Quantitative Marketing SIG: A Gentle Introduction to Estimation Bayesian Models Using Stan

Jason M.T. Roos

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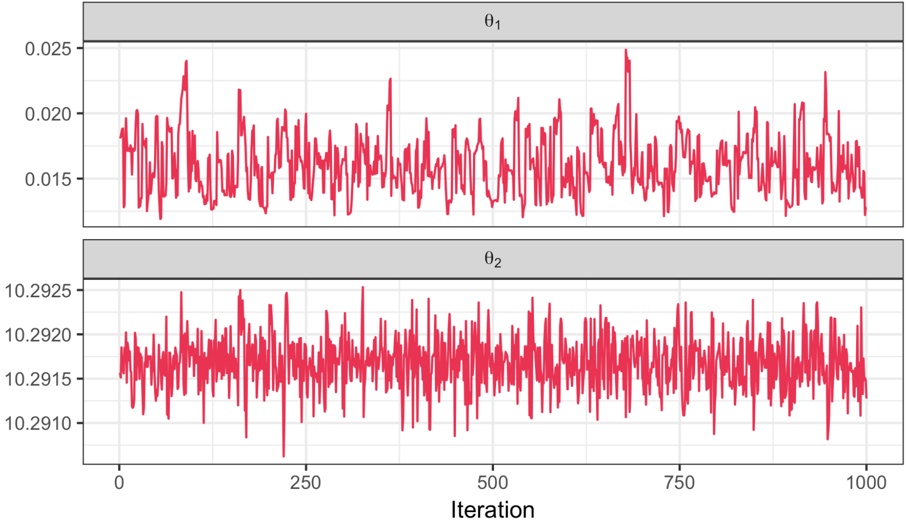
Motivation

Why we're talking about Stan today



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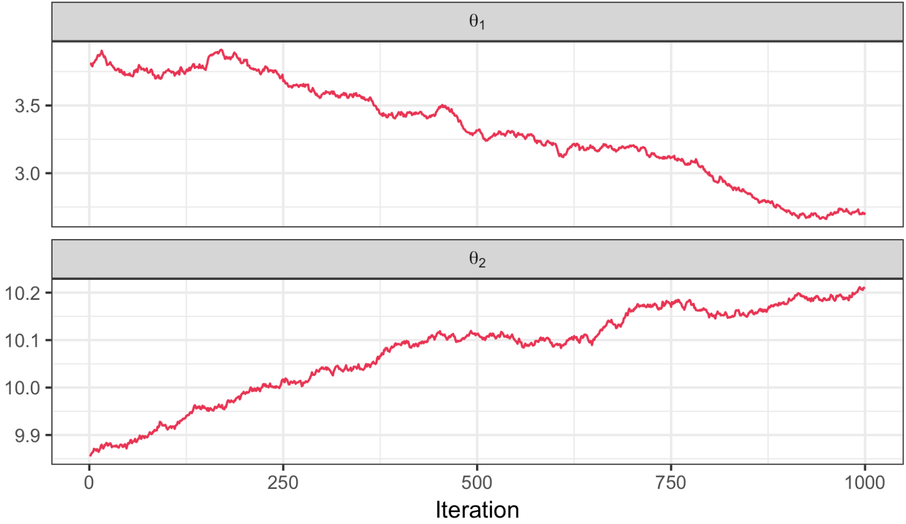

Why we're talking about Stan today

- Highly efficient sampling from complex Bayesian models that Gibbs and Metropolis-Hastings might fail at
- Interfaces to R, Python, Matlab, etc.
- Coding errors limited to the model (not sampling algorithm)
- Diagnostic tools to evaluate if your sampler works
- Might require you to learn a new programming language (not necessarily)

Roadmap

Part 1: Introduction to Hamiltonian Monte Carlo and Stan

- Sampling from complex Bayesian models using standard methods is inefficient and error-prone
- Hamiltonian Monte Carlo (HMC) offers huge improvements
- Intuition for how HMC works
- Implementing an HMC sampler in Stan

Part 2: Alina Ferecatu on hierarchical logit and models of bounded rationality

Part 3: Hernan Bruno on multivariate Tobit and two-stage "hurdle" models

Setup

- **Goal:** Sample from some distribution (the target)
  - Typically a Bayesian posterior distribution, $\pi(\theta|y, x)$
  - But generally any distribution $\pi(\theta)$
- **Requirements:**
  - All elements $\theta_i \in \theta$ (parameters) are continuous
    - Discrete parameters cannot be sampled
    - Usually they can be integrated out before sampling
  - Target distribution can be evaluated at any permitted value of θ
    - With or without normalizing constant

Common approaches for Bayesian models

- Metropolis-Hastings (MH) or Gibbs sampling
- Typical problems:
  - High parameter correlation kills efficiency
  - Finite chains may dramatically over- and under-sample certain regions, with biased inferences
    - Convergence guaranteed *asymptotically*
- Many alternatives alleviate these problems
  - One discussed today: Hamiltonian Monte Carlo (HMC)

Hamiltonian Monte Carlo

Hamiltonian mechanics

- Idealized physical model of random particle motion
- A particle's potential energy is $-\log \pi(\theta)$
  - Start thinking of θ as the parameter vector and $\pi(\theta)$ its density
- Particle has mass M, momentum p, and position θ
  - Start thinking of p as the random step in standard random-walk Metropolis, and M as its step size
- Total energy of the physical system is constant

Hamiltonian equations

- Hamilton's equations describe the particle's motion in continuous time

$$\text{Change in position:} \quad \frac{\mathrm{d}\theta}{\mathrm{d}t} = M^{-1}p$$

$$\text{Change in momentum:} \quad \frac{\mathrm{d}p}{\mathrm{d}t} = \nabla_\theta \log\left[\pi\left(\theta\right)\right]$$

- Motion is like "a frictionless puck that slides over a surface of varying height" (Neal 2011, p.2)
- I prefer: "a frictionless skateboarder in an empty swimming pool"

one_particle.mp4

Idealized version of Hamiltonian MC (HMC) sampling

- Take a particle and give it a random shove (momentum p)
  - Let it move for a while and then stop it
  - Record its position (value of the parameter vector θ)
- Give it another random shove
  - Let it more for a while and then stop it
  - Record its position again
- Repeat

Idealized version of Hamiltonian MC (HMC) sampling

hmct1.mp4...

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hmct2.mp4...

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Idealized version of Hamiltonian MC (HMC) sampling

hmct3.mp4...

Idealized version of Hamiltonian MC (HMC) sampling

hmct4.mp4...

Idealized version of HMC is just that…an ideal

- It would generate exact samples from target distribution
- However:
  - Analytical solutions to this continuous time model aren't available
  - Numerical approximation is necessary
- Solution:
  - Discretize the model by dividing time into discrete steps
  - Simulate the particle's motion in discrete time

Discretized version of HMC

- Discretize time into small steps of length ϵ, leading to sampling trajectories

$$\theta^{(t)} \rightarrow \theta^{(t+\epsilon)} \rightarrow \theta^{(t+2\epsilon)} \rightarrow \theta^{(t+3\epsilon)} \rightarrow \theta^{(t+4\epsilon)} \rightarrow \cdots \rightarrow \theta^{(t+1)}$$

  - Monte Carlo samples are t and $t+1$
  - $t+\epsilon$, $t+2\epsilon$, etc. are intermediate "leapfrog" steps
- No longer a trajectory in $\pi(\theta)$, but close
  - Must correct for discrepancy between continuous model and discrete approximation
  - Occasionally reject samples (as in MH) to correct for discrepancy

ani.mp4

Costs and benefits of standard HMC

- Benefits:
  - Rarely rejects proposals, lower autocorrelation
  - Almost always more efficient than Gibbs or MH
- Costs:
  - Need to compute $\nabla_\theta \log \pi(\theta)$, the gradient (first derivative) of the log of the target density, with respect to the parameters θ, for all L intermediate steps
  - Calculus is hard
    - However: Automatic differentiation will save us

Detour: What is automatic differentiation?

- While computing the value of a function, obtain exact values of derivatives of that function
- Not magic: Exploit the chain rule from calculus:

$$(f \circ g)' = (f' \circ g)g' \qquad \text{...or...}$$

$$\frac{\partial}{\partial x} f(g(x)) = f'(g(x))g'(x)$$

- Example: mean μ of normal distribution:

$$\begin{array}{ccccccccc} -\frac{1}{2}(y-\mu)^2 & = & \mu & \rightarrow & y-(\cdot) & \rightarrow & (\cdot)^2 & \rightarrow & -\frac{1}{2}(\cdot) \\ & & & & \downarrow & & \downarrow & & \downarrow \\ \frac{\partial}{\partial \mu} & = & & & -1 & \times & 2(y-\mu) & \times & -\frac{1}{2} \end{array}$$

Comparison of HMC and RW Metropolis

hmc.rw.mp4

Stan

Stan for Hamiltonian Monte Carlo

- In its simplest form, Stan implements an HMC sampler
  - You specify the target distribution $\pi(\theta)$ in a way Stan can understand
  - Stan generates and compiles C++ code to evaluate $\pi(\theta)$ *and* $\nabla_\theta \log \pi(\theta)$
  - Stan adapts the HMC step size during a burn-in phase
- HMC samplers are (notoriously?) difficult to tune
  - The the total length of the path followed by the particle (integration length) affects sampling efficiency

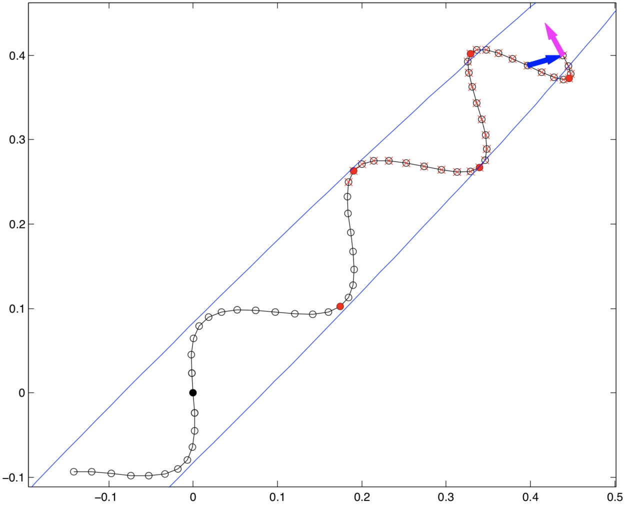
An inefficient HMC sampler

badL.mp4

Stan's NUTS sampler

- Stan also implements the No U-Turn Sampler
- Stops the particle when the sampler detects it has started making a U-Turn
- Only tuning parameter needed is ϵ (the step size) which Stan tunes during burn-in

Stopping before a U-turn



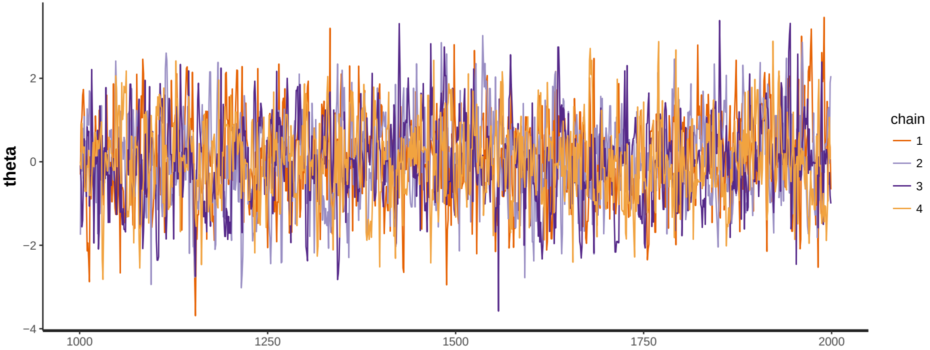
Basics of a Stan model

```
parameters {
  real theta;
}
model {
  theta ~ normal(0, 1);
}
```

```
sm <- stan_model(model_code = ...)
fit <- sampling(sm)
```

Output from a basic Stan model

```
stan_trace(fit)
```



Bayesian linear regression example

- Data y and X
  - n observations in y and X
  - p columns in X
- Likelihood: $y|X \sim N(\alpha + X\beta, \sigma^2)$
- Priors:
  - $\alpha, \beta \sim N(0, 1)$
  - $\sigma \sim Expo(1)$

Stan model for linear regression

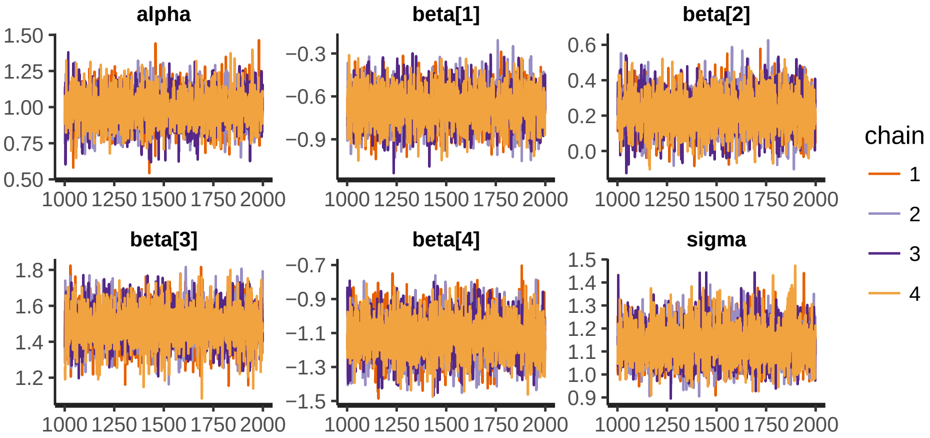
```
data {
  int<lower = 0> n;
  int<lower = 0> p;
  vector[n] y;
  matrix[n, p] X;
}
parameters {
  real alpha;
  vector[p] beta;
  real<lower = 0> sigma;
}
model {
  alpha ~ normal(0, 1);
  beta ~ normal(0, 1);
  sigma ~ exponential(1);

  y ~ normal(alpha + X * beta, sigma);
}
```

Compiling and sampling from R

```r
library(rstan)
sm <- stan_model(file = 'my_model.stan')

X <- ...
y <- ...
d <- list(n = nrow(X), p = ncol(X),
          X = X, y = y)

fit <- sampling(sm, data = d)
```

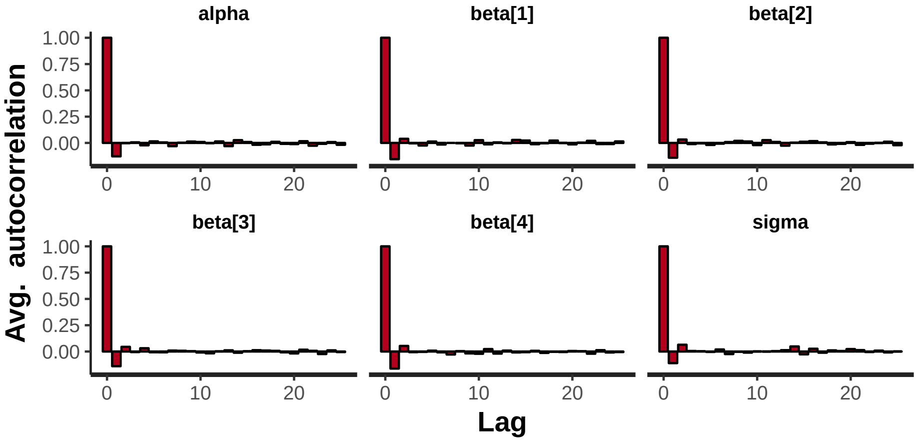
Trace plots

```
stan_trace(fit)
```



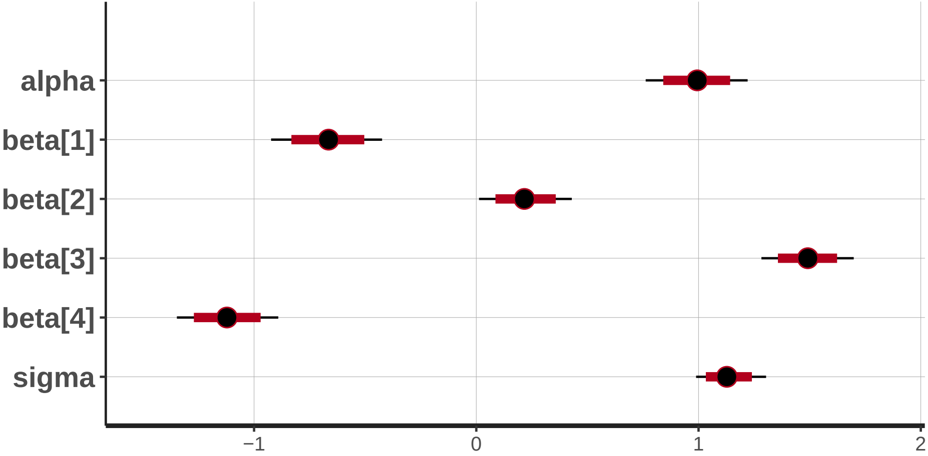
Sample autocorrelation

```
stan_ac(fit)
```



Posterior means and intervals

```
stan_plot(fit)
```



Parts of a Stan model

```
functions { ... }

data { ... }

transformed data { ... }

parameters { ... }

transformed parameters { ... }

model { ... }

generated quantities { ... }
```

Stan Inside™

What if I don't want to write my own Stan code?

```
library(rstanarm)
fit <- stan_glm(y ~ 1 + X1 + X2 + X3 + X4, data = d,
                prior = normal(0, 1),
                prior_intercept = normal(0, 1),
                prior_aux = exponential(1))
```

- `rstanarm` uses Stan to estimate complex hierarchical and non-gaussian models
- Created by Stan team, integrates nicely with `bayesplot`
  - Another alternative is `brms`, but `rstanarm` seems better so far

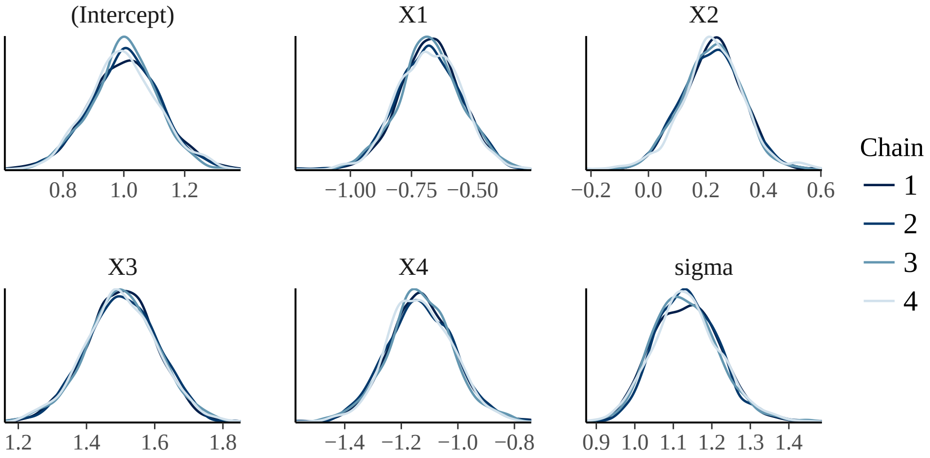
```r
summary(fit)
```

```
Model Info:

 function:     stan_glm
 family:       gaussian [identity]
 formula:      y ~ 1 + X1 + X2 + X3 + X4
 algorithm:    sampling
 priors:       see help('prior_summary')
 sample:       4000 (posterior sample size)
 observations: 100
 predictors:   5

Estimates:
                mean   sd     2.5%   25%    50%    75%    97.5%
(Intercept)     1.0    0.1    0.8    0.9    1.0    1.1    1.2
X1             -0.7    0.1   -0.9   -0.8   -0.7   -0.6   -0.4
X2              0.2    0.1    0.0    0.2    0.2    0.3    0.4
X3              1.5    0.1    1.3    1.4    1.5    1.6    1.7
X4             -1.1    0.1   -1.3   -1.2   -1.1   -1.1   -0.9
sigma           1.1    0.1    1.0    1.1    1.1    1.2    1.3
mean_PPD        1.1    0.2    0.8    1.0    1.1    1.2    1.4
log-posterior -161.3    1.8 -165.8 -162.2 -161.0 -160.0 -158.9
```

```
Diagnostics:
              mcse Rhat n_eff
(Intercept)   0.0  1.0  4000
X1            0.0  1.0  4000
X2            0.0  1.0  4000
X3            0.0  1.0  4000
X4            0.0  1.0  4000
sigma         0.0  1.0  4000
mean_PPD      0.0  1.0  4000
log-posterior 0.0  1.0  1724

For each parameter, mcse is Monte Carlo standard error, n_eff is a crude
measure of effective sample size, and Rhat is the potential scale reduction
factor on split chains (at convergence Rhat=1).
```

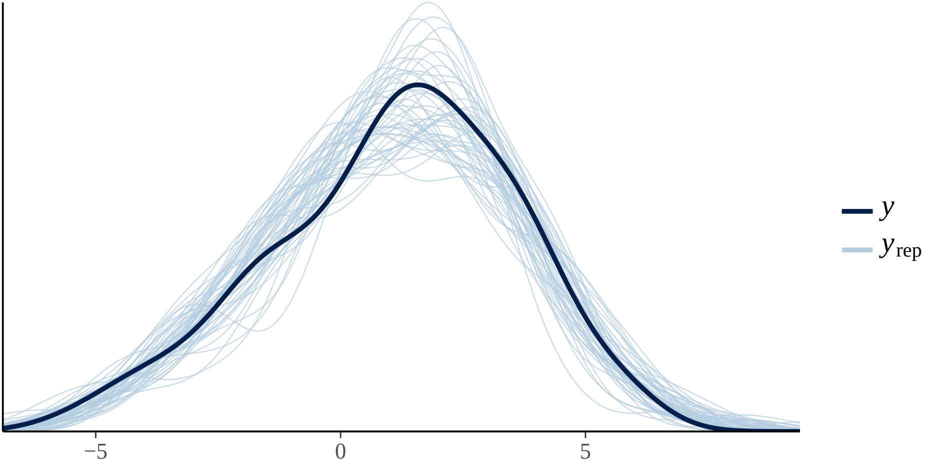
Density overlays

```
fit %>% as.array() %>% bayesplot::mcmc_dens_overlay()
```



Posterior predictive checks

```
pp_check(fit)
```



Automatic integration with loo

```
loo(fit)

Computed from 4000 by 100 log-likelihood matrix

         Estimate   SE
elpd_loo   -157.0  5.4
p_loo         5.5  0.7
looic       314.1 10.9
------
Monte Carlo SE of elpd_loo is 0.0.

All Pareto k estimates are good (k < 0.5).
See help('pareto-k-diagnostic') for details.
```

Conclusion

Why Stan is so important

- Coding errors confined to model specification
- If Stan fails, more likely due to a problem with your model than Stan
  - Numerically ill-conditioned
  - Non-identified
  - Improper posterior
- Nothing privileged about conjugacy
  - Choose priors based on what makes sense for the model
- Stan best practices and defaults should be MCMC best practices and defaults
  - Sampling diagnostics based on output from HMC
  - $\hat{R}$ for assessing convergence
  - Model comparison via the `loo` package

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