binomial}(y|N,\theta) \\
&= \frac{1}{\text{B}(\alpha,\beta)}\theta^{\alpha-1}\,(1-\theta)^{\beta-1}\;\binom{N}{y}\theta^{y}\,(1-\theta)^{N-y} \\
&\propto \theta^{y+\alpha-1}\,(1-\theta)^{N-y+\beta-1} \\
&\propto \text{Beta}(\theta|\alpha+y,\;\beta+(N-y))
\end{aligned}
$$

Chaining Updates

- Start with prior Beta$(\theta|\alpha, \beta)$
- Receive binomial data in K statges $(y_1, N_1), \ldots, (y_K, N_K)$
- After (y_1, N_1), posterior is Beta$(\theta|\alpha + y_1,\ \beta + N_1 - y_1)$
- Use as prior for (y_2, N_2), with posterior
  Beta$(\theta|\alpha + y_1 + y_2,\ \ \beta + (N_1 - y_1) + (N_2 - y_2))$
- Lather, rinse, repeat, until final posterior
  Beta$(\theta|\alpha + y_1 + \cdots + y_K,\ \ \beta + (N_1 + \cdots + N_K) - (y_1 + \cdots + y_K))$
- Same result as if we'd updated with combined data
  Beta$(y_1 + \cdots + y_K,\ \ N_1 + \cdots + N_K)$

Part II

(Un-)Bayesian Point Estimation

MAP Estimator

- For a Bayesian model $p(y, \theta) = p(y|\theta)\, p(\theta)$, the max a posteriori (MAP) estimate maximizes the posterior,

$$\begin{aligned}
\theta^* &= \text{arg max}_\theta \; p(\theta|y) \\
&= \text{arg max}_\theta \; \frac{p(y|\theta)p(\theta)}{p(y)} \\
&= \text{arg max}_\theta \; p(y|\theta)p(\theta). \\
&= \text{arg max}_\theta \; \log p(y|\theta) + \log p(\theta).
\end{aligned}$$

- *not* Bayesian because it doesn't integrate over uncertainty
- *not* frequentist because of distributions over parameters

MAP and the MLE

- MAP estimate reduces to the MLE if the prior is uniform, i.e.,

  $$p(\theta) = c$$

  because

  $$\begin{aligned} \theta^* &= \arg\max_\theta \, p(y|\theta)\, p(\theta) \\ &= \arg\max_\theta \, p(y|\theta)\, c \\ &= \arg\max_\theta \, p(y|\theta). \end{aligned}$$

Penalized Maximum Likelihood

- The MAP estimate can be made palatable to frequentists via philosophical sleight of hand
- Treat the negative log prior $-\log p(\theta)$ as a "penalty"
- e.g., a Normal$(\theta|\mu,\sigma)$ prior becomes a penalty function

$$\lambda_{\theta,\mu,\sigma} \; = \; -\left(\log\sigma + \frac{1}{2}\left(\frac{\theta-\mu}{\sigma}\right)^2\right)$$

- Maximize sum of log likelihood and negative penalty

$$\begin{aligned}\theta^* &= \text{arg max}_\theta \; \log p(y|\theta,x) - \lambda_{\theta,\mu,\sigma} \\ &= \text{arg max}_\theta \; \log p(y|\theta,x) + \log p(\theta|\mu,\sigma)\end{aligned}$$

Proper Bayesian Point Estimates

- Choose estimate to minimize some loss function
- To minimize expected squared error (L2 loss), $\mathbb{E}[(\theta - \theta')^2 \mid y]$, use the posterior mean

$$\hat{\theta} \;=\; \text{arg min}_{\theta'} \mathbb{E}[(\theta - \theta')^2 \mid y] \;=\; \int_{\Theta} \theta \times p(\theta|y)\, d\theta.$$

- To minimize expected absolute error (L1 loss), $\mathbb{E}[|\theta - \theta'|]$, use the posterior median.
- Other loss (utility) functions possible, the study of which falls under decision theory
- All share property of involving full Bayesian inference.

Point Estimates for Inference?

- Common in machine learning to generate a point estimate θ^*, then use it for inference, $p(\tilde{y}|\theta^*)$

- This is **defective** because it

  underestimates uncertainty.

- To properly estimate uncertainty, apply full Bayes

- A major focus of statistics and decision theory is estimating uncertainty in our inferences

Philosophical Interlude

What is Statistics?

Exchangeability

- Roughly, an exchangeable probability function is such that for a sequence of random variables $y = y_1, \ldots, y_N$,

  $$p(y) = p(\pi(y))$$

  for every N-permutation π (i.e, a one-to-one mapping of $\{1, \ldots, N\}$)

- i.i.d. implies exchangeability, but not vice-versa

Exchangeability Assumptions

- Models almost always make some kind of exchangeability assumption
- Typically when other knowledge is not available
  - e.g., treat voters as conditionally i.i.d. given their age, sex, income, education level, religous affiliation, and state of residence
  - But voters have many more properties (hair color, height, profession, employment status, marital status, car ownership, gun ownership, etc.)
  - Missing predictors introduce additional error (on top of measurement error)

Random Parameters: Doxastic or Epistemic?

- Bayesians treat distributions over parameters as epistemic (i.e., about knowledge)
- They do *not* treat them as being doxastic (i.e., about beliefs)
- Priors encode our knowledge before seeing the data
- Posteriors encode our knowledge after seeing the data
- Bayes’s rule provides the way to update our knowledge
- People like to pretend models are ontological (i.e., about what exists)

Arbitrariness: Priors vs. Likelihood

- Bayesian analyses often criticized as subjective (arbitrary)
- Choosing priors is no more arbitrary than choosing a likelihood function (or an exchangeability/i.i.d. assumption)
- As George Box famously wrote (1987),

"All models are wrong, but some are useful."

- This does not just apply to Bayesian models!

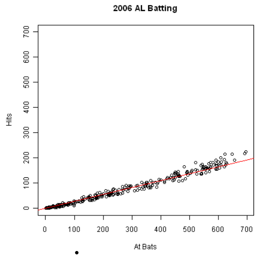
Part III
Hierarchical Models

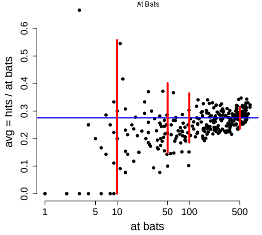
Baseball At-Bats

- For example, consider baseball batting ability.
  - Baseball is sort of like cricket, but with round bats, a one-way field, stationary "bowlers", four bases, short games, and no draws
- Batters have a number of "at-bats" in a season, out of which they get a number of "hits" (hits are a good thing)
- Nobody with higher than 40% success rate since 1950s.
- No player (excluding "bowlers") bats much less than 20%.
- Same approach applies to hospital pediatric surgery complications (a BUGS example), reviews on Yelp, test scores in multiple classrooms, . . .

Baseball Data

- Hits versus at bats for the 2006 American League season
- Not much variation in ability!
- Ignore skill vs. at-bats relation
- Note uncertainty of MLE





Pooling Data

- How do we estimate the ability of a player who we observe getting 6 hits in 10 at-bats? Or 0 hits in 5 at-bats? Estimates of 60% or 0% are absurd!
- Same logic applies to players with 152 hits in 537 at bats.
- *No pooling*: estimate each player separately
- *Complete pooling*: estimate all players together (assume no difference in abilities)
- *Partial pooling*: somewhere in the middle
  - use information about other players (i.e., the population) to estimate a player's ability

Hierarchical Models

- Hierarchical models are principled way of determining how much pooling to apply.
- Pull estimates toward the population mean based on amount of variation in population
  - low variance population: more pooling
  - high variance population: less pooling
- In limit
  - as variance goes to 0, get complete pooling
  - as variance goes to ∞, get no pooling

Hierarchical Batting Ability

- Instead of fixed priors, estimate priors along with other parameters
- Still only uses data once for a single model fit
- Data: y_n, B_n: hits, at-bats for player n
- Parameters: θ_n: ability for player n
- Hyperparameters: α, β: population mean and variance
- Hyperpriors: fixed priors on α and β (hardcoded)

Hierarchical Batting Model (cont.)

$$\begin{aligned}
y_n &\sim \text{Binomial}(B_n, \theta_n) \\
\theta_n &\sim \text{Beta}(\alpha, \beta) \\
\frac{\alpha}{\alpha + \beta} &\sim \text{Uniform}(0, 1) \\
(\alpha + \beta) &\sim \text{Pareto}(1.5)
\end{aligned}$$

- Sampling notation syntactic sugar for:

  $p(y, \theta, \alpha, \beta) = \text{Pareto}(\alpha+\beta|1.5) \prod_{n=1}^{N} \left(\text{Binomial}(y_n|B_n, \theta_n)\ \text{Beta}(\theta_n|\alpha, \beta)\right)$

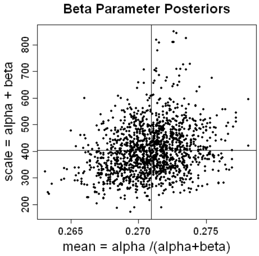
- Pareto provides power law: $\text{Pareto}(u|\alpha) \propto \frac{\alpha}{u^{\alpha+1}}$
- Should use more informative hyperpriors!

Stan Program

```
data {
  int<lower=0> N;                 // items
  int<lower=0> K[N];              // initial trials
  int<lower=0> y[N];              // initial successes
}
parameters {
  real<lower=0, upper=1> phi;          // population chance of suc
  real<lower=1> kappa;                 // population concentration
  vector<lower=0, upper=1>[N] theta;   // chance of success
}
model {
  kappa ~ pareto(1, 1.5);                          // hyperprior
  theta ~ beta(phi * kappa, (1 - phi) * kappa);    // prior
  y ~ binomial(K, theta);                          // likelihood
}
```

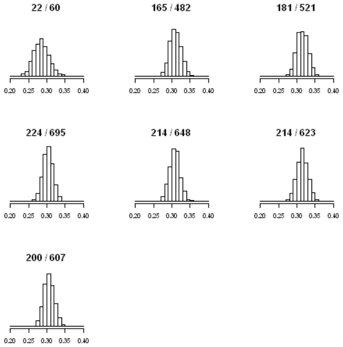
Hierarchical Prior Posterior

- Draws from posterior (crosshairs at posterior mean)
- Prior population mean: 0.271
- Prior population scale: 400
- Together yield prior std dev of 0.022
- Mean is better estimated than scale (typical)



Posterior Ability (High Avg Players)

- Histogram of posterior draws for high-average players
- Note uncertainty grows with lower at-bats



Multiple Comparisons

- Who has the highest ability (based on this data)?
- Probabilty player n is best is

Average	*At-Bats*	Pr[best]
.347	521	0.12
.343	623	0.11
.342	482	0.08
.330	648	0.04
.330	607	0.04
.367	60	0.02
.322	695	0.02

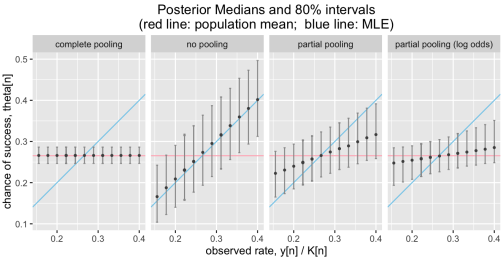
- No clear winner—sample size matters.
- In last game (of 162), Mauer (Minnesota) edged out Jeter (NY)

Efron & Morris (1975) Data

```
   FirstName   LastName Hits At.Bats Rest.At.Bats Rest.Hits
1    Roberto   Clemente   18      45          367       127
2      Frank   Robinson   17      45          426       127
3      Frank     Howard   16      45          521       144
4        Jay  Johnstone   15      45          275        61
5        Ken      Berry   14      45          418       114
6        Jim    Spencer   14      45          466       126
7        Don  Kessinger   13      45          586       155
8       Luis   Alvarado   12      45          138        29
9        Ron      Santo   11      45          510       137
10       Ron    Swaboda   11      45          200        46
11      Rico Petrocelli   10      45          538       142
```

Pooling Estimates

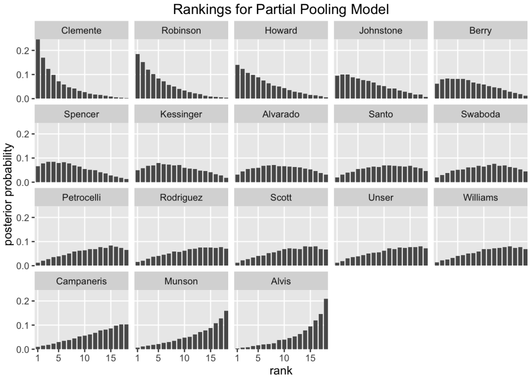
- Case Study: Repeated Binary Trials (mc-stan.org)



Ranking

```
generated quantities {
  int<lower=1, upper=N> rnk[N];      // rank of player n
  {
    int dsc[N];
    dsc <- sort_indices_desc(theta);
    for (n in 1:N)
      rnk[dsc[n]] <- n;
  }
```

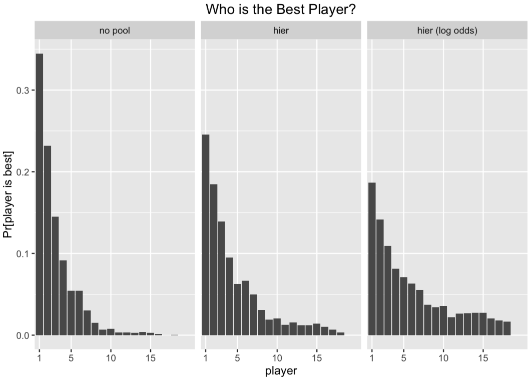
Posterior Ranks



Who is Best? Stan Code

```
generated quantities {
  ...
  int<lower=0, upper=1> is_best[N];  // Pr[player n highest chanc
  ...
  for (n in 1:N)
    is_best[n] <- (rnk[n] == 1);
  ...
```

Who is Best? Posterior

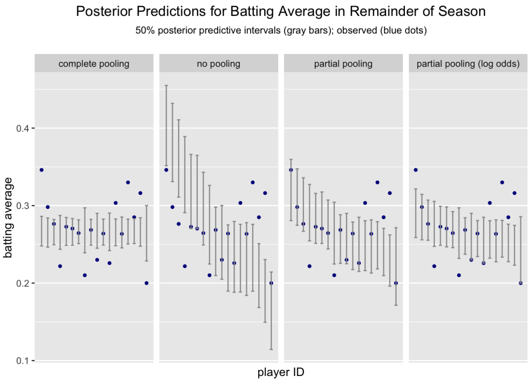


Posterior Predictive Inference

- How do we predict new outcomes (e.g., rest of season)?

```
data {
  int<lower=0> K_new[N];       // new trials
  int<lower=0> y_new[N];       // new successes
  ...
generated quantities {
  int<lower=0> z[N];  // posterior prediction
  for (n in 1:N)
    z[n] <- binomial_rng(K_new[n], theta[n]);
```

Posterior Predictions

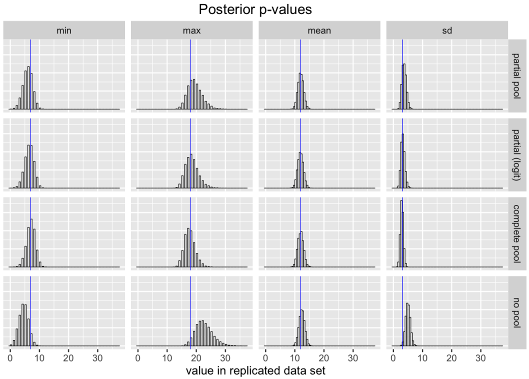


Posterior Predictive Check

- Replicate data from paraemters

```
generated quantities {
  ...
  for (n in 1:N)
    y_rep[n] <- binomial_rng(K[n], theta[n]);
  for (n in 1:N)
    y_pop_rep[n] <- binomial_rng(K[n],
                                 beta_rng(phi * kappa,
                                          (1 - phi) * kappa));
  min_y_rep <- min(y_rep);
  sd_y_rep <- sd(to_vector(y_rep));
  p_min <- (min_y_rep >= min_y);
  p_sd <- (sd_y_rep >= sd_y);
}
```

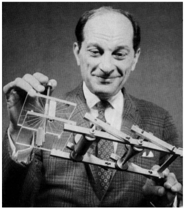
Posterior p-Values



Part IV
Stan Overview

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

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)
- **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

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?

- 1600+ **users group** registrations; 10,000 manual **downloads** (2.5.0); 300+ 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

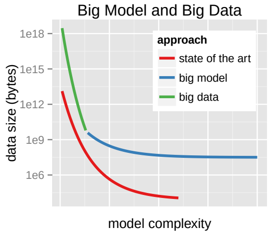
Documentation

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

Books and Model Sets

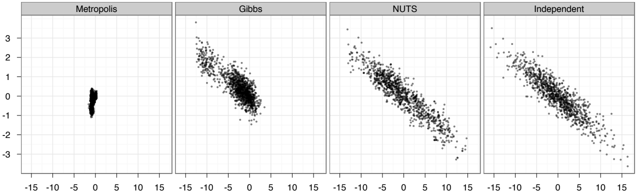
- **Model Sets** Translated to Stan
  - BUGS and JAGS examples (most of all 3 volumes)
  - Gelman and Hill (2009) *Data Analysis Using Regression and Multilevel/Hierarchical Models*
  - Wagenmakers and Lee (2014) *Bayesian Cognitive Modeling*
- **Books** with Sections on Stan
  - Gelman et al. (2013)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

Scaling and Evaluation



- Types of Scaling: 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

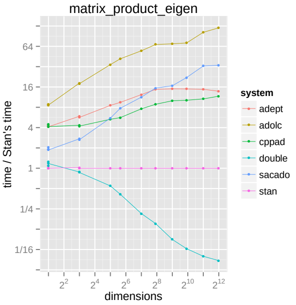
NUTS vs. Gibbs and Metropolis

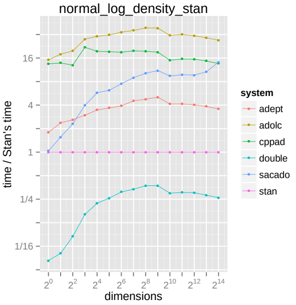


- Two dimensions of highly correlated 250-dim normal
- **1,000,000 draws** from Metropolis and Gibbs (thin to 1000)
- **1000 draws** from NUTS; 1000 independent draws

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 is a Programming Language

- **Not** a graphical specification language like BUGS or JAGS
- Stan is a Turing-complete imperative programming langauge 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

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,

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

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);`
- **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);
  ```

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)

Transforms: Precision

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

Transforms: “Matt Trick”

```
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);
}
```

Linear Regression (Normal Noise)

- **Likelihood**:
  - $y_n = \alpha + \beta x_n + \epsilon_n$
  - $\epsilon_n \sim \text{Normal}(0, \sigma)$ for $n \in 1{:}N$
- Equivalently,
  - $y_n \sim \text{Normal}(\alpha + \beta x_n, \sigma)$
- **Priors** (improper)
  - $\sigma \sim \text{Uniform}(0, \infty)$
  - $\alpha, \beta \sim \text{Uniform}(-\infty, \infty)$
- Stan allows **improper prior**; requires **proper posterior**.

Linear Regression: Stan Code

```
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

```
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 {
  for (n in 2:N)
    y[n] ~ normal(alpha + beta * y[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);
}
```

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);
}
```

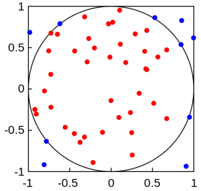
- Must include noise for predictive uncertainty
- PRNGs only allowed in generated quantities block
  - more computationally efficient per iteration
  - more statistically efficient with i.i.d. samples (i.e., MC, not MCMC)

Part V

Monte Carlo Integration

Monte Carlo Calculation of π

- Computing $\pi = 3.14\ldots$ via simulation is *the* textbook application of Monte Carlo methods.
- Generate points uniformly at random within the square
- Calculate proportion within circle ($x^2 + y^2 < 1$) and multiply by square's area (4) to produce the area of the circle.
- This area is π (radius is 1, so area is $\pi r^2 = \pi$)



Plot by Mysid Yoderj courtesy of Wikipedia.

Monte Carlo Calculation of π (cont.)

- R code to calcuate π with Monte Carlo simulation:

```
> x <- runif(1e6,-1,1)
> y <- runif(1e6,-1,1)

> prop_in_circle <- sum(x^2 + y^2 < 1) / 1e6

> 4 * prop_in_circle
[1] 3.144032
```

Accuracy of Monte Carlo

- Monte Carlo is *not* an approximation!
- It can be made exact to within any ϵ
- Monte Carlo draws are i.i.d. by definition
- Central limit theorem: expected error decreases at rate of

$$\frac{1}{\sqrt{N}}$$

- 3 decimal places of accuracy with sample size 1e6
- Need $100\times$ larger sample for each digit of accuracy

General Monte Carlo Integration

- MC can calculate arbitrary definite integrals,

$$\int_a^b f(x)\,dx$$

- Let d upper bound $f(x)$ in (a,b); tightness determines computational efficiency
- Then generate random points uniformly in the rectangle bounded by (a,b) and $(0,d)$
- Multiply proportion of draws (x,y) where $y < f(x)$ by area of rectangle, $d \times (b-a)$.
- Can be generalized to multiple dimensions in obvious way

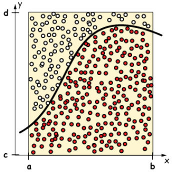


Image courtesy of Jeff Cruzan, http://www.drcruzan.com/NumericalIntegration.html

Expectations of Function of R.V.

- Suppose $f(\theta)$ is a function of random variable vector θ
- Suppose the density of θ is $p(\theta)$
  - *Warning*: θ overloaded as random and bound variable
- Then $f(\theta)$ is also random variable, with expectation

$$\mathbb{E}[f(\theta)] = \int_{\Theta} f(\theta)\; p(\theta)\; d\theta.$$

  - where Θ is support of $p(\theta)$ (i.e., $\Theta = \{\theta \mid p(\theta) > 0\}$

QoI as Expectations

- Most Bayesian quantities of interest (QoI) are expectations over the posterior $p(\theta \mid y)$ of functions $f(\theta)$
- **Bayesian parameter estimation**: $\hat{\theta}$
  - $f(\theta) = \theta$
  - $\hat{\theta} = \mathbb{E}[\theta|y]$ minimizes expected square error
- **Bayesian parameter (co)variance estimation**: $\mathrm{var}[\theta \mid y]$
  - $f(\theta) = (\theta - \hat{\theta})^2$
- **Bayesian event probability**: $\Pr[A \mid y]$
  - $f(\theta) = \mathrm{I}(\theta \in A)$

Expectations via Monte Carlo

- Generate draws $\theta^{(1)}, \theta^{(2)}, \ldots, \theta^{(M)}$ drawn from $p(\theta)$
- Monte Carlo Estimator **plugs in average** for expectation:

$$\mathbb{E}[f(\theta)|y] \approx \frac{1}{M} \sum_{m=1}^{M} f(\theta^{(m)})$$

- Can be made **as accurate as desired**, because

$$\mathbb{E}[f(\theta)] = \lim_{M \to \infty} \frac{1}{M} \sum_{m=1}^{M} f(\theta^{(m)})$$

- *Reminder*: By CLT, error goes down as $1 \,/\, \sqrt{M}$

Part VI
Markov Chain Monte Carlo

Markov Chain Monte Carlo

- Standard Monte Carlo draws i.i.d. draws

  $$\theta^{(1)}, \dots, \theta^{(M)}$$

  according to a probability function $p(\theta)$

- Drawing an i.i.d. sample is often impossible when dealing with complex densities like Bayesian posteriors $p(\theta|y)$

- So we use Markov chain Monte Carlo (MCMC) in these cases and draw $\theta^{(1)}, \dots, \theta^{(M)}$ from a Markov chain

Markov Chains

- A Markov Chain is a sequence of random variables

$$\theta^{(1)}, \theta^{(2)}, \ldots, \theta^{(M)}$$

such that $\theta^{(m)}$ only depends on $\theta^{(m-1)}$, i.e.,

$$p(\theta^{(m)}|y, \theta^{(1)}, \ldots, \theta^{(m-1)}) \ = \ p(\theta^{(m)}|y, \theta^{(m-1)})$$

- Drawing $\theta^{(1)}, \ldots, \theta^{(M)}$ from a Markov chain according to $p(\theta^{(m)} \mid \theta^{(m-1)}, y)$ is more tractable
- Require marginal of each draw, $p(\theta^{(m)}|y)$, to be equal to true posterior

Applying MCMC

- Plug in just like ordinary (non-Markov chain) Monte Carlo
- Adjust standard errors for dependence in Markov chain

MCMC for Posterior Mean

- Standard Bayesian estimator is posterior mean

$$\hat{\theta} \;=\; \int_{\Theta} \theta \, p(\theta|y)\, d\theta$$

  - Posterior mean minimizes expected square error

- Estimate is a conditional expectation

$$\hat{\theta} = \mathbb{E}[\theta|y]$$

- Compute by averaging

$$\hat{\theta} \;\approx\; \frac{1}{M} \sum_{m=1}^{M} \theta$$

MCMC for Posterior Variance

- Posterior variance works the same way,

$$\begin{aligned}\mathbb{E}[(\theta - \mathbb{E}[\theta \mid y])^2 \mid y] &= \mathbb{E}[(\theta - \hat{\theta})^2] \\ &\approx \frac{1}{M} \sum_{m=1}^{M} (\theta^{(m)} - \hat{\theta})^2\end{aligned}$$

MCMC for Event Probability

- Event probabilities are also expectations, e.g.,

$$\mathsf{Pr}[\theta_1 > \theta_2] \ = \ \mathbb{E}[\mathsf{I}[\theta_1 > \theta_2]] \ = \ \int_\Theta \mathsf{I}[\theta_1 > \theta_2]\, p(\theta|y) d\theta.$$

- Estimation via MCMC just another plug-in:

$$\mathsf{Pr}[\theta_1 > \theta_2] \approx \frac{1}{M} \sum_{m=1}^{M} \mathsf{I}[\theta_1^{(m)} > \theta_2^{(m)}]$$

- Again, can be made as accurate as necessary

MCMC for Quantiles (incl. median)

- These are not expectations, but still plug in
- Alternative Bayesian estimator is posterior median
  - Posterior median minimizes expected absolute error
- Estimate as median draw of $\theta^{(1)}, \ldots, \theta^{(M)}$
  - just sort and take halfway value
  - e.g., Stan shows 50% point (or other quantiles)
- Other quantiles including interval bounds similar
  - estimate with quantile of draws
  - estimation error goes up in tail (based on fewer draws)

Part VII

MCMC Algorithms

Random-Walk Metropolis

- Draw random initial parameter vector $\theta^{(1)}$ (in support)
- For $m \in 2{:}M$
  - Sample proposal from a (symmetric) jumping distribution, e.g.,
    $$\theta^* \sim \text{MultiNormal}(\theta^{(m-1)}, \sigma \mathbf{I})$$
    where $\mathbf{I}$ is the identity matrix
  - Draw $u^{(m)} \sim \text{Uniform}(0,1)$ and set
    $$\theta^{(m)} = \begin{cases} \theta^* & \text{if } u^{(m)} < \dfrac{p(\theta^*|y)}{p(\theta^{(m-1)}|y)} \\ \theta^{(m-1)} & \text{otherwise} \end{cases}$$

Metropolis and Normalization

- Metropolis only uses posterior in a ratio:

$$\frac{p(\theta^* \mid y)}{p(\theta^{(m)} \mid y)}$$

- This **allows** the use of **unnormalized densities**
- Recall Bayes's rule:

$$p(\theta|y) \propto p(y|\theta)\, p(\theta)$$

- Thus we only need to evaluate sampling (likelihood) and prior
  - i.e., no need to compute normalizing integral for $p(y)$,

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

Metropolis-Hastings

- Generalizes Metropolis to asymmetric proposals
- Acceptance ratio is

$$\frac{J(\theta^{(m)}|\theta^{*}) \ \times \ p(\theta^{*}|y)}{J(\theta^{*}|\theta^{(m-1)}) \ \times \ p(\theta^{(m)}|y)}$$

  where J is the (potentially asymmetric) proposal density

- i.e.,

$$\frac{\text{probabilty of being at } \theta^{*} \text{ and jumping to } \theta^{(m-1)}}{\text{probability of being at } \theta^{(m-1)} \text{ and jumping to } \theta^{*}}$$

Metropolis-Hastings (cont.)

- General form ensures equilibrium by maintaining *detailed balance*
- Like Metropolis, only requires ratios
- Many algorithms involve a Metropolis-Hastings “correction”
    - Including vanilla HMC and RHMC and ensemble samplers

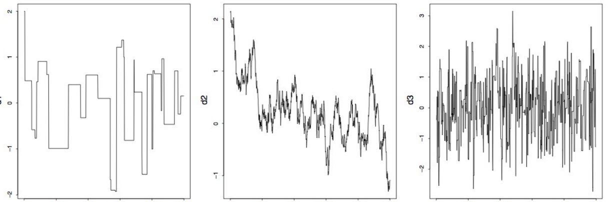
Detailed Balance & Reversibility

- Definition is measure theoretic, but applies to densities
  - just like Bayes's rule
- Assume Markov chain has stationary density $p(a)$
- Suppose $\pi(a|b)$ is density of transitioning from b to a
  - use of π to indicates different measure on Θ than p
- Detailed balance is a reversibility equilibrium condition

$$p(a)\,\pi(b|a) \;=\; p(b)\,\pi(a|b)$$

Optimal Proposal Scale?

- Proposal scale σ is a free; too low or high is inefficient



(a) Proposal variance too large (b) Proposal variance too small (c) Proposal variance approximately optimised

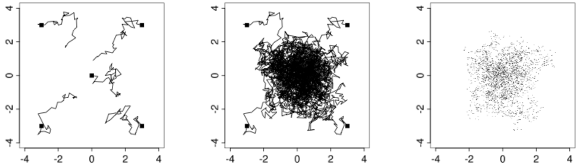
- *Traceplots* show parameter value on y axis, iterations on x
- Empirical tuning problem; theoretical optima exist for some cases

Roberts and Rosenthal (2001) Optimal Scaling for Various Metropolis-Hastings Algorithms. *Statistical Science*.

Convergence

- Imagine releasing a hive of bees in a sealed house
  - they disperse, but eventually reach equilibrium where the same number of bees leave a room as enter it (on average)
- May take many iterations for Markov chain to reach equilibrium

Convergence: Example



- Four chains with different starting points
  - *Left*: 50 iterations
  - *Center*: 1000 iterations
  - *Right*: Draws from second half of each chain

Gelman et al., *Bayesian Data Analysis*

Potential Scale Reduction ($\hat{R}$)

- Gelman & Rubin recommend M chains of N draws with **diffuse initializations**
- Measure that each chain has same posterior mean and variance
- If not, may be stuck in multiple modes or just not converged yet
- Define statistic $\hat{R}$ of chains s.t. **at convergence**, $\hat{R} \to 1$
  - $\hat{R} >> 1$ implies non-convergence
  - $\hat{R} \approx 1$ **does not guarantee convergence**
  - Only measures marginals

Split $\hat{R}$

- Vanilla $\hat{R}$ may not diagnose non-stationarity
  - e.g., a sequence of chains with an increasing parameter
- **Split $\hat{R}$**: Stan splits each chain into first and second half
  - start with M Markov chains of N draws each
  - split each in half to creates $2M$ chains of $N/2$ draws
  - then apply $\hat{R}$ to the $2M$ chains

Calculating $\hat{R}$ Statistic: Between

- M chains of N draws each
- **Between-sample variance** estimate

$$B = \frac{N}{M-1} \sum_{m=1}^{M} (\bar{\theta}_m^{(\bullet)} - \bar{\theta}_{\bullet}^{(\bullet)})^2,$$

where

$$\bar{\theta}_m^{(\bullet)} = \frac{1}{N} \sum_{n=1}^{N} \theta_m^{(n)} \quad \text{and} \quad \bar{\theta}_{\bullet}^{(\bullet)} = \frac{1}{M} \sum_{m=1}^{M} \bar{\theta}_m^{(\bullet)}.$$

Calculating $\hat{R}$ (cont.)

- M chains of N draws each
- **Within-sample variance** estimate:

$$W = \frac{1}{M} \sum_{m=1}^{M} s_m^2,$$

where

$$s_m^2 = \frac{1}{N-1} \sum_{n=1}^{N} (\theta_m^{(n)} - \bar{\theta}_m^{(\bullet)})^2.$$

Calculating $\hat{R}$ Statistic (cont.)

- **Variance** estimate:

$$\widehat{\text{var}}^{+}(\theta|y) = \frac{N-1}{N} W + \frac{1}{N} B.$$

  recall that W is within-chain variance and B between-chain

- **Potential scale reduction** statistic (“R hat”)

$$\hat{R} = \sqrt{\frac{\widehat{\text{var}}^{+}(\theta|y)}{W}}.$$

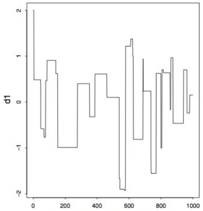
Correlations in Posterior Draws

- Markov chains typically display autocorrelation in the series of draws $\theta^{(1)}, \ldots, \theta^{(m)}$
- Without i.i.d. draws, central limit theorem *does not apply*
- Effective sample size N_{eff} divides out autocorrelation
- N_{eff} must be estimated from sample
  - Fast Fourier transform computes correlations at all lags
- Estimation accuracy proportional to

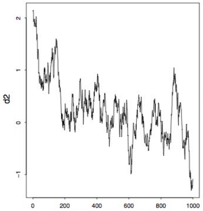
$$\frac{1}{\sqrt{N_{\text{eff}}}}$$

Reducing Posterior Correlation

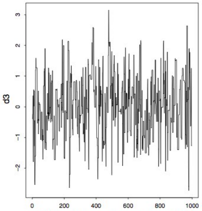
- Tuning algorithm parameters to ensure good mixing
- Recall Metropolis traceplots of Roberts and Rosenthal:



(a) Proposal variance too large



(b) Proposal variance too small



(c) Proposal variance approximately optimised

- Good jump scale σ produces good mixing and high N_{eff}

Effective Sample Size

- Autocorrelation at lag t is correlation between subseqs
  - $(\theta^{(1)}, \ldots, \theta^{(N-t)})$ and $(\theta^{(1+t)}, \ldots, \theta^{(N)})$
- Suppose chain has density $p(\theta)$ with
  - $\mathbb{E}[\theta] = \mu$ and $\mathrm{Var}[\theta] = \sigma^2$
- Autocorrelation ρ_t at lag $t \geq 0$:

$$\rho_t = \frac{1}{\sigma^2} \int_\Theta (\theta^{(n)} - \mu)(\theta^{(n+t)} - \mu)\, p(\theta)\, d\theta$$

- Because $p(\theta^{(n)}) = p(\theta^{(n+t)}) = p(\theta)$ at convergence,

$$\rho_t = \frac{1}{\sigma^2} \int_\Theta \theta^{(n)}\, \theta^{(n+t)}\, p(\theta)\, d\theta$$

Estimating Autocorrelations

- Effective sample size (N draws in chain) is defined by

$$N_{\text{eff}} \;=\; \frac{N}{\sum_{t=-\infty}^{\infty} \rho_t} \;=\; \frac{N}{1 + 2\sum_{t=1}^{\infty} \rho_t}$$

- Estimate in terms of variograms (M chains) at lag t
  - Calculate with fast Fourier transform (FFT)

$$V_t = \frac{1}{M} \sum_{m=1}^{M} \left(\frac{1}{N_m - t} \sum_{n=t+1}^{N_m} \left(\theta_m^{(n)} - \theta_m^{(n-t)} \right)^2 \right)$$

- Adjust autocorrelation at lag t using cross-chain variance as

$$\hat{\rho}_t = 1 - \frac{V_t}{2\,\widehat{\text{var}}^{+}}$$

- If not converged, $\widehat{\text{var}}^{+}$ overestimates variance

Estimating N_{eff}

- Let T' be first lag s.t. $\rho_{T'+1} < 0$,
- Estimate autocorrelation by

$$\hat{N}_{\text{eff}} = \frac{MN}{1 + \sum_{t=1}^{T'} \hat{\rho}_t}.$$

- NUTS avoids negative autocorrelations, so first negative autocorrelation estimate is reasonable
- For basics (not our estimates), see

  Charles Geyer (2013) Introduction to MCMC. In *Handbook of MCMC*.

  (free online at `http://www.mcmchandbook.net/index.html`)

Gibbs Sampling

- Draw random initial parameter vector $\theta^{(1)}$ (in support)
- For $m \in 2{:}M$
  - For $n \in 1{:}N$:
    - draw $\theta_n^{(m)}$ according to conditional

      $$p(\theta_n | \theta_1^{(m)}, \ldots, \theta_{n-1}^{(m)}, \theta_{n+1}^{(m-1)}, \ldots, \theta_N^{(m-1)}, y).$$
- e.g, with $\theta = (\theta_1, \theta_2, \theta_3)$:
  - draw $\theta_1^{(m)}$ according to $p(\theta_1 | \theta_2^{(m-1)}, \theta_3^{(m-1)}, y)$
  - draw $\theta_2^{(m)}$ according to $p(\theta_2 | \theta_1^{(m)}, \theta_3^{(m-1)}, y)$
  - draw $\theta_3^{(m)}$ according to $p(\theta_3 | \theta_1^{(m)}, \theta_2^{(m)}, y)$

Generalized Gibbs

- "Proper" Gibbs requires conditional Monte Carlo draws
  - typically works only for conjugate priors
- In general case, may need to use less efficient conditional draws
  - Slice sampling is a popular general technique that works for discrete or continuous θ_n (JAGS)
  - Adaptive rejection sampling is another alternative (BUGS)
  - Very difficult in more than one or two dimensions

Sampling Efficiency

- We care only about N_{eff} per second
- Decompose into
  1. Iterations per second
  2. Effective sample size per iteration
- Gibbs and Metropolis have high iterations per second (especially Metropolis)
- But they have low effective sample size per iteration (especially Metropolis)
- Both are particular weak when there is high correlation among the parameters in the posterior

Hamiltonian Monte Carlo & NUTS

- Slower iterations per second than Gibbs or Metropolis
- Much higher effective sample size per iteration for complex posteriors (i.e., high curvature and correlation)
- Overall, much higher $N_{1\text{ff}}$ per second

- Details in the next talk . . .
- Along with details of how Stan implements HMC and NUTS

Part VIII

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 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 draws in sample 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
- **Standard errors** on unconstrained scale
  (estimated using curvature of penalized log likelihood function
- Models, data, initialization as in MCMC
- **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

Posterior Analysis: Estimates

- For each parameter (and `lp__`)
  - Posterior mean
  - Posterior standard deviation
  - Posterior MCMC error esimate: sd$/N_{\text{eff}}$
  - Posterior quantiles
  - Number of effective samples
  - $\hat{R}$ convergence statistic

- . . . and much much more in ShinyStan

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** (soon: Hessian)
  - data I/O and parameter initialization
  - model provides variable names and dimensionalities
  - transforms to and from constrained representation (with or without Jacobian)

Part IX
How Stan Works

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)

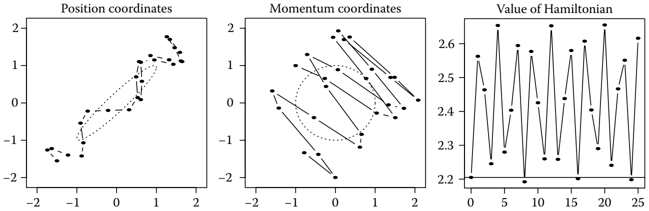
Optimize: L-BFGS

- Initialize unconstrained parameters and Hessian
  - Random values on unconstrained scale uniform in $(-2, 2)$
    - or user specified on constrained scale, transformed
  - Hessian approximation initialized to unit matrix
- While not converged
  - Move unconstrained parameters toward optimum based on Hessian approximation and step size (Newton step)
  - If diverged (arithmetic, support), reduce step size, continue
  - else if converged (parameter change, log density change, gradient value), return value
  - else update Hessian approx. based on calculated gradient

Sample: Hamiltonian Flow

- Generate random **kinetic energy**
  - random Normal$(0, 1)$ in each parameter
- Use negative log posterior as **potential energy**
- Hamiltonian is kinetic plus potential energy
- **Leapfrog Integration**: for *fixed* stepsize (time discretization), number of steps (total time), and mass matrix,
  - update momentum half-step based on potential (gradient)
  - update position full step based on momentum
  - update momentum half-step based on potential
- Numerical solution of Hamilton's first-order version of Newton's second-order diff-eqs of motion (force $=$ mass $\times$ acceleration)

Sample: Leapfrog Example



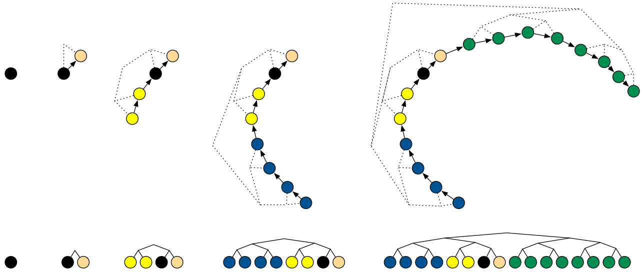
- Trajectory of 25 leapfrog steps for correlated 2D normal (ellipses at 1 sd from mean), stepsize of 0.25, initial state of $(-1, 1)$, and initial momentum of $(-1.5, -1.55)$.

Radford Neal (2013) MCMC using Hamiltonian Dynamics. In *Handbook of MCMC*. (free online at http://www.mcmchandbook.net/index.html)

Sample: No-U-Turn Sampler (NUTS)

- Adapts Hamiltonian simulation time
  - goal to maximize mixing, maintaining detailed balance
  - too short devolves to random walk
  - too long does extra work (i.e., orbits)
- For exponentially increasing number of steps up to max
  - Randomly choose to extend forward or backward in time
  - Move forward or backward in time number of steps
    - stop if any subtree (size 2, 4, 8, ...) makes U-turn
    - remove all current steps if subtree U-turns (not ends)
- Randomly select param with density above slice (or reject)

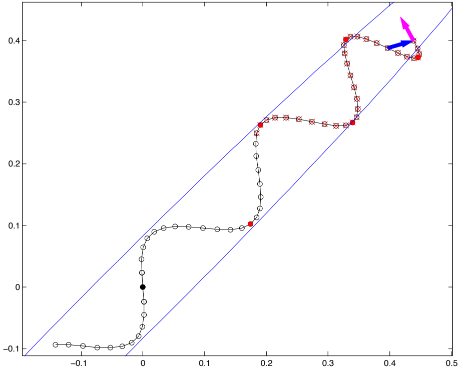
Sample: NUTS Binary Tree



- Example of repeated doubling building binary tree forward and backward in time until U-turn.

  Hoffman and Gelman. 2014. The No-U-Turn Sampler. *JMLR*. (free online at http://jmlr.org/papers/v15/hoffman14a.html)

Sample: NUTS U-Turn



- Example of trajectory from one iteration of NUTS.
- Blue ellipse is contour of 2D normal.
- Black circles are leapfrog steps.
- Solid red circles excluded below slice
- U-turn made with blue and magenta arrows
- Red crossed circles excluded for detailed balance

Sample: HMC/NUTS Warmup

- Estimate stepsize
  - too small requires too many leapfrog steps
  - too large induces numerical inaccuracy
  - need to balance
- Estimate mass matrix
  - Diagonal accounts for parameter scales
  - Dense optionally accounts for rotation

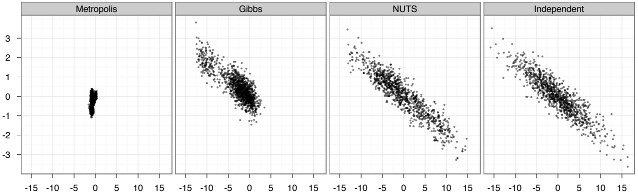
Sample: Warmup (cont.)

- Initialize unconstrained parameters as for optimization
- For exponentially increasing block sizes
  - for each iteration in block
    - generate random kinetic energy
    - simulate Hamiltonian flow (HMC fixed time, NUTS adapts)
    - choose next state (Metroplis for HMC, slice for NUTS)
  - update regularized point estimate of mass matrix
    - use parameter draws from current block
    - shrink diagonal toward unit; dense toward diagonal
  - tune stepsize (line search) for target acceptance rate

Sample: HMC/NUTS Sampling

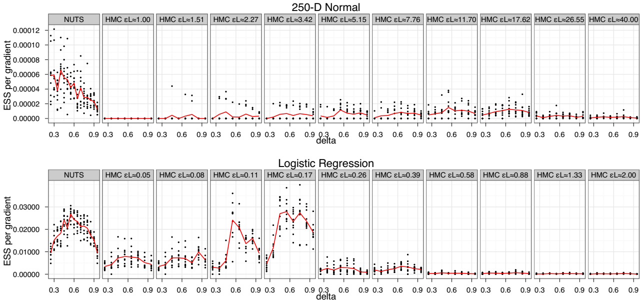
- Fix stepsize and and mass matrix
- For sampling iterations
  - generate random kinetic energy
  - simulate Hamiltonian flow
  - apply Metropolis accept/reject (HMC) or slice (NUTS)

NUTS vs. Gibbs and Metropolis



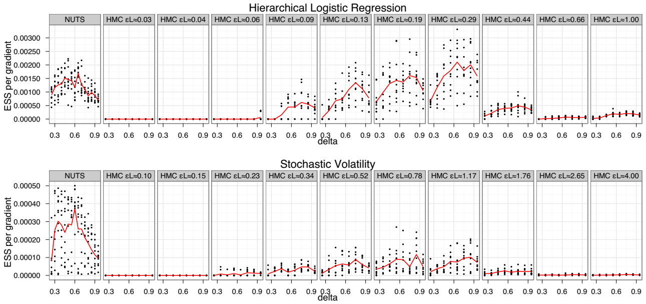
- Two dimensions of highly correlated 250-dim normal
- **1,000,000 draws** from Metropolis and Gibbs (thin to 1000)
- **1000 draws** from NUTS; 1000 independent draws

NUTS vs. Basic HMC



- 250-D normal and logistic regression models
- Vertical axis is effective sample size per sample (bigger better)
- Left) NUTS; Right) HMC with increasing $t = \epsilon L$

NUTS vs. Basic HMC II



- Hierarchical logistic regression and stochastic volatility
- Simulation time t is $\epsilon\, L$, step size (ϵ) times number of steps (L)
- NUTS can beat optimally tuned HMC (latter very expensive)

Part X
Under Stan’s Hood

Euclidean Hamiltonian

- **Phase space**: q position (parameters); p momentum
- **Posterior density**: $\pi(q)$
- **Mass matrix**: M
- **Potential energy**: $V(q) = -\log \pi(q)$
- **Kinetic energy**: $T(p) = \frac{1}{2} p^\top M^{-1} p$
- **Hamiltonian**: $H(p, q) = V(q) + T(p)$
- **Diff eqs**:

$$\frac{dq}{dt} = +\frac{\partial H}{\partial p} \qquad \frac{dp}{dt} = -\frac{\partial H}{\partial q}$$

Leapfrog Integrator Steps

- Solves Hamilton's equations by **simulating dynamics**
  (symplectic [volume preserving]; ϵ^3 error per step, ϵ^2 total error)
- Given: **step size** ϵ, **mass matrix** M, **parameters** q
- **Initialize kinetic** energy, $p \sim \text{Normal}(0, \mathbf{I})$
- **Repeat** for L leapfrog steps:

$$p \leftarrow p - \frac{\epsilon}{2} \frac{\partial V(q)}{\partial q} \qquad \text{[half step in momentum]}$$

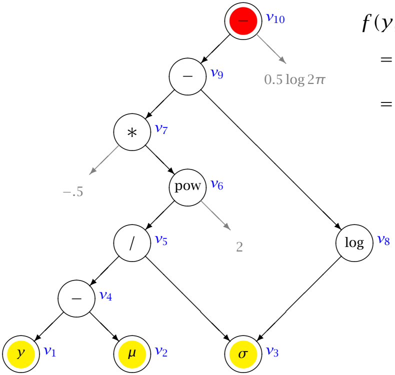
$$q \leftarrow q + \epsilon M^{-1} p \qquad \text{[full step in position]}$$

$$p \leftarrow p - \frac{\epsilon}{2} \frac{\partial V(q)}{\partial q} \qquad \text{[half step in momentum]}$$

Reverse-Mode Auto Diff

- Eval gradient in (usually small) multiple of function eval time
  - independent of dimensionality
  - time proportional to number of expressions evaluated
- Result accurate to machine precision (cf. finite diffs)
- Function evaluation builds up **expression tree**
- Dynamic program propagates **chain rule** in reverse pass
- Reverse mode computes ∇g in one pass for a function $f : \mathbb{R}^N \rightarrow \mathbb{R}$

Autodiff Expression Graph



$$f(y,\mu,\sigma)$$

$$= \log\left(\text{Normal}(y|\mu,\sigma)\right)$$

$$= -\frac{1}{2}\left(\frac{y-\mu}{\sigma}\right)^2 - \log\sigma - \frac{1}{2}\log(2\pi)$$

$$\frac{\partial}{\partial y} f(y,\mu,\sigma)$$

$$= -(y-\mu)\sigma^{-2}$$

$$\frac{\partial}{\partial \mu} f(y,\mu,\sigma)$$

$$= (y-\mu)\sigma^{-2}$$

$$\frac{\partial}{\partial \sigma} f(y,\mu,\sigma)$$

$$= (y-\mu)^2\sigma^{-3} - \sigma^{-1}$$

Autodiff Partials

var	*value*	*partials*	
v_1	y		
v_2	μ		
v_3	σ		
v_4	$v_1 - v_2$	$\partial v_4/\partial v_1 = 1$	$\partial v_4/\partial v_2 = -1$
v_5	v_4/v_3	$\partial v_5/\partial v_4 = 1/v_3$	$\partial v_5/\partial v_3 = -v_4 v_3^{-2}$
v_6	$(v_5)^2$	$\partial v_6/\partial v_5 = 2v_5$	
v_7	$(-0.5)v_6$	$\partial v_7/\partial v_6 = -0.5$	
v_8	$\log v_3$	$\partial v_8/\partial v_3 = 1/v_3$	
v_9	$v_7 - v_8$	$\partial v_9/\partial v_7 = 1$	$\partial v_9/\partial v_8 = -1$
v_{10}	$v_9 - (0.5 \log 2\pi)$	$\partial v_{10}/\partial v_9 = 1$	

Autodiff: Reverse Pass

var	*operation*	*adjoint*	*result*
$a_{1:9}$	$=$	0	$a_{1:9} = 0$
a_{10}	$=$	1	$a_{10} = 1$
a_9	$+=$	$a_{10} \times (1)$	$a_9 = 1$
a_7	$+=$	$a_9 \times (1)$	$a_7 = 1$
a_8	$+=$	$a_9 \times (-1)$	$a_8 = -1$
a_3	$+=$	$a_8 \times (1/v_3)$	$a_3 = -1/v_3$
a_6	$+=$	$a_7 \times (-0.5)$	$a_6 = -0.5$
a_5	$+=$	$a_6 \times (2v_5)$	$a_5 = -v_5$
a_4	$+=$	$a_5 \times (1/v_3)$	$a_4 = -v_5/v_3$
a_3	$+=$	$a_5 \times (-v_4 v_3^{-2})$	$a_3 = -1/v_3 + v_5 v_4 v_3^{-2}$
a_1	$+=$	$a_4 \times (1)$	$a_1 = -v_5/v_3$
a_2	$+=$	$a_4 \times (-1)$	$a_2 = v_5/v_3$

Stan’s Reverse-Mode

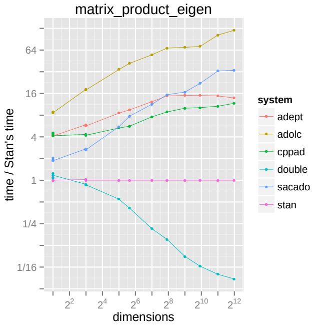
- Easily extensible **object-oriented** design
- **Code nodes** in expression graph for primitive functions
  - requires **partial derivatives**
  - built-in flexible abstract base classes
  - **lazy evaluation** of chain rule saves memory
- Autodiff through templated C++ functions
  - templating on each argument avoids excess promotion

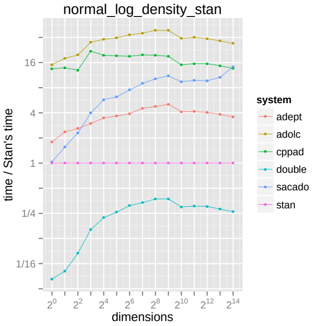
Stan’s Reverse-Mode (cont.)

- Arena-based **memory management**
  - specialized C++ `operator new` for reverse-mode variables
  - custom functions inherit memory management through base
- Nested application to support ODE solver

Stan’s Autodiff vs. Alternatives

- Stan is **fastest** (and uses least memory)
  - among open-source C++ alternatives





Forward-Mode Auto Diff

- Evaluates expression graph forward from one independent variable to any number of dependent variables
- Function evaluation propagates **chain rule** forward
- In one pass, computes $\frac{\partial}{\partial x} f(x)$ for a function $f : \mathbb{R} \rightarrow \mathbb{R}^N$
  - derivative of N outputs with respect to a single input

Stan’s Forward Mode

- Templated scalar type for value and tangent
  - allows higher-order derivatives
- Primitive functions propagate derivatives
- No need to build expression graph in memory
  - much less memory intensive than reverse mode
- Autodiff through templated functions (as reverse mode)

Second-Order Derivatives

- Compute Hessian (matrix of second-order partials)

$$H_{i,j} = \frac{\partial^2}{\partial x_i \partial x_j} f(x)$$

- Required for Laplace covariance approximation (MLE)
- Required for curvature (Riemannian HMC)
- Nest reverse-mode in forward for **second order**
- N forward passes: takes gradient of derivative

Third-Order Derivatives

- Compute gradients of Hessians (tensor of third-order partials)

$$\frac{\partial^3}{\partial x_i \partial x_j \partial x_k} f(x)$$

  - Required for SoftAbs metric (Riemannian HMC)
  - N^2 forward passes: gradient of derivative of derivative

Jacobians

- Assume function $f : \mathbb{R}^N \rightarrow \mathbb{R}^M$
- Partials for multivariate function (matrix of first-order partials)

$$J_{i,j} = \frac{\partial}{\partial x_i} f_j(x)$$

- Required for stiff ordinary differential equations
  - differentiate is coupled sensitivity autodiff for ODE system
- Two execution strategies
  1. Multiple reverse passes for rows
  2. Forward pass per column (required for stiff ODE)

Autodiff Functionals

- Functionals map templated functors to derivatives
  - fully encapsulates and hides all autodiff types
- Autodiff functionals supported
  - gradients: $\mathcal{O}(1)$
  - Jacobians: $\mathcal{O}(N)$
  - gradient-vector product (i.e., directional derivative): $\mathcal{O}(1)$
  - Hessian-vector product: $\mathcal{O}(N)$
  - Hessian: $\mathcal{O}(N)$
  - gradient of trace of matrix-Hessian product: $\mathcal{O}(N^2)$
    (for SoftAbs RHMC)

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

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

Coding Probability Functions

- **Vectorized** to allow scalar or container arguments
  (containers all same shape; scalars broadcast as necessary)

- Avoid **repeated computations**, e.g. $\log \sigma$ in

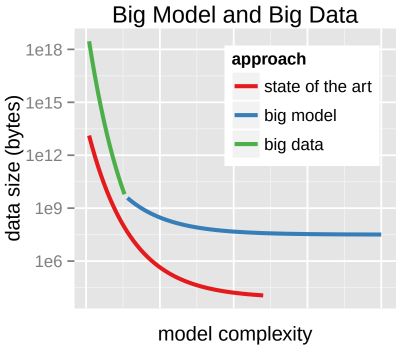
$$\begin{aligned} \log \mathsf{Normal}(y|\mu,\sigma) &= \textstyle\sum_{n=1}^{N} \log \mathsf{Normal}(y_n|\mu,\sigma) \\ &= \textstyle\sum_{n=1}^{N} -\log\sqrt{2\pi} \;-\log\sigma \;-\frac{y_n-\mu}{2\sigma^2} \end{aligned}$$

- recursive **expression templates** to broadcast and cache scalars, generalize containers (arrays, matrices, vectors)

- **traits** metaprogram to **drop constants** (e.g., $-\log\sqrt{2\pi}$ or $\log\sigma$ if constant) and calculate intermediate and return types

Part XI
Stan for Big Data

Scaling and Evaluation



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

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

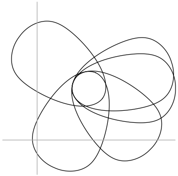
“Black Box” Variational Inference

- **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

“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 Cavity Distribution



- Two parameters, with data split into $y_1, \ldots, y_5$
- Contours of likelihood $p(y_k|\theta)$ for $k \in 1{:}5$
- $g_{-k}(\theta)$ is **cavity distribution** (current approx. without y_k)
- Separately computing for y_k reqs each partition to cover its area
- Combining likelihood with cavity **focuses on overlap**

Maximum Marginal Likelihood

- Fast, approx. inference for hierarchical models: $p(\phi, \alpha)$
- Marginalize out lower-level params: $p(\phi) = \int p(\phi, \alpha) d\alpha$
- Optimize higher-level parameters ϕ^* and fix
- Optimize lower-level parameters given higher-level: $p(\phi^*, \alpha)$
- Errors estimated as in MLE
- aka "empirical Bayes"
  - but not fully Bayesian
  - and no more empirical than full Bayes
- Design complete; awaiting parameter tagging

Part XII

Posterior Modes & Laplace Approximation

Laplace Approximation

- Multivariate normal approximation to posterior
- Compute posterior mode via optimization

$$\theta^* = \text{arg max}_\theta \; p(\theta|y)$$

- Laplace approximation to the posterior is

$$p(\theta|y) \approx \text{MultiNormal}(\theta^* | -H^{-1})$$

- H is the Hessian of the log posterior

$$H_{i,j} = \frac{\partial^2}{\partial\theta_i \, \partial\theta_j} \log p(\theta|y)$$

Stan's Laplace Approximation

- Operates on unconstrained parameters
- L-BFGS to compute posterior mode $\theta*$
- Automatic differentiation to compute H
  - current R: finite differences of gradients
  - soon: second-order automatic differentiation
- Draw a sample from approximate posterior
  - transfrom back to constrained scale
  - allows Monte Carlo computation of expectations

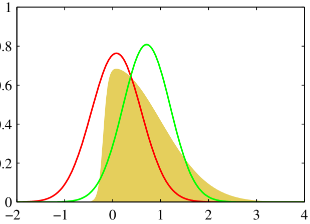
Part XIII
Variational Bayes

VB in a Nutshell

- y is observed data, θ parameters
- Goal is to approximate posterior $p(\theta|y)$
- with a convenient approximating density $g(\theta|\phi)$
  - ϕ is a vector of parameters of approximating density
- Given data y, VB computes ϕ^* minimizing KL-divergence
  - from approximation $g(\theta \mid \phi)$ to posterior $p(\theta \mid y)$

$$\begin{aligned} \phi^* &= \text{arg min}_\phi \ \text{KL}[g(\theta|\phi) \ || \ p(\theta|y)] \\ &= \text{arg max}_\phi \ -\int_\Theta \log\left(\frac{p(\theta \mid y)}{g(\theta \mid \phi)}\right) \ g(\theta|\phi) \ \mathrm{d}\theta \end{aligned}$$

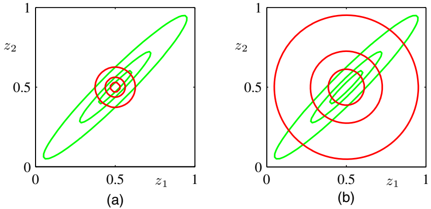
VB vs. Laplace



- *solid yellow*: target; *red*: Laplace; *green*: VB
- **Laplace** located at posterior mode
- **VB** located at approximate posterior mean

— Bishop (2006) *Pattern Recognition and Machine Learning*, fig. 10.1

KL-Divergence Example



- **Green**: true distribution p; **Red**: best approximation g
  (a) VB-like: KL$[g \,||\, p]$
  (b) EP-like: KL$[p \,||\, g]$
- VB systematically **understimates posterior variance**

— Bishop (2006) *Pattern Recognition and Machine Learning*, fig. 10.2

Stan's "Black-Box" VB

- Typically custom $g()$ per model
  - based on conjugacy and analytic updates
- Stan uses "black-box VB" with multivariate Gaussian g

$$g(\theta|\phi) = \text{MultiNormal}(\theta \mid \mu, \Sigma)$$

  for the **unconstrained posterior**
  - e.g., scales σ log-transformed with Jacobian
- Stan provides two versions
  - Mean field: Σ diagonal
  - General: Σ dense

Stan’s VB: Computation

- Use L-BFGS optimization to optimize θ^*
- Requires differentiable $\mathrm{KL}[g(\theta|\phi) \mid\mid p(\theta|y)]$
  - only up to constant (i.e., use evidence lower bound (ELBO))
- Approximate KL-divergence and gradient via Monte Carlo
  - KL divergence is an expectation w.r.t. approximation $g(\theta|\phi)$
  - Monte Carlo draws i.i.d. from approximating multi-normal
  - only need approximate gradient calculation for soundness
  - so only a few Monte Carlo iterations are enough

Stan’s VB: Computation (cont.)

- To support compatible plug-in inference
  - draw Monte Carlo sample $\theta^{(1)}, \ldots, \theta^{(M)}$ with

$$\theta^{(m)} \sim \mathsf{MultiNormal}(\theta \mid \mu^*, \Sigma^*)$$

  - inverse transfrom from unconstrained to constrained scale
  - report to user in same way as MCMC draws

- Future: reweight $\theta^{(m)}$ via importance sampling
  - with respect to true posterior
  - to improve expectation calculations

Near Future: Stochastic VB

- Data-streaming form of VB
  - Scales to billions of observations
  - Hoffman et al. (2013) Stochastic variational inference. *JMLR* 14.
- Mashup of stochastic gradient (Robbins and Monro 1951) and VB
  - subsample data (e.g., stream in minibatches)
  - upweight each minibatch to full data set size
  - use to make unbiased estimate of true gradient
  - take gradient step to minimimize KL-divergence
- Prototype code complete