Pathologies in hierarchical models

FW 891

Click here to view presentation online

Christopher Cahill

16 October 2023

Quantitative Fisheries Center
MICHIGAN STATE UNIVERSITY

Purpose

- Introduce some background and theoretical concepts
- The Devil's funnel (spooky seaz'n )
- What to do about it
- Example
- Example #2 (Eight schools)

Background

- Many of the most exciting problems in applied statistical ecology involve intricate, high-dimensional models, and sparse data (at least relative to model complexity)

Betancourt and Girolami 2013

Background

- Many of the most exciting problems in applied statistical ecology involve intricate, high-dimensional models, and sparse data (at least relative to model complexity)
- In situations where the data alone cannot identify a model, significant prior information is required to draw valid inference

Betancourt and Girolami 2013

Background

- Many of the most exciting problems in applied statistical ecology involve intricate, high-dimensional models, and sparse data (at least relative to model complexity)
- In situations where the data alone cannot identify a model, significant prior information is required to draw valid inference
- Such prior information is not limited to an explicit prior distribution, but instead can be encoded in the model construction itself 🤯

Betancourt and Girolami 2013

A one level hierarchical model

$$\pi(\theta, \phi \mid \mathcal{D}) \propto \prod_{i=1}^{n} \pi\left(\mathcal{D}_i \mid \theta_i\right) \pi\left(\theta_i \mid \phi\right) \pi(\phi)$$

Betancourt and Girolami 2013

A one level hierarchical model

$$\pi(\theta, \phi \mid \mathcal{D}) \propto \prod_{i=1}^{n} \pi\left(\mathcal{D}_i \mid \theta_i\right) \pi\left(\theta_i \mid \phi\right) \pi(\phi)$$

- Hierarchical models are defined by the organization of a model's parameters into exchangeable groups, and the resulting conditional independencies between those groups

Betancourt and Girolami 2013

A one level hierarchical model

$$\pi(\theta, \phi \mid \mathcal{D}) \propto \prod_{i=1}^{n} \pi\left(\mathcal{D}_i \mid \theta_i\right) \pi\left(\theta_i \mid \phi\right) \pi(\phi)$$

- Hierarchical models are defined by the organization of a model's parameters into exchangeable groups, and the resulting conditional independencies between those groups
- Can also visualize this as a directed acyclic graph (DAG)

Betancourt and Girolami 2013

Hierarchical DAG

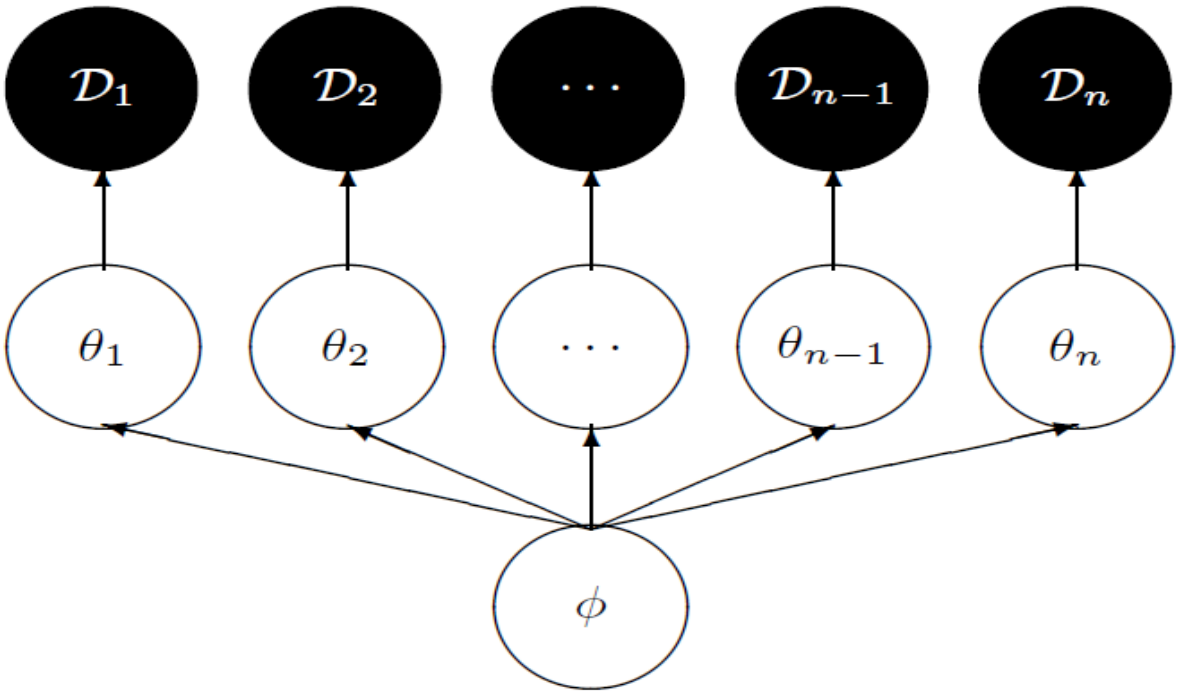


FIG. 1. In hierarchical models "local" parameters, θ, interact via a common dependency on "global" parameters, ϕ. The interactions allow the measured data, $\mathcal{D}$, to inform all of the θ instead of just their immediate parent. More general constructions repeat this structure, either over different sets of parameters or additional layers of hierarchy.

Betancourt and Girolami 2013

A one-level hierarchical model

$$y_i \sim N\left(\theta_i, \sigma_i^2\right)$$
$$\theta_i \sim N\left(\mu, \tau^2\right), \text{ for } i = 1, \ldots, I$$

Betancourt and Girolami 2013

A one-level hierarchical model

$$y_i \sim N\left(\theta_i, \sigma_i^2\right)$$
$$\theta_i \sim N\left(\mu, \tau^2\right), \text{ for } i = 1, \ldots, I$$

- In terms of the previous equations,
  $\mathcal{D} = (y_i, \sigma_i), \phi = (\mu, \tau), \text{ and } \theta = (\theta_i)$

Betancourt and Girolami 2013

A one-level hierarchical model

$$y_i \sim N\left(\theta_i, \sigma_i^2\right)$$
$$\theta_i \sim N\left(\mu, \tau^2\right), \text{ for } i = 1, \ldots, I$$

- In terms of the previous equations, $\mathcal{D} = \left(y_i \sigma_i\right), \phi = (\mu, \tau), \text{ and } \theta = \left(\theta_i\right)$
- Call any elements of ϕ *global* parameters

Betancourt and Girolami 2013

A one-level hierarchical model

$$y_i \sim N\left(\theta_i, \sigma_i^2\right)$$
$$\theta_i \sim N\left(\mu, \tau^2\right), \text{ for } i = 1, \ldots, I$$

- In terms of the previous equations, $\mathcal{D} = \left(y_i, \sigma_i\right), \phi = (\mu, \tau), \text{ and } \theta = \left(\theta_i\right)$
- Call any elements of ϕ *global* parameters
- Call any elements of θ *local* parameters

Betancourt and Girolami 2013

A one-level hierarchical model

$$y_i \sim N\left(\theta_i, \sigma_i^2\right)$$
$$\theta_i \sim N\left(\mu, \tau^2\right), \text{ for } i = 1, \ldots, I$$

- In terms of the previous equations, $\mathcal{D} = \left(y_i \sigma_i\right), \phi = (\mu, \tau), \text{ and } \theta = \left(\theta_i\right)$
- Call any elements of ϕ *global* parameters
- Call any elements of θ *local* parameters
- However, recognize this nomencalture breaks down in situations with more levels

Betancourt and Girolami 2013

A key pathology

- Unfortunately, this one-level model exhibits some of the typical pathologies of hierarchical models
- Small changes in ϕ induce large changes in density
- When data are sparse, the density of these models looks like a “funnel”
  - Region of high density but low volume, and a region of low density but high volume
- However, the probability mass of these two regions is the same (or nearly so)
- Any algorithm must be able to manage the dramatic variations in curvature to fully map out the posterior

Betancourt and Girolami 2013

Naive model implementations

- Assuming a normal model with no data, a latent mean μ set at zero, and a lognormal prior on the variance $\tau^2 = e^{v^2}$

Betancourt and Girolami 2013

Naive model implementations

- Assuming a normal model with no data, a latent mean μ set at zero, and a lognormal prior on the variance $\tau^2 = e^{v^2}$

$$\pi\left(\theta_1, \ldots, \theta_n, v\right) \propto \prod_{i=1}^{n} N\left(x_i \mid 0, \left(e^{-v/2}\right)^2\right) N\left(v \mid 0, 3^2\right)$$

Betancourt and Girolami 2013

Naive model implementations

- Assuming a normal model with no data, a latent mean μ set at zero, and a lognormal prior on the variance $\tau^2 = e^{v^2}$

$$\pi\left(\theta_1, \ldots, \theta_n, v\right) \propto \prod_{i=1}^{n} N\left(x_i \mid 0, \left(e^{-v/2}\right)^2\right) N\left(v \mid 0, 3^2\right)$$

- This hierarchical structure induces large correlations between v and each θ_i

Betancourt and Girolami 2013

Visualizing the pathology 😈

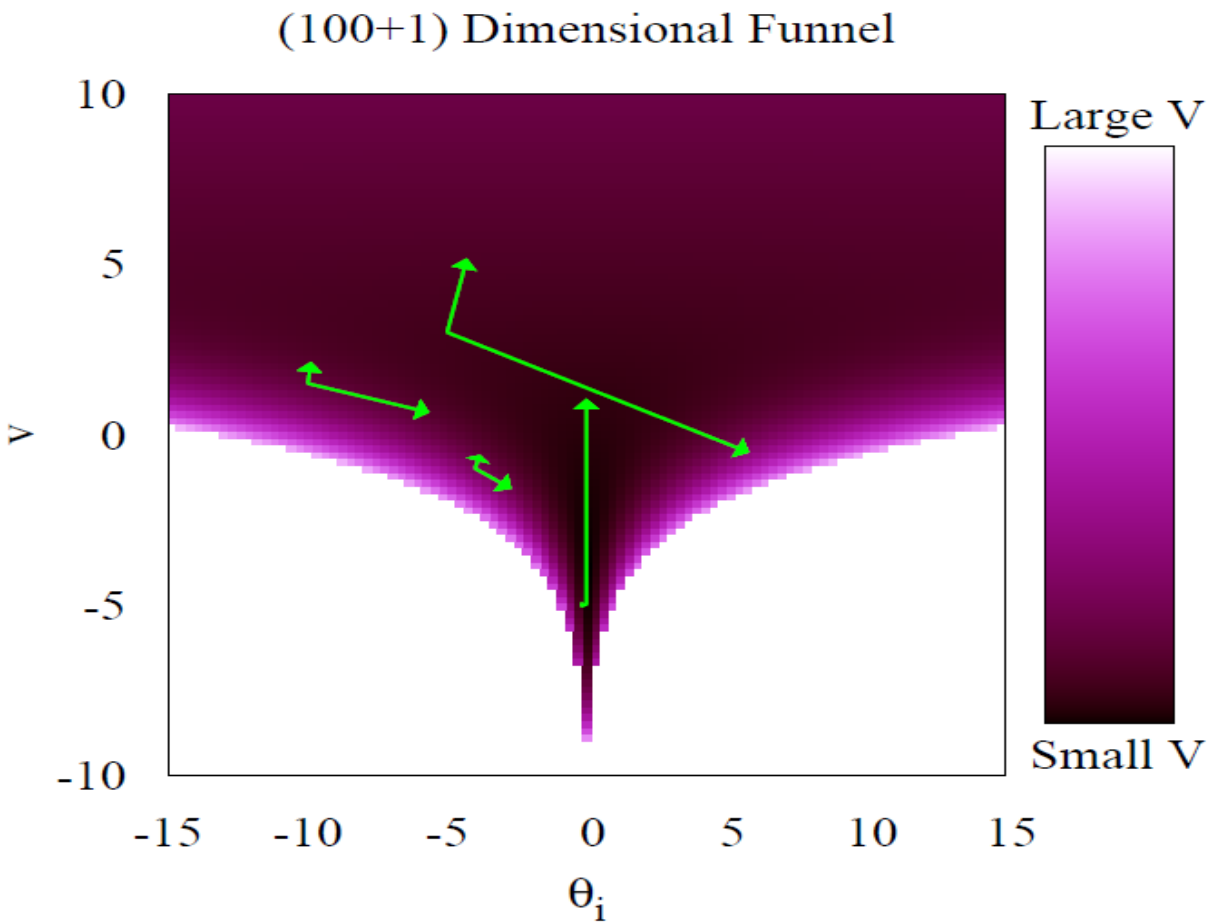


FIG. 2. Typical of hierarchical models, the curvature of the funnel distribution varies strongly with the parameters, taxing most algorithms and limiting their ultimate performance.

Some things worth noting

- There is position dependence in the correlation structure, i.e., correlation changes depending on where you are located in the posterior

Betancourt and Girolami 2013

Some things worth noting

- There is position dependence in the correlation structure, i.e., correlation changes depending on where you are located in the posterior
- No global correction, like rotating or rescaling will solve this problem!

Betancourt and Girolami 2013

Some things worth noting

- There is position dependence in the correlation structure, i.e., correlation changes depending on where you are located in the posterior
- No global correction, like rotating or rescaling will solve this problem!
- Often manifests as a divergent transition in Stan, as HMC cannot accurately explore the posterior

Betancourt and Girolami 2013

How can we fix this problem?

- Remember that the prior information we include in an analysis is not only limited to the choice of an explict prior distribution

Betancourt and Girolami 2013

How can we fix this problem?

- Remember that the prior information we include in an analysis is not only limited to the choice of an explict prior distribution
- The dependence between layers in our model can actually be broken up by reparameterizing the existing parameters into a so-called “non-centered” parameterization
  - Think about the DAG

Betancourt and Girolami 2013

How can we fix this problem?

- Remember that the prior information we include in an analysis is not only limited to the choice of an explict prior distribution
- The dependence between layers in our model can actually be broken up by reparameterizing the existing parameters into a so-called “non-centered” parameterization
  - Think about the DAG
- Non-centered parameterizations factor certain dependencies into deterministic transformations between the layers, leaving the actively sampled variables uncorrelated

Betancourt and Girolami 2013

Centered vs. non-centered model maths

Centered model:

$$y_i \sim N\left(\theta_i, \sigma_i^2\right)$$
$$\theta_i \sim N\left(\mu, \tau^2\right),$$

Non-centered analog:

Betancourt and Girolami 2013

Centered vs. non-centered model maths

Centered model:

$$
\begin{aligned}
y_i &\sim N\left(\theta_i, \sigma_i^2\right) \\
\theta_i &\sim N\left(\mu, \tau^2\right),
\end{aligned}
$$

Non-centered analog:

$$
\begin{aligned}
y_i &\sim N\left(\vartheta_i \tau + \mu, \sigma_i^2\right) \\
\vartheta_i &\sim N(0, 1).
\end{aligned}
$$

Betancourt and Girolami 2013

Centered vs. non-centered model maths

Centered model:

$$
\begin{aligned}
y_i &\sim N\left(\theta_i, \sigma_i^2\right) \\
\theta_i &\sim N\left(\mu, \tau^2\right),
\end{aligned}
$$

Non-centered analog:

$$
\begin{aligned}
y_i &\sim N\left(\vartheta_i \tau + \mu, \sigma_i^2\right) \\
\vartheta_i &\sim N(0, 1).
\end{aligned}
$$

Key point: NCP shifts correlation from the latent parameters to data

Betancourt and Girolami 2013

Centered vs. non-centered model DAG

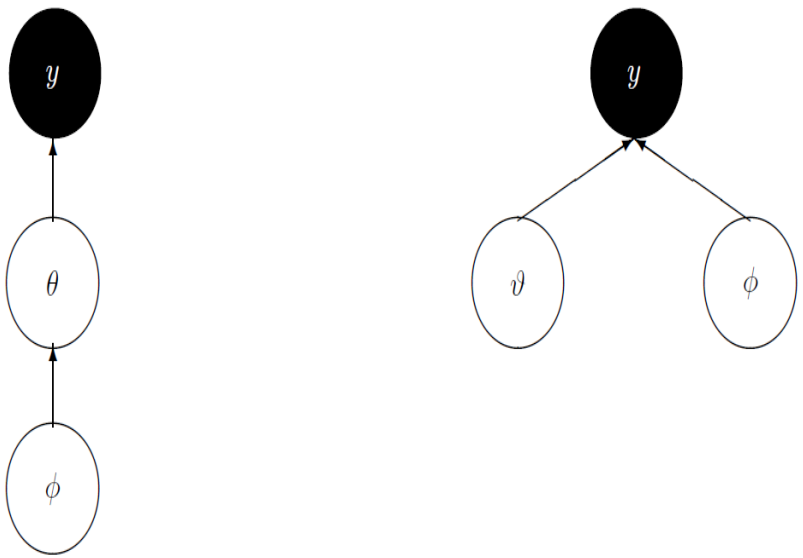


FIG. 4. In one-level hierarchical models with global parameters, ϕ, local parameters, θ, and measured data y, correlations between parameters can be mediated by different parameterizations of the model. Non-centered parameterizations exchange a direct dependence between ϕ and θ for a dependence between ϕ and y; the reparameterized ϑ and ϕ become independent conditioned on the data. When the data are weak these non-centered parameterizations yield simpler posterior geometries.

Betancourt and Girolami 2013

When does NCP help?

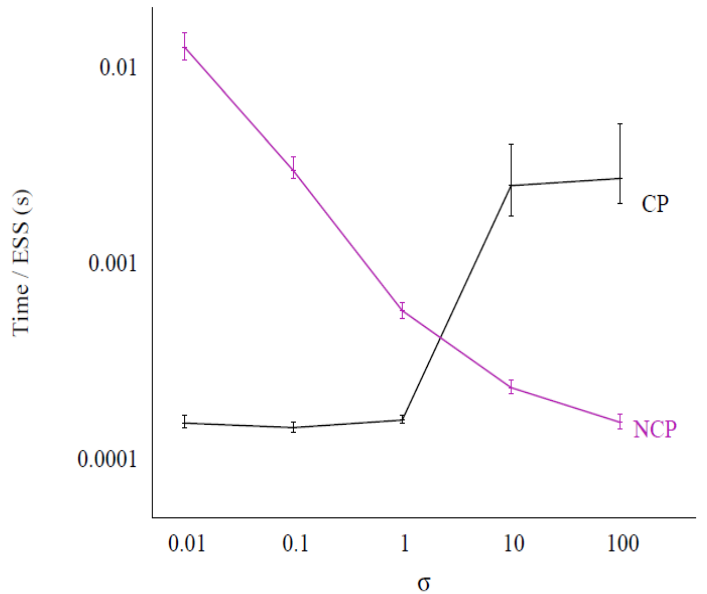


FIG. 8. Depending on the common variance, σ^2, from which the data were generated, the performance of a 10-dimensional one-way normal model (2) varies drastically between centered (CP) and non-centered (NCP) parameterizations of the latent parameters, θ_i. As the variance increases and the data become effectively more sparse, the non-centered parameterization yields the most efficient inference and the disparity in performance increases with the dimensionality of the model.

Betancourt and Girolami 2013

Example

Example

- consider the one-way normal model with 800 latent θ_i
- constant measurement error $\sigma_i = \sigma = 10$
- latent parameters are $\mu = 8, \tau = 3$
- θ_i and y_i sampled randomly

Betancourt and Girolami 2013

Example

- consider the one-way normal model with 800 latent θ_i
- constant measurement error $\sigma_i = \sigma = 10$
- latent parameters are $\mu = 8, \tau = 3$
- θ_i and y_i sampled randomly

Add weakly informative priors to this generative likelihood

$$\pi(\mu) = N\left(0, 5^2\right)$$
$$\pi(\tau) = \text{Half-Cauchy}\left(0, 2.5\right).$$

Betancourt and Girolami 2013

Example, centered vs. noncentered

The centered parameterization of this model can be written as

$$
\begin{aligned}
y_i &\sim N\left(\theta_i, \sigma_i^2\right) \\
\theta_i &\sim N\left(\mu, \tau^2\right), \text{ for } i = 1, \ldots, 800
\end{aligned}
$$

Betancourt and Girolami 2013

Example, centered vs. noncentered

The centered parameterization of this model can be written as

$$
\begin{aligned}
y_i &\sim N\left(\theta_i, \sigma_i^2\right) \\
\theta_i &\sim N\left(\mu, \tau^2\right), \text{ for } i = 1, \ldots, 800
\end{aligned}
$$

and it should have inferior performance relative to the noncentered model:

$$
\begin{aligned}
y_i &\sim N\left(\tau\vartheta_i + \mu, \sigma_i^2\right) \\
\vartheta_i &\sim N(0, 1), \text{ for } i = 1, \ldots, 800
\end{aligned}
$$

Betancourt and Girolami 2013

Using Stan to simulate fake data

```
transformed data {
  real mu;
  real<lower=0> tau;
  real alpha;
  int N;
  mu = 8;
  tau = 3;
  alpha = 10;
  N = 800;
}
generated quantities {
  real mu_print;
  real tau_print;
  vector[N] theta;
  vector[N] sigma;
  vector[N] y;
  mu_print = mu;
  tau_print = tau;
  for (i in 1:N) {
    theta[i] = normal_rng(mu, tau);
    sigma[i] = alpha;
    y[i] = normal_rng(theta[i], sigma[i]);
  }
}
```

Calling that from R

```r
library("cmdstanr")

one_level <- cmdstan_model("src/sim_one_level.stan")

# simulate data
sim <- one_level$sample(
  fixed_param = T, # look here
  iter_warmup = 0, iter_sampling = 1,
  chains = 1, seed = 1
)
```

```
Running MCMC with 1 chain...

Chain 1 Iteration: 1 / 1 [100%]  (Sampling)
Chain 1 finished in 0.0 seconds.
```

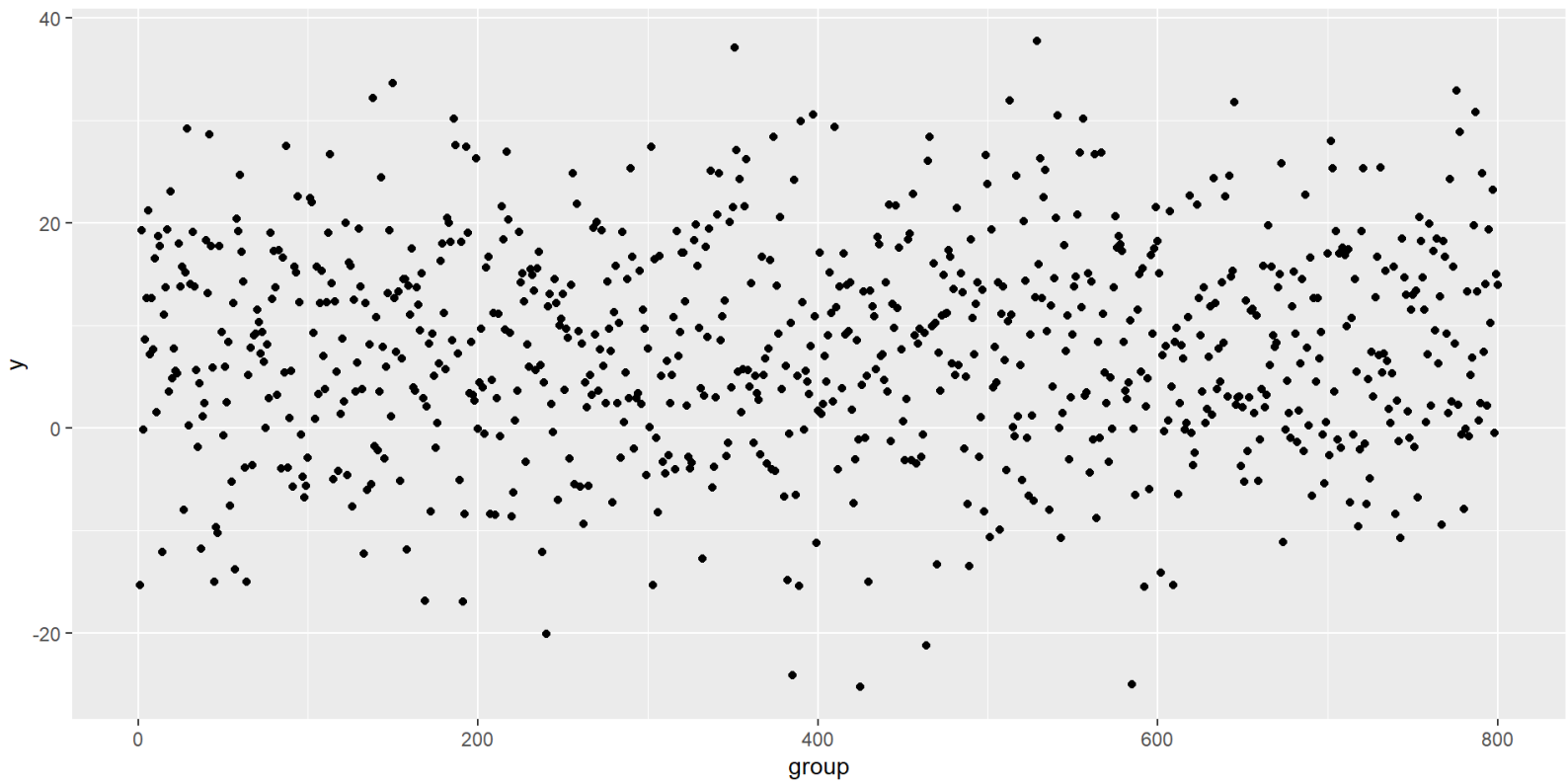
- Note the fixed_param and iters

Extract the relevant quantities

```r
# extract it
y <- as.vector(sim$draws("y", format = "draws_matrix"))
sigma <- as.vector(sim$draws("sigma", format = "draws_matrix"))
theta <- as.vector(sim$draws("theta", format = "draws_matrix"))
mu <- as.vector(sim$draws("mu_print", format = "draws_matrix"))
tau <- as.vector(sim$draws("tau_print", format = "draws_matrix"))
```

Look at it (duh)

```
1  library(tidyverse)
2  my_data <- data.frame(y, group = 1:length(y))
3  my_data %>%
4      ggplot(aes(x = group, y = y)) +
5      geom_point()
```



The centered parameterization in code

```
data {
  int<lower=0> J;
  array[J] real y;
  array[J] real sigma;
}
parameters {
  real mu;
  real<lower=0> tau;
  array[J] real theta;
}
model {
  mu ~ normal(0, 5);
  tau ~ cauchy(0, 2.5);
  theta ~ normal(mu, tau);
  y ~ normal(theta, sigma);
}
```

The noncentered parameterization in code

```
data {
  int<lower=0> J;
  array[J] real y;
  array[J] real sigma;
}
parameters {
  real mu;
  real<lower=0> tau;
  array[J] real var_theta;
}
transformed parameters {
  array[J] real theta;
  for (j in 1:J) theta[j] = tau * var_theta[j] + mu;
}
model {
  mu ~ normal(0, 5);
  tau ~ cauchy(0, 2.5);
  var_theta ~ normal(0, 1);
  y ~ normal(theta, sigma);
}
```

Running things from R

```r
# Centered estimation model:
stan_data <- list(
  J = length(y), y = y, sigma = sigma
)
one_level_cp <- cmdstan_model("src/one_level_cp.stan")

fit_cp <- one_level_cp$sample(
  data = stan_data,
  iter_warmup = 1000, iter_sampling = 1000,
  chains = 4, parallel_chains = 4,
  seed = 13, refresh = 0, adapt_delta = 0.99
)
```

```
Running MCMC with 4 parallel chains...

Chain 1 finished in 10.3 seconds.
Chain 4 finished in 11.1 seconds.
Chain 3 finished in 12.7 seconds.
Chain 2 finished in 18.0 seconds.

All 4 chains finished successfully.
Mean chain execution time: 13.0 seconds.
Total execution time: 18.3 seconds.
```

Checking diagnostics

```
1  fit_cp$cmdstan_diagnose()
```

```
Processing csv files: C:/Users/Chris/AppData/Local/Temp/RtmpGQ8KIl/one_level_cp-
202310152158-1-3442a5.csv, C:/Users/Chris/AppData/Local/Temp/RtmpGQ8KIl/one_level_cp-
202310152158-2-3442a5.csv, C:/Users/Chris/AppData/Local/Temp/RtmpGQ8KIl/one_level_cp-
202310152158-3-3442a5.csv, C:/Users/Chris/AppData/Local/Temp/RtmpGQ8KIl/one_level_cp-
202310152158-4-3442a5.csv

Checking sampler transitions treedepth.
Treedepth satisfactory for all transitions.

Checking sampler transitions for divergences.
No divergent transitions found.

Checking E-BFMI - sampler transitions HMC potential energy.
The E-BFMI, 0.00, is below the nominal threshold of 0.30 which suggests that HMC may have
trouble exploring the target distribution.
If possible, try to reparameterize the model.

The following parameters had fewer than 0.001 effective draws per transition:
```

Running things from R

```r
# noncentered estimation model:
one_level_ncp <- cmdstan_model("src/one_level_ncp.stan")

fit_ncp <- one_level_ncp$sample(
  data = stan_data,
  iter_warmup = 1000, iter_sampling = 1000,
  chains = 4, parallel_chains = 4,
  seed = 13, refresh = 0, adapt_delta = 0.99
)
```

```
Running MCMC with 4 parallel chains...

Chain 2 finished in 15.5 seconds.
Chain 4 finished in 16.1 seconds.
Chain 1 finished in 16.4 seconds.
Chain 3 finished in 23.4 seconds.

All 4 chains finished successfully.
Mean chain execution time: 17.8 seconds.
Total execution time: 23.5 seconds.
```

Checking diagnostics

```
1  fit_ncp$cmdstan_diagnose()
```

```
Processing csv files: C:/Users/Chris/AppData/Local/Temp/RtmpGQ8KIl/one_level_ncp-
202310152159-1-847b44.csv, C:/Users/Chris/AppData/Local/Temp/RtmpGQ8KIl/one_level_ncp-
202310152159-2-847b44.csv, C:/Users/Chris/AppData/Local/Temp/RtmpGQ8KIl/one_level_ncp-
202310152159-3-847b44.csv, C:/Users/Chris/AppData/Local/Temp/RtmpGQ8KIl/one_level_ncp-
202310152159-4-847b44.csv

Checking sampler transitions treedepth.
Treedepth satisfactory for all transitions.

Checking sampler transitions for divergences.
No divergent transitions found.

Checking E-BFMI - sampler transitions HMC potential energy.
E-BFMI satisfactory.

Effective sample size satisfactory.

Split R-hat values satisfactory all parameters.
```

Comparing the two models

```
1 fit_cp$summary(c("mu", "tau"))
```

```
# A tibble: 2 × 10
  variable  mean median    sd   mad    q5   q95  rhat ess_bulk ess_tail
  <chr>    <num>  <num> <num> <num> <num> <num> <num>    <num>    <num>
1 mu        7.79   7.76 0.373 0.413 7.25   8.45  1.19    15.0     152.
2 tau       1.82   1.94 1.09  1.31  0.251  3.45  2.02     5.50     12.2
```

```
1 fit_ncp$summary(c("mu", "tau"))
```

```
# A tibble: 2 × 10
  variable  mean median    sd   mad    q5   q95  rhat ess_bulk ess_tail
  <chr>    <num>  <num> <num> <num> <num> <num> <num>    <num>    <num>
1 mu        7.88   7.87 0.355 0.340 7.28   8.47  1.00    6132.    2937.
2 tau       1.68   1.65 0.994 1.16  0.177  3.34  1.01     479.    1147.
```

First example wrap up

- The centered parameterization throws low-EBFMI warnings, occasional divergent transition warnings, and maximum treedepth reached warnings
- NCP increases efficiency (measured as ESS / run time)

Eight schools in class demo

Centered model:

$$
\begin{aligned}
y_j &\sim \text{Normal}(\theta_j, \sigma_j), \quad j = 1, \ldots, J \\
\theta_j &\sim \text{Normal}(\mu, \tau), \quad j = 1, \ldots, J \\
\mu &\sim \text{Normal}(0, 10) \\
\tau &\sim \text{half} - \text{Cauchy}(0, 10)
\end{aligned}
$$

Non-centered analog:

$$
\begin{aligned}
\theta_j &= \mu + \tau\eta_j, \quad j = 1, \ldots, J \\
\eta_j &\sim N(0, 1), \quad j = 1, \ldots, J.
\end{aligned}
$$

Rubin 1981, Gelman et al. 2013; Stan Development Team 2023

Key thing to note about Eight Schools NCP vs. CP

- NCP replaces the vector θ with a vector η of i.i.d. standard normal parameters and then constructs θ deterministically from η by scaling by τ and shifting by μ

Rubin 1981, Gelman et al. 2013; Stan Development Team 2023

Key thing to note about Eight Schools NCP vs. CP

- NCP replaces the vector θ with a vector η of i.i.d. standard normal parameters and then constructs θ deterministically from η by scaling by τ and shifting by μ
- To the code!

Rubin 1981, Gelman et al. 2013; Stan Development Team 2023

References

- Betancourt, M. and Girolami, M. 2013. Hamiltonian Monte Carlo for hierarchical models. https://arxiv.org/abs/1312.0906
- Gelman, A., Carlin, J. B., Stern, H. S., Dunson, D. B., Vehtari, A., and Rubin, D. B. 2013. Bayesian Data Analysis. Chapman & Hall/CRC Press, London, third edition.
- Rubin, D. B. 1981. Estimation in Parallel Randomized Experiments. Journal of Educational and Behavioral Statistics. 6:377–401.
- Stan Development Team. 2023. Stan Modeling Language Users Guide and Reference Manual. https://mc-stan.org/users/documentation/