Graphical Models and Variational Inference

Demian Wassermann, Inria

Graphical Models: Discrete Inference and Learning

And the Usual Graph Slide

Image credit: Medium

Social Networks

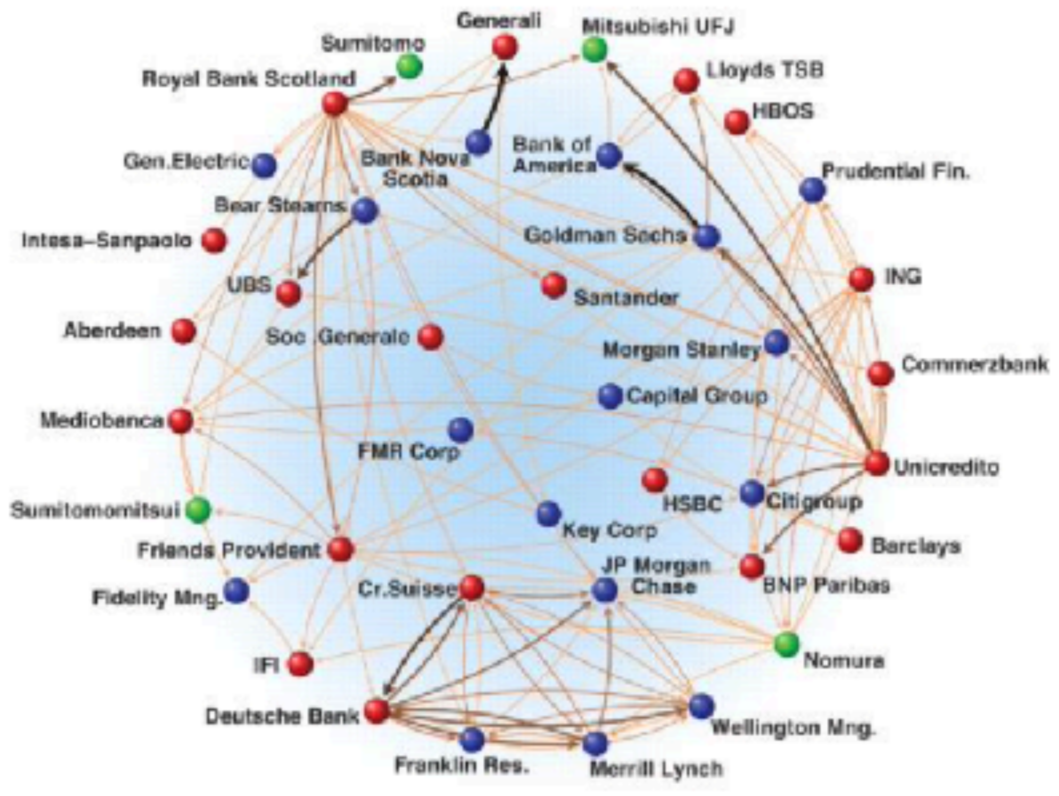

Image credit: Science

Economic Networks

Image credit: Lumen Learning

Communication Networks

Citation Networks

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Internet

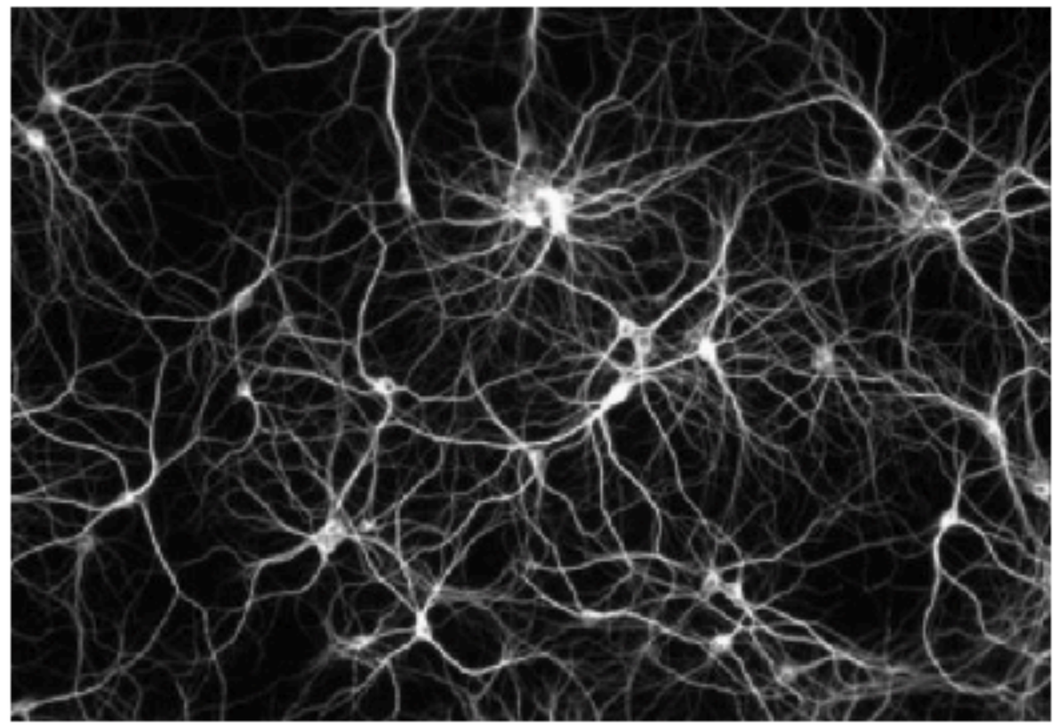
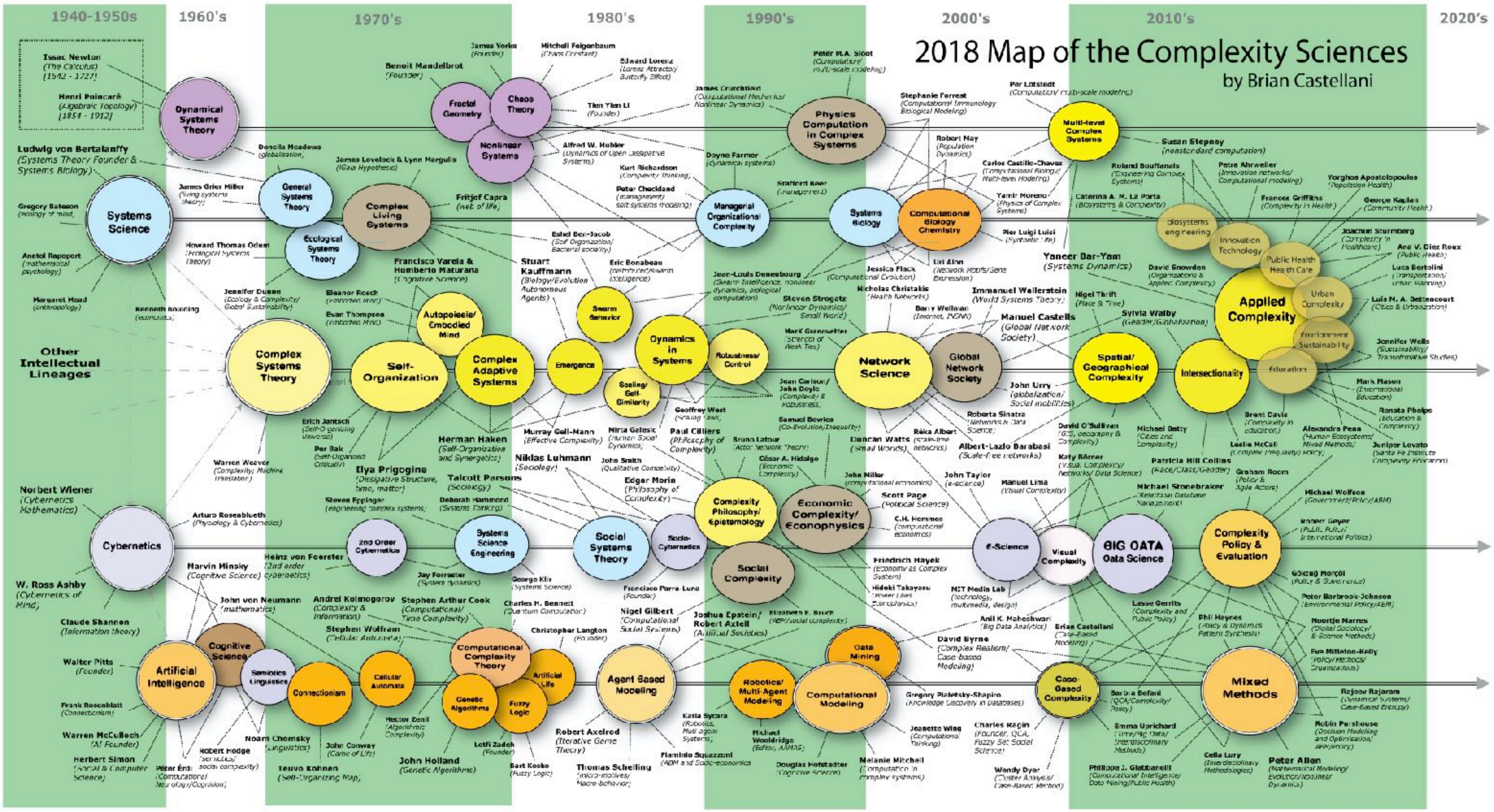


Image credit: The Conversation

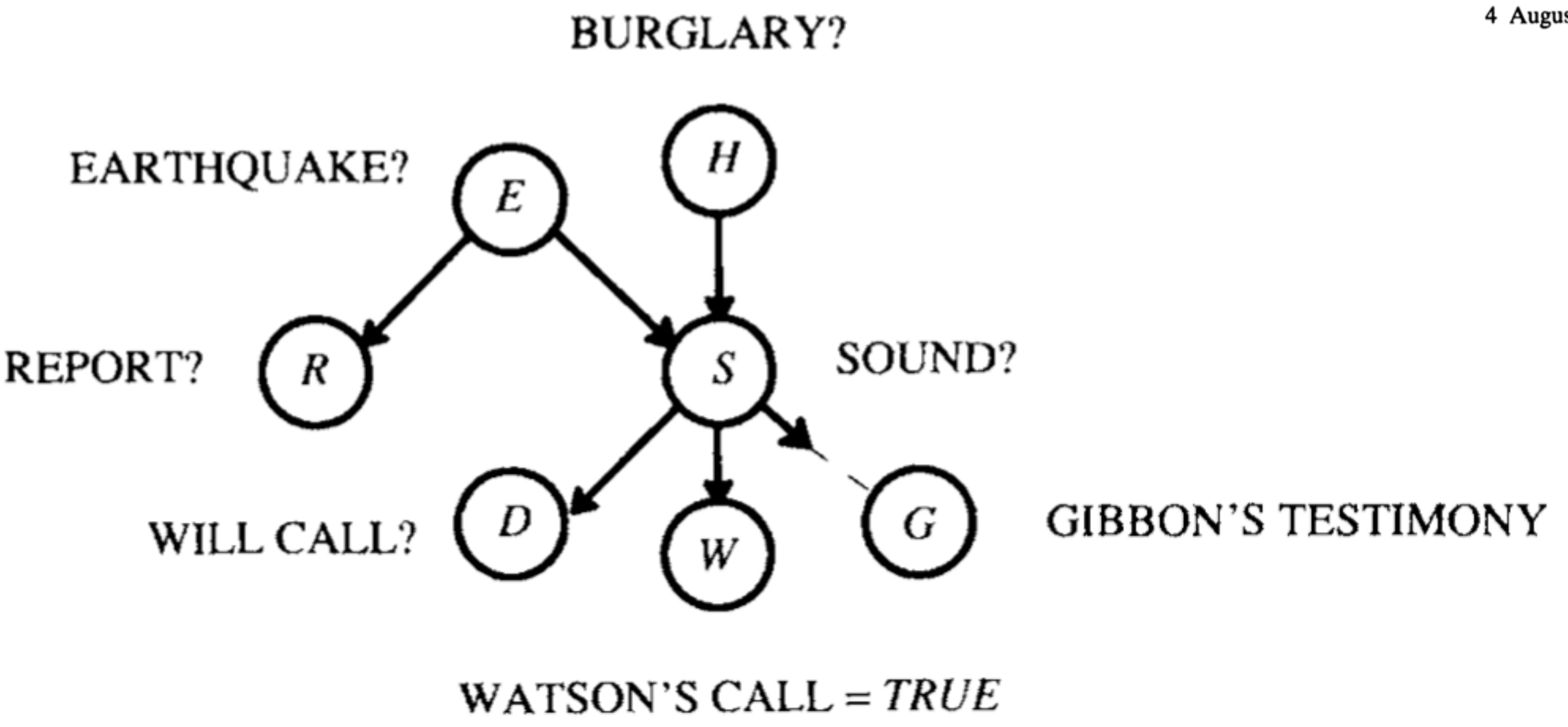
Networks of Neurons

Complex Systems to Understand the World



Wikipedia

Main Epistemological Angles on Graphs and Knowledge



[Pearl 1987]

4 August 1972, Volume 177, Number 4047 **SCIENCE**

More Is Different

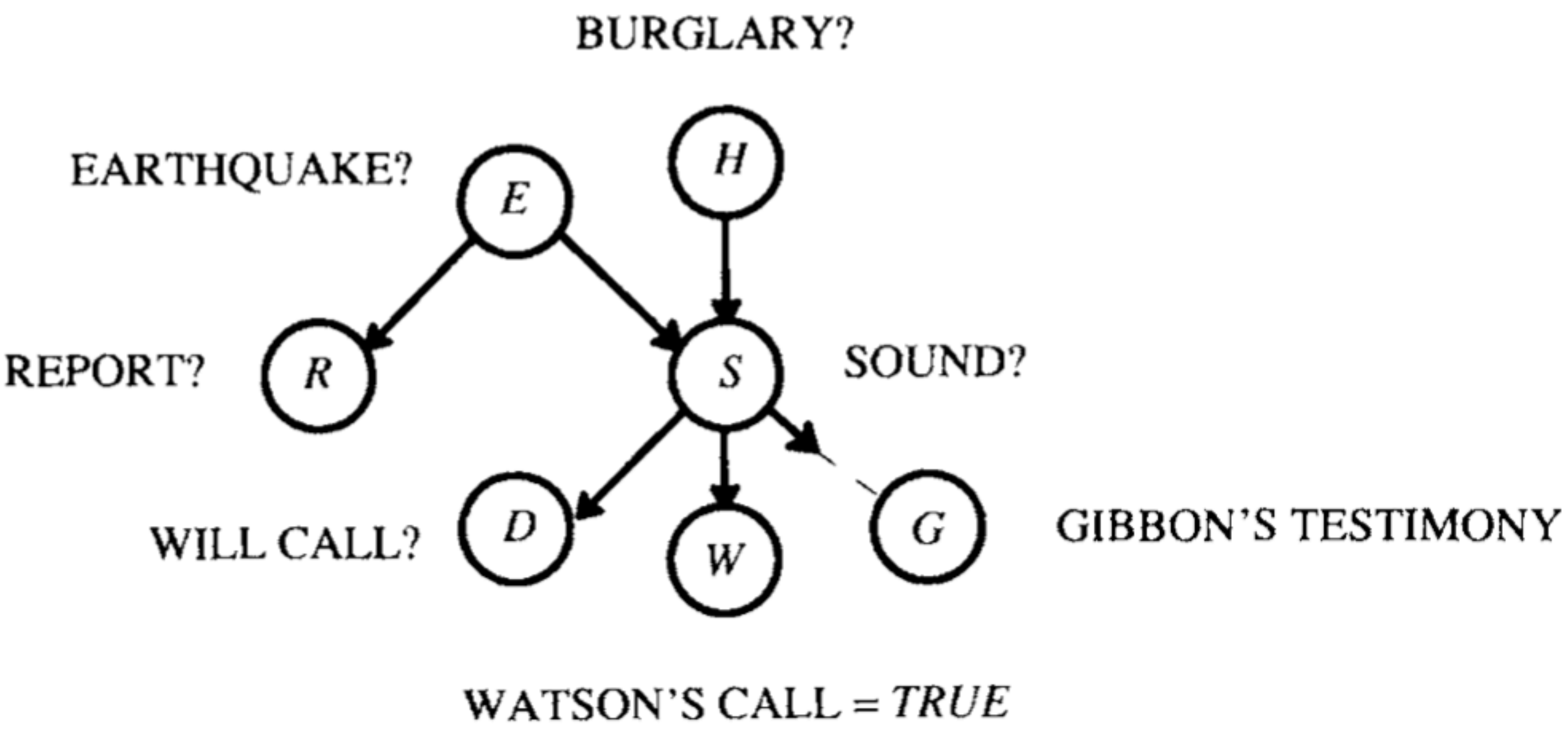
Broken symmetry and the nature of the hierarchical structure of science.

P. W. Anderson

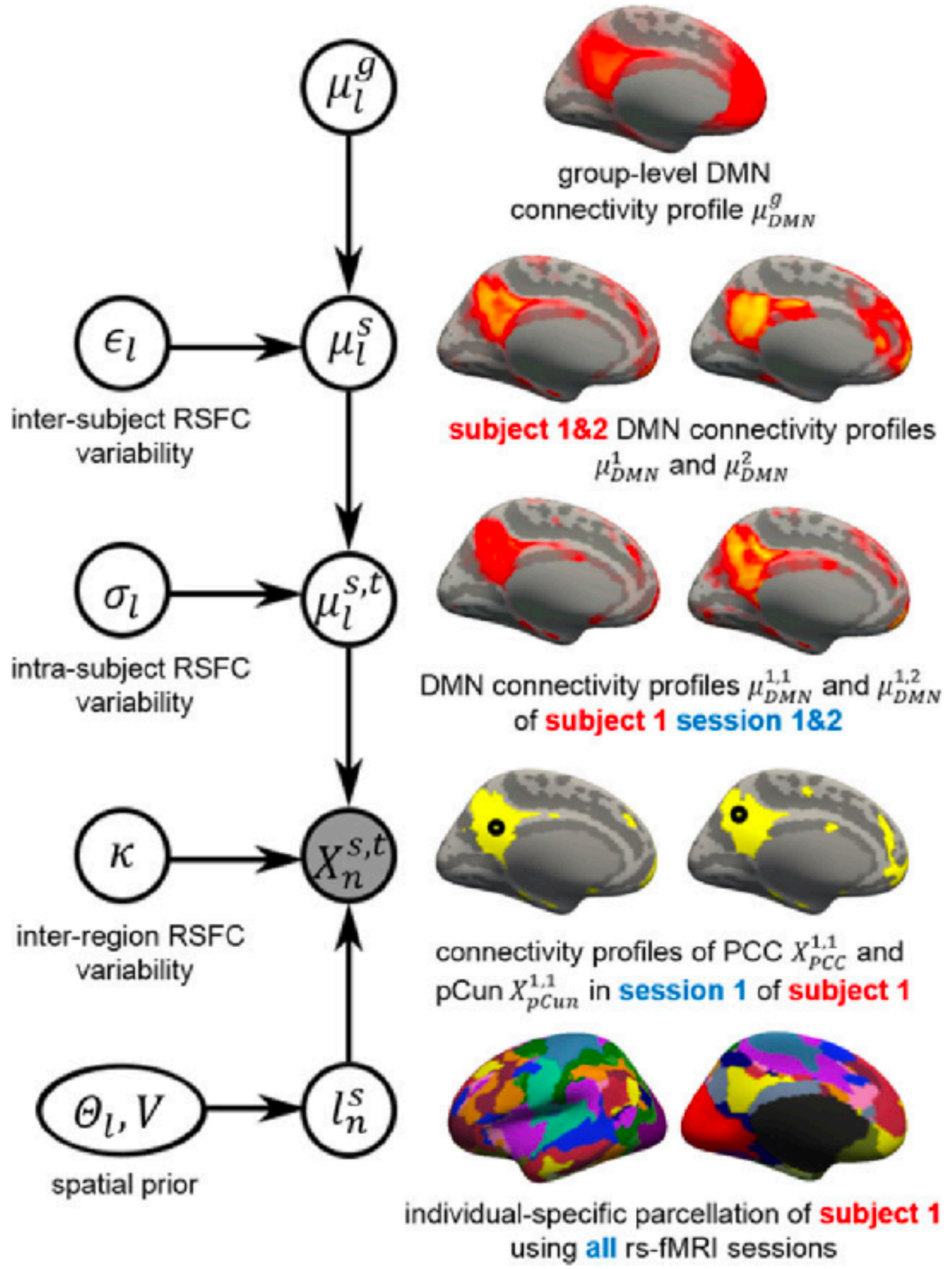
Introduction to DAG and their relationship with Probability Functions (Pearl)

- Show examples of the above, Yeo, RE, etc
- Show the formal relationship between graphs and probs
- Show the discrete case and mention solving algorithms
- Show the continuous case and state the problem is too complex, we need approximations

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



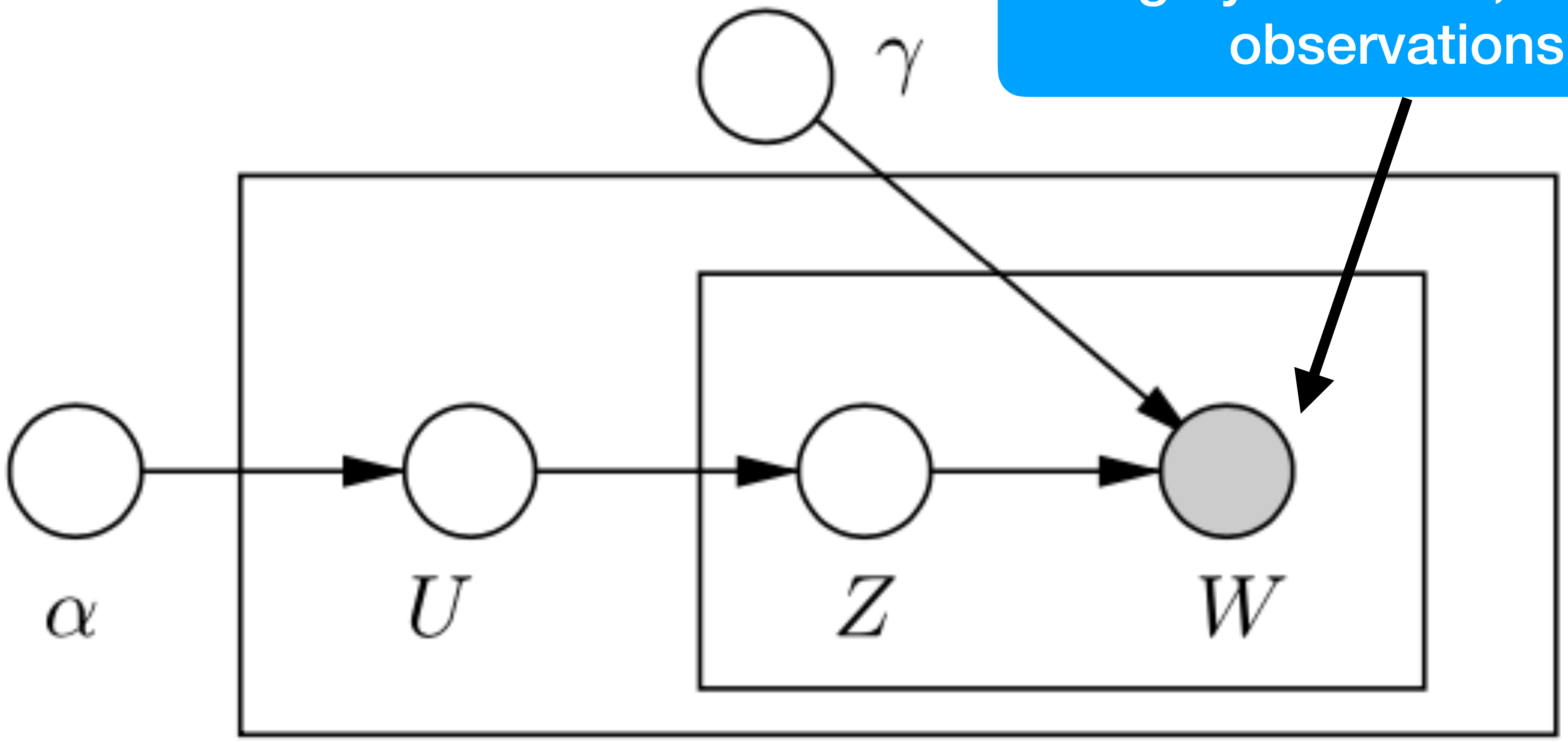
[Pearl 1987]



[Kong et al 2019]

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

The greyed nodes, represent observations



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

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

"Arts"	"Budgets"	"Children"	"Education"
NEW	MILLION	CHILDREN	SCHOOL
FILM	TAX	WOMEN	STUDENTS
SHOW	PROGRAM	PEOPLE	SCHOOLS
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LOVE	CONGRESS	LIFE	HAITI

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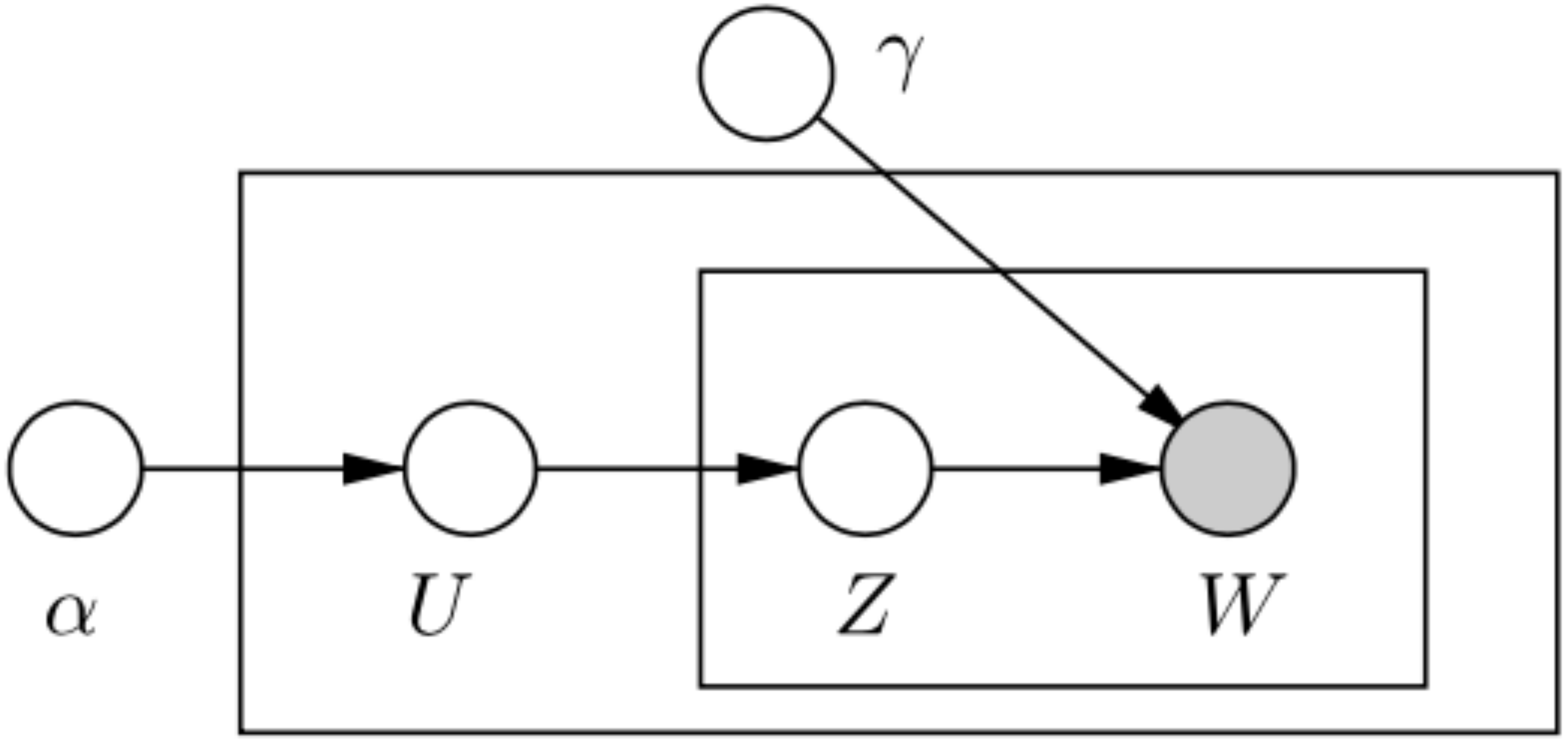

$$U_j \sim Dirichlet(\alpha), \alpha < 1$$

$$Z_{i,j} \sim Multinomial(U_j)$$

$$W_{i,j} \sim Multinomial\left(\gamma_{Z_{i,j}}\right)$$

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

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

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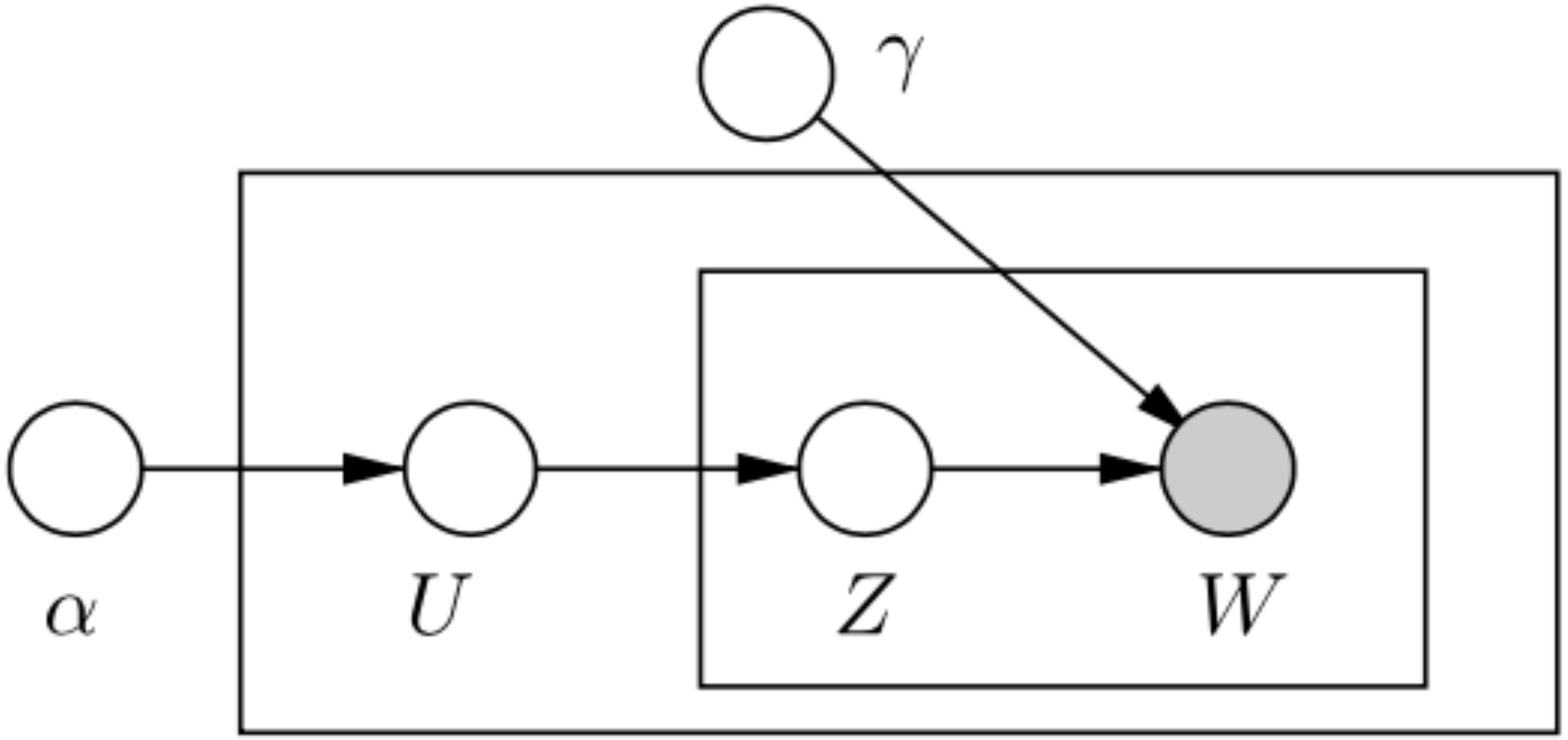

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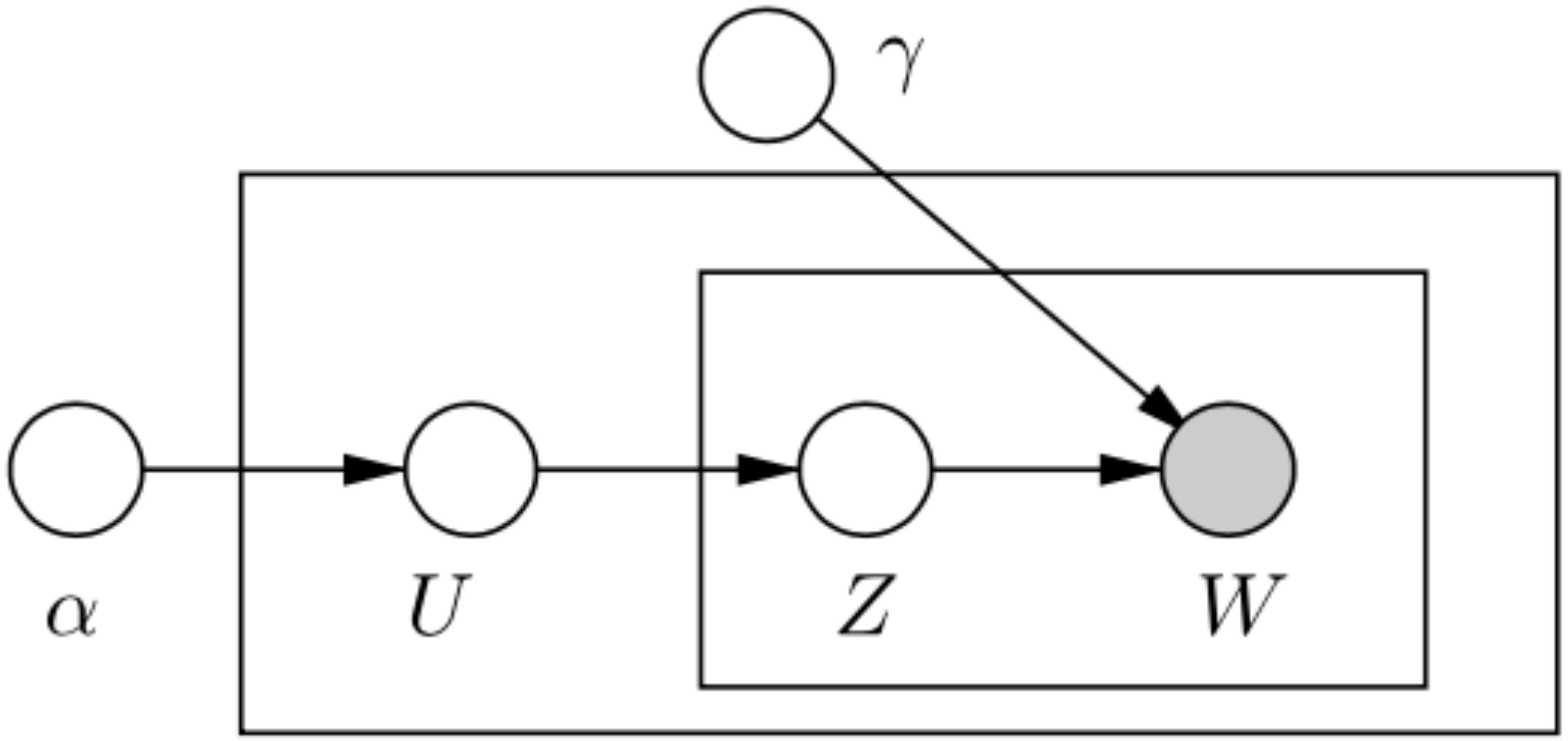
No analytical solution

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

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



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$$P(W_1, \ldots, W_I, Z_1, \ldots, Z_I, U_1 \ldots, U_J, \alpha, \gamma) = \Pi_j \Pi_i P(W_i \,|\, Z_i, \gamma) P(Z_i \,|\, U_j) P(U_j \,|\, \alpha)$$

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

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

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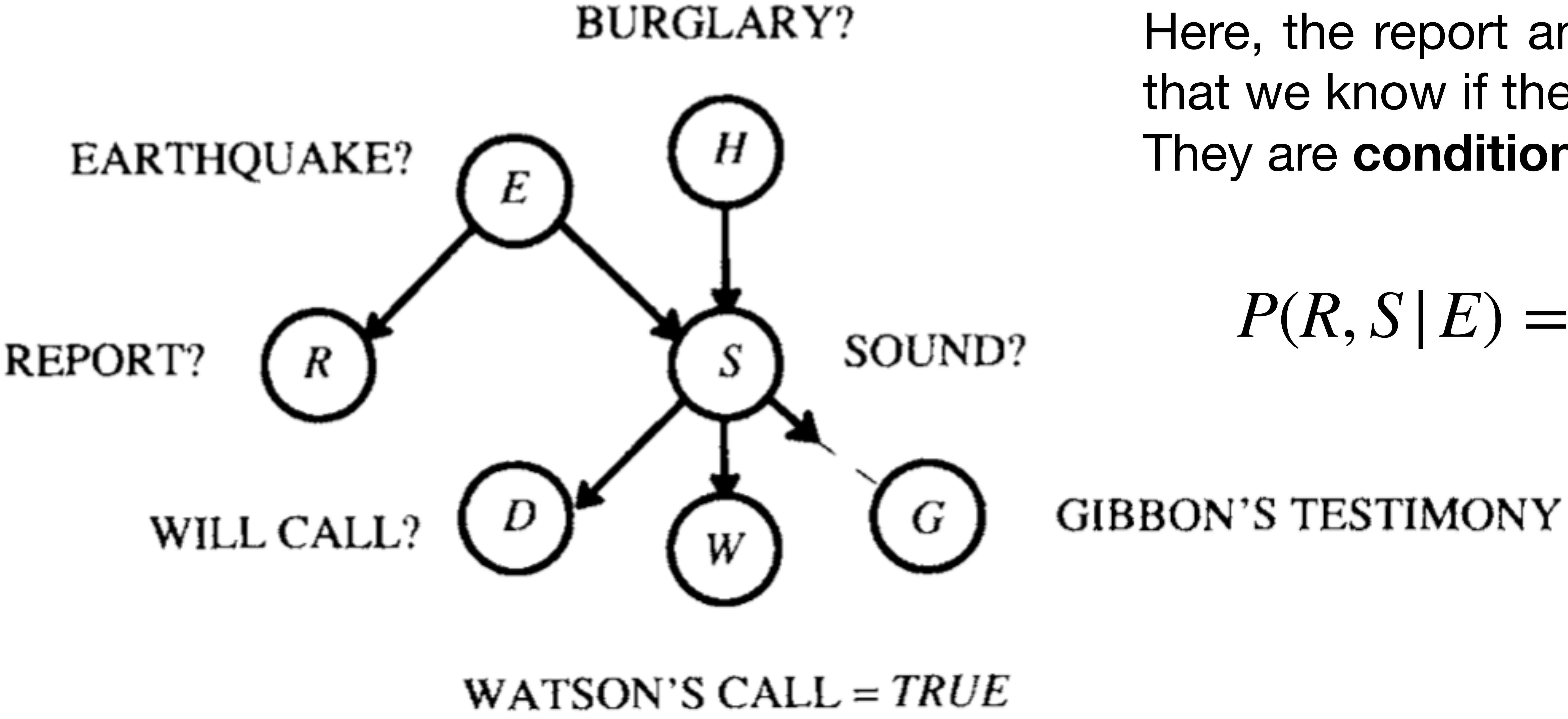

Here, the report and the sound are independent, given that we know if there was an earthquake:
They are **conditionally** independent

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

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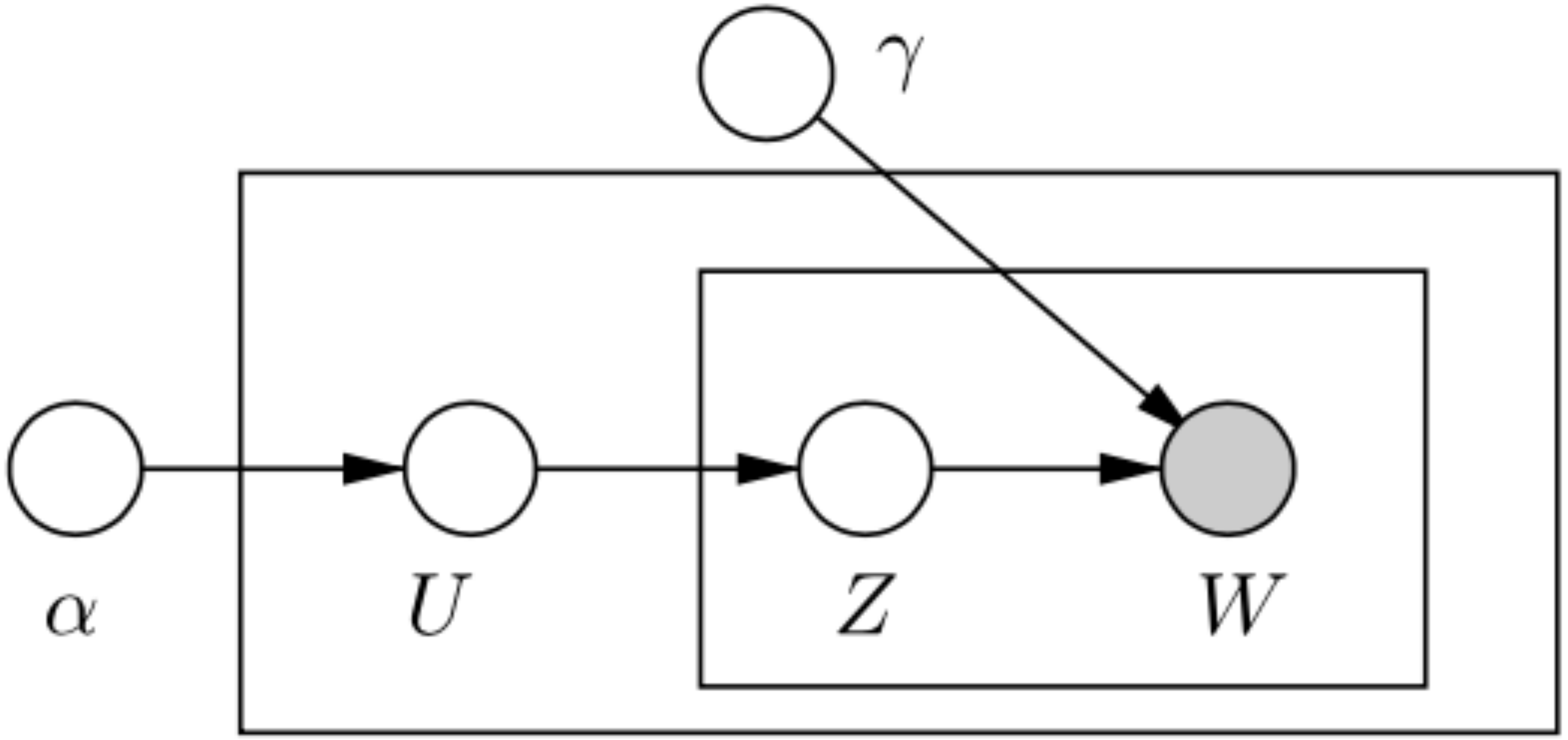

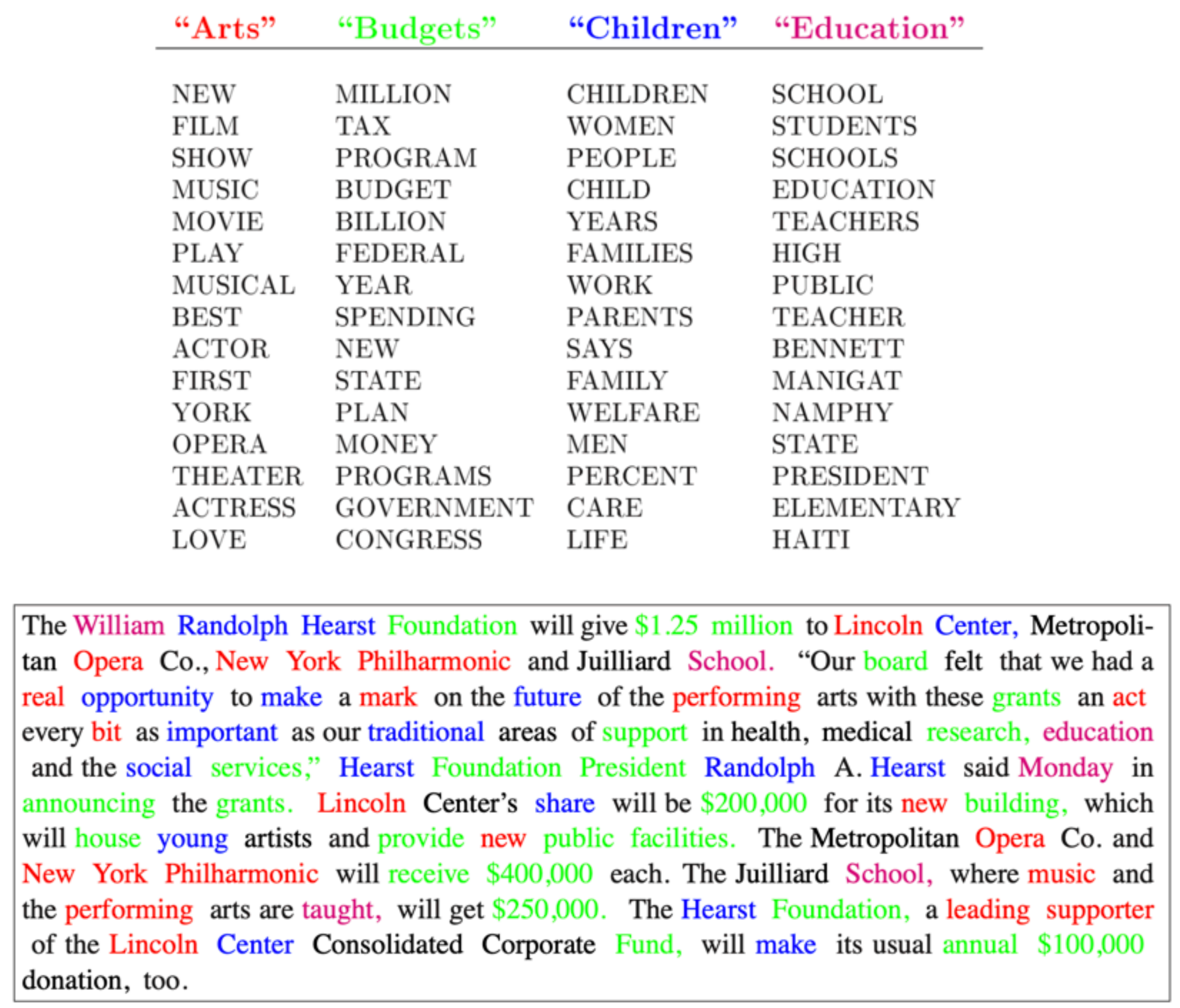

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However, our usual problem is: given observed variables O and latent variables L, to compute the posterior $P(L \mid O)$

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

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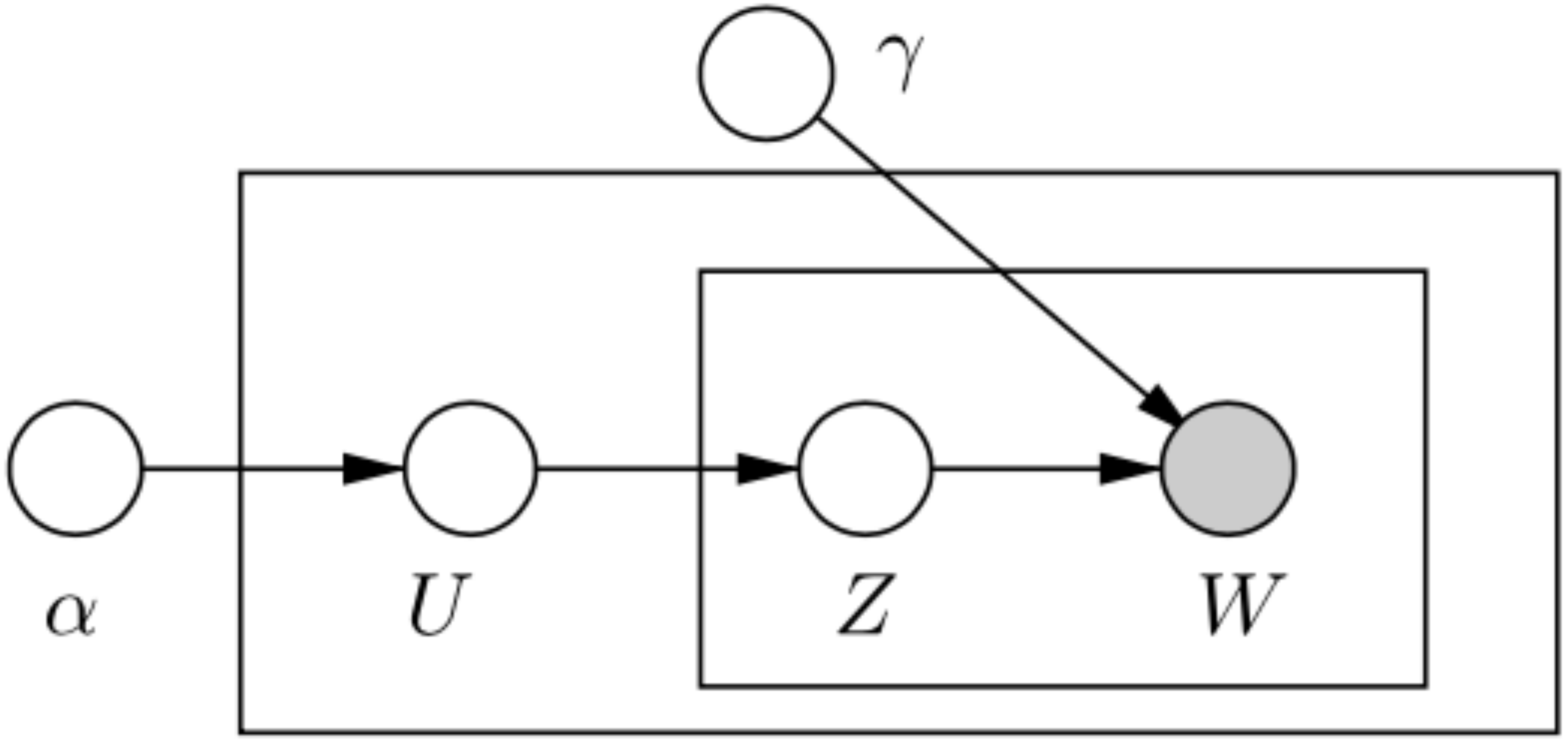

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In the case of continuous variables this is

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

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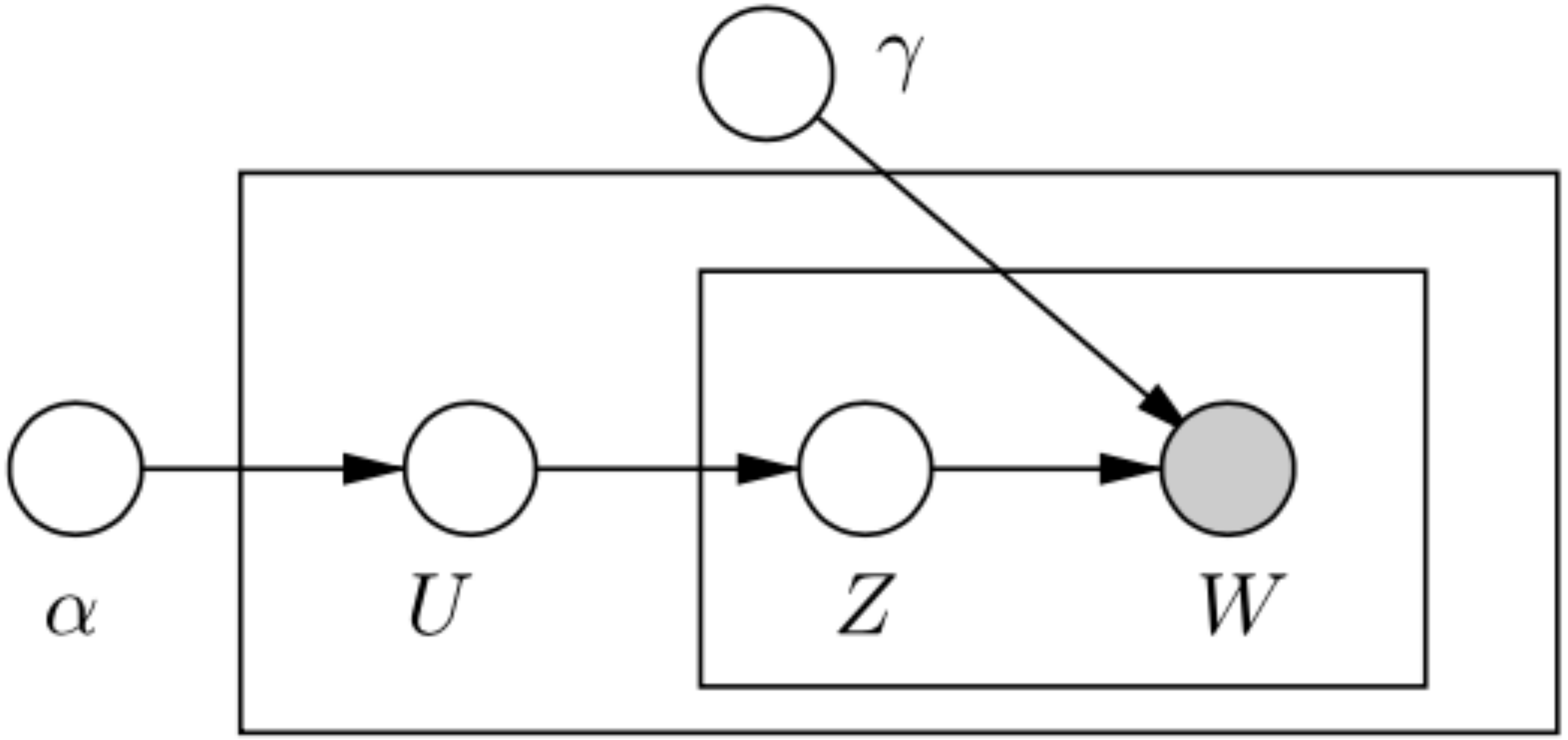

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No analytical solution, for the general case

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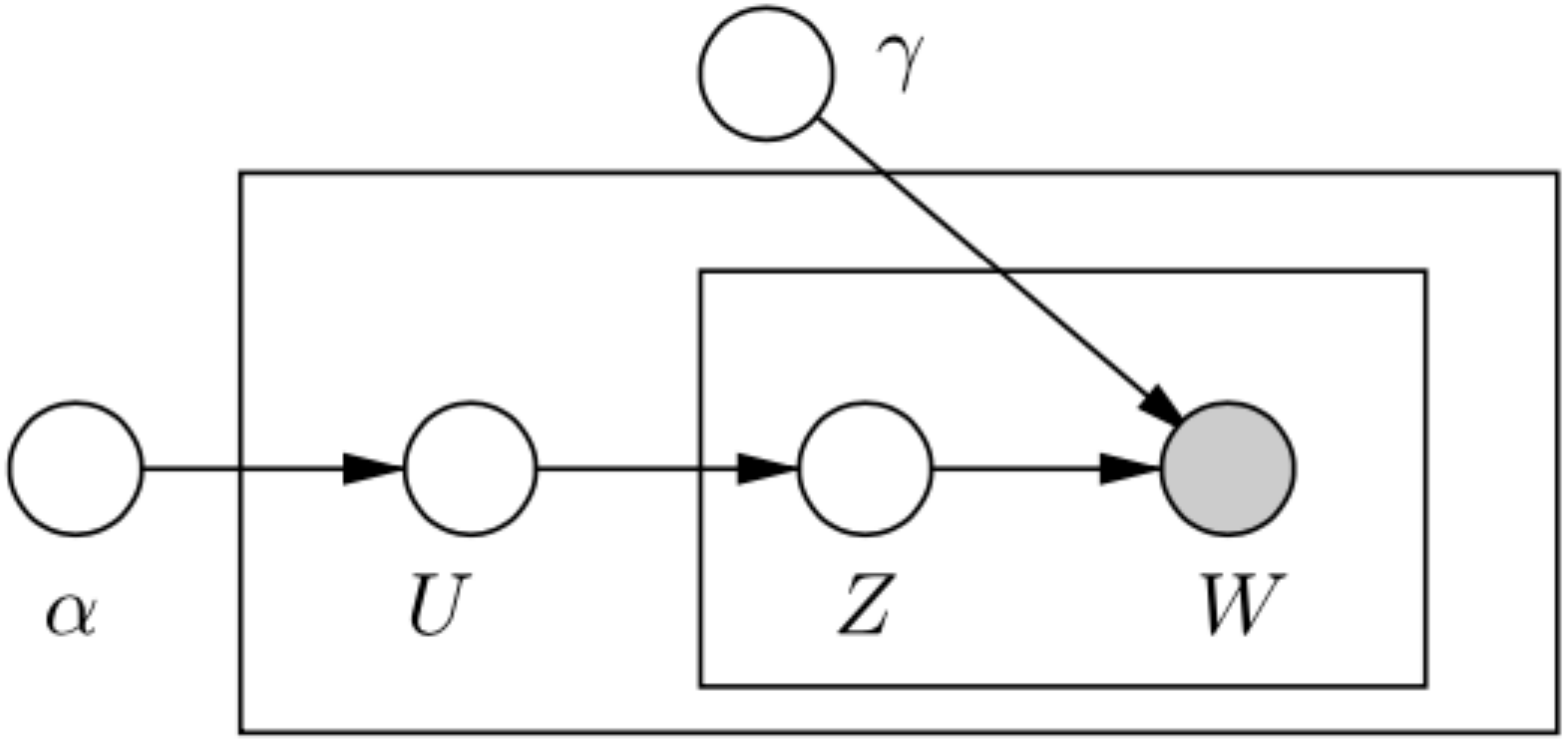

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Can we approximate $P(L\,|\,O)$?

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

Approximations to Density Laws

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

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

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

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

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

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

Approximations to Density Laws

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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 $P(L \mid O)$?

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

- So? What do we do?
  - We choose an approximate distribution $Q_\theta(X) = Q_\theta(L)$ from a given family, with parameters θ. Then

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

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 Density Laws

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

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

This is what we call Variational Inference

- So? What do we do?
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so we need to define the right similarity measurement D to compare distributions. And in standard Variational Inference (VI), Z is notation for O

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 $\Sigma = \sigma^2 \text{Id}$, which boils down to $Q_\mu(X) = \Pi_i Q_{\mu_i}(X_i)$

So Which D and Q Should We Choose?

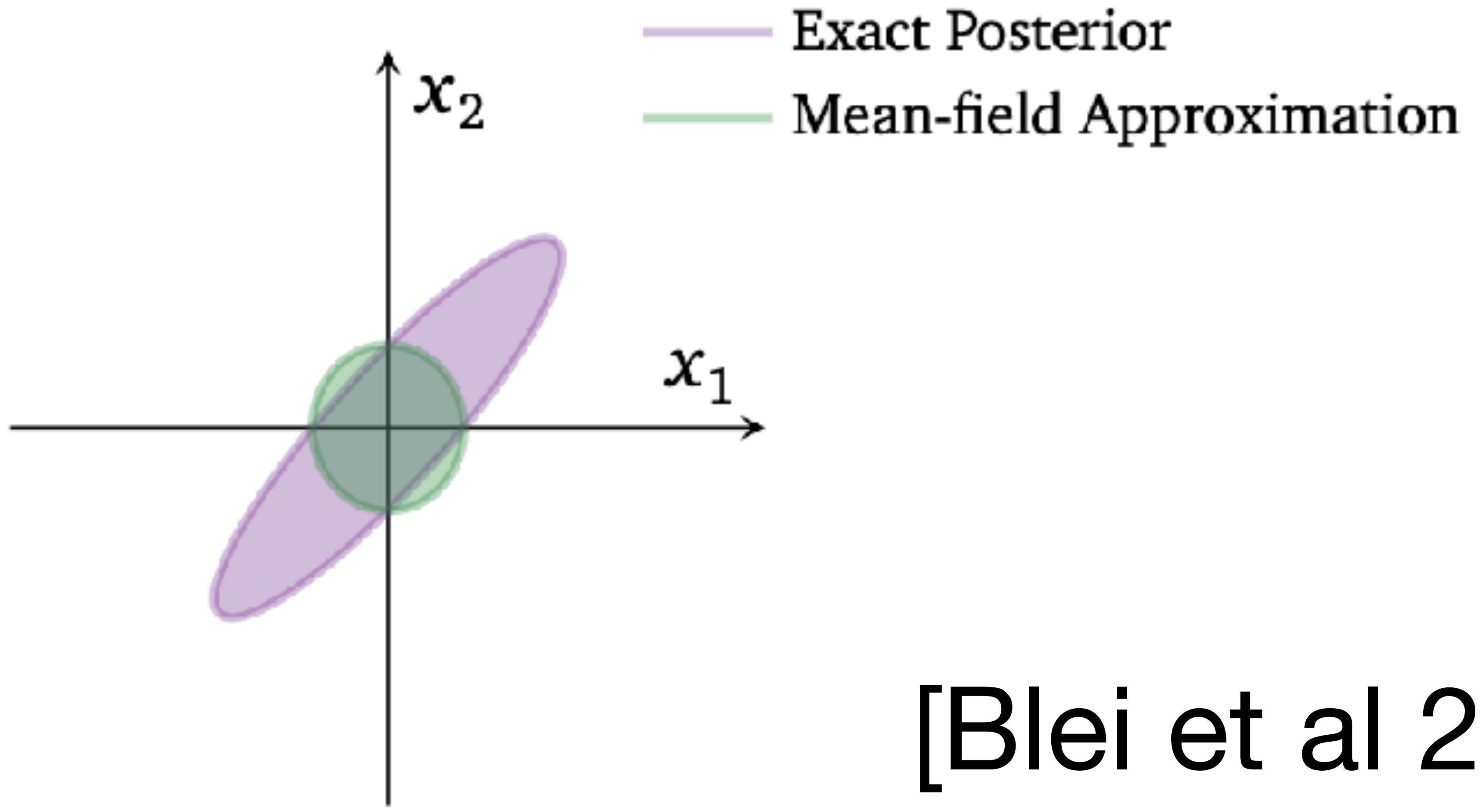
$$Q^* = Q_{\theta^*} : \theta^* = \arg\min_{\theta} D(Q_\theta(X), P(X|Z))$$

X the latent variables and Z the observations

More Information theoretic

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

Journal of Artificial Intelligence Research 4 (1996) 61—76 Submitted 11/95; published 3/96

Mean Field Theory for Sigmoid Belief Networks

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Massachusetts Institute of Technology
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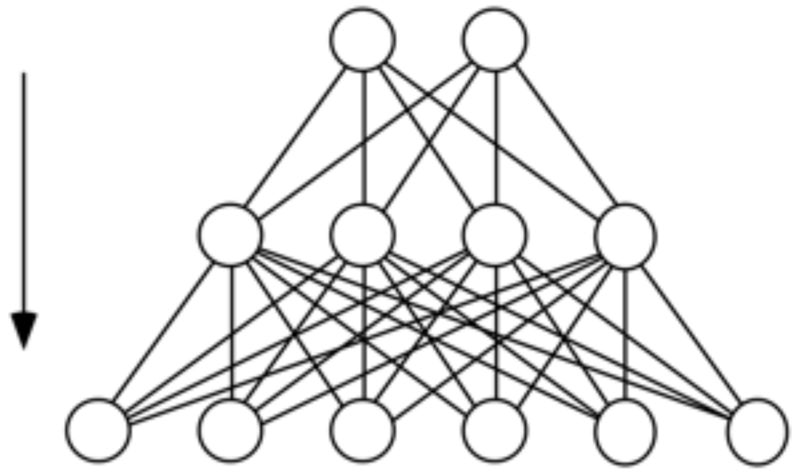
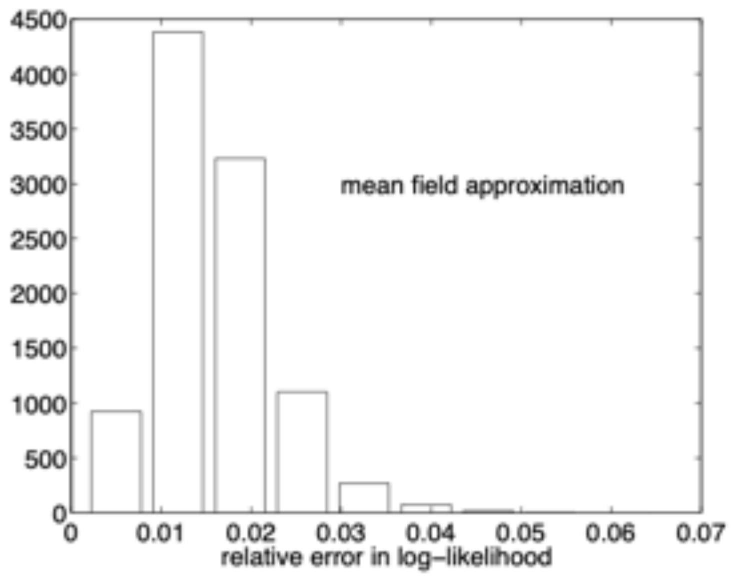
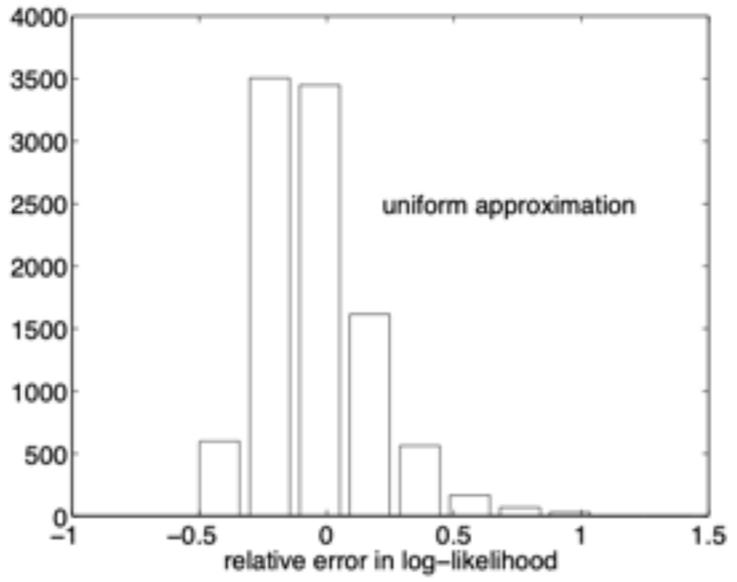
Cambridge, MA 02139

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.







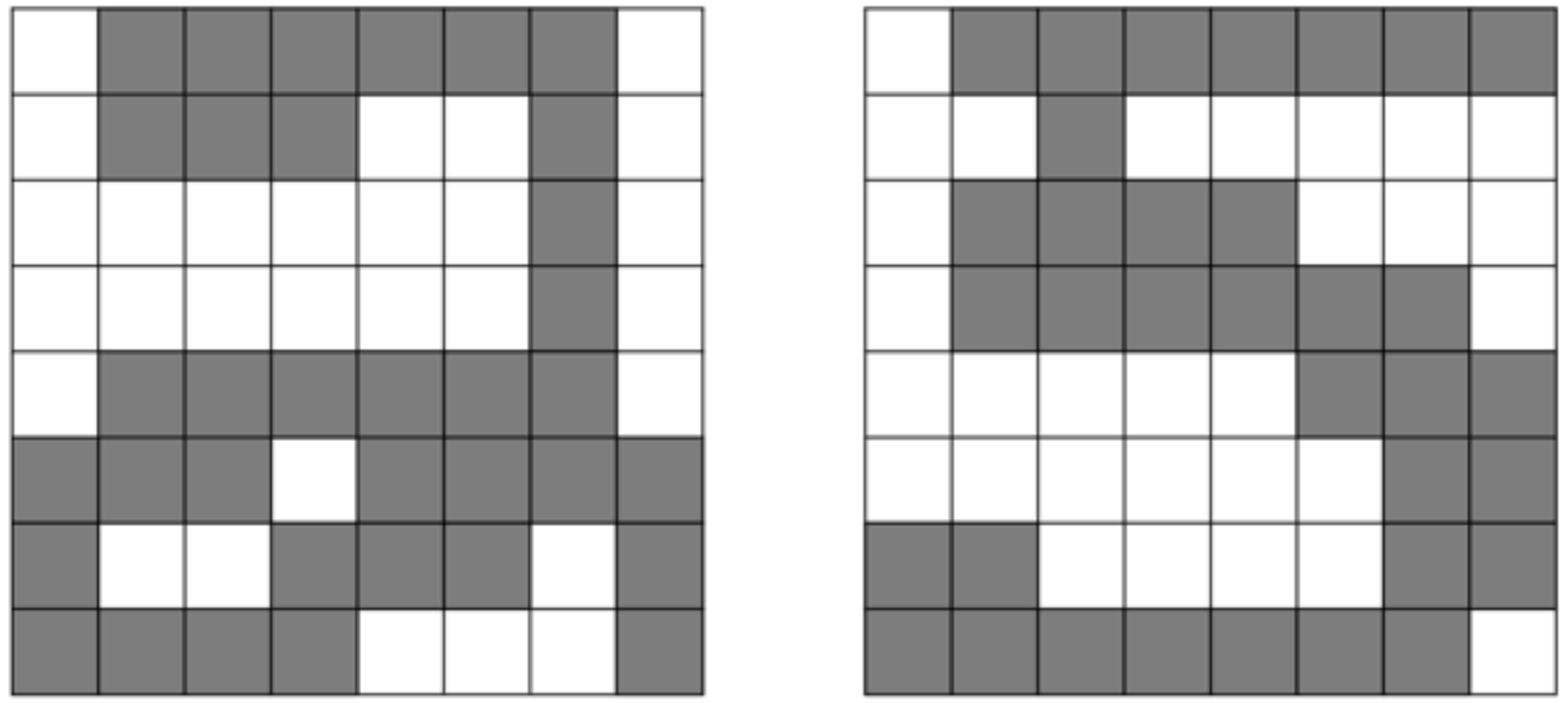


Figure 7: Binary images of handwritten digits: two and five.

	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

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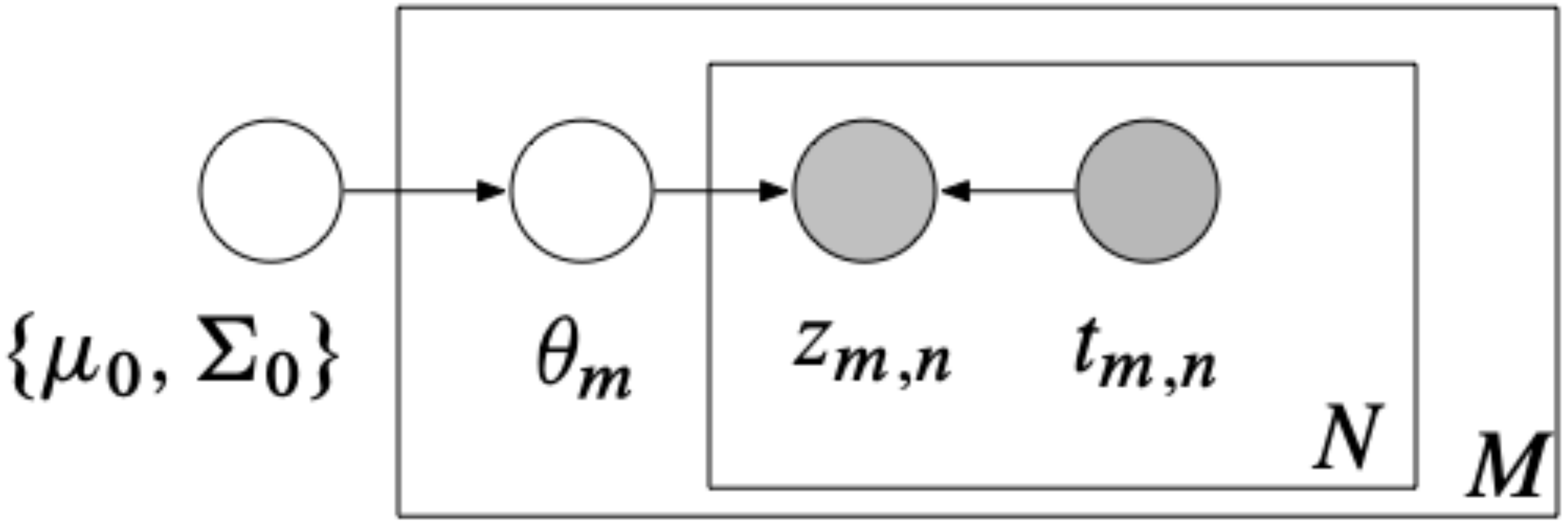

Variational Inference in Nonconjugate Models

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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

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

	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?

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

X the latent variables and Z the observations

A second order information-theoretic model

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

So Which D Should We Choose? Finding Bounds

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

And we know that $\log P(X) = \log \mathbb{E}_O[P(X, O)] = \log \int dP(o) P(X, o)$

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

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

using Jensen's $\log \mathbb{E}_{X\sim Q_\theta}\left[\frac{P(O, X)}{Q_\theta(X)}\right] \geq \mathbb{E}_{X\sim Q_\theta}\left[\log \frac{P(O, X)}{Q_\theta(X)}\right] = \mathscr{L}(\theta)$

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

So Which D and Q Should We Choose?

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

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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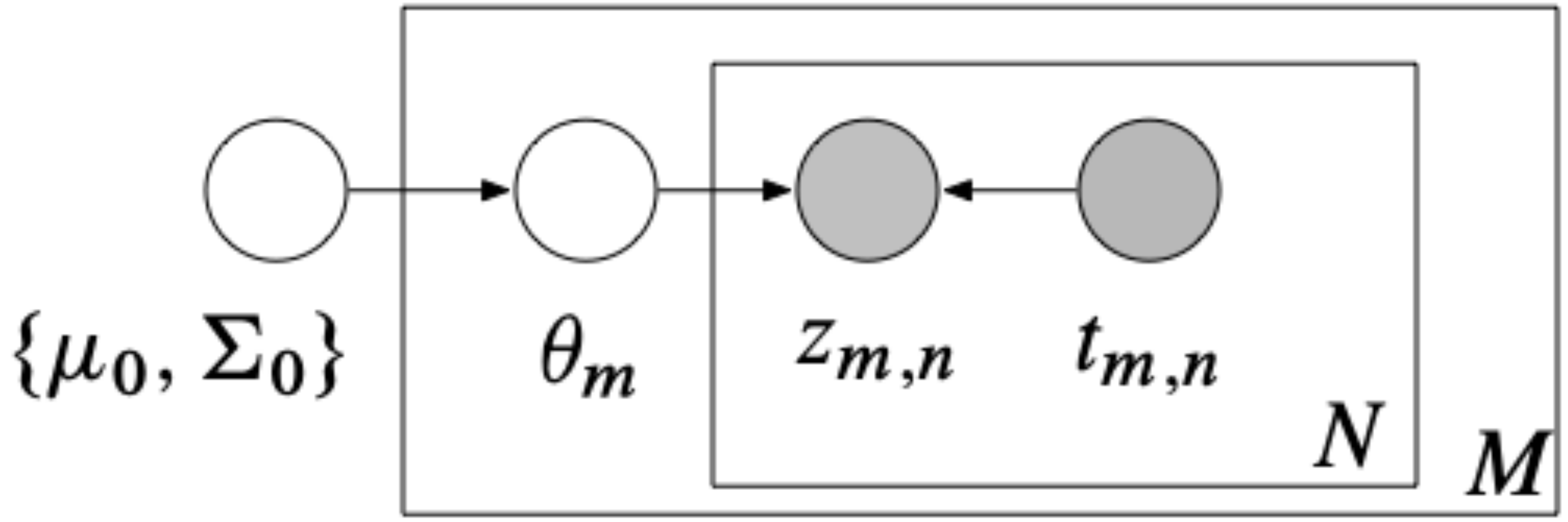

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More General Q_θ

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

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.

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

- Normalised Flows: $Q_\theta(X) \triangleq \phi_\theta(X)$

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

Current Problems in VI

- Scalability
- Amortization
- Preservation of dependencies
- Auto-regressive models

Other Modern Bayesian Techniques

- Variational AutoEncoders
- Likelihood-free Inference