Stan: Under the Bonnet

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34 active devs, ≈ 10 *full-time equivalents*

Stan 2.18.0 (June 2018) http://mc-stan.org

Linear Regression with Prediction

```
data {
  int<lower = 0> K;          int<lower = 0> N;
  matrix[N, K] x;            vector[N] y;
  int<lower = 0> N_p;        matrix[N_tilde, K] x_p;
}
parameters {
  vector[K] beta;            real<lower = 0> sigma;
}
model {
  y ~ normal(x * beta, sigma);
}
generated quantities {
  vector[N_p] y_p = normal_rng(x_p * beta, sigma);
}
```

Stan Language

Stan is a Programming Language

- **Not** a graphical specification language like BUGS or JAGS
- Stan is a Turing-complete imperative programming language for specifying differentiable log densities
  - reassignable local variables and scoping
  - full conditionals and loops
  - functions (including recursion)
- With automatic "black-box" inference on top (though even that is tunable)
- Programs computing same thing may have different efficiency

Basic Program Blocks

- **`data`** (once)
  - *content*: declare data types, sizes, and constraints
  - *execute*: read from data source, validate constraints
- **`parameters`** (every log prob eval)
  - *content*: declare parameter types, sizes, and constraints
  - *execute*: transform to constrained, Jacobian
- **`model`** (every log prob eval)
  - *content*: statements defining posterior density
  - *execute*: execute statements

Derived Variable Blocks

- **`transformed data`** (once after data)
  - *content*: declare and define transformed data variables
  - *execute*: execute definition statements, validate constraints
- **`transformed parameters`** (every log prob eval)
  - *content*: declare and define transformed parameter vars
  - *execute*: execute definition statements, validate constraints
- **`generated quantities`** (once per draw, `double` type)
  - *content*: declare and define generated quantity variables; includes pseudo-random number generators
    (for posterior predictions, event probabilities, decision making)
  - *execute*: execute definition statements, validate constraints

Model: Read and Transform Data

- Only done once for optimization or sampling (per chain)
- Read data
  - read data variables from memory or file stream
  - validate data
- Generate transformed data
  - execute transformed data statements
  - validate variable constraints when done

Model: Log Density

- *Given* parameter values on unconstrained scale
- Builds expression graph for log density (start at 0)
- Inverse transform parameters to constrained scale
  - constraints involve non-linear transforms
  - e.g., positive constrained x to unconstrained $y = \log x$
- account for curvature in change of variables
  - e.g., unconstrained y to positive $x = \log^{-1}(y) = \exp(y)$
  - e.g., add log Jacobian determinant, $\log \left| \frac{d}{dy} \exp(y) \right| = y$
- 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 evaluate log density

Model: Generated Quantities

- **Given** parameter values
- Once per iteration (not once per leapfrog step)
- May involve (pseudo) random-number generation
  - Executed generated quantity statements
  - Validate values satisfy constraints
- Typically used for
  - Event probability estimation
  - Predictive posterior estimation
- Efficient because evaluated with `double` types (no autodiff)

Variable Transforms

- Code HMC and optimization with $\mathbb{R}^n$ **support**
- Transform constrained parameters to unconstrained
  - lower (upper) bound: offset (negated) log transform
  - lower and upper bound: scaled, offset logit transform
  - simplex: centered, stick-breaking logit transform
  - ordered: free first element, log transform offsets
  - unit length: spherical coordinates
  - covariance matrix: Cholesky factor positive diagonal
  - correlation matrix: rows unit length via quadratic stick-breaking

Variable Transforms (cont.)

- Inverse transform from unconstrained $\mathbb{R}^n$
- Evaluate log probability in model block on natural scale
- Optionally adjust log probability for change of variables
  - adjustment for MCMC and variational, not MLE
  - add log determinant of inverse transform Jacobian
  - automatically differentiable

Variable and Expression Types

Variables and expressions are **strongly, statically typed**.

- **Primitive**: `int, real`
- **Matrix**: `matrix[M,N], vector[M], row_vector[N]`
- **Bounded**: primitive or matrix, with
  `<lower=L>, <upper=U>, <lower=L,upper=U>`
- **Constrained Vectors**: `simplex[K], ordered[N], positive_ordered[N], unit_length[N]`
- **Constrained Matrices**: `cov_matrix[K], corr_matrix[K], cholesky_factor_cov[M,N], cholesky_factor_corr[K]`
- **Arrays:** of any type (and dimensionality)

Integers vs. Reals

- Different types (conflated in BUGS, JAGS, and R)
- Distributions and assignments care
- Integers may be assigned to reals but not vice-versa
- Reals have not-a-number, and positive and negative infinity
- Integers single-precision up to +/- 2 billion
- Integer division rounds (Stan provides warning)
- Real arithmetic is inexact and reals should not be (usually) compared with ==

Arrays vs. Vectors & Matrices

- Stan separates arrays, matrices, vectors, row vectors
- Which to use?
- Arrays allow most efficient access (no copying)
- Arrays stored first-index major (i.e., 2D are row major)
- Vectors and matrices required for matrix and linear algebra functions
- Matrices stored column-major (memory locality matters)
- Are not assignable to each other, but there are conversion functions

"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, lambda));`
- * up to a constant
- Sampling statement drops constant terms

What Stan Does

Full Bayes: No-U-Turn Sampler

- Adaptive **Hamiltonian Monte Carlo** (HMC)
  - **Potential Energy**: negative log posterior
  - **Kinetic Energy**: random standard normal per iteration
- Adaptation **during warmup**
  - step size adapted to target total acceptance rate
  - mass matrix (scale/rotation) estimated with regularization
- Adaptation **during sampling**
  - simulate forward and backward in time until U-turn
  - **discrete sample** along path prop to density

(Hoffman and Gelman 2011, 2014)

Adaptation During Warmup

- (I) initial fast interval to find typical set
  (adapt step size, default 75 iterations)
- (II) expanding memoryless windows to estimate metric
  (adapt step size & metric, initial 25 iterations)
- (III) final fast interval for final step size
  (adapt step size, default 50 iterations)

Posterior Inference

- Generated quantities block for **inference**:
  predictions, decisions, and event probabilities
- **Extractors** for samples in RStan and PyStan
- Coda-like **posterior summary**
  - posterior mean w. MCMC std. error, std. dev., quantiles
  - split-$\hat{R}$ multi-chain convergence diagnostic (Gelman/Rubin)
  - multi-chain effective sample size estimation (FFT algorithm)
- Model comparison with approximate or exact leave-one-out cross-validation

MAP / Penalized MLE

- Posterior **mode finding** via L-BFGS optimization
  (uses model gradient, efficiently approximates Hessian)
- **Disables Jacobians** for parameter inverse transforms
- Models, data, initialization as in MCMC
- **Standard errors** on unconstrained scale
  (estimated using curvature of penalized log likelihood function)
- Standard errors **on constrained scale**
  (sample unconstrained approximation and inverse transform)
- From Bayesian perspective, Laplace approximation to posterior

“Black Box” Variational Inference

- **Black box** so can fit any Stan model
- Multivariate **normal approx to unconstrained** posterior
  - covariance: diagonal (aka mean-field) or full rank
  - like Laplace approx, but around posterior mean, not mode
- **Gradient-descent** optimization
  - ELBO gradient estimated via Monte Carlo + autodiff
- Returns **approximate posterior** mean / covariance
- Returns **sample** transformed to constrained space

Stan as a Research Tool

- Stan can be used to **explore algorithms**
- Models transformed to **unconstrained support** on $\mathbb{R}^n$
- Once a model is compiled, have
  - **log probability, gradient, and Hessian**
  - data I/O and parameter initialization
  - model provides variable names and dimensionalities
  - transforms to and from constrained representation (with or without Jacobian)

Under Stan's Hood

Euclidean Hamiltonian Monte Carlo

- **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:

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

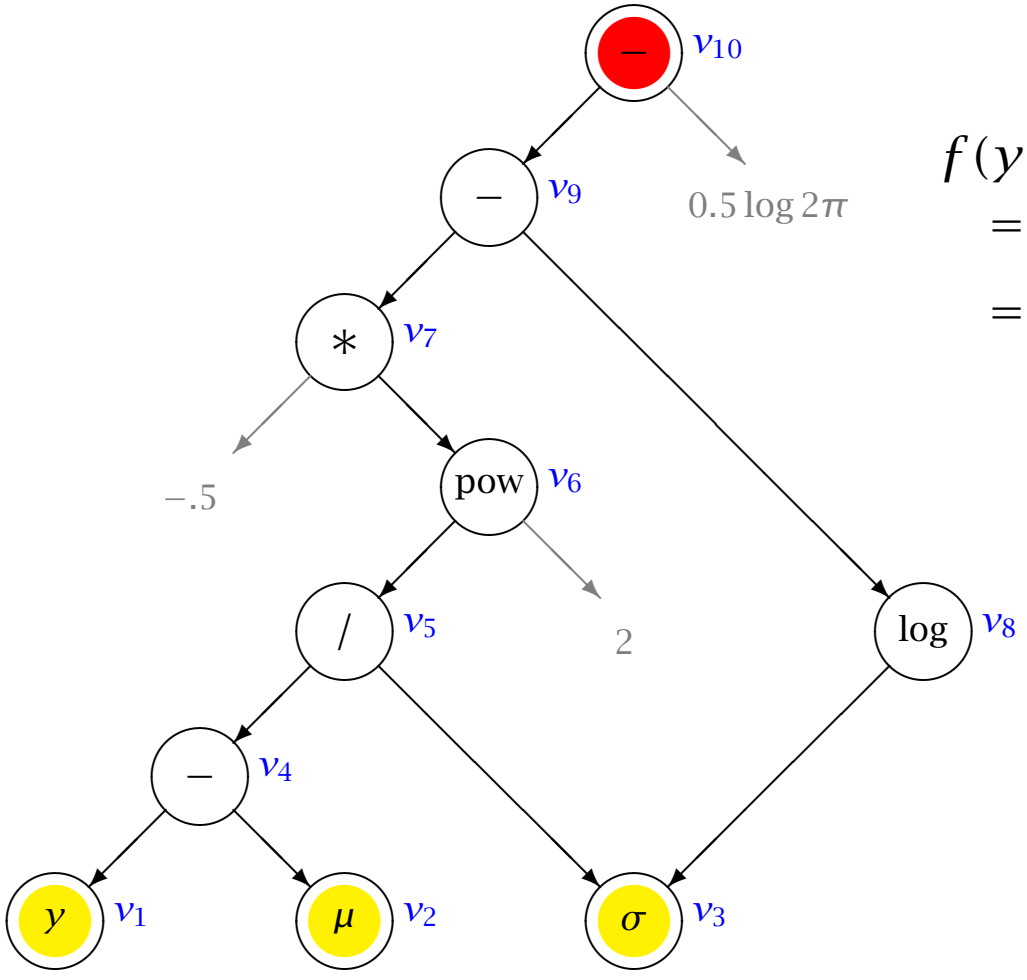
$$q \leftarrow q + \epsilon M^{-1} p \qquad \text{[full step in position]}$$

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

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



$$
\begin{aligned}
f(y, \mu, \sigma) &= \log\left(\text{Normal}(y|\mu, \sigma)\right) \\
&= -\frac{1}{2}\left(\frac{y-\mu}{\sigma}\right)^2 - \log\sigma - \frac{1}{2}\log(2\pi)
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial}{\partial y} f(y, \mu, \sigma) &= -(y-\mu)\sigma^{-2} \\
\frac{\partial}{\partial \mu} f(y, \mu, \sigma) &= (y-\mu)\sigma^{-2} \\
\frac{\partial}{\partial \sigma} f(y, \mu, \sigma) &= (y-\mu)^2\sigma^{-3} - \sigma^{-1}
\end{aligned}
$$

Autodiff Partials

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

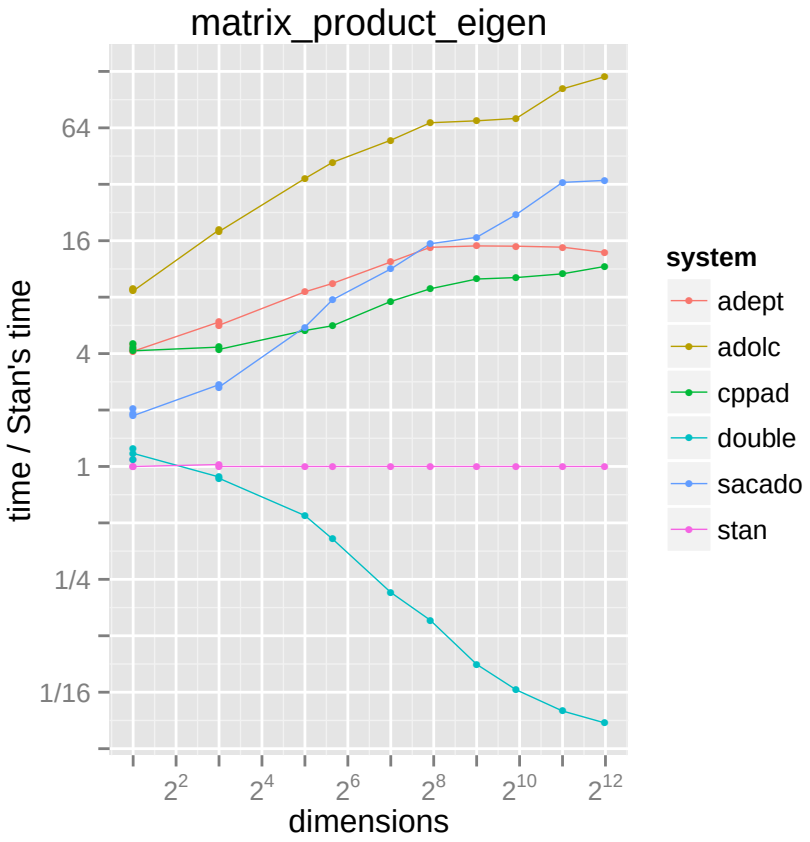
- Easily extensible **object-oriented** design
- **Code nodes** in expression graph for primitive functions
  - requires **partial derivatives**
  - built-in flexible abstract base classes
  - **lazy evaluation** of chain rule saves memory
- Autodiff through templated C++ functions
  - templating each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

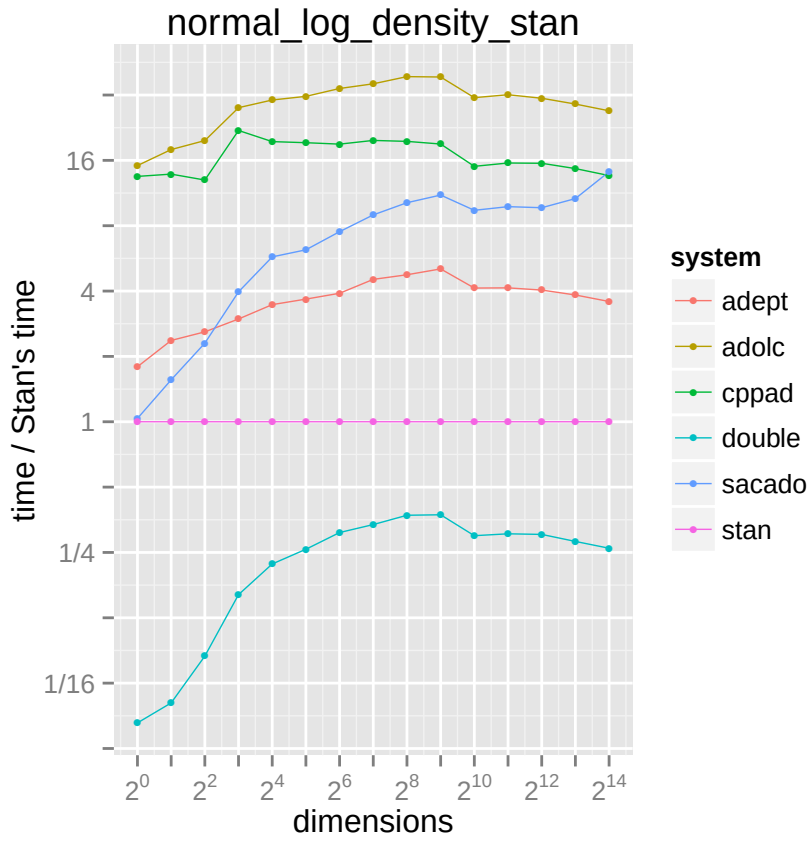
Stan's Reverse-Mode (cont.)

- 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**
- Adjoint-vector product formulation for **multivariates**
  - avoids N^2 memory cost of storing Jacobian
  - minimizes autodiff nodes and virtual function calls

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

- Required for Riemannian HMC
- Gradients of Hessians (tensor of third-order partials)

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

  - N^2 forward passes: gradient of derivative of derivative

Third-order Derivatives (cont.)

- Gradient of trace of Hessian times matrix
  - $\nabla \mathrm{tr}(H\,M)$, or
  - needed for Riemannian Hamiltonian Monte Carlo
  - computable in quadratic time for fixed M

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 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)

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

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

- Based on Eigen's Odeint package (RK45 non-stiff solver)

Stiff Diff Eqs

- Based on CVODES implementation of BDF (Sundials)
- CVODES builds-in efficient structure for sensitivity
- More nested autodiff required for system Jacobian
  - algebraic reductions save a lot of work

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
- Moving to **OCaml**—nearly complete
  - much cleaner and easier to manage than the C++
  - optimize by tranforming intermediate representations
- **Next**: tuples, ragged arrays, lambdas (closures)

Coding Probability Functions

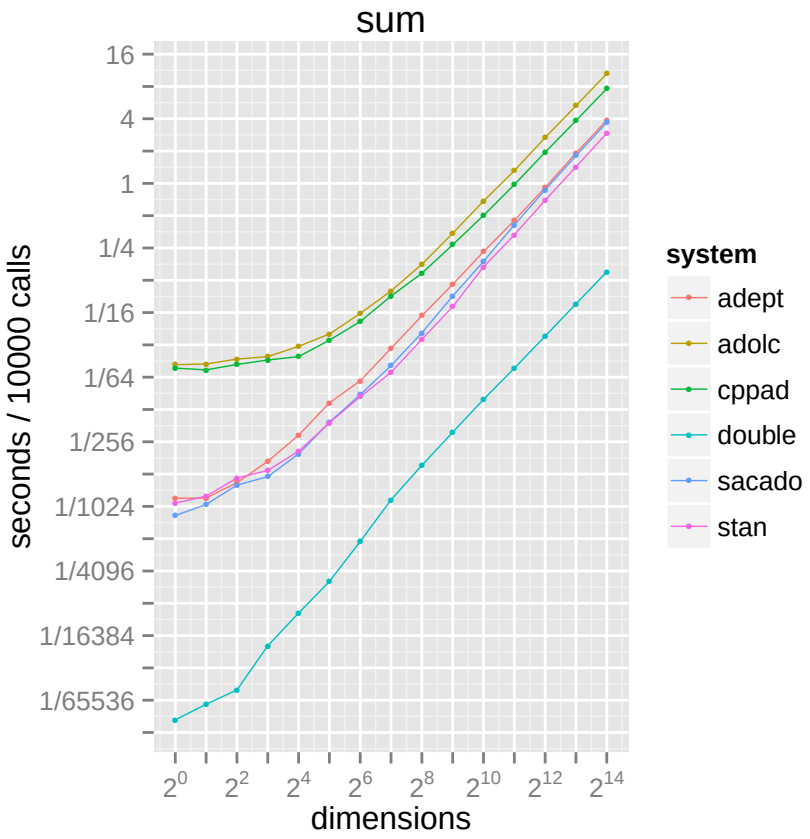
- **Vectorized** to allow scalar or container arguments
  (containers all same shape; scalars broadcast as necessary)
- Avoid **repeated computations**, e.g. $\log \sigma$ in

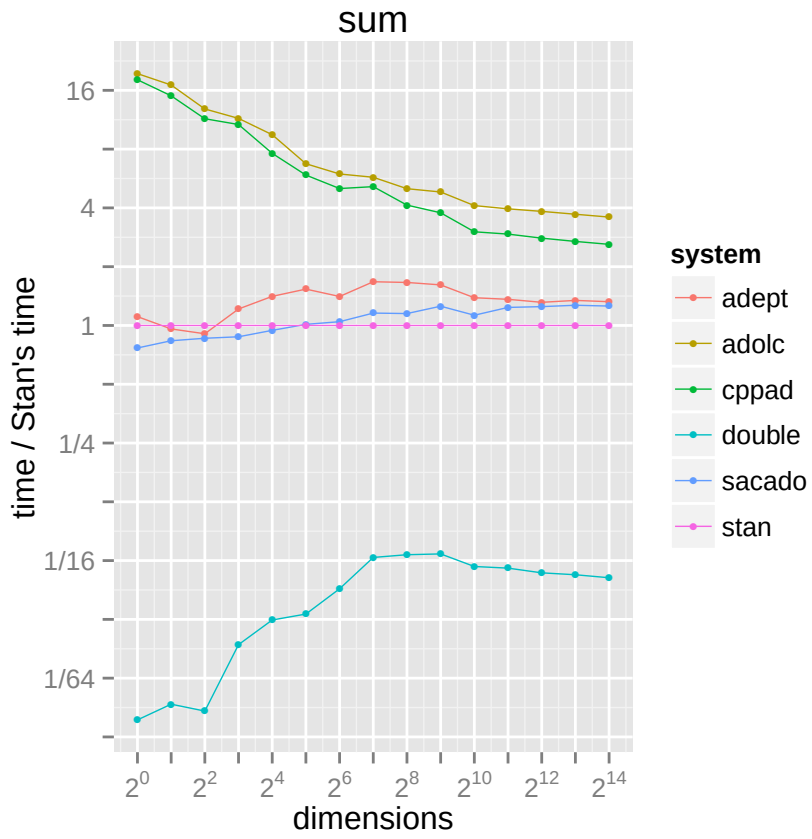
$$\begin{aligned} \log \text{Normal}(y|\mu,\sigma) &= \sum_{n=1}^{N} \log \text{Normal}(y_n|\mu,\sigma) \\ &= \sum_{n=1}^{N} -\log\sqrt{2\pi} \; - \log\sigma \; - \frac{y_n - \mu}{2\sigma^2} \end{aligned}$$

- 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

Stan's Autodiff vs. Alternatives

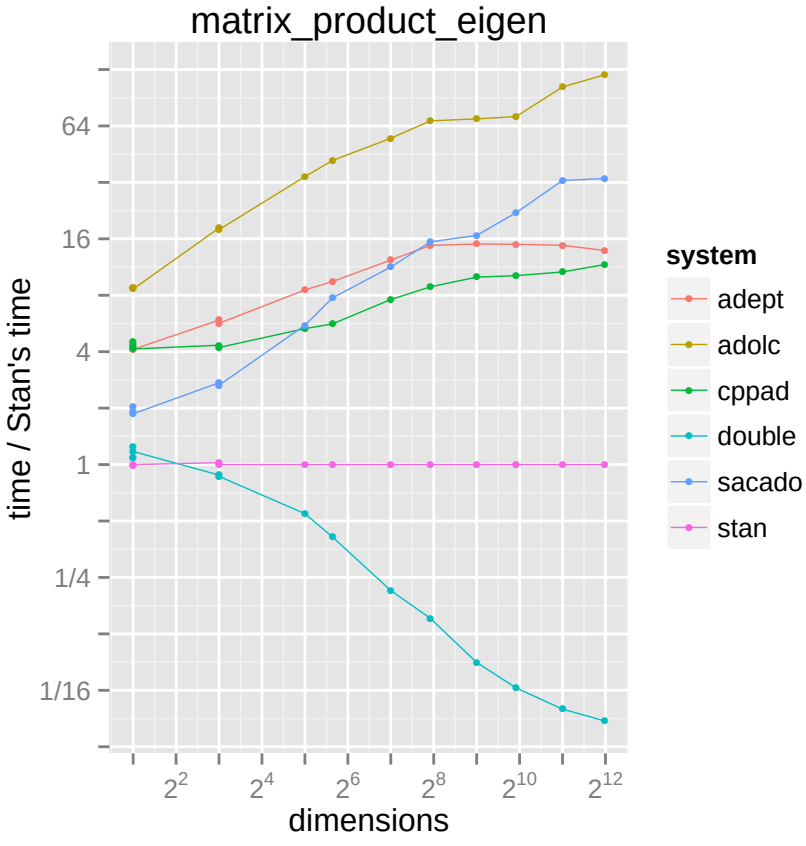
- Stan is **fastest** and uses least memory
  - among open-source C++ alternatives we managed to install

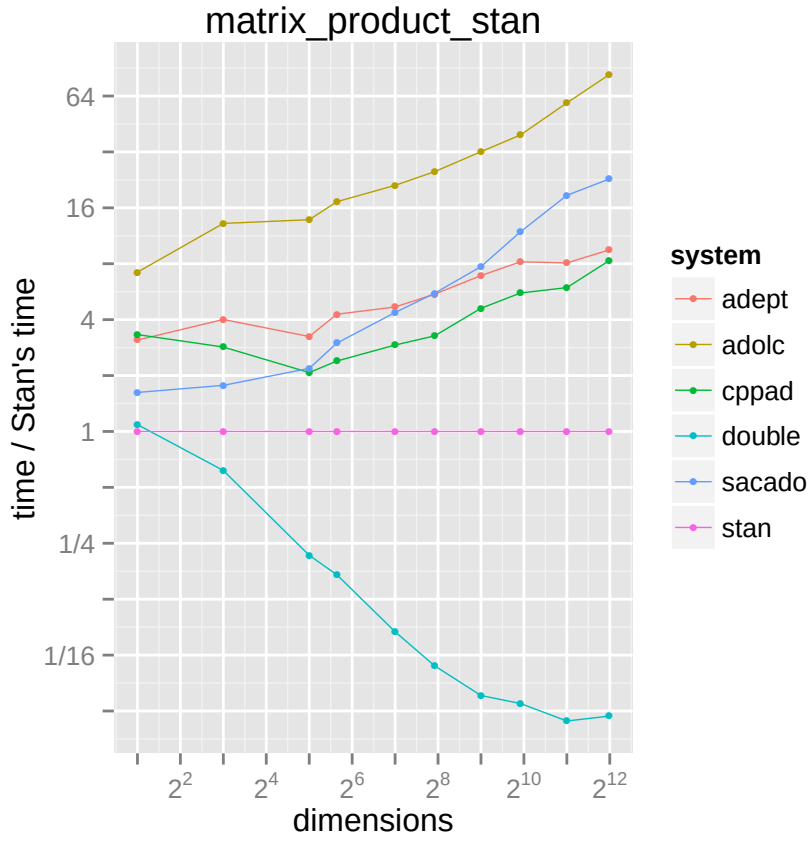




Stan's Matrix Calculations

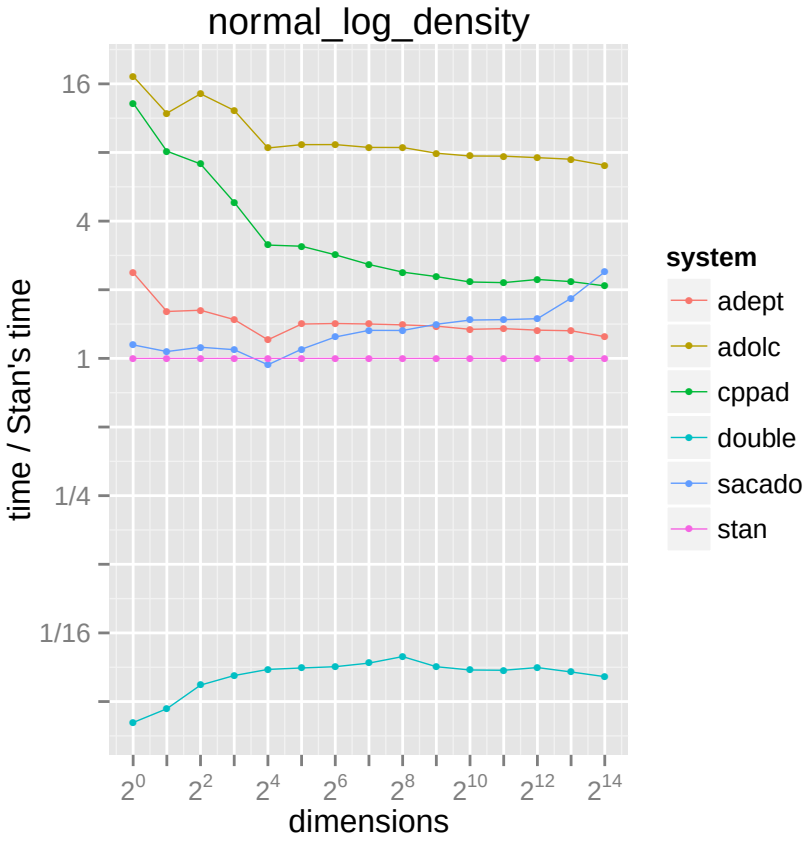
- Faster in Eigen, but takes more memory
- Best of both worlds coming soon

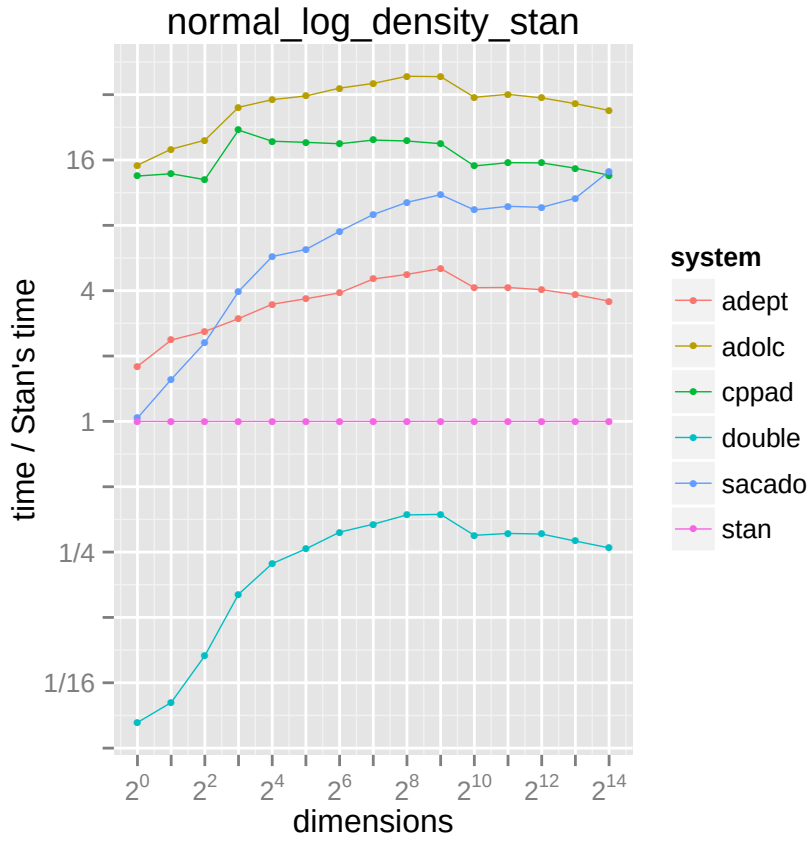




Stan's Density Calculations

- Vectorization a huge win





Hard Models, Big Data

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
- merged with develop branch

Laplace Approximation

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

$$\theta^* = \arg\max_\theta \, p(\theta|y)$$

- 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 θ^*
- 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

“Black Box” Variational Inference

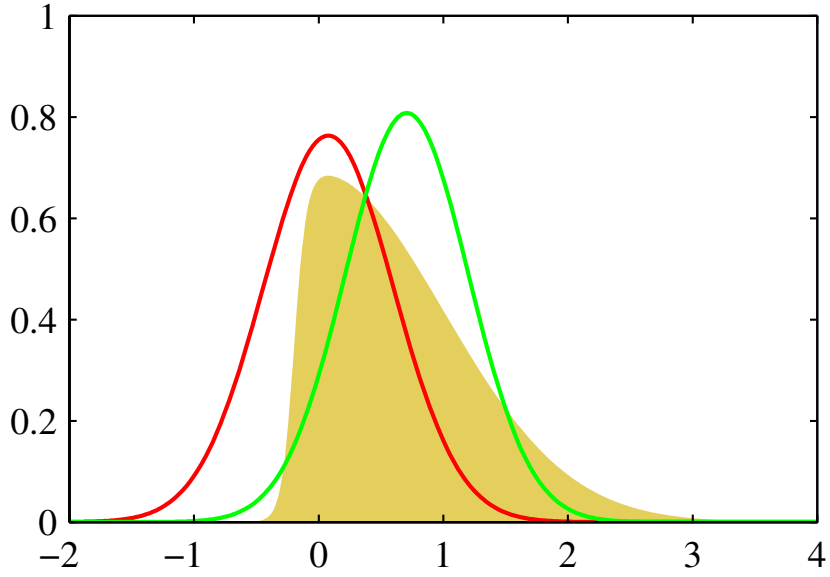
- **Black box** so can fit any Stan model
- Multivariate **normal approx to unconstrained** posterior
  - covariance: diagonal mean-field or full rank
  - not Laplace approx — around posterior mean, not mode
  - transformed back to constrained space (built-in Jacobians)
- Stochastic **gradient-descent** optimization
  - ELBO gradient estimated via Monte Carlo + autodiff
- Returns **approximate posterior** mean / covariance
- Returns **sample** transformed to constrained space

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

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

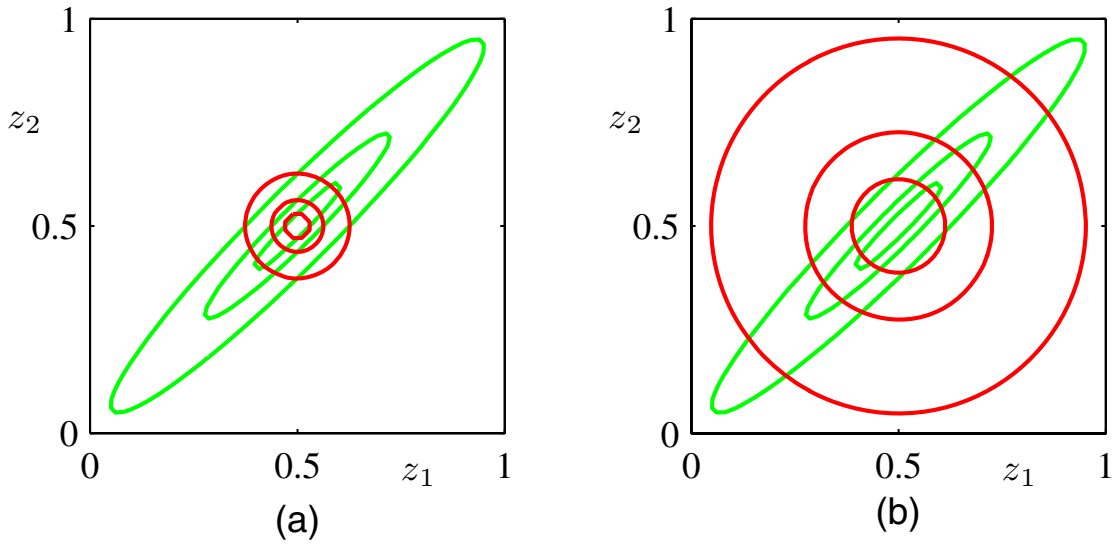
VB vs. Laplace



- *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 **underestimates 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 gradient of KL-divergence w.r.t. θ up to constant
- Approximate KL-divergence and gradient via Monte Carlo
  - only need approximate gradient calculation for soundness of L-BFGS
  - KL divergence is an expectation w.r.t. approximation $g(\theta|\phi)$
  - Monte Carlo draws i.i.d. from approximating multi-normal
  - derivatives with respect to true model log density via reverse-mode autodiff
  - 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

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

  - 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

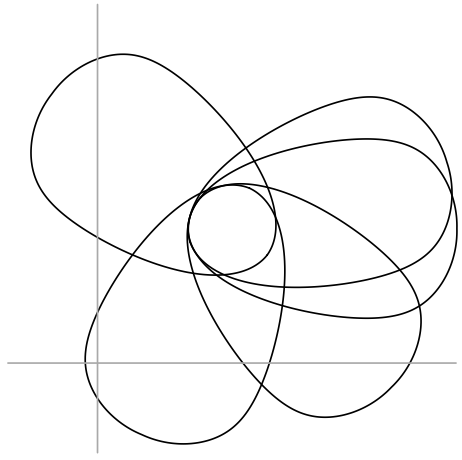
Near Future: Stochastic VB

- 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 minimize KL-divergence
- Prototype code complete

“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
- Prototype 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**

Challenges

Discrete Parameters

- e.g., simple mixture models, survival models, HMMs, discrete measurement error models, missing data
- **Marginalize out** discrete parameters
- Efficient sampling due to **Rao-Blackwellization**
- Inference straightforward with expectations

- Too **difficult** for many of our users
  (exploring encapsulation options)

Models with Missing Data

- In principle, missing data just **additional parameters**
- In practice, how to declare?
  - **observed** data as data variables
  - **missing** data as parameters
  - combine into single vector

    (in transformed parameters or local in model)

Position-Dependent Curvature

- Mass matrix does **global** adaptation for
  - parameter scale (diagonal) and rotation (dense)
- Dense mass matrices hard to estimate ($\mathcal{O}(N^2)$ estimands)
- **Problem**: Position-dependent curvature
  - Example: banana-shaped densities
    - arise when parameter is product of other parameters
  - Example: hierarchical models
    - hierarchical variance controls lower-level parameters
- Mitigate by reducing stepsize
  - initial (`stepsize`) and target acceptance (`adapt_delta`)

The End