Machine Learning for Graphs and Sequential Data

Recap: Bayesian Networks

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Data Analytics and
Machine Learning

Challenge

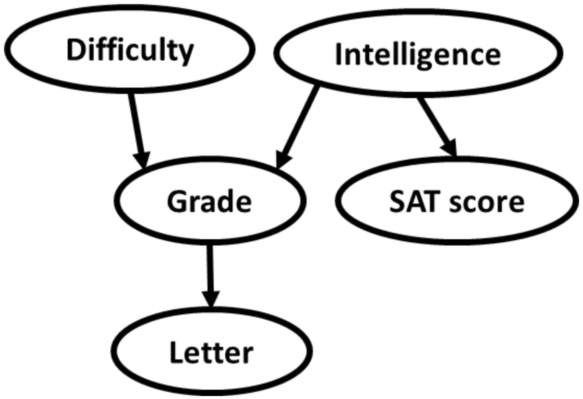
How to model $\Pr(X_1, \ldots, X_T)$, e.g. a distribution over sequences?

- Assume that X_t can take, e.g., values in $\{1, \ldots, K\}$.
- Challenge: In general, we need $K^T - 1$ parameters to specify a distribution over the sequence $X_1, \ldots, X_T$.

- To have a more compact representation and to reduce the number of parameters, we make additional assumptions about the joint distribution $\Pr(X_1, \ldots, X_T)$.
  - These assumptions should be a natural-fit for the data/task.
  - We use **Bayesian networks** (i.e. directed graphical models) to illustrate the assumptions on $\Pr(X_1, \ldots, X_T)$.

Directed Graphical Models (Bayesian Networks)

- Bayesian network is a way to represent a joint distribution via a directed acyclic graph $G = (V, E)$.
  - Each node represents a random variable.
  - Directed edges are often interpreted as causal relations.



$variables \in \{0\!: low, 1\!: high\}$

- Graph G provides:

  1) a particular factorization for the joint distribution $Pr(X_1, \dots, X_{|V|})$.

  2) a set of conditional independencies, inferred by a routine $d\_separation(G)$.

Example from: [Daphne Koller and Nir Friedman. 2009. Probabilistic Graphical Models: Principles and Techniques. The MIT Press].

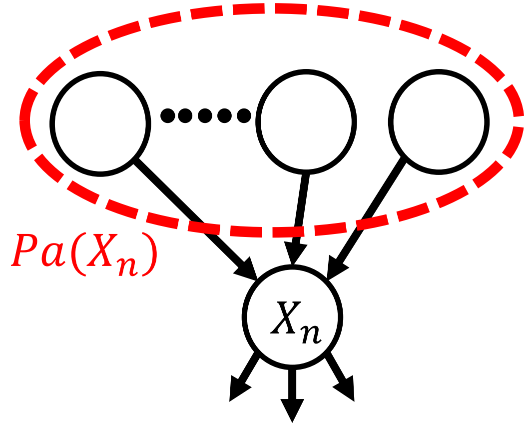
Recall: $X \perp Y | Z \iff \Pr(X, Y|Z) = \Pr(X|Z) \Pr(Y|Z)$

Bayesian Networks - Factorization

- A Bayesian network specifies the following factorization for the joint distribution $\Pr(X_1, \dots, X_{|V|})$.

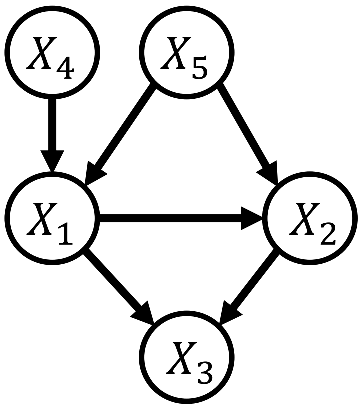
$$\Pr(X_1, \dots, X_{|V|}) = \prod_{n=1}^{|V|} \Pr(X_n | Pa(X_n))$$

  – $Pa(X_n)$: parents of node X_n in Graph G.



- Example:

$$\Pr(X_1, X_2, X_3, X_4, X_5) =$$



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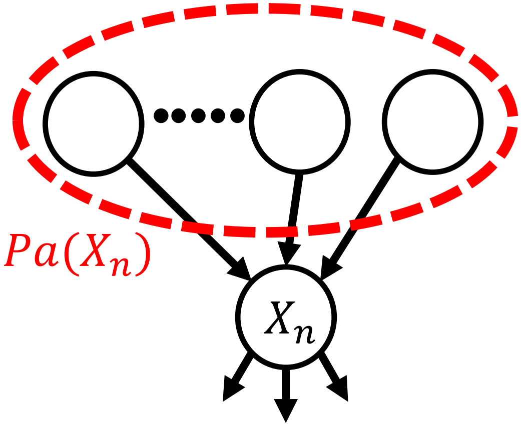

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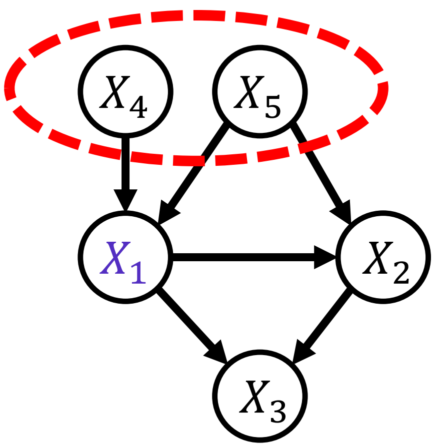

$$\Pr(X_1, X_2, X_3, X_4, X_5) =$$

$$\Pr(X_1 | X_4, X_5) \times$$

$$\boxed{Pa(X_1) = \{X_4, X_5\}}$$

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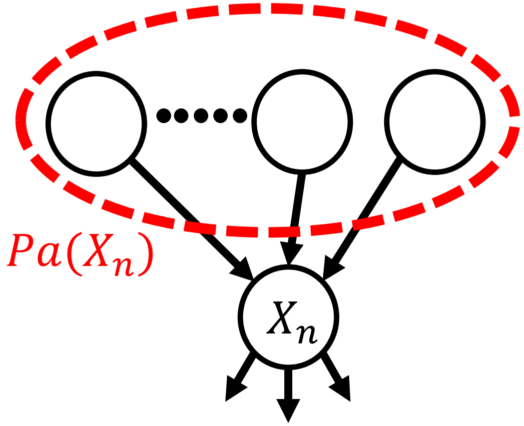

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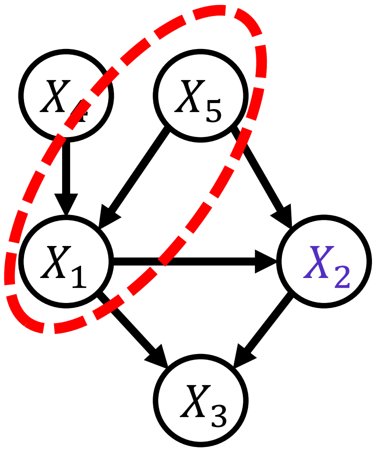

$\Pr(X_1, X_2, X_3, X_4, X_5) =$

$\Pr(X_1 | X_4, X_5) \times \Pr(X_2 | X_1, X_5) \times$

$\boxed{Pa(X_2) = \{X_1, X_5\}}$

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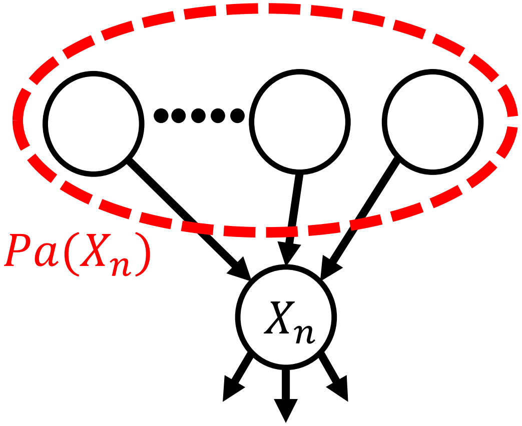

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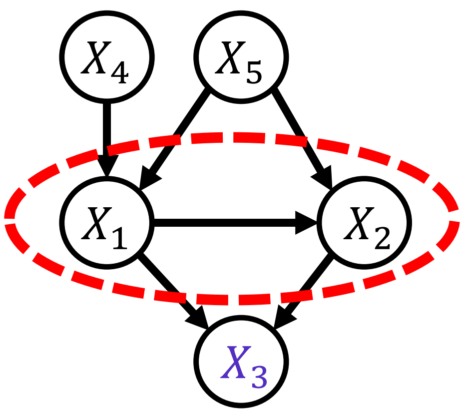

$$\Pr(X_1, X_2, X_3, X_4, X_5) =$$

$$\Pr(X_1 | X_4, X_5) \times \Pr(X_2 | X_1, X_5) \times \Pr(X_3 | X_1, X_2) \times$$

$$\boxed{Pa(X_3) = \{X_1, X_2\}}$$

Bayesian Networks - Factorization

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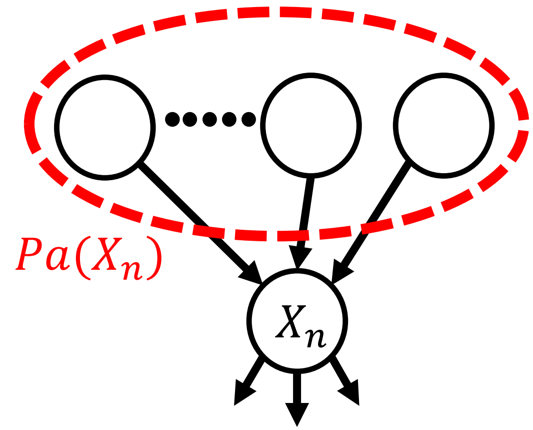
  - $Pa(X_n)$: parents of node X_n in Graph G.



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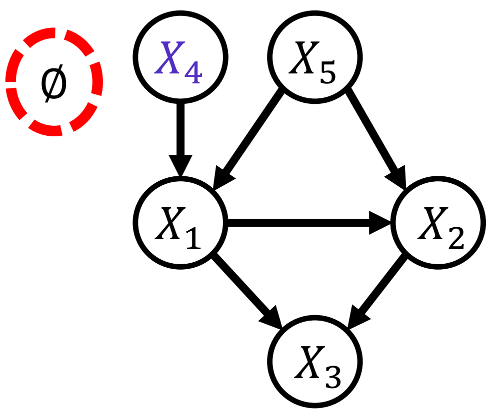

$$\Pr(X_1, X_2, X_3, X_4, X_5) =$$

$$\Pr(X_1|X_4, X_5) \times \Pr(X_2|X_1, X_5) \times \Pr(X_3|X_1, X_2) \times \Pr(X_4) \times$$

$$\boxed{Pa(X_4) = \emptyset}$$

Bayesian Networks - Factorization

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$$\Pr(X_1, \dots, X_{|V|}) = \prod_{n=1}^{|V|} \Pr(X_n | Pa(X_n))$$

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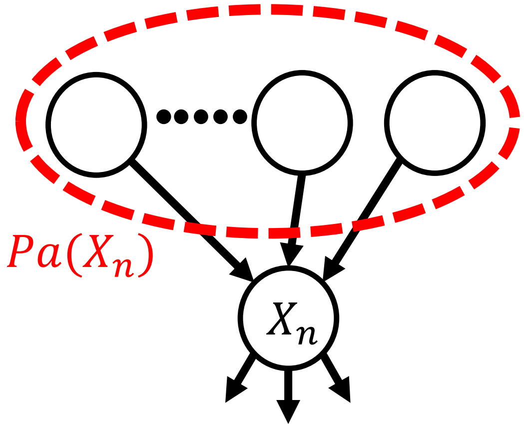

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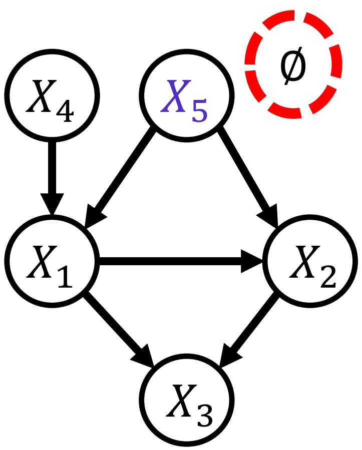


$$\Pr(X_1, X_2, X_3, X_4, X_5) =$$

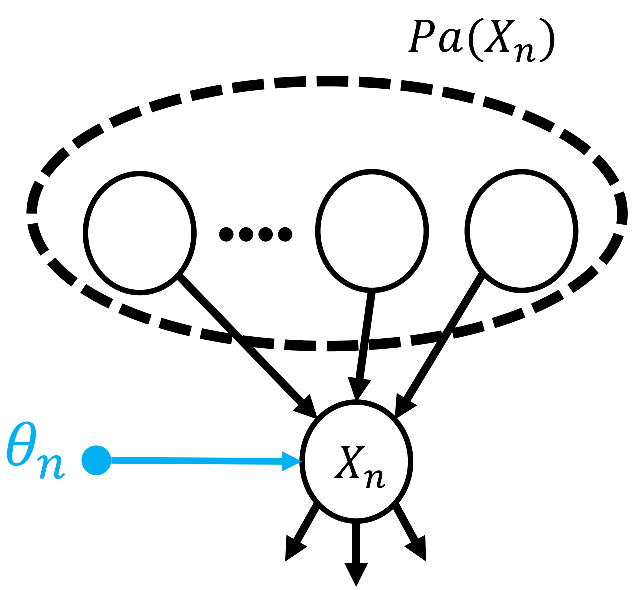
$$\Pr(X_1 | X_4, X_5) \times \Pr(X_2 | X_1, X_5) \times \Pr(X_3 | X_1, X_2) \times \Pr(X_4) \times \Pr(X_5)$$

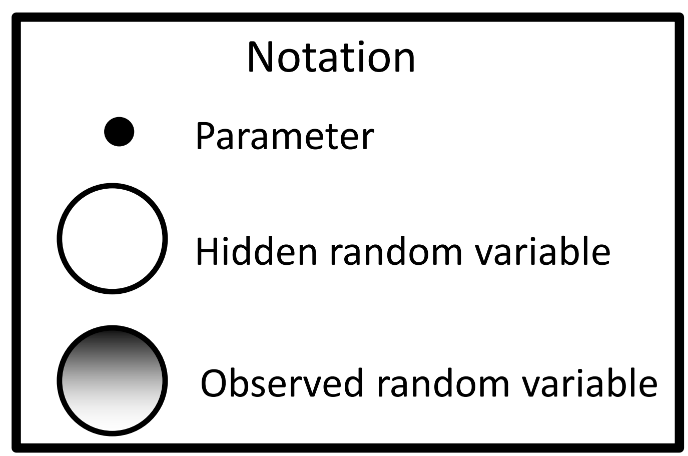
$$\boxed{Pa(X_5) = \emptyset}$$

Bayesian Networks - Model Parameters

- A set of parameters $\{\theta_1, \dots, \theta_{|V|}\}$ parametrizes the joint distribution.
- θ_n parametrizes the factor $\Pr\big(X_n | Pa(X_n)\big)$
  - Indeed, the factor is a function of θ_n as well.

    We can write $\Pr(X_n | Pa(X_n)\ ; \theta_n\ )$.
  - In a graphical model, we show θ_n using a filled circle connected to X_n.





$P(D) \cdot P(I) \cdot P(G|D,I) \cdot P(S|I) \cdot P(L|G)$

Bayesian Networks - Model Parameters

NAIV 2^5-1

- Example:

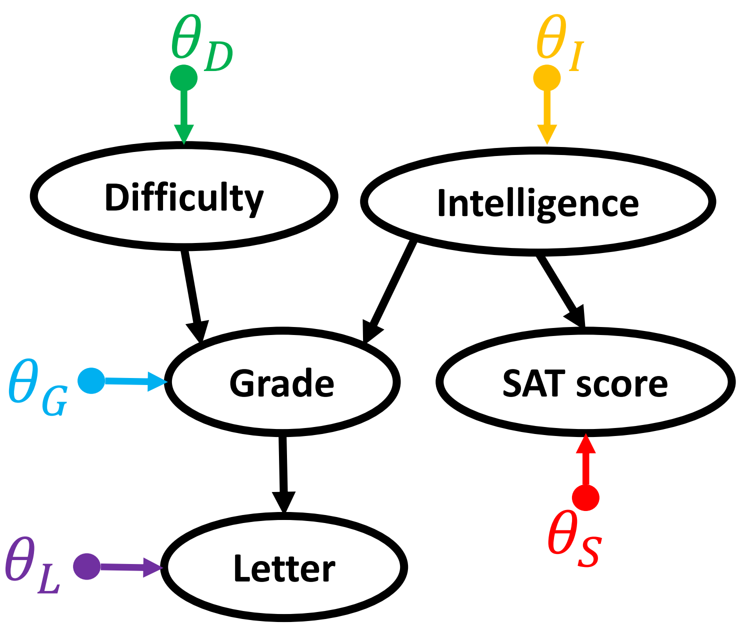
vs 10

$\Pr(D=0)$	$\Pr(D=1)$
0.5	0.5

$\Pr(I=0)$	$\Pr(I=1)$
0.5	0.5

$variables \in \{0: low, 1: high\}$

D	I	$\Pr(G=0 \mid D,I)$	$\Pr(G=1 \mid D,I)$
0	0	0.5	0.5
0	1	0.1	0.9
1	0	0.9	0.1
1	1	0.5	0.5



I	$\Pr(S=0 \mid I)$	$\Pr(S=1 \mid I)$
0	0.9	0.1
1	0.1	0.9

G	$\Pr(L=0 \mid G)$	$\Pr(L=1 \mid G)$
0	0.9	0.1
1	0.1	0.9

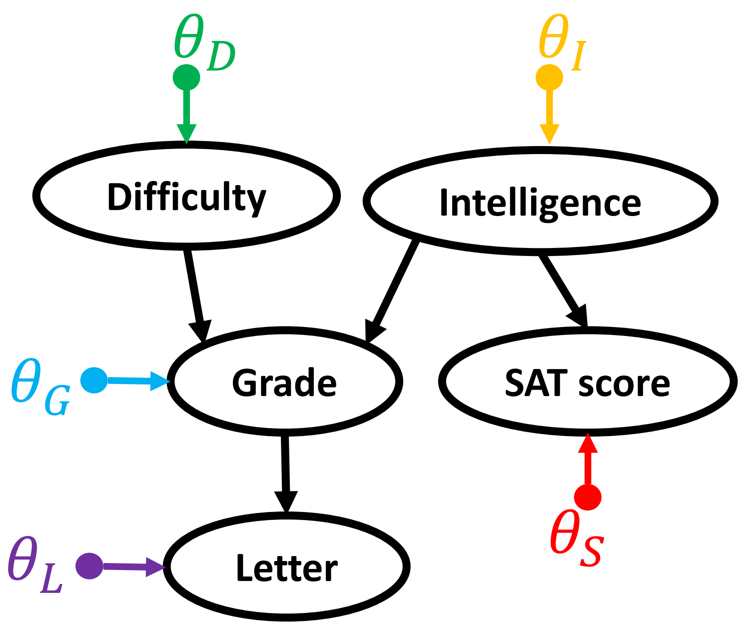
Example from: [Daphne Koller and Nir Friedman. 2009. Probabilistic Graphical Models: Principles and Techniques. The MIT Press].

Bayesian Networks – Generative Process

$z \sim \mathcal{N}(0,1)$

$x \sim \mathcal{N}(f(z),1)$

- We can think of the model as a generative process



$$
\begin{aligned}
Difficulty &\sim p(D|\theta_D)\\
Intelligence &\sim p(I|\theta_I)\\
Grade &\sim p(G|D, I,\ \theta_G)\\
SAT &\sim p(S|I,\ \theta_S)\\
Letter &\sim p(L|G,\ \theta_L)
\end{aligned}
$$

Example from: [Daphne Koller and Nir Friedman. 2009. Probabilistic Graphical Models: Principles and Techniques. The MIT Press].