Solving Inverse Problems with Bayesian Inference

Bob Carpenter

Center for Computational Mathematics

Flatiron Institute

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https://mc-stan.org

Uncertainty

- permeates **science** and **decision making**
- in the form of
  - **sampling** uncertainty,
  - **measurement** uncertainty, and
  - **modeling** uncertainty.

- The **alternative to good statistics** is
  - not no statistics,
  - but **bad statistics**. (Bill James)

Probability & Statistics

- Probability theory uses math to **quantify uncertainty**.
- **Bayesian statistics** applies probability theory to
  - data analysis,
  - prediction & forecasting,
  - model evaluation, and
  - decision theory.
- The **computational bottlenecks** are
  - model expression and
  - posterior inference.

Probability is ...

Every event is in itself certain, not probable; if we knew all, we should either know positively that it will happen, or positively that it will not. But its **probability** to us means the **degree of expectation of its occurrence, which we are warranted in entertaining by our present evidence**.

– **John Stuart Mill**. 1882. *A System of Logic: Ratiocinative and Inductive*. Eighth edition. III:18.

The chance of rain in Edinburgh?

- What's the chance of rain in Edinburgh, Scotland?
  - if it could be any day of the year: 52%
  - if I know the month is October: 55%
  - if I also know it's 24h from now: 55%
  - if I also have today's weather report: 80%
  - if it's now and I see rain: 100%
- The world didn't change, our knowledge of it did.
- Coin flips are the same!

Simulate some Baseball (or clinical trials)

- True .300 on base percentage (OBP) then simulate
  - **10 at bats** (.000 to .600 OBP)

    1 1 2 6 2 0 4 4 4 2
  - **100 at bats** (0.220 to 0.330 OBP)

    22 34 30 26 25 31 31 28 27 33
  - **1000 at bats** (.294 to .320 OBP)

    296 307 302 298 290 297 303 294 280 320
  - **10,000 at bats** (.295 to .305 OBP)

    3022 2953 2987 2946 2994 2989 3052 3024 3038 2938

Bayesian Inference

Notation

- Variables
  - y : **data** (observed)
  - θ : **parameters** (unknown)

- Probability functions
  - $p(y, \theta)$: **joint** density
  - $p(y \mid \theta)$: **sampling** density (**likelihood** as fun of θ)
  - $p(\theta)$: **prior** (parameter marginal)
  - $p(\theta \mid y)$: **posterior**
  - $p(y)$: **evidence** (data marginal)

Bayes's rule

$$
\begin{aligned}
p(\theta \mid y) &= \frac{p(y,\theta)}{p(y)} \\
&= \frac{p(y \mid \theta) \cdot p(\theta)}{p(y)} \\
&= \frac{p(y \mid \theta) \cdot p(\theta)}{\int_{\Theta} p(y,\theta)\,\mathrm{d}\theta} \\
&= \frac{p(y \mid \theta) \cdot p(\theta)}{\int_{\Theta} p(y \mid \theta) \cdot p(\theta)\,\mathrm{d}\theta} \\
&\propto p(y \mid \theta) \cdot p(\theta).
\end{aligned}
$$

- **Posterior** proportional to **likelihood times prior**

Estimates, events, and predictions

- **Parameter estimate**

$$\hat{\theta} \;=\; \mathbb{E}[\theta \mid y] \;=\; \int_{\Theta} \theta \cdot p(\theta \mid y)\,\mathrm{d}\theta$$

- **Event probability** ($A \subseteq \Theta$, e.g., $A = \{\theta \,.\, \theta > 0\}$)

$$\Pr[A \mid y] \;=\; \mathbb{E}[\mathrm{I}_A(\theta) \mid y] \;=\; \int_{\Theta} \mathrm{I}_A(\theta) \cdot p(\theta \mid y)\,\mathrm{d}\theta$$

- **Predictive inference**

$$p(\tilde{y} \mid y) \;=\; \mathbb{E}[p(\tilde{y} \mid \theta) \mid y] \;=\; \int_{\Theta} p(\tilde{y} \mid \theta) \cdot p(\theta \mid y)\,\mathrm{d}\theta$$

(Markov chain) Monte Carlo

- Given **sample** $\theta^{(1)}, \ldots, \theta^{(M)} \sim p(\theta \mid y)$.
- General **plug-in expectation** calculations,

$$\begin{aligned}
\mathbb{E}[f(\theta) \mid y] &= \int_\Theta f(\theta) \cdot p(\theta \mid y)\, \mathrm{d}\theta \\
&= \lim_{M \to \infty} \frac{1}{M} \sum_{m=1}^{M} f\left(\theta^{(m)}\right) \\
&\approx \frac{1}{M} \sum_{m=1}^{M} f\left(\theta^{(m)}\right).
\end{aligned}$$

- (MCMC) central limit theorem **approx. error** $\propto \dfrac{1}{\sqrt{M_{(\mathrm{eff})}}}$

Example 1

Birth Ratio

Birth ratio (Laplace, 1781)

- **Live births** in Paris, 1745–1770
  - $y = 251,527$ male, $N = 493,472$ total
- **Sampling**: $p(y \mid N, \theta) = \text{binomial}(y \mid N, \theta)$.
- **Prior**: $p(\theta) = \text{uniform}(\theta \mid 0, 1)$
- **Posterior**: $p(\theta \mid y) = \text{beta}(\theta \mid 1 + y,\ 1 + N - y)$.

- $\Pr[\theta \in (0.508, 0.512)] = 0.99$ (estimated **male birth rate**)
- $\Pr[\theta > 0.5] \approx 1 - 10^{-42}$ (“morally certain” **more boys**)

Coding in Stan

```
data {
  int y;  // boys = 251527
  int N;  // total = 493472
}
parameters {
  real<lower=0, upper=1> theta;
}
model {
  y ~ binomial(N, theta);
  theta ~ uniform(0, 1);
}
generated quantities {
  int<lower=0, upper=1> theta_gt_half = (theta > 0.5);
  int<lower = 0> y_sim = binomial_rng(100, theta);
}
```

Executing

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

                mean se_mean   0.5%   99.5%
theta          0.510   0.000  0.508   0.512
theta_gt_half  1.000     NaN  1.000   1.000
y_sim         50.902   0.081 38.000  64.000
```

- **estimate** $\hat{\theta}$ is posterior sample **mean** for θ;
- 99% **interval** for θ estimated by sample **quantiles**
- $\Pr[\theta > 0.5]$ estimated by sample **mean of indicator**
- y_sim estimated **forecast** for next 100 births

Workflow

Bayesian Workflow

1. Design experiment & **collect data** (its own workflow)

2. Model evaluation

   - **prior predictive checks**: is the prior sensible?
   - **simulation-based calibration**: does the algorithm work on data simulated from the model?
   - **posterior predictive checks**: does model capture relevant aspects of real data?
   - **hold out/cross-validation**: does model predict well?

3. If model is lacking, **improve model and repeat (2)**

   - and if data is lacking, collect more and repeat (1)

Calibration

Calibration

- Empirical (frequentist) evaluation of **probabilistic forecasts**
- Of the days on which a 75% of rain is forecast, roughly 75% of them should be rainy.
  - for N **calibrated predictions** of probability θ, $Y \sim \mathrm{binomial}(N, \theta)$ will obtain
- Calibrated predictions for **rain in Edinburgh**:
  - 52% is calibrated if evaluated over random days of the year.
  - Prediction based on average for day of month is calibrated (i.e., 65% for December)
  - Is `weather.com`'s forecast calibrated? Empirical question.

Sharpness

- Sharp probabilistic predictions have **low entropy**.
- **Narrowly concentrated** predictions are sharper
  - $\Pr[\alpha \in (.58, .59)] = .9$ sharper than $\Pr[\alpha \in (.5, .6)] = .9$
- Probabilistic predictions **nearer 0 or 1** are sharper
  - $\Pr[z_i = 1] = 0.95$ sharper than $\Pr[z_i = 1] = 0.6$

Inference evaluation criterion

- For probabilistic forecasts:

  Maximize sharpness subject to calibration.

- **Goal**: consistent, useful inference from **finite data**.
  - cf. minimize variance subject to zero bias for estimators
- Bayesian models are calibrated if they are **well-specified**
  - i.e., they capture the true data-generating process.
  - But, models are always approximate.
  - So, need to test fit to real data and predictions.

Example 2

Population Dynamics

Population Dynamics (Volterra 1926)

- populations at time t of prey $u(t)$ & predator $v(t)$
- Volterra's mechanistic model

$$\frac{\mathrm{d}}{\mathrm{d}t}u = (\alpha - \beta \cdot v) \cdot u \qquad \frac{\mathrm{d}}{\mathrm{d}t}v = (-\gamma + \delta \cdot u) \cdot v$$

  – α: prey growth rate; β: predation shrinkage
  – γ: predator shrinkage; δ: predation growth

Analytic solution (Volterra 1926)

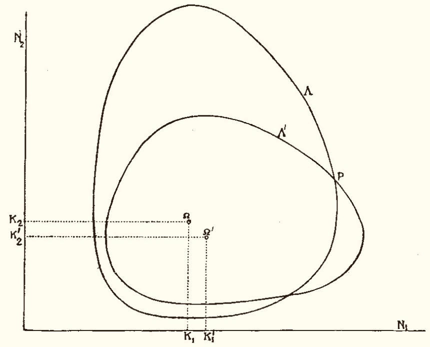


FIG. 1.

Knowns and Unknowns

- **Knowns**
  - number of pelts collected at each time
- **Unknowns**
  - initial populations
  - subsequent populations
  - growth and shrinkiage parameters $\alpha, \beta, \gamma, \delta$

Measurement/model error

- u, v are observed
- $\hat{u}, \hat{v}$ predicted by mechanistic model
- Independent **error proportional to population** size
  - $u_t \sim \text{lognormal}(\hat{u}_t, \sigma_1)$
  - $v_t \sim \text{lognormal}(\hat{v}_t, \sigma_2)$
- Weakly informative **priors determine scale**
  - $\alpha, \gamma \sim \text{normal}(1, 0.5); \quad \beta, \delta \sim \text{normal}(0.05, 0.05)$
  - $\sigma_1, \sigma_2 \sim \text{lognormal}(-1, 1)$

Assumptions

- pelts are a reasonable proxy for the populations
  - could try to validate with mark/recapture
- population only depends on population of predator and prey
  - no outside shocks like weather, epidemics, other predators, etc.
- rough scale of solutions known ahead of time
- measurement error is proportional to population size

Normal and log normal

- Normal density is the usual bell curve, with

$$\text{normal}(y \mid \mu, \sigma) \propto \frac{1}{\sigma} \exp\left(-\frac{1}{2}\left(\frac{y-\mu}{\sigma}\right)^2\right)$$

- If y has a $\text{normal}(\mu, \sigma)$ distribution, then $\exp(y)$ has a $\text{lognormal}(\mu, \sigma)$ distribution.

- 95% intervals for normal are roughly $\mu \pm 2\sigma$

- 95% intervals for lognormal are roughly

$$\exp(\mu \pm 2\sigma) = \exp(\mu) \overset{\times}{\div} \exp(2\sigma)$$

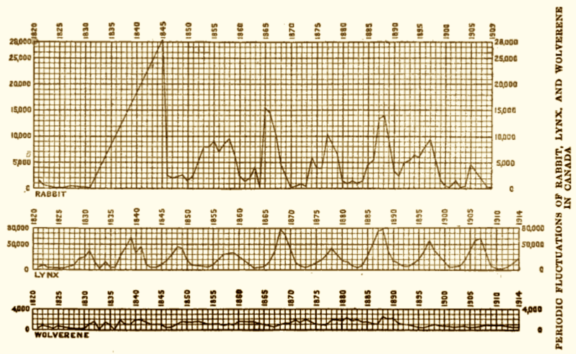
The Lynx and the Hare

- **Lynx** (left) are predators who prey almost exclusively on **snowshoe hares** (right)

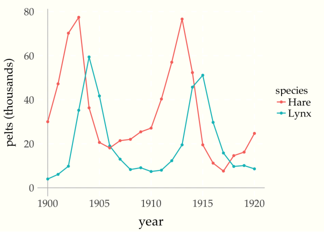
- But it's very labor intensive to count animals with standard mark/recapture techniques

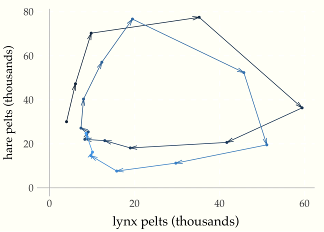
Hudson's Bay Co. pelts (Hewitt 1921)

- A proxy is the number of animals captured for pelts.



Plotted pelt data





- *left)* pelts vs. time (line per species)

  right) hare vs. lynx pelts (over time)

- pelt data assumed proportional to population

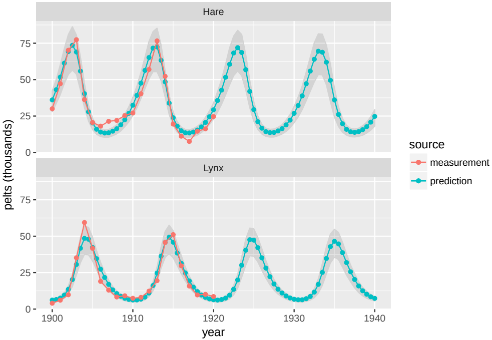
- w/o modeling relation, **model predicts pelts**

Stan dynamics & error

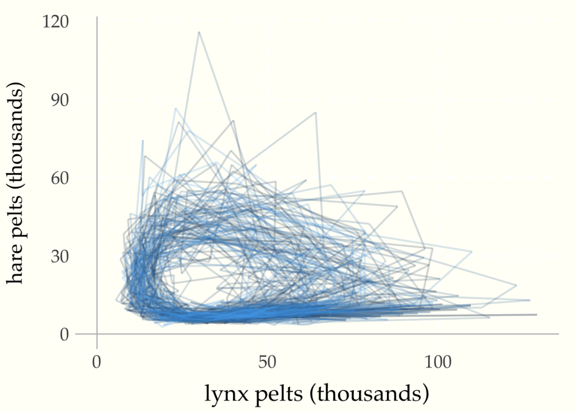
```
real[] duv_dt(real t, real[] uv, real[] theta,
              real[] theta, real[] x_r, int[] x_i) {
  return { (theta[1] - theta[2] * uv[2]) * uv[1],
           (-theta[3] + theta[4] * uv[1]) * uv[2] };
}
...
real uv_hat[T, 2]
  = integrate_ode(duv_dt, z0, t0, sol_ts[1:T], theta,
                  rep_array(0.0, 0), rep_array(0, 0));
...
y[1:T, 1] ~ lognormal(uv_hat[1:T, 1], sigma_u);  // prey
y[1:T, 2] ~ lognormal(uv_hat[1:T, 2], sigma_v);  // predator
```

Measurements & predictions

- measured pelts (red) vs. fitted model and predictions (blue)



100 predictive draws



Identification of parameters?

- Posterior mean estimates minimize expected square error,

$$\hat{\alpha} = \mathbb{E}[\alpha \mid y] = \arg\min_{\alpha'} \mathbb{E}[(\alpha' - \alpha)^2 \mid y].$$

- Given the Hudson's Bay data, the estimates are

$$\hat{\alpha} = 0.55 \quad \hat{\beta} = 0.028 \quad \hat{\gamma} = 0.80 \quad \hat{\delta} = 0.024$$

$$\hat{\sigma}_1 = 0.25 \qquad \hat{\sigma}_2 = 0.25$$

- Posterior intervals are quite wide
  - $\Pr[0.45 \leq \alpha \leq 0.63] = 0.8 \quad \Pr[0.023 \leq \beta \leq 0.033] = 0.8$
  - $\Pr[0.69 \leq \gamma \leq 0.91] = 0.8 \quad \Pr[0.020 \leq \delta \leq 0.029] = 0.8$
  - $\Pr[0.20 \leq \sigma_1 \leq 0.31] = 0.8 \quad \Pr[0.20 \leq \sigma_2 \leq 0.31] = 0.8$

Summary

- mechanistic forward model of dynamics (Lotka 1926)
  - $\hat{y} = f(\theta)$
- error model $y_{t,k} \sim \mathrm{lognormal}(\hat{y}_{t,k}, \sigma_k)$
- added weakly informative priors $p(\theta)$ (fixing scale)
- Stan turns the Bayesian crank to sample from posterior
  - $\theta^{(1)}, \ldots, \theta^{(M)} \sim p(\theta \mid y)$.
- Estimates are sample means; intervals are sample quantiles; predictions are plug-in estimates
- This methodology **works for many scientific models**.

AI, ML, and Statistics

What is Artificial Intelligence (AI)?

- AI is about pushing frontier of “thinking” computers
  - playing Go, driving a car, translating natural language, recognizing images, . . .
- AI is not about a technique
  - according to Google and the European Union, regression is AI!
- machine learning (ML) is more difficult to characterize

Machine Learning (ML) and Stats (1)

- Traditional stats focuses on data analysis
- Traditional ML focuses on prediction
  - this is why ML is eating stats' lunch
- Bayesian stats is about data analysis *and* prediction

ML and Stats (2)

- Models
  - Stats focuses on interpretable, tractable parametric models
  - ML focuses on black-box, intractable, non-parametric models
- Inference
  - ML focuses on prediction based on plug-in point estimates
  - traditional stats focuses on estimates, confidence intervals, and hypothesis tests
  - Bayesian stats focuses on calibrated posterior uncertainty and uses probability for everything

ML and Stats (3)

- Scale
  - ML focuses largely on “big” data
  - Stats tries to squeeze info out of small data
  - Stats can build more model with more data (spatio-temporal, sub-population, etc.)
  - ML models tend to be more flexible and also scale with data

Questions / Comments?

Stan

What is Stan?

- a domain-specific **probabilistic programming language**
- Stan **program** defines a **differentiable** probability model
  - declares data and (constrained) parameter variables
  - defines log posterior (or penalized likelihood)
  - defines predictive quantities
- Stan **inference** fits model & makes predictions
  - MCMC for full Bayesian inference
  - variational and Laplace for approximate Bayes
- Carpenter, B., Gelman, A., Hoffman, M. D., Lee, D., Goodrich, B., Betancourt, M., Marcus Brubaker, Jiqiang Guo, Peter Li, Riddell, A. (2017). Stan: A probabilistic programming language. *J. Stat. Soft.* 76(1).

Availability & Usage

- *Platforms:* Linux, Mac OS X, Windows
- *Interfaces:* R, Python, Julia, MATLAB, Mathematica
- *Developers (academia & industry):* 40+ (15+ FTEs)
- *Users:* tens or hundreds of thousands
- *Companies using:* hundreds or thousands
- *Downloads:* millions
- *User's Group:* 3000+ registered; 6000+ non-bot views/day
- *Books using:* 10+
- *Courses using:* 100+
- *Case studies about:* 100+
- *Articles using:* 3000+
- *Conferences:* 4 (800+ attendance)

Some published applications

- **Physical sciences**: astrophysics, statistical mechanics, particle physics, (organic) chemistry, geology, oceanography, climatology, biogeochemistry, materials science, ...
- **Biological sciences**: molecular biology, clinical drug trials, entomology, pharmacology, toxicology, opthalmology, neurology, genomics, agriculture, botany, fisheries, epidemiology, population ecology, neurology, psychiatry, ...
- **Social sciences**: econometrics (macro and micro), population dynamics, cognitive science, psycholinguistics, social networks, political science, survey sampling, anthropology, sociology, social work, ...
- **Other**: education, public health, A/B testing, government, finance, machine learning, logistics, electrical engineering, transportation, actuarial science, sports, advertising, marketing, ...

Industries using Stan

- **marketing attribution**: Google, Domino's Pizza, Legendary Ent.
- **demand forecasting**: Facebook, Salesforce
- **financial modeling**: Two Sigma, Point72
- **pharmacology & CTs**: Novartis, Pfizer, Astra Zeneca
- **(e-)sports analytics**: Tampa Bay Rays, NBA, Sony Playstation
- **survey sampling**: YouGov, Catalist
- **agronomy**: Climate Corp., CiBO Analytics
- **real estate pricing models**: Reaktor
- **industrial process control**: Fero Labs

Why is Stan so Popular?

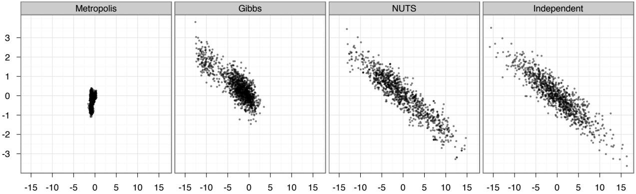
- **Community**: large, friendly, helpful, and sharing
- **Documentation**: novice to expert; breadth of fields
- **Robustness**: industrial-strength code; user diagnostics
- **Flexibility**: highly expressive language; large math lib
- **Portability**: popular OS, language, and cloud support
- **Extensibility**: developer friendly; derived packages
- **Speed**: $2 - \infty$ orders of magnitude faster
- **Scalability**: 2+ orders of magnitude more scalable
- **Openness**: permissive code and doc licensing

What Stan Does

No-U-turn sampler

- **Hamiltonian Monte Carlo** (HMC)
  - **Potential Energy**: negative log posterior $-\log p(\theta \mid y)$
  - **Kinetic Energy**: random standard normal each iteration
  - **geometric ergodicity** for wider range of models & data
- Adapt leapfrog algorithm **during warmup**
  - step size adapted to target acceptance rate
  - Euclidean metric estimated w. sample covariance
- Adapt leapfrog algorithm **during sampling**
  - simulate forward and backward in time until U-turn
  - multinomial sample trajectory propto energy; bias furthest
- developed concurrently w. Stan (Hoffman & Gelman 2011)

NUTS vs. Gibbs and Metropolis



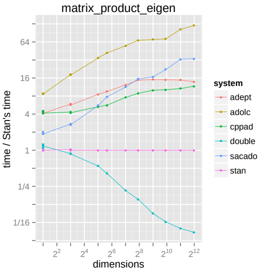
- Two dimensions from highly correlated 250-dim normal
- **1,000,000 draws** from Metropolis and Gibbs (thinned to 1000)
- **1000 draws** from NUTS; 1000 independent draws

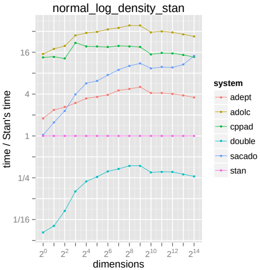
Reverse-mode autodiff (adjoint)

- Build up expression graph with values x and adjoints $\overline{x}$
- Differentiating $f . \mathbb{R}^N \rightarrow \mathbb{R}$ is additional $\mathcal{O}(1)$
- Set final result y's adjoint $\overline{y} = 1$ and proceed in reverse
- Example: scalar $c = \log a$
  - $\overline{a} \mathrel{+}= \overline{c} \cdot \frac{1}{a}$
- Example: scalar $c = a \cdot b$
  - $\overline{a} \mathrel{+}= \overline{c} \cdot b; \qquad \overline{b} \mathrel{+}= \overline{c} \cdot a$
- Example: matrix $C = A^{-1}$
  - $\overline{A} \mathrel{+}= -C^\top \cdot \overline{C} \cdot C^\top$

Stan's Autodiff vs. Alternatives

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





- Carpenter, B. et al. (2015). The Stan math library: Reverse-mode automatic differentiation in C++. *arXiv:*1509.07164

Forward-mode autodiff (tangent)

- Build tangents forward with values x and tangents $\dot{x}$
- Differentiating $f\,.\,\mathbb{R} \to \mathbb{R}^M$ is additional $\mathcal{O}(1)$
- To differentiate w.r.t. x, set $\dot{x} = 1$ and work forward
- Example: scalar $c = \log a$
  - $\dot{c} = \dot{a} \cdot \frac{1}{a}$
- Example: scalar $c = a \cdot b$
  - $\dot{c} = \dot{a} \cdot b + \dot{b} \cdot a$
- Example: matrix $C = A^{-1}$
  - $\dot{C} = -C \cdot \dot{A} \cdot C$

Higher-order autodiff

- Open up new algorithms exploiting curvature
  - Riemannian HMC, nested Laplace approximations (ala INLA), nested Jacobians for ODE solver, Newton solvers for optimizers and nested algebraic equations

- Considering log densities $f . \mathbb{R}^N \to \mathbb{R}$

- Second-order derivatives
  - nest reverse in forward adds $\mathcal{O}(N)$
  - nest forward in forward $\mathcal{O}(N^2)$

- Third-order derivatives
  - nest reverse in forward in forward $\mathcal{O}(N^2)$
  - nest forward in forward in forward $\mathcal{O}(N^3)$

Stan's shortcomings

- Failures
  - extreme varying posterior curvature (stiff—can't adapt)
  - floating point (e.g., log cdfs and ccdfs, gradients)
  - scalability of data and parameters
- Missing features
  - black-box log densities (cf. emcee in Python)
  - checkpointed autodiff for large Gaussian processes
  - filtering (online model updating)
  - stochastic algebraic & differential eqs, PDEs
  - structured data types, sparse data types & closures

Discrete parameters?

- **Stan's focus**: tractably **marginalized**
  - e.g., mixtures, HMMs, state-space models
  - **efficient** in theory due to Rao-Blackwell; in practice by eliminating combinatorics; much better tail behavior
  - marginalizations available wherever you find EM & MML
- **Out of scope**: combinatorially **intractable**
  - e.g., selection, clustering, random trees, neural nets
  - optimization is NP-hard or worse
  - thus **nobody knows how to get right** answer in general
  - some special cases can be fit
- **In between**: missing count data