香港科技大學
THE HONG KONG
UNIVERSITY OF SCIENCE
AND TECHNOLOGY

COMP 5212
Machine Learning
Lecture 14

Probabilistic Graphical Models

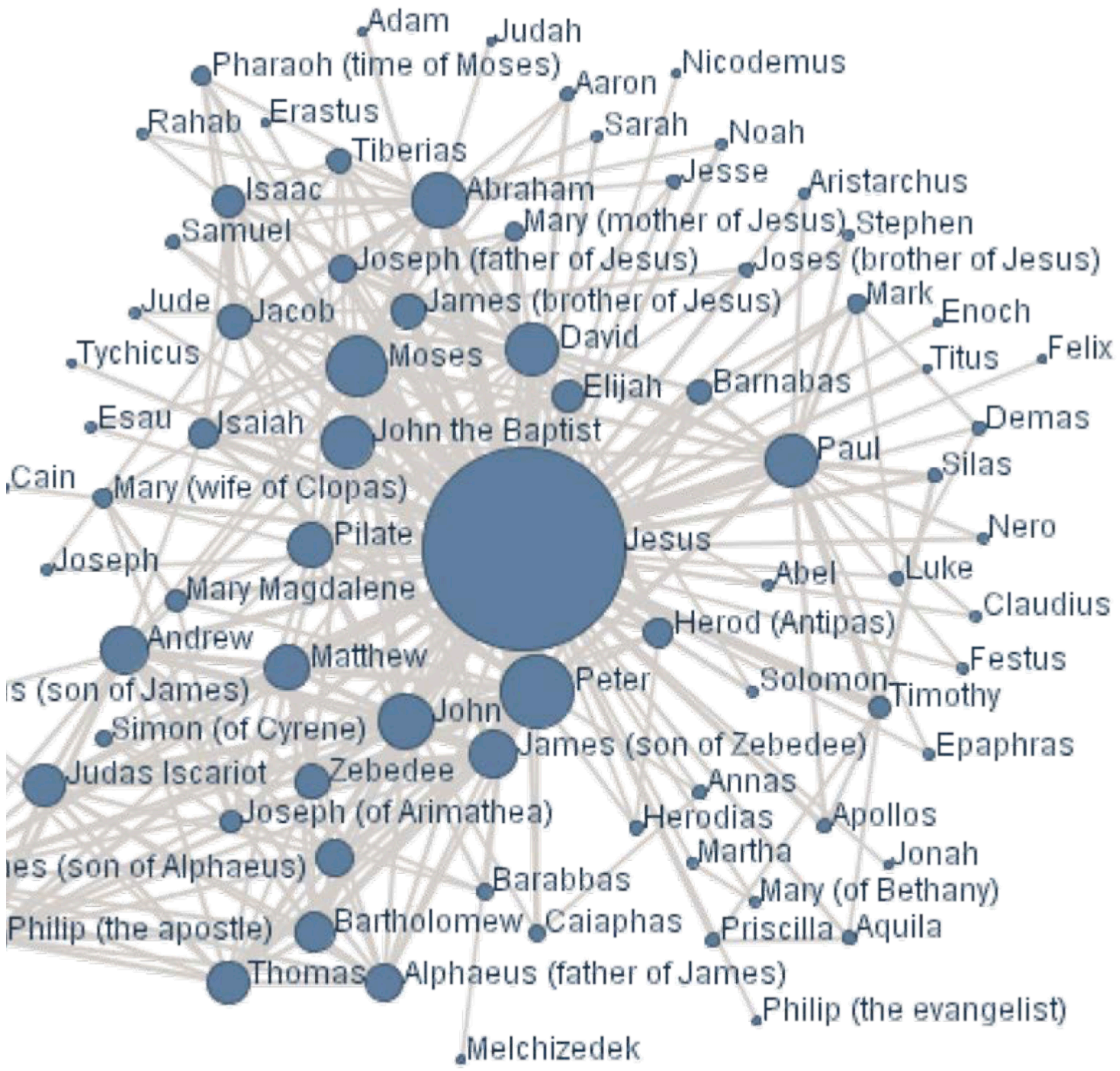
Junxian He
Oct 31, 2024

Some Announcements

- Don’t worry too much on midterm exam, it is only 20%

- We have a makeup lecture on Nov 7, 7pm-820pm, at Room 2303 after we finish HMM. Attendance is not required, zoom recording will be released

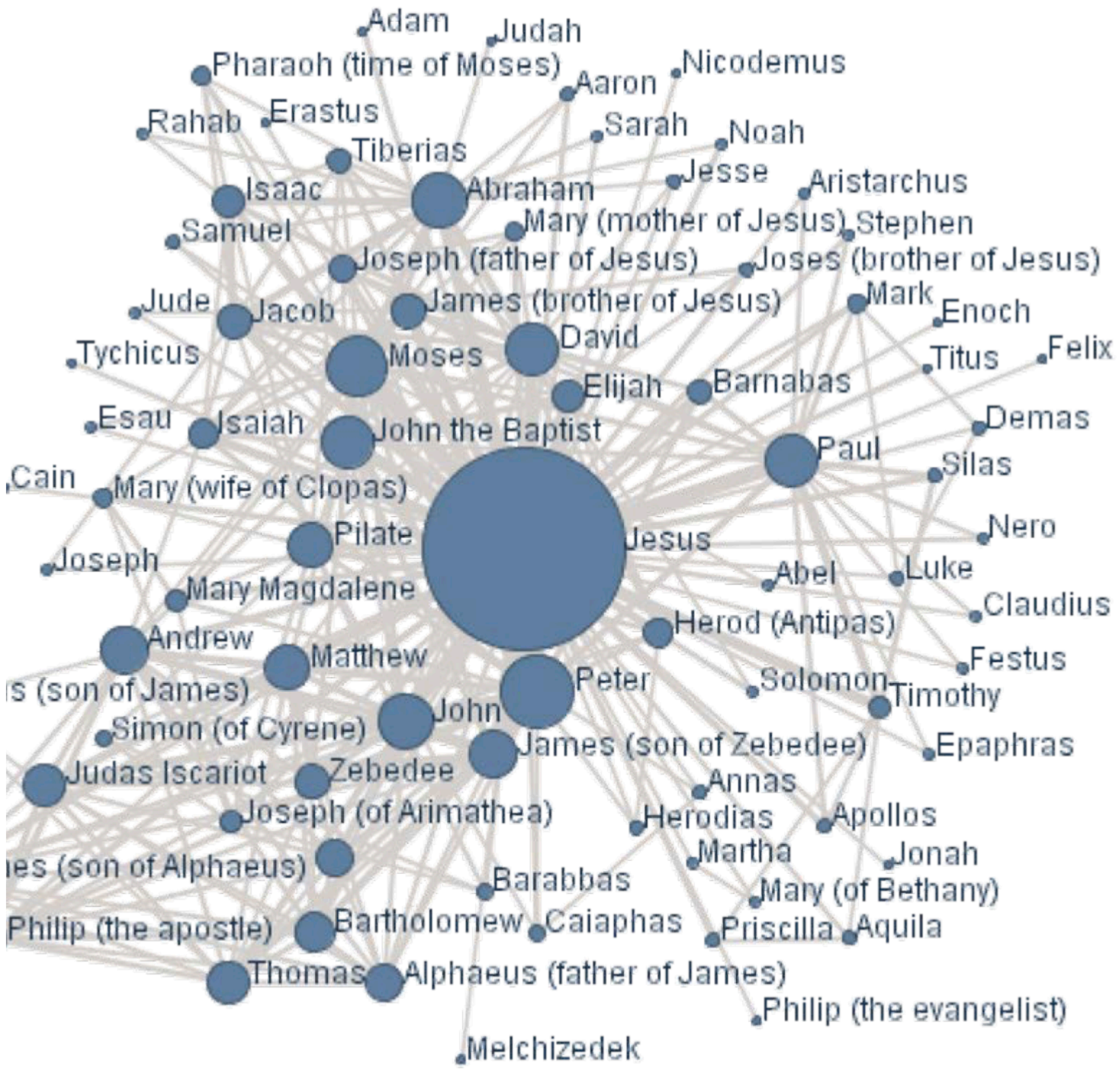
What Are Graphical Models?



What Are Graphical Models?

GNN

- Informally, a GM is just a graph representing relationship among random variables
  - Nodes: random variables (features, not examples)
  - Edges (or absence of edges): relationship



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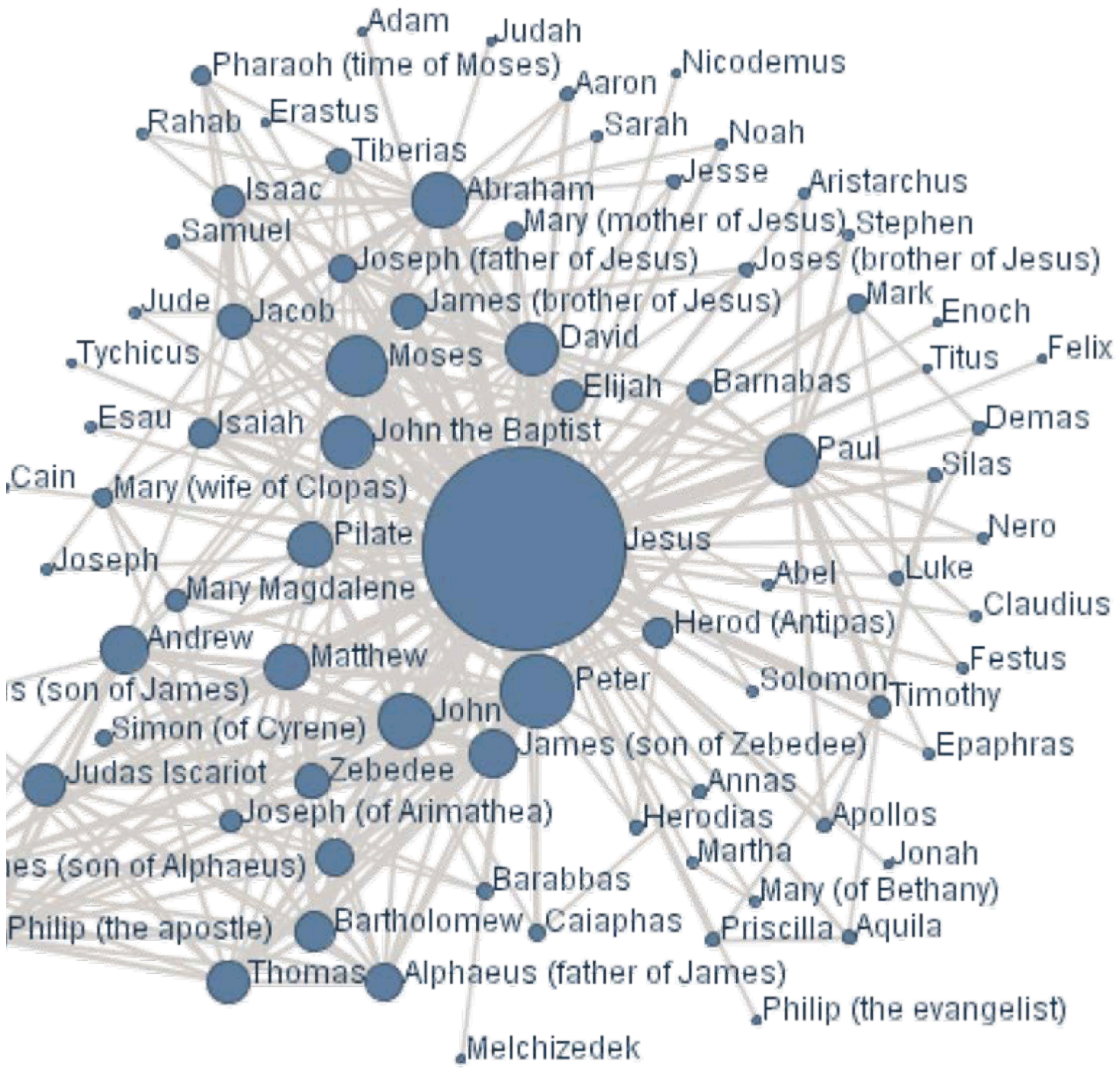

- Looks simple!
  - But detail matters, as always.
  - What exactly do we mean by relationship?

Relationship between two random variables

- Many types of relationships exist:
  - X and Y are correlated
  - X and Y are dependent
  - X and Y are independent
  - X and Y are partially correlated given Z
  - X and Y are conditionally dependent given Z
  - X and Y are conditionally independent given Z
  - X causes Y
  - Y causes X
  - ...

causation

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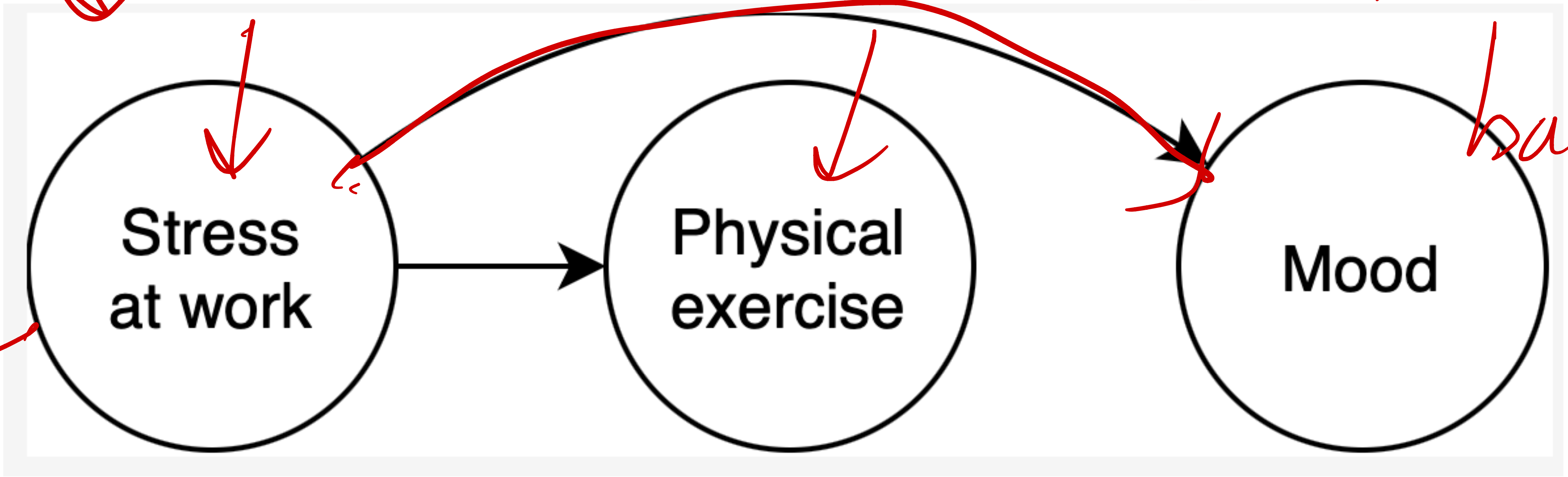
  - ...

X = physical exercise

Y = bad mood

correlated

Correlation does not imply causation



bad

Stress work

physical exercise

What is a Graphical Model?

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Graphical model represents a multivariate distribution in High-D space

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A possible world for celluar signal transduction:

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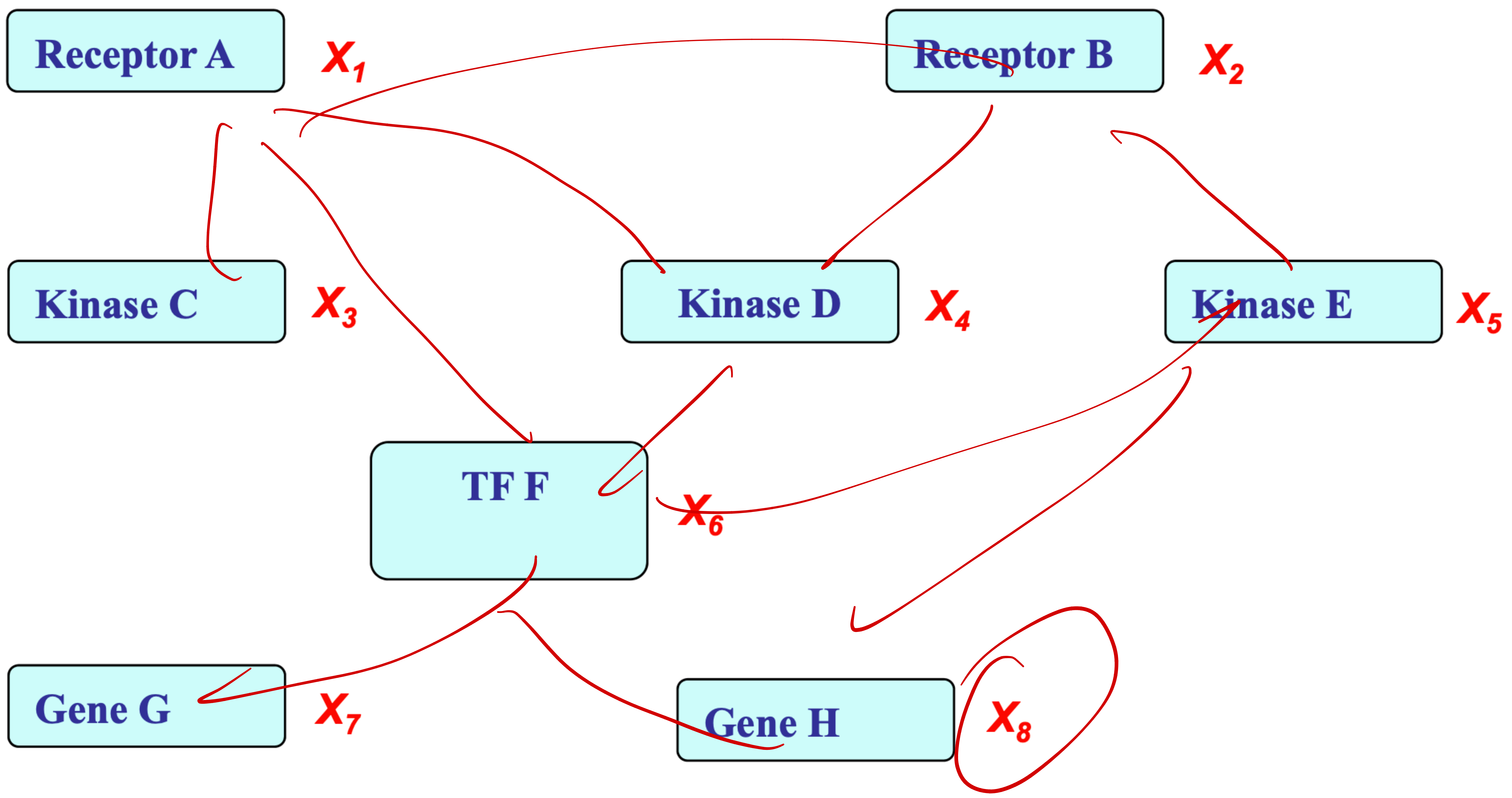
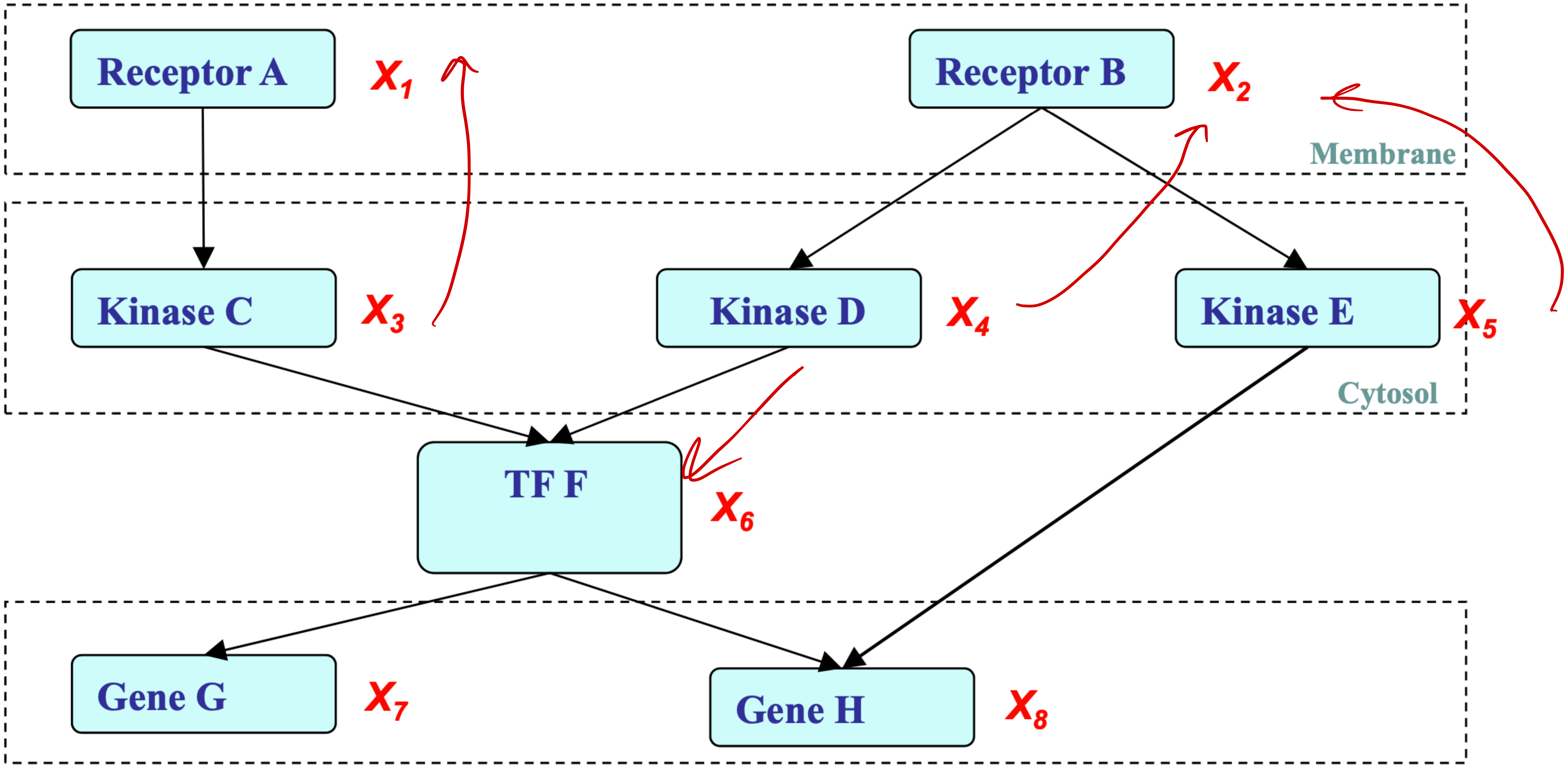


Structure Simplifies Representation

$P(X_1, X_2)$

$P(X_1)$ $P(X_2)$

Dependencies among variables



Probabilistic Graphical Models

Probabilistic Graphical Models

- If X_i's are **conditionally independent** (as described by a **PGM**), the joint can be factored to a product of simpler terms, e.g., naive bayes: $P(x_1, \dots, x_8) = P(x_1) P(x_2) \dots P(x_8)$

Probabilistic Graphical Models

x_i, y

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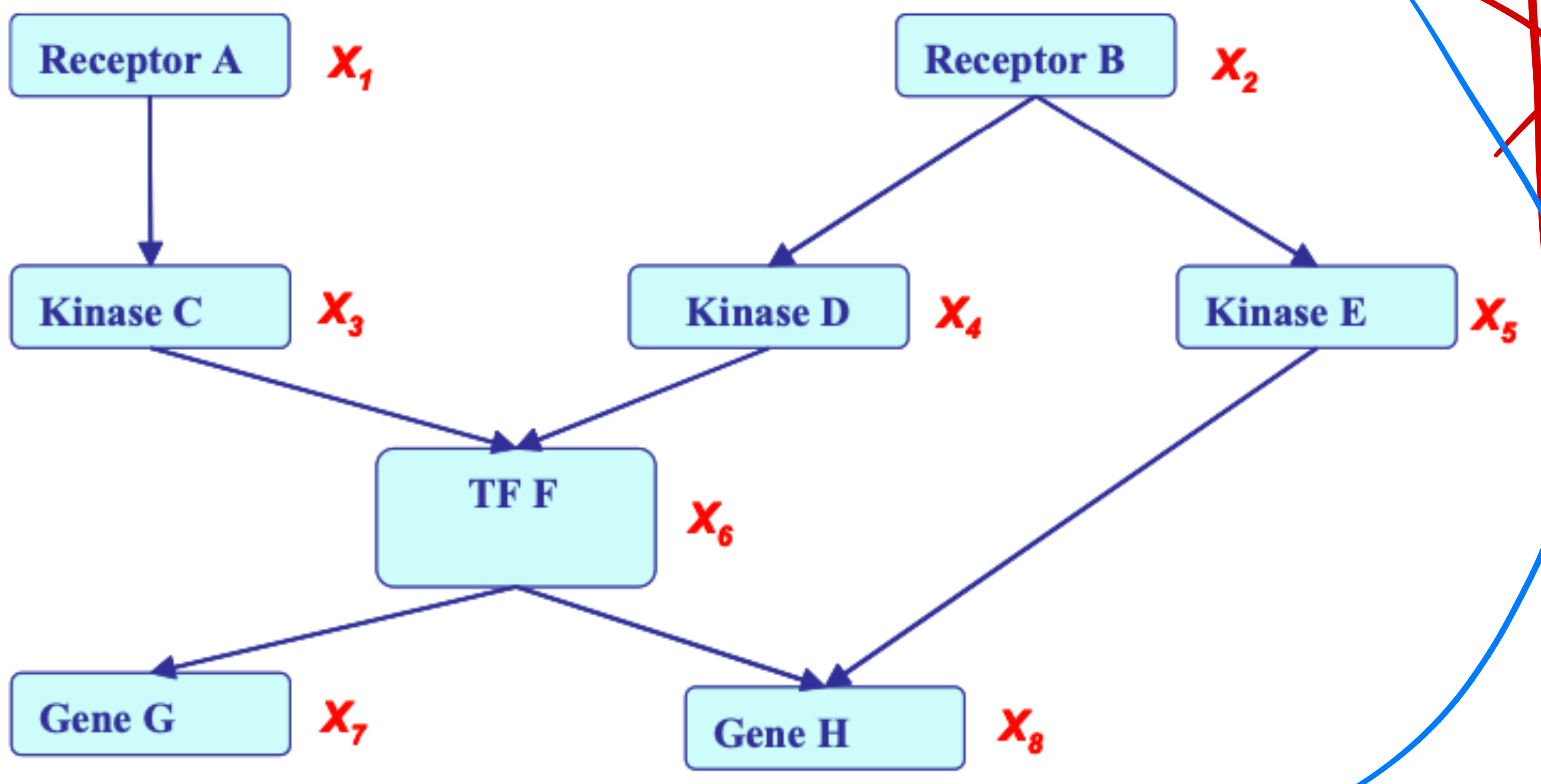


100 →

K^{100}

2^{100}

$$P(X_1, X_2, X_3, X_4, X_5, X_6, X_7, X_8)$$

$$= P(X_1)\, P(X_2)\, P(X_3 | X_1)\, P(X_4 | X_2)\, P(X_5 | X_2)\, P(X_6 | X_3, X_4)\, P(X_7 | X_6)\, P(X_8 | X_5, X_6)$$

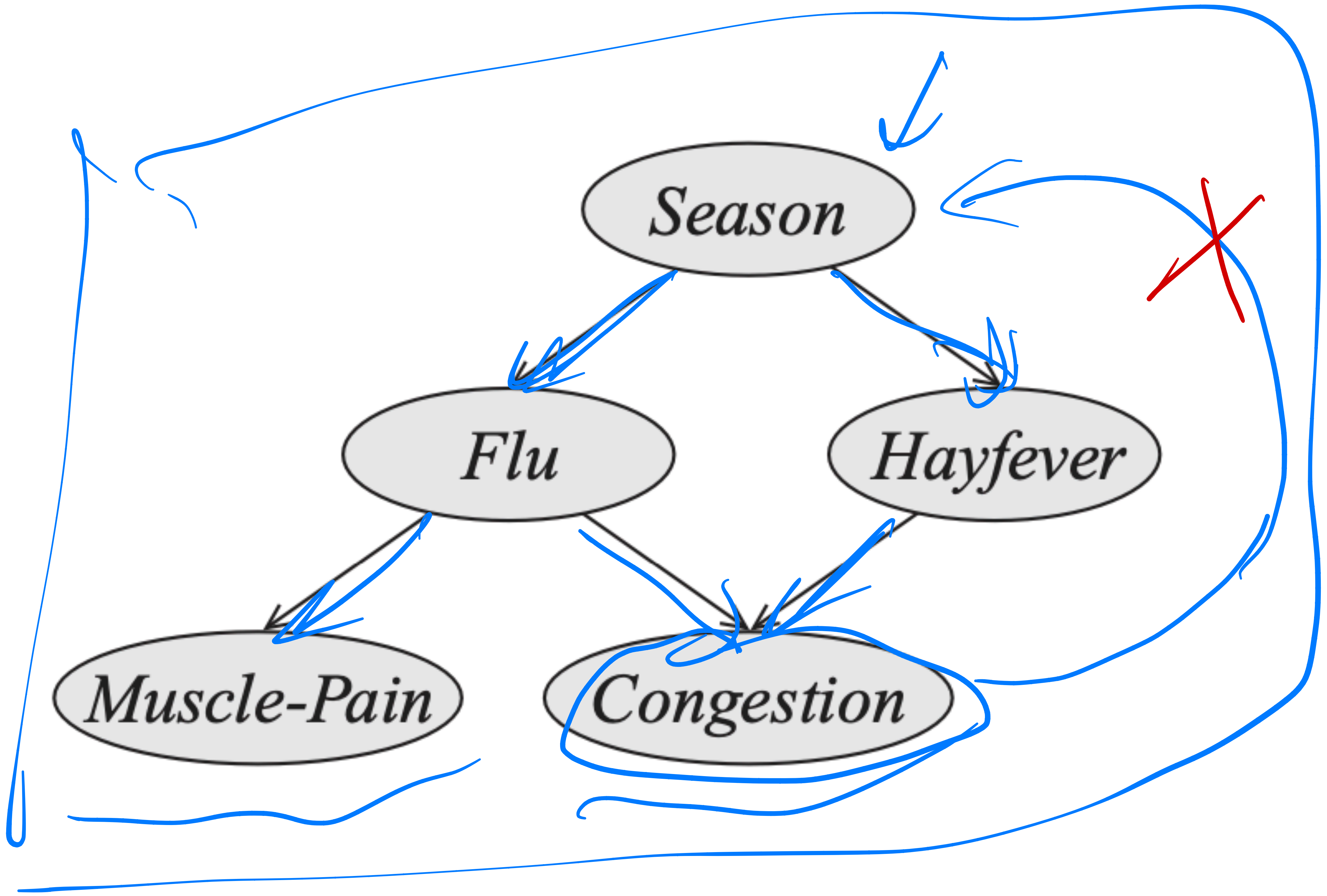
Stay tune for what are these independencies!

$O(K^3)$

$x_i = \{1, \dots, K\}$ $P(x_1, x_2, \dots, x_8) = P(x_1)\, P(x_2 | x_1)\, P(x_3 | x_1, x_2) \dots P(x_8 | x_1, x_2, \dots, x_7)$

K^8 K^{100}

Another Example



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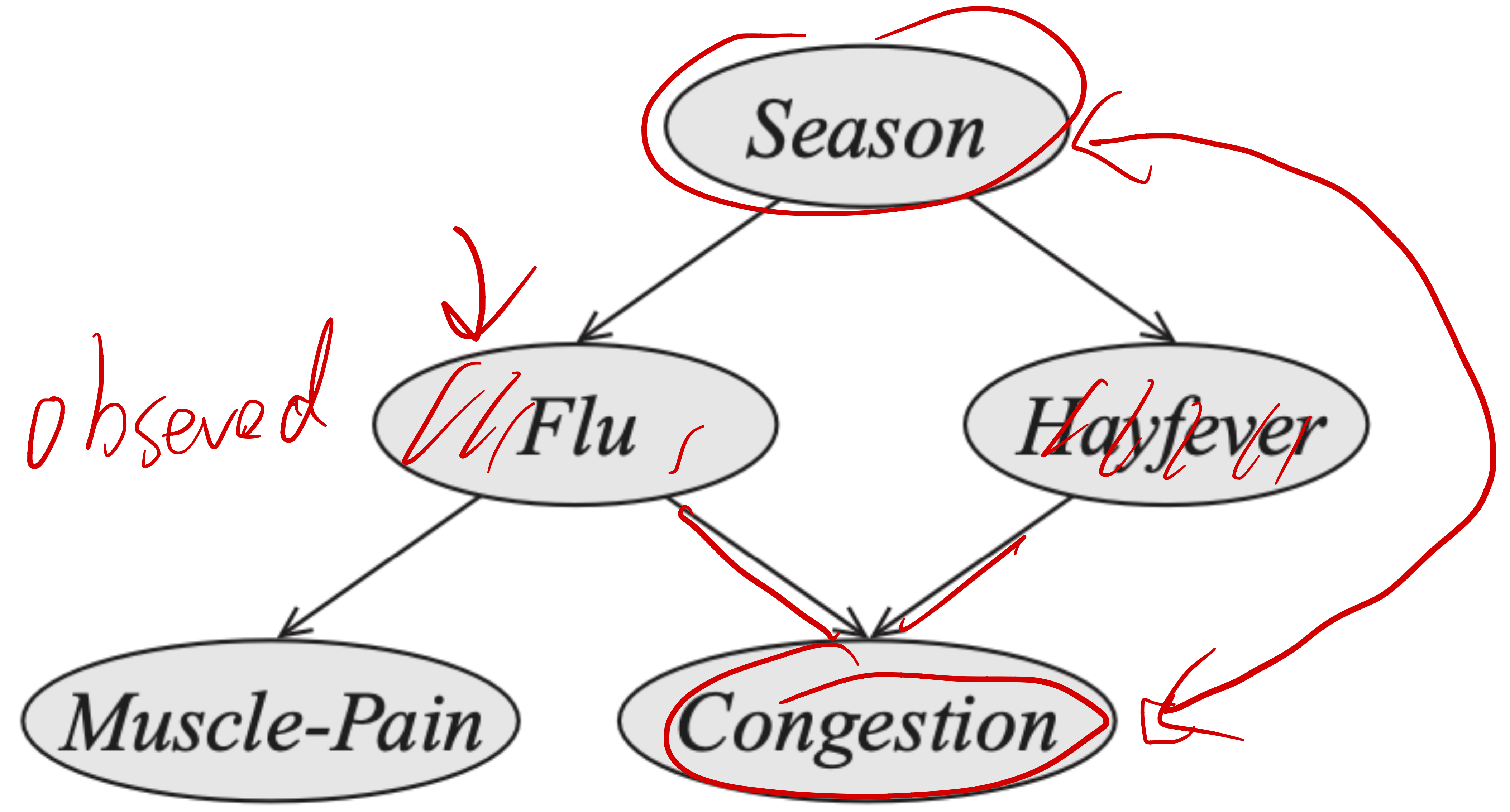

$$P(Congestion \mid Flu, Hayfever, Season) = P(Congestion \mid Flu, Hayfever);$$

What is a PGM After All

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It is a smart way to write/specify/compose/design exponentially-large probability distributions without paying an exponential cost, and at the same time endow the distributions with ***structured semantics***

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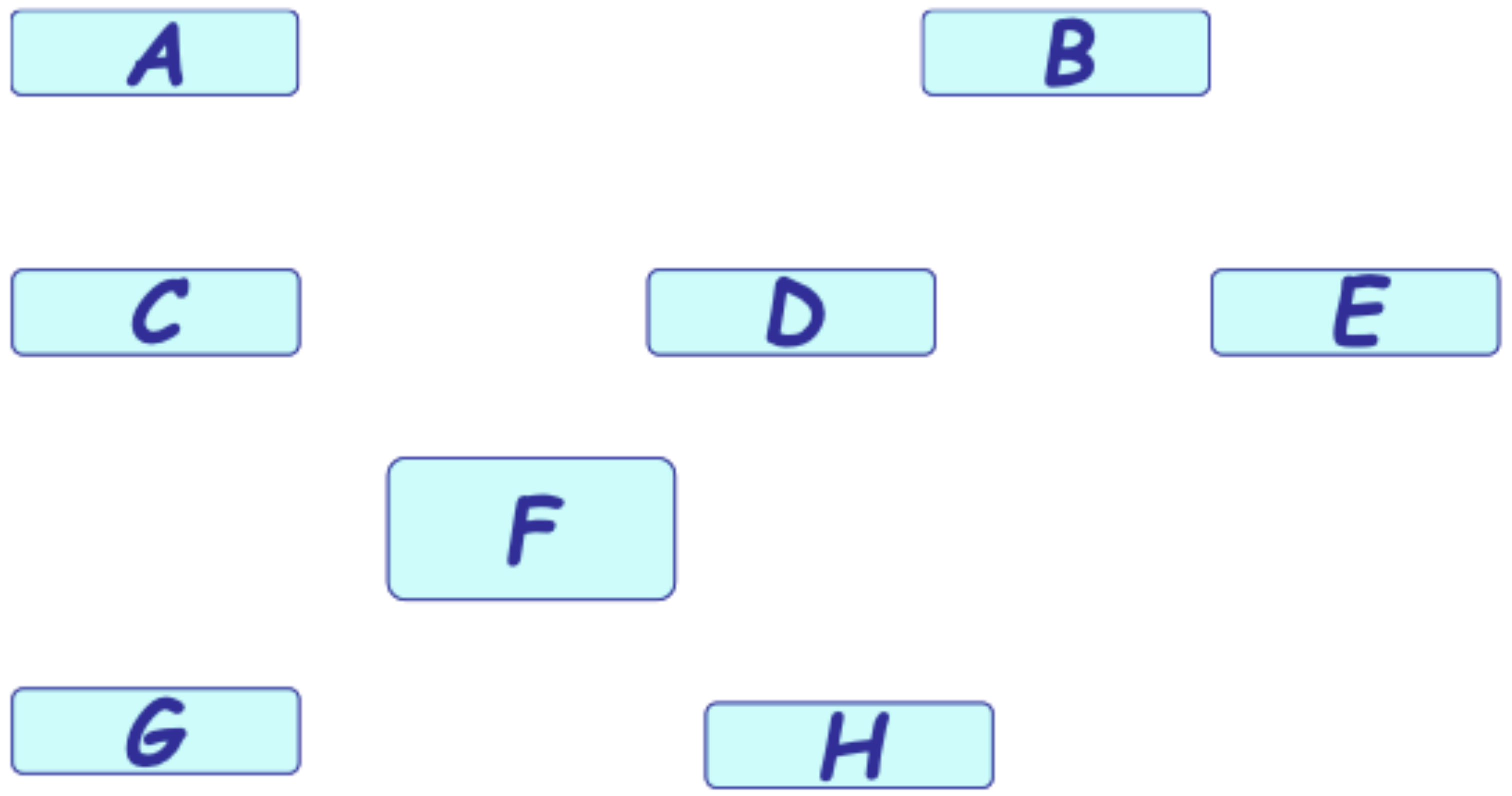

$$P(X_1, X_2, X_3, X_4, X_5, X_6, X_7, X_8)$$

$O(k^8)$

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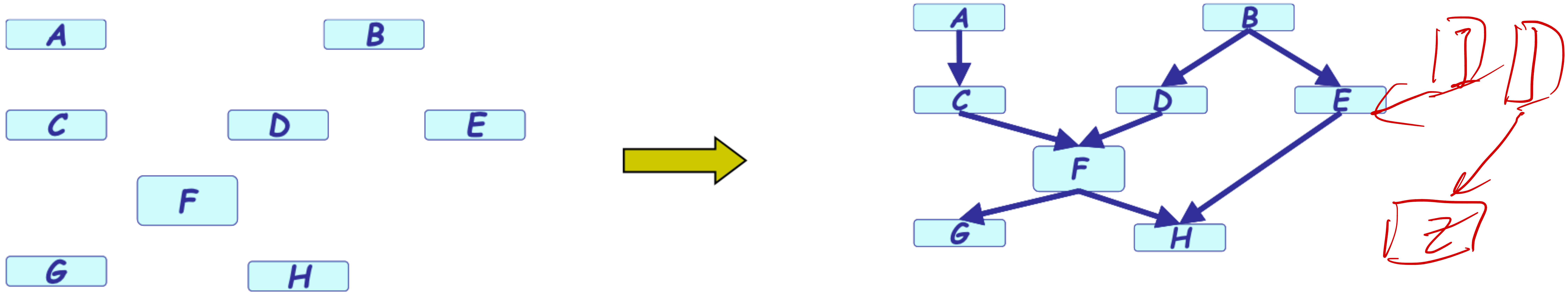

$$P(X_1, X_2, X_3, X_4, X_5, X_6, X_7, X_8)$$

$$P(X_{1:8}) = P(X_1)P(X_2)P(X_3 \mid X_1 X_2)P(X_4 \mid X_2)P(X_5 \mid X_2)$$
$$P(X_6 \mid X_3, X_4)P(X_7 \mid X_6)P(X_8 \mid X_5, X_6)$$

$O(K^8)$ $\longrightarrow$ $O(K^3)$

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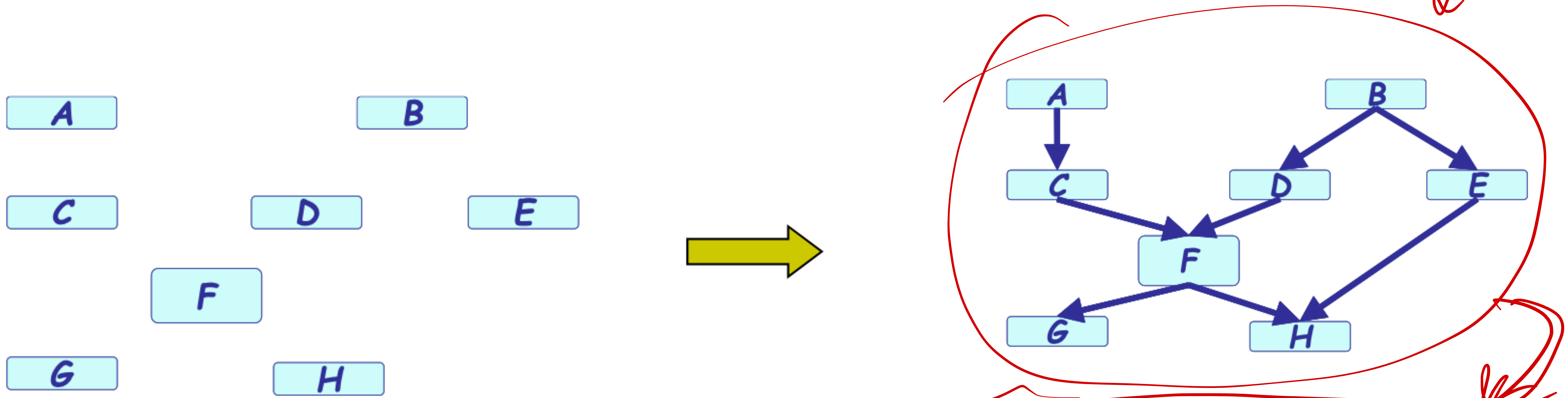

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More formal definition: It refers to a family of distributions on a set of random variables that are compatible with all the probabilistic independence propositions encoded by a graph that connects these variables

$x_1 \perp x_2$ given x_4, x_5

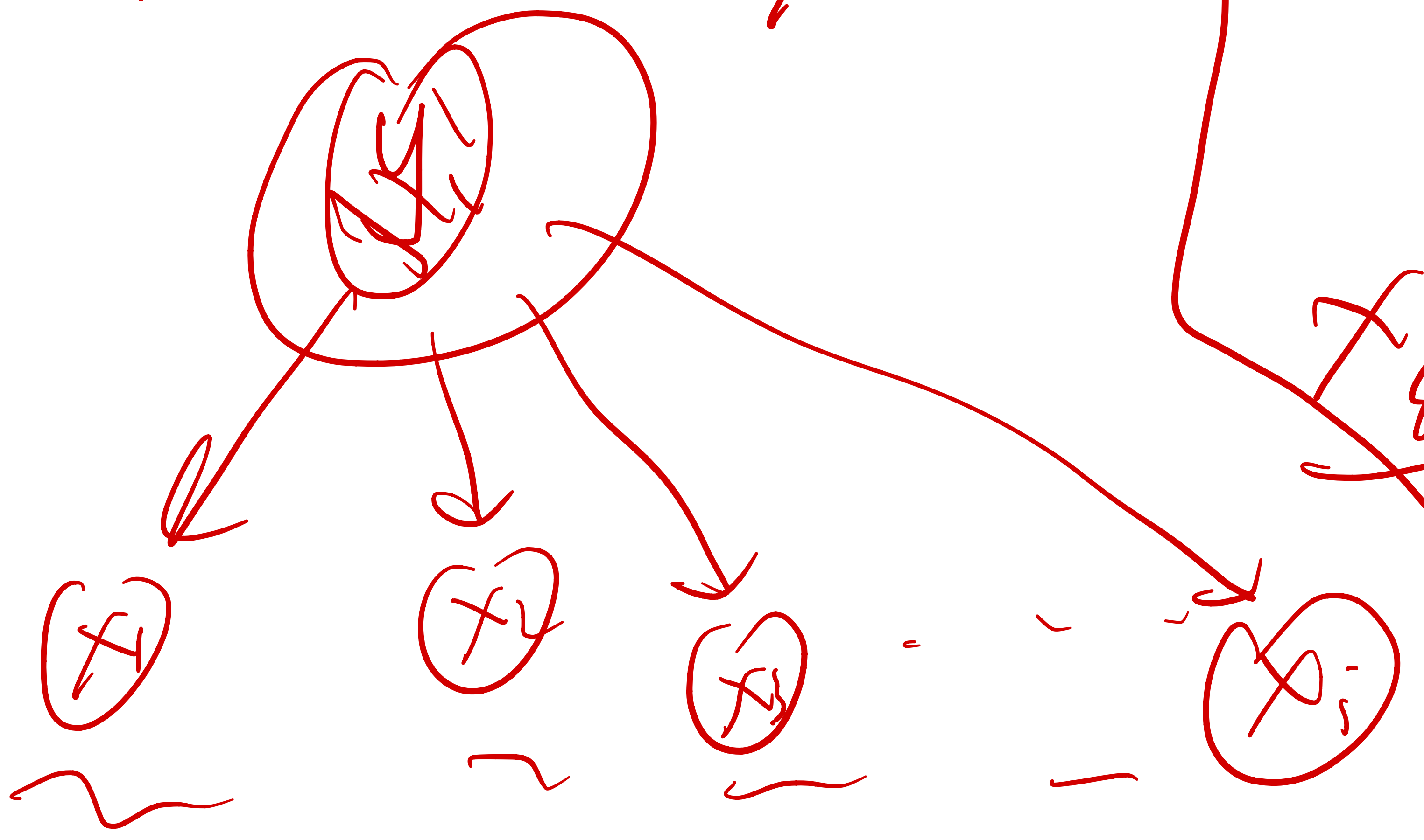
$x_3 \perp x_4$ given x_8

Probabilistic Graphical Model is a graphical language to express conditional independence

naive bayes:

y

Naive bayes



x_8

$x_i \perp x_j$ given y

$x_1, x_2 \cdots x_3$

Two types of Graphical Models

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- Directed edges give causality relationships (**Bayesian Network** or **Directed Graphical Model**): DGM

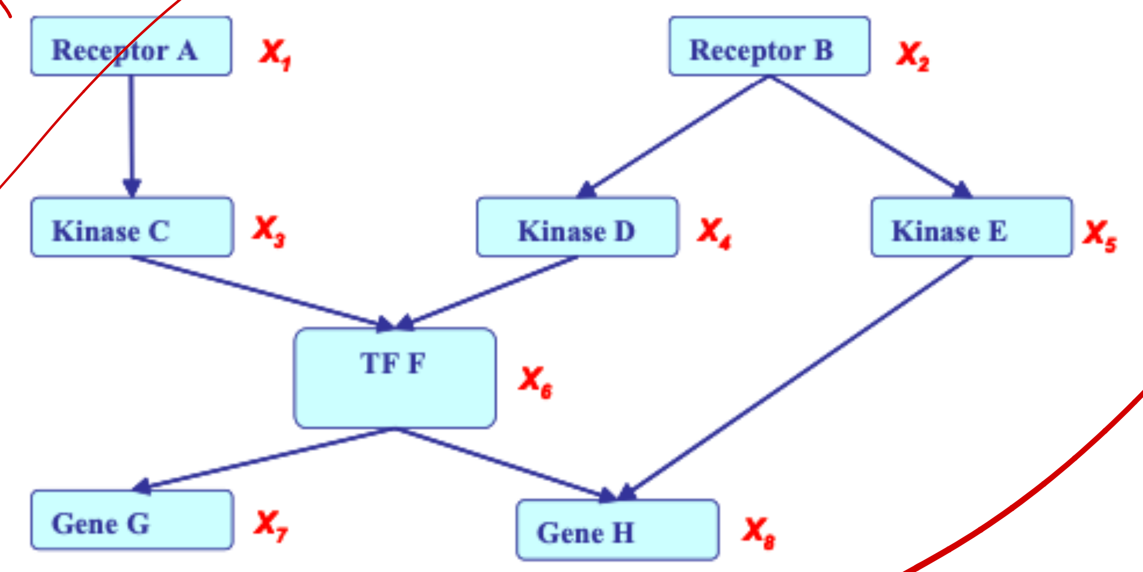
Two types of Graphical Models

DGM

VAE diffusion

- Directed edges give causality relationships (**Bayesian Network** or **Directed Graphical Model**):

DGM



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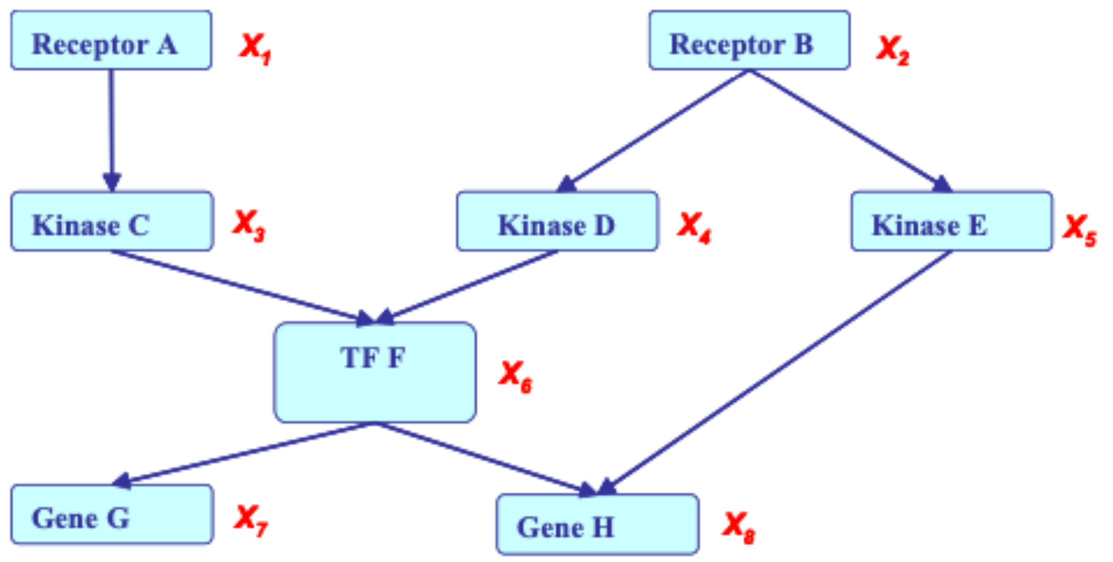

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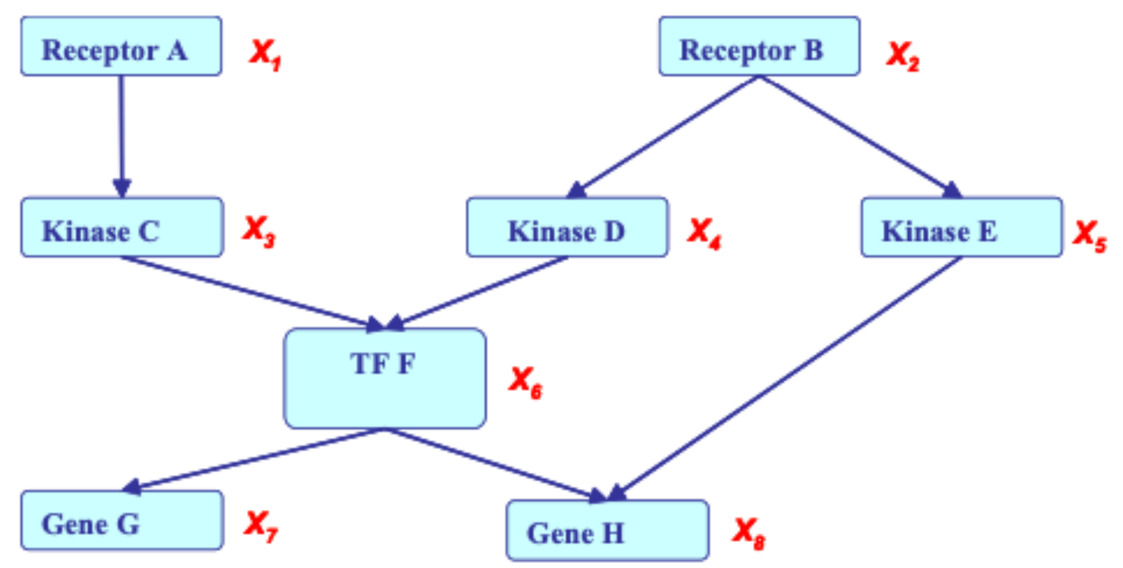

- Undirected edges simply give correlations between variables (**Markov Random Field** or **Undirected Graphical model**):

MRF

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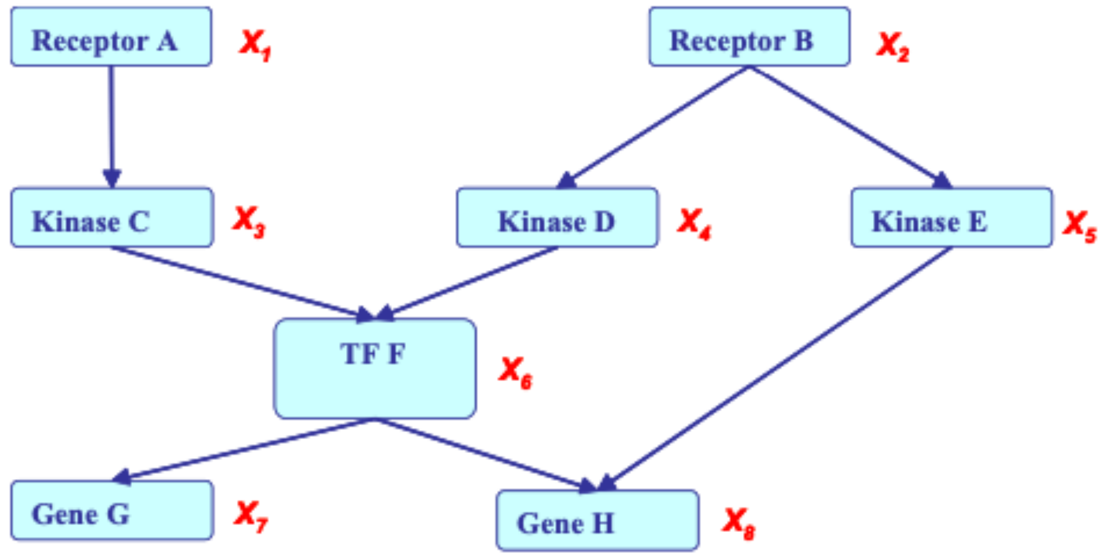

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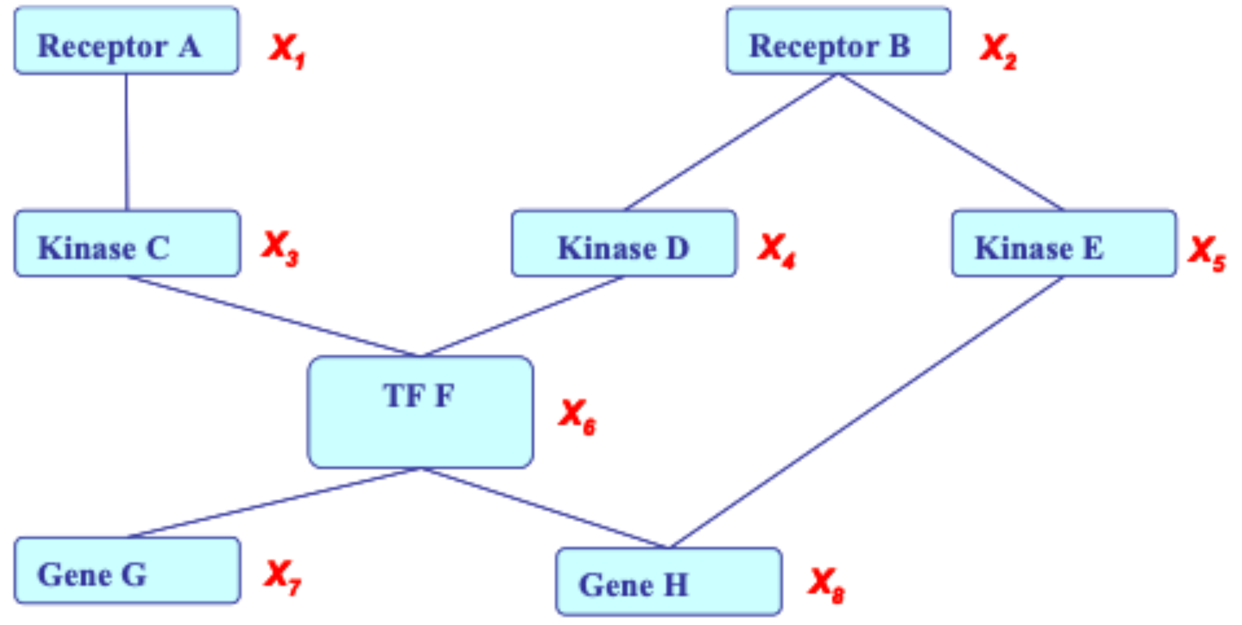

Two types of Graphical Models

locally normalized

$P(x_1, \ldots, x_8) = P(x_1)\, P(x_2|x_1)\, P(x_3|x_1,x_2) \ldots$

- **Directed edges** give **causality** relationships (**Bayesian Network** or **Directed Graphical Model**):

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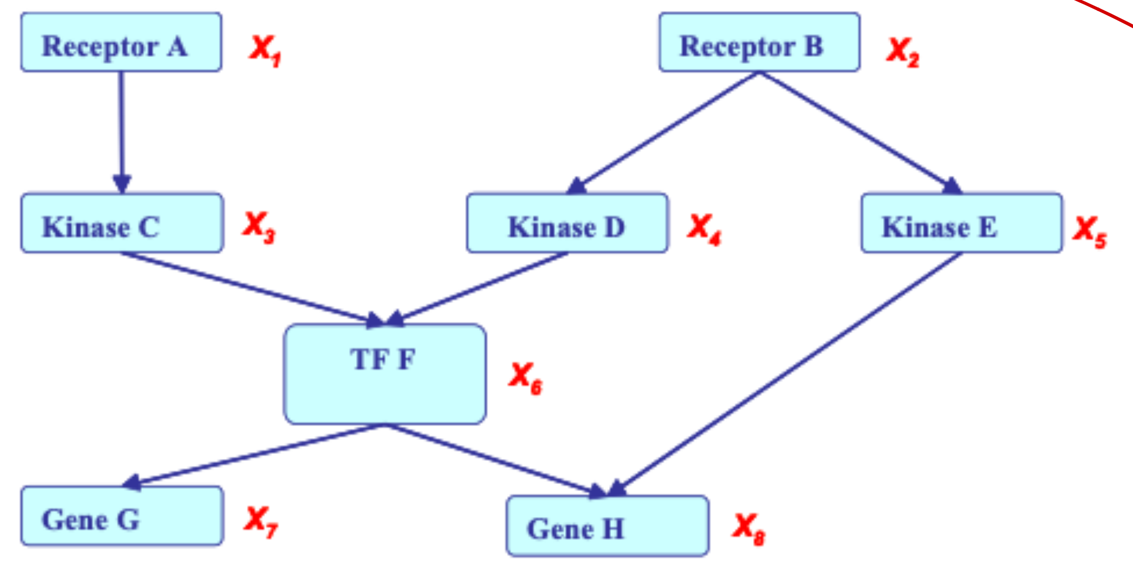
normalized

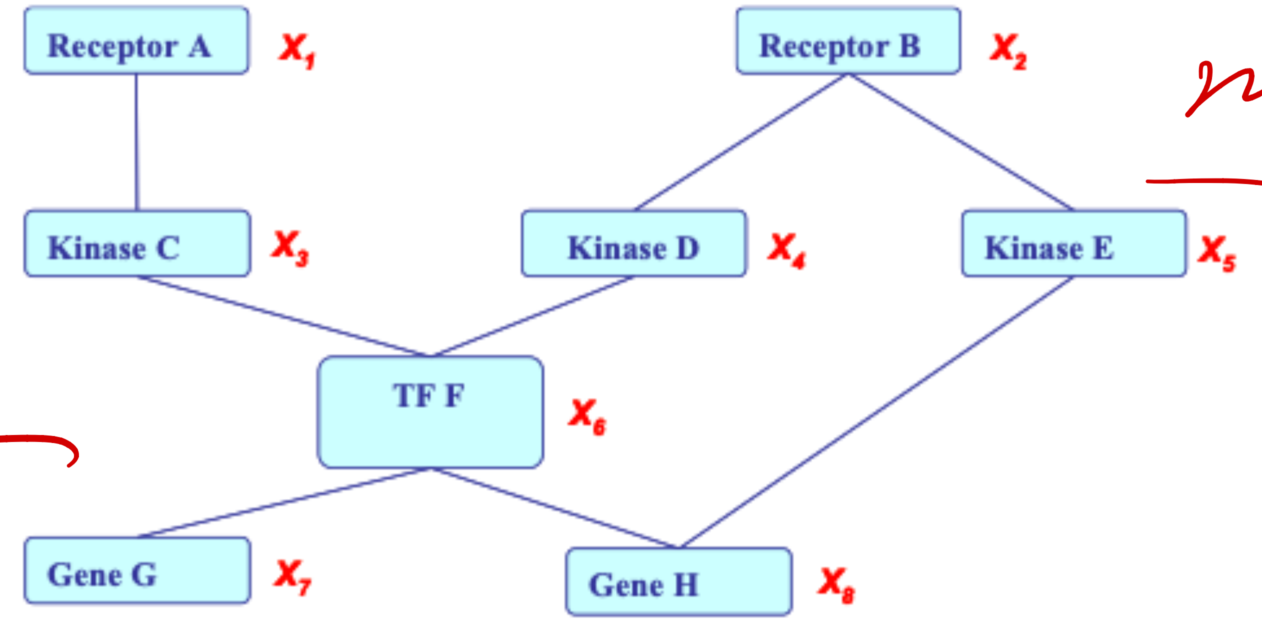


- **Undirected edges** simply give **correlations** between variables (**Markov Random Field** or **Undirected Graphical model**):

globally normalized models

energy

$$P(X_1, X_2, X_3, X_4, X_5, X_6, X_7, X_8)$$
$$= 1/Z \exp\{E(X_1)+E(X_2)+E(X_3, X_1)+E(X_4, X_2)+E(X_5, X_2) + E(X_6, X_3, X_4)+E(X_7, X_6)+E(X_8, X_5, X_6)\}$$



$Z = ?$

energy-based model

PGMs are Structural Specification of Probability Distribution

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- Separation properties in the graph imply independence properties about the associated variables

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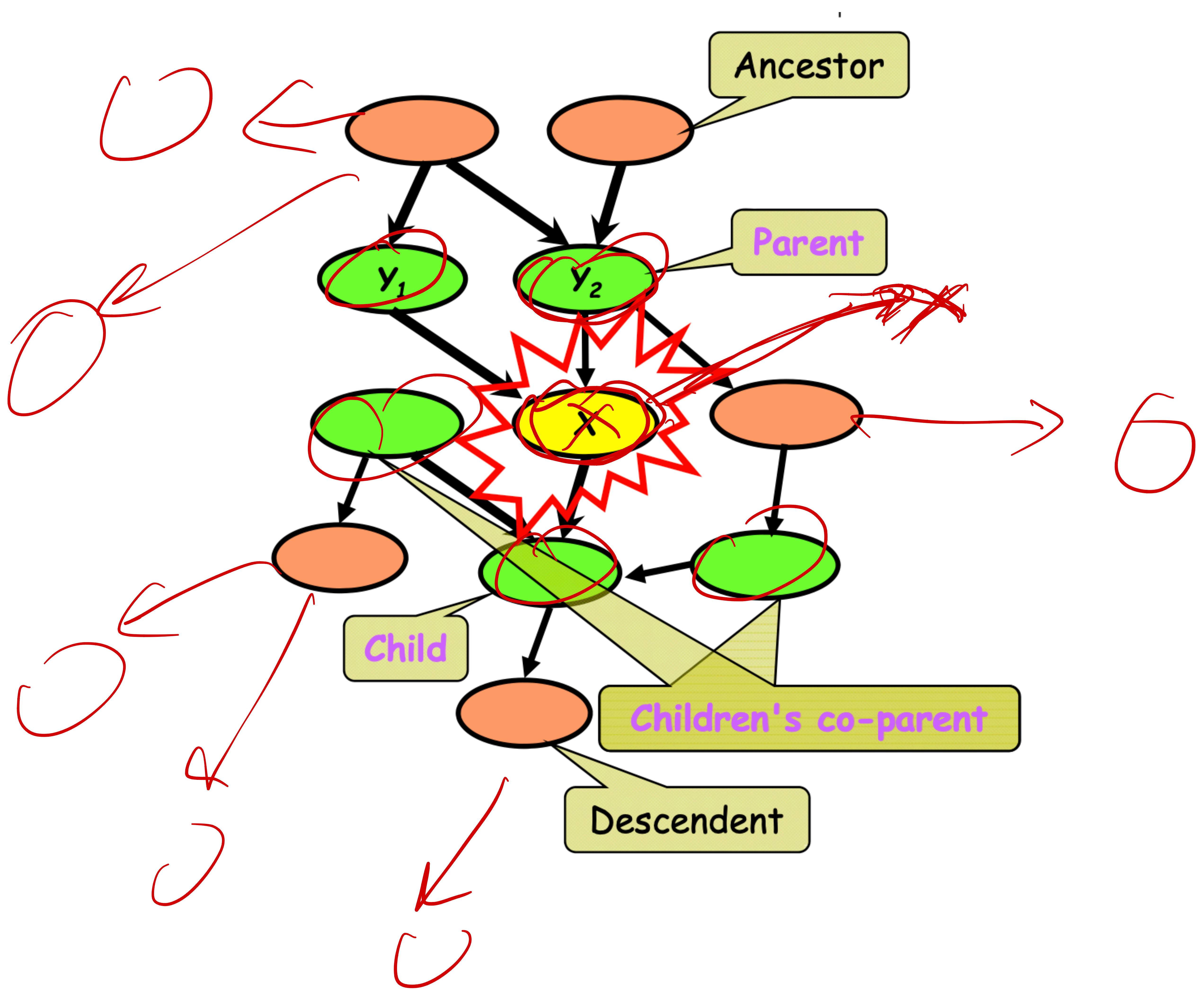
- Separation properties in the graph imply independence properties about the associated variables

- For the graph to be useful, any conditional independence properties we can derive from the graph should hold for the probability distribution that the graph represents

Markov Blanket for Directed Acyclic Graph (DAG)

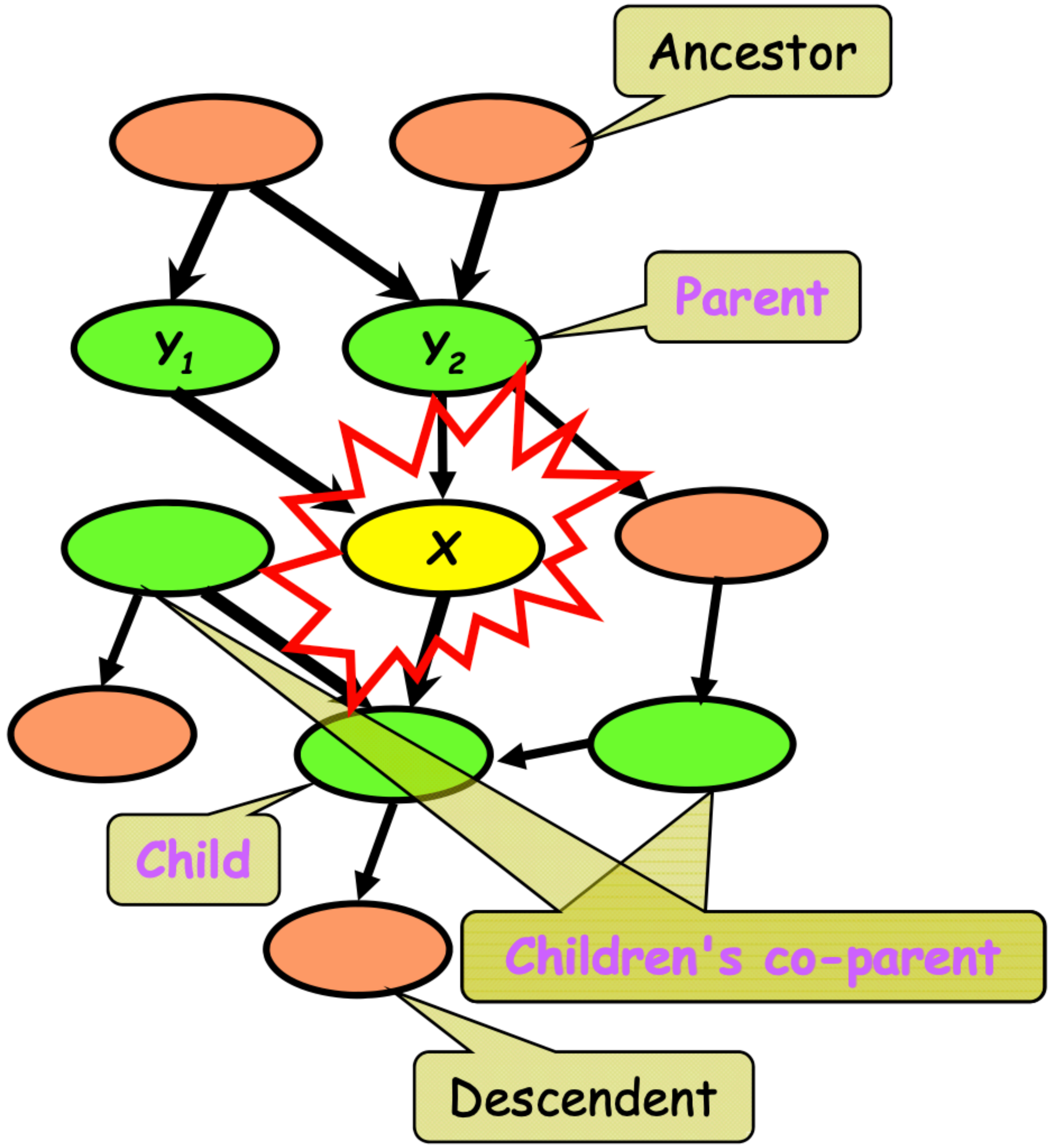
no ~~cycle~~ cycle

Markov Blanket for Directed Acyclic Graph (DAG)



Markov Blanket for Directed Acyclic Graph (DAG)

- Meaning: a node is **conditionally independent** of every other node in the network outside its **Markov blanket**



Markov Blanket for Directed Acyclic Graph (DAG)

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Struct

given z

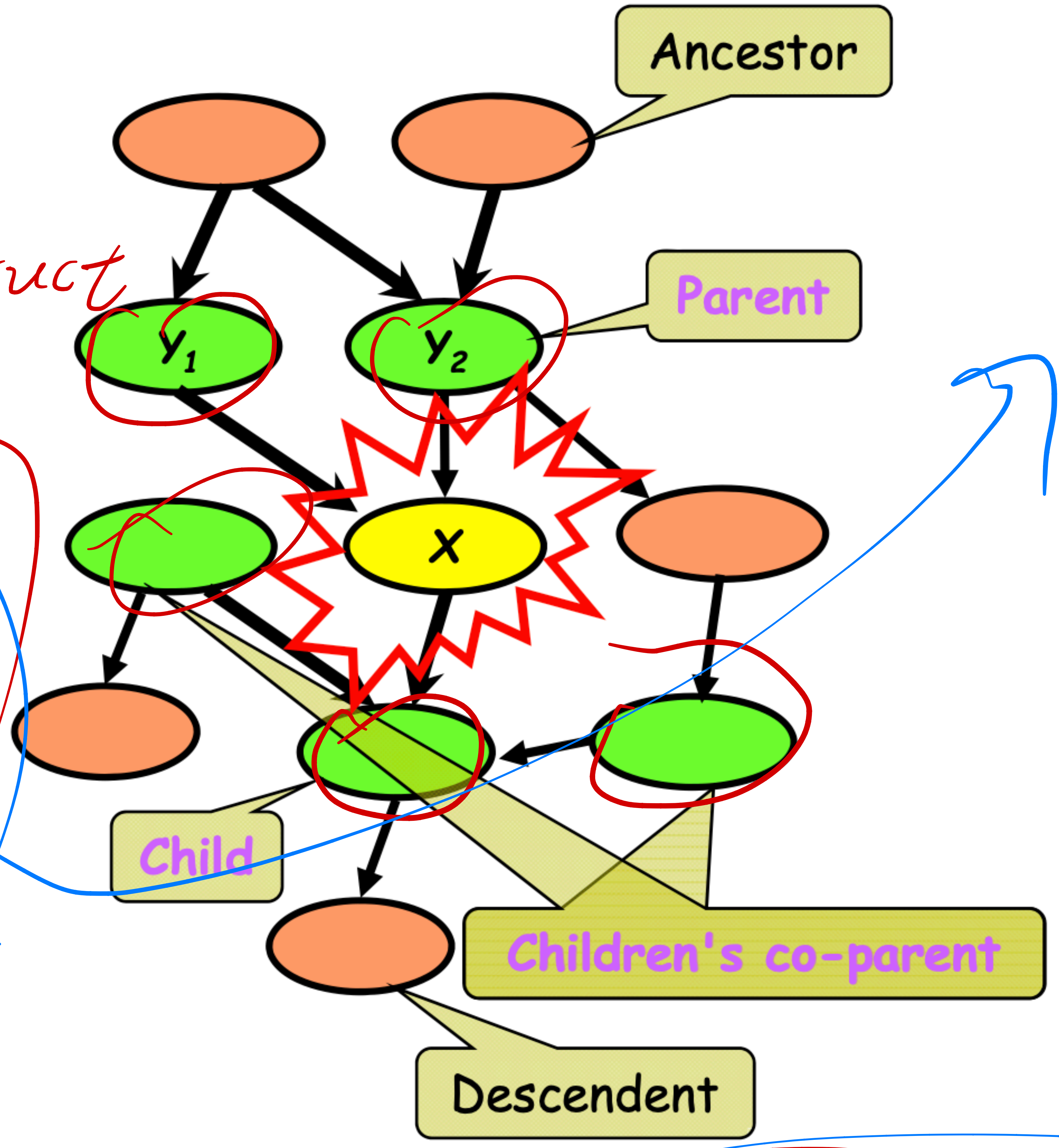
⊥ y

flu

hayfever

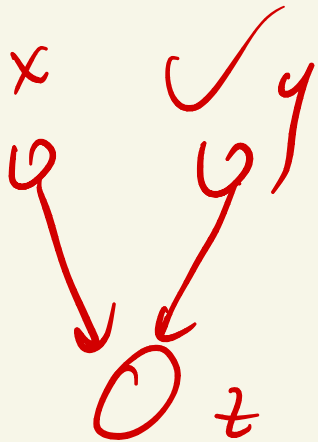
congestion

observed



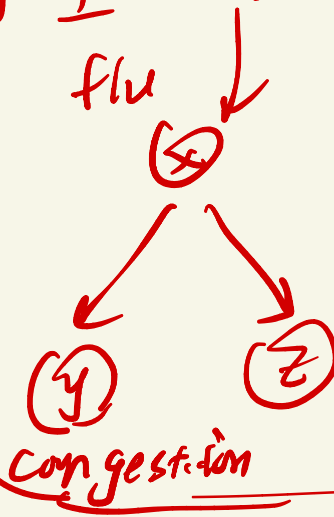
Markov blanket of a node is its parents + child + children’s co-parent

$x \not\perp y$ given z



common effect

given x. $y \perp z$?



$y \perp z$ given x

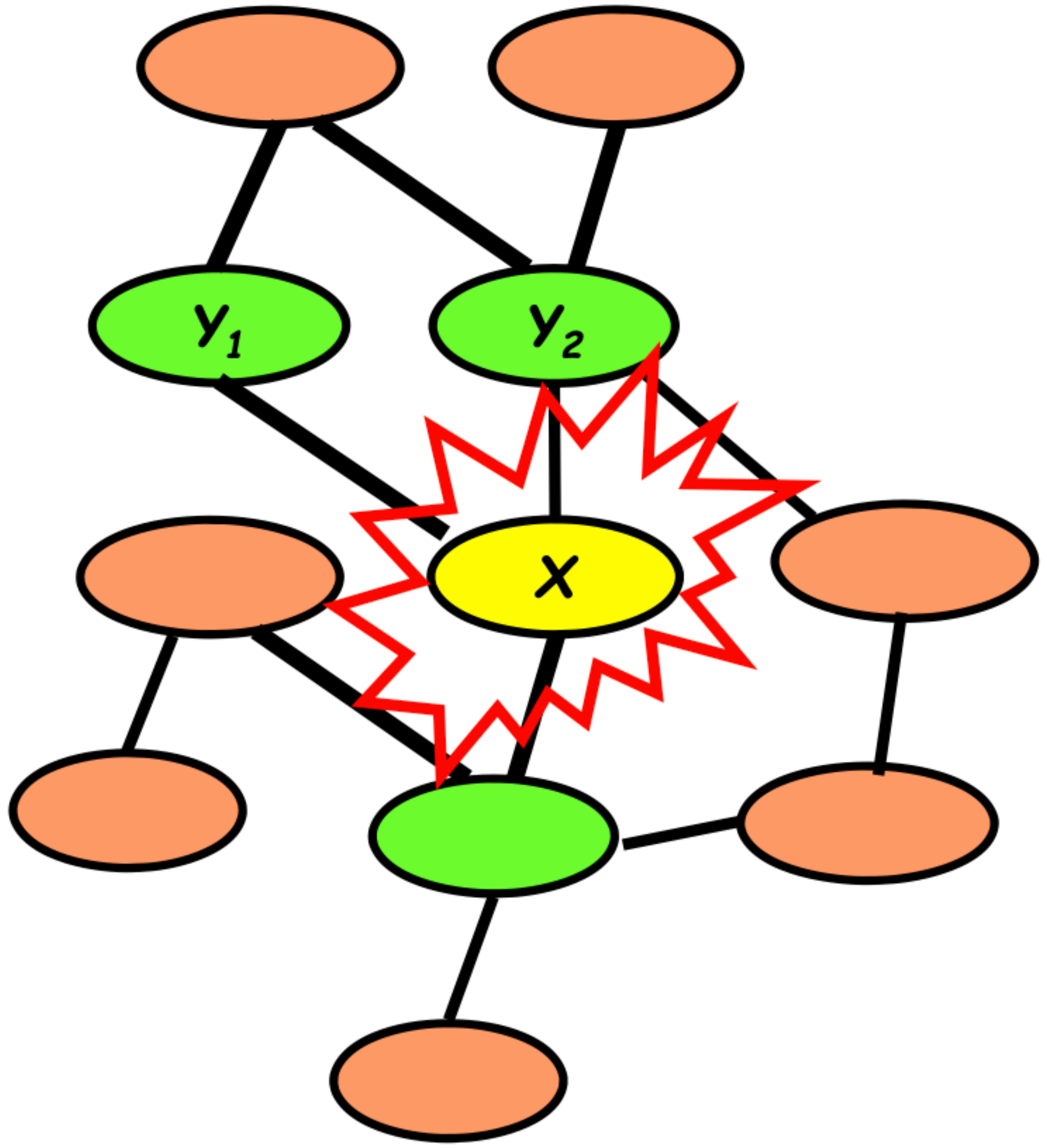
common cause

x is correlated with y given z

NN ← ?

Conditional Independence of Undirected Graph

- Meaning: a node is **conditionally independent** of every other node in the network given its **Directed neighbors**



GMs are your old friends

Probabilistic Graphical Model is a language to express distributions

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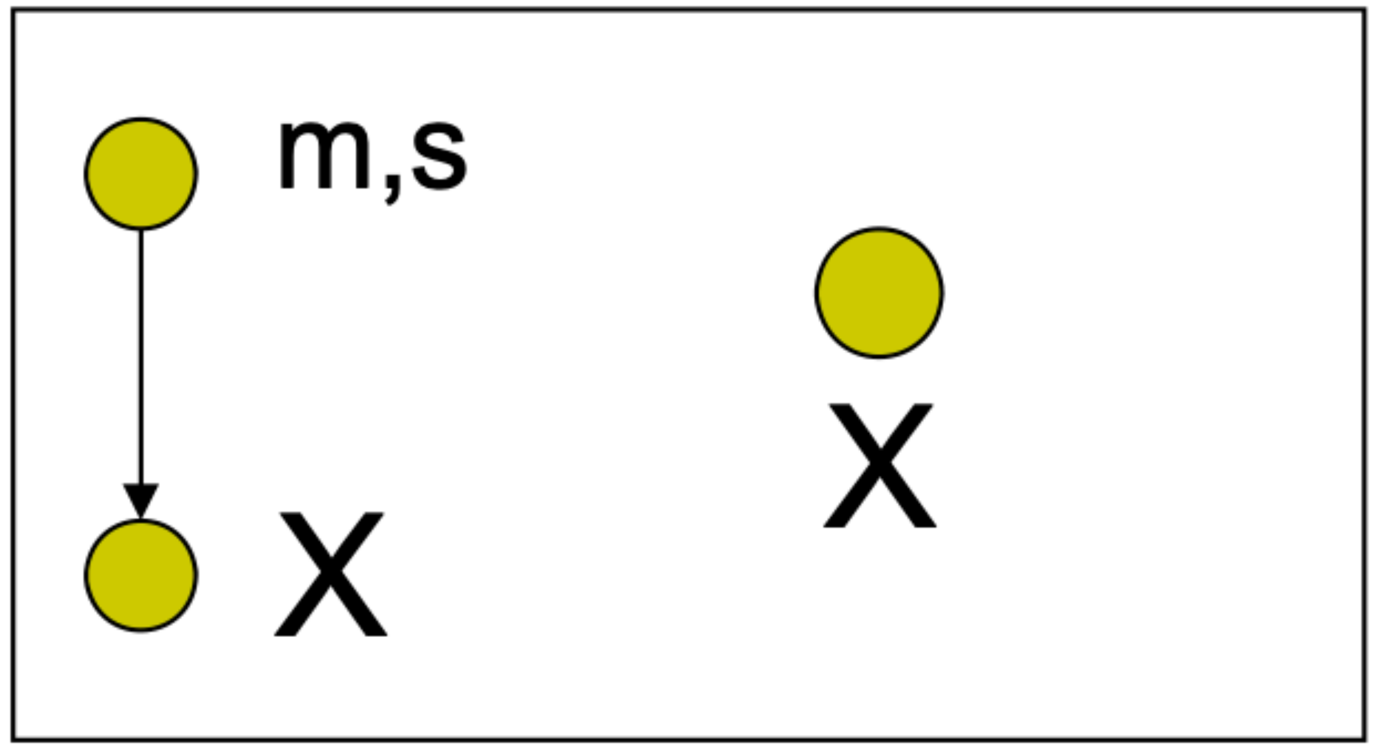

P(x)

p(x)

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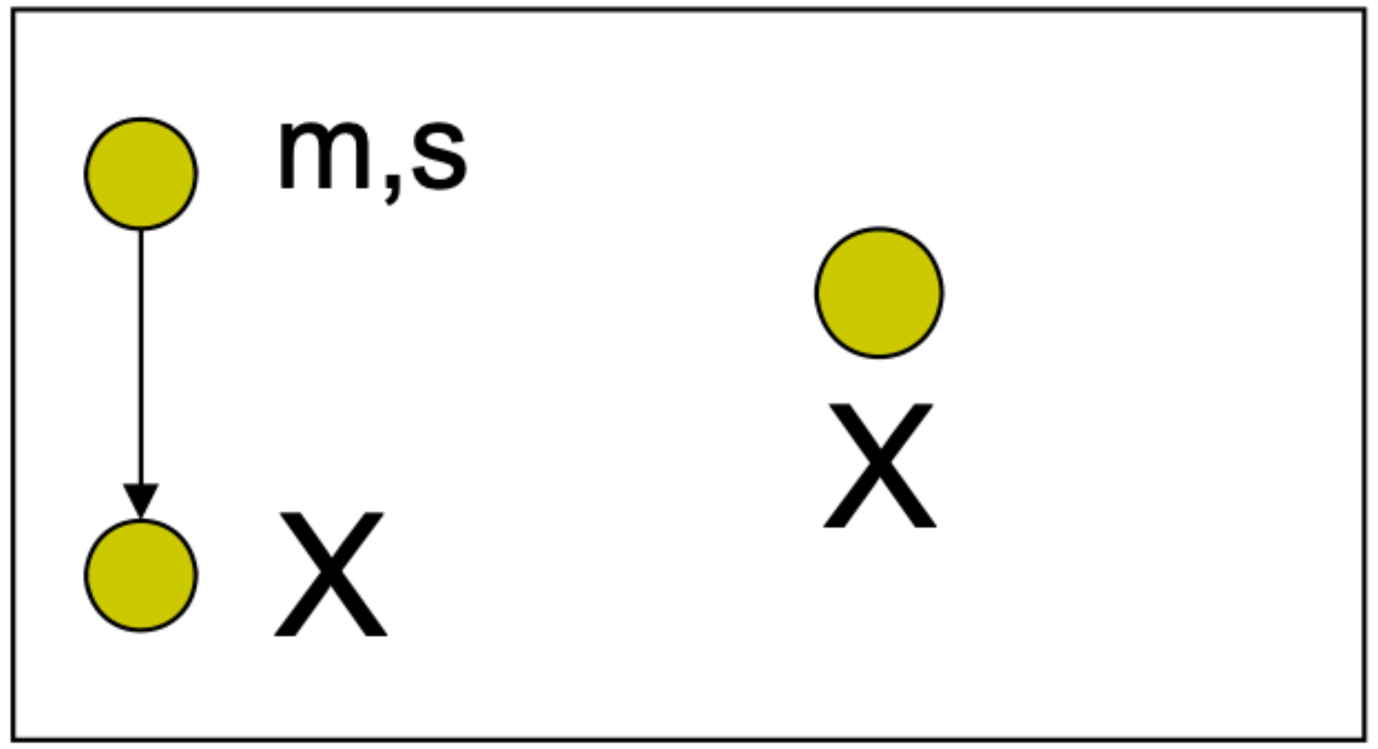

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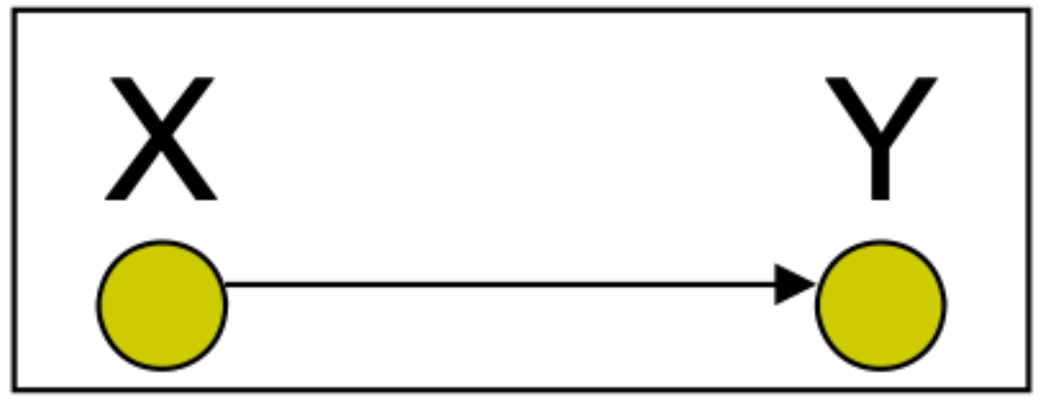

Regression, classification

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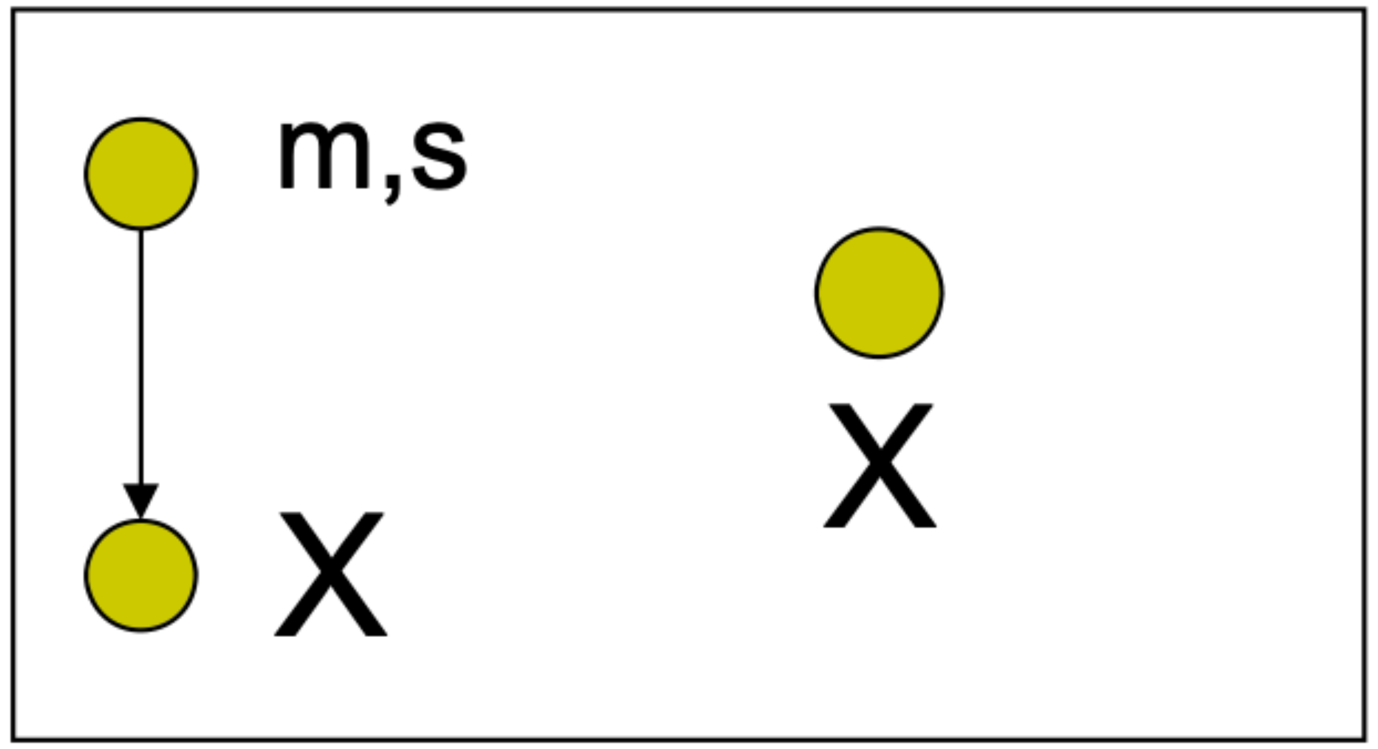

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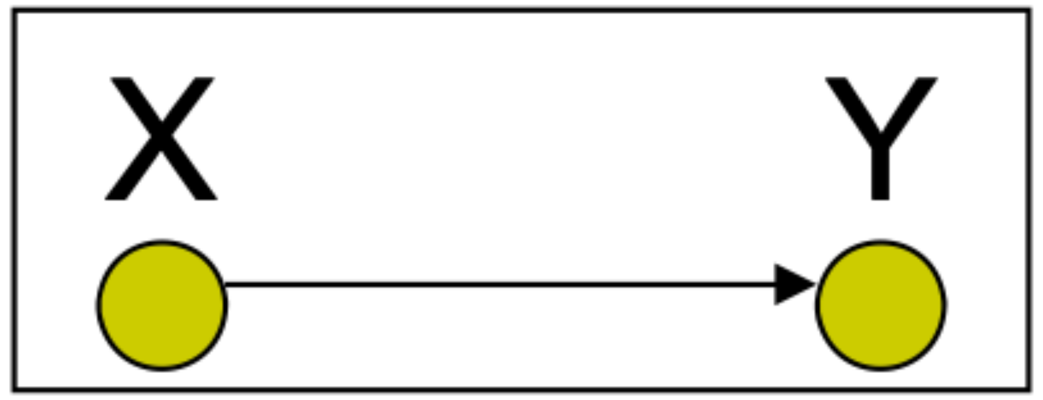

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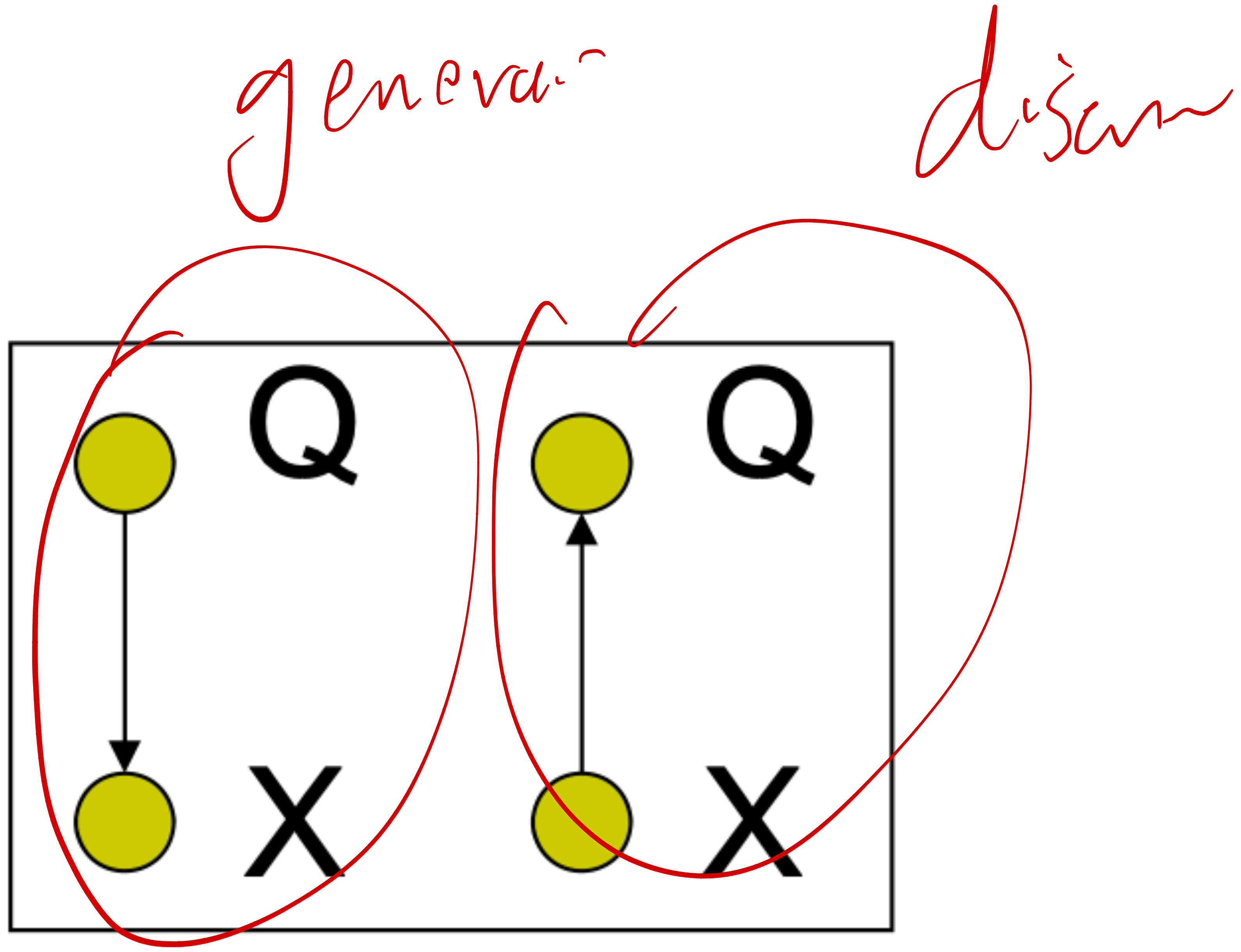

Generative vs
Discriminative Classification

Probabilistic Graphical Model is a language to express distributions

Fancier GMs: Solid State Physics

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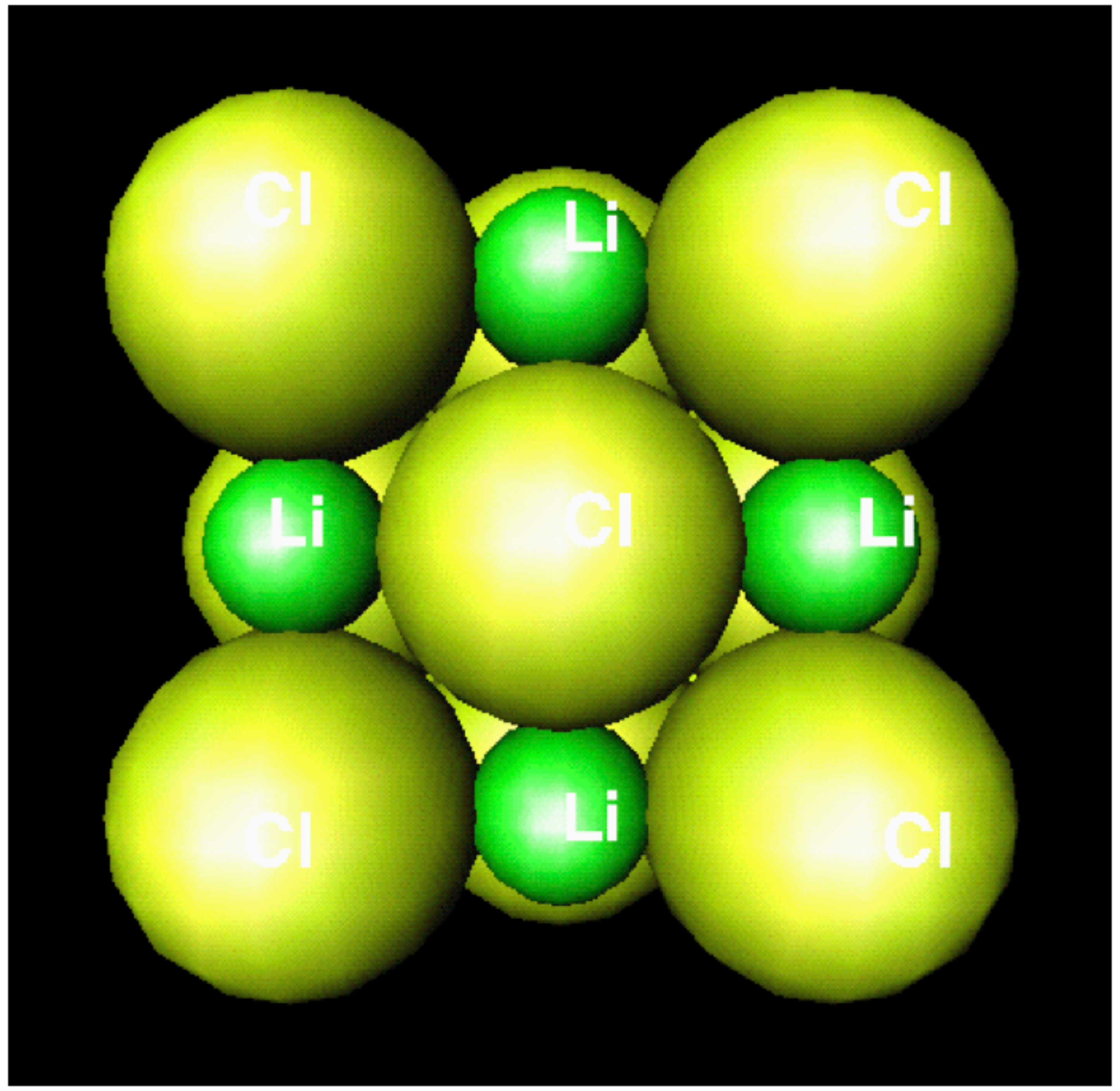
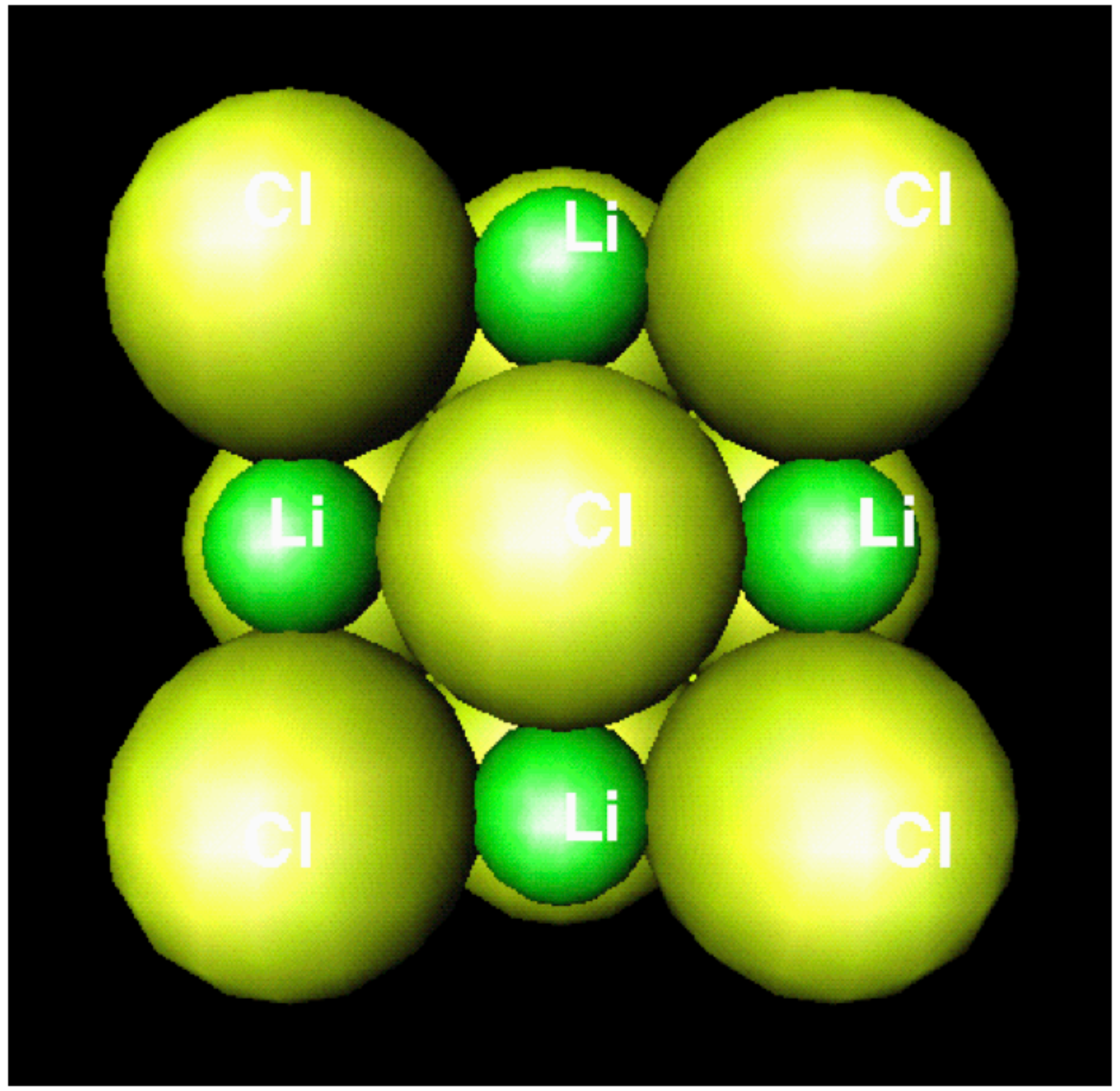
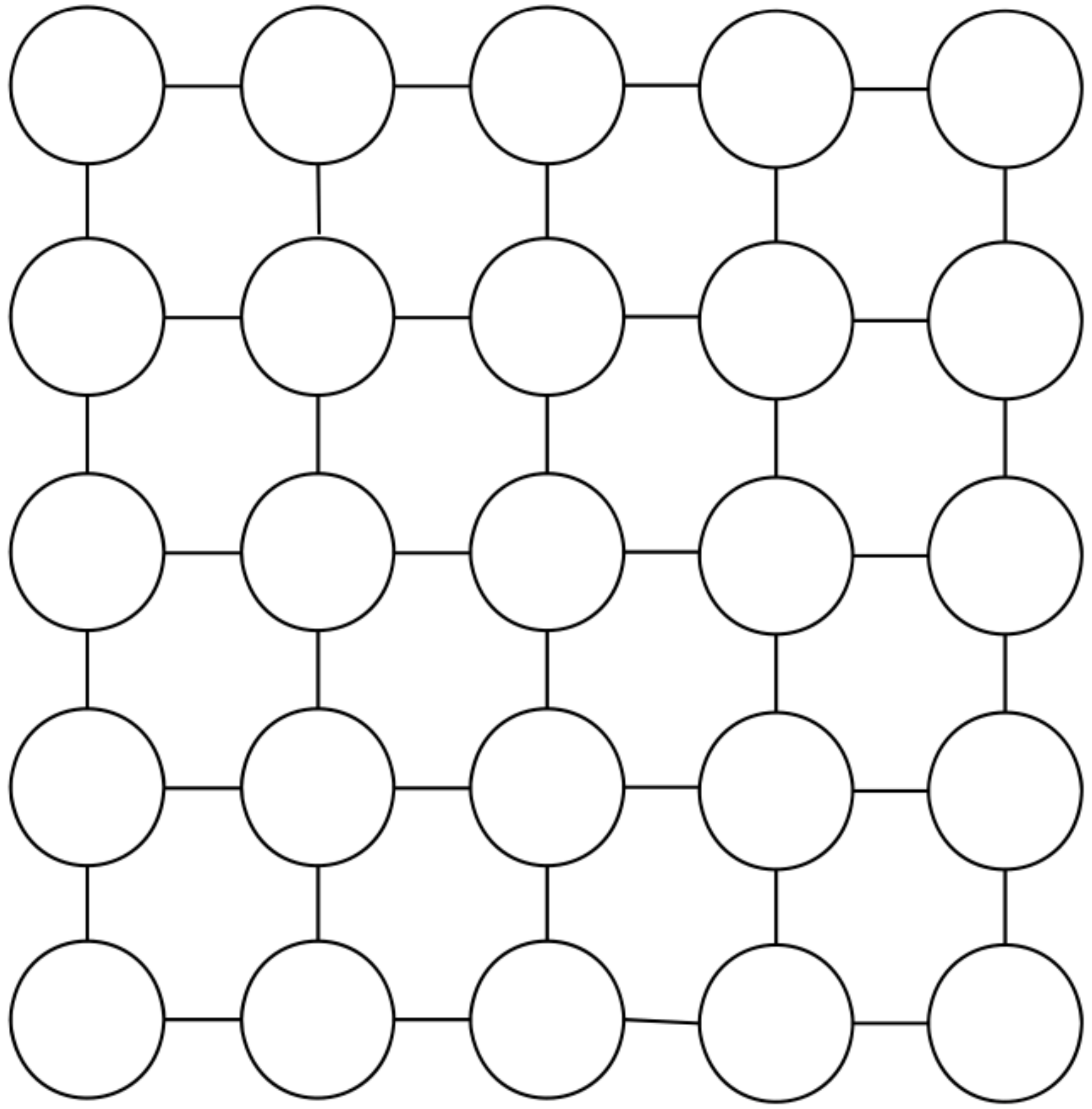


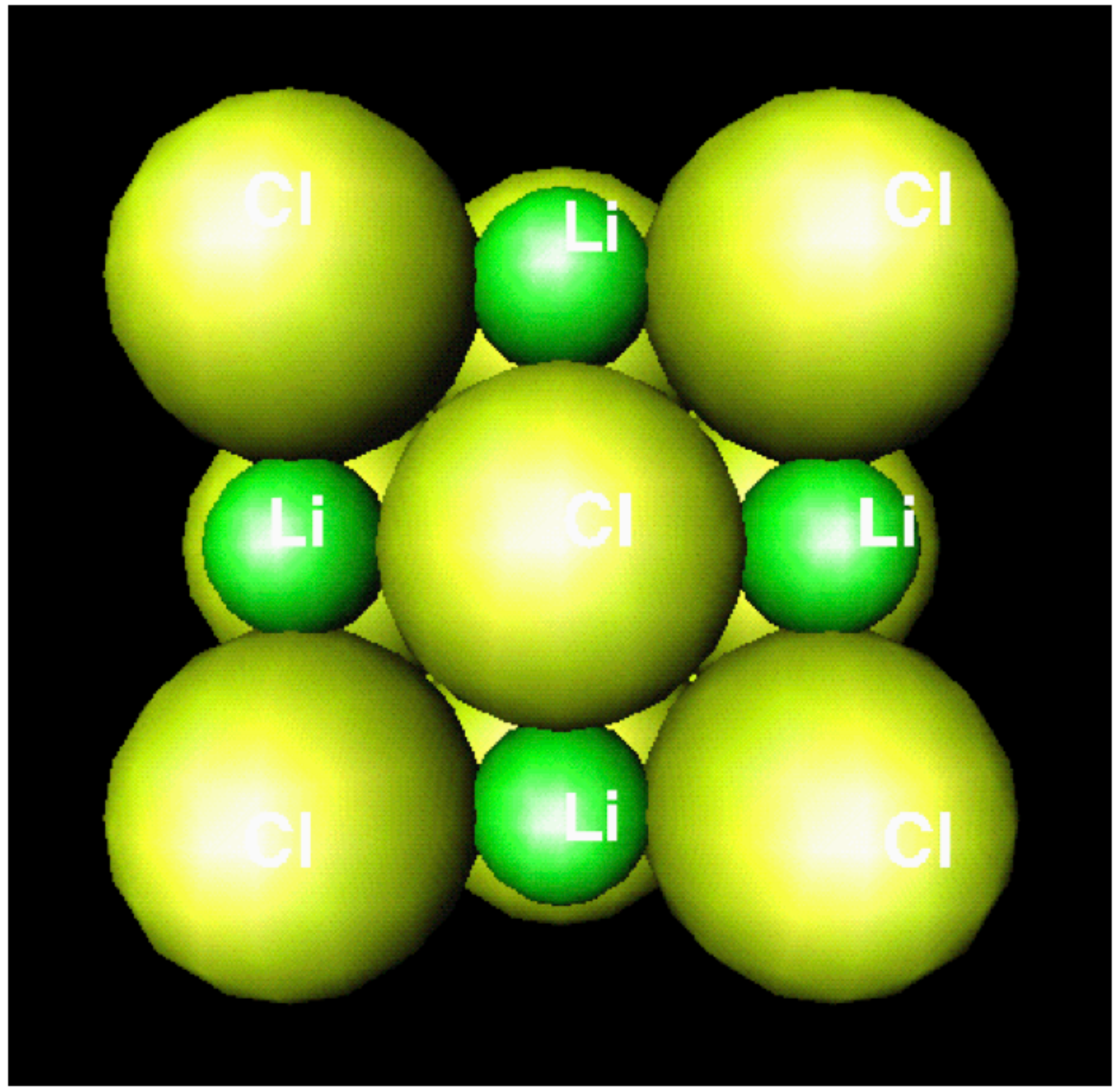
Fancier GMs: Solid State Physics

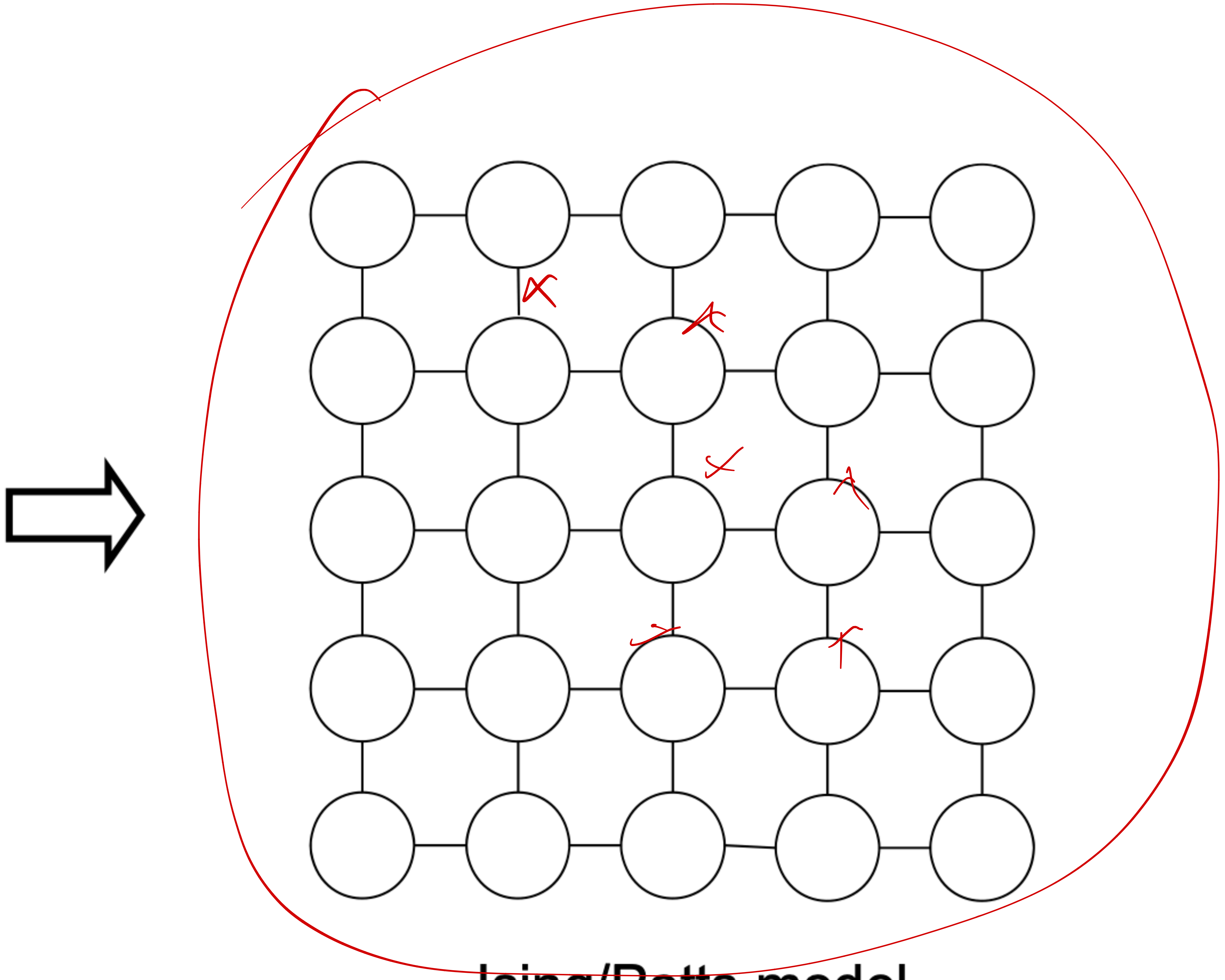




Ising/Potts model

Fancier GMs: Solid State Physics





Ising/Potts model

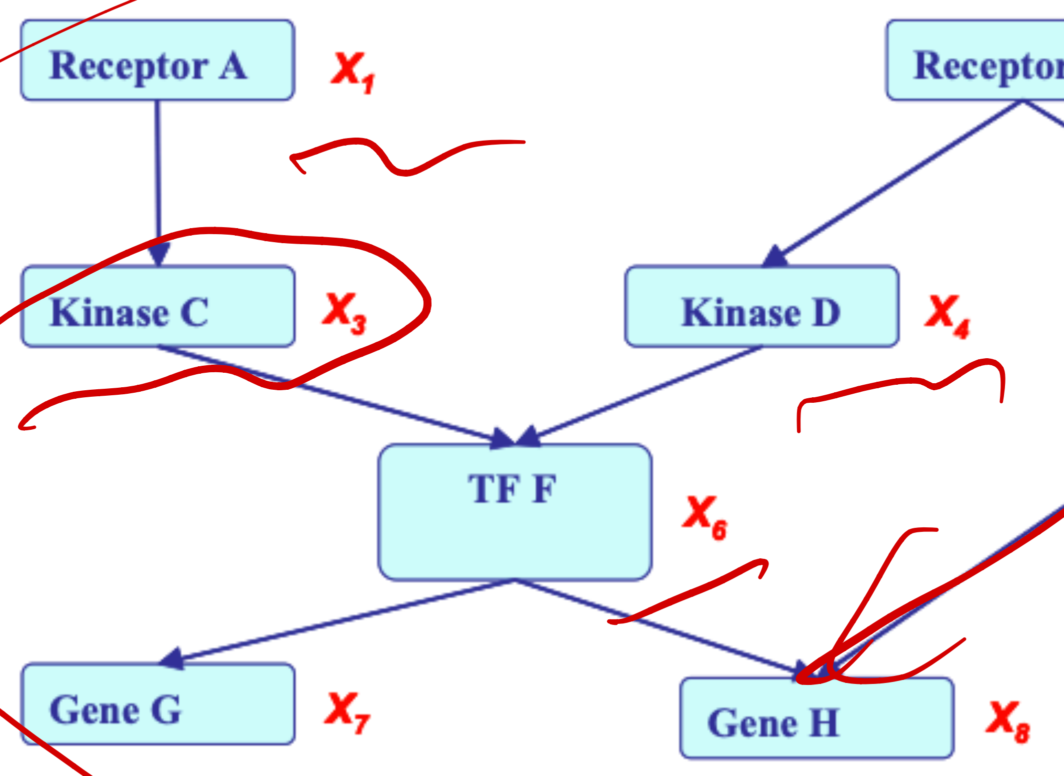
Define the strengths/correlation between different atoms

Why Graphical Models

- A language for communication
- A language for computation
- A language for development

How to Factor a Distribution Given a DAG

How to Factor a Distribution Given a DAG



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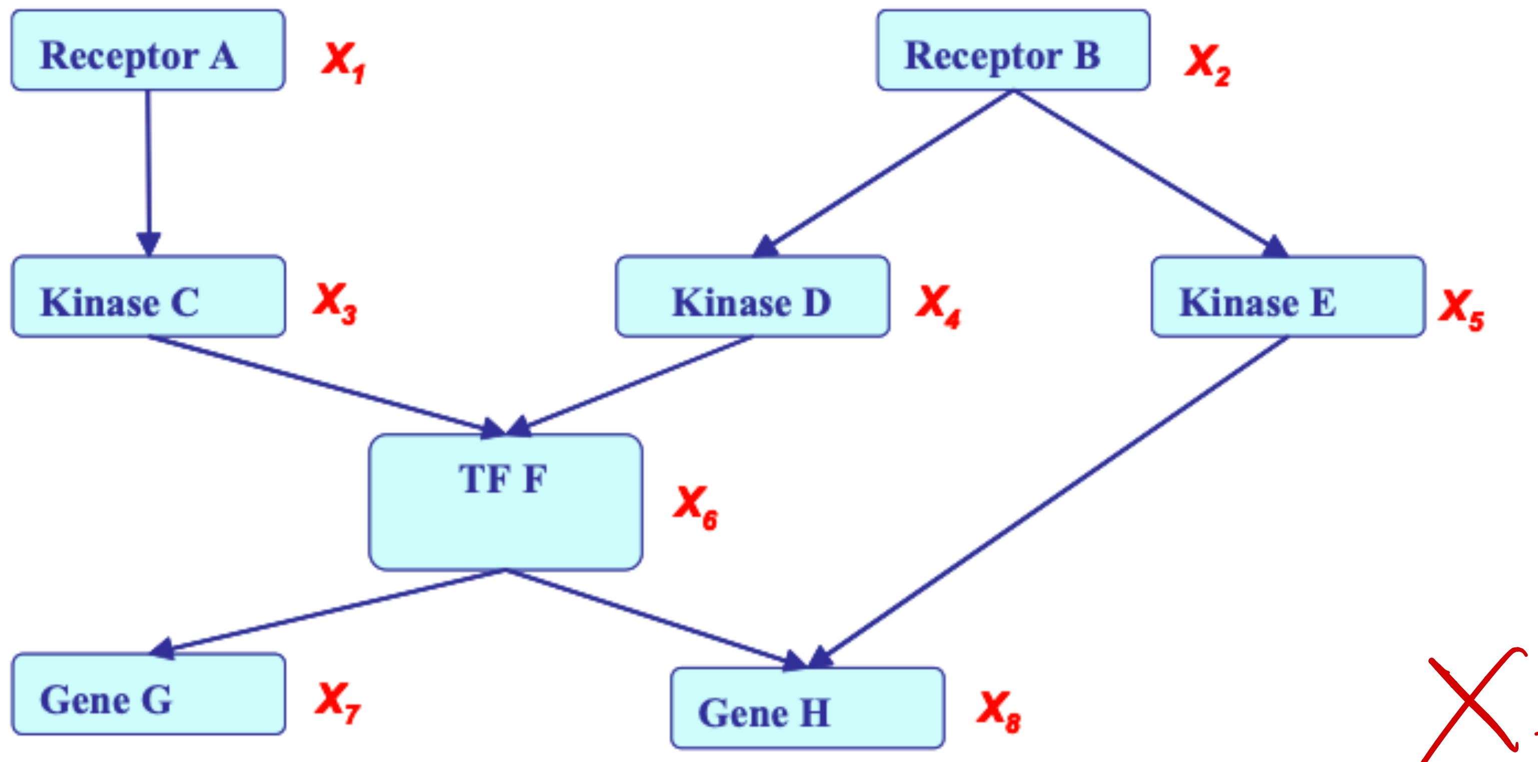
$$P(X_6 | X_3, X_4)\, P(X_7 | X_6)\, P(X_8 | X_5, X_6)$$

$P(x_1)\, P(x_2)\, P(x_3 | x_1)$

$P(x_6 | x_3, x_4)\, P(x_7 | x_6)$

$P(x_8 | x_6, x_5)$

How to Factor a Distribution Given a DAG



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X_1 X_2

- **Theorem:**

  Given a DAG, The most general form of the probability distribution that is consistent with the (probabilistic independence properties encoded in the) graph factors according to "node given its parents":

$$P(\mathbf{X}) = \prod_i P(X_i \,|\, \mathbf{X}_{\pi_i})$$

where $\mathbf{X}_{\pi_i}$ is the set of parents of xi. d is the number of nodes (variables) in the graph.

Local Structures & Independence

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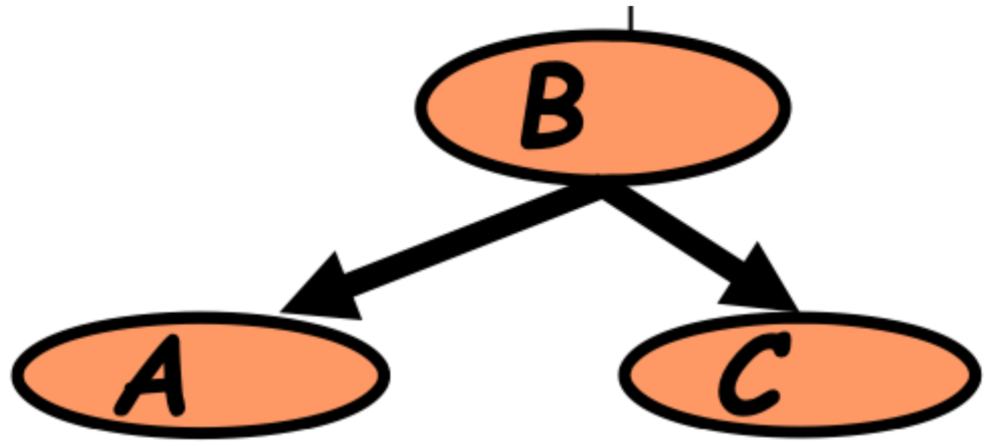

Local Structures & Independence

- Common parent
  - Fixing B decouples A and C
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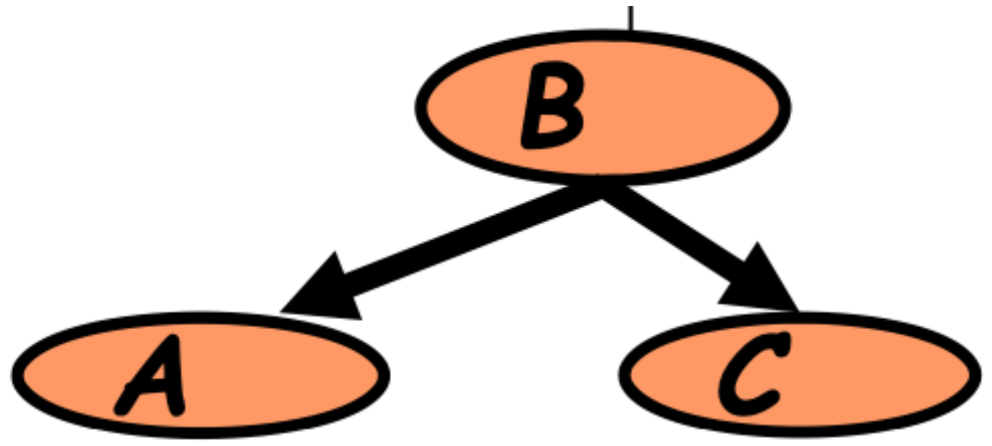

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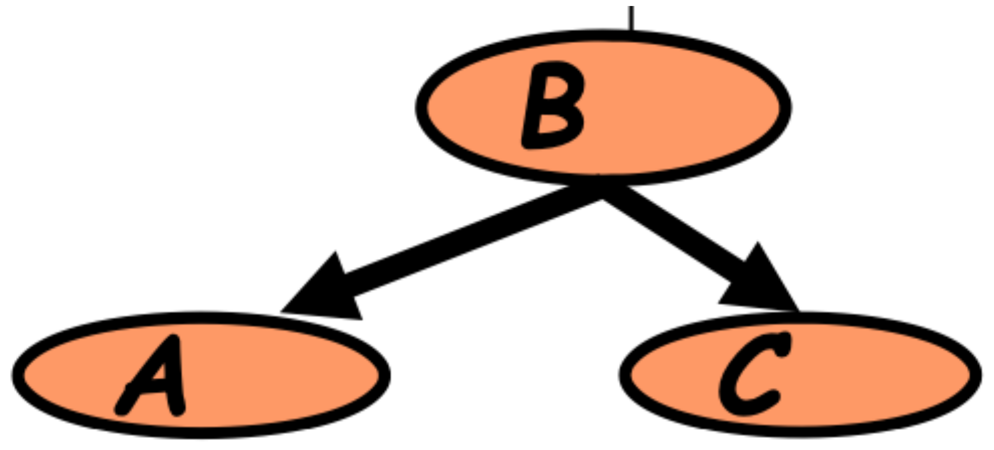

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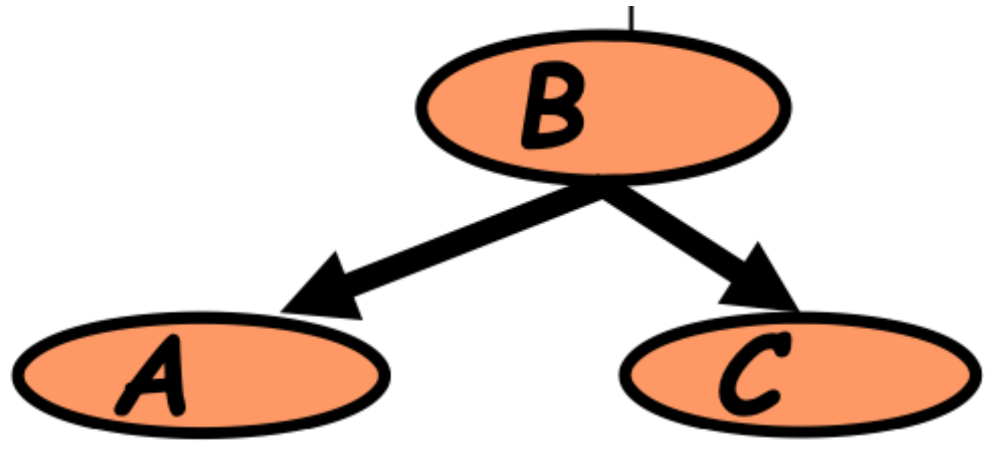

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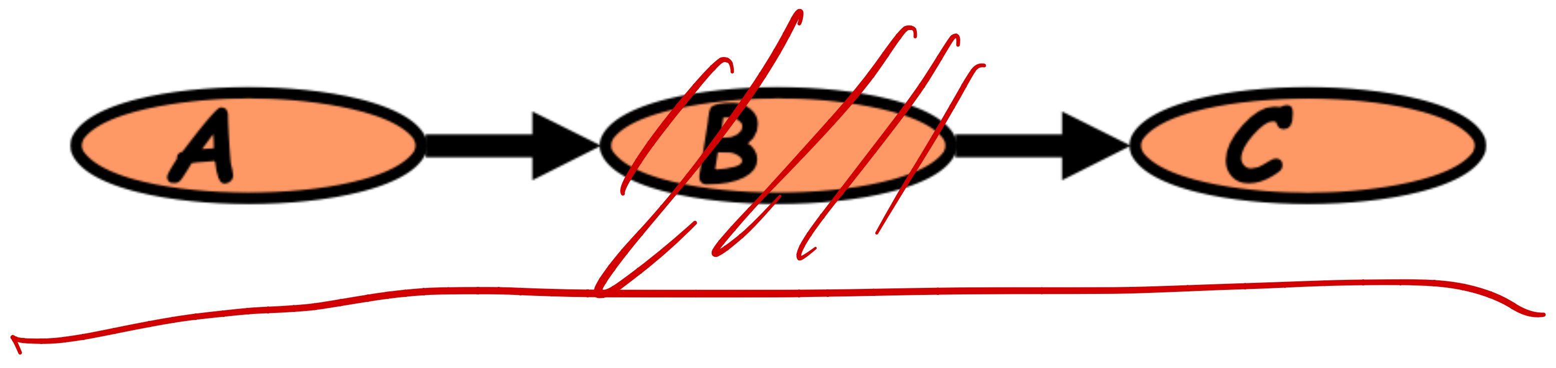

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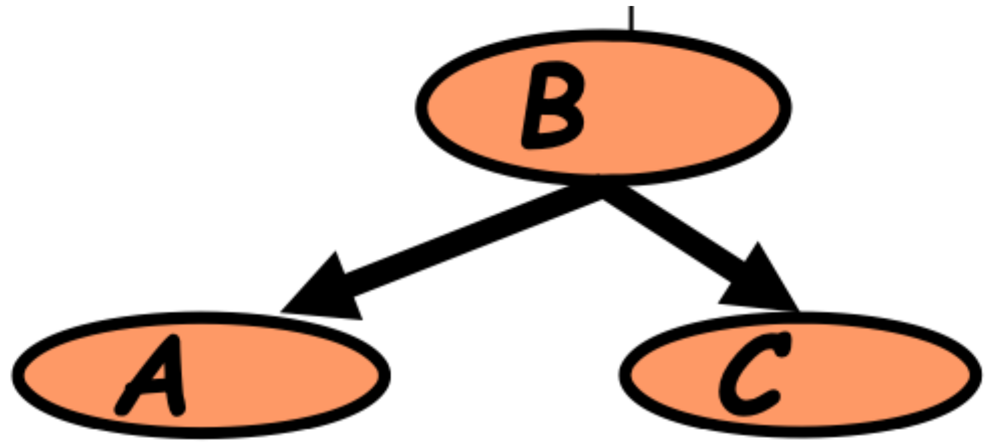

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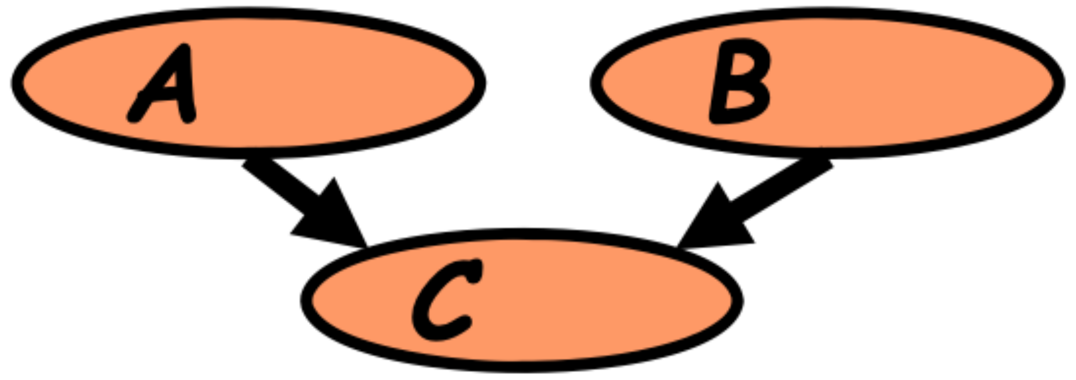

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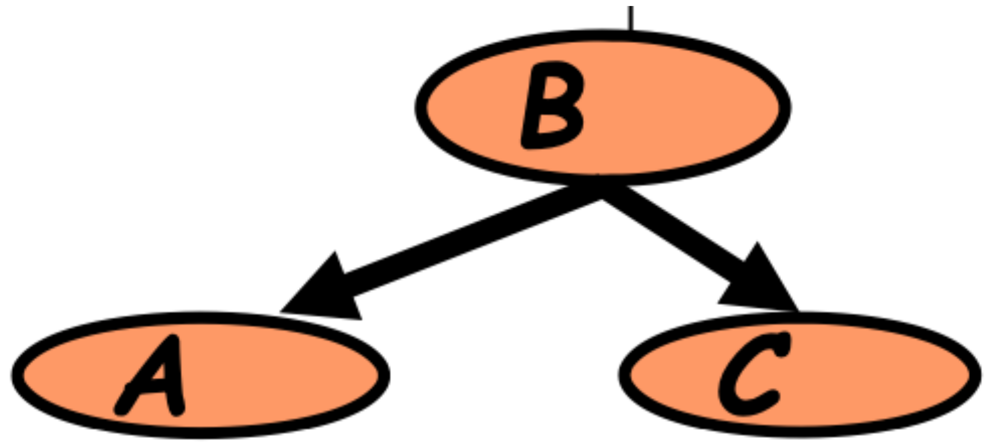

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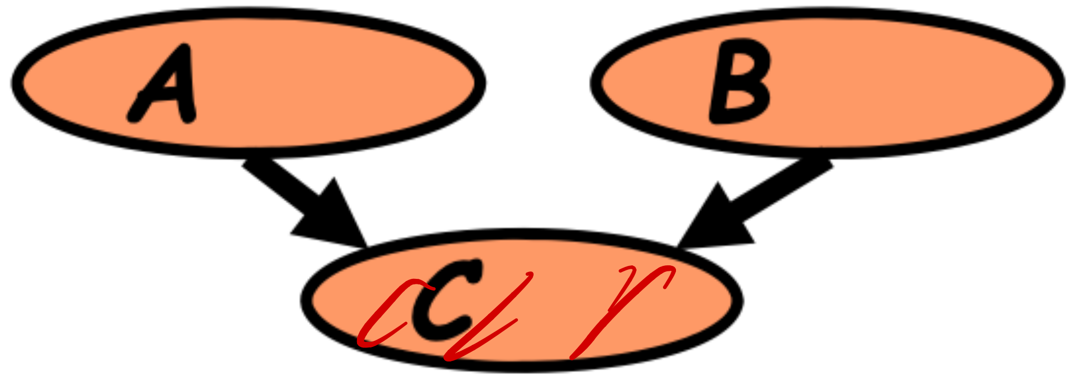

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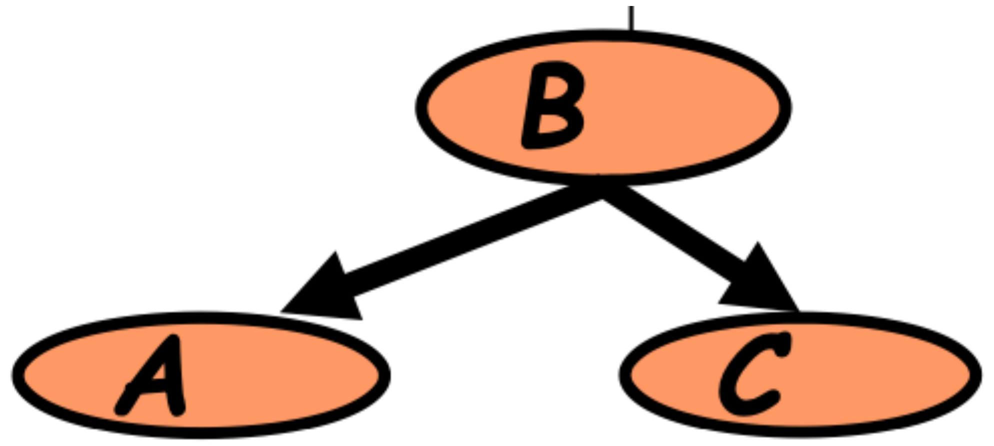

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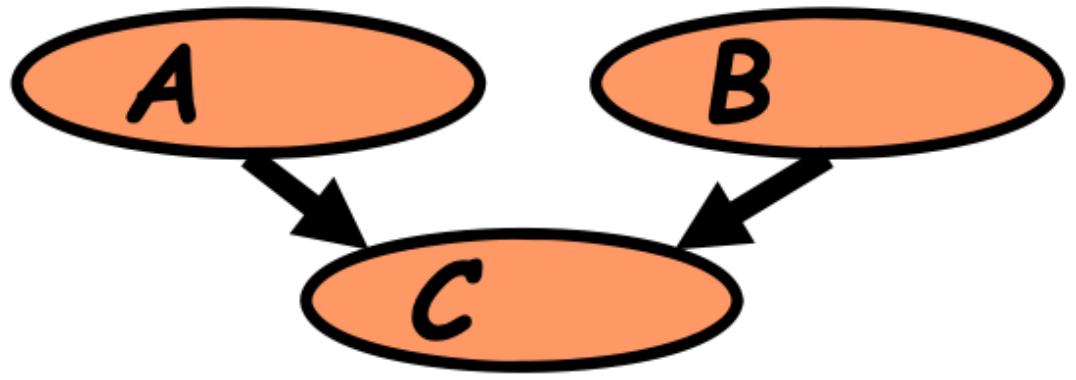

The language is compact, the concepts are rich!

Global Markov Properties of DAGs

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How to determine two variables are conditionally independent given another variable?

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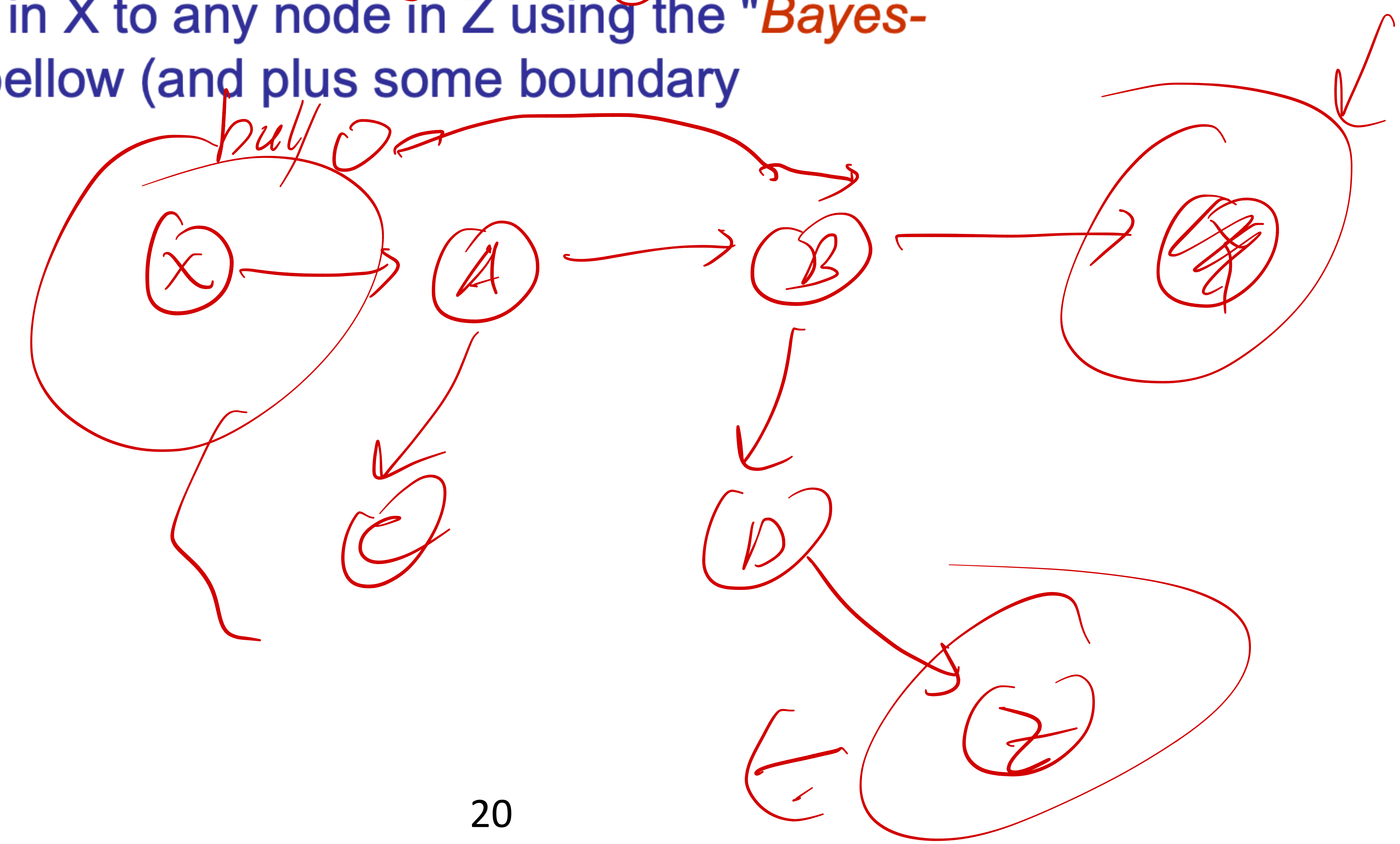

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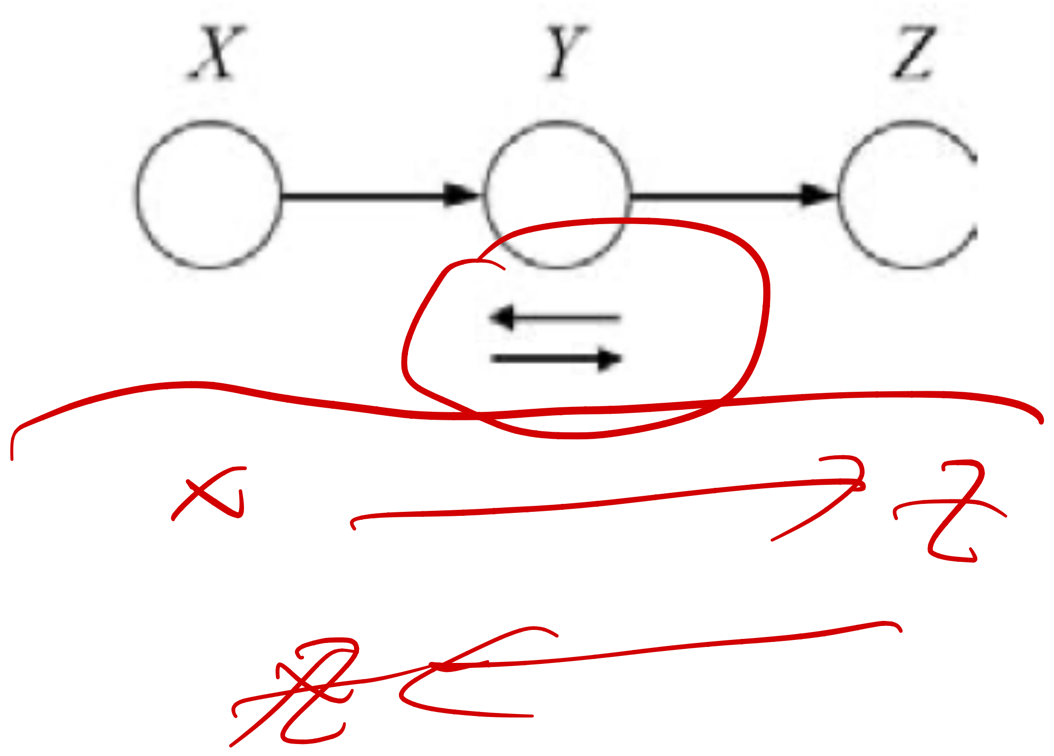

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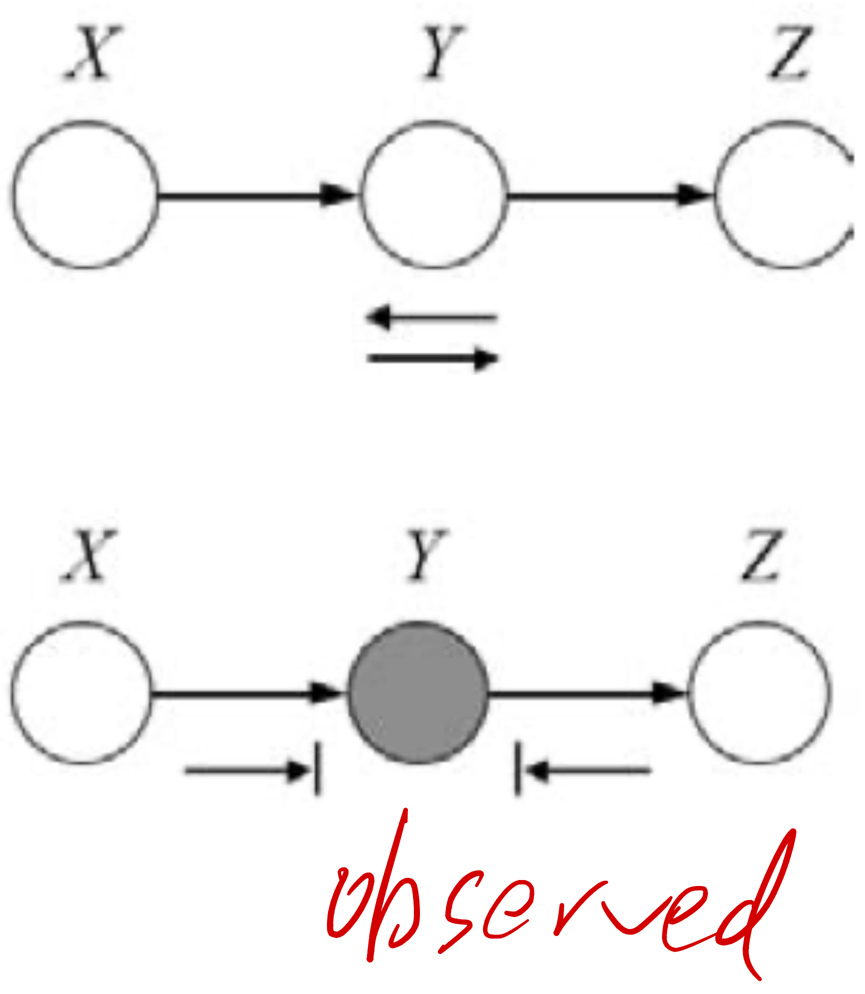

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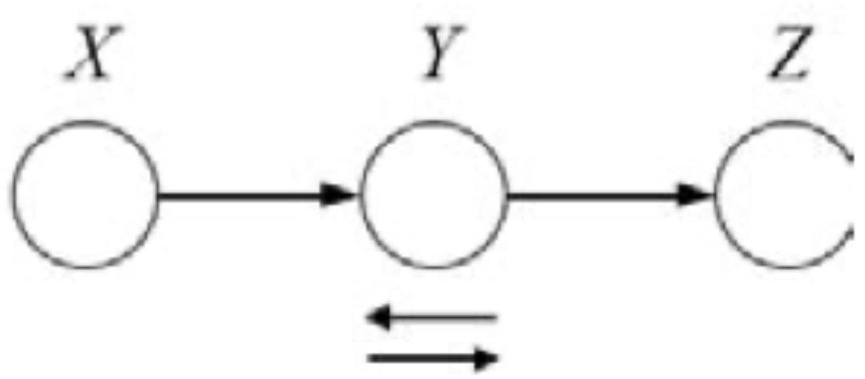

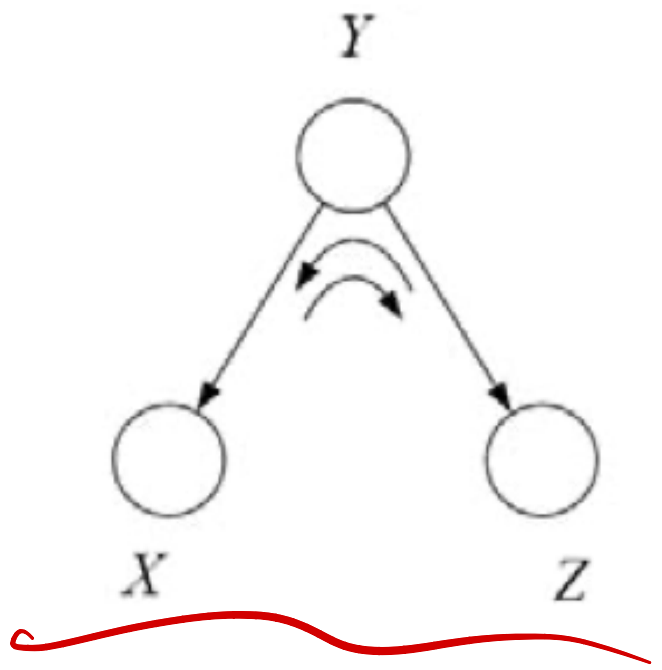

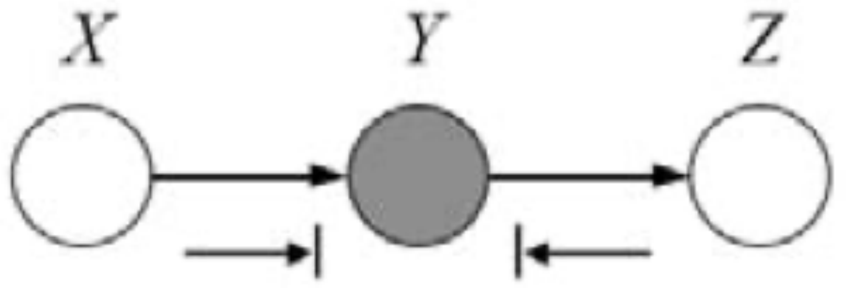

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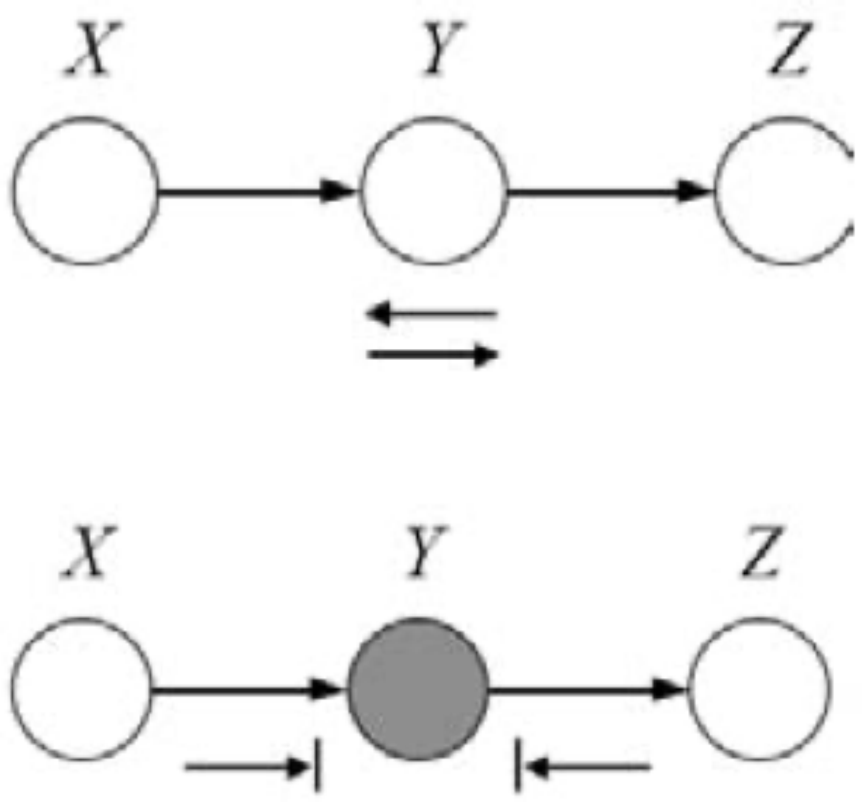

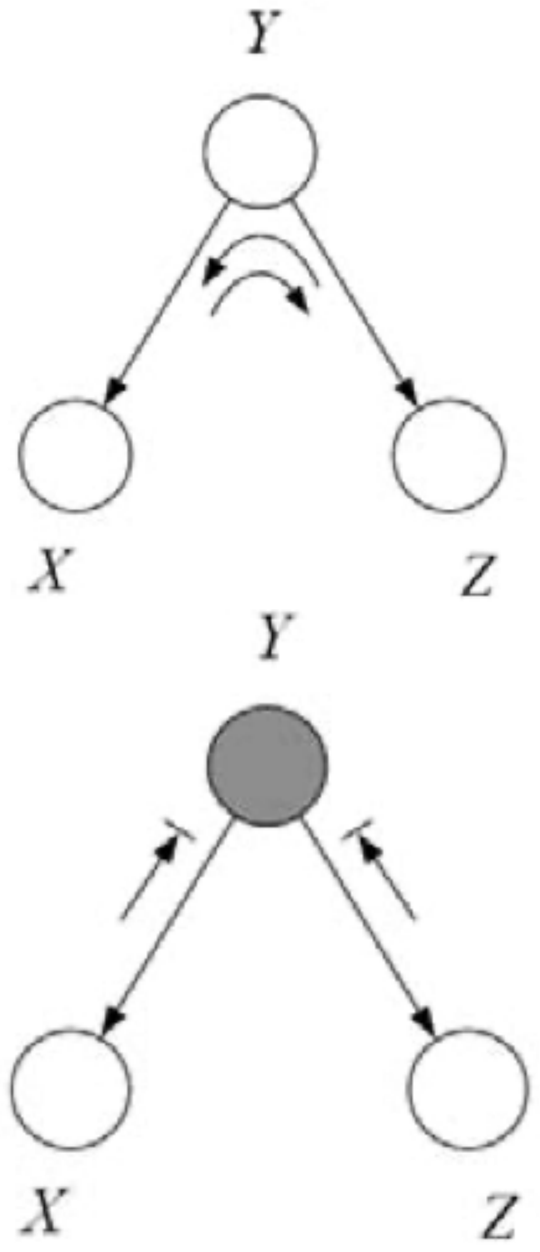

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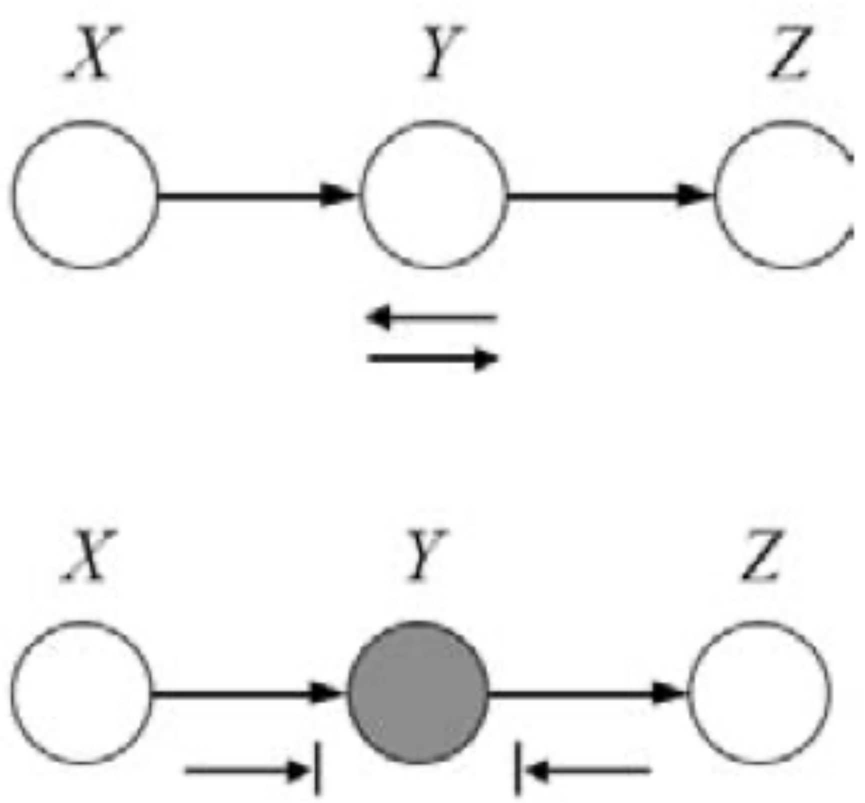

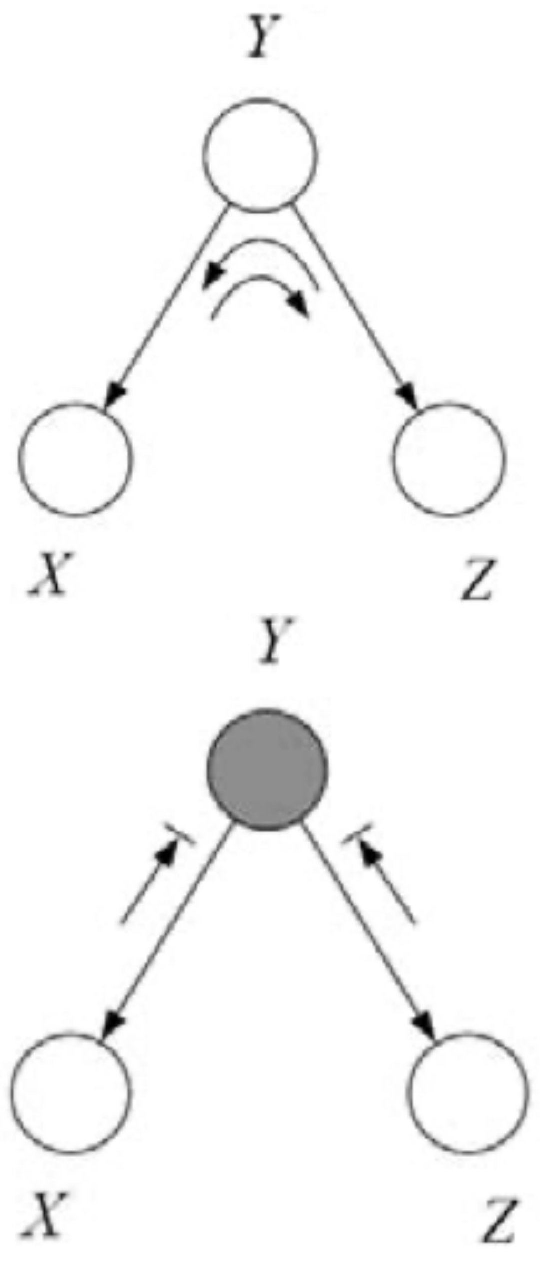

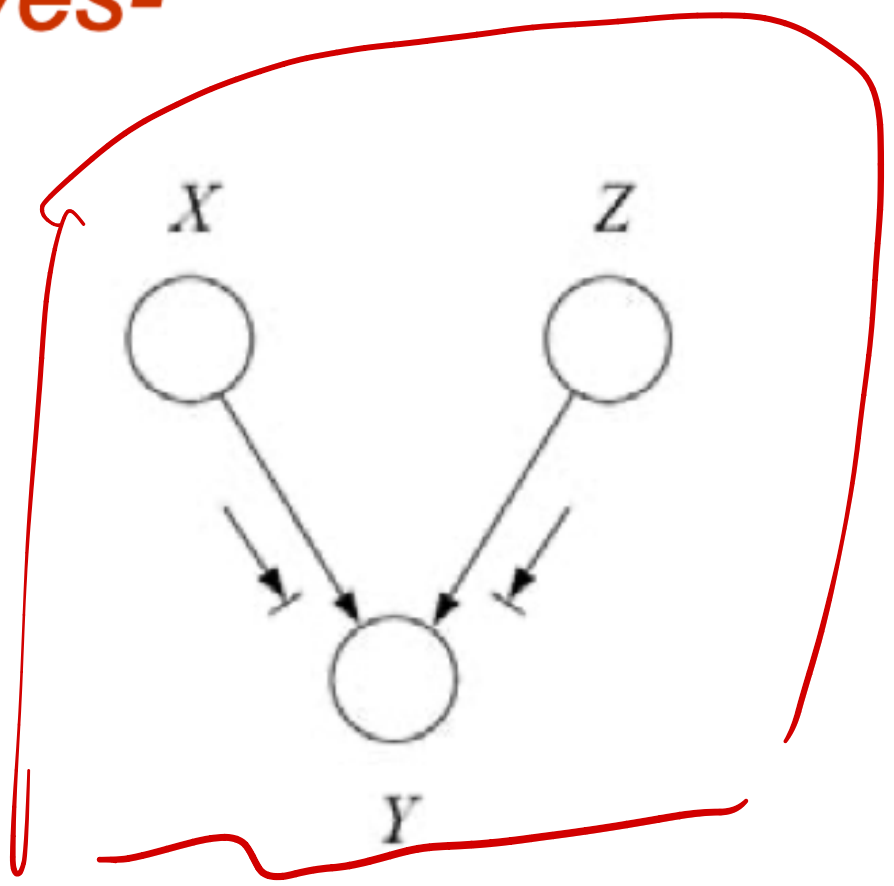

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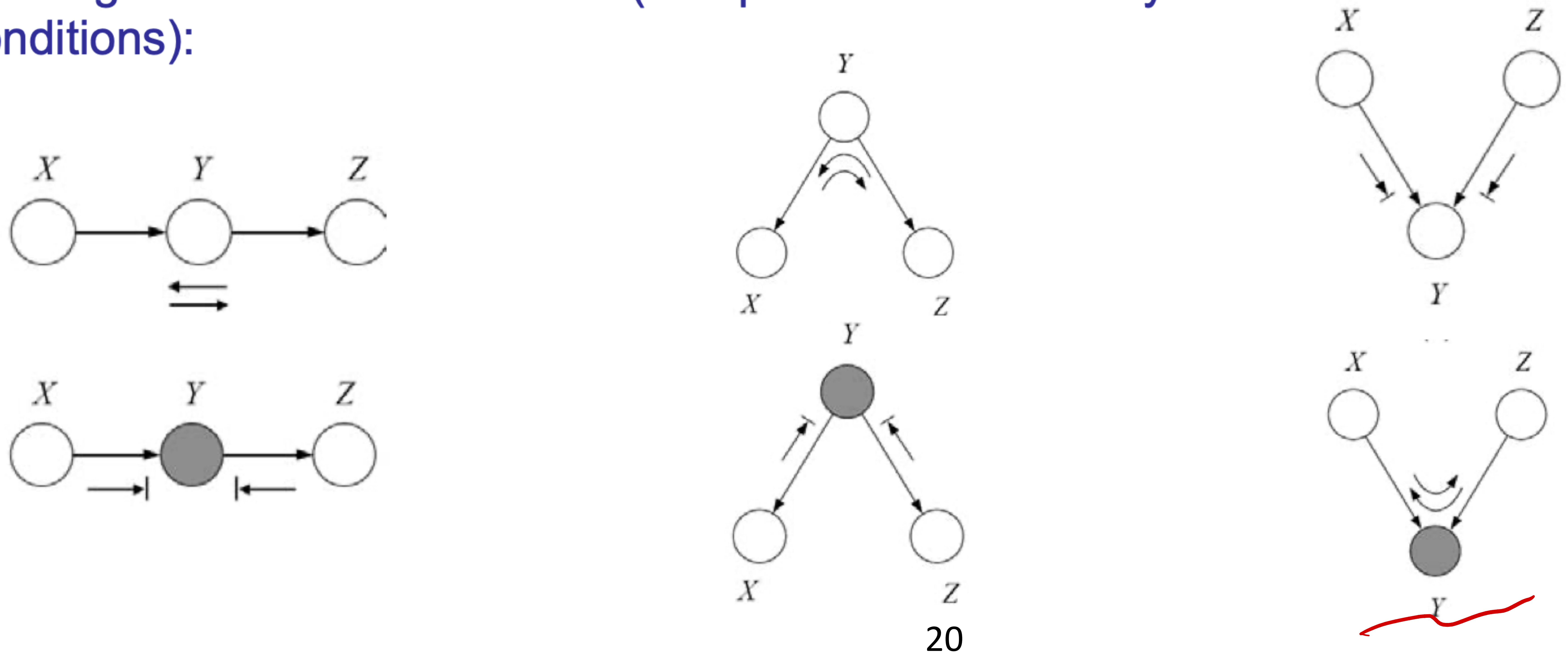
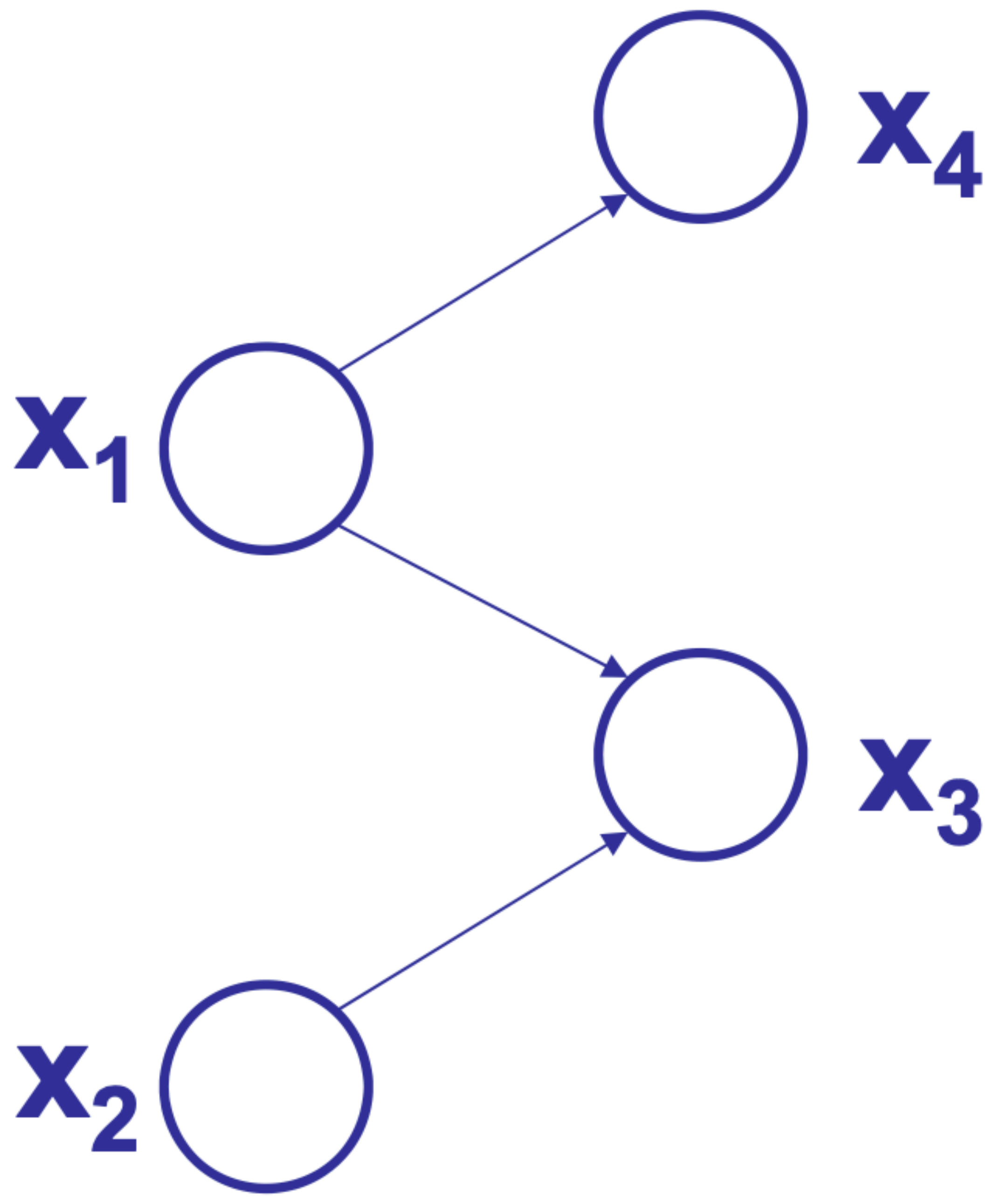


Example



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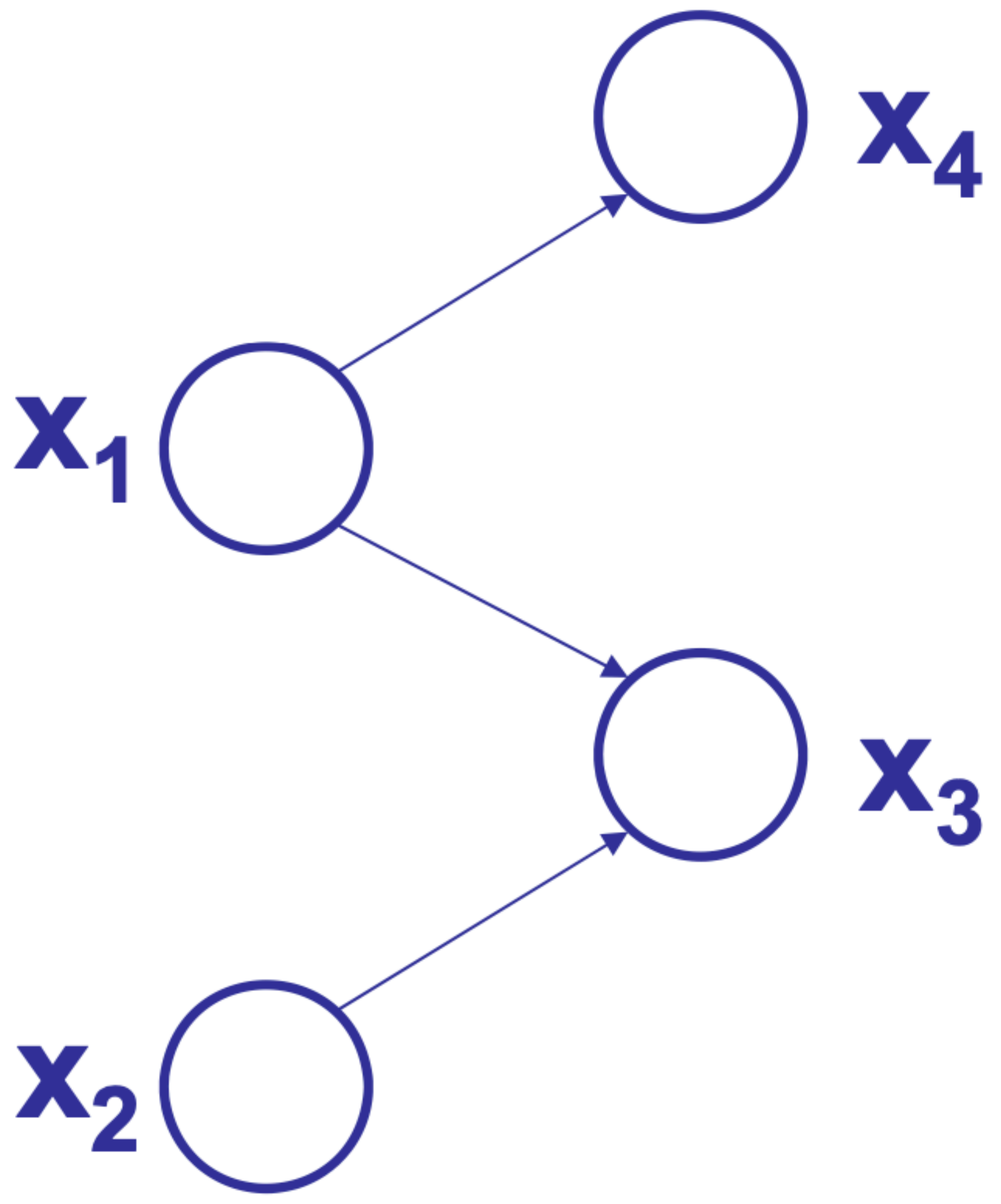

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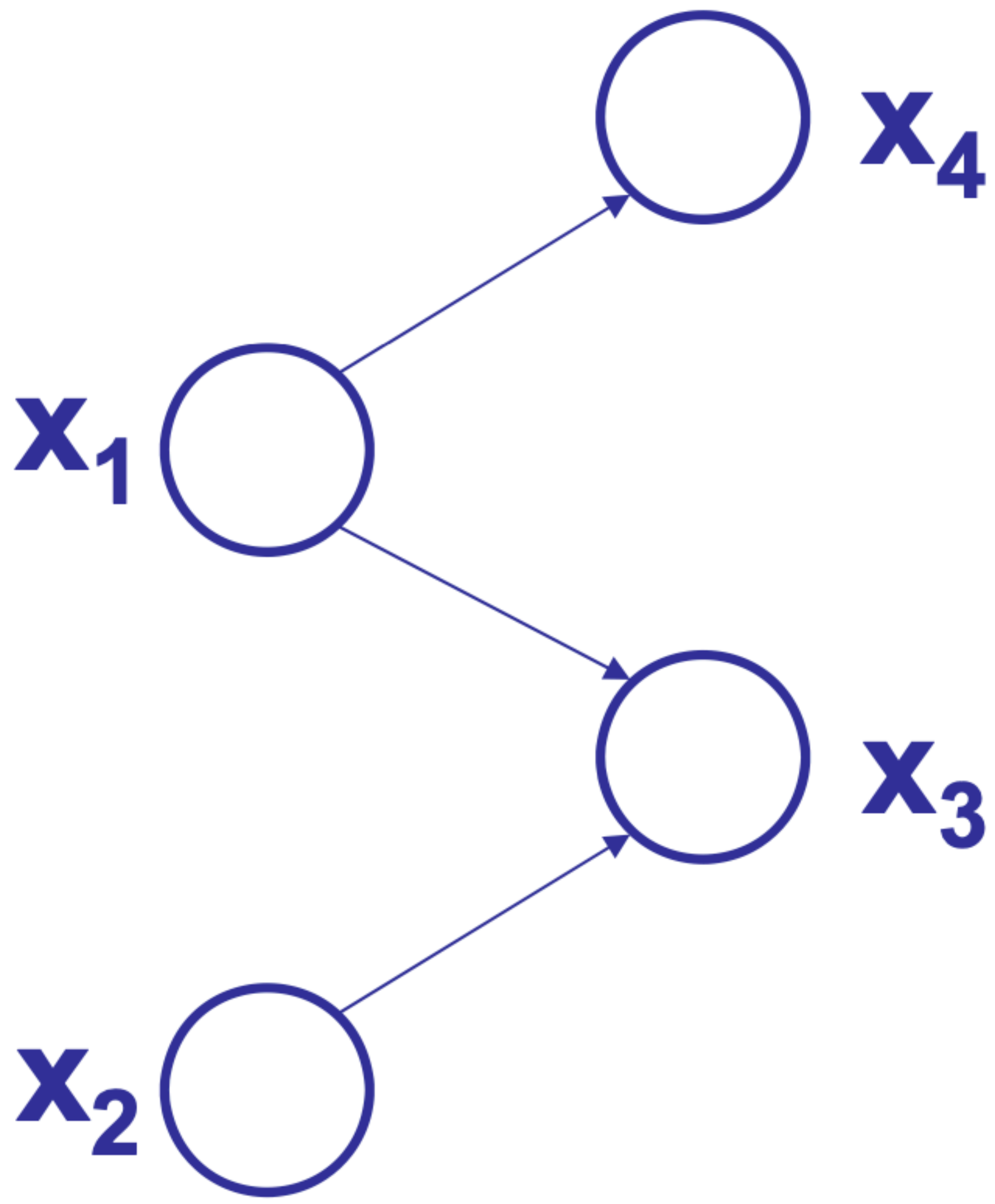

1. Are X2 and X4 independent?

2. Are X2 and X4 conditionally independent given X1?

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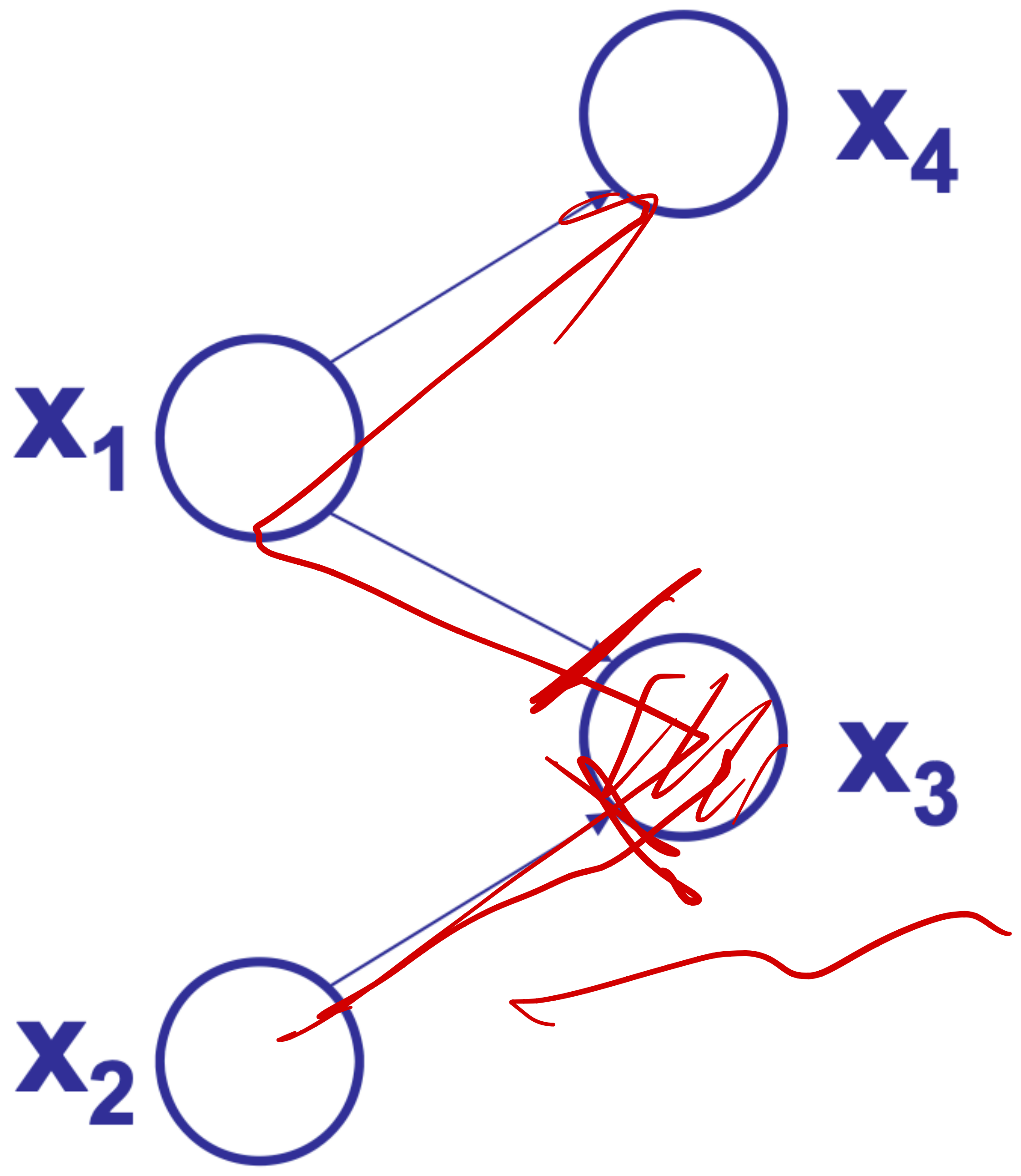

1. Are X2 and X4 independent? Yes

2. Are X2 and X4 conditionally independent given X1? yes

3. Are X2 and X4 conditionally independent given X3?

No

Conditional Probability Density Func

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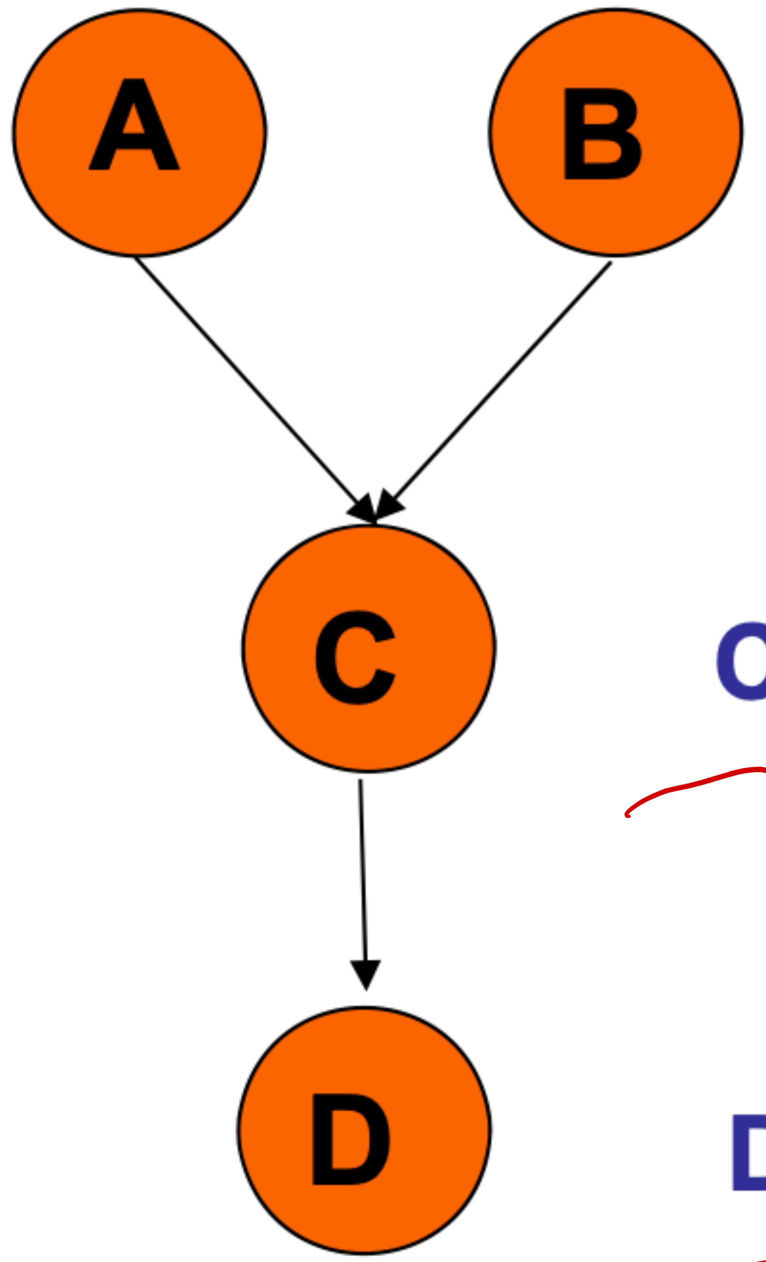
$A \sim N(\mu_a, \Sigma_a)$ $B \sim N(\mu_b, \Sigma_b)$



$C \sim N(A+B, \Sigma_c)$

$D \sim N(\mu_a+C, \Sigma_a)$

BMM

$P(z) \sim$ Bernoulli

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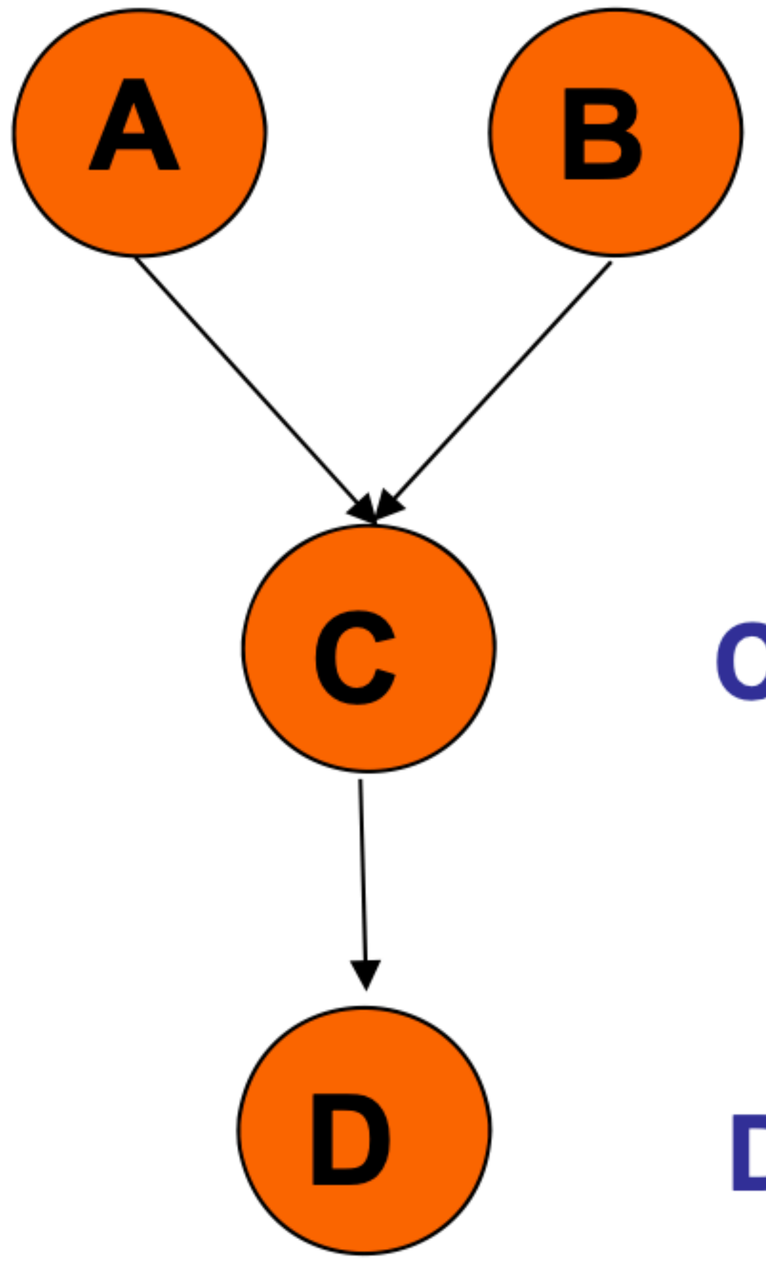

$C \sim N(A+B, \Sigma_c)$

$D \sim N(\mu_a + C, \Sigma_a)$

$$P(a,b,c.d) = P(a)P(b)P(c|a,b)P(d|c)$$

$P(a)P(b)P(c|a,b)P(d|c)$

Conditional Independencies

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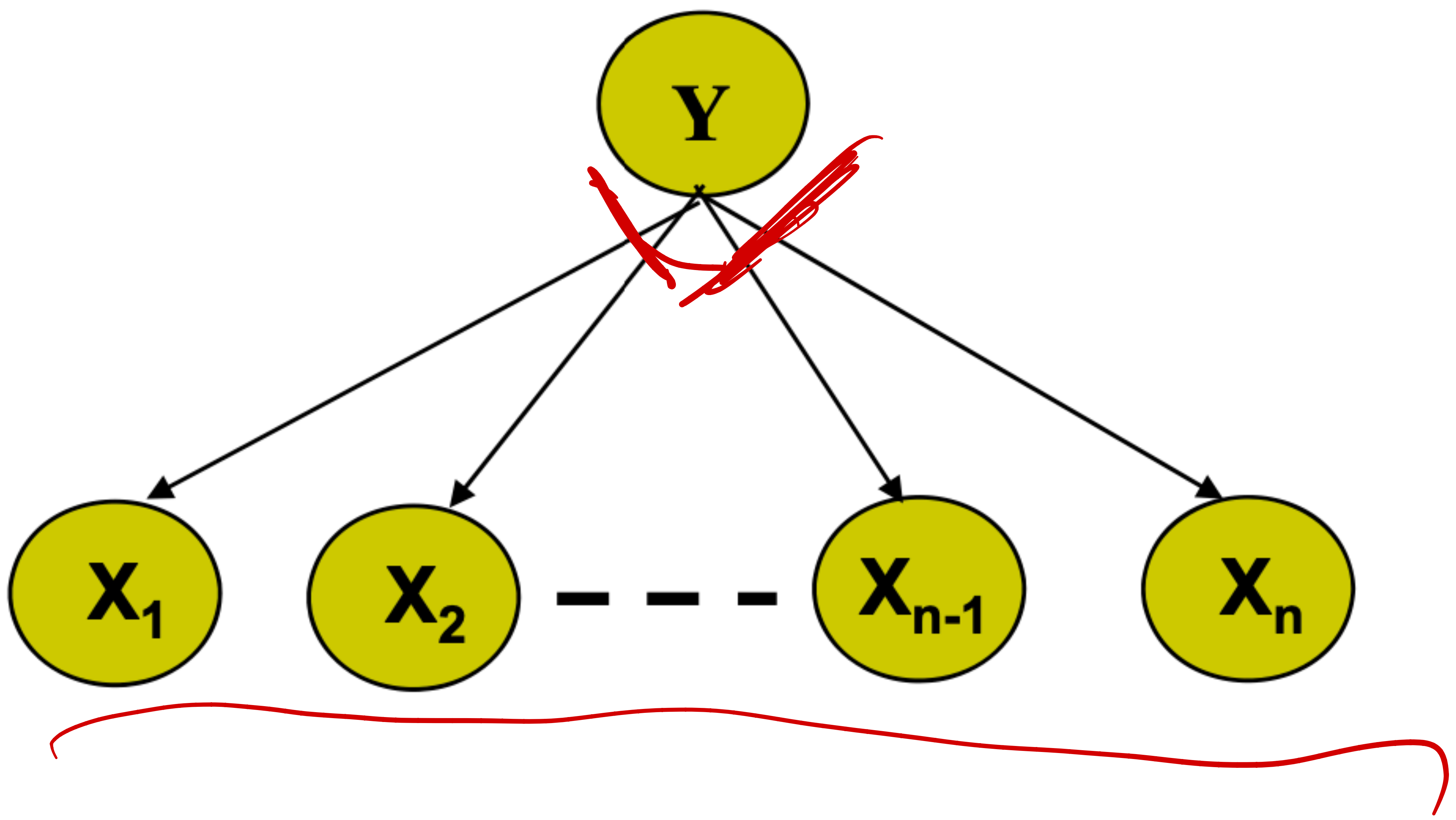
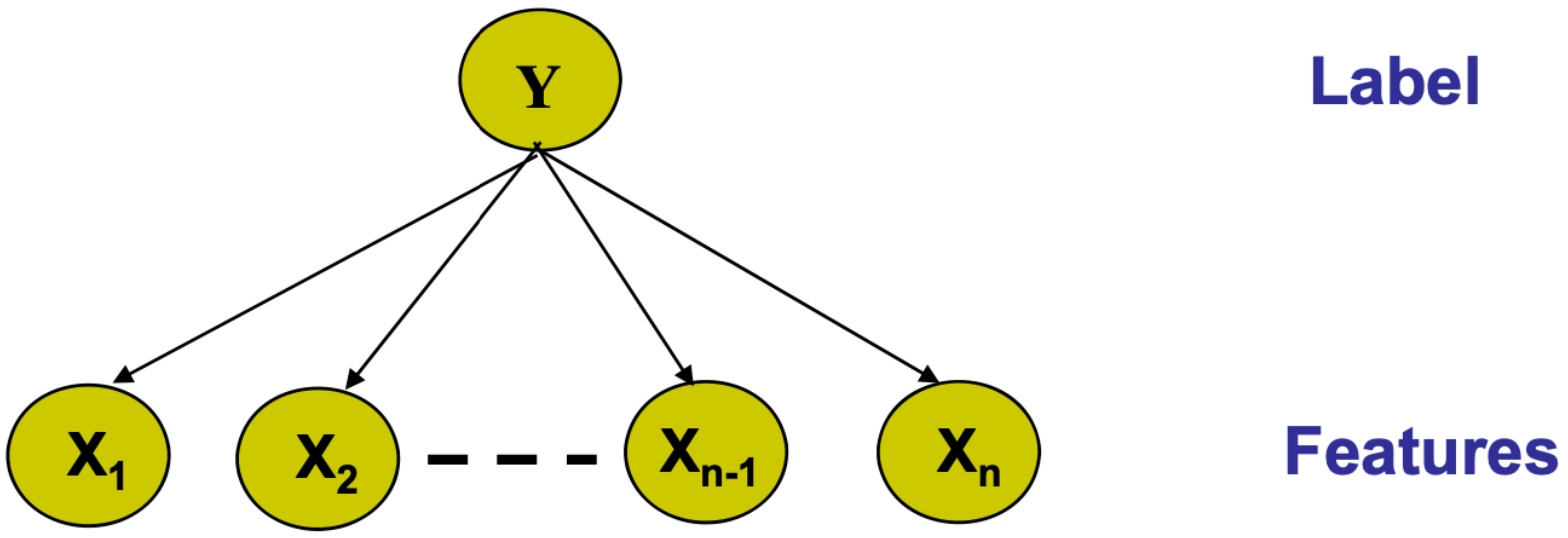


Label

Features

Conditional Independencies



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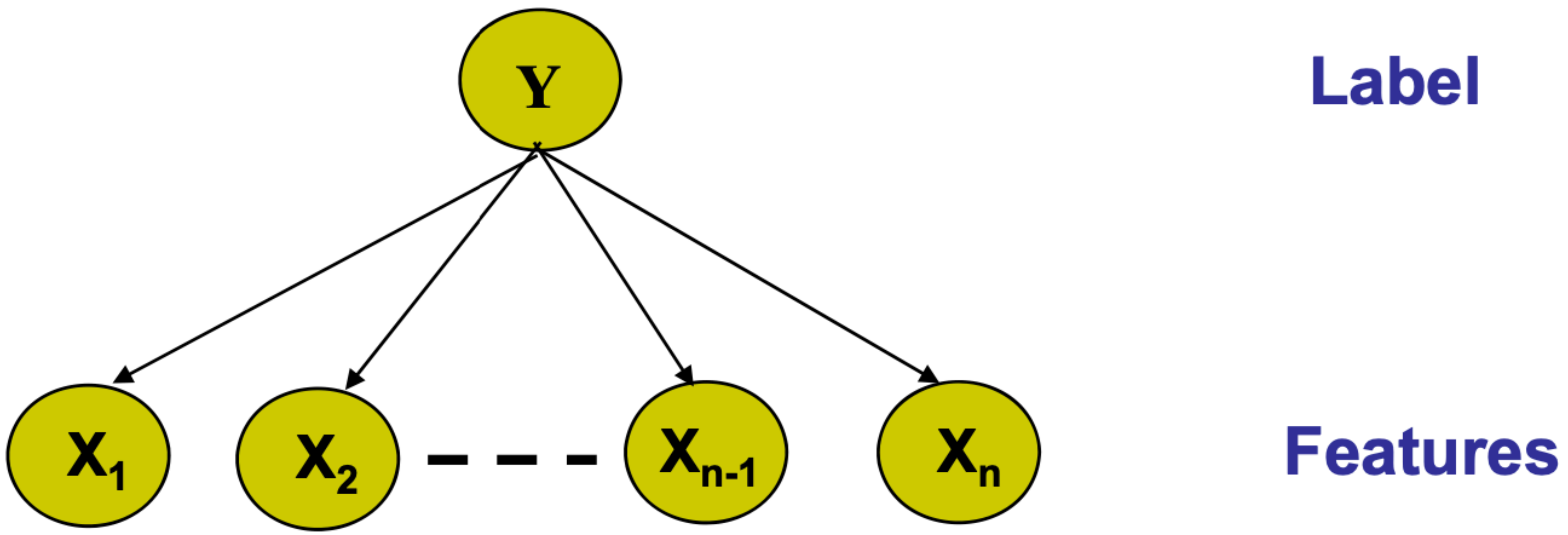

Are Xi D-separated from Xj given Y?

What is this model when Y is observed? naive bayes

Conditionally Independent Observations

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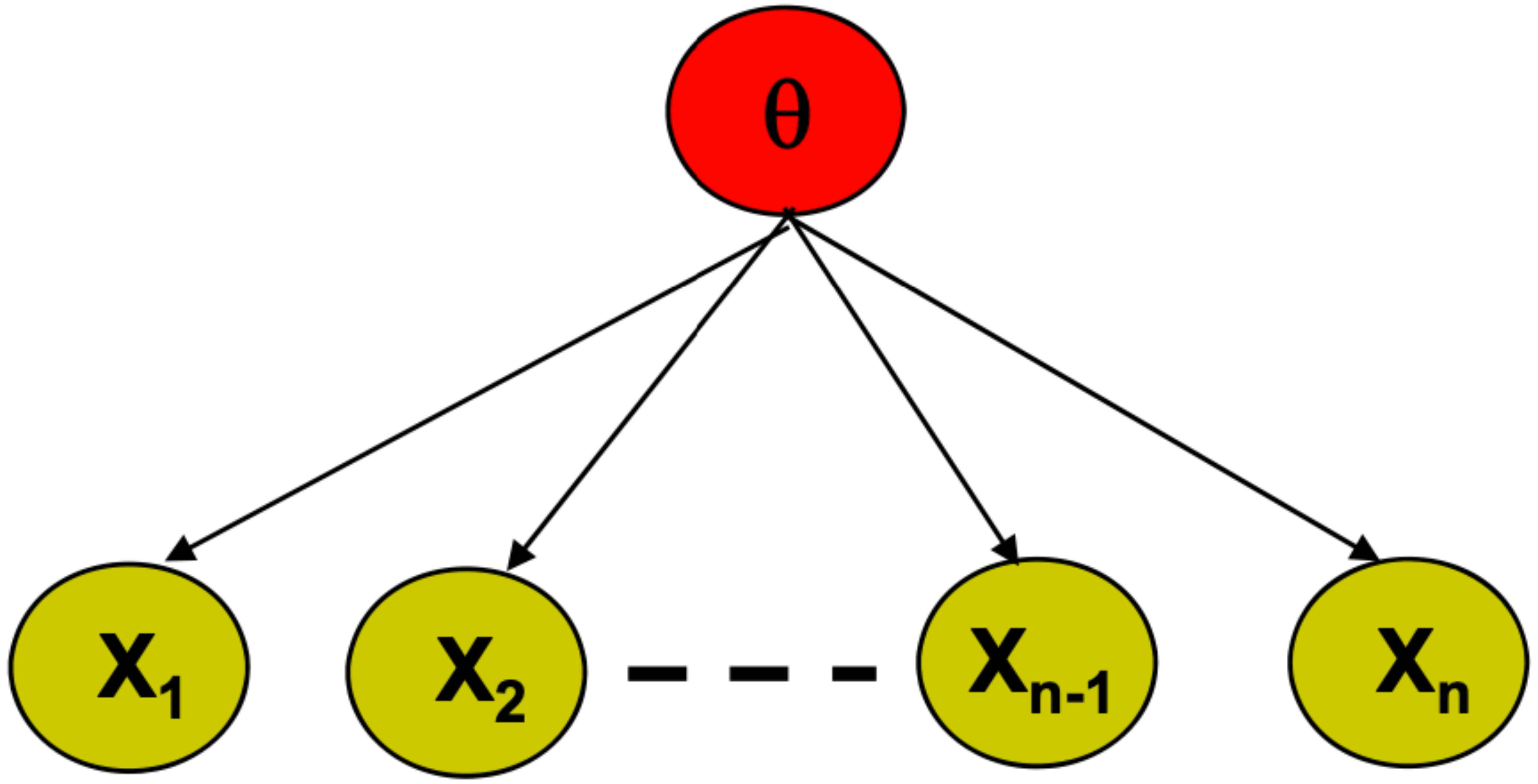

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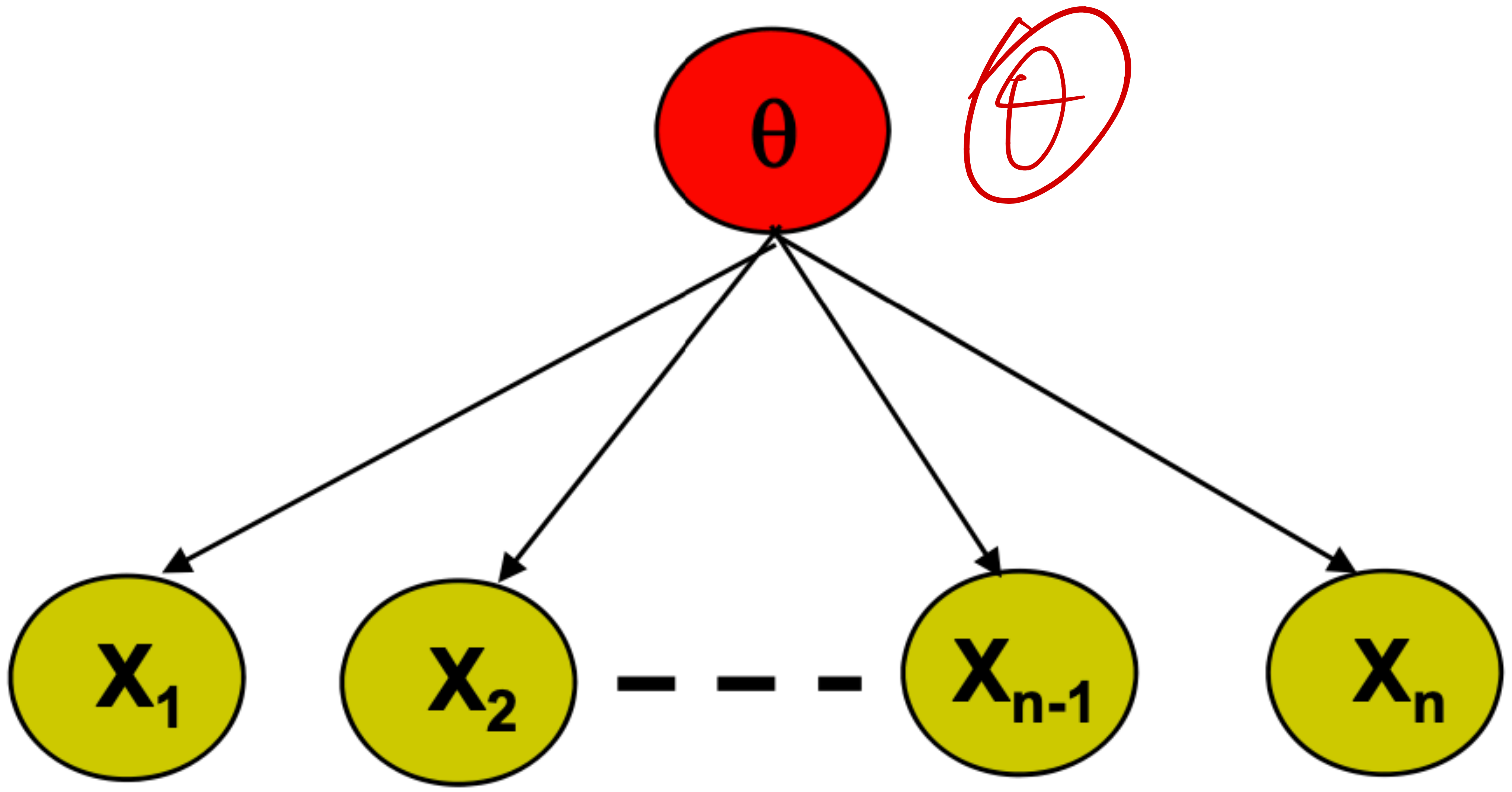

Model parameters

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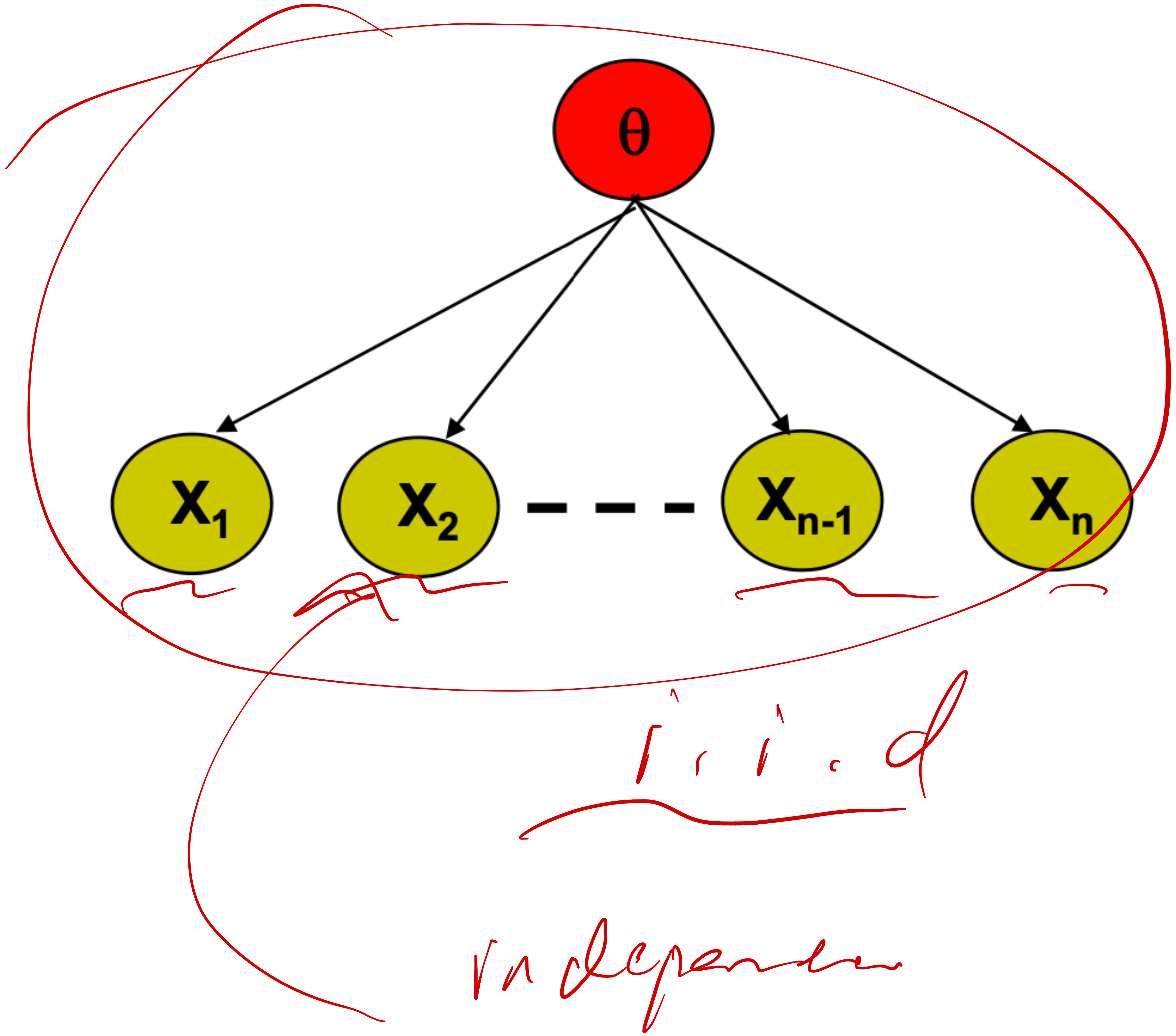

Model parameters

Data {X1, X2 …. Xn}

“Plate” Notation

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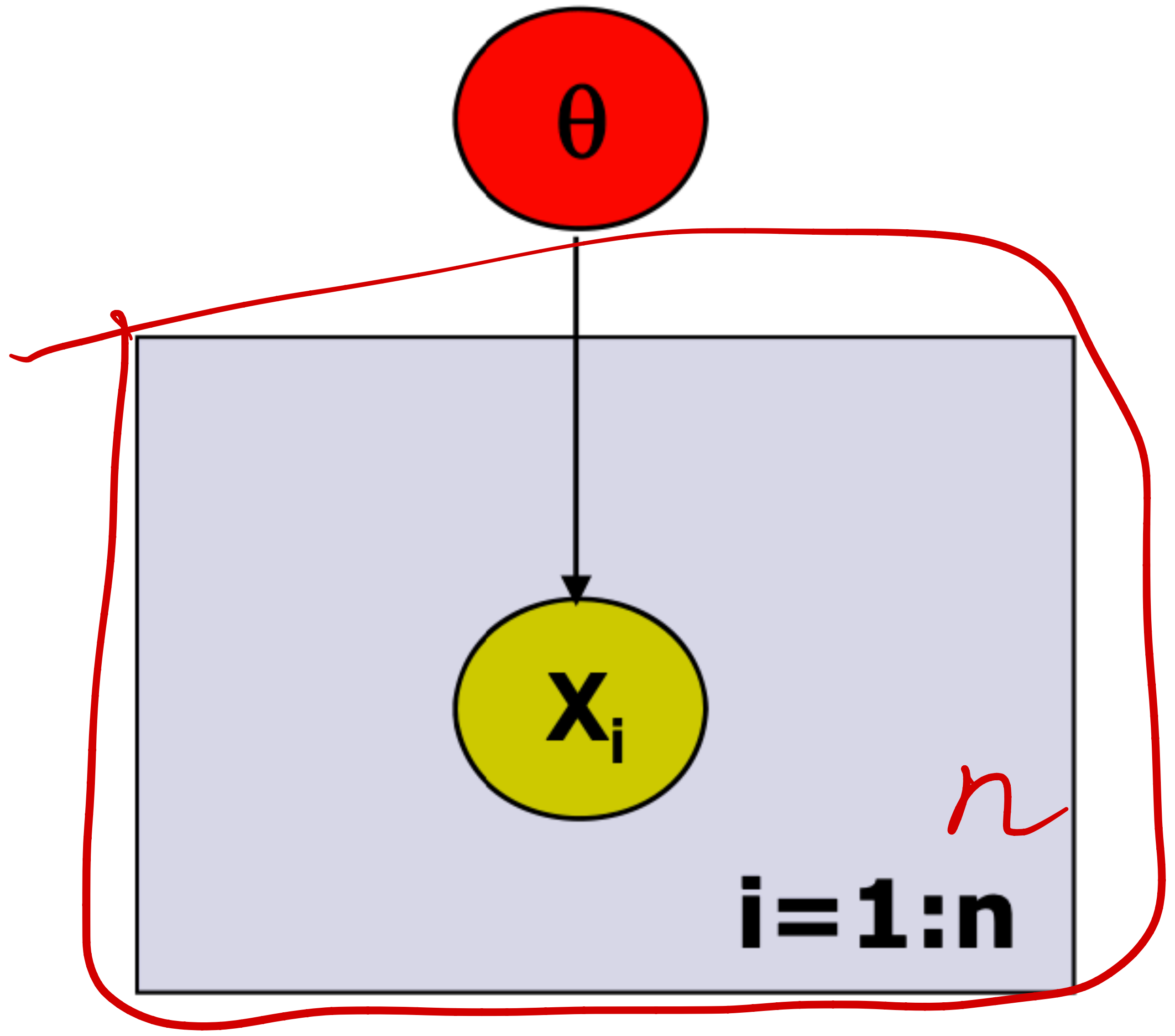

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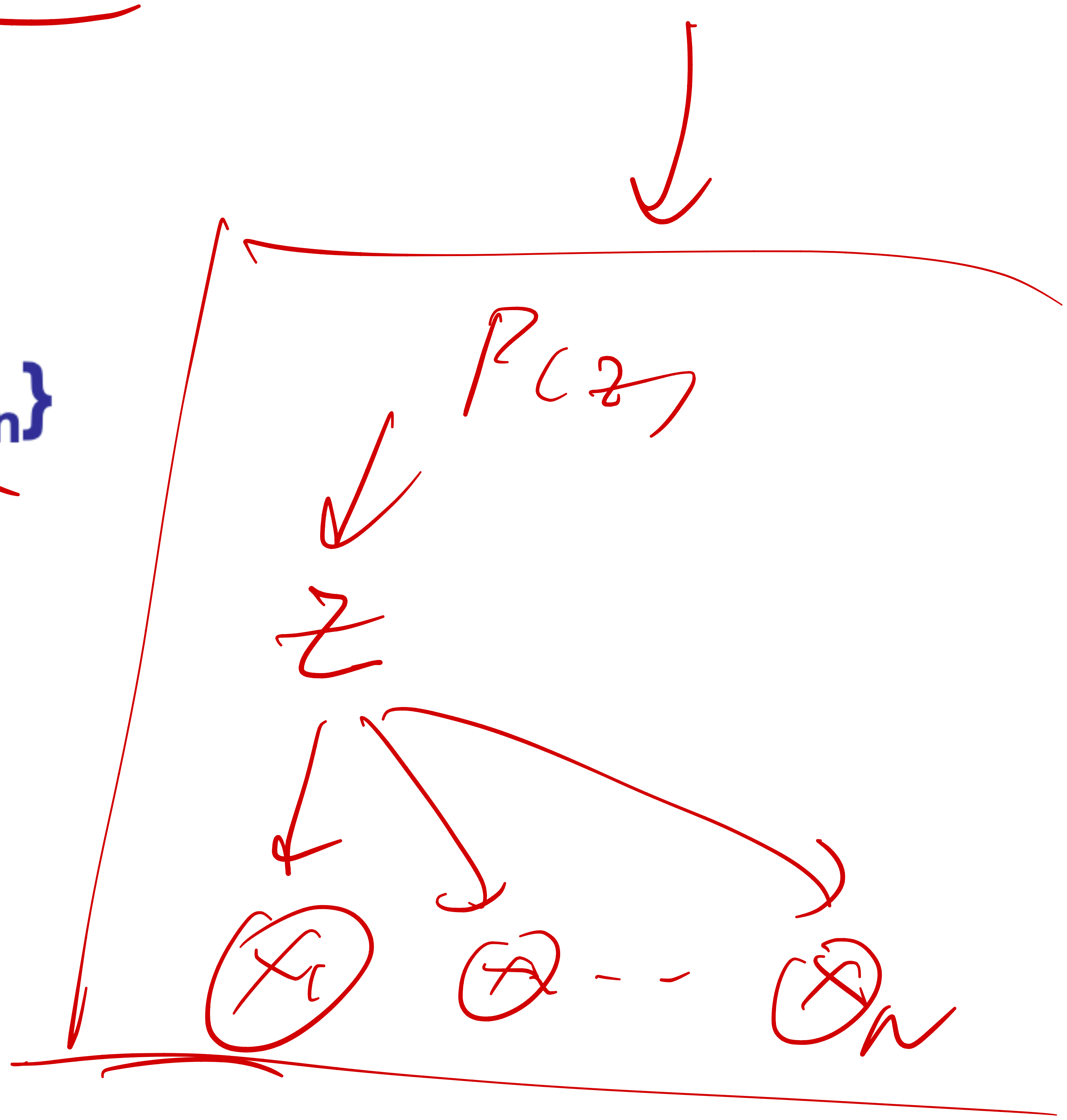

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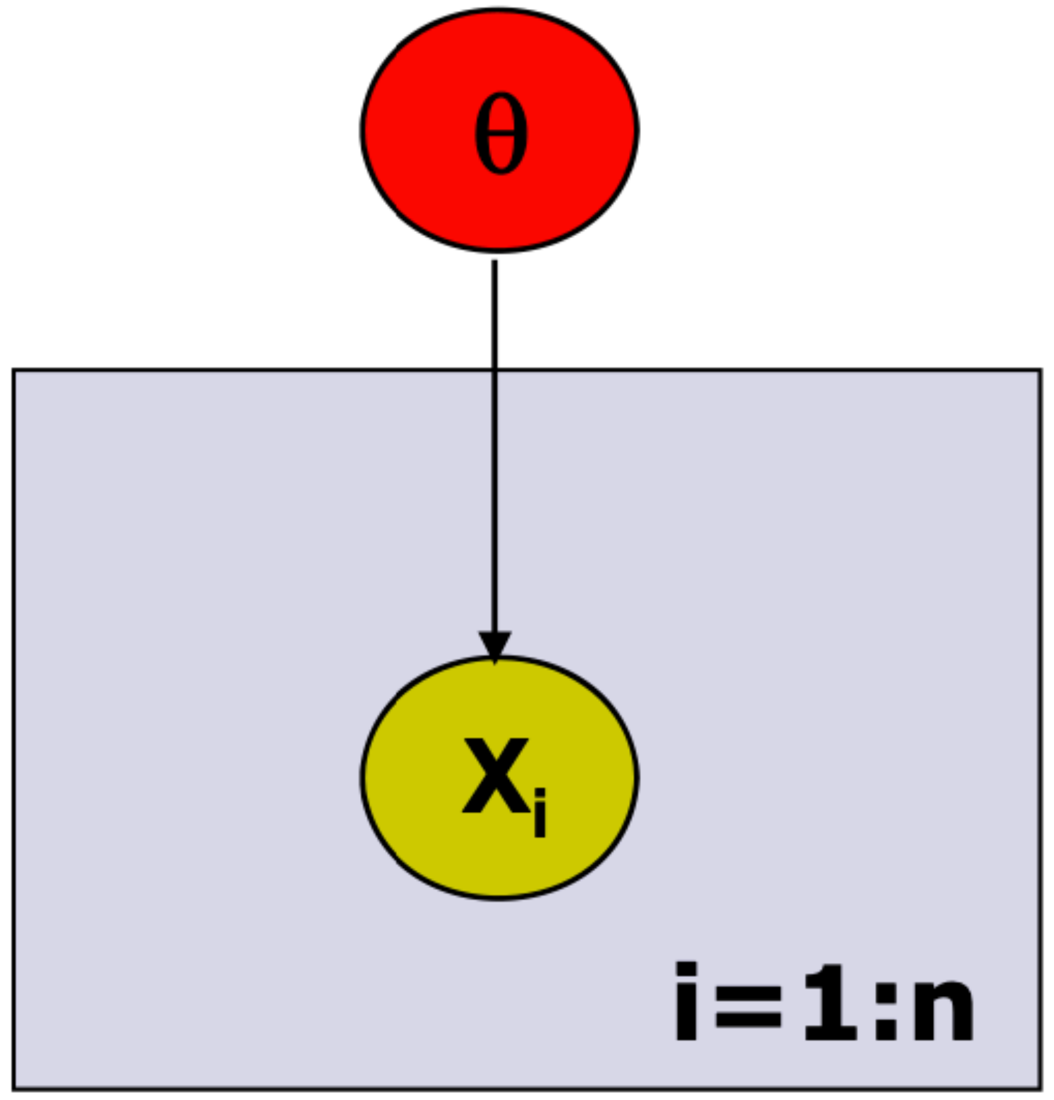

Model parameters

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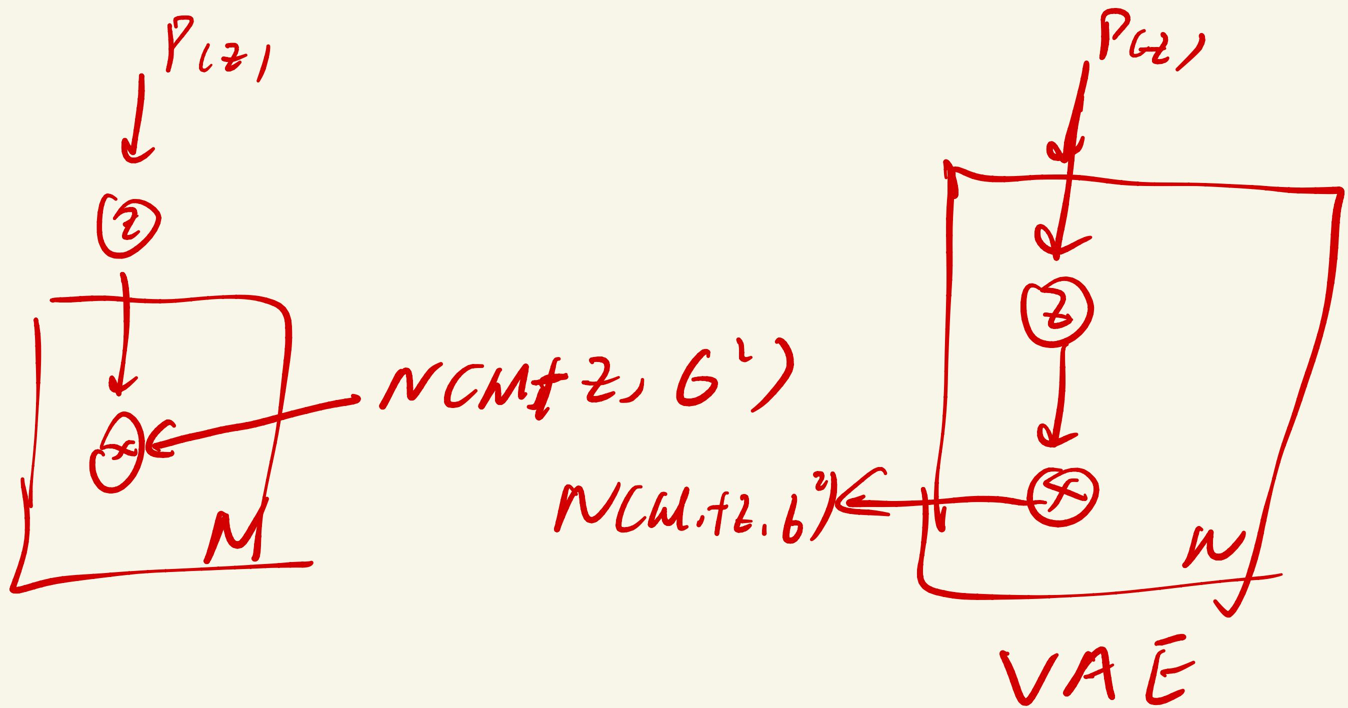
variables within a plate are replicated
in a conditionally independent manner



P(z)
N(Mf(z), σ²)
M
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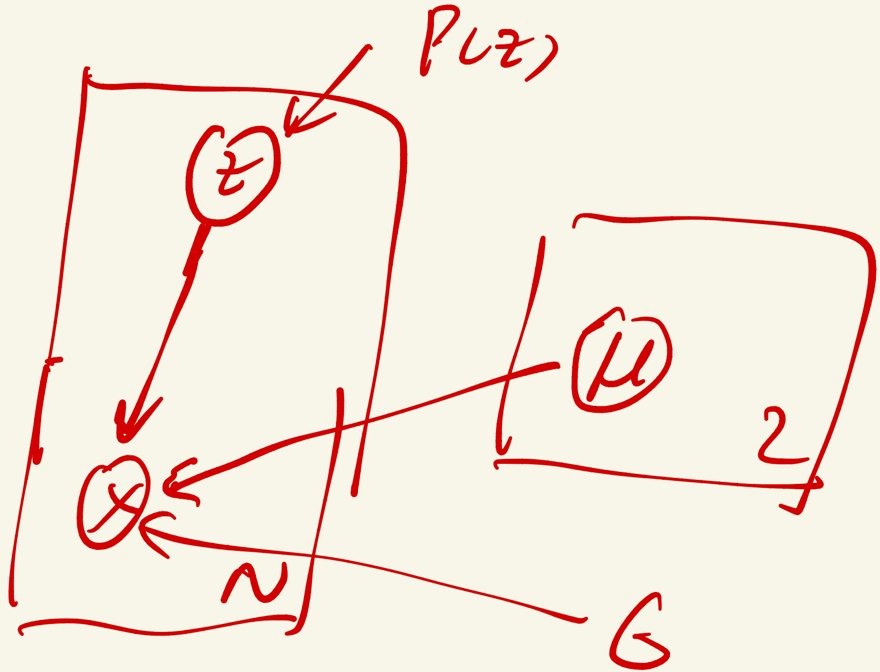
N
VAE

midterm clust BMM

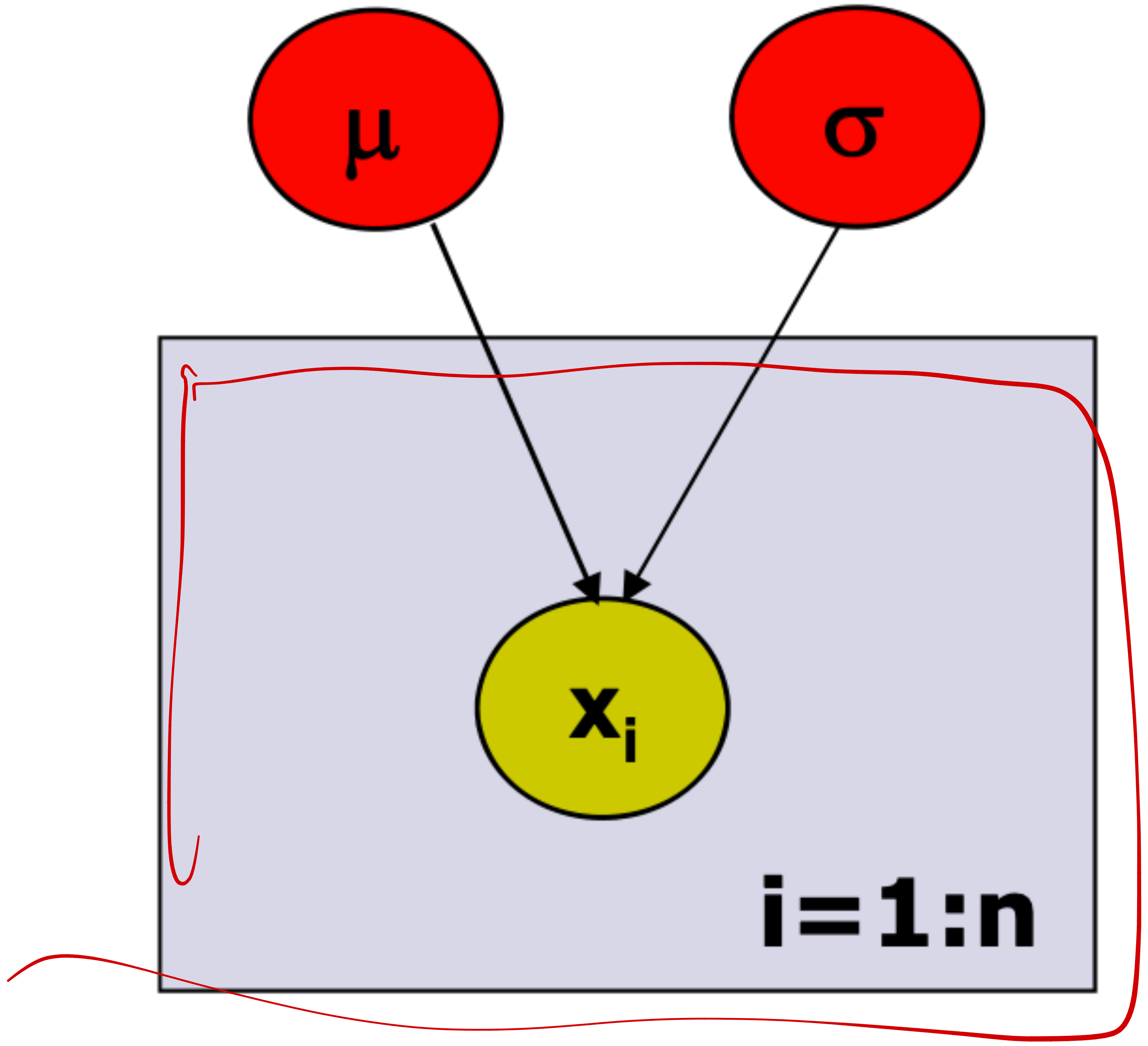


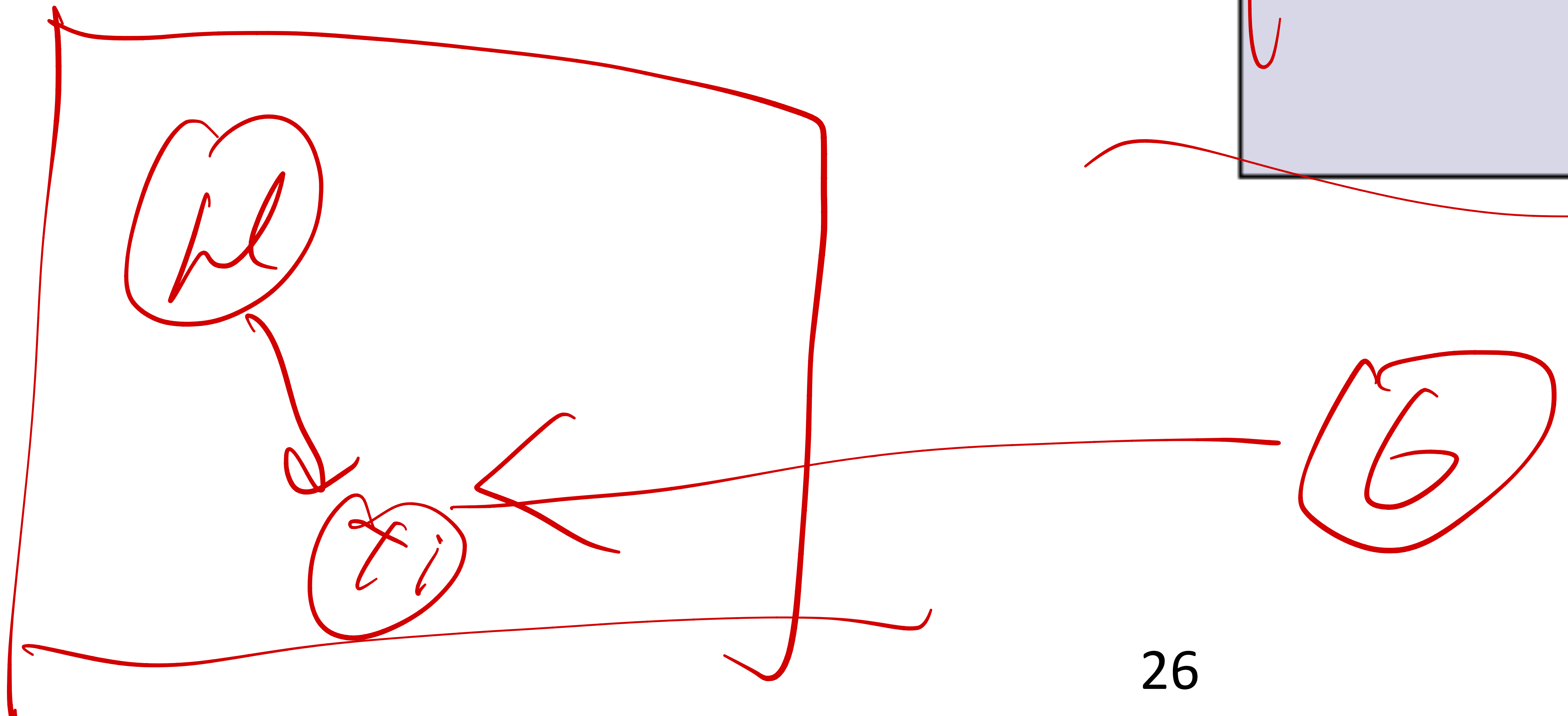
Example: Gaussian Model

Generative model:

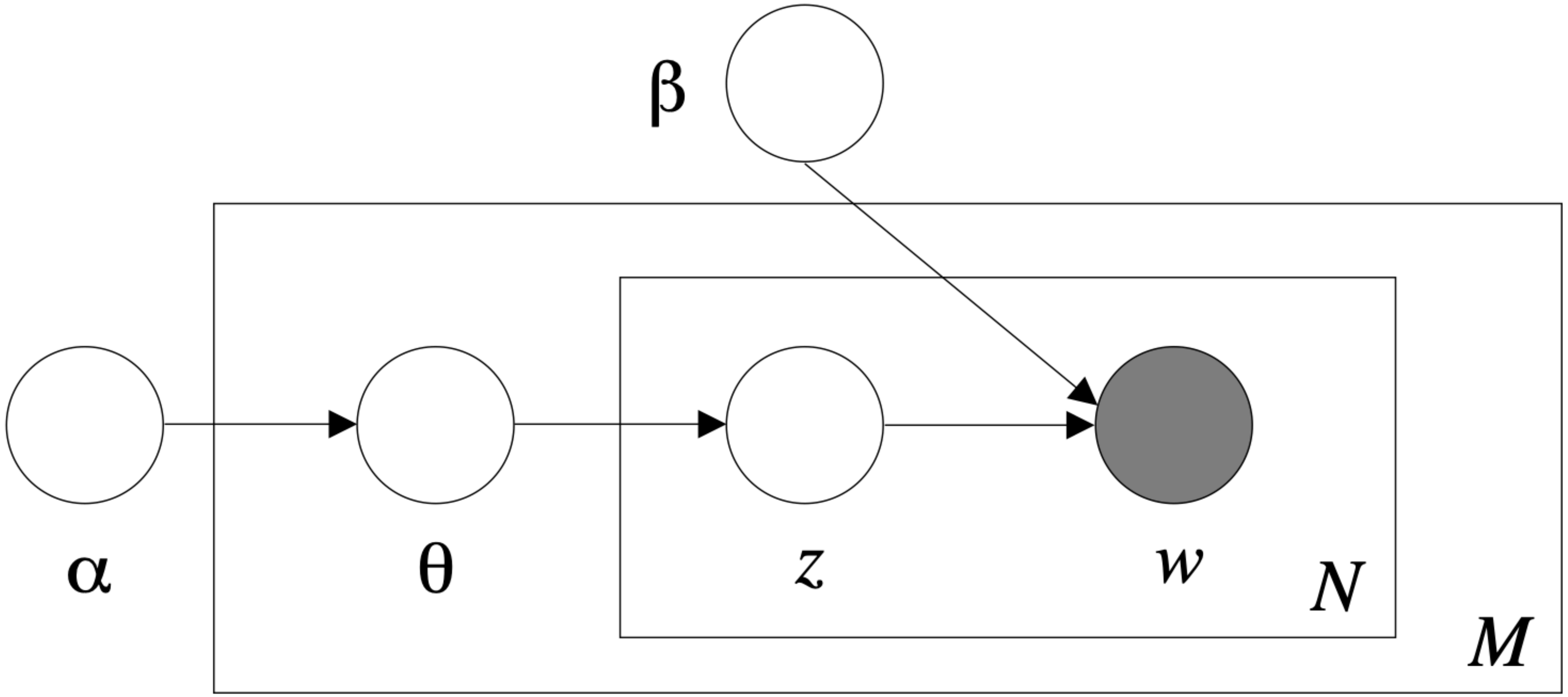
$$p(x_1,\ldots x_n \mid \mu, \sigma) = \prod p(x_i \mid \mu, \sigma)$$
$$= p(\text{data} \mid \text{parameters})$$
$$= p(D \mid \theta)$$

where $\theta = \{\mu, \sigma\}$





Observed Variable and Latent Variable Notations



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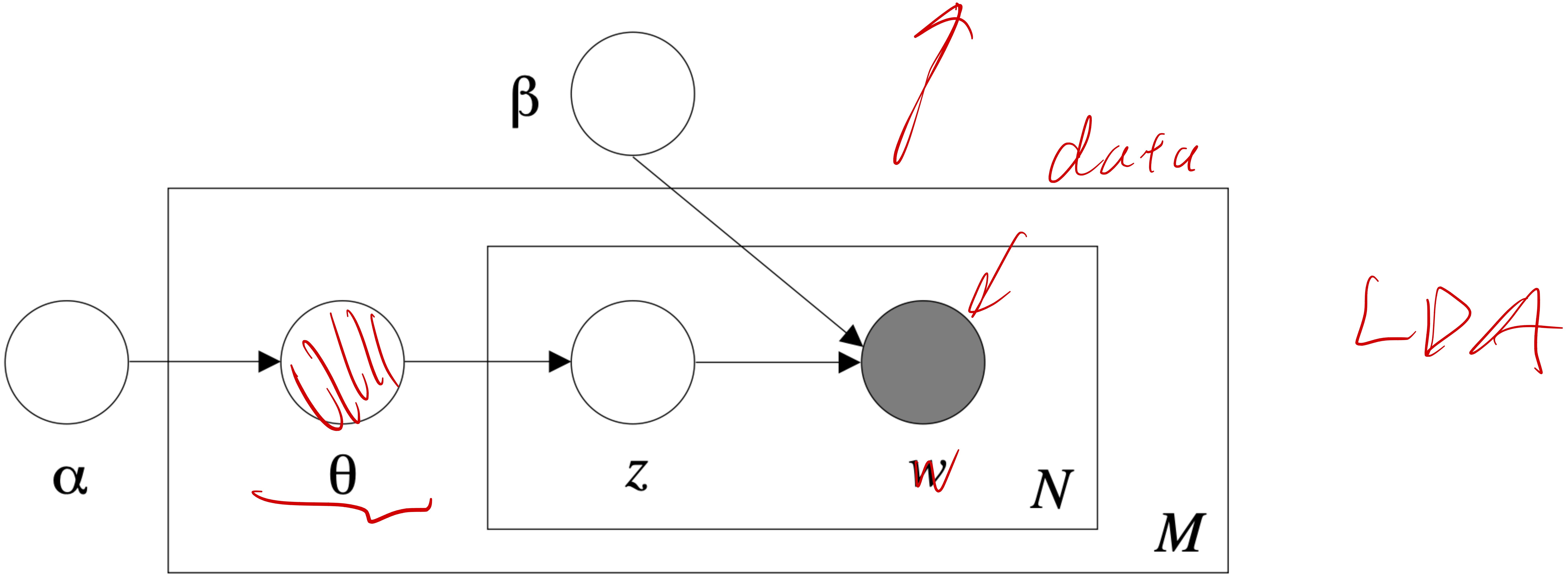

We typically use gray variables to denote observed variables

Gaussian Mixture Model / Gaussian Discriminative Analysis in PGMs

Inference and Learning

Inference and Learning

- Task 1: How do we answer **queries** about P?
  - We use **inference** as a name for the process of computing answers to such queries

Inference and Learning

Query a node (random variable) in the graph

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- Task 2: How do we estimate a **plausible model** M from data D?

  i. We use **learning** as a name for the process of obtaining point estimate of M.

Examples

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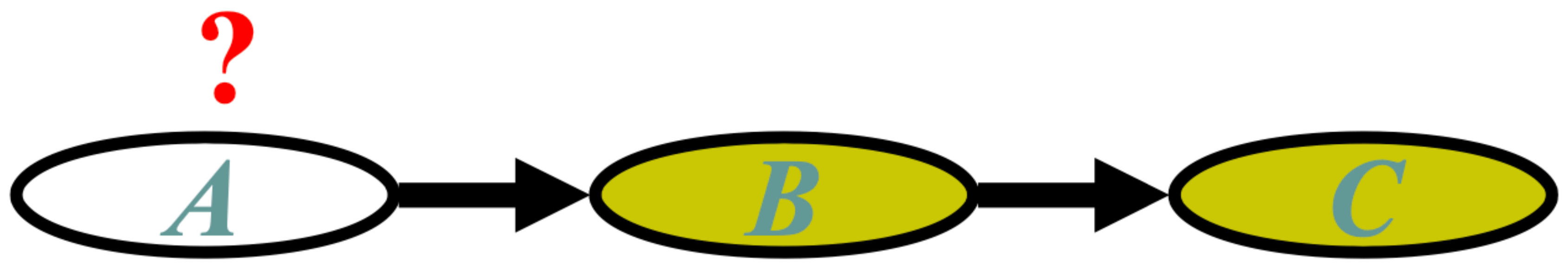

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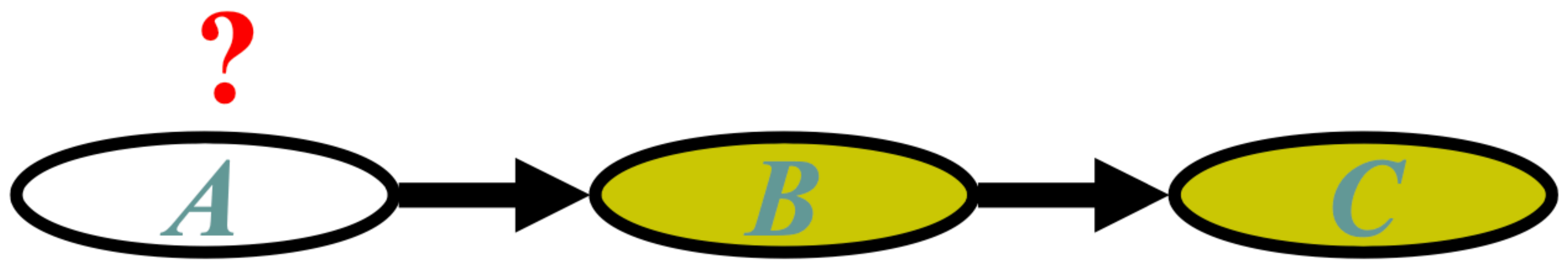

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In practice, the observed variable is often the data that is on the leaf nodes

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1. When θ is the parameter and does not have prior —> MLE

$$p(x, z; \theta)$$

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$$p(x, z; \theta)$$

2. When we add the prior over θ —> MAP (Bayesian)

$$p(x, z, \theta)$$

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Expectation Maximization!

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This process is referred to as inference

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Variational Autoencoders

Elimination Algorithm/ Marginalization

$$P(h) = \sum_{g} \underbrace{\sum_{f}\sum_{e}\sum_{d}\sum_{c}\sum_{b}}\sum_{a} P(a,b,c,d,e,f,g,h)$$

a naïve summation needs to enumerate over an exponential number of terms

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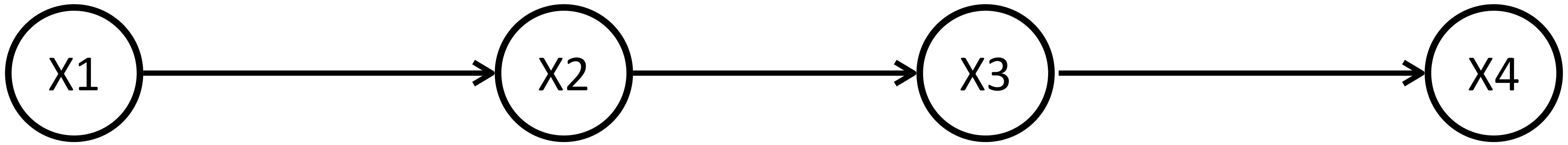

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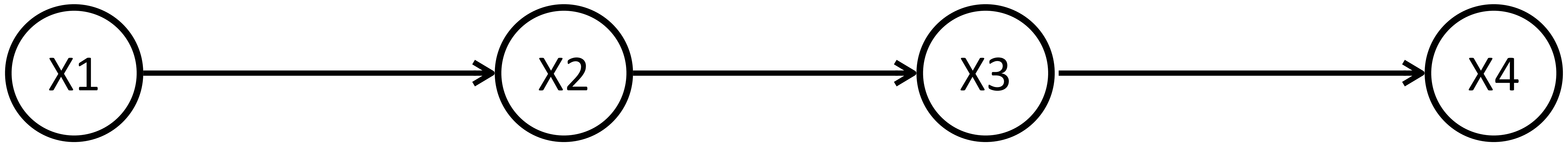

What if the random variables follow this chain structure?

Thank You!
Q & A