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Bayesian Statistics and Data Analysis

Lecture 6

Måns Magnusson

Department of Statistics, Uppsala University
Thanks to Aki Vehtari, Aalto University

- MCMC recap
- Hamiltonian Monte Carlo
- Dynamic HMC and NUTS
- HMC diagnostics
- Probabilistic Programming
- Stan



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Recap: MCMC, Gibbs and Metropolis

- Markov Chain Monte Carlo
 - A **transition distribution** $T(\theta_0 \rightarrow \theta_1)$ with a unique **stationary distribution**
 - Target: setup T so that $p(\theta|y)$ is the stationary distribution

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 - Conditional (or block) sampling of θ

$$\theta_j \sim p(\theta_j | \theta_{-j}, y)$$

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 - Proposal distribution J (i.e. T)



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 - Proposal distribution J (i.e. T)
 - + better for correlated posteriors
 - scale need to be tuned for efficient sampling
 - hard to propose in high dimensions (many small steps or many rejections)



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- MCMC recap
- **Hamiltonian Monte Carlo**
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Section 2

Hamiltonian Monte Carlo



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Why Hamiltonian Monte Carlo?

- MCMC recap
 - **Hamiltonian Monte Carlo**
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- Want to build an **efficient** Markov Chain
 - We want to sample jointly all θ
 - We know the **unnormalized** posterior $q(\theta|y) = Z \cdot p(\theta|y)$, where Z is the normalization constant.
 - Can we use this to create a good **proposal** distribution J ?



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 - **Hamiltonian Monte Carlo!**



What is Hamiltonian Monte Carlo?

- Add momentum variables to our posterior (**canonical** distribution)

$$p(\psi, \theta|y) = p(\psi|\theta, y) \cdot p(\theta|y),$$

in practice we let $p(\psi|\theta, y) = p(\psi)$

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- Idea from Physics (Mechanics):
 - θ : position
 - ψ : momentum

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in practice we let $p(\psi|\theta, y) = p(\psi)$

- Idea from Physics (Mechanics):
 - θ : position
 - ψ : momentum
- Define the Hamiltonian as

$$H(\psi, \theta) = -\log(p(\psi)) - \log(p(\theta|y)) \quad (1)$$

$$= K(\psi) + V(\theta), \quad (2)$$

where $K(\psi)$ is the **kinetic** energy and $V(\theta)$ is the **potential** energy

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What is Hamiltonian Monte Carlo?

- Hamiltonian Dynamics (**preserve energy**)

$$\frac{d\theta}{dt} = \frac{\partial H}{\partial \psi} = \frac{\partial K}{\partial \psi} \quad (3)$$

$$\frac{d\psi}{dt} = -\frac{\partial H}{\partial \theta} = -\frac{\partial V}{\partial \theta} \quad (4)$$

- Let $V(\theta) = -\log(q(\theta|y)) = -\log p(\theta) - \log p(y|\theta)$
- Let $\psi \sim N(0, M)$ where M is the **mass matrix**
- Hence, $K(\psi) = -\log p(\psi) \propto 0.5\psi^T M^{-1}\psi + C$

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- Let $V(\theta) = -\log(q(\theta|y)) = -\log p(\theta) - \log p(y|\theta)$
- Let $\psi \sim N(0, M)$ where M is the **mass matrix**
- Hence, $K(\psi) = -\log p(\psi) \propto 0.5\psi^T M^{-1}\psi + C$
- We need to choose M in a smart way.
 1. Ideally, $M^{-1} = \text{Cov}(\theta|y)$
 2. In practice, $M^{-1} = V(\theta|y)$



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The leapfrog integrator

- We want to simulate Hamiltonian dynamics

$$\frac{d\theta}{dt} = M^{-1}\psi \quad (5)$$

$$\frac{d\psi}{dt} = \frac{\partial \log q(\theta|y)}{\partial \theta} \quad (6)$$

- A **discrete** approximation: **the leapfrog integrator**



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- A **discrete** approximation: **the leapfrog integrator**
- We take L leapfrog steps with step size ϵ as

$$\psi \leftarrow \psi + \frac{1}{2}\epsilon \frac{d \log q(\theta|y)}{d\theta} \quad (7)$$

$$\theta \leftarrow \theta + \epsilon M^{-1}\psi \quad (8)$$

$$\psi \leftarrow \psi + \frac{1}{2}\epsilon \frac{d \log q(\theta|y)}{d\theta} \quad (9)$$



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The leapfrog integrator

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- Discretization introduce a error depending on ϵ (not $L\epsilon$)



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Hamiltonian Monte Carlo Algorithm

1. Sample momentum

$$\psi_0 \sim N(0, M)$$

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1. Sample momentum

$$\psi_0 \sim N(0, M)$$

2. Simulate values (θ^*, ψ^*) using the leapfrog integrator L steps with stepsize ϵ , starting from (θ_{t-1}, ψ_0)



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1. Sample momentum

$$\psi_0 \sim N(0, M)$$

- ## 2. Simulate values (θ^*, ψ^*) using the leapfrog integrator L steps with stepsize ϵ , starting from (θ_{t-1}, ψ_0)
- ## 3. Accept the proposed values (θ^*, ψ^*) with probability

$$r = \min \left(1, \frac{q(\theta^*|y)}{q(\theta_{t-1}|y)} \frac{p(\psi^*)}{p(\psi_0)} \right)$$



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Hamiltonian Monte Carlo

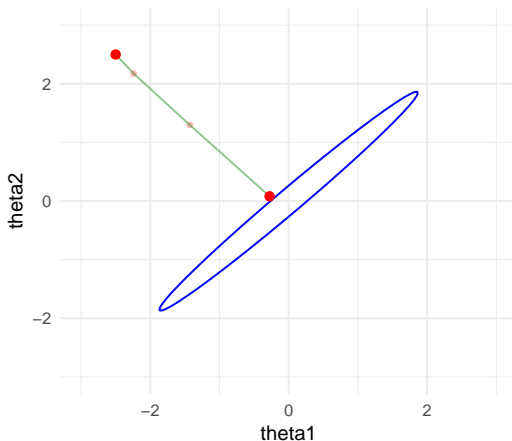
- Bivariate Normal HMC example

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Hamiltonian Monte Carlo

- Bivariate Normal HMC example



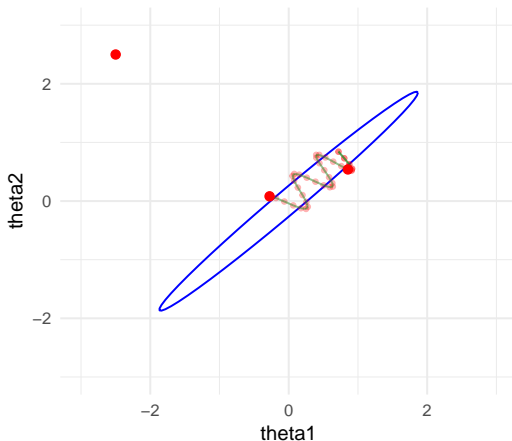
• Samples — Steps of the sampler — 90% HPD

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Hamiltonian Monte Carlo

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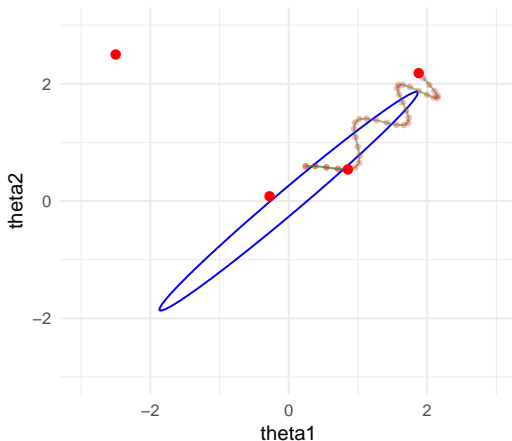


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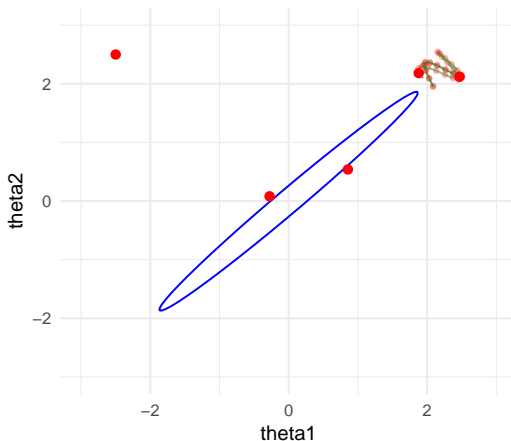


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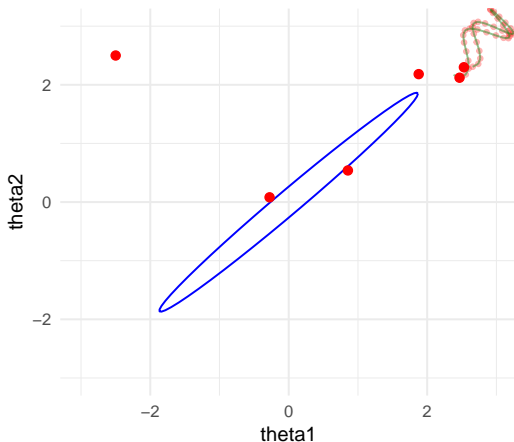
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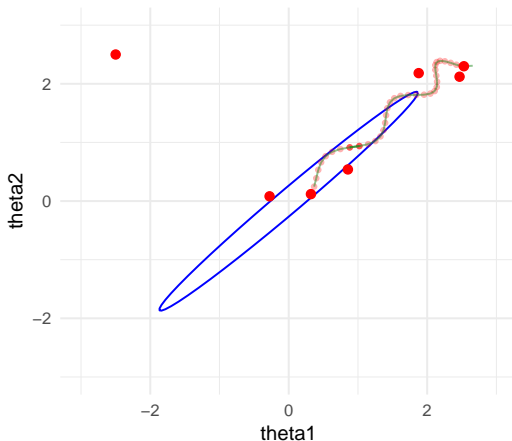


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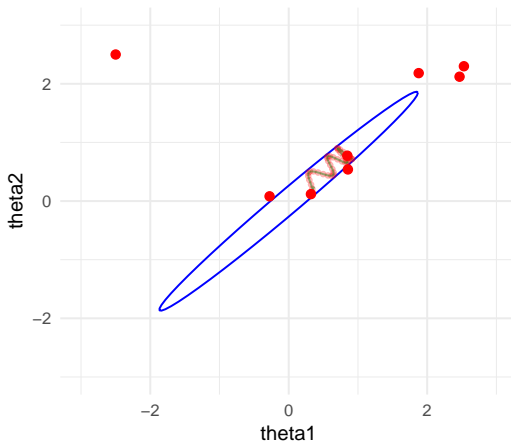
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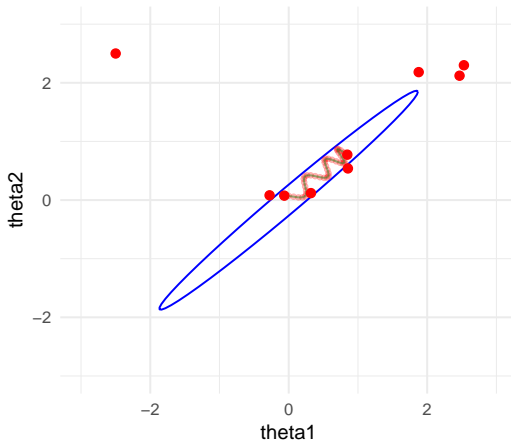
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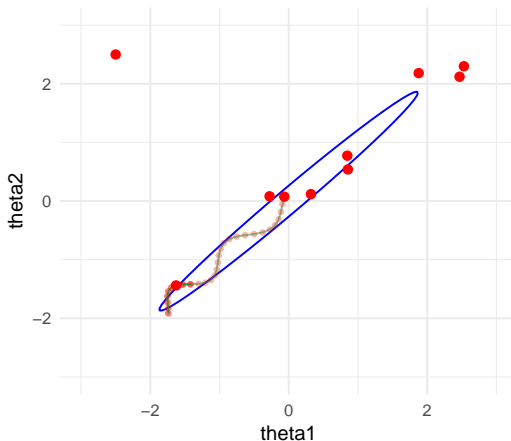


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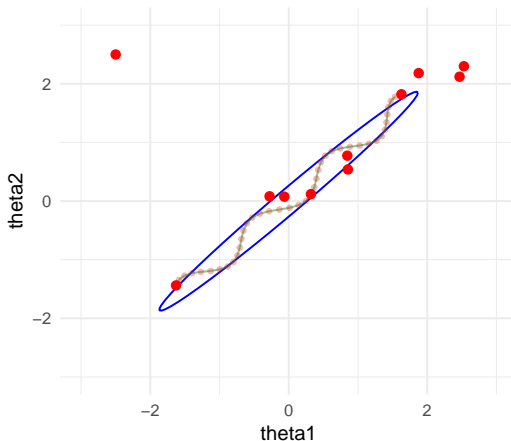
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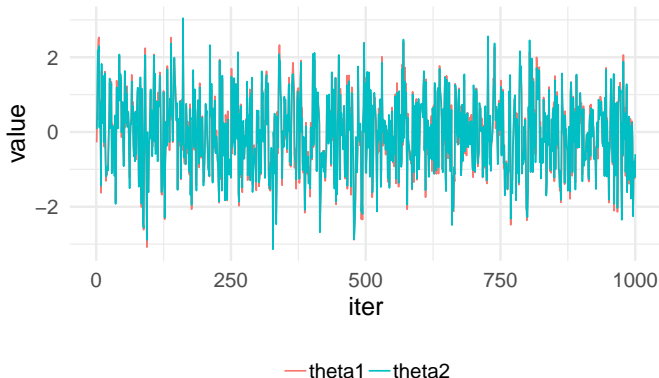
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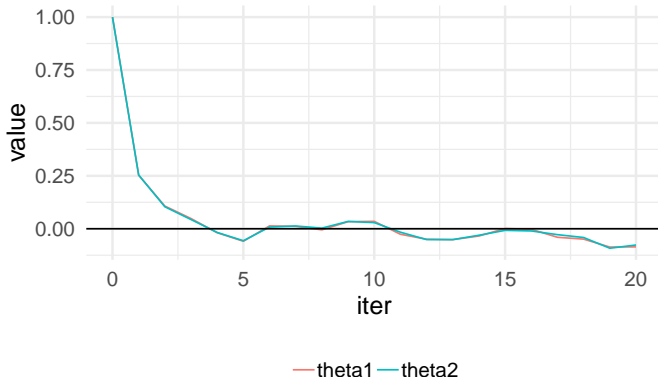
Trends





- Bivariate Normal HMC example

Autocorrelation function





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Hamiltonian Monte Carlo Summary

- Parameters:

- ϵ step size

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Hamiltonian Monte Carlo Summary

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Hamiltonian Monte Carlo Summary

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- + Can be very efficient (S_{eff})

- + Additional diagnostics

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- Can be difficult to tune (U-turns)
 - Bounded parameters needs handling
 - Ideally, we should adapt ϵL
 - Costly to run each iteration (L log density gradient evaluations)



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demo



Dynamic HMC

- **Goal:** Simplify/adapt the tuning of HMC
- **Dynamic** HMC refers to **dynamic** trajectory length of the leapfrog integrator (i.e. L is chosen on the fly)

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- The NUTS/dynamic algorithm:
 1. Grow a binary tree of leapfrog steps L
 2. Grow (randomly) in two directions (to keep reversibility of Markov chain)
 3. Stop to grow tree when encounter a U-turn
$$(\theta_L - \theta_{start}) \cdot \psi_L < 0$$
 4. Sample one of the step at the trajectory (higher probability further away)



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$$(\theta_L - \theta_{start}) \cdot \psi_L < 0$$

4. Sample one of the step at the trajectory (higher probability further away)
- Dynamic simulation is discretized
 - small ϵ gives accurate simulation, but requires more log density evaluations
 - large ϵ reduces computation, but increases simulation error



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Dynamic Hamiltonian Monte Carlo Summary

- MCMC recap
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- Parameters:
 - step size



Dynamic Hamiltonian Monte Carlo Summary

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- Parameters:
 - ϵ step size
 - M mass matrix



Dynamic Hamiltonian Monte Carlo Summary

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- + Additional diagnostics



Dynamic Hamiltonian Monte Carlo Summary

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- Parameters:
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 - + Can be very efficient (S_{eff})
 - + Additional diagnostics
 - Bounded parameters needs handling
 - Costly to run each iteration (L log density gradient evaluations)



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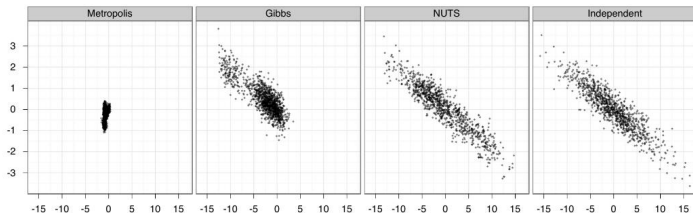
- Costly to run each iteration (L log density gradient evaluations)

demo



Comparison of algorithms on **highly correlated** 250-dimensional Gaussian distribution

- MCMC recap
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- Do **1,000,000** draws with both Random Walk Metropolis and Gibbs, thinning by 1000
 - Do **1,000** draws using Stan's NUTS algorithm (no thinning)
 - Do 1,000 independent draws (we can do this for multivariate normal)



Source: Jonah Gabry



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Section 4

HMC diagnostics



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Max tree depth

- MCMC recap
 - Hamiltonian Monte Carlo
 - Dynamic HMC and NUTS
 - **HMC diagnostics**
 - Probabilistic Programming
 - Stan
- Dynamic HMC specific diagnostic
 - Indicates inefficiency in sampling leading to higher autocorrelations and lower ESS (n_{eff})
 - Different parameterizations can help/matter



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Divergent transitions

- HMC specific diagnostic

- MCMC recap
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- HMC specific diagnostic
- The Hamiltonian $H(\theta, \psi)$ should remain roughly constant throughout the trajectory:

$$H(\theta_{start}, \psi_{start}) \approx H(\theta_{end}, \psi_{end})$$

- A large difference between the initial and final Hamiltonian indicates a divergent transition:

$$H(\theta_{start}, \psi_{start}) - H(\theta_{end}, \psi_{end}) \gg 0$$

- indicates that Hamiltonian dynamic simulation has problems with unexpected fast changes in log-density
- possibility of biased estimates



Divergent transitions

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- Why do we get divergent transitions?
 1. Step size too large
 - Do not approximate the trajectory



- Why do we get divergent transitions?
 1. Step size too large
 - Do not approximate the trajectory
 2. Highly curved posterior geometry
 - Small changes in position can result in very large changes in the gradient (momentum)
 - Unstable trajectory
 - Common in hierarchical models

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 1. Step size too large
 - Do not approximate the trajectory
 2. Highly curved posterior geometry
 - Small changes in position can result in very large changes in the gradient (momentum)
 - Unstable trajectory
 - Common in hierarchical models
 3. Tight correlations between parameters
 - Small changes in position can result in very large changes in the gradient (momentum)
 - small movements in one parameter may cause disproportionately large movements in another



Divergent transitions

- MCMC recap
- Hamiltonian Monte Carlo
- Dynamic HMC and NUTS
- HMC diagnostics
- Probabilistic Programming
- Stan

- Solutions:

1. Decrease step size/Increase number of leapfrog steps



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- Solutions:
 1. Decrease step size/Increase number of leapfrog steps
 2. Reparameterization
 - Reparameterizing the model to reduce correlations between parameters or to make the posterior geometry more regular can help, e.g. in hierarchical models



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 1. Decrease step size/Increase number of leapfrog steps
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 3. Use a better Metric (Mass Matrix)



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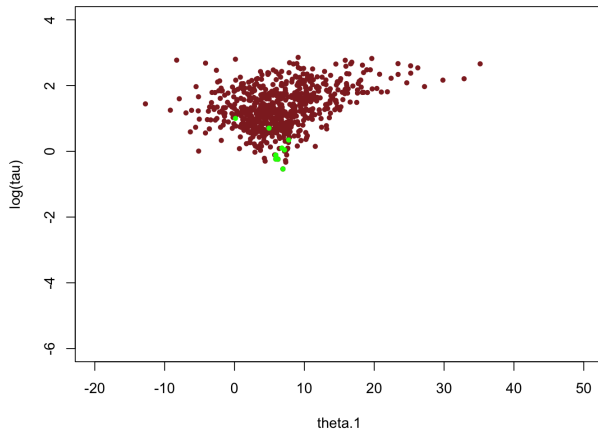
- **Solutions:**
 1. Decrease step size/Increase number of leapfrog steps
 2. Reparameterization
 - Reparameterizing the model to reduce correlations between parameters or to make the posterior geometry more regular can help, e.g. in hierarchical models
 3. Use a better Metric (Mass Matrix)
 4. Use other samplers that uses the Hessian, e.g. Riemannian Manifold HMC (but it has its own drawbacks)



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Divergences (Betancourt, 2017)

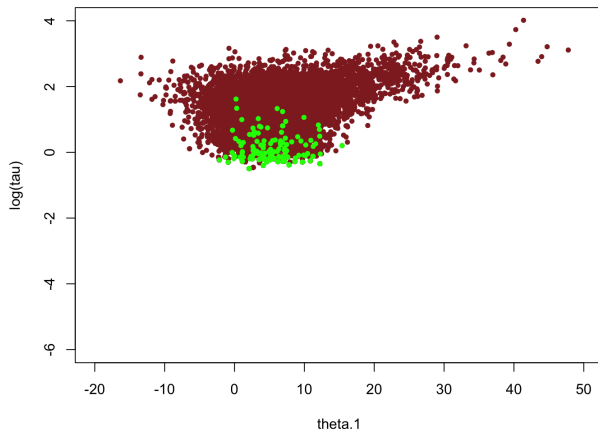




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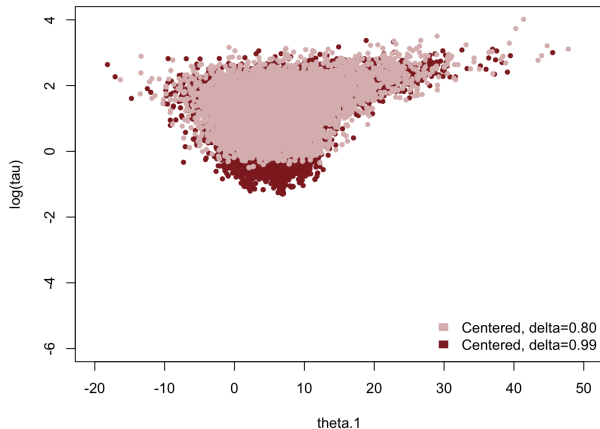




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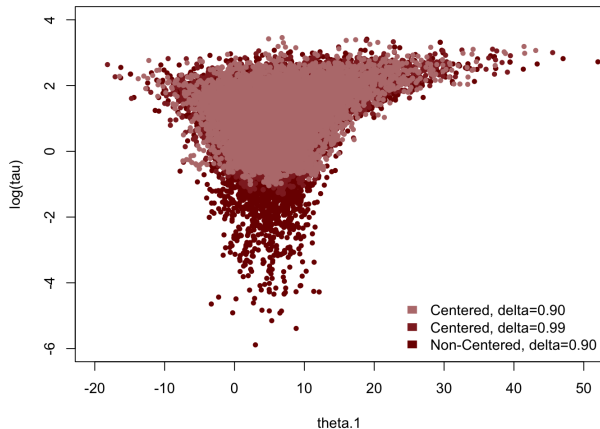




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Divergences (Betancourt, 2017)





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Problematic distributions

- MCMC recap
 - Hamiltonian Monte Carlo
 - Dynamic HMC and NUTS
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 - Stan
- Nonlinear dependencies
 - simple mass matrix scaling doesn't help



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Problematic distributions

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 - Funnels
 - optimal step size depends on location



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 - Funnels
 - optimal step size depends on location
 - Multimodal
 - difficult to move from one mode to another



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 - Hamiltonian Monte Carlo
 - Dynamic HMC and NUTS
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- Nonlinear dependencies
 - simple mass matrix scaling doesn't help
 - Funnels
 - optimal step size depends on location
 - Multimodal
 - difficult to move from one mode to another
 - Long-tailed with non-finite variance and mean
 - efficiency of exploration is reduced
 - central limit theorem doesn't hold for mean and variance



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Extra (optional) material for HMC

- MCMC recap
- Hamiltonian Monte Carlo
- Dynamic HMC and NUTS
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- Stan

- Michael Betancourt (2018). A Conceptual Introduction to Hamiltonian Monte Carlo.
<https://arxiv.org/abs/1701.02434>
- Michael Betancourt (2017). Diagnosing Biased Inference with Divergences.
https://mc-stan.org/users/documentation/case-studies/divergences_and_bias.html



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Section 5

Probabilistic Programming



- MCMC recap
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The Box process: Probabilistic modeling

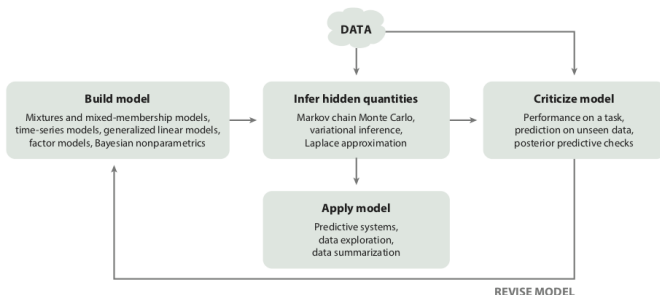


Figure: The Box approach (Box, 1976, Blei, 2014)



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Probabilistic programming languages

- MCMC recap
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 - Stan
- Wikipedia “A probabilistic programming language (PPL) is a programming language designed to describe probabilistic models and then perform inference in those models”



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Probabilistic programming languages

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- Wikipedia “A probabilistic programming language (PPL) is a programming language designed to describe probabilistic models and then perform inference in those models”
 - To make probabilistic programming useful
 - easy workflow to build and revise models
 - inference has to be as automatic as possible
 - diagnostics for telling if the automatic inference doesn't work



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Probabilistic programming

- MCMC recap
 - Hamiltonian Monte Carlo
 - Dynamic HMC and NUTS
 - HMC diagnostics
 - Probabilistic Programming
 - Stan
- Enables agile (incremental) workflow for developing probabilistic models
 - language
 - automated inference
 - diagnostics
 - Many frameworks Stan, PyMC3, Pyro (Uber), Edward (Google), Birch (Uppsala), ...



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- MCMC recap
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Section 6

Stan



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Stan - probabilistic programming framework

- Language, inference engine, user interfaces, documentation, case studies, diagnostics, packages, ...
 - autodiff to compute gradients of the log density



mc-stan.org



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- Language, inference engine, user interfaces, documentation, case studies, diagnostics, packages, ...
 - autodiff to compute gradients of the log density
- More than ten thousand users in social, biological, and physical sciences, medicine, engineering, and business



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- More than ten thousand users in social, biological, and physical sciences, medicine, engineering, and business
- Several full time developers, 40+ developers, more than 100 contributors
- R, Python, Julia, Scala, Stata, Matlab, command line interfaces
- More than 100 R packages using Stan



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Stan

- MCMC recap
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- Stanislaw Ulam (1909-1984)
 - Monte Carlo method
 - H-Bomb



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Adaptive dynamic HMC in Stan

- Dynamic HMC using growing tree to increase simulation trajectory until no-U-turn criterion stopping
 - max treedepth to keep computation in control

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Adaptive dynamic HMC in Stan

- Dynamic HMC using growing tree to increase simulation trajectory until no-U-turn criterion stopping
 - max treedepth to keep computation in control
 - pick a draw along the trajectory with probabilities adjusted to take into account the error in the discretized dynamic simulation

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 - mass matrix refers to having different scaling for different parameters and optionally also rotation to reduce correlations



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 - mass matrix and step size adjustment and are estimated during initial adaptation phase



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 - step size is adjusted to be as big as possible while keeping discretization error in control (adapt_delta)



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- After adaptation the algorithm parameters are fixed



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- After adaptation the algorithm parameters are fixed
- After warmup store iterations for inference



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- After adaptation the algorithm parameters are fixed
- After warmup store iterations for inference
- See more details in Stan reference manual



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Binomial model - Stan code

```
data {  
  int<lower=0> N;          // number of experiments  
  int<lower=0,upper=N> y;  // number of successes  
}  
  
parameters {  
  real<lower=0,upper=1> theta; // parameter of the  
}  
  
model {  
  theta ~ beta(1,1);        //prior  
  y ~ binomial(N,theta);    // observation model  
}
```



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```
data {  
  int<lower=0> N;      // number of experiments  
  int<lower=0,upper=N> y; // number of successes  
}
```

- Data type and size are declared
- Stan checks that given data matches type and constraints



```
data {  
  int<lower=0> N;      // number of experiments  
  int<lower=0,upper=N> y; // number of successes  
}
```

- Data type and size are declared
- Stan checks that given data matches type and constraints
 - If you are not used to strong typing, this may feel annoying, but it will reduce the probability of coding errors, which will reduce probability of data analysis errors



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- **Stan**

Binomial model - Stan code

```
parameters {  
  real<lower=0,upper=1> theta;  
}
```

- Parameters may have constraints
- Stan makes transformation to unconstrained space and samples in unconstrained space
 - e.g. log transformation for `<lower=a>`
 - e.g. logit transformation for `<lower=a,upper=b>`



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Binomial model - Stan code

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- Parameters may have constraints
- Stan makes transformation to unconstrained space and samples in unconstrained space
 - e.g. log transformation for `<lower=a>`
 - e.g. logit transformation for `<lower=a,upper=b>`
- For these declared transformation Stan automatically takes into account the Jacobian of the transformation (see BDA3 p. 21)



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```
model {  
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Binomial model - Stan code

```
model {  
  theta ~ beta(1,1);    // prior  
  y ~ binomial(N,theta); // likelihood  
}
```

- \sim is syntactic sugar and this is equivalent to

```
model {  
  target += beta_lpdf(theta | 1, 1);  
  target += binomial_lpmf(y | N, theta);  
}
```



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- target is the log posterior density



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  target += beta_lpdf(theta | 1, 1);  
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}
```

- `target` is the log posterior density
- `_lpdf` for continuous, `_lpmf` for discrete distributions (discrete for the left hand side of `|`)



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- `_lpdf` for continuous, `_lpmf` for discrete distributions (discrete for the left hand side of `|`)
- for Stan sampler there is no difference between prior and likelihood, all that matters is the final `target`



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```

- target is the log posterior density
- `_lpdf` for continuous, `_lpmf` for discrete distributions (discrete for the left hand side of `|`)
- for Stan sampler there is no difference between prior and likelihood, all that matters is the final target
- you can write in Stan language any program to compute the log density (Stan language is Turing complete)



- MCMC recap
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 - Stan
- Stan compiles (transpiles) the model written in Stan language to C++
 - this makes the sampling for complex models and bigger data faster
 - also makes Stan models easily portable, you can use your own favorite interface



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RStan

RStan

```
library(rstan)
rstan_options(auto_write = TRUE)
options(mc.cores = parallel::detectCores())

d_bin <- list(N = 10, y = 7)
fit_bin <- stan(file = 'binom.stan', data = d_bin)
```



- MCMC recap
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RStan

RStan

```
library(rstan)
rstan_options(auto_write = TRUE)
options(mc.cores = parallel::detectCores())

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```



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PyStan

PyStan

```
import pystan
import stan_utility

data = dict(N=10, y=8)
model = stan_utility.compile_model('binom.stan')
fit = model.sampling(data=data)
```



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PyStan

PyStan

```
import pystan
import stan_utility
```

```
data = dict(N=10, y=8)
model = stan_utility.compile_model('binom.stan')
fit = model.sampling(data=data)
```



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Stan

- MCMC recap
 - Hamiltonian Monte Carlo
 - Dynamic HMC and NUTS
 - HMC diagnostics
 - Probabilistic Programming
 - Stan
- Compilation (unless previously compiled model available)
 - Warm-up including adaptation
 - Sampling
 - Generated quantities
 - Save posterior draws
 - Report divergences, $n_{E_{\max}}$, \hat{R}



Difference between proportions

- MCMC recap
 - Hamiltonian Monte Carlo
 - Dynamic HMC and NUTS
 - HMC diagnostics
 - Probabilistic Programming
 - Stan
- An experiment was performed to estimate the effect of beta-blockers on mortality of cardiac patients
 - A group of patients were randomly assigned to treatment and control groups:
 - out of 674 patients receiving the control, 39 died
 - out of 680 receiving the treatment, 22 died



- MCMC recap
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Difference between proportions

```
data {  
  int<lower=0> N1;  
  int<lower=0> y1;  
  int<lower=0> N2;  
  int<lower=0> y2;  
}  
parameters {  
  real<lower=0, upper=1> theta1;  
  real<lower=0, upper=1> theta2;  
}  
model {  
  theta1 ~ beta(1,1);  
  theta2 ~ beta(1,1);  
  y1 ~ binomial(N1, theta1);  
  y2 ~ binomial(N2, theta2);  
}  
  
generated quantities {  
  real oddsratio;  
  oddsratio = (theta2/(1-theta2))/(theta1/(1-theta1));  
}
```



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Difference between proportions

```
data {  
  int<lower=0> N1;  
  int<lower=0> y1;  
  int<lower=0> N2;  
  int<lower=0> y2;  
}  
parameters {  
  real<lower=0, upper=1> theta1;  
  real<lower=0, upper=1> theta2;  
}  
model {  
  theta1 ~ beta(1,1);  
  theta2 ~ beta(1,1);  
  y1 ~ binomial(N1, theta1);  
  y2 ~ binomial(N2, theta2);  
}  
  
generated quantities {  
  real oddsratio;  
  oddsratio = (theta2/(1-theta2))/(theta1/(1-theta1));  
}
```



Difference between proportions

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```
generated quantities {  
  real oddsratio;  
  oddsratio = (theta2/(1-theta2))/(theta1/(1-theta1))  
}
```

- generated quantities is run after the sampling



- MCMC recap
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Difference between proportions

```
d_bin2 <- list(N1 = 674, y1 = 39, N2 = 680, y2 = 20)
fit_bin2 <- stan(file = 'binom2.stan', data = d_bin2)
```

```
starting worker pid=10151 on localhost:11783 at 10:03:27.872
starting worker pid=10164 on localhost:11783 at 10:03:28.087
starting worker pid=10176 on localhost:11783 at 10:03:28.295
starting worker pid=10185 on localhost:11783 at 10:03:28.461
```

SAMPLING FOR MODEL 'binom2' NOW (CHAIN 1).

Gradient evaluation took 6e-06 seconds
1000 transitions using 10 leapfrog steps per transition would take 0.06 seconds.
Adjust your expectations accordingly!

```
Iteration:    1 / 2000 [  0%] (Warmup)
Iteration:   200 / 2000 [ 10%] (Warmup)
...
Iteration:  1000 / 2000 [ 50%] (Warmup)
Iteration:  1001 / 2000 [ 50%] (Sampling)
...
Iteration:  2000 / 2000 [100%] (Sampling)
```

```
Elapsed Time: 0.012908 seconds (Warm-up)
              0.017027 seconds (Sampling)
              0.029935 seconds (Total)
```

SAMPLING FOR MODEL 'binom2' NOW (CHAIN 2).

...



Difference between proportions

```
monitor(fit_bin2, probs = c(0.1, 0.5, 0.9))
```

Inference for the input samples
(4 chains: each with iter=1000; warmup=0):

	mean	se_mean	sd	10%	50%	90%	n_eff	Rhat
theta1	0.1	0	0.0	0.0	0.1	0.1	3280	1
theta2	0.0	0	0.0	0.0	0.0	0.0	3171	1
oddsratio	0.6	0	0.2	0.4	0.6	0.8	3108	1
lp_	-253.5	0	1.0	-254.8	-253.2	-252.6	1922	1

For each parameter, `n_eff` is a crude measure of effective samples and `Rhat` is the potential scale reduction factor on split chain convergence, `Rhat=1`).



Difference between proportions

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For each parameter, `n_eff` is a crude measure of effective samples and `Rhat` is the potential scale reduction factor on split chain convergence, `Rhat=1`).

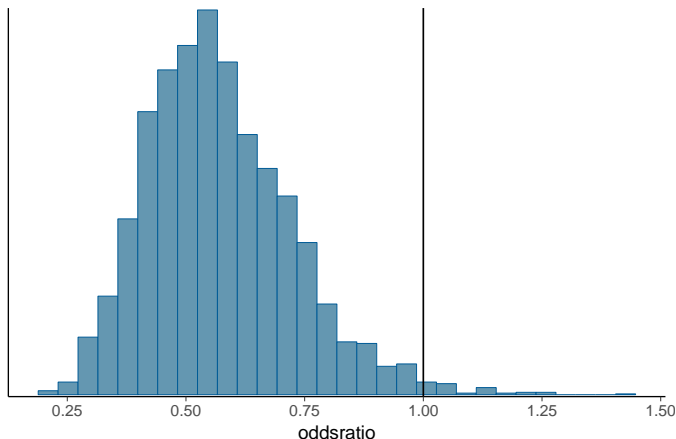
- `lp__` is the log density, ie, same as target



- MCMC recap
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Difference between proportions

```
draws <- as.data.frame(fit_bin2)
mcmc_hist(draws, pars = 'oddsratio') +
  geom_vline(xintercept = 1) +
  scale_x_continuous(breaks = c(seq(0.25, 1.5, by=0.25)))
```





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```
check_treedepth(fit_bin2)  
check_div(fit_bin2)
```

```
[1] "0 of 4000 iterations saturated the maximum tree depth of 1  
[1] "0 of 4000 iterations ended with a divergence (0%)"
```

```
get_num_leapfrog_per_iteration(fit_bin2)
```




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Shinystan

- MCMC recap
 - Hamiltonian Monte Carlo
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 - Stan
- Graphical user interface for analysing MCMC results



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Gaussian linear model

```
data {  
  int<lower=0> N; // number of data points  
  vector[N] x; //  
  vector[N] y; //  
}  
parameters {  
  real alpha;  
  real beta;  
  real<lower=0> sigma;  
}  
transformed parameters {  
  vector[N] mu;  
  mu <- alpha + beta*x;  
}  
model {  
  y ~ normal(mu, sigma);  
}
```



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```
data {  
  int<lower=0> N; // number of data points  
  vector[N] x; //  
  vector[N] y; //  
}
```

- difference between `vector[N] x` and `real x[N]`



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Gaussian linear model

```
parameters {  
  real alpha;  
  real beta;  
  real<lower=0> sigma;  
}  
transformed parameters {  
  vector[N] mu;  
  mu <- alpha + beta*x;  
}
```

- transformed parameters are deterministic transformations of parameters and data



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Priors for Gaussian linear model

```
data {  
  int<lower=0> N; // number of data points  
  vector[N] x; //  
  vector[N] y; //  
  real pmualpha; // prior mean for alpha  
  real psalpha; // prior std for alpha  
  real pmubeta; // prior mean for beta  
  real psbeta; // prior std for beta  
}  
...  
transformed parameters {  
  vector[N] mu;  
  mu <- alpha + beta*x;  
}  
model {  
  alpha ~ normal(pmualpha, psalpha);  
  beta ~ normal(pmubeta, psbeta);  
  y ~ normal(mu, sigma);  
}
```



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Student-t linear model

```
...
parameters {
  real alpha;
  real beta;
  real<lower=0> sigma;
  real<lower=1,upper=80> nu;
}
transformed parameters {
  vector[N] mu;
  mu <- alpha + beta*x;
}
model {
  nu ~ gamma(2,0.1);
  y ~ student_t(nu, mu, sigma);
}
```



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- **Stan**

Linear regression model in Stan

```
data {  
  int<lower=0> N; // number of data points  
  vector[N] x; //  
  vector[N] y; //  
  real xpred; // input location for prediction  
}  
transformed data {  
  vector[N] x_std;  
  vector[N] y_std;  
  real xpred_std;  
  x_std = (x - mean(x)) / sd(x);  
  y_std = (y - mean(y)) / sd(y);  
  xpred_std = (xpred - mean(x)) / sd(x);  
}
```



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- **Stan**

- RStanARM provides simplified model description with pre-compiled models
 - no need to wait for compilation
 - a restricted set of models

Two group Binomial model:

```
d_bin2 <- data.frame(N = c(674, 680), y = c(39,22), grp2 = c(0,1))
fit_bin2 <- stan_glm(y/N ~ grp2, family = binomial(), data = d_bin2, weights = N)
```




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- RStanARM provides simplified model description with pre-compiled models
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 - a restricted set of models

Two group Binomial model:

```
d_bin2 <- data.frame(N = c(674, 680), y = c(39,22), grp2 = c(0,1))
fit_bin2 <- stan_glm(y/N ~ grp2, family = binomial(), data = d_bin2, weights = N)
```

Gaussian linear model

```
fit_lin <- stan_glm(temp ~ year, data = d_lin)
```



- MCMC recap
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- BRMS provides simplified model description
 - a larger set of models than RStanARM, but still restricted
 - need to wait for the compilation

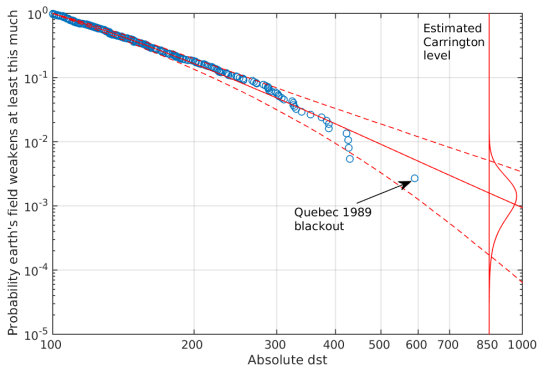
```
fit_bin2 <- brm(y/N ~ grp2, family = binomial(), data = d_bin2,  
               weights = N)
```

```
fit_lin_t <- brm(temp ~ year, data = d_lin, family = student())
```



Geomagnetic storms

- MCMC recap
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Extreme value analysis

```
data {  
  int<lower=0> N;  
  vector<lower=0>[N] y;  
  int<lower=0> Nt;  
  vector<lower=0>[Nt] yt;  
}  
transformed data {  
  real ymax;  
  ymax <- max(y);  
}  
parameters {  
  real<lower=0> sigma;  
  real<lower=-sigma/ymax> k;  
}  
model {  
  y ~ gpareto(k, sigma);  
}  
generated quantities {  
  vector[Nt] predccdf;  
  predccdf<-gpareto_ccdf(yt, k, sigma);  
}
```



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Functions

```
functions {  
  real gpareto_lpdf(vector y, real k, real sigma) {  
    // generalised Pareto log pdf with  $\mu=0$   
    // should check and give error if  $k < 0$   
    // and  $\max(y)/\sigma > -1/k$   
    int N;  
    N <- dims(y)[1];  
    if (fabs(k) > 1e-15)  
      return  $-(1+1/k) * \text{sum}(\log1pv(y*k/\sigma)) - N * \log(\sigma)$   
    else  
      return  $-\text{sum}(y/\sigma) - N * \log(\sigma)$ ; // limit  $k \rightarrow 0$   
  }  
  vector gpareto_ccdf(vector y, real k, real sigma) {  
    // generalised Pareto log ccdf with  $\mu=0$   
    // should check and give error if  $k < 0$   
    // and  $\max(y)/\sigma < -1/k$   
    if (fabs(k) > 1e-15)  
      return  $\exp((-1/k) * \log1pv(y/\sigma * k))$ ;  
    else  
      return  $\exp(-y/\sigma)$ ; // limit  $k \rightarrow 0$   
  }  
}
```



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Other packages

- MCMC recap
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- R
 - shinystan — interactive diagnostics
 - bayesplot — visualization and model checking (see model checking in Ch 6)
 - loo — cross-validation model assessment, comparison and averaging (see Ch 7)
 - projpred — projection predictive variable selection
- Python
 - ArviZ — visualization, and model checking and assessment (see Ch 6 and 7)



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- RStan / PyStan
 - C++ functions of Stan are called directly from R / Python
 - Higher integration between R/Python and Stan, but maybe more difficult to install due to more requirements of compatible C++ compilers and libraries
- CmdStanR / CmdStanPy
 - Lightweight interface on top of commandline program CmdStan
 - Lacks some features that are not needed in this course, but is usually easier to install
- More recent useful R packages
 - posterior: for handling posterior draws, convergence diagnostics, and summaries
 - tidybayes + ggdist: pretty plots



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Extra material for Stan

- Andrew Gelman, Daniel Lee, and Jiqiang Guo (2015) Stan: A probabilistic programming language for Bayesian inference and optimization.
http://www.stat.columbia.edu/~gelman/research/published/stan_jebbs_2.pdf
- Carpenter et al (2017). Stan: A probabilistic programming language. Journal of Statistical Software 76(1).
<https://doi.org/10.18637/jss.v076.i01>
- Stan User's Guide, Language Reference Manual, and Language Function Reference (in html and pdf)
<https://mc-stan.org/users/documentation/>
 - easiest to start from Example Models in User's guide
- Basics of Bayesian inference and Stan, part 1 Jonah Gabry & Lauren Kennedy (StanCon 2019 Helsinki tutorial)
 - <https://www.youtube.com/watch?v=ZRpo41l02KQ&index=6&list=PLuwyh42iHquU4hUBQs20hkBsKSMrp6H0J>
 - <https://www.youtube.com/watch?v=6cc4N1vT8pk&index=7&list=PLuwyh42iHquU4hUBQs20hkBsKSMrp6H0J>