Wednesday 14:00-17:30

Part 7

Bayesian hierarchical modelling, simulation and MCMC

by Gero Walter

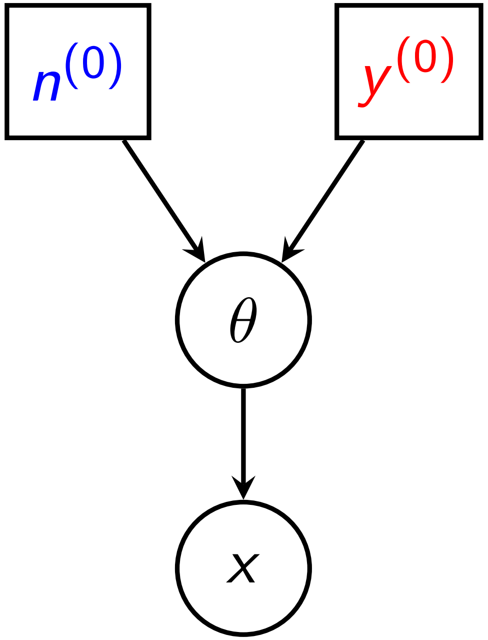
Bayesian hierarchical modelling, simulation and MCMC

Outline

Bayesian Hierarchical Modelling, a.k.a. Bayesian (Belief) Networks, a.k.a. Graphical Models

- many names for the same thing (it's a powerful tool),
  I will use the term Bayesian Networks (BNs)
- BNs as a unifying way to think about (Bayesian) statistical models
- how to build complex Bayesian models out of simple building blocks
- how to specify joint distributions (over many variables)
  via univariate distributions
  using conditional independence assumptions
- conditional independence assumptions are visualized by a graph
- the graph can establish a hierarchy between variables

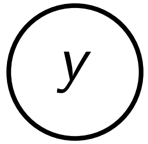
Bayesian Networks: Simple Example



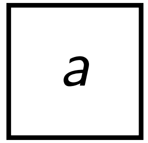
$$f(x \mid \theta) \sim \text{Binomial}(n, \theta)$$

$$f(\theta \mid n^{(0)}, y^{(0)}) \sim \text{Beta}(n^{(0)}, y^{(0)})$$

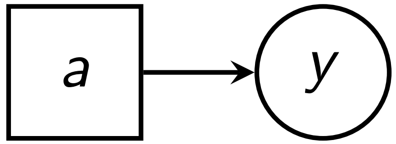
variables / parameters



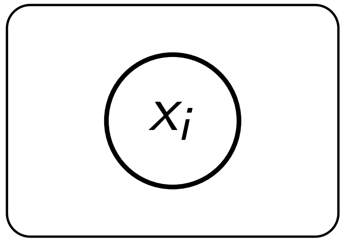
fixed values



y depends on a

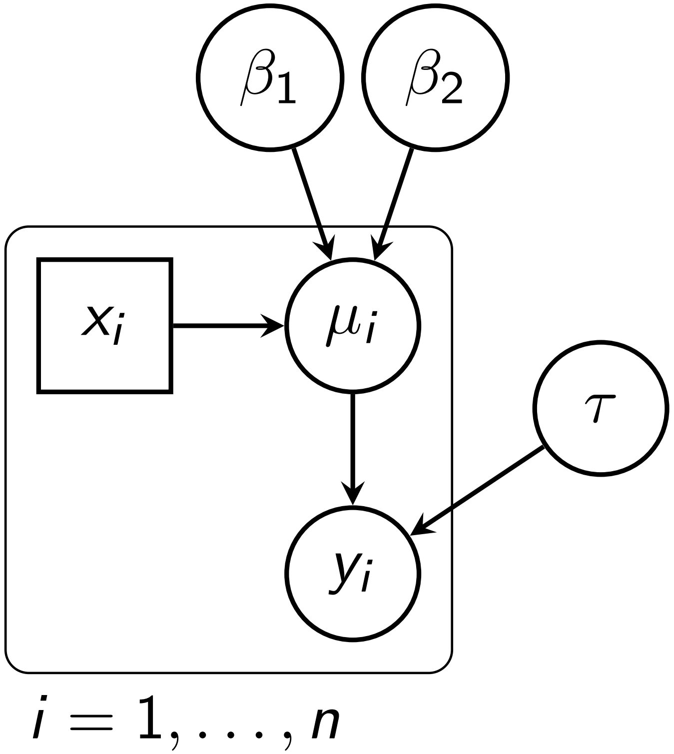


repeated nodes



$i = 1, \ldots, n$

Another Example: Linear Regression



$$y_i = \beta_1 + x_i\beta_2 + \varepsilon_i, \quad \text{where } \varepsilon_i \overset{\text{iid}}{\sim} \mathrm{N}(0, \sigma^2)$$

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$$\tau \mid a, b \sim \mathrm{Gamma}(a, b)$$

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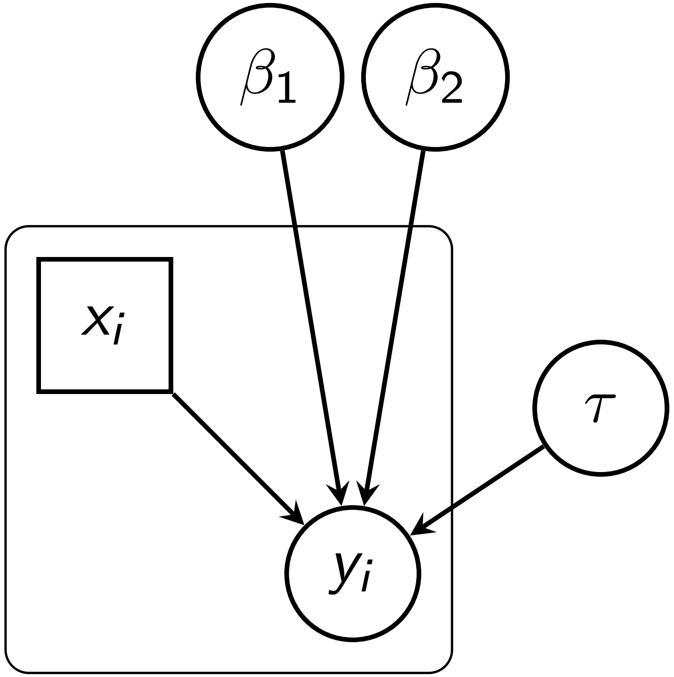

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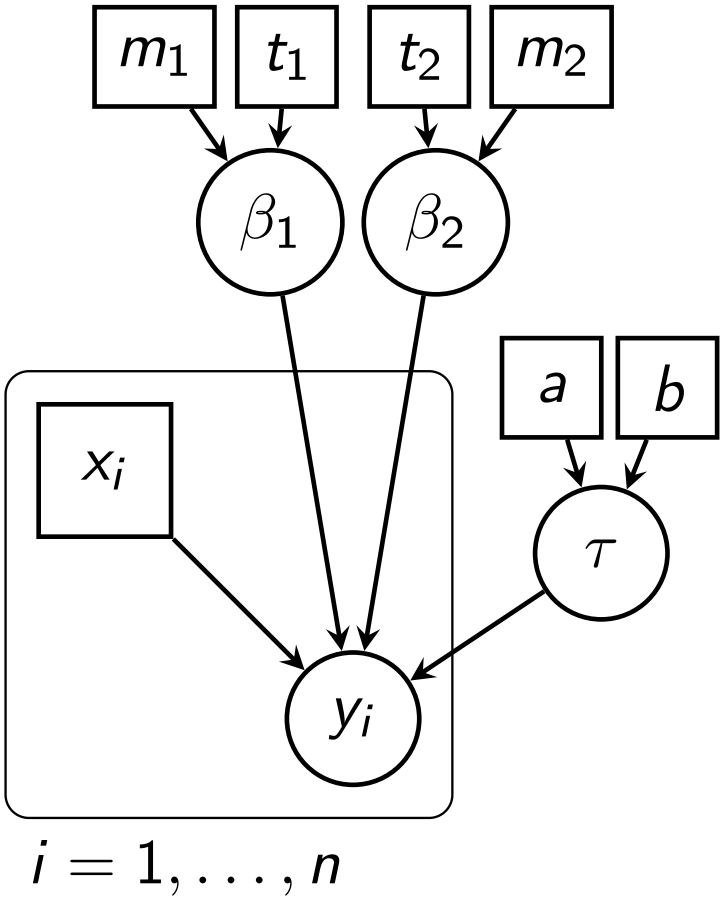

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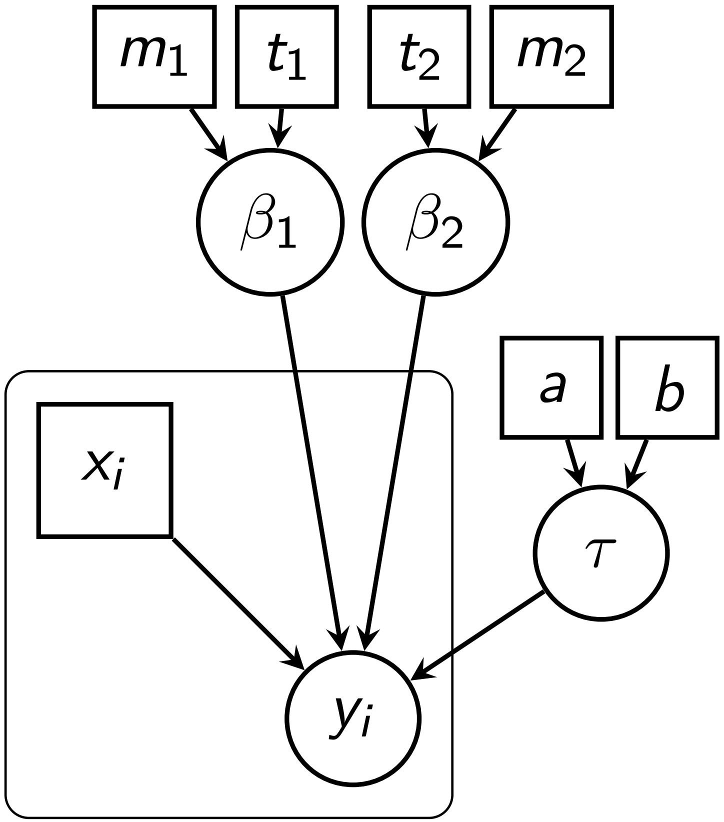

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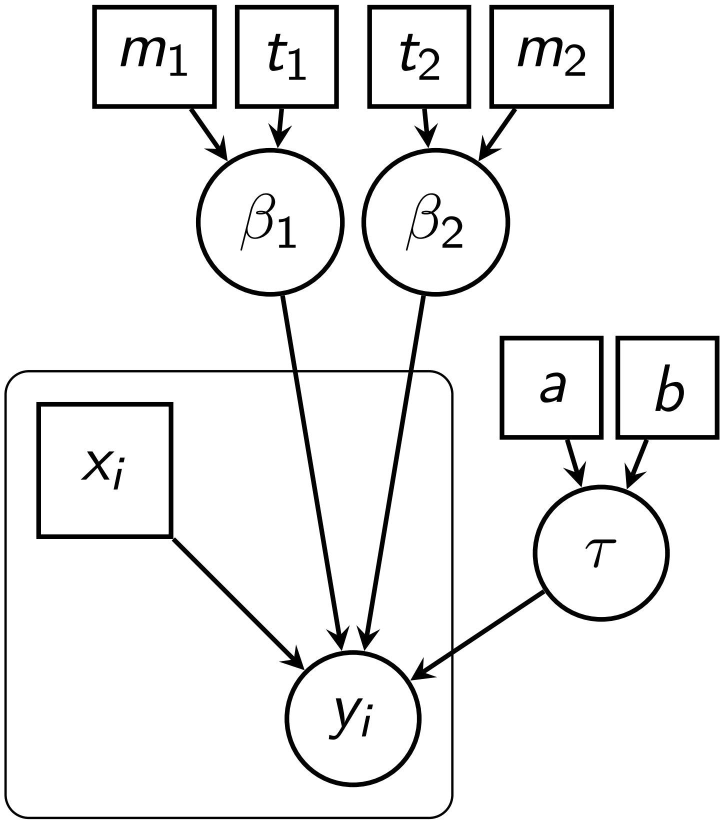

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cond. indep. relations

variables:
conditional distributions

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- often: BN = discrete variables only, distributions defined via conditional probability tables (CPTs)
- What kind of graphs work for expressing conditional independence relations?

Bayesian Networks: Directed Acyclic Graphs

Definition (Directed Graph)

A *directed graph* $G = (V, E)$ consists of a set of vertices V and a set of edges E, where $E \subset V \times V$. An arrow leads from $u \in V$ to $v \in V$ if and only if $(u, v) \in E$; u is the *source* and v is the *target* of edge (u, v).

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Definition (Directed Acyclic Graph)

A *directed acyclic graph (DAG)* is a directed graph that does not contain a cycle, i.e. there does not exist a subset of edges that forms a cycle.

Bayesian Networks: Formal Definition

Definition (Bayesian Network)

Given a DAG $G = (V, E)$, and variables $x_V = \{x_v\}_{v \in V}$, a *Bayesian network* with respect to G and x_V is a joint probability distribution for the x_V of the form:

$$f(x_V) = \prod_{v \in V} f\left(x_v \mid x_{\mathrm{pa}(v)}\right)$$

where $\mathrm{pa}(v)$ is the set of parents of v, i.e. the set of vertices u such that (u, v) is an edge.

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- joint distribution factorizes according to the graph!

Bayesian Networks: Factorization of the joint

One can always factorize a joint distribution by

$$f(x_1, \ldots, x_K) = f(x_K \mid x_1, \ldots, x_{K-1})\, f(x_{K-1} \mid x_1, \ldots, x_{K-2}) \cdots f(x_3 \mid x_1, x_2)\, f(x_2 \mid x_1)\, f(x_1)$$

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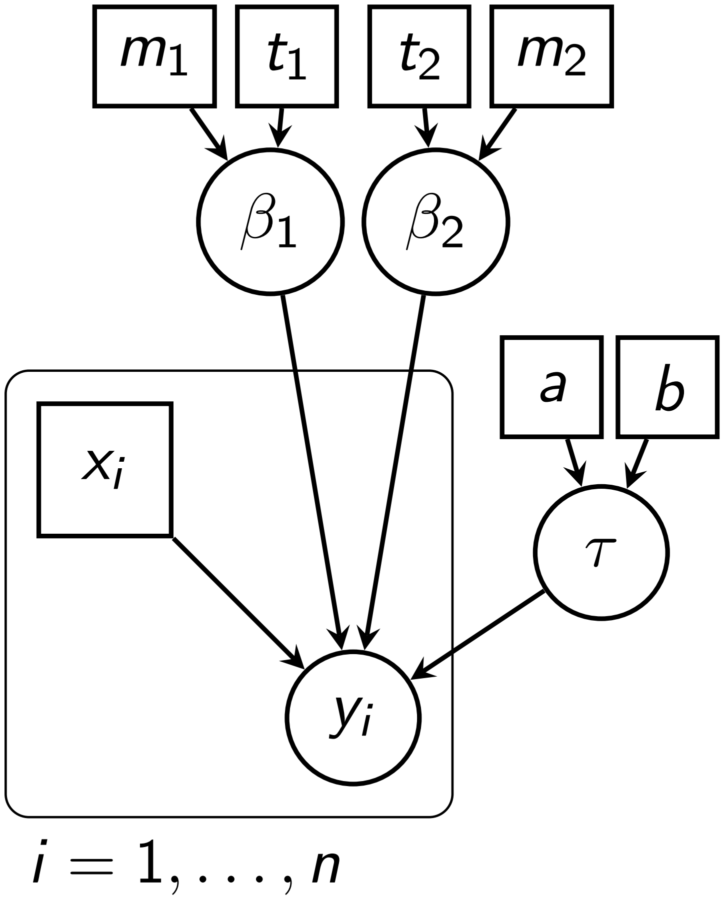
- sparser graph $\implies$ nodes have fewer parents
  $\implies$ less complex joint

Factorization of the joint: Example



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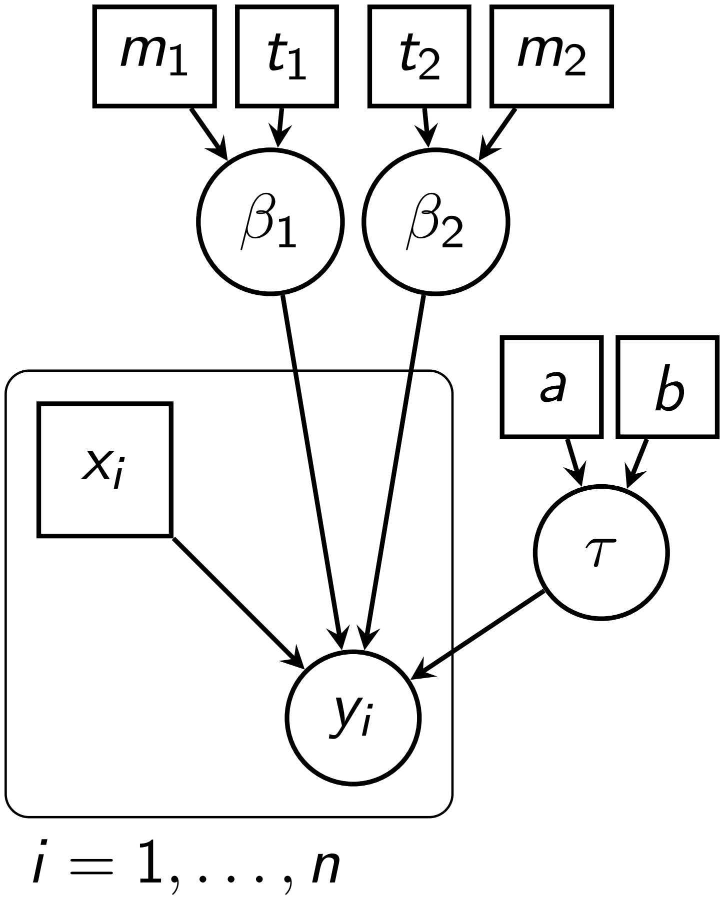

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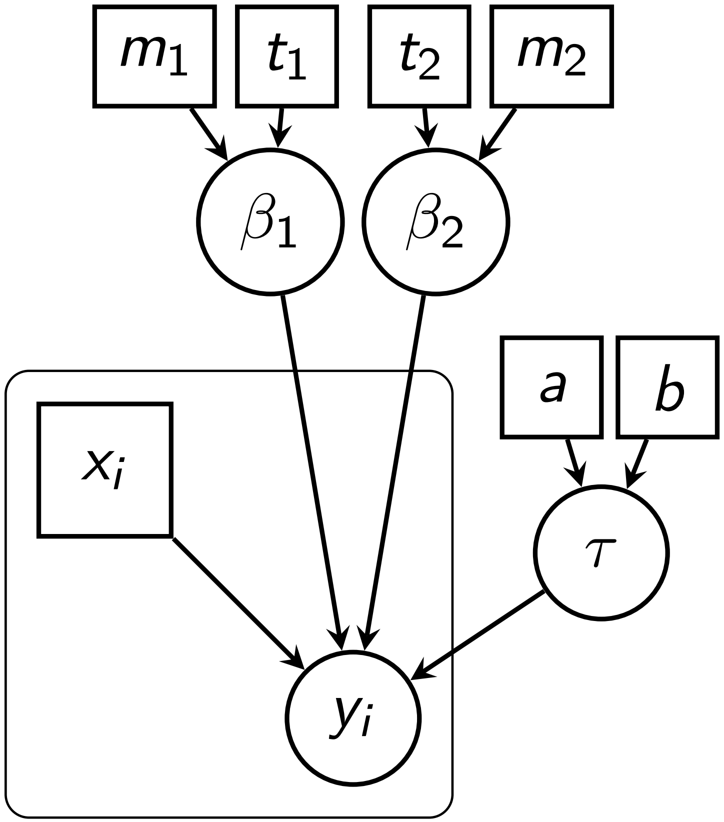

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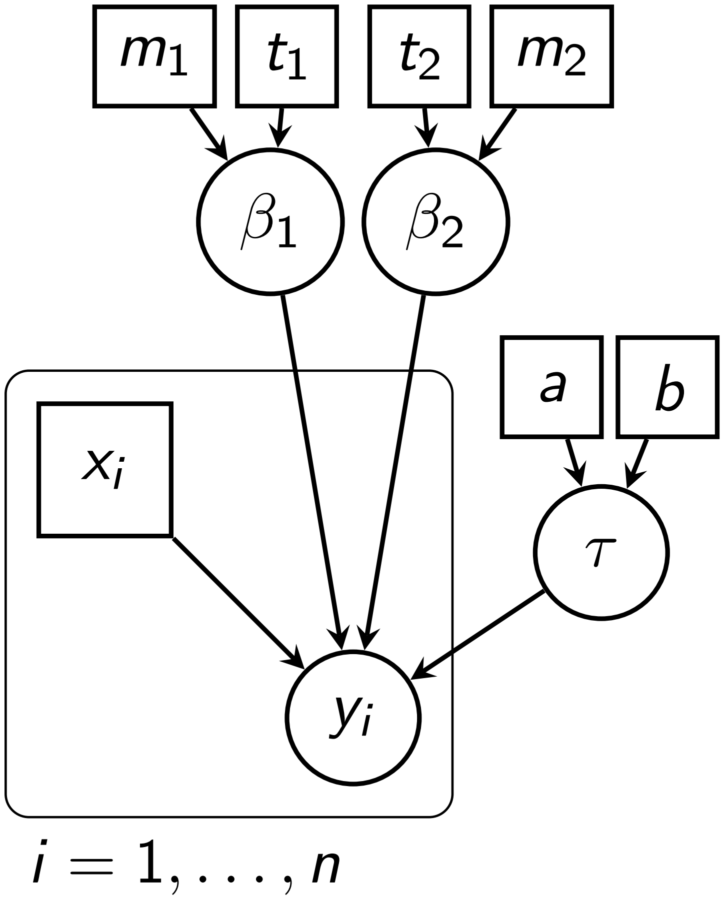

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- it would be really useful to get posterior estimates based on the non-normalized density $f(y_1, \ldots, y_n, \beta_1, \beta_2, \tau)$!

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  - marginalizing = use only, e.g., $\{\beta_1^m\}, m = 1, \ldots, M$
  - conditioning = use only samples m with the right value of the conditioning parameter(s)
    (or redo the sampling with fixed conditioned values)

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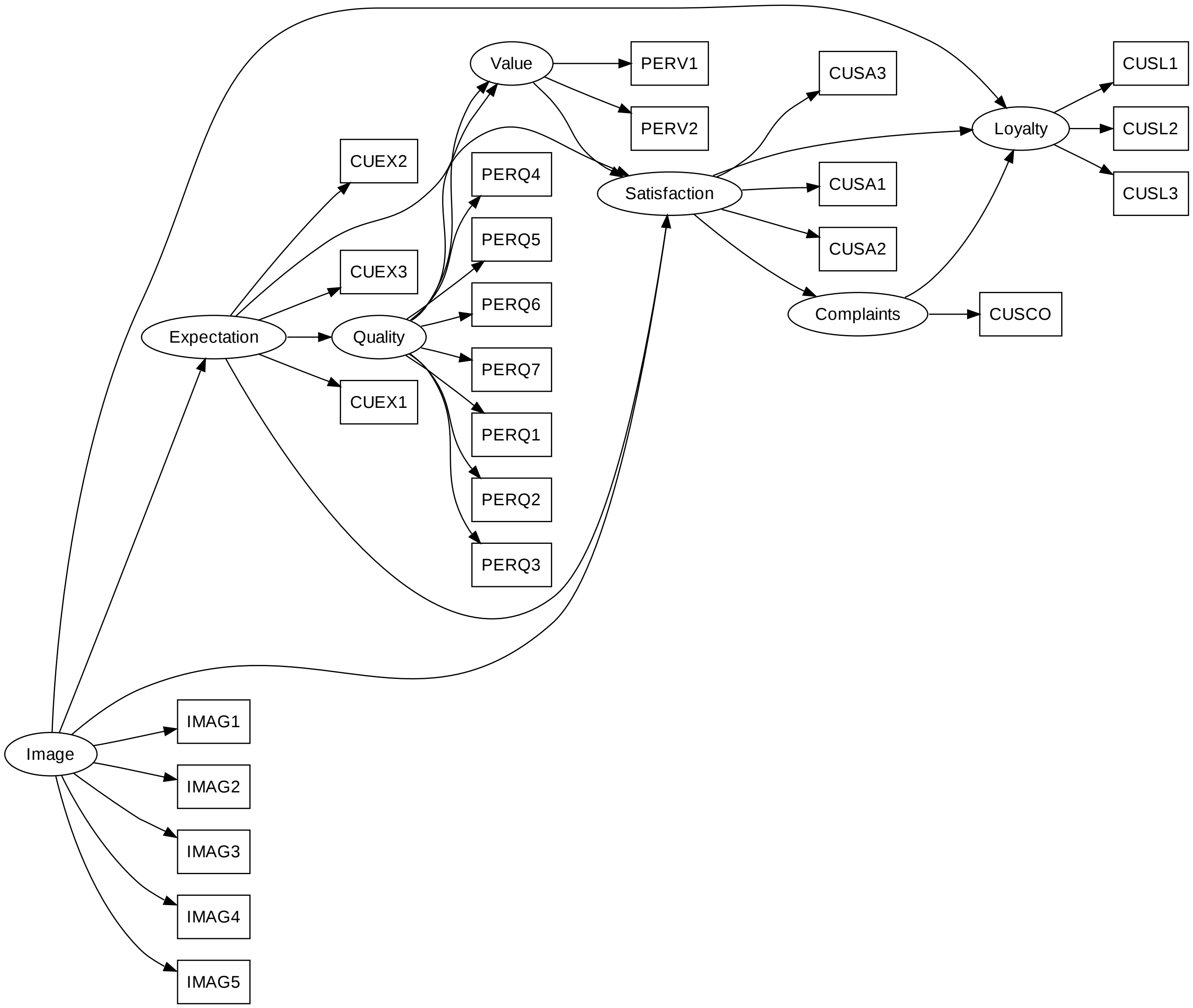
- conditional independence with IP gets very non-trivial (see, e.g., [2, §4] for the gory details)
- here: do sensitivity analysis by varying prior distributions in sets: $f(\beta_1) \in \mathcal{M}_{\beta_1}, \ldots$

Other Graph-Based Methods: SEM, Path Analysis



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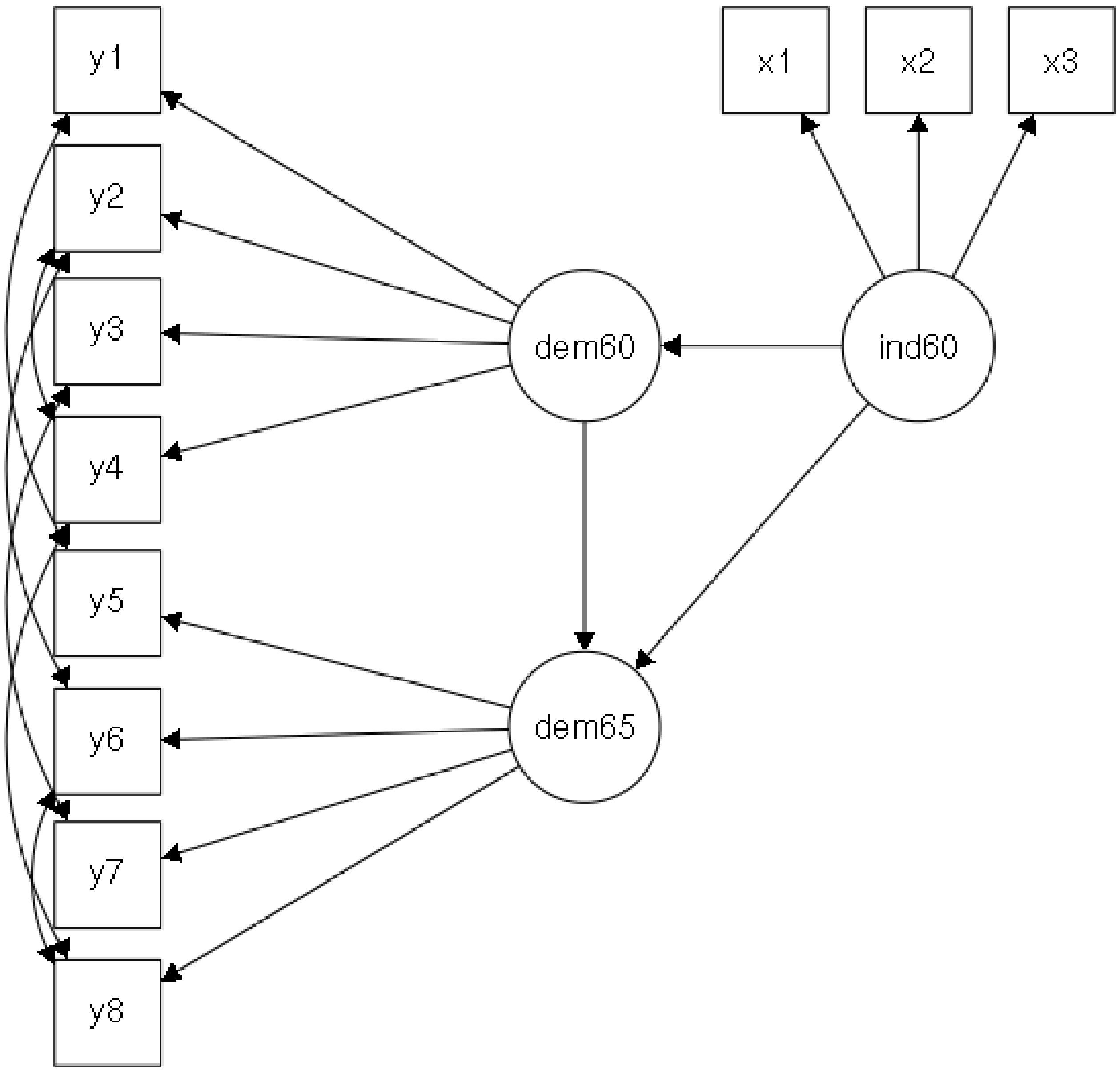

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  - Bayesian SEM: (**R** package `blavaan`)

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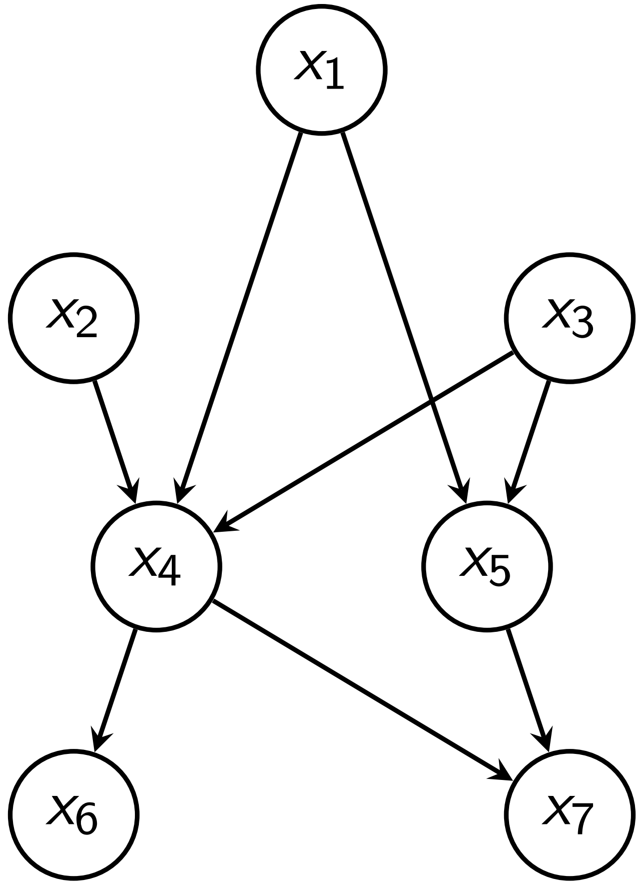
  - partial least squares (**R** package `semPLS`):
    iterative fitting of latent variable values
    and regression coefficients via least squares
- path analysis: special case where a measurement can be linked to only one construct

Exercise 1: Factorization of a Joint

Which factorization of
$f\left(\{x_i\}_{i\in[1,\ldots,7]}\right)$
does this graph encode?



Exercise 2: Naive Bayes Classifier

The naive Bayes classifier from Part 6 assumes that the joint distribution of class c and attributes $a_1, \ldots, a_k$ can be factorized as

$$p(c, a) = p(c)p(a \mid c) = p(c) \prod_{i=1}^{k} p(a_i \mid c).$$

Draw the corresponding DAG!
(Hint: use either a plate or consider two attributes a_1 and a_2 only.)

Exercise 3: Naive Bayes Classifier with Dirichlet Priors

We can introduce parameters for $p(c)$ and $p(a_i \mid c)$:

$$(n(c))_{c\in\mathcal{C}} \sim \text{Multinomal}(\theta_c; c \in \mathcal{C}) \tag{36}$$

$$\forall c \in \mathcal{C}\colon (n(a_i, c))_{a_i\in\mathcal{A}_i} \mid c \sim \text{Multinomal}(\theta_{a_i|c}; a_i \in \mathcal{A}_i) \tag{37}$$

where $\mathcal{C}$ denotes the set of all possible class values, and $\mathcal{A}_i$ denotes the set of all possible values of attribute i.

The θ parameters can be estimated using a Dirichlet prior:

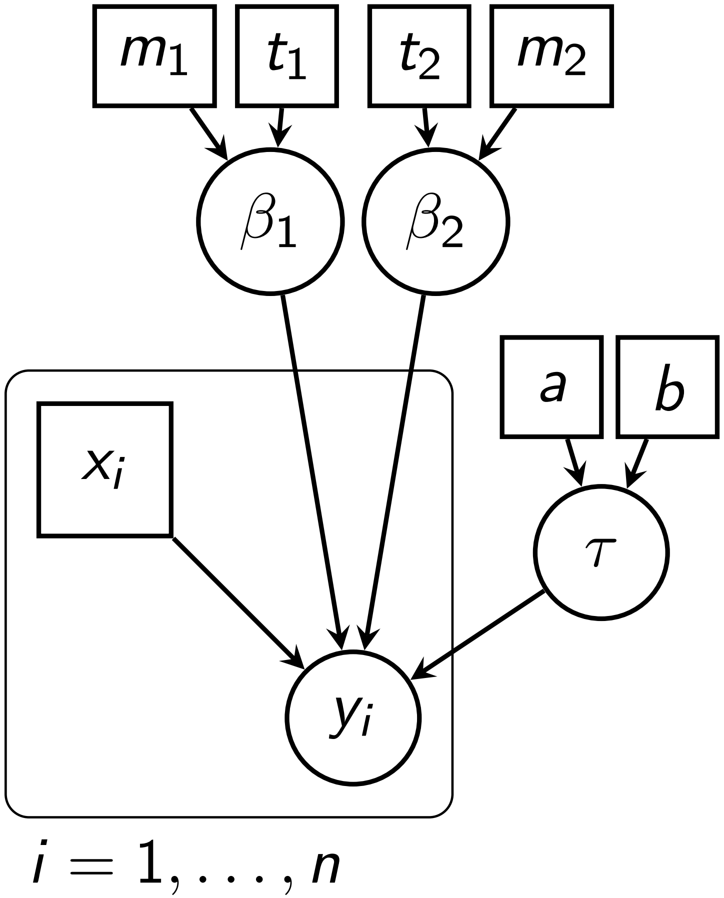
$$(\theta_c)_{c\in\mathcal{C}} \sim \text{Dir}(s, (t(c))_{c\in\mathcal{C}}) \tag{38}$$

$$\forall c \in \mathcal{C}\colon (\theta_{a_i|c})_{a_i\in\mathcal{A}_i} \mid c \sim \text{Dir}(s, (t(a_i, c))_{a_i\in\mathcal{A}_i}) \tag{39}$$

where we must have that $\sum_{a_i\in\mathcal{A}_i} t(a_i, c) = t(c)$. [Note that $t(c)$ is the prior expectation of θ_c and $t(a_i, c)/t(c)$ is the prior expectation of $\theta_{a_i|c}$.]

Draw the corresponding graph!

Exercise 4: Sensitivity Analysis



In the linear regression example there are 6 hyperparameters m_1, t_1, m_2, t_2, a, b.

How would you do sensitivity analysis over the prior in that example? What problems do you foresee?

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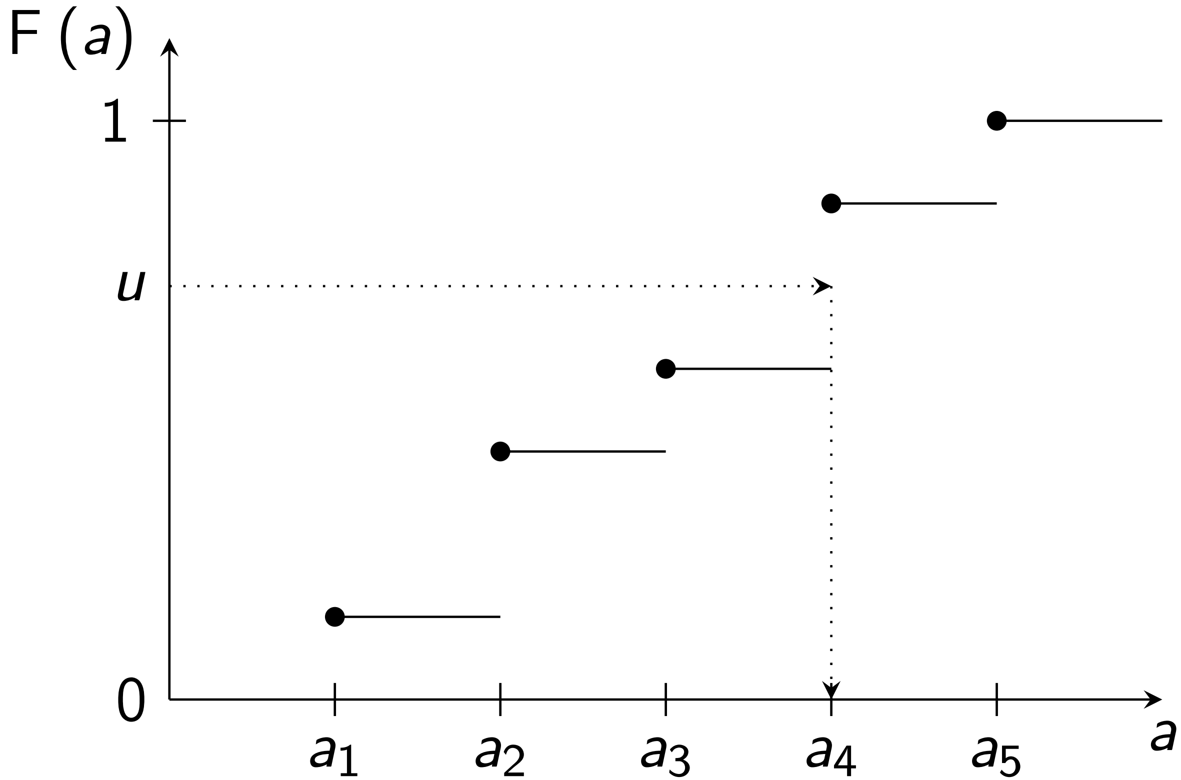

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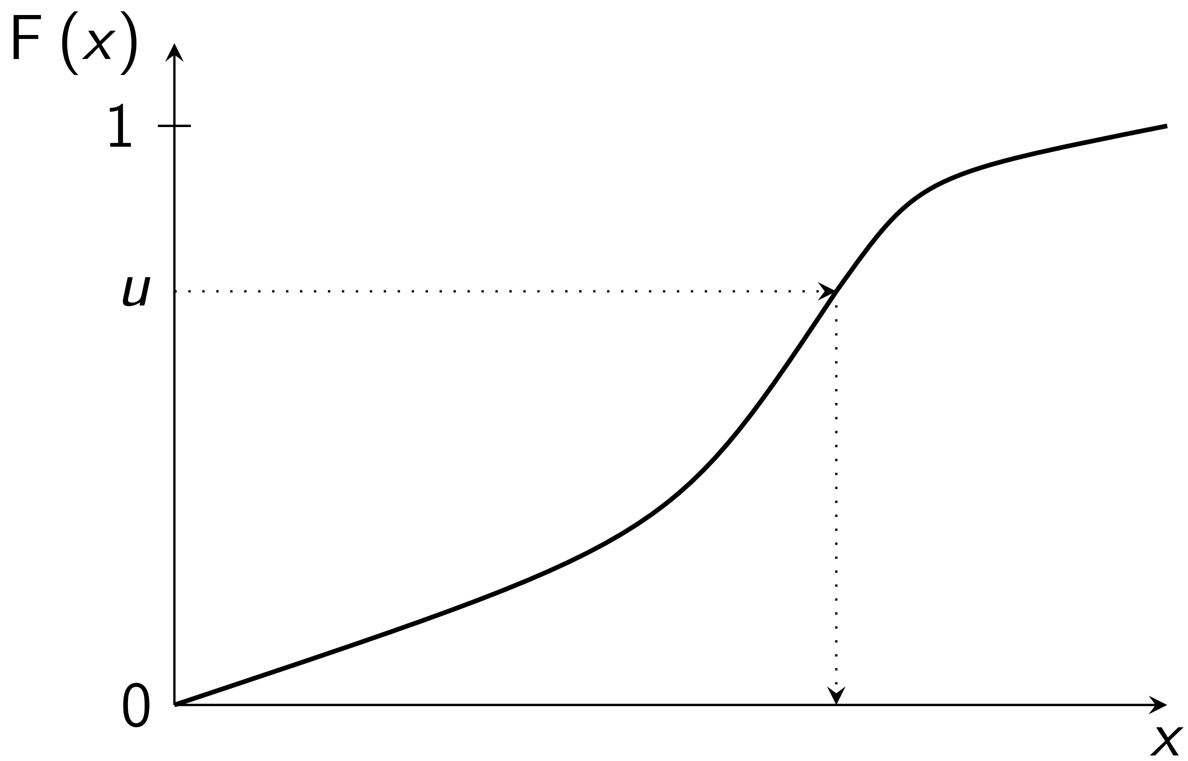

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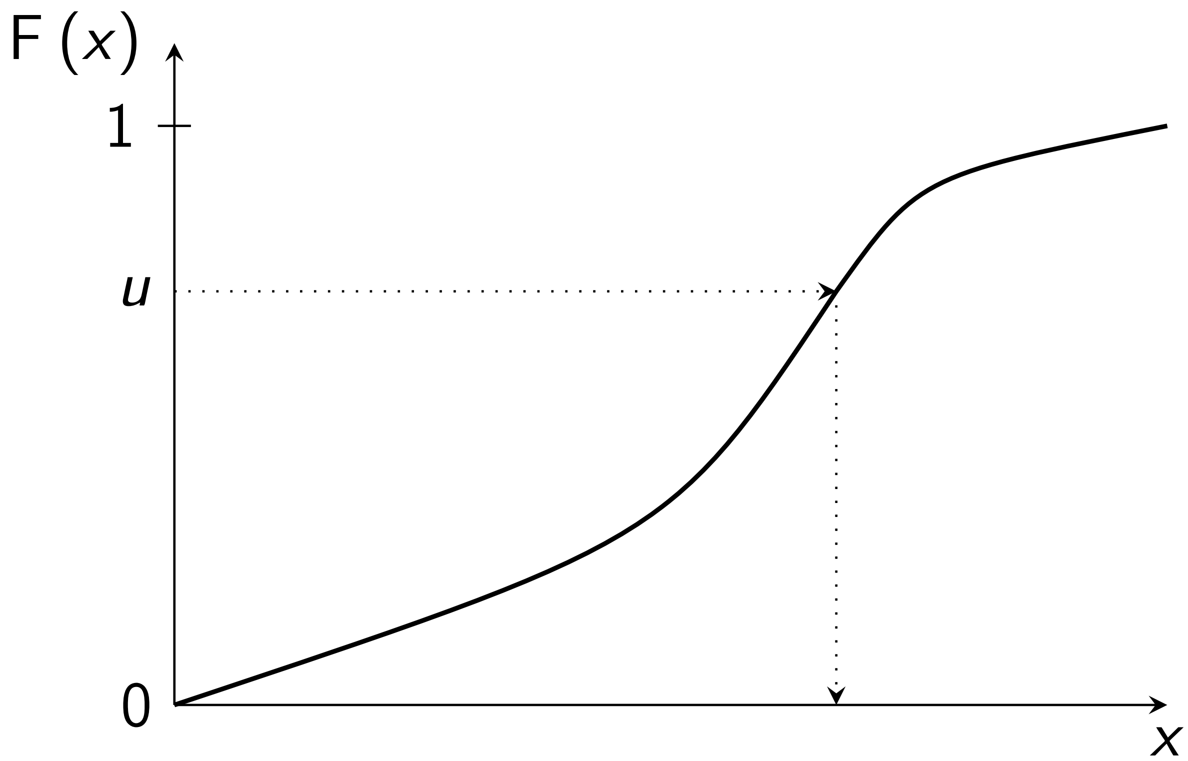

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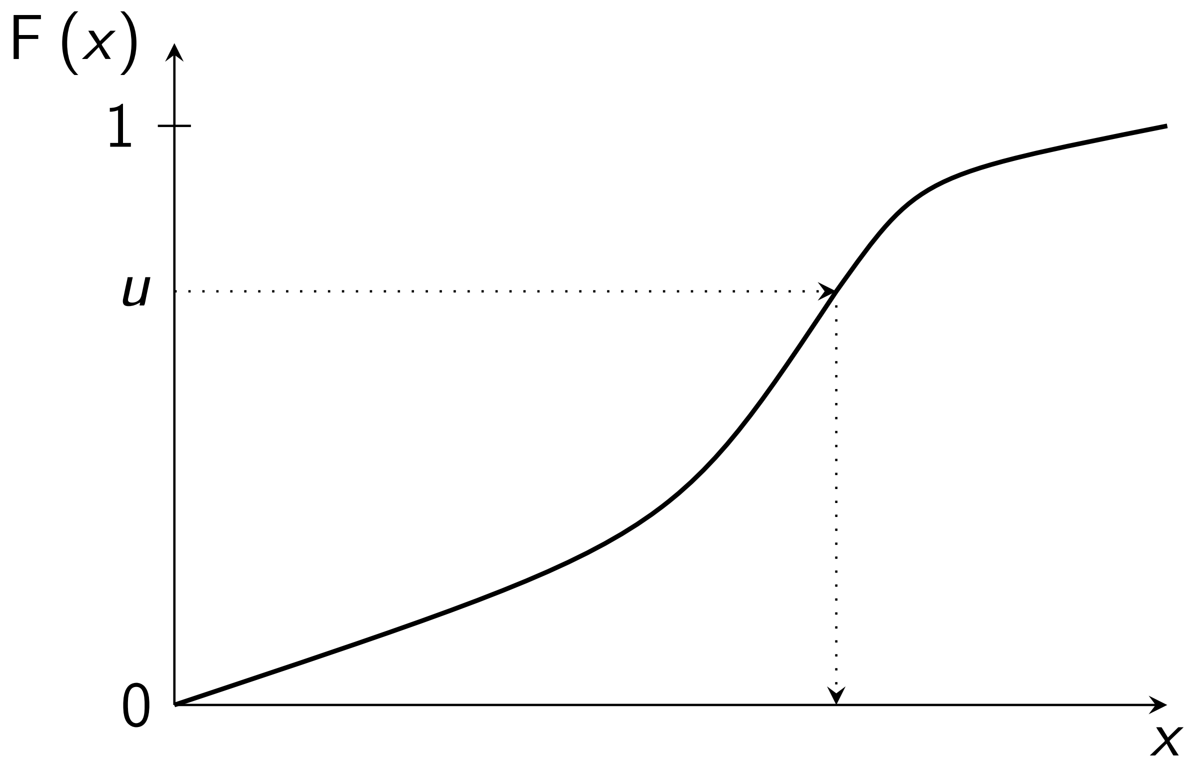

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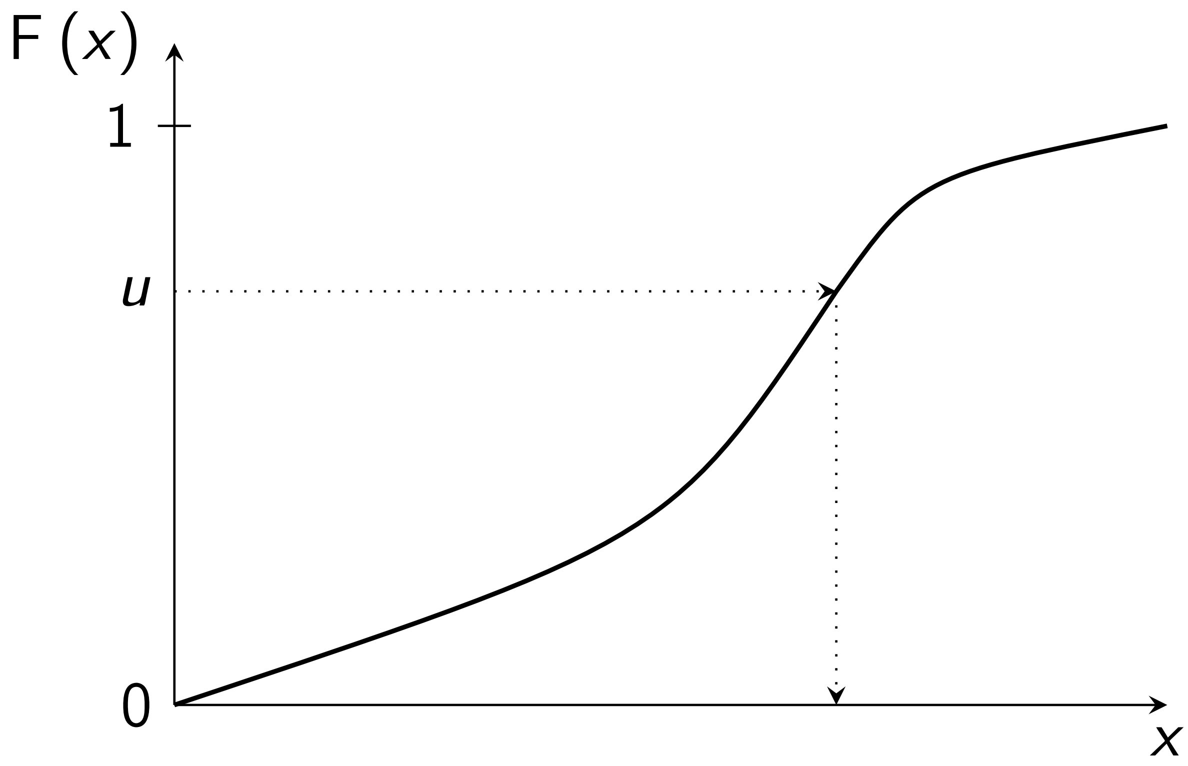

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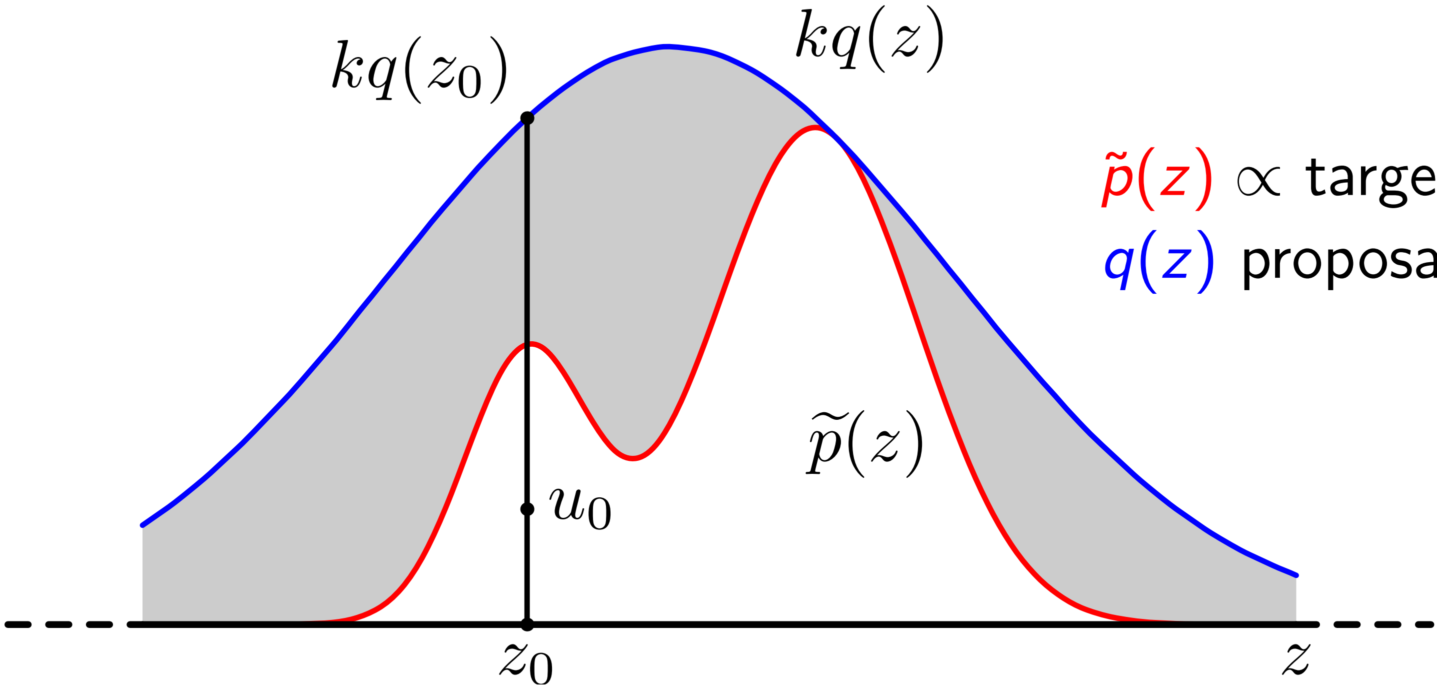

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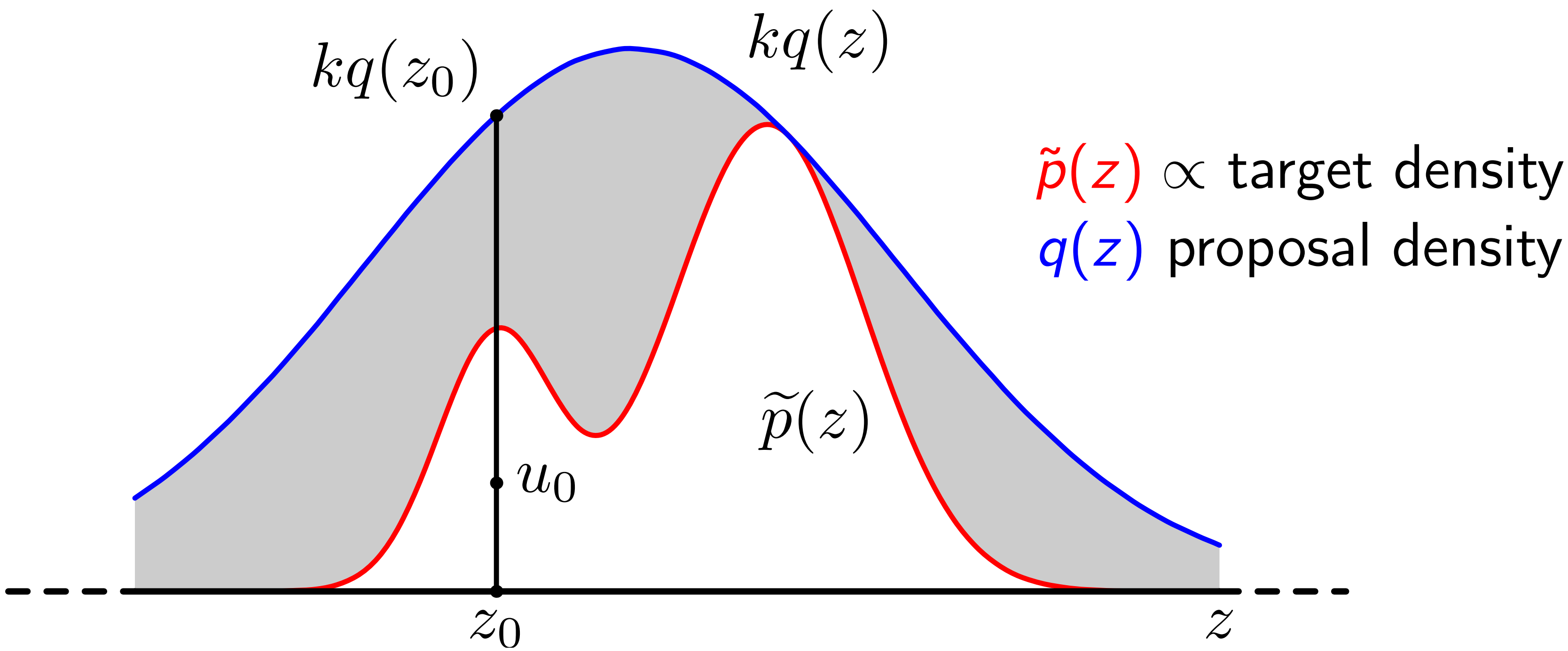

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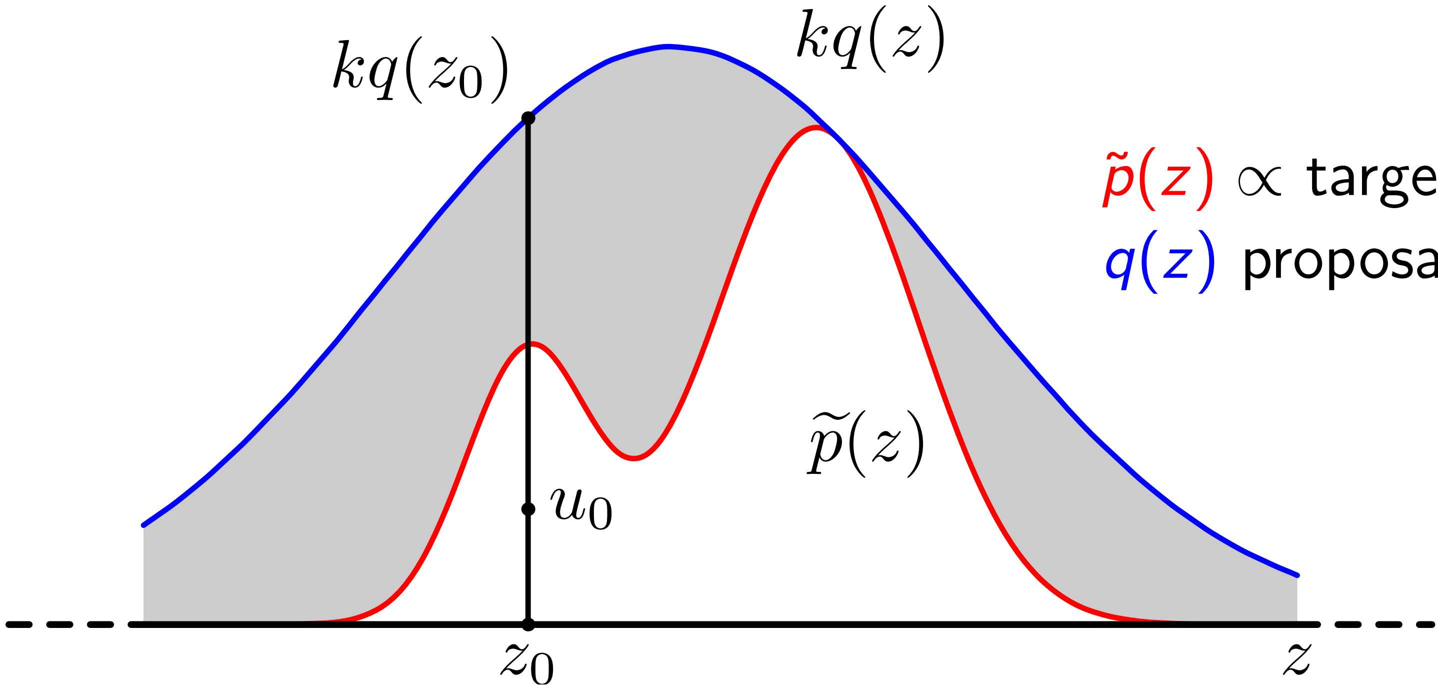

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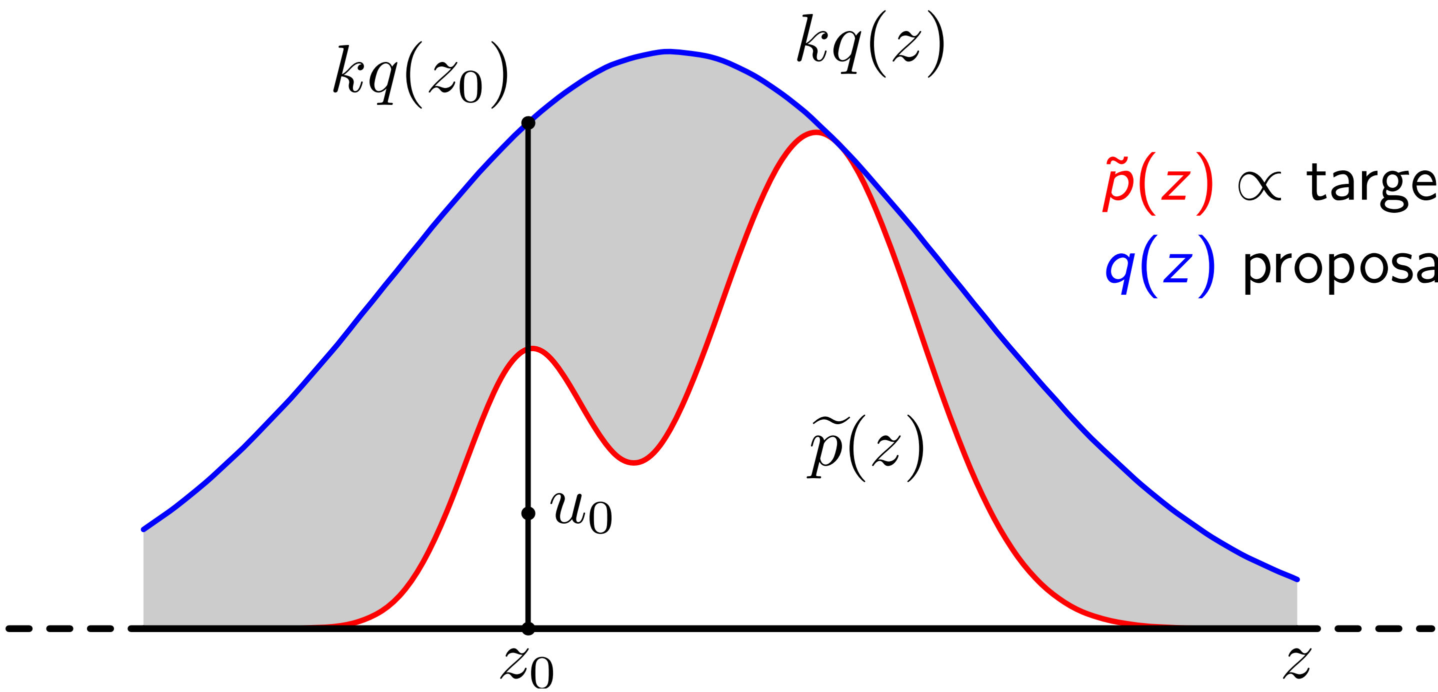

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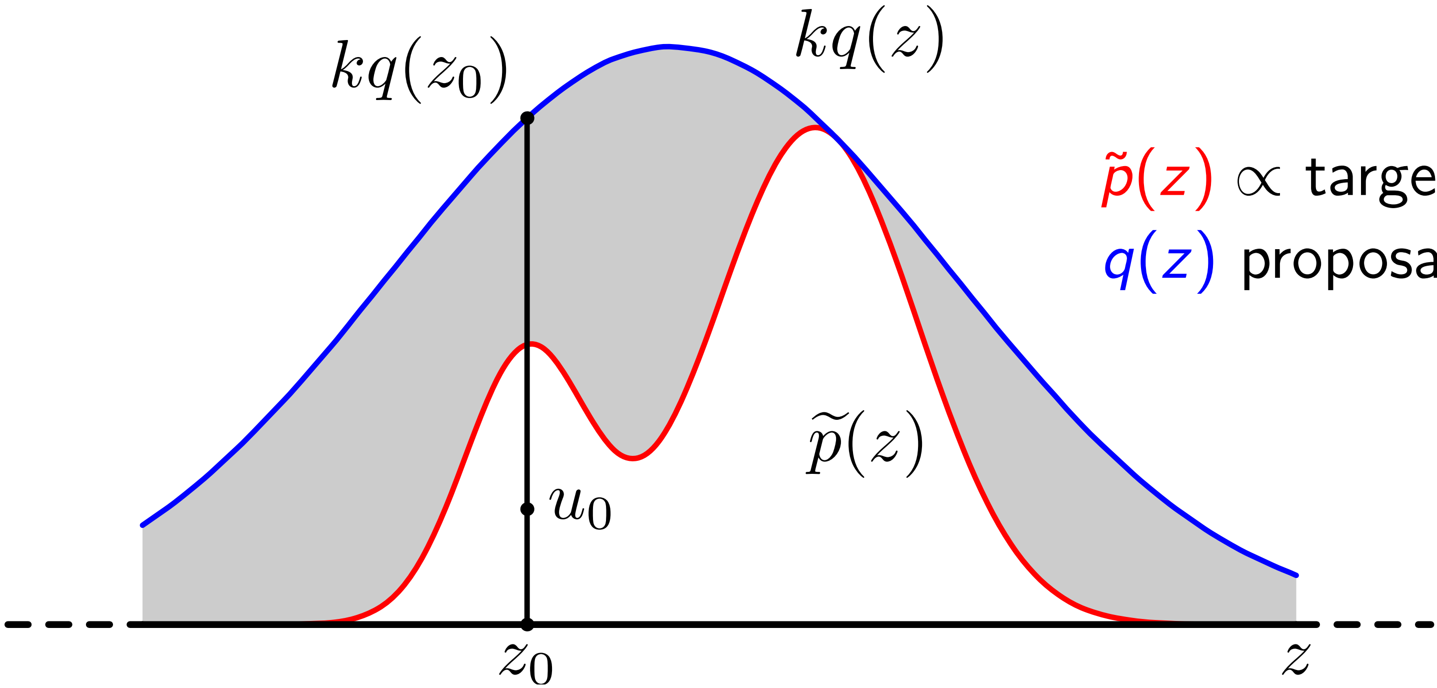

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Steps 1–2: sample points uniformly from union of white and grey areas

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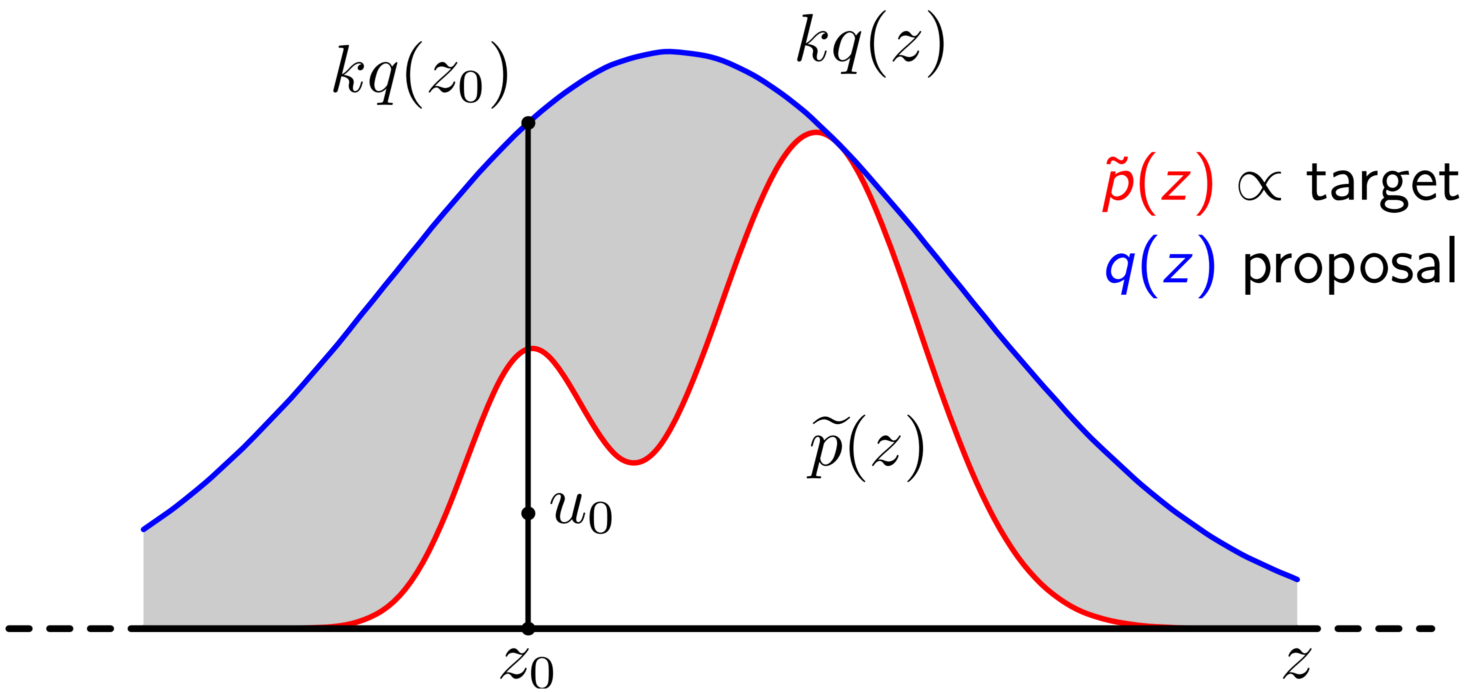

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4. forget about u: z distributed $\propto \tilde{p}(z)$!

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  - special case of MH where proposals are always accepted

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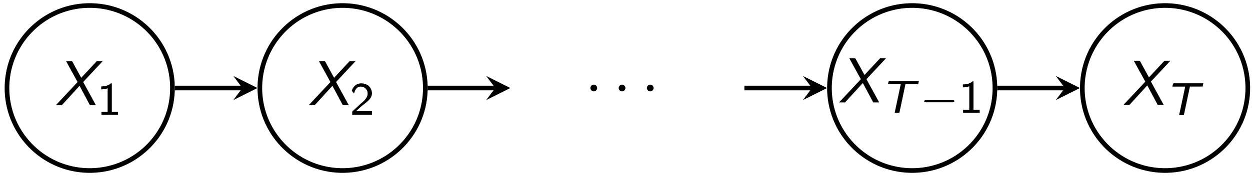

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$$f(x_2 \mid x_1) = \cdots = f(x_n \mid x_{n-1})$$

$$X_1 \rightarrow X_2 \rightarrow \cdots \rightarrow X_{T-1} \rightarrow X_T$$

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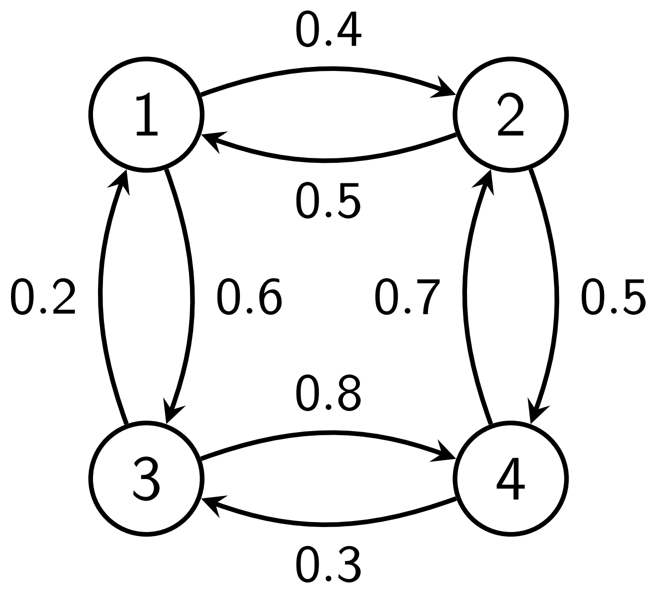

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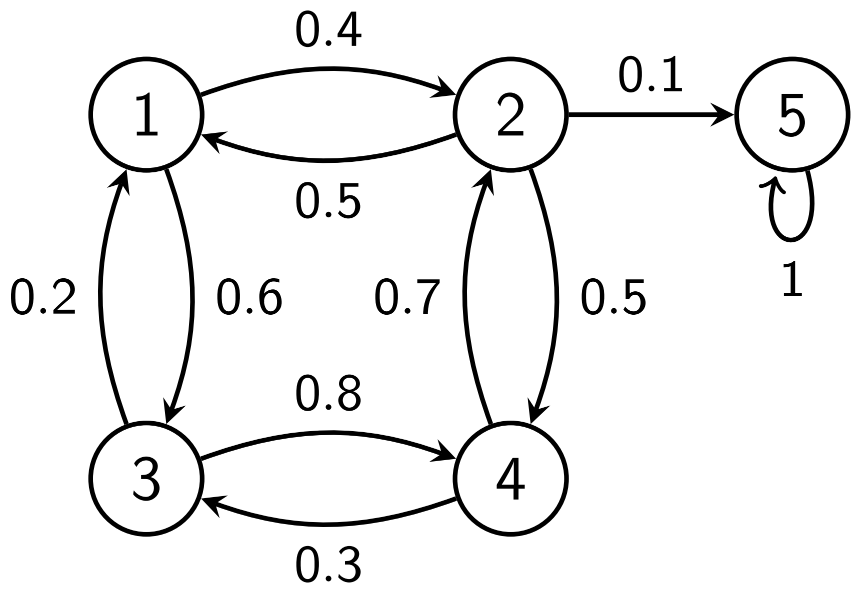

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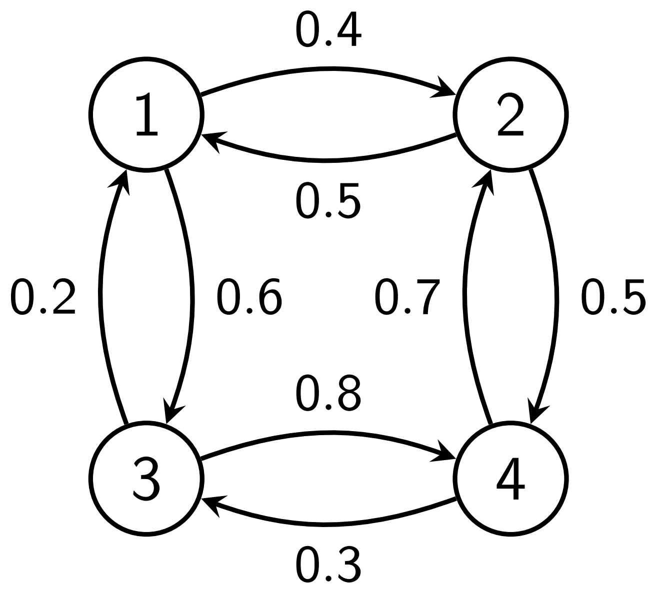

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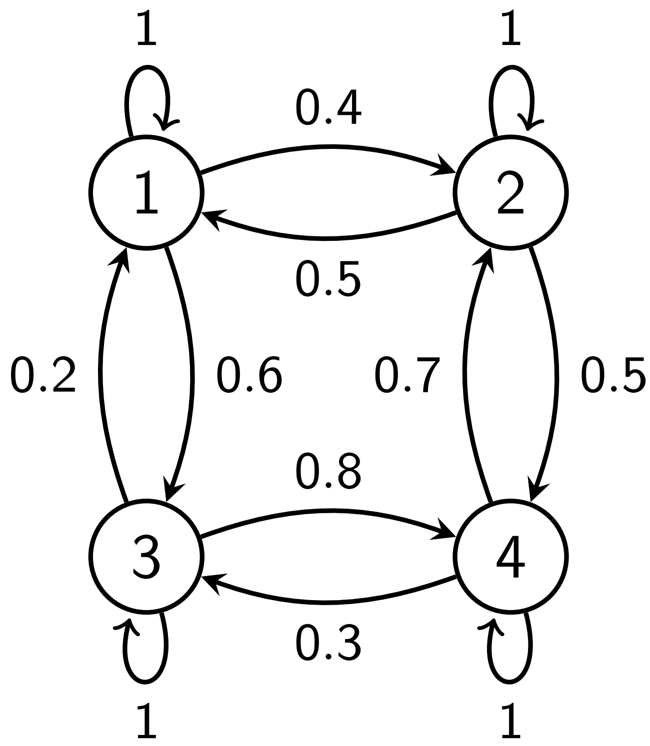

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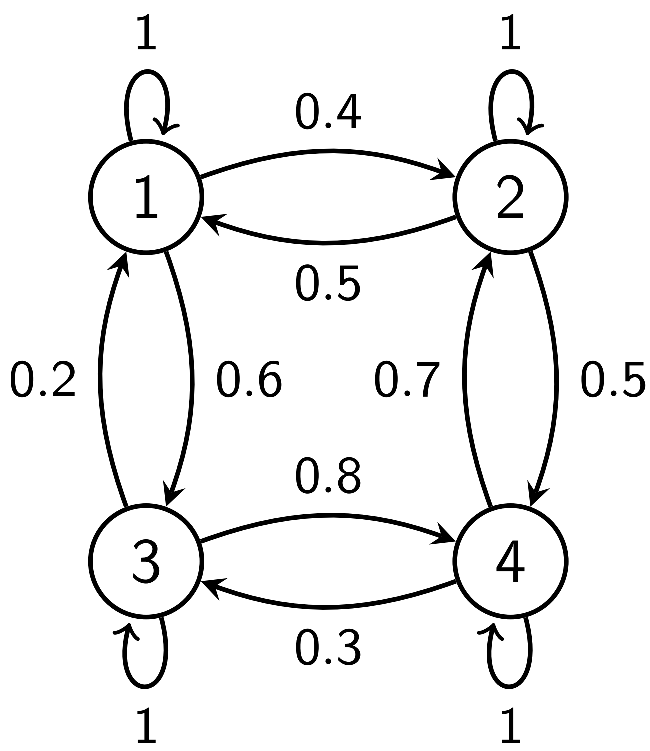

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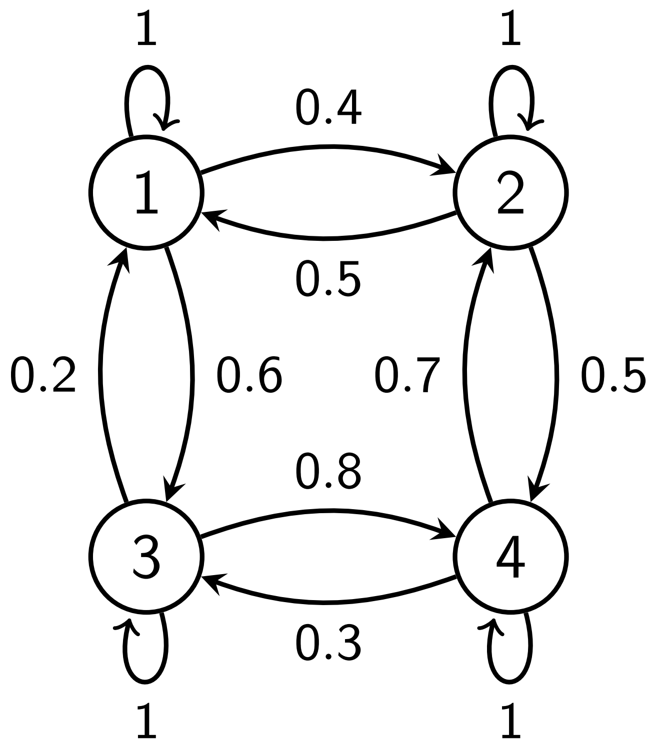
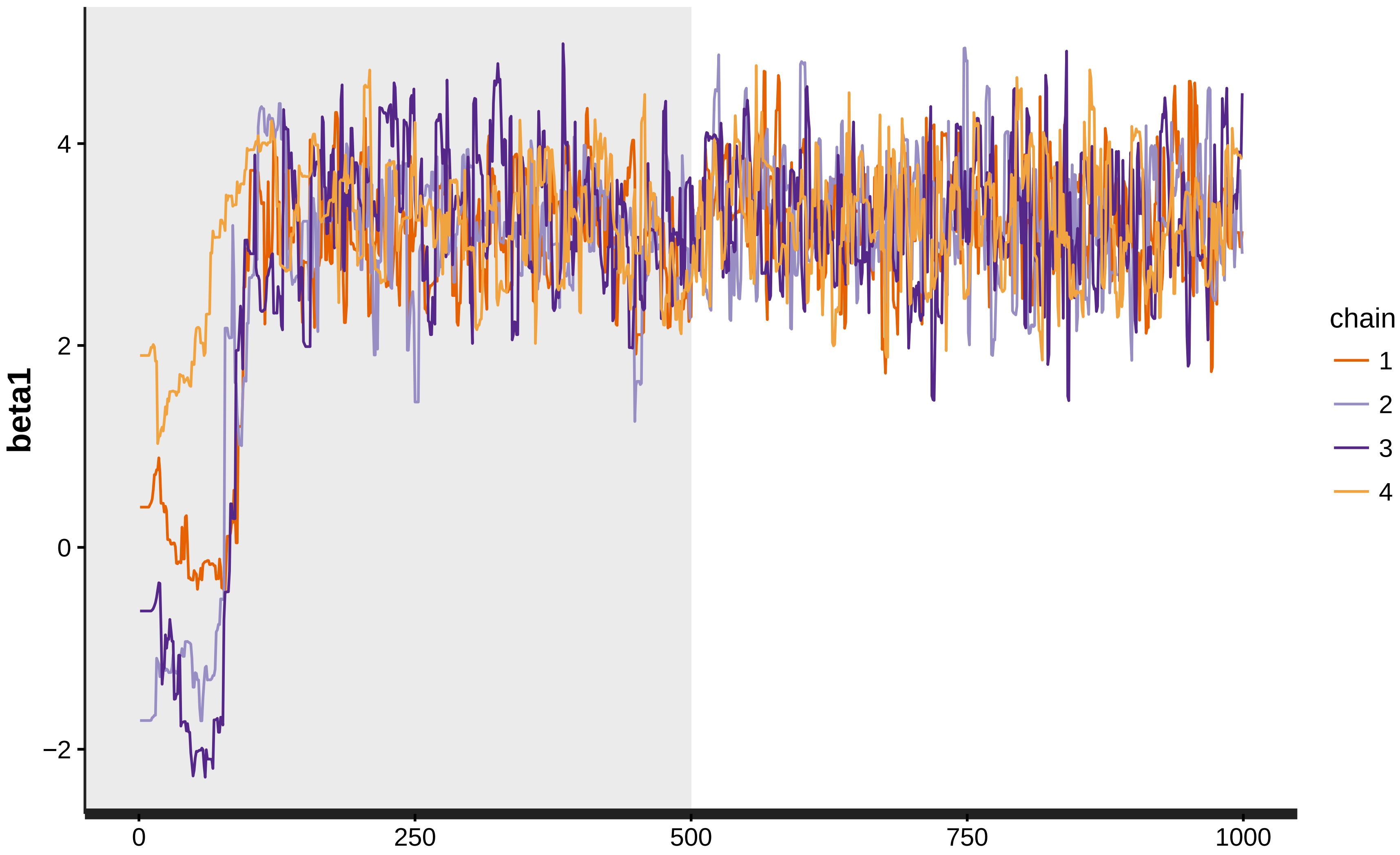


$$\big(p_1(t), p_2(t), p_3(t), p_4(t)\big) \xrightarrow{t \to \infty} \big(p_1, p_2, p_3, p_4\big)$$

MCMC: Warm-Up (= Burn-In), Mixing, Thinning



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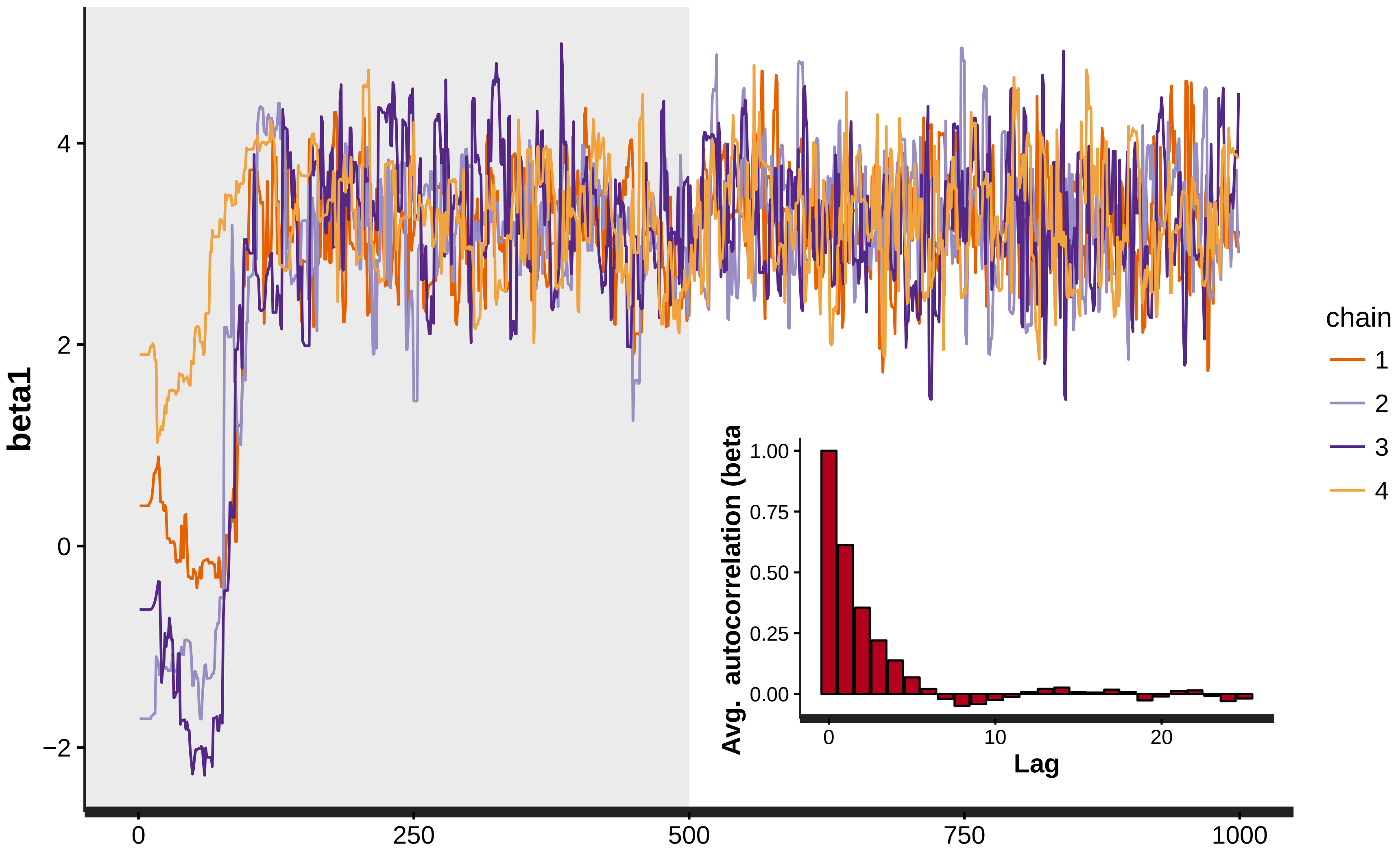

Bayesian hierarchical modelling / Bayesian networks / graphical models

Exercises I

Simulation & MCMC

Exercises II

Exercise: Quick start RStan

A Stan model is defined by five program blocks:

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model1 <- "
data {
   ...
}
transformed data {
   ...
}
parameters {
   ...
}
transformed parameters {
   ...
}
model {
   ...
}
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   ...
}"
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Exercise: Quick start RStan

A Stan model is defined by five program blocks:

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}
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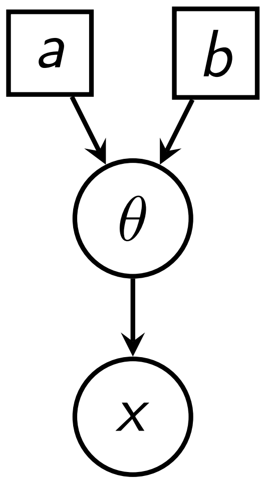

$$f(x \mid \theta) \sim \text{Binomial}(n, \theta)$$

$$f(\theta \mid a, b) \sim \text{Beta}(a, b)$$

```
library(rstan)
model0 <- "
data {
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  int<lower=0> x;
}
parameters {
  real<lower=0,upper=1> theta;
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model {
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data0 <- list(n=10, x=5)
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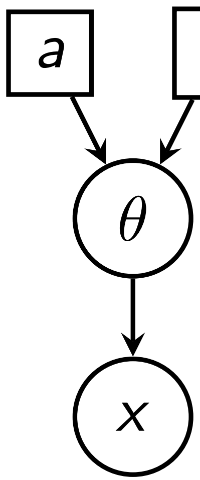

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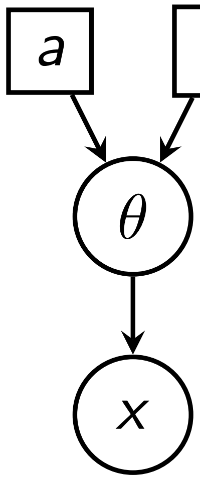

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fit0 <- stan(model_code=model0, data=data0, iter=1000, chains=4)
print(fit0); plot(fit0)
```
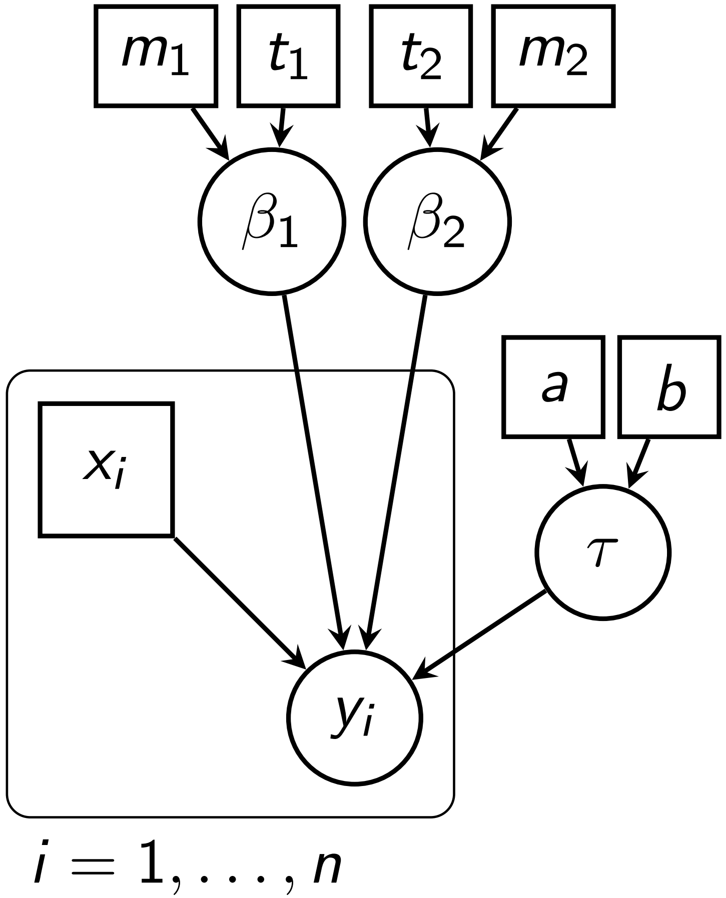

The samples can be extracted by `samples0 = extract(fit0, c("theta"))`

http://mc-stan.org/documentation/

http://github.com/stan-dev/rstan/wiki/RStan-Getting-Started#how-to-use-rstan

Exercise: Linear regression in RStan



We want to estimate the parameters in the linear regression example, using RStan to sample from the posterior.

The model assumptions are:

$$
\begin{aligned}
y_i \mid \beta_1, \beta_2, \tau &\sim \mathrm{N}(\beta_1 + x_i\beta_2, 1/\tau) \\
\tau \mid a, b &\sim \mathrm{Gamma}(a, b), \quad a = b = 10^{-3} \\
\beta_1 \mid m_1, t_1 &\sim \mathrm{N}(m_1, 1/t_1), \quad m_1 = 0, t_1 = 10^4 \\
\beta_2 \mid m_2, t_2 &\sim \mathrm{N}(m_2, 1/t_2), \quad m_2 = 0, t_2 = 10^4
\end{aligned}
$$

Exercise: Linear regression in RStan

- Create an artificial data set $x_1, \ldots, x_n, y_1, \ldots, y_n$ by

  ```
  data <- list()
  data$N <- 50
  data$x <- rnorm(data$N)+30
  data$y <- 3 + 5*data$x + rnorm(data$N, sd=1/10)
  ```

  What are thus the 'true' parameter values?
- *Define the model in* `Stan`. *Include a* `transformed parameters` *block where you define $\sigma = \sqrt{1/\tau}$.* (In `Stan`, the Normal distribution is parametrized with the standard deviation σ!)
- *Simulate four chains with 1000 iterations each and use* `plot()` *and* `print()` *to get a first impression of the results. What point estimates do you get for β_1, β_2 and σ?*

Exercise: Linear regression in `RStan`

- The functions `stan_trace()`, `stan_dens()` and `stan_ac()` allow you to analyze your sample from the posterior distribution more closely. (You can include the warm-up phase in your plots by setting `inc_warmup = TRUE`.)
  How long is the warm-up phase? Do your chains mix well? Is thinning necessary?
- The function `pairs()` also works on `stanfit` objects.
  Plot pairwise scatterplots of your sample using `pairs()`.
  What do you observe about the relation between β_1 and β_2?

Exercise: Linear regression in RStan

- The high correlation between β_1 and β_2 indicates that the Markov chain cannot move around freely. You can mitigate this problem by centering the data $x_1, \ldots, x_n$. The mean for the Normal distribution of y_i is then given by $\beta_1^c + \beta_2(x_i - \bar{x})$, where $\beta_1^c = \beta_1 + \beta_2\bar{x}$.
  Add the following block to your `stan` *model definition,*

  ```
  transformed data {
    vector[N] xcentered;
    xcentered=x-mean(x);
  }
  ```

  and edit the `parameters` *and* `model` *blocks such that the model generates samples from β_1^c instead of β_1.*
- *Edit the* `transformed parameters` *block to define β_1 as $\beta_1 = \beta_1^c + \beta_2\bar{x}$.*
- *Simulate four chains with 1000 iterations each from this new model, and analyze your sample from the posterior distribution like for the first model. What has changed?*

Exercise: Linear regression in `RStan`

- *Choose an informative prior for one or both of β_1 and β_2. Try out different values for mean and standard deviation. What is the effect on the chains and the posterior densities?*