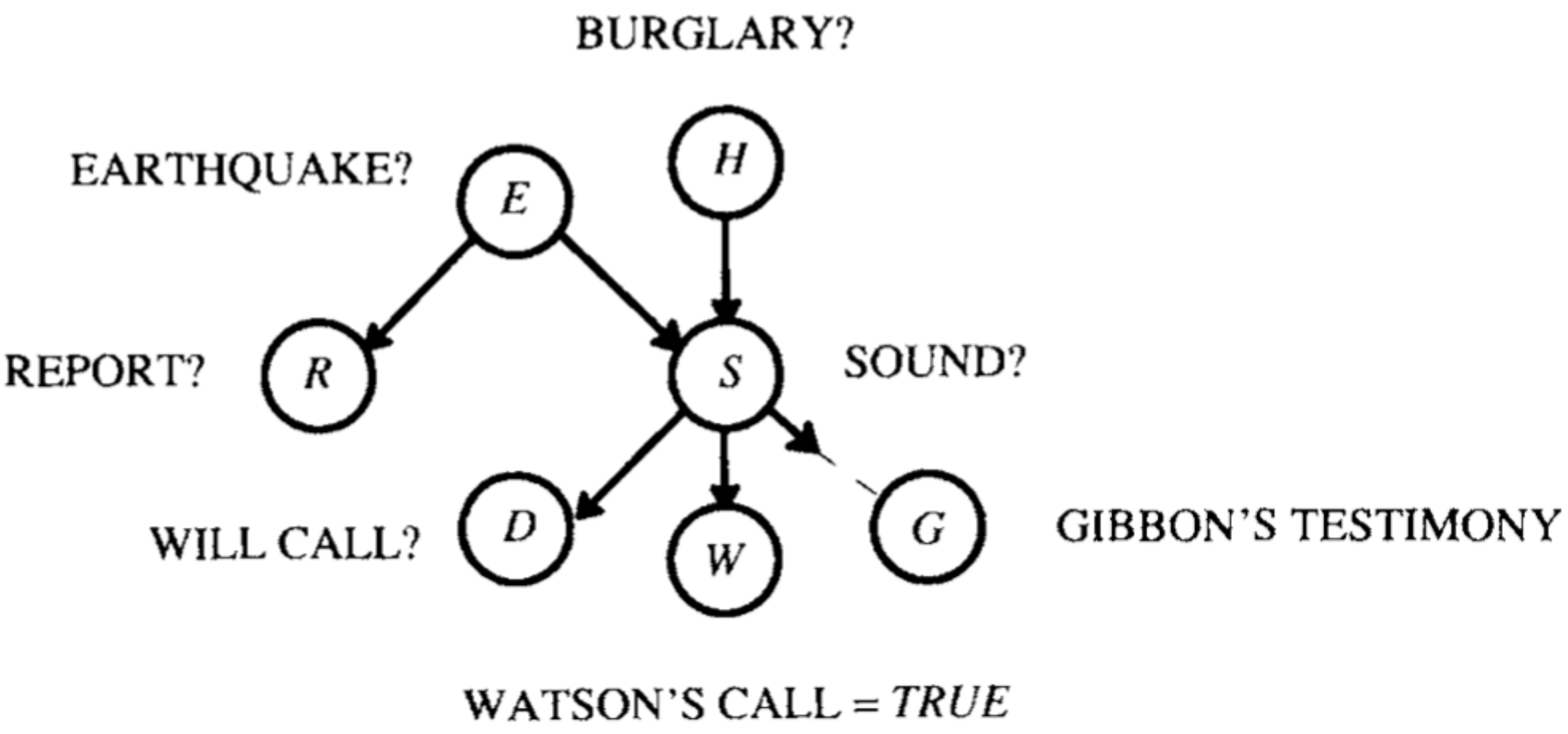
# Graphical Models and Variational Inference

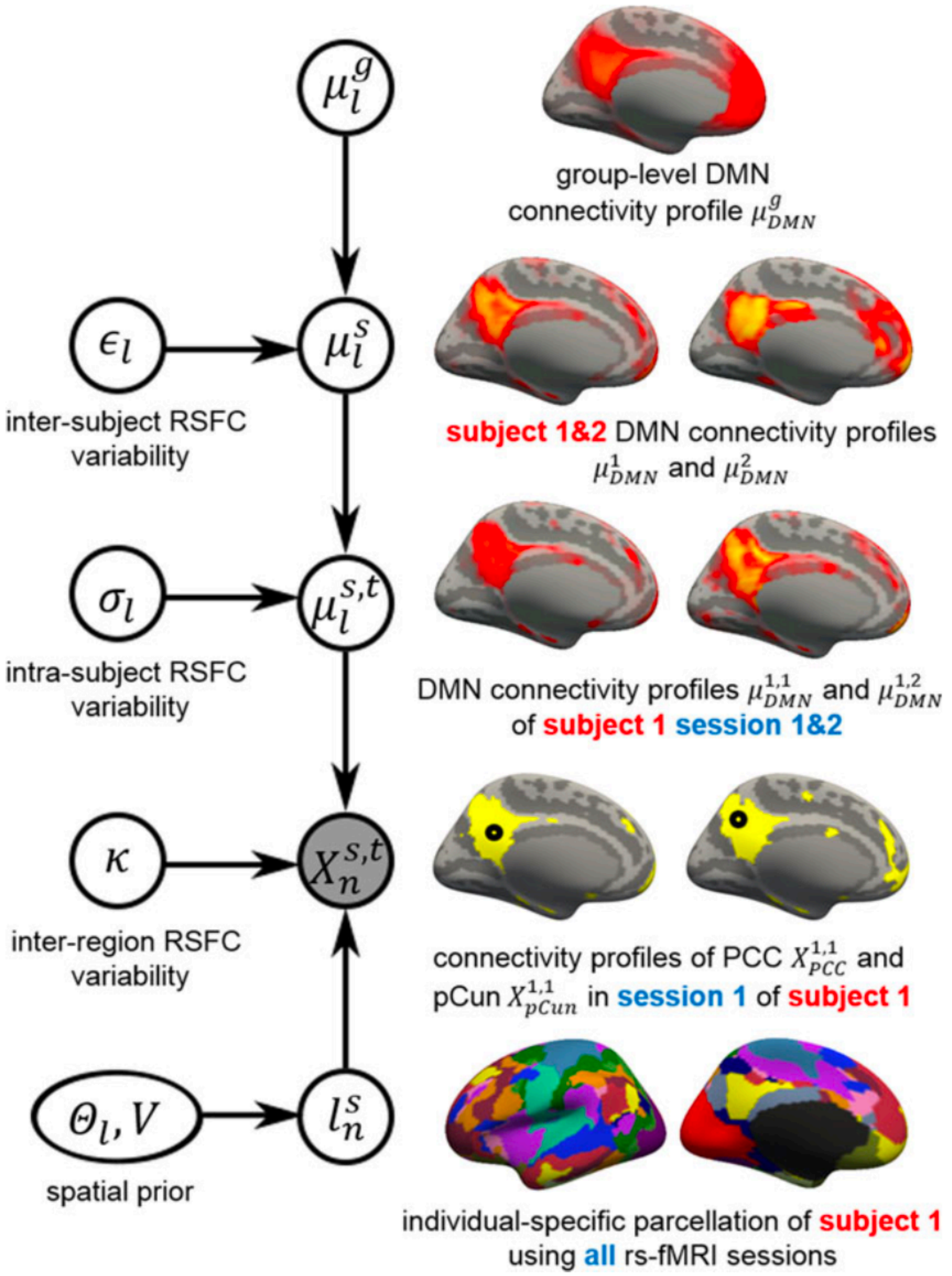
Demian Wassermann, Inria

Graphical Models: Discrete Inference and Learning

# Introduction to DAG and their relationship with Probability Functions (Pearl)




[Pearl 1987]




[Kong et al 2019]

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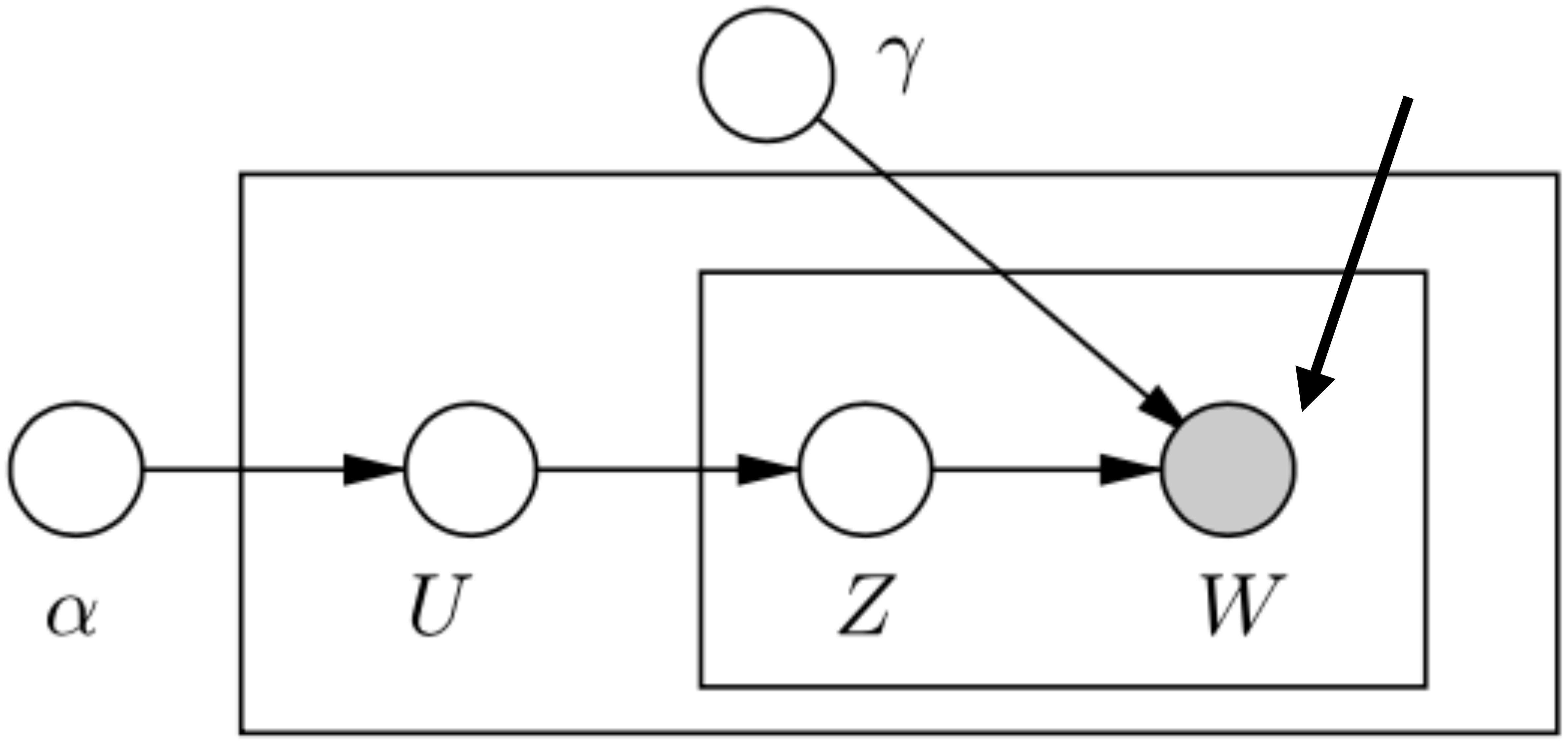


U: is a Dirichlet or "clustering variable"
Z: is a "Topic"
W: is an *observed* "Word"
[Blei et al 2003]

Each "box" or template represents a set of i.i.d. random variables with the same distribution

| "Arts" | "Budgets" | "Children" | "Education" |
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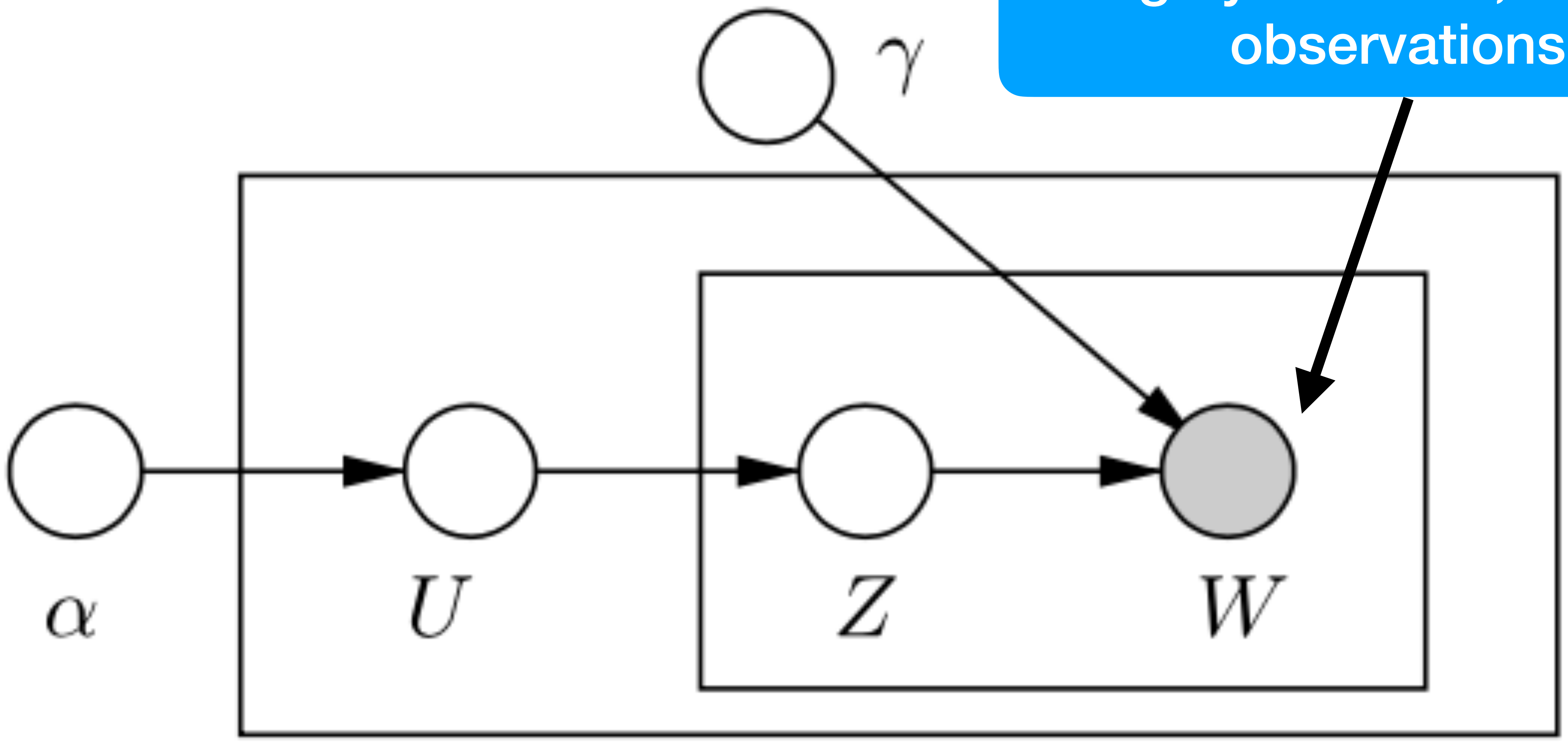
The greyed nodes, represent observations

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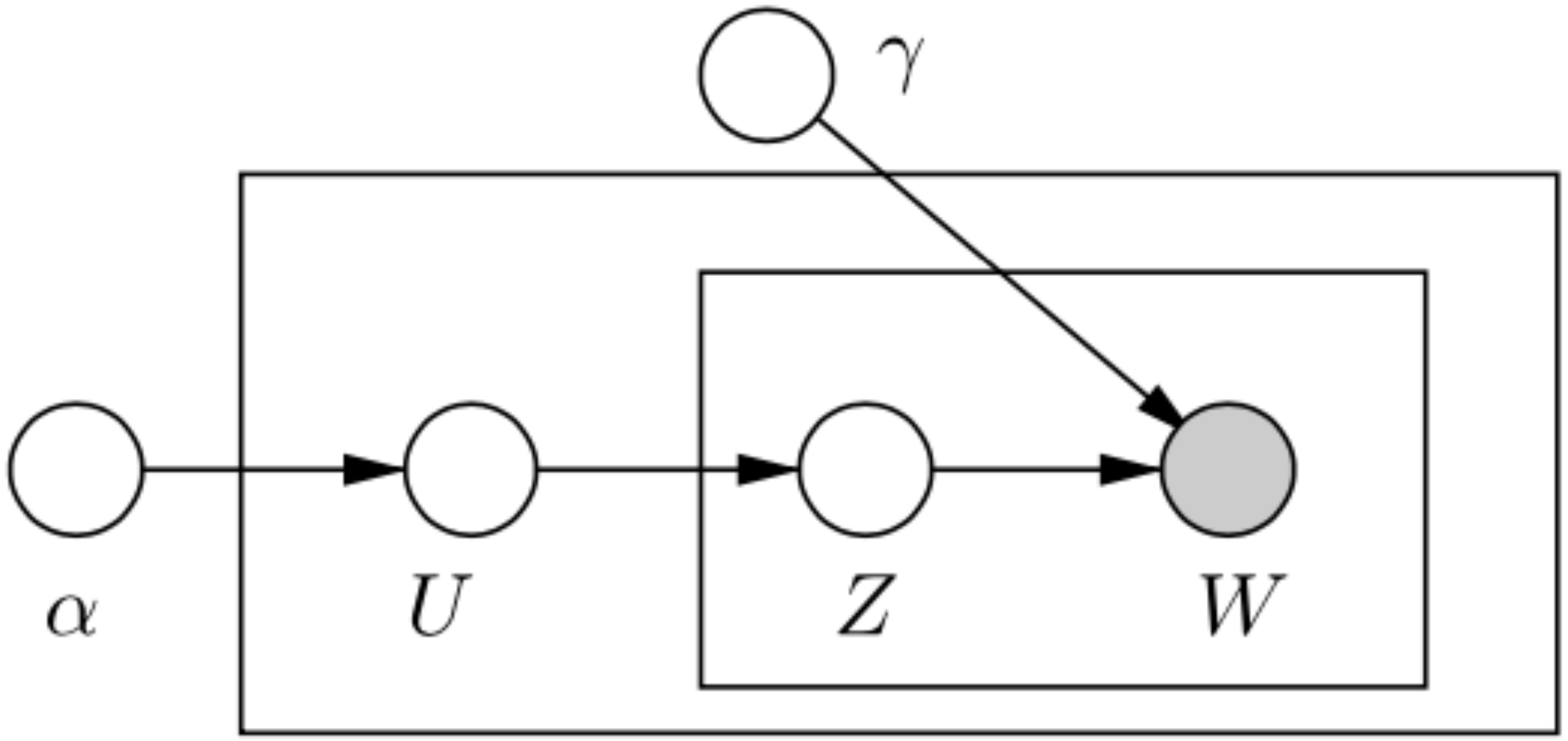


$$U_j \sim Dirichlet(\alpha), \alpha < 1$$
$$Z_{i,j} \sim Multinomial(U_j)$$
$$W_{i,j} \sim Multinomial\left(\gamma_{Z_{i,j}}\right)$$

Then, we are looking for the posterior $P(U, Z \mid W, \alpha, \gamma) = \dfrac{P(U, Z, W \mid \alpha, \gamma)}{P(W \mid \alpha, \gamma)}$

$$P(U, Z, W \mid \alpha, \gamma) = \Pi_j \int P(U_j \mid \alpha) \left( \Pi_i \sum_{Z_{i,j}} P(Z_{i,j} \mid U_j) P(W_{i,j} \mid Z_{i,j}, \gamma) \right) dU_j$$

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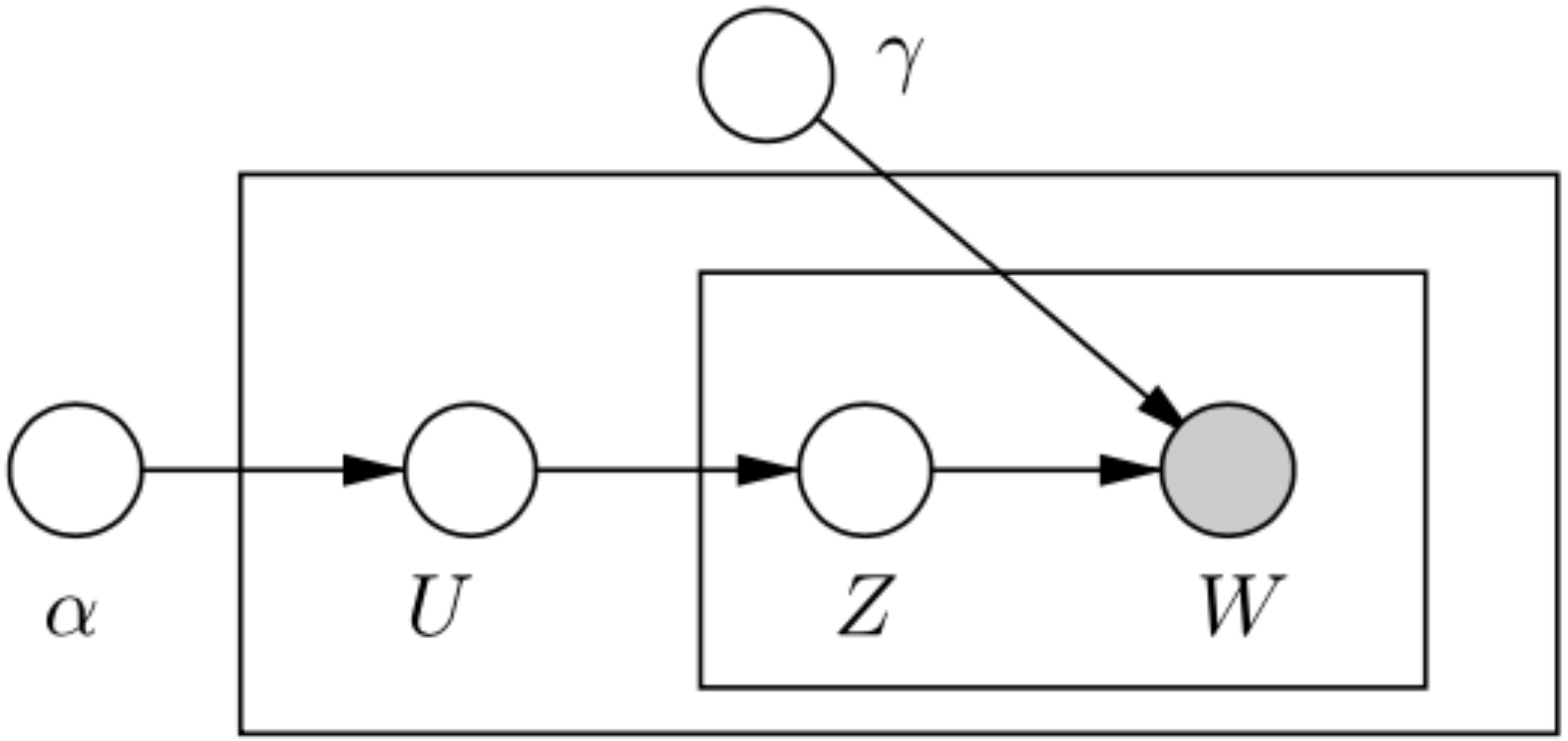


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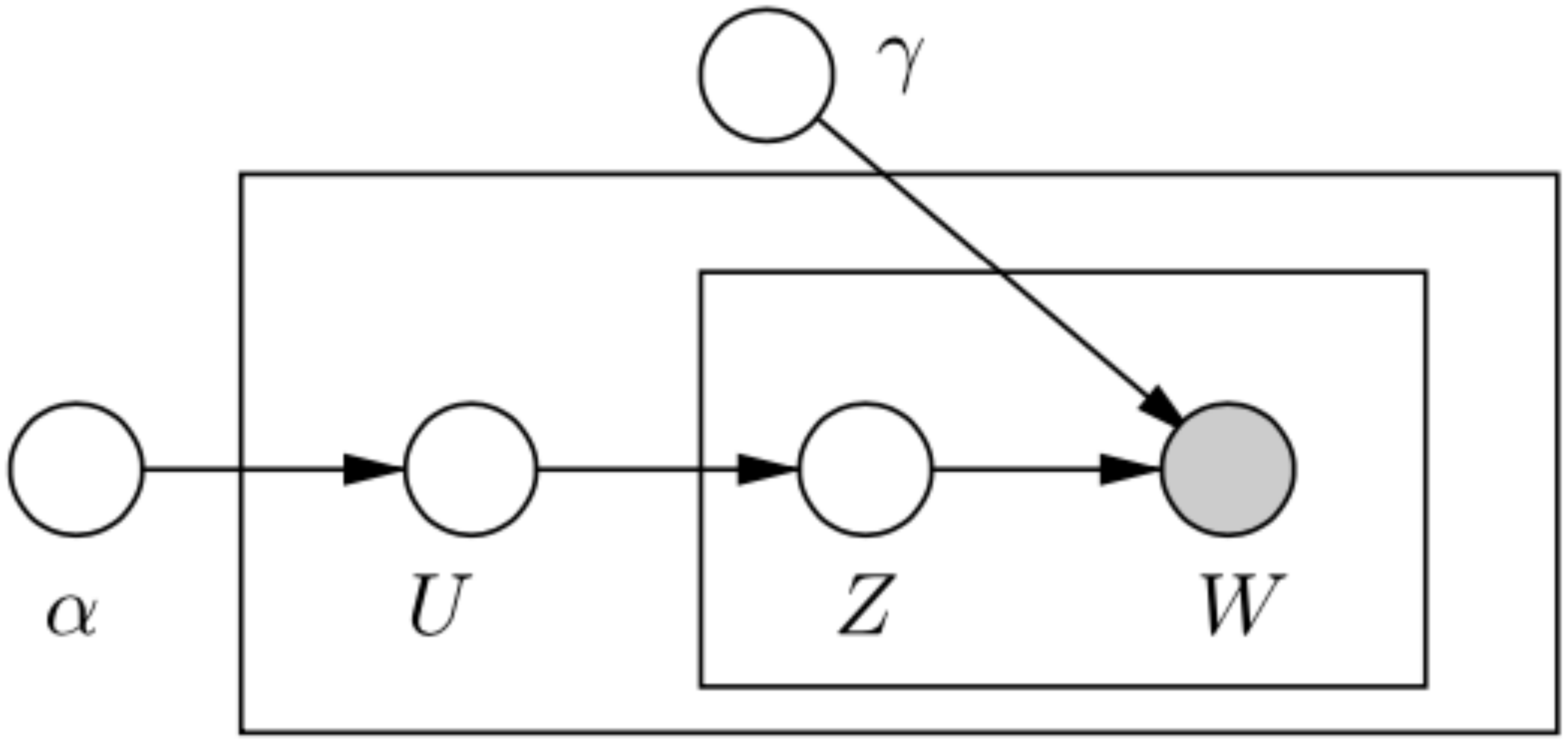


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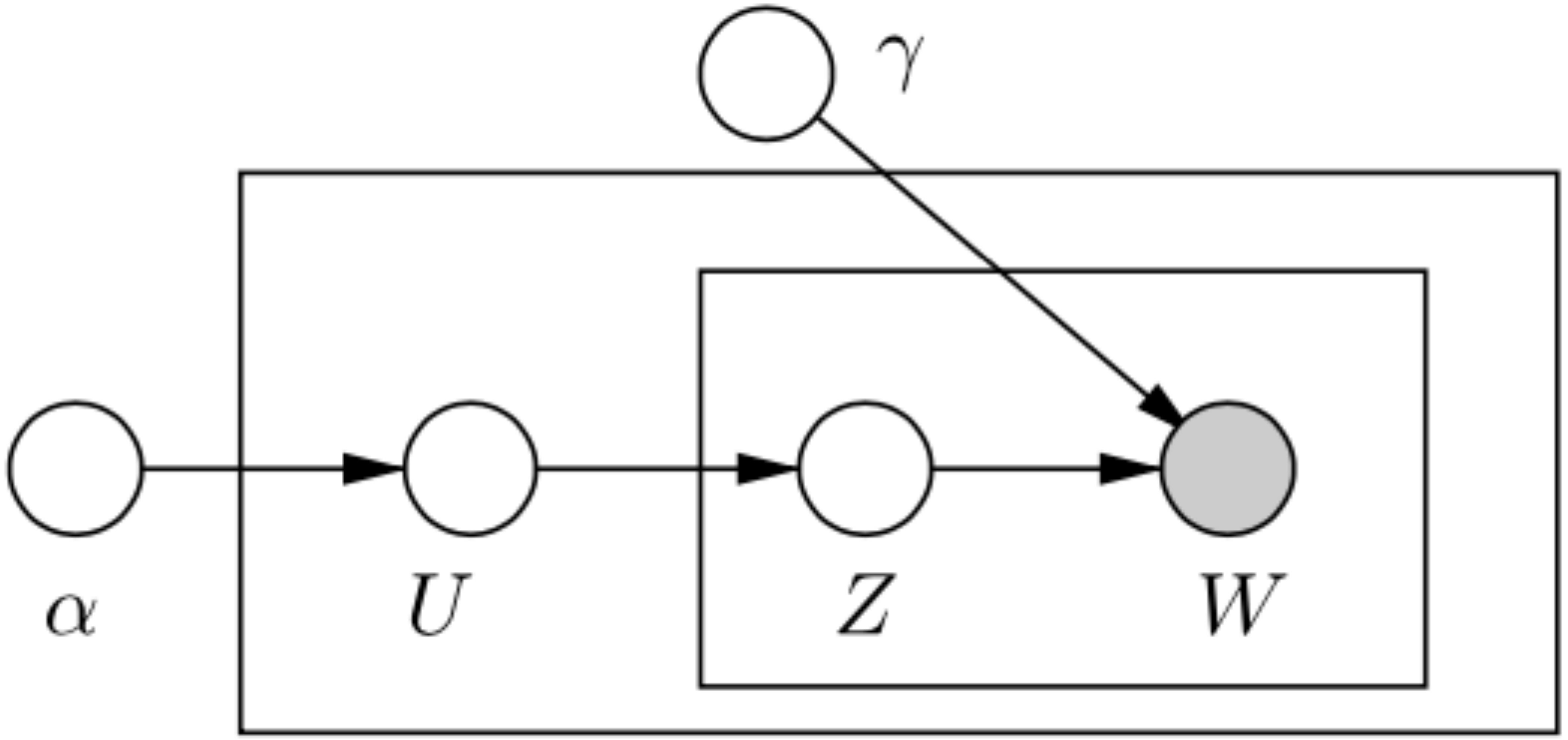
No analytical solution

$$P(U, Z, W \mid \alpha, \gamma) = \Pi_j \int P(U_j \mid \alpha) \left( \Pi_i \sum_{Z_{i,j}} P(Z_{i,j} \mid U_j) P(W_{i,j} \mid Z_{i,j}, \gamma) \right) dU_j$$

# Relationship between a Directed Graphical Model and its Probability Law (Pearl and Paz 1985)

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In general, for a graphical model Graphical Model with vertices V and edges E

$$GM = (V, E), P(V) = \Pi_{v \in V} P(v \mid Pa(v)), Pa(v) = \{v' : v' \to v \in E\}$$

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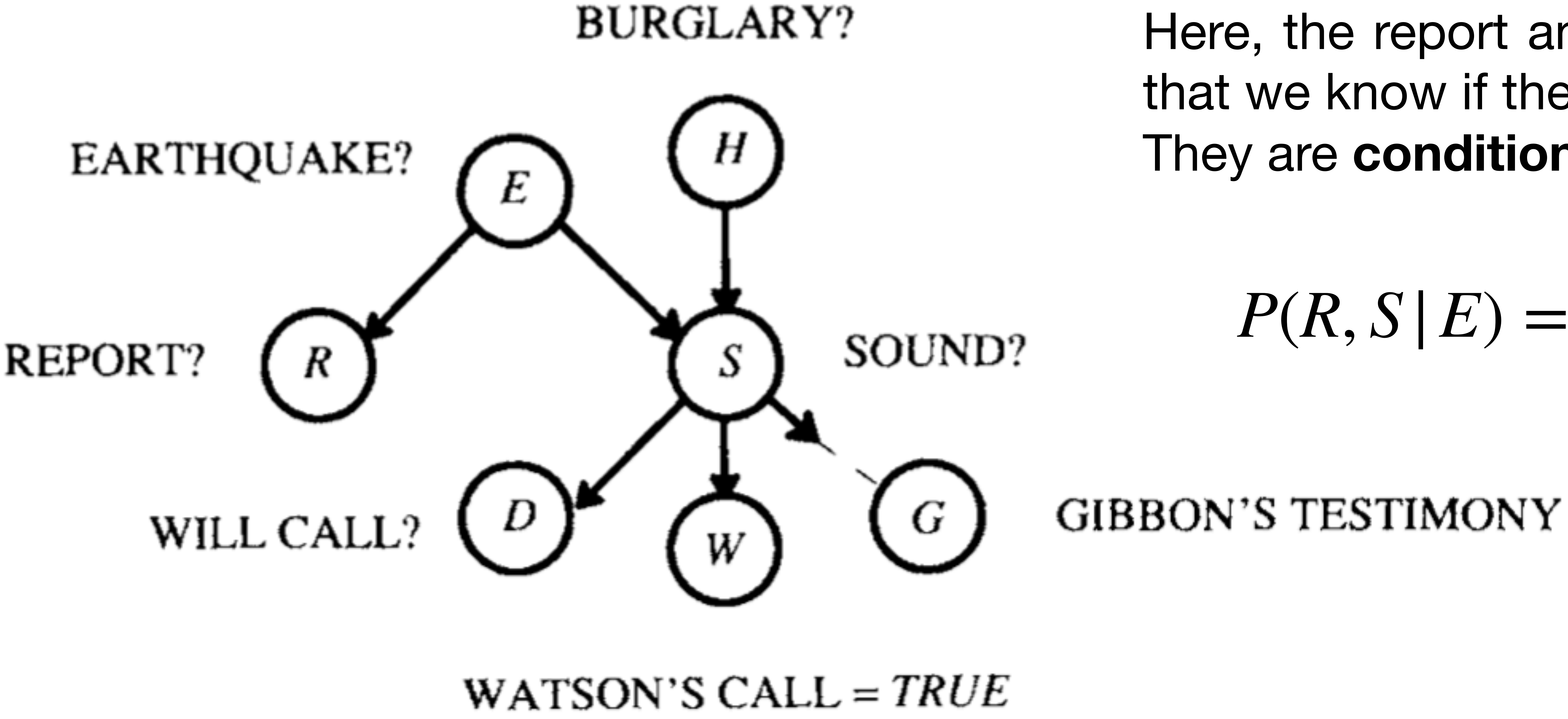


Here, the report and the sound are independent, given that we know if there was an earthquake:
They are **conditionally** independent

$$P(R, S \mid E) = P(R \mid E)P(S \mid E) \text{ iif } I(R, S, E)$$

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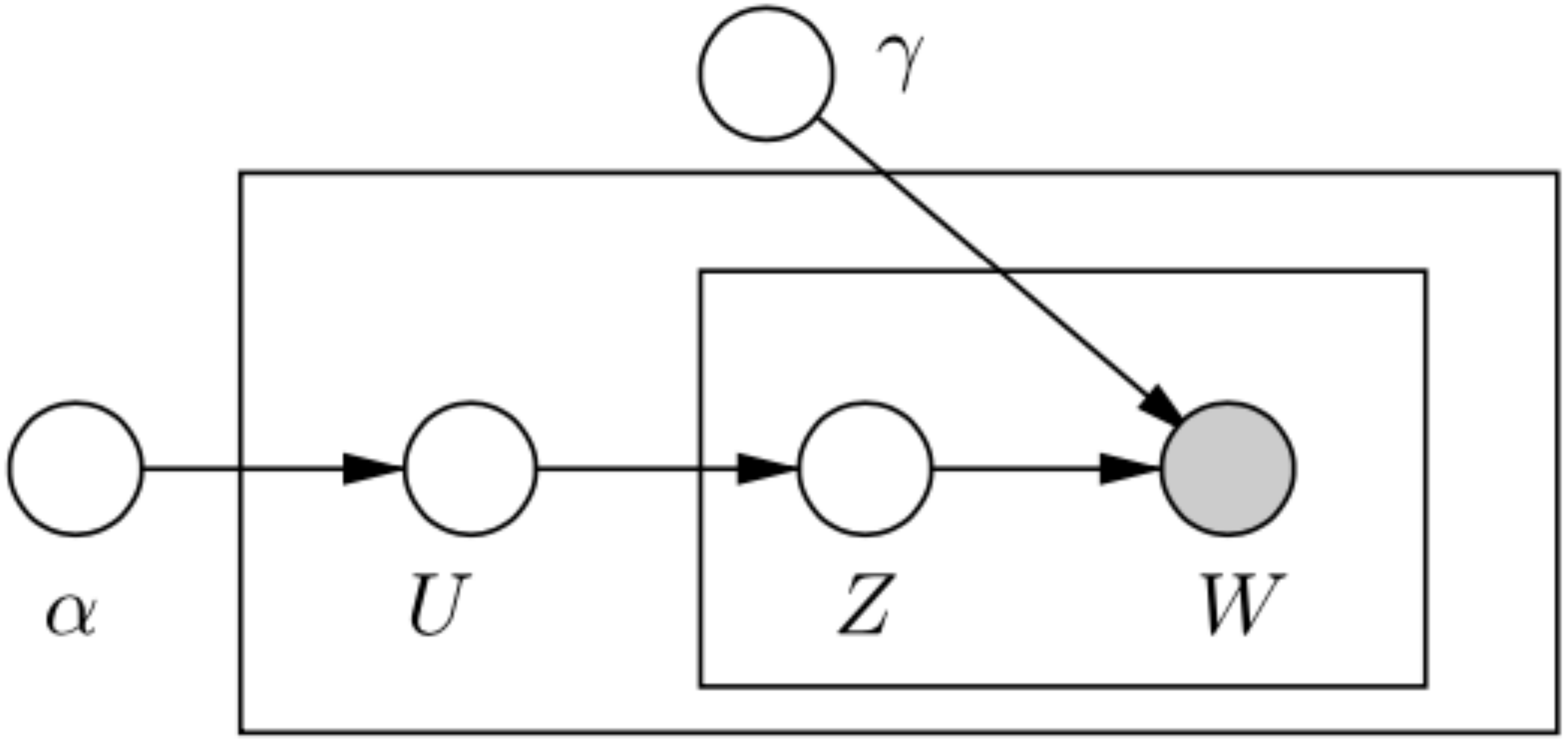


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However, our usual problem is: given observed variables O and latent variables L, to compute the posterior $P(L \mid O)$

$$P(L \mid O) = \frac{\Pi_{v \in V} P(v \mid Pa(v))}{\Pi_o P(o \mid Pa(o))}, GM = (V = L \cup O, E), \;\; \nexists l \in L : o \to l \in E$$

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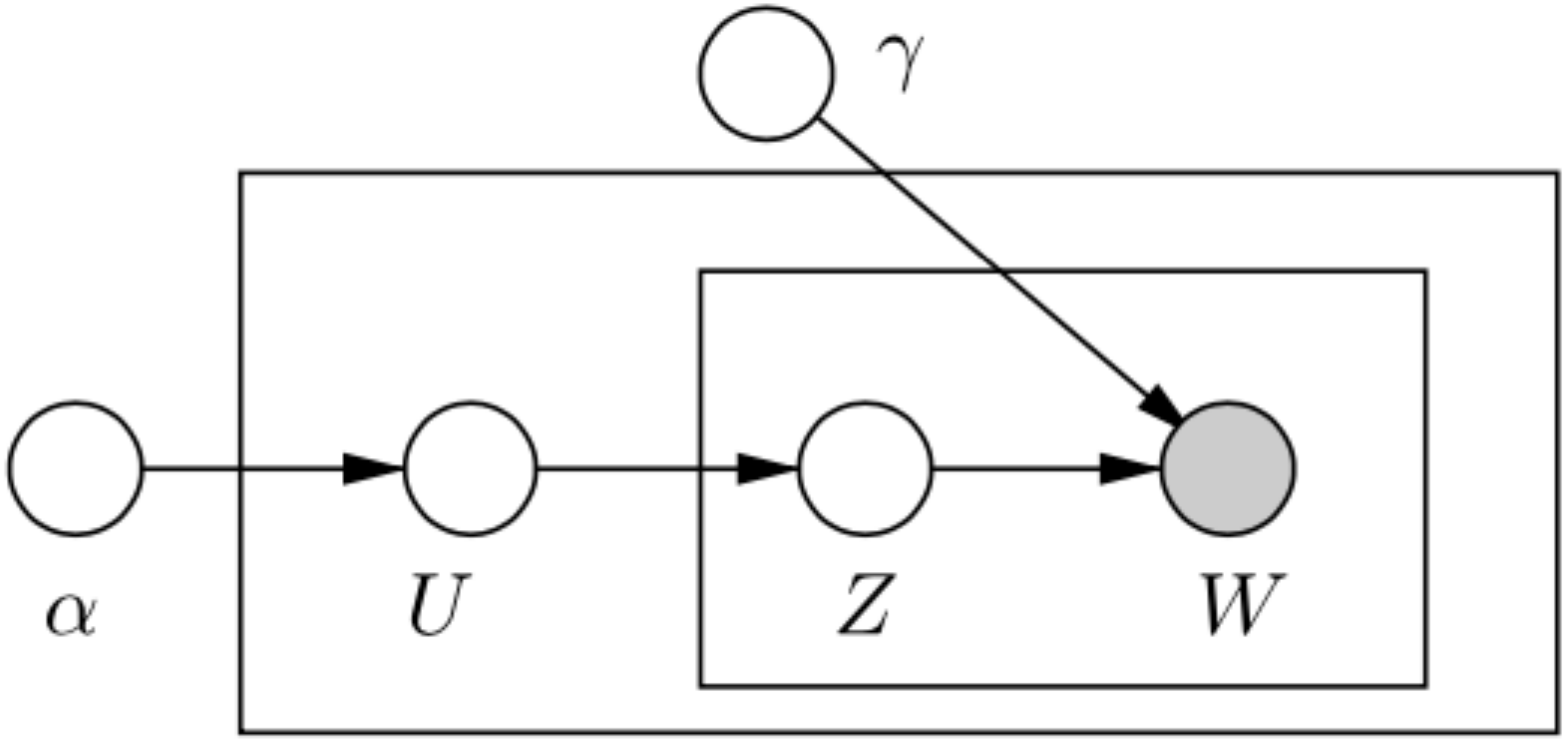


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In the case of continuous variables this is

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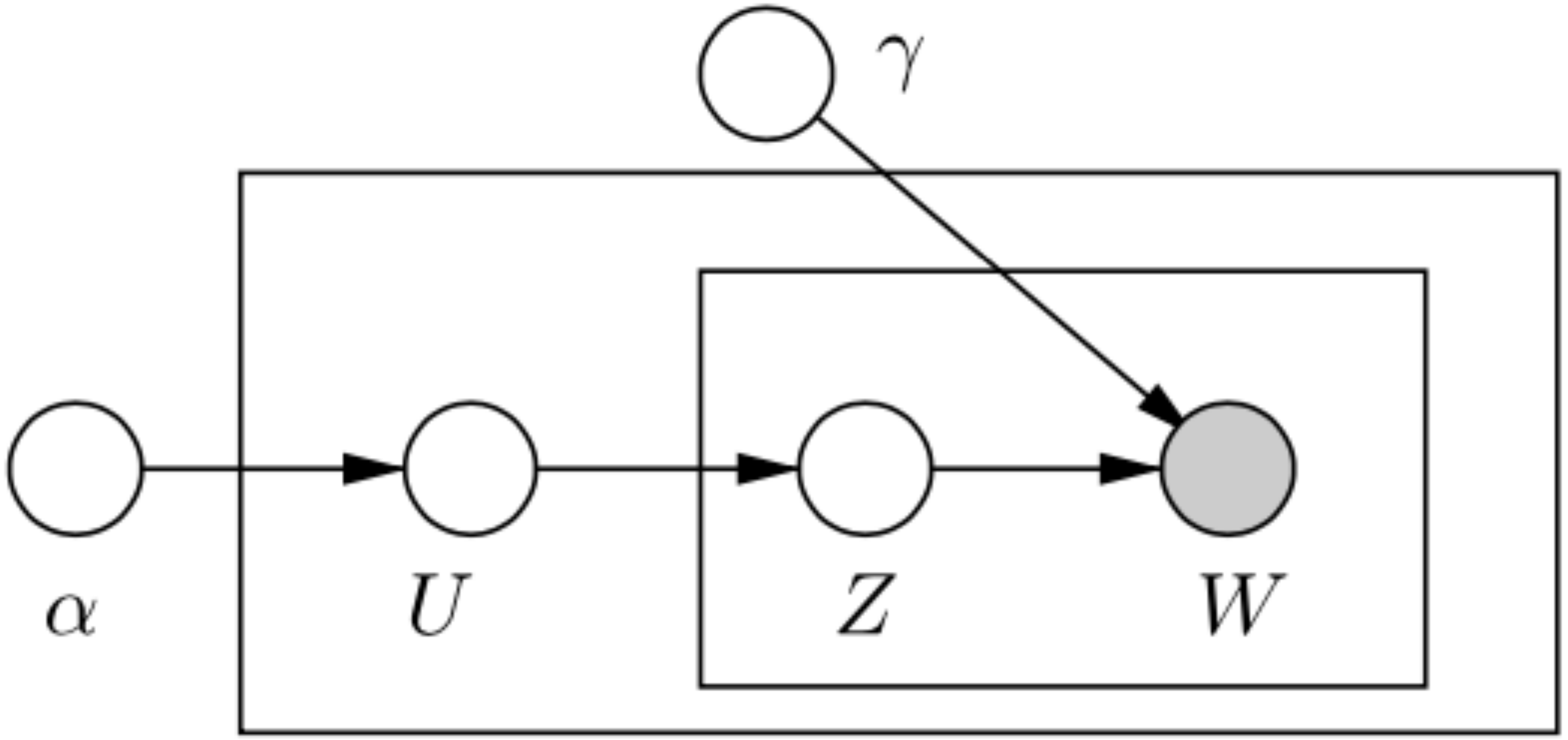


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**No analytical solution, for the general case**

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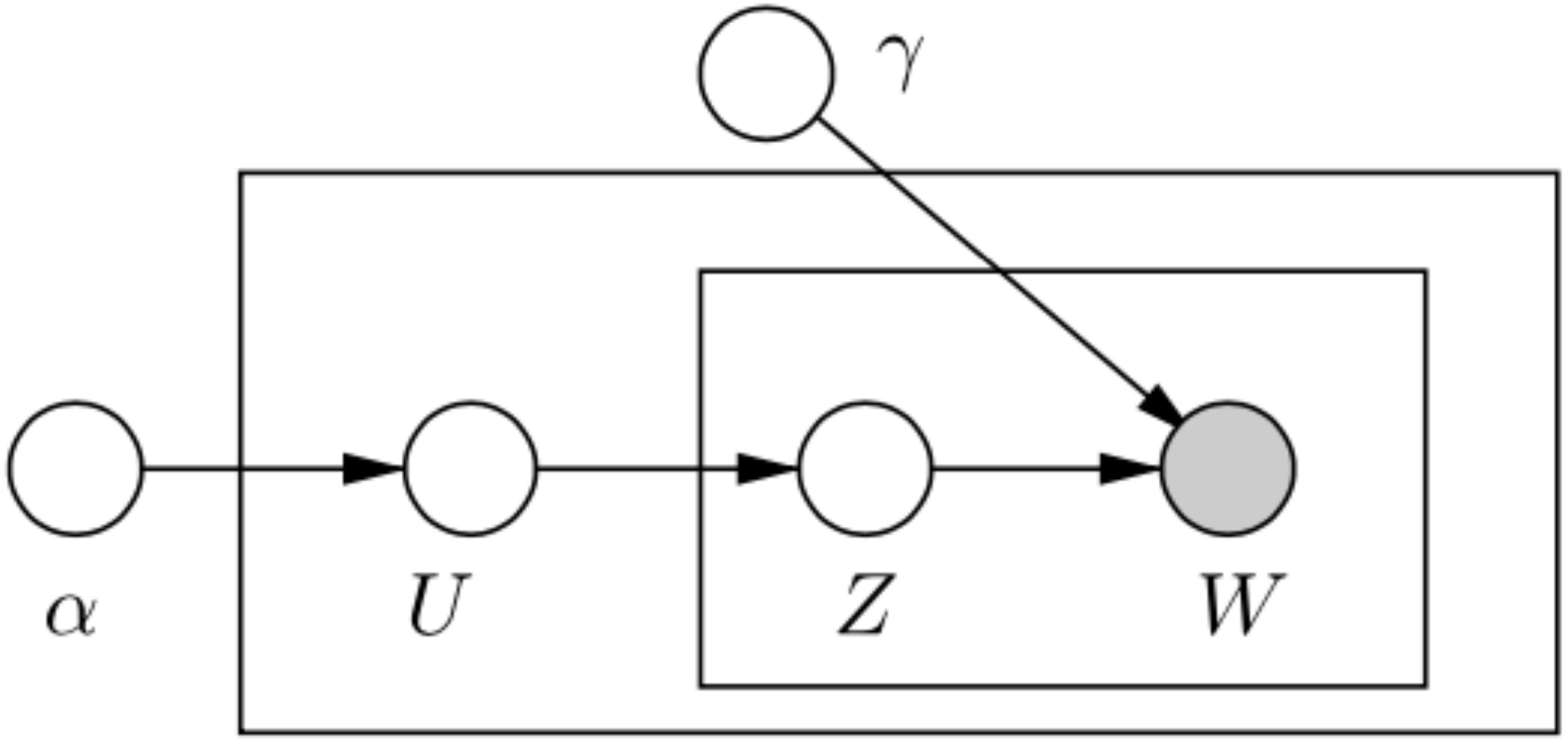


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Can we approximate $P(L\,|\,O)$?

$$\color{blue}{Q(L)} \simeq P(L\,|\,O) = \frac{P(L, O)}{\int P(L, O) dO}$$

# Approximations to Density Laws

Can we approximate $P(L \mid O)$? $\quad Q(L) \simeq P(L \mid O) = \dfrac{P(L,O)}{\int P(L,O)dO}$

- First try: MacLaurin $Q(L) = \sum P(L = l \mid O) + P'(L = l \mid O)(l - L) + \dots$

  problem: how to guarantee that $Q(L)$ is a probability law?

- Second try: cumulant approximations (changing the random $L$ by $X$)

$$\phi(t) = \log \mathbb{E}_{X \sim Q(X)}[\exp(tX)] = \sum_n \kappa_n \frac{t^n}{n!} = \kappa_1 t + \kappa_2 \frac{t^2}{2!} + \dots = \mu t + \sigma^2 \frac{t^2}{2!} + \dots$$

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- However, a probability law has either up to two moments, or an infinite number (Cramèr 1938)

# Approximations to Density Laws

Can we approximate $P(L \mid O)$?

$$Q(L) \simeq P(L \mid O) = \frac{P(L, O)}{\int P(L, O) dO}$$

- Other options: Edgesworth, approximations which come from this identity

$$\phi(t) = \log \mathbb{E}_X[\exp(itX)] = \sum_n \kappa_n \frac{(it)^n}{n!},$$

$$\psi(t) = \log \mathbb{E}_X[\exp(itX)] = \sum_n \gamma_n \frac{(it)^n}{n!}$$

$$\hat{\phi}(t) = \sum_n (\kappa_n - \gamma_n) \frac{(it)^n}{n!} + \log \psi(t)$$

however, they are not guaranteed to be probability laws for finite samples.

# Approximations to Density Laws

Can we approximate $P(L \,|\, O)$?

$$\color{blue}{Q(L)} \simeq P(L \,|\, O) = \frac{P(L, O)}{\int P(L, O) dO}$$

- So? What do we do?
  - We choose an approximate distribution $Q_\theta(X)$ —replacing $L$ by $X$ and $O$ by $Z$ for notation— from a given family, with parameters $\theta$. Then
    $$Q* = Q_{\theta*} : \theta* = \arg\min_\theta D(Q_\theta(X), P(X \,|\, Z))$$
    so we need to define the right similarity measurement $D$ to compare distributions. And in standard Variational Inference (VI), $Z$ is notation for $O$

# Approximations to Dens… …aws

Can we approximate $P(L|O)$?

$\color{blue}{Q(L)} \simeq P(L|O)$ …

This is what we call Variational Inference

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# So Which $D$ and $Q$ Should We Choose?

$$Q* = Q_{\theta*} : \theta* = \arg\min_{\theta} D(Q_\theta(X), P(X|Z))$$

$X$ the latent variables and $Z$ the observations

Let's start with "analytical" ideas:

- $D(Q_\theta(X), P(X|Z)) = \int (Q_\theta(x) - P(x|Z))^2 dx$
  - What does it mean for two distributions to be close in the $L_2$ sense?
  - How easy is to obtain bounds and closed form solutions?

- $Q_\theta(X) : X \sim \mathcal{N}(\mu, \Sigma), \theta = (\mu, \Sigma)$ : This is called the Laplace approximation
  - Even simpler $\Sigma = \sigma^2$Id, which boils down to $Q_\mu(X) = \Pi_i Q_{\mu_i}(X_i)$

# So Which $D$ and $Q$ Should We Choose?

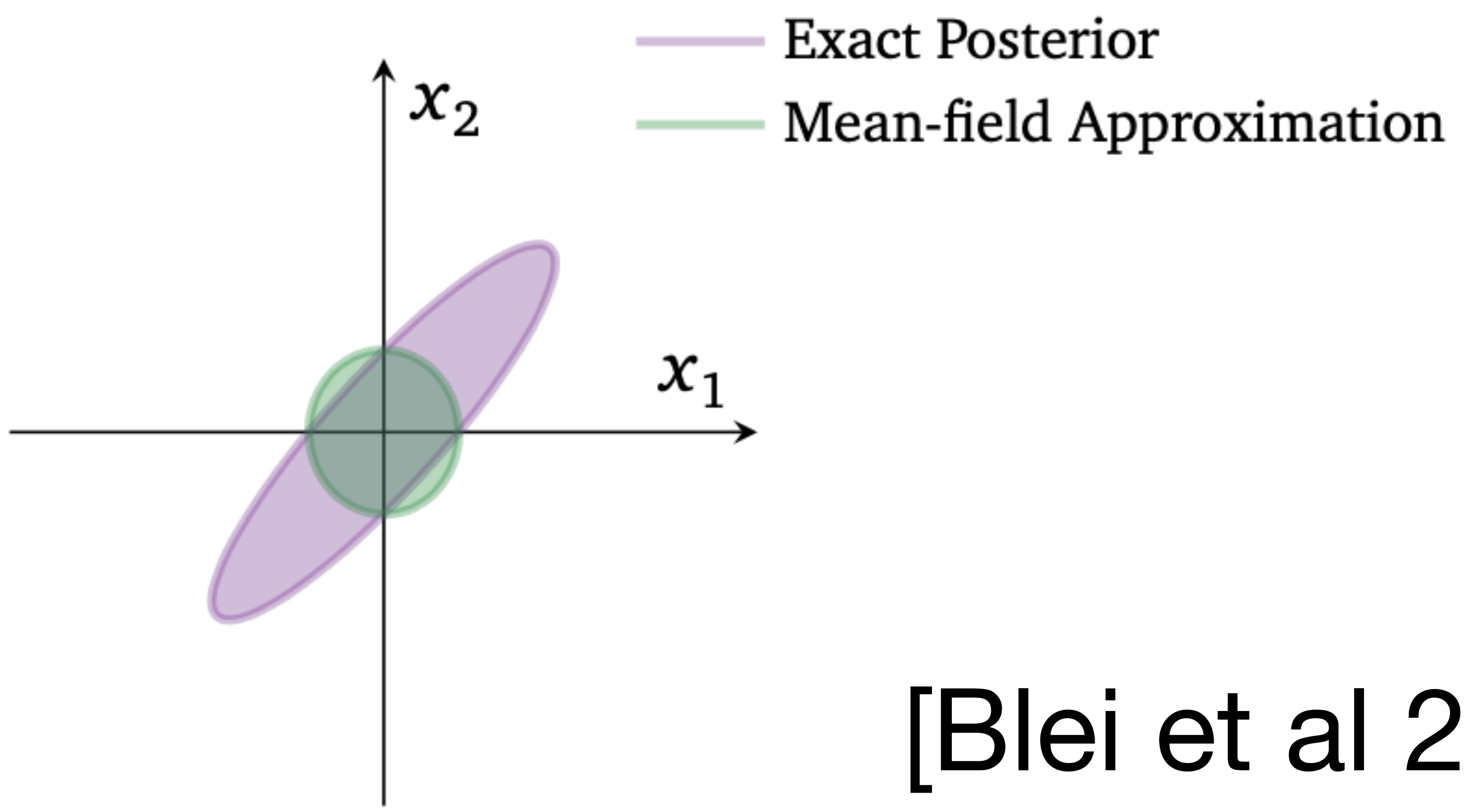
$$Q^* = Q_{\theta^*} : \theta^* = \arg\min_{\theta} D(Q_\theta(X), P(X|Z))$$

$X$ the latent variables and $Z$ the observations

More Information theoretic

- $$D_{KL}(Q_\theta(X), P(X|Z)) = \mathbb{E}_{X \sim Q_\theta}\left[-\log \frac{P(X|Z)}{Q_\theta(X)}\right] = -\int dQ_\theta(x) \log \frac{P(x|Z)}{Q_\theta(x)}$$
  - The Kullback-Leibler divergence is based on information theory
  - Known formulations for common cases

- Mean field $Q_{\theta=\mu}(X) = \Pi_i Q_{\mu_i}(X_i)$




[Blei et al 2017]

# A Case for Mean Field KL-based VI

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## Mean Field Theory for Sigmoid Belief Networks

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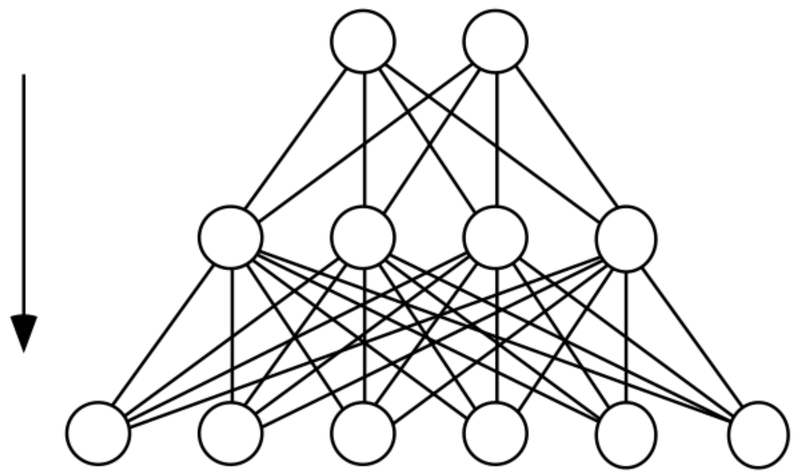
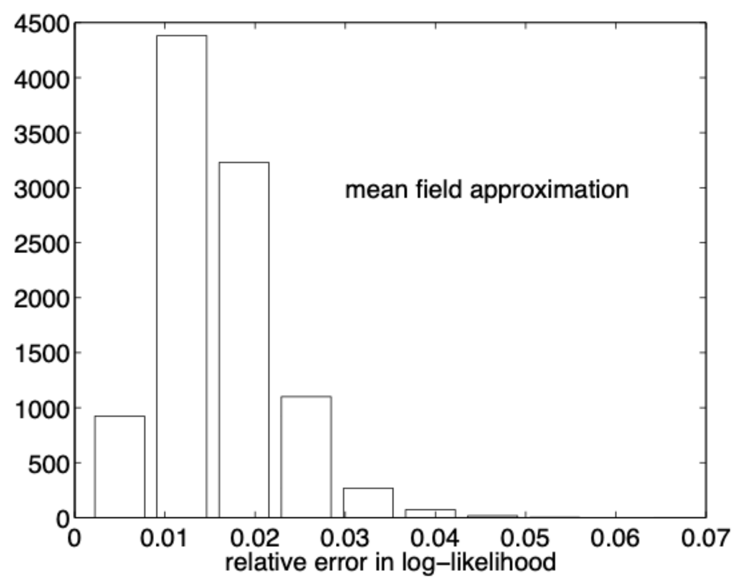
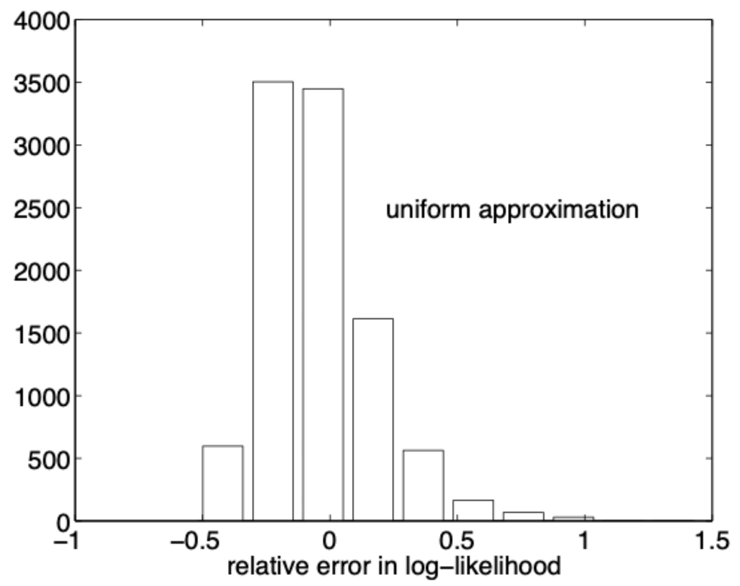
**Abstract**

We develop a mean field theory for sigmoid belief networks based on ideas from statistical mechanics. Our mean field theory provides a tractable approximation to the true probability distribution in these networks; it also yields a lower bound on the likelihood of evidence. We demonstrate the utility of this framework on a benchmark problem in statistical pattern recognition—the classification of handwritten digits.





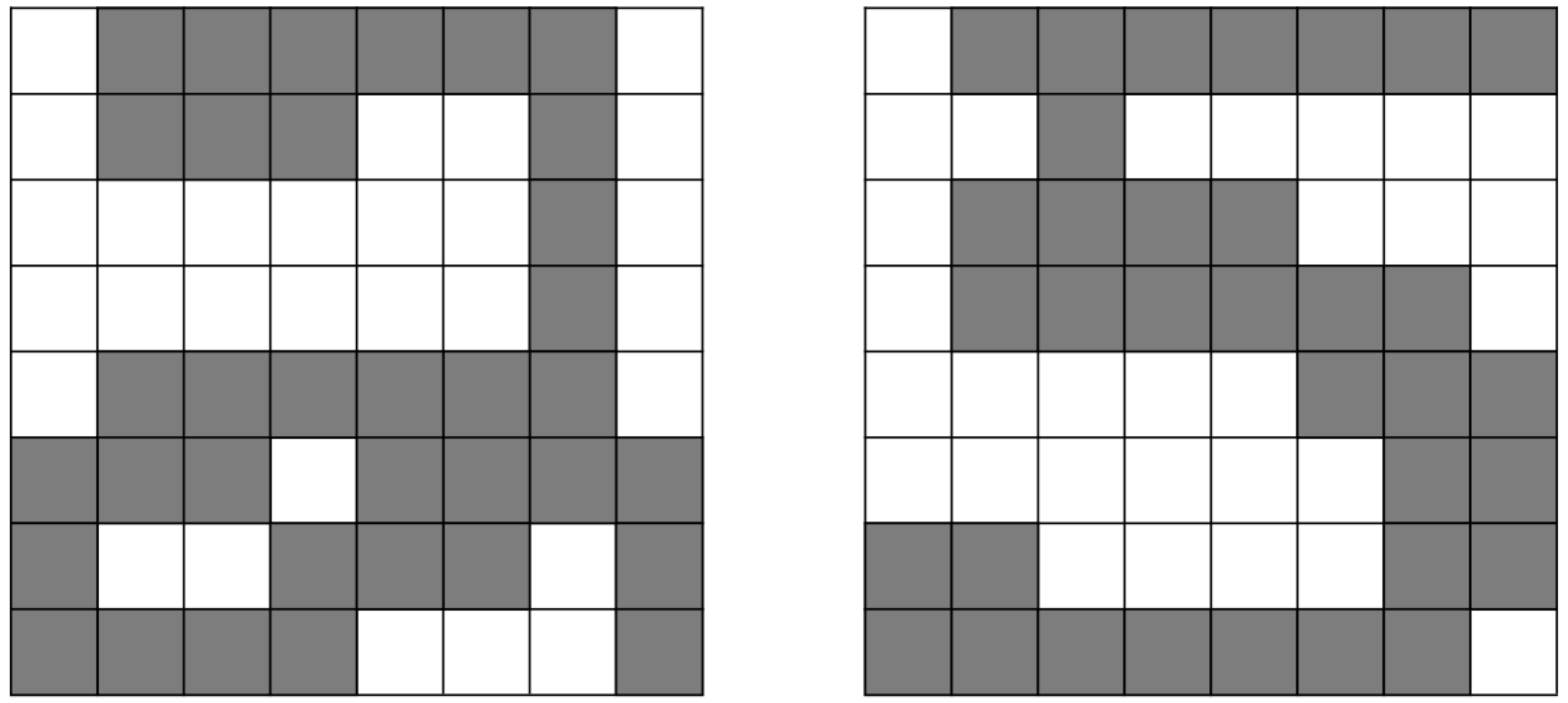



Figure 7: Binary images of handwritten digits: two and five.

| | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 388 | 2 | 2 | 0 | 1 | 3 | 0 | 0 | 4 | 0 |
| 1 | 0 | 393 | 0 | 0 | 0 | 1 | 0 | 0 | 6 | 0 |
| 2 | 1 | 2 | 376 | 1 | 3 | 0 | 4 | 0 | 13 | 0 |
| 3 | 0 | 2 | 4 | 373 | 0 | 12 | 0 | 0 | 6 | 3 |
| 4 | 0 | 0 | 2 | 0 | 383 | 0 | 1 | 2 | 2 | 10 |
| 5 | 0 | 2 | 1 | 13 | 0 | 377 | 2 | 0 | 4 | 1 |
| 6 | 1 | 4 | 2 | 0 | 1 | 6 | 386 | 0 | 0 | 0 |
| 7 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 388 | 3 | 8 |
| 8 | 1 | 9 | 1 | 7 | 0 | 7 | 1 | 1 | 369 | 4 |
| 9 | 0 | 4 | 0 | 0 | 0 | 0 | 0 | 8 | 5 | 383 |

# So Which $D$ and $Q$ Should We Choose?

$$Q^* = Q_{\theta^*} : \theta^* = \arg\min_{\theta} D(Q_\theta(X), P(X|Z))$$

$X$ the latent variables and $Z$ the observations

A second order information-theoretic model

- $D_{KL}(Q_\theta(X), P(X|Z)) = \mathbb{E}_{X\sim Q_\theta}\left[-\log \frac{P(X|Z)}{Q_\theta(X)}\right] = -\int dQ_\theta(x)\log \frac{P(x|Z)}{Q_\theta(x)}$
- $Q_\theta(X) : X \sim \mathcal{N}(\mu, \Sigma), \theta = (\mu, \Sigma)$ : This is called the Laplace approximation

# But Laplace is Better

Journal of Machine Learning Research (2013) Submitted 00/00; Published 00/00

## Variational Inference in Nonconjugate Models

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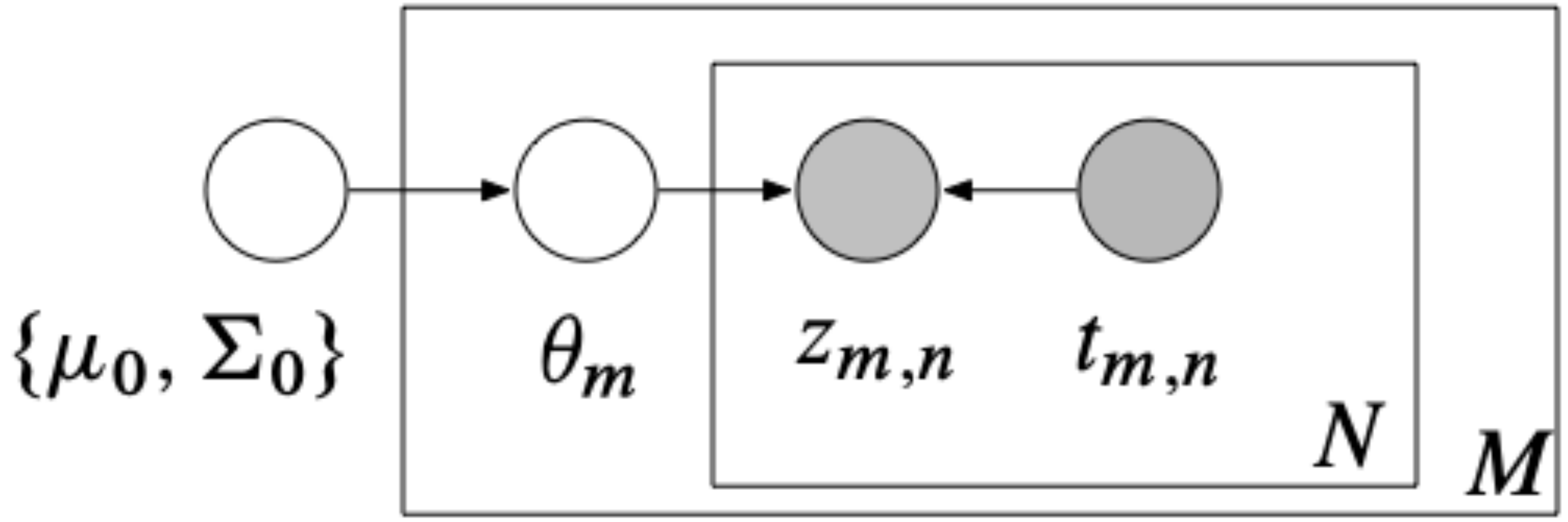
*Princeton University*
*Princeton, NJ, 08540, USA*


1. Draw coefficients $\theta \sim \mathcal{N}(\mu_0, \Sigma_0)$.
2. For each data point $n$ and its covariates $t_n$, draw its class label from

$$z_n \,|\, \theta, t_n \sim \text{Bernoulli}\left(\sigma(\theta^\top t_n)^{z_{n,1}} \sigma(-\theta^\top t_n)^{z_{n,2}}\right),$$

| | *Yeast* | | *Scene* | |
|---|---|---|---|---|
| | Accuracy | Log Likelihood | Accuracy | Log Likelihood |
| Jaakkola and Jordan (1996) | 79.7% | -0.678 | 87.4% | -0.670 |
| Laplace inference | **80.1%** | **-0.449** | **89.4%** | **-0.259** |

# So Which $D$ and $Q$ Should We Choose?

$$Q^* = Q_{\theta^*} : \theta^* = \arg\min_{\theta} D(Q_\theta(X), P(X|Z))$$

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A second order information-theoretic model

- $D_{KL}(Q_\theta(X), P(X|Z)) = \mathbb{E}_{X \sim Q_\theta}\left[-\log \frac{P(X|Z)}{Q_\theta(X)}\right] = -\int dQ_\theta(x) \log \frac{P(x|Z)}{Q_\theta(x)}$
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# So Which $D$ Should We Choose? Finding Bounds

$$D_{KL}(Q_\theta(X), P(X|Z)) = \mathbb{E}_{X\sim Q_\theta}\left[-\log \frac{P(X|Z)}{Q_\theta(X)}\right] = -\int dQ_\theta(x) \log \frac{P(x|Z)}{Q_\theta(x)}$$

But our graphical model is more adapted to sample from $P(X,Z)$ than from $P(X|Z)$.

Then, can we find a way to efficiently minimise $D_{KL}\left(Q_\theta(X), \frac{P(X,Z)}{P(Z)}\right)$

when, in general, we don't know the probability of "evidence" $P(Z)$?

Let's see in the next slide….

# So Which $D$ Should We Choose? Finding Bounds

$$D_{KL}(Q_\theta(X), P(X|Z)) = \mathbb{E}_{X \sim Q_\theta}\left[-\log \frac{P(X|Z)}{Q_\theta(X)}\right] = -\int dQ_\theta(x) \log \frac{P(x|Z)}{Q_\theta(x)}$$

And we know that

$$\log P(Z) = \log \int dx P(x, Z) = \log \int \frac{dQ_\theta(x) P(x, Z)}{Q_\theta(x)} = \log \mathbb{E}_{X \sim Q_\theta}\left[\frac{P(X, Z)}{Q_\theta(X)}\right]$$

with $Z$ being the observed data ($O$ before) and $X$ our latent variables ($L$)

then, $P(Z) = \log \mathbb{E}_{X \sim Q_\theta}\left[\frac{P(X, Z)}{Q_\theta(X)}\right] \geq E_{X \sim Q_\theta}\left[\frac{P(X, Z)}{Q_\theta(X)}\right] \triangleq \mathscr{L}(\theta)$

$$\min_\theta D_{KL}(Q_\theta(X), P(X|Z)) = \log P(Z) - \max_\theta \mathscr{L}(\theta)$$

Hence, it is enough to maximise the Evidence Lower Bound (ELBO): $\mathscr{L}(\theta)$

# So Which $D$ and $Q$ Should We Choose?

$$Q^* = Q_{\theta^*} : \theta^* = \arg\min_{\theta} D(Q_\theta(X), P(X \mid Z))$$

$X$ the latent variables and $Z$ the observations

A simplified second order information-theoretic model

- $\theta = \arg\max_{\theta} \mathscr{L}(\theta) = \mathbb{E}_{X \sim Q_\theta}\left[\log \frac{P(X, Z)}{Q_\theta(X)}\right]$
- $Q_\theta(X) : X \sim \mathcal{N}(\mu, \Sigma), \theta = (\mu, \Sigma)$ : This is called the Laplace approximation

# But Laplace is Better (they use ELBO)

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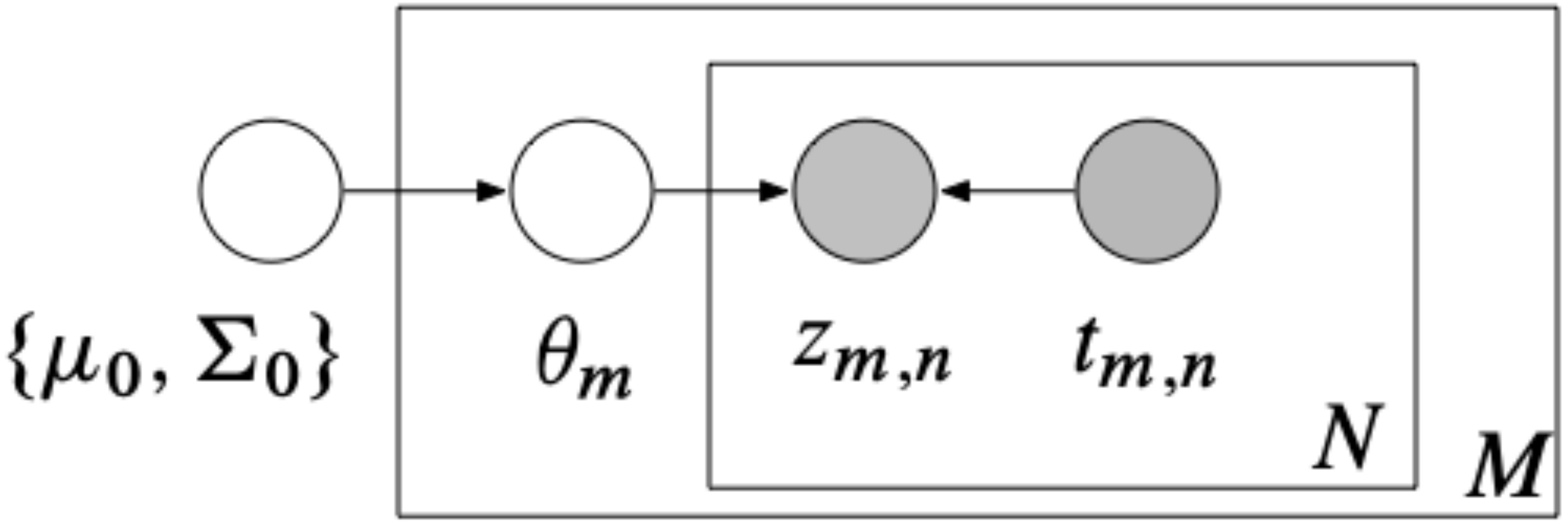


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# More General $Q_\theta$

$$Q^* = Q_{\theta^*} : \theta^* = \arg\min_\theta D(Q_\theta(X), P(X|Z))$$

$X$ the latent variables and $Z$ the observations

- Gaussian Processes: A measure over continuous functions where any discrete sample of the domain follows a Gaussian law.

  $P(f(x)) : (f(x_1), \ldots, f(x_N)) \sim N(\mu_{x_1,\ldots,x_N}, \Sigma_{x_1,\ldots,x_N})$

- Support Transformations: $Q_\theta(X) \triangleq \phi_\theta(X)$

  $X \sim \mathcal{N}(\mu, \Sigma), \phi_\theta$ a parametric mass-preserving diffeomorphism

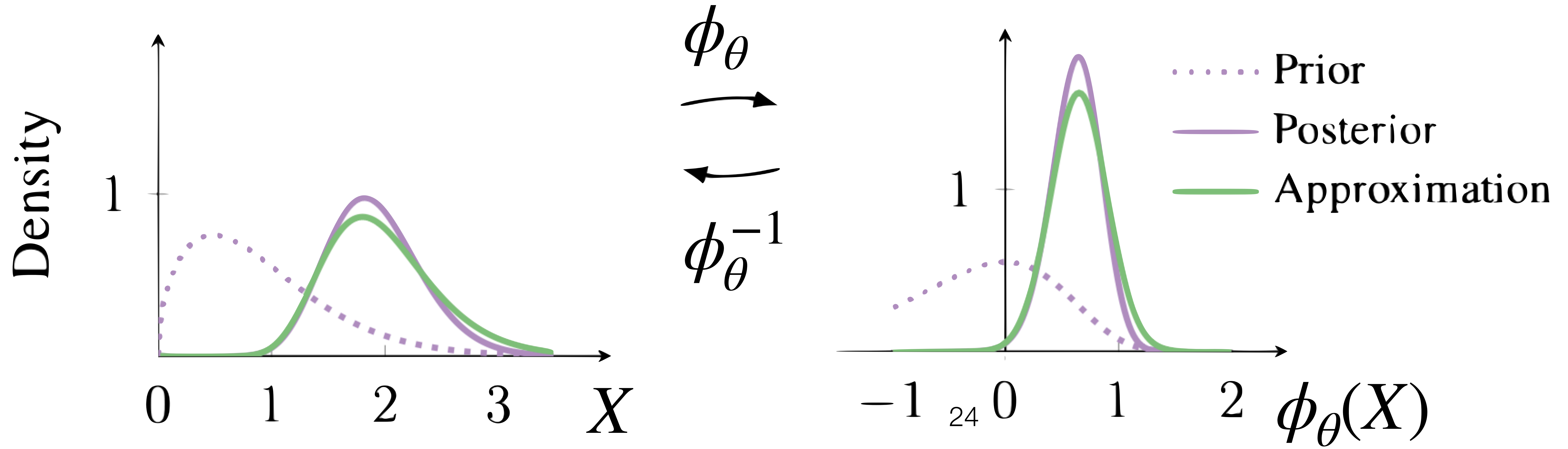
# More General $Q_\theta$

$$Q^* = Q_{\theta^*} : \theta^* = \arg\min_\theta D(Q_\theta(X), P(X\,|\,Z))$$

$X$ the latent variables and $Z$ the observations

- Support Transformations: $Q_\theta(X) \triangleq N_{\mu,\Sigma}(\phi_\theta(X))\left|J_{\phi_\theta}(X)\right|$

$X \sim \mathcal{N}(\mu, \Sigma)$, $\phi_\theta$ a parametric mass-preserving diffeomorphism




[Kucukelbir etal 17]

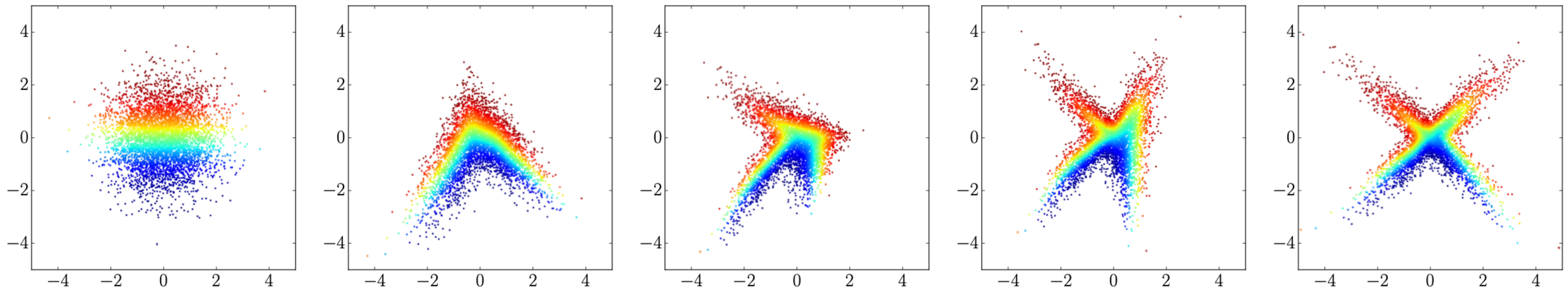
# More General $Q_\theta$

$$Q^* = Q_{\theta^*} : \theta^* = \arg\min_\theta D(Q_\theta(X), P(X \mid Z))$$

$X$ the latent variables and $Z$ the observations

- Support Transformations: $Q_\theta(X) \triangleq N_{\mu,\Sigma}(\phi_\theta(X)) \left| J_{\phi_\theta}(X) \right|$

$\phi_\theta(X) \sim \mathcal{N}(\mu, \Sigma)$, $\phi_\theta$ a stochastic flow or learnable diffeomorphism

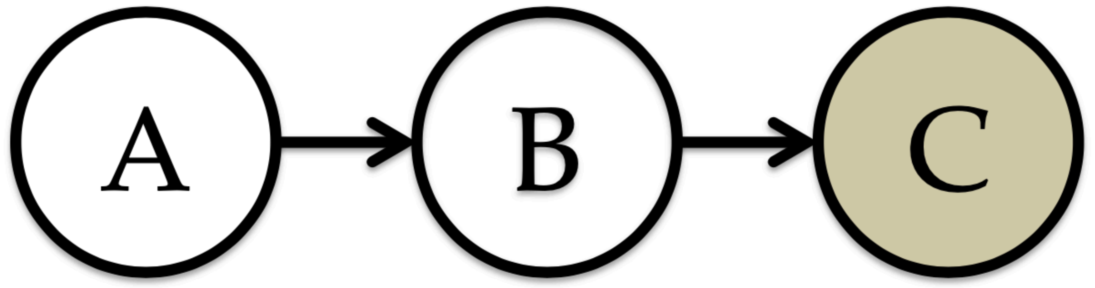





[Papamakarios etal 21]

# Current Problems in VI

- Scalability
- Amortization [Gershman et al 2014]
- Preservation of dependencies
- Auto-regressive models




Query 1: $P(B|C) = P(C|B)P(B)/P(C)$

Query 2: $P(A|C) = \sum_{B} P(A|B)P(B|C)$

Amortisation, reused probability in blue

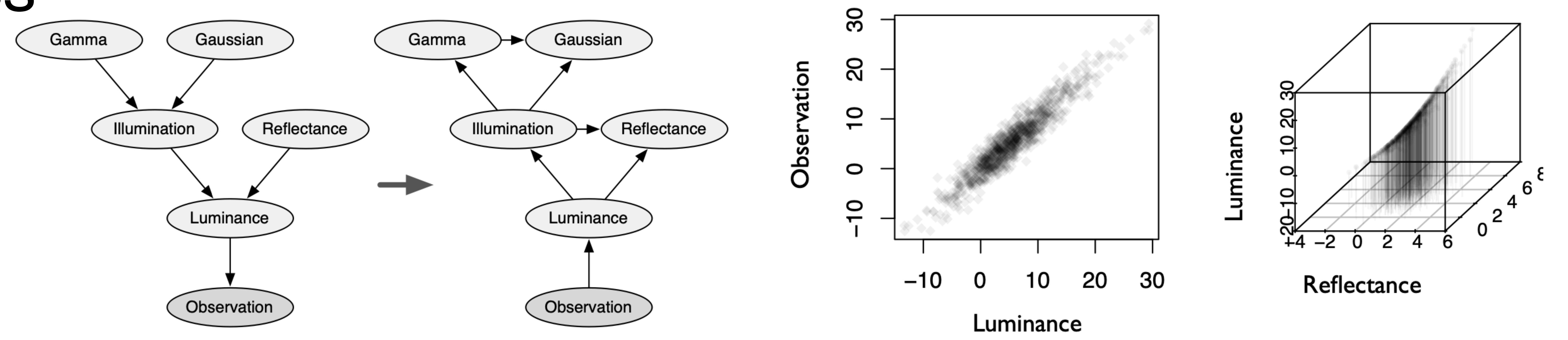


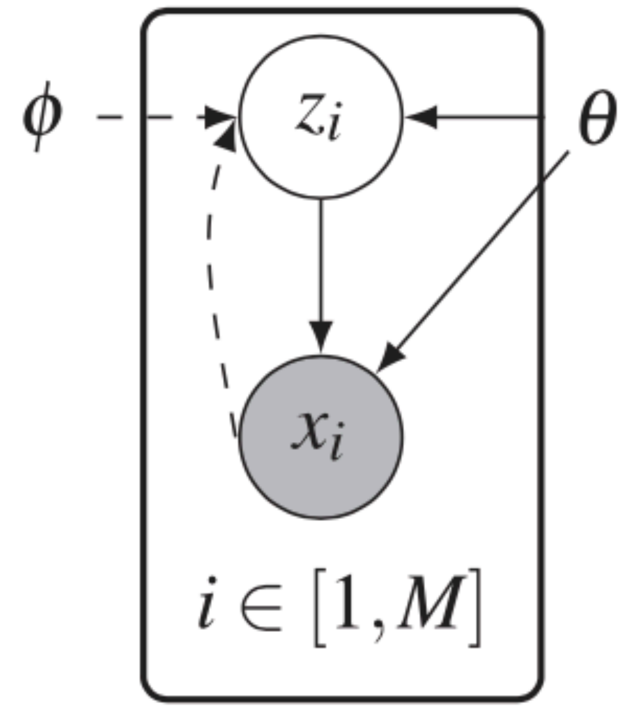

Figure 1: A Bayesian network modeling brightness constancy in visual perception, a possible invers
factorization, and two of the local joint distributions that determine the inverse conditionals.



[Stuhlmüller et al 14]

# Other Modern Bayesian Techniques

- Variational AutoEncoders
- Likelihood-free Inference



(b) VAE

$$\theta = \arg\max_{\theta} \mathscr{L}(\theta) = \mathbb{E}_{X \sim Q_\theta}\left[\log \frac{P(X,Z)}{Q_\theta(X)}\right]$$

$$VAE : Z \sim N(\mu(X), \Sigma(X))$$

Likelihood

Prior

$$P(Z|X) = \frac{P(X|Z)P(Z)}{P(X)}$$

Evidence