Bayesian Modeling

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Agenda

Sampling from a distribution

Conjugate models

- Limited set of applications
- Lack of flexibility
- They are scalable

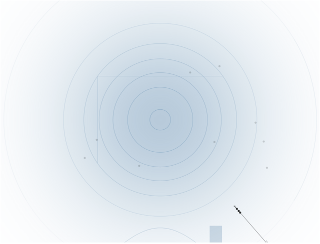


Figure: Easy distribution

Most models

- No closed form solution
- Posterior distributions is complicated
- Less scalable
- Flexible

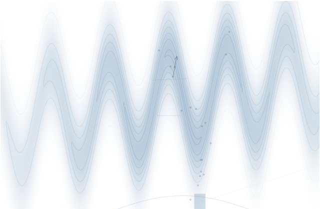


Figure: Complicated distribution

Hamiltonian Monte Carlo Intuition

HMC samples from a complicated distribution

1. Ideas from physics
2. Requires gradient
3. Requires numerical integration

Tuned HMC converges to the target distribution

Warning

I promised a not math heavy course. But this is important for debugging your models.

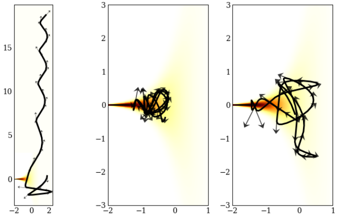


Figure: Leapfrog Integration

HMC Distributions

- $p(\Theta)$ - Target distribution, $\Theta \in \mathbb{R}^d$ (Θ aka **Position**)
- $p(\Delta \mid \Theta)$ - Momentum distribution, $\Delta \in \mathbb{R}^d$ (Δ aka **Velocity**)

Hamiltonian

$$H(\Delta, \Theta) = -\log p(\Delta, \Theta)$$

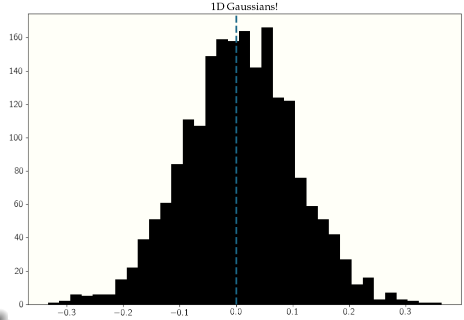


Figure: $p(\Theta) = \text{Normal}(0, 1)$

Notes

- $p(\Delta \mid \Theta) = \text{Normal}(0, M)$, usually a Normal distibution
- Δ and Θ have same dimensions

HMC Differential Equation

$$
\begin{aligned}
H(\Delta, \Theta) &= -\log p(\Delta, \Theta) \\
&= -\log p(\Delta \mid \Theta) \quad -\log p(\Theta) \\
&= \underbrace{K(\Delta, \Theta)}_{\text{Kinetic E}} \quad + \underbrace{V(\Theta)}_{\text{Potential E}}
\end{aligned}
$$

The Physical **motion** equation

$$
\frac{\partial \Theta}{\partial t} = \frac{\partial H}{\partial \Delta}
$$

$$
\frac{\partial \Delta}{\partial t} = -\frac{\partial H}{\partial \Theta}
$$

Motion preserves total energy $H(\Delta, \Theta)$

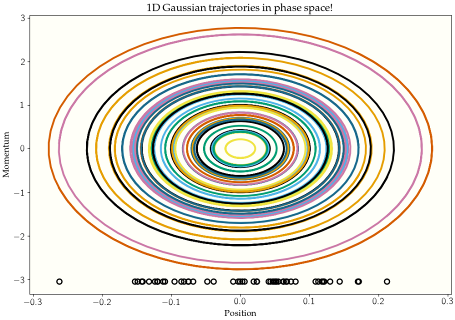


Figure: Momentum, Position trajectories

HMC Divergences

A divergence is a huge integration error solving the differential equation.

When HMC Fails

Bad geometry for Hamiltonian

Bad geometry comes from a lot of things

1. Strong correlations
2. Narrow funnels in the posterior
3. Strong likelihood
4. Non homogeneous posterior

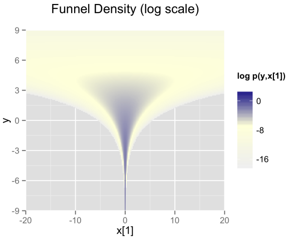


Figure: Neal's Funnel

HMC Reading Materials

Advanced Reading

1. Interactive Demo
2. A tutorial from Colin Carroll
3. A paper from Michael Betancourt
4. NUTS paper from Matthew D. Hoffman, Andrew Gelman

Example

Toy example - Cobb-Douglas with Simpson Paradox

You should all know the Cobb-Douglas function

$$Y \approx A \cdot L^{\beta}$$

In our example:

1. data has 6 groups (hierarchical)
2. We know the groups
3. We know the total factor productivity A is different per group (different equipment)
4. Labour productivity β does not differ much

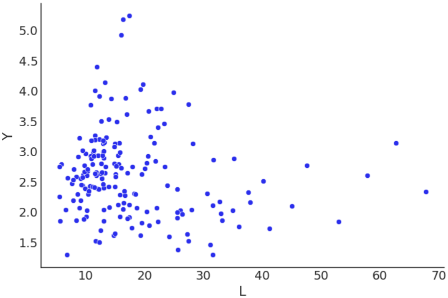


Figure: Example Data (aggregated)

Toy example - Carpet Knitters

Let's put more interpretation in the example

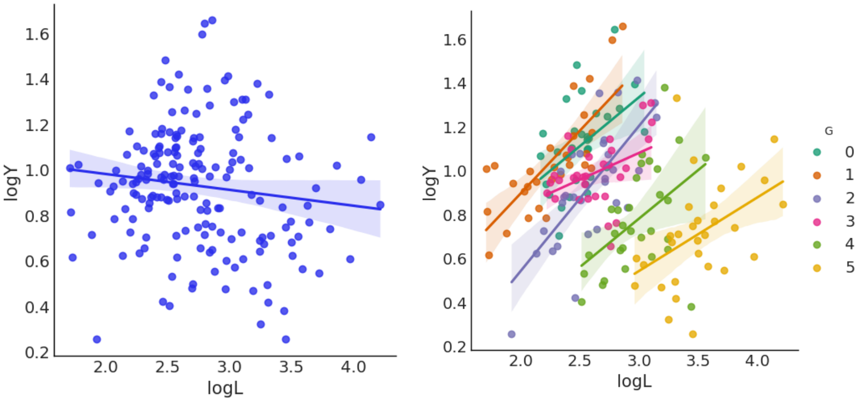
$$Y_g \approx A_g \cdot L^\beta$$

In our example we have a carpet manufacturing plant with 6 workers (groups):

1. Workers make different carpets, thus have total factor productivity A
2. Labour productivity β is like concentration, the more you work the less productive you are
3. Workers produce carpets individually

Figure: Example Y

The paradox



One group model

Best practices when you start.

- Start with a most simple model
- Make sure simple model converges well
- Write a more complex model

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Best practices when you start.

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  - You have groups, start with one
  - Make sure priors are well specified, do checks
- Make sure simple model converges well
  - If one group model fails, all fail
  - There are simple checks to verify your model samples well
- Write a more complex model
  - Try several parametrizations
  - Check how model samples
  - Compare models (out of scope for now)

Starting with a simple model

To get an idea why we start simple

$$Y_{g=0} \approx A_{g=0} \cdot L^{\beta}$$

1. What is prior for A?
2. What is prior for β?
3. What is prior predictive for $Y_{g=0}$?

Writing a model

$$
\begin{aligned}
Y_{g=0} &\approx A_{g=0} \cdot L^{\beta} \\
\log Y_{g=0} &\approx \log A_{g=0} + \log L \cdot \beta
\end{aligned}
$$

Introducing distributions

$$
\begin{aligned}
\log Y_{g=0} &\sim \text{Normal}(\log A_{g=0} + \log L \cdot \beta, \epsilon) \\
\epsilon &\sim ??? \\
\beta &\sim ??? \\
A_{g=0} &\sim ???
\end{aligned}
$$

Prior for β

What is a reasonable prior for labour productivity (elasticity) β? Questions to ask yourself

1. Can it be < 0?
2. Can it be large?
3. Can it be > 1?

Prior for β

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Conclusion: It is bounded by $(0, 1)$

The prior is subjective!

Who can argue these bounds do not make sense?

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Not yet a prior

To get a prior we need a distribution that fits the reasoning

Prior for β

What we know:

- $\beta \in (0, 1)$
- Less probable to be close to the boundary
- Nothing specific about exact value in the range.

In the mind

Enumerate possible distributions that fit the reasoning

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1. Beta(a, b), $a > 0, b > 0$ with some a, b avoids boundaries
2. LogitNormal(μ, σ) - always avoids boundaries

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3. Uniform$(0, 1)$ - a special case of Beta$(1, 1)$

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1. Beta(a, b), $a > 0, b > 0$ with some a, b avoids boundaries
2. LogitNormal(μ, σ) - always avoids boundaries
3. Uniform$(0, 1)$ - a special case of Beta$(1, 1)$
4. Kumaraswamy(a, b), $a > 0, b > 0$ you do not need to know that

Visualize your prior

Before writing a line of code, visualise your prior. What do you like more?

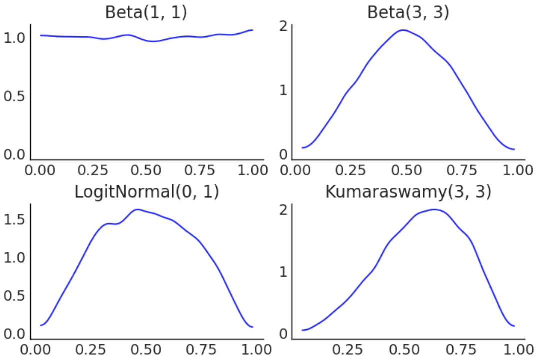

Figure: Visualized Priors

You can choose the form with theory in mind

Setting a prior

I prefer LogitNormal$(0, 1)$ in this situation. It has a good functional form.

To remember

- Prior is **your** modelling choice
- The choice has to be motivated
- The choice should make sense given practical constraints
- You should always be able to defend your choice
- **Prior is what you do not know, the uncertainty**

The model so far

$$
\begin{aligned}
\log Y_{g=0} &\sim \text{Normal}(\log A_{g=0} + \log L \cdot \beta, \epsilon) \\
\epsilon &\sim ??? \\
\beta &\sim \text{LogitNormal}(0, 1) \\
A_{g=0} &\sim ???
\end{aligned}
$$

Prior for ϵ

Rule of thumb

Error term is something small. Usually avoids zero.

In our case;

- small is "orders of 0.1-0.5"

Let it be

$$\epsilon \sim \mathrm{LogNormal}(-2, 1)$$

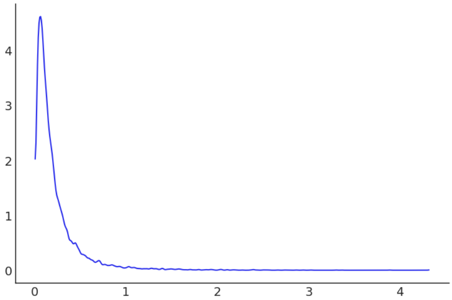

Figure: Prior for ϵ

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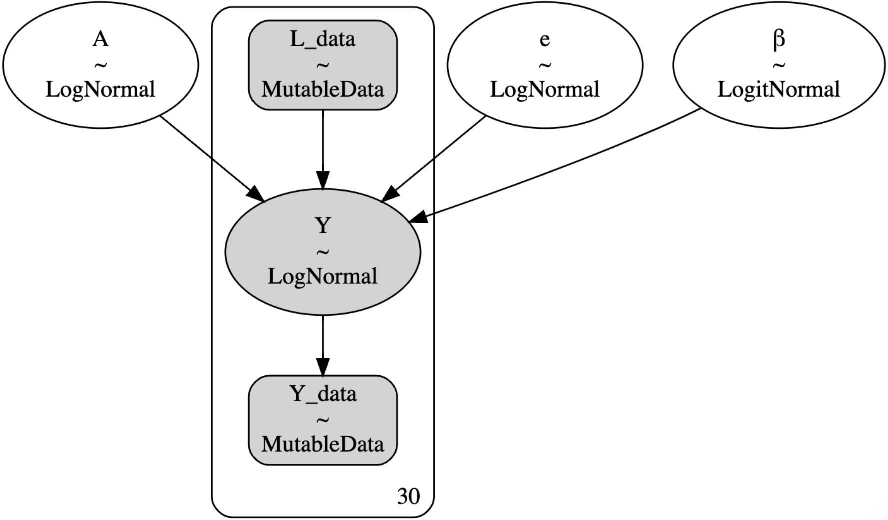
Visual Model



Prior Predictive

Prior for β is an easy one. We need one for $A_{g=0}$

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Definition

Prior predictive is simulated observation model given no data.

The truth

Nobody said setting priors is easy. It is the most work.

Random prior

Why not using e.g.

$$A \sim \mathrm{LogNormal}(0, 1)$$

Random prior

Why not using e.g.

$$A \sim \text{LogNormal}(0, 1)$$

Nonsense

Workers do not produce 800 carpets per week.

That's why

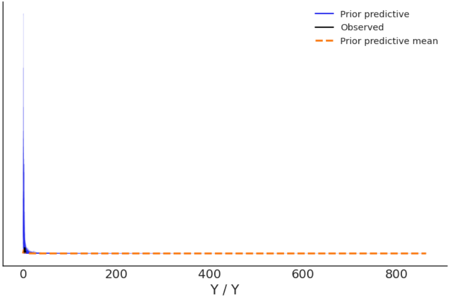

Figure: Prior predictive for Y vs data

Analysing the prior predictive

Getting back to a full model

$$\begin{aligned}
\log Y_{g=0} &\sim \text{Normal}(\log A_{g=0} + \log L \cdot \beta, \epsilon) \\
\epsilon &\sim \text{LogNormal}(-2, 1) \\
\beta &\sim \text{LogitNormal}(0, 1) \\
A_{g=0} &\sim \text{LogNormal}(0, 1)
\end{aligned}$$

- We see over dispersion in predictions
- Variance may come from A or ϵ

Actions

1. Try reducing A variance
2. Try reducing ϵ variance

What can we read here?

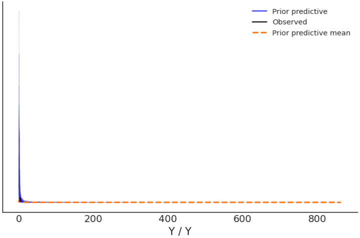

Figure: Prior predictive for Y vs data

Good prior predictive

Seminar

You will play with the example at the seminar.

A good looking prior predictive was with the definition below

$$\log Y_{g=0} \sim \text{Normal}(\log A_{g=0} + \log L \cdot \beta, \epsilon)$$
$$\epsilon \sim \text{LogNormal}(-2, 0.1)$$
$$\beta \sim \text{LogitNormal}(0, 1)$$
$$A_{g=0} \sim \text{LogNormal}(-0.5, 0.1)$$

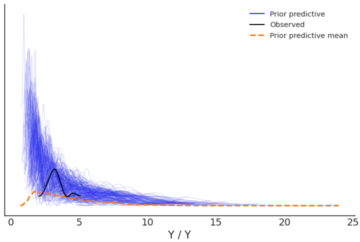

Figure: Prior predictive for Y vs data

What is a good prior predictive?

- Prior predictive covers **reasonable** range for observed data.

- **Data is reference**, not your objective.

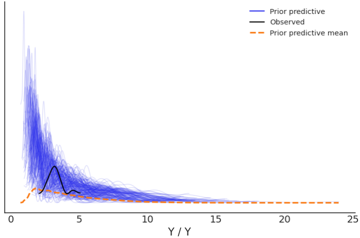

Figure: Prior predictive for Y vs data

What is a good prior predictive?

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  - no astronomic speeds
  - no microscopic distances
  - no black hole densities
  - no superpower workers
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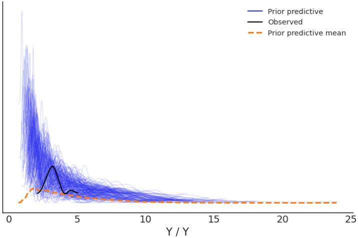

Figure: Prior predictive for Y vs data

What is a good prior predictive?

- Prior predictive covers **reasonable** range for observed data.
    - no astronomic speeds
    - no microscopic distances
    - no black hole densities
    - no superpower workers
- **Data is reference**, not your objective.
    - do not overfit priors on data.
    - in 90% cases you do not need data for prior predictive
    - in 90% cases common sense should work just fine
    - in 10% cases you can ask experts and adjust the priors
    - data is your last resort

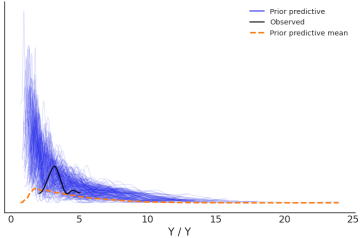

Figure: Prior predictive for Y vs data

HMC in action

Sampling

After we've checked the priors it is time to sample.

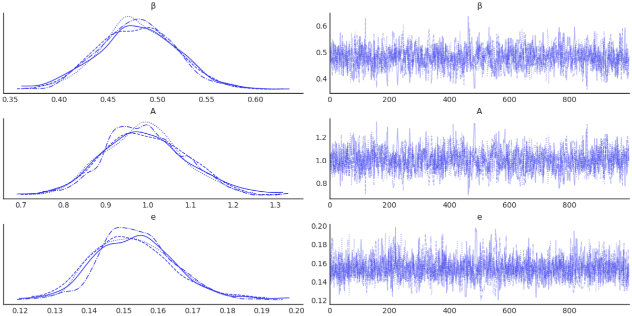

Figure: Posterior MCMC trace

Hierarchies

Hierarchies

Initial data has groups. How to take them in account?

$$
\begin{aligned}
\log Y_{\mathbf{g}} &\sim \text{Normal}(\log A_{\mathbf{g}} + \log L \cdot \beta, \epsilon) \\
\epsilon &\sim \text{LogNormal}(-2, 1) \\
\beta &\sim \text{LogitNormal}(0, 1) \\
A_{\mathbf{g}} &\sim \text{???}
\end{aligned}
$$

What is Hierarchy?

Hierarchy

Once you have similar groups in your data, you have hierarchy.

Examples:

1. Countries, Regions
2. User groups: by age, by profession, etc
3. Treatment groups
4. Time dependent effects
5. Panel Data

Our Example

Workers make different carpets and have total factor productivity A

Treating Hierarchy

Classical Econometrics view:

1. All the groups are independent and treated similarly. **Pooled Model**

$$y_{k,i} = \alpha + \beta x_{k,i} + \varepsilon_{i,k}$$

2. Groups have significant differences. **Fixed Effect Model**

$$y_{k,i} = \alpha_k + \beta x_{k,i} + \varepsilon_{i,k}$$

3. Groups have non significant, random differences. **Random Effects Model**

$$y_{k,i} = \alpha + \beta x_{k,i} + u_k + \varepsilon_{i,k}$$

Where

$$\mathbb{E} u_{k,i} = 0, \quad \mathbb{E} \varepsilon_{k,i} = 0$$

Bayesian Hierarchy

In

$$y_{k,i} = \alpha + \beta x_{k,i} + u_k + \varepsilon_{i,k}$$

Let's rearrange terms

$$y_{k,i} = (\alpha + u_k) + \beta x_{k,i} + \varepsilon_{i,k}$$

- α - population mean
- $\alpha_k = \alpha + u_k$ - group mean

In a Bayesian analysis we need priors. There is more than one way

$$\begin{aligned} \alpha &\sim \text{Normal}(\bar{\mu}, \bar{\sigma}) \\ u_k &\sim \text{Normal}(0, 1) \\ \alpha_k &= \alpha + u_k \cdot \sigma \end{aligned}$$

$$\begin{aligned} \alpha &\sim \text{Normal}(\bar{\mu}, \bar{\sigma}) \\ \alpha_k &\sim \text{Normal}(\alpha, \sigma) \end{aligned}$$

More on priors

Non centered parametrization

$$\alpha \sim \text{Normal}(\bar{\mu}, \bar{\sigma})$$
$$u_k \sim \text{Normal}(0, 1)$$
$$\alpha_k = \alpha + u_k \cdot \sigma$$

Group specific parameter u_k is disentangled

Centered parametrization

$$\alpha \sim \text{Normal}(\bar{\mu}, \bar{\sigma})$$
$$\alpha_k \sim \text{Normal}(\alpha, \sigma)$$

σ is a measure of group differences

1. $\sigma \to 0$: Pooled Model
2. Small σ: Random Effects / Partial Pooling
3. Large σ: Fixed Effects / Unpooled Model

σ interpolates between the models

Degeneracy

TODO: improve the visualization

Centered parametrization

$$\alpha \sim \text{Normal}(\bar{\mu}, \bar{\sigma})$$
$$\alpha_k \sim \text{Normal}(\alpha, \sigma)$$

Warning

Centered parametrization creates funnel geometry with few data

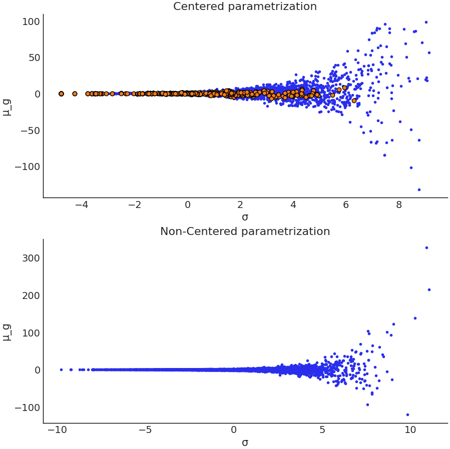

Figure: Divergences appear in the Centered Parametrization

Why Funnel is created?

Geometry is important

1. Sampler has adaptive step size
2. With bad geometry Sampler can't find a good one

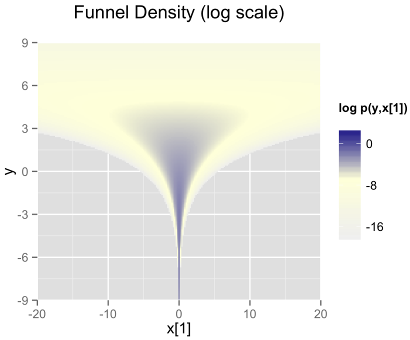

Figure: Funnel Geometry

Suggested reading

Read more on reparametrization in Stan's Guide

Inverted Funnel degeneracy

A "nice" parametrization does have issues as well.

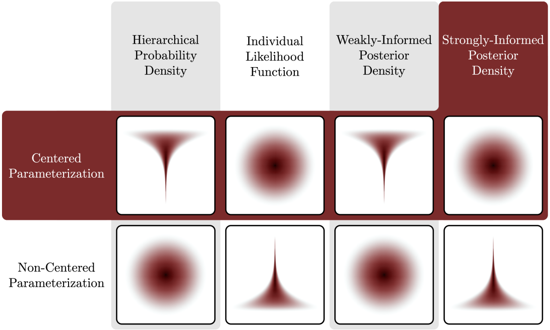

Figure: Inverted Funnel Degeneracy

Advanced Reading

Read more from Michael Betancourt

Setting a Hierarchical Prior

1. Start with a Pooled or Single group model

2. Add Hierarchy

Setting a Hierarchical Prior

1. Start with a Pooled or Single group model
    - You get an idea of prior parameter scales
    - You get a decent model structure
    - Do not care about predictions
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    - Decide on which parameters to share
    - Decide on allowed variability for the rest parameters
    - Debug divergences, reparametrize if required

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Best Practice

Do not hard-code the parametrization, toggle it in the code

The Cobb-Douglas Case

Single group model

$$
\begin{aligned}
\log Y_0 &\sim \text{Normal}(\log A_0 + \log L \cdot \beta, \epsilon) \\
\epsilon &\sim \text{LogNormal}(-2, 0.1) \\
\beta &\sim \text{LogitNormal}(0, 1) \\
A_0 &\sim \text{LogNormal}(-0.5, 0.1)
\end{aligned}
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Hierarchical model

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\beta &\sim \text{LogitNormal}(0, 1) \\
A_k &\sim \text{LogNormal}(\log A_{\text{pop}}, \sigma_A) \\
A_{\text{pop}} &\sim \text{LogNormal}(-0.5, 0.1) \\
\sigma_A &\sim \text{LogNormal}(-2, 0.1)
\end{aligned}
$$

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\beta &\sim \text{LogitNormal}(0, 1)\\
A_k &\sim \text{LogNormal}(\log A_{\text{pop}}, \sigma_A)\\
A_{\text{pop}} &\sim \text{LogNormal}(-0.5, 0.1)\\
\sigma_A &\sim \text{LogNormal}(-2, 0.1)
\end{aligned}
$$

Hint

You can reuse some parameters, just add reasonable variability σ_A

Discussion Time

Setting priors

- Sometimes you do not have expert knowledge
- Sometimes parametrization does not allow you to set a good prior
- Sometimes prior predictive depends on many parameters
- You are limited in time
- Using hyperpriors