CPSC 540: Machine Learning

Directed Acyclic Graphical Models

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University of British Columbia

Winter 2016

Admin

- Assignment 3:
  - Due today, 1 late day to hand it in Thursday.
- Assignment 4:
  - Out, due in 2 weeks.
- Thursday;
  - Rich Sutton in DMP 110 at 3:30 (cancelling class):
    "The Future of Artificial Intelligence"
- Friday:
  - Julien Mairal in ICICS 146 at 5:00.
- Monday:
  - Monday: CVPR Area Chair Workshop;
    `http://cvpr2016.thecvf.com/events/ac_workshop`.

Course Roadmap

- Topic 1 was supervised learning: modeling $p(y^i|x^i)$.
  - Regresion models, change of basis, cross-validation, regularization/MAP.
  - Robust/logistic losses, structured sparisty, convex optimization, kernels, duality.

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  - We'll start clarifying this in topic 5, where we'll also start relaxing IID...

Independence of Random Variables

- Let A and B are random variables taking values $a \in \mathcal{A}$ and $b \in \mathcal{B}$.
- We say that A and B are independent if we have

$$p(a, b) = p(a)p(b),$$

  for all a and b.
- This is true iff $p(a, b) = f(a)g(b)$ for some functions f and g.

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$$p(a) = \frac{p(a, b)}{p(b)} = p(a|b).$$

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  for all a and b.
- By the same logic it's also equivalently to $p(b|a) = p(b)$.
- We sometimes write this as $A \perp B$.

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- If we are talking about d variables x_j, we say they're mutually independent if

$$p(x_1, x_2, \dots, x_d) = \prod_{j=1}^{d} p(x_j), \text{ or } p(x_j | x_{-j}) = p(x_j) \text{ for all } j.$$

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    so the x_j are independent and $p(x_j|x_{-j}) = p(x_j)$.
  - In a mixture of (product of Bernoullis) the x_j are not independent:
    - Knowing x_{-j} can tell you something about x_j.

Conditional Independence

- We say that A is conditionally independent of B given C if

$$p(a, b|c) = p(a|c)p(b|c),$$

or equivalently we have

$$p(a|b, c) = p(a|c) \quad \left(\text{both equal } \frac{p(a, b|c)}{p(b|c)}\right).$$

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- If you know C, then *also* knowing B would tell you nothing about A.
- We often write this as $A \perp B \mid C$ or equivalently $B \perp A \mid C$.
- In a mixture of (product of Bernoullis) model
$$p(x) = \sum_{c=1}^{k} p(z = c) \prod_{j=1}^{d} p(x_j|z = c),$$
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- In particular, we can show that

$$p(x_i, x_j|z) = p(x_i|z)p(x_j|z) \text{ and } p(x_i|x_j, z) = p(x_i|z).$$

Outline

DAG Models

- Directed acyclic graphical (DAG) use product rule, $p(a, b, c) = p(b, c|a)p(a)$, to write

$$\begin{aligned} p(x_1, x_2, \ldots, x_d) &= p(x_1)p(x_2, x_3, \ldots, x_d|x_1) \\ &= p(x_1)p(x_2|x_1)p(x_3, x_4, \ldots, x_d|x_1, x_2) \\ &= p(x_1)p(x_2|x_1)p(x_3|x_2, x_1)p(x_4, x_5, \ldots, x_d|x_1, x_2, x_3) \end{aligned}$$

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- The above always holds, but it has too many parameters:
  - For binary x_i, we need 2^d parameters for $p(x_j|x_1, x_2, \ldots, x_{j-1})$ alone

DAG Models: Parsimonious Parameterization

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- Approach 1: we can treat $p(x_j | x_{1:j-1})$ as supervised learning problem.
    - The features are $x_{1:j-1}$ and the label is x_j.
    - If we use linear model, only need $(j-1)$ parameters.
    - We can apply our tricks from Topic 1 to Topic 2.
        - Nonlinear bases, robust/logistic losses, structured sparsity, kernels, etc.

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$$p(x_j | x_{1:j-1}) = p(x_j | x_{\mathsf{pa}(j)}),$$

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  where $\text{pa}(j)$ are the parents of j.
- Specifically, we assume that $x_j \perp x_{\text{np}(j)} | x_{\text{pa}(j)}$, where $\text{np}(j)$ are non-parents.
- In binary case, if we have k parents then only need 2^{k+1} parameters.
  - We can also combine both approaches: use regression on parents.

Special Cases of DAG Models

- We can write a lot of models as special cases DAG models,

$$p(x) = \prod_{j=1}^{d} p(x_j | x_{\mathsf{pa}(j)}).$$

  - Product of independent: if $\mathsf{pa}(j) = \varnothing$ then all variables are independent,

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  - Naive Bayes: Add an extra variable y with $\text{pa}(y) = \emptyset$ and $\text{pa}(x_j) = y$,

$$p(y, x) = p(y) \prod_{j=1}^{n} p(x_j | y).$$

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  - Discriminative models (Classification using topic 1): $\text{pa}(y) = x$ and $\text{pa}(x) = \emptyset$,

$$p(y,x) = p(y|x)p(x).$$

  - Mixture models: $\text{pa}(z) = \emptyset$ and $\text{pa}(x) = z$,

$$p(x,z) = p(z)p(x|z).$$

From Probability Factorizations to Graphs

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  - By construction, the graph will be acyclic.
- Two interesting properties of the structure of this graph:
  1. Can be used to test conditional independence between arbitrary sets.
  2. Nice structures allow efficient calculation using dynamic programming.

Graph Structure Examples

With product of independent we have

$$p(x) = \prod_{j=1}^{d} p(x_j).$$

The corresponding graph structure is:

Graph Structure Examples

With Markov chain we have

$$p(x) = p(x_1) \prod_{j=2}^{d} p(x_j | x_{j-1}).$$

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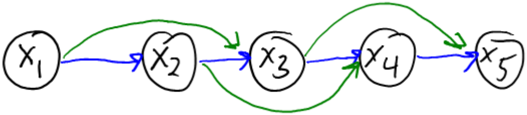
Graph Structure Examples

With second-order Markov chain we have

$$p(x) = p(x_1)p(x_2|x_1)\prod_{j=3}^{d} p(x_j|x_{j-1}, x_{j-2}).$$

The corresponding graph structure is:

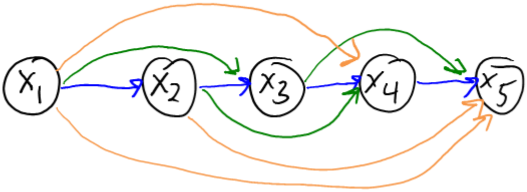


Graph Structure Examples

With general distribution we have

$$p(x) = \prod_{j=1}^{d} p(x_j | x_{1:j-1}).$$

The corresponding graph structure is:

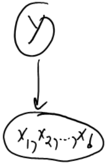


Graph Structure Examples

With Gaussian generative classifier we have

$$p(y, x) = p(y)p(x|y).$$

The corresponding graph structure is:



Graph Structure Examples

With naive Bayes or diagonal Gaussian generative classifier we have

$$p(y, x) = p(y) \prod_{j=1}^{d} p(x_j | y).$$

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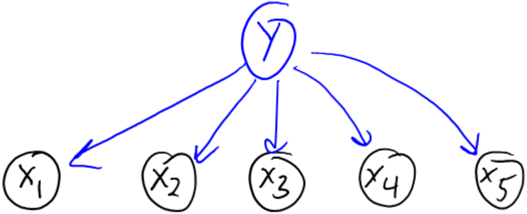
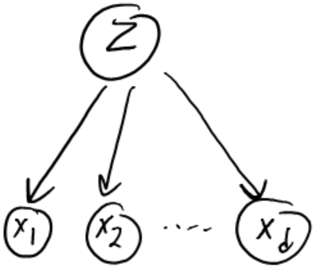


Graph Structure Examples

With mixture of independent we have

$$p(z, x) = p(z) \prod_{j=1}^{d} p(x_j | z).$$

The corresponding graph structure is:



Graph Structure Examples

With mixture of Gaussian we have

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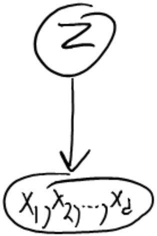
The corresponding graph structure is:



Graph Structure Examples

With probabilistic PCA we have

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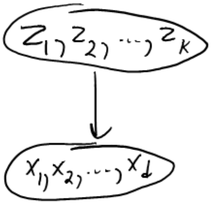
The corresponding graph structure is:



Graph Structure Examples

With hidden Markov models we have

$$p(z, x) = p(z_1) \left(\prod_{j=2}^{d} p(z_j | z_{j-1}) \right) \left(\prod_{j=1}^{n} p(x_j | z_j) \right).$$

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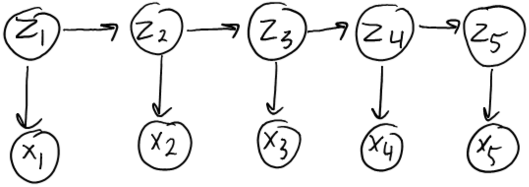

Graph Structure Examples

We can do multi-output regression/classification via conditional DAGs,

$$p(y, x) = p(x) \prod_{c=1}^{k} p(y_c | y_{\text{pa}(c)}, x)$$

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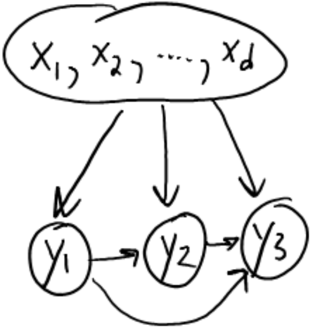
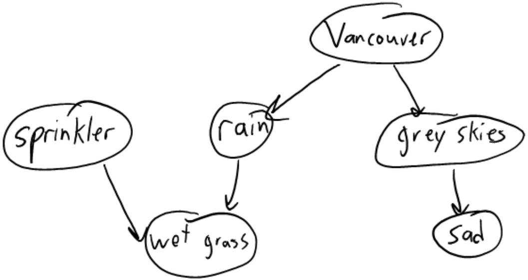


Graph Structure Examples

We can consider less-structured examples,

$$p(S, V, R, W, G, D) = p(S)p(V)p(R|V)p(W|S, R)p(G|V)p(D|G).$$

The corresponding graph structure is:

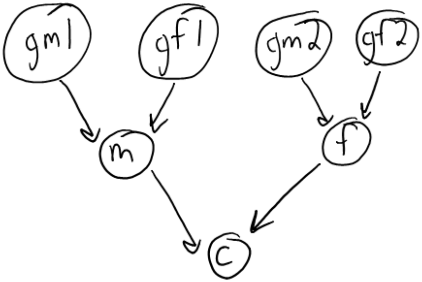


Graph Structure Examples

We can consider phylogeny (family trees):

$$
\begin{aligned}
&p(gm1, gf1, gm2, gf2, m, f, c) \\
&= p(gm1)p(gf1)p(gm2)p(gf2)p(m|gm1, gf1)p(f|gm2, gf2)p(c|m, f).
\end{aligned}
$$

The corresponding graph structure is:



Outline

D-Separation: From Graphs to Conditional Independence

- The graph represents conditional independence implied by factorization.
- Can we use the graph to test generic conditional independence statements?
  - Yes, variables are independent if all paths are block by d-separation.
- The rules are best illustrated by example...

D-Separation Case 0 (No Paths and Direct Links)

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- Direct link: x is the parent of y,

  We have $x \not\perp y$: knowing x tells you about y (direct paths aren't blockable).

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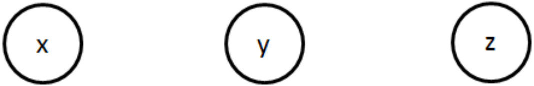

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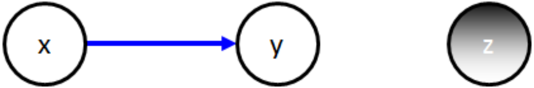

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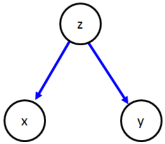

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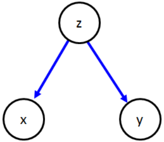

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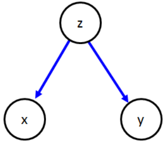

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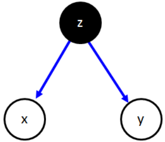

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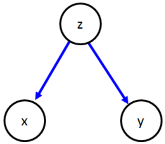

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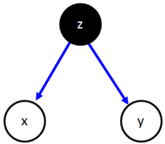

    In this case $x \perp y \mid z$: knowing z "breaks" dependence between x and y.

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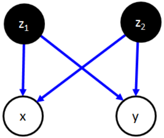

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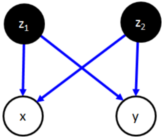

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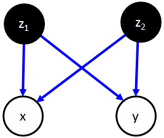

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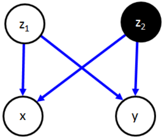
  - But if we only observe z_2:



Then we have $x \not\perp y \mid z_2$: dependence still "flows" through z_1.

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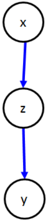

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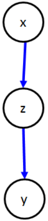

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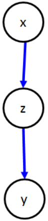

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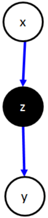

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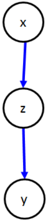

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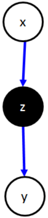

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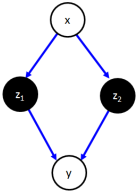

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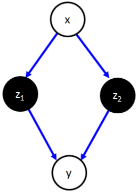

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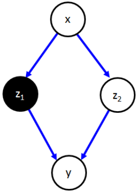

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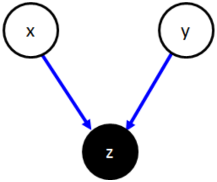

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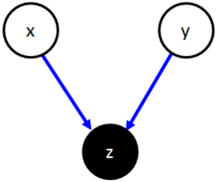

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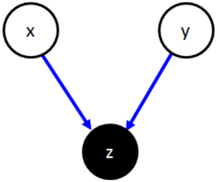

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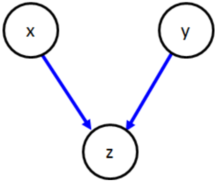

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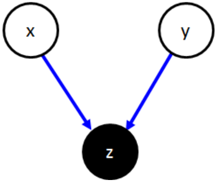

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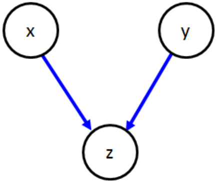

    We have $x \perp y$: if you don't observe z then x and y are independent.
- Different from Case 1 and Case 2: not observing the child blocks path.

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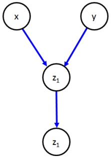

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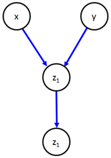

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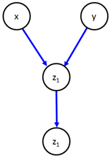

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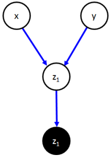

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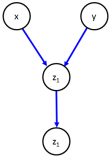

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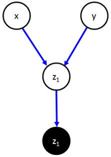

    We have $x \not\perp y \mid z_2$: grandchild creates dependence even with unobserved parent.
- Case 3 needs to consider descendants of child.

D-Separation

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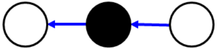

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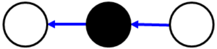
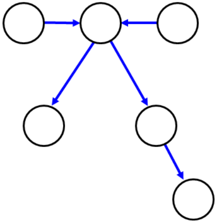


  3. P includes a "collider":



where C and all its descendants are unobserved.

Alarm Example

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- Earthquake $\not\perp$ Call.

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Alarm Example

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Outline

Discussion of D-Separation

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$$(A \text{ and } B \text{ are d-separated given } E) \Rightarrow A \perp B \mid E.$$

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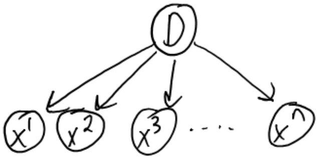
  - Or some orderings may to non-equivalent graphs.
- Nevertheless, we can do a lot with d-separation:
  - Implies every instance of independence/conditional-independence/IID we've used.

IID Assumption in DAG and Plate Notation

- Graphical representation of the IID assumption:



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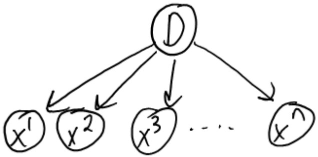

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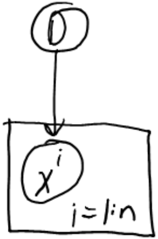
- We can concisely represent repeated parts of graphs using plate notation:



Tilde Notation in DAG and Plate Notation

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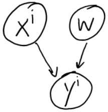
$$y^i \sim \mathcal{N}(w^T x^i, 1),$$
we can interpret it as the DAG model:



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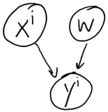
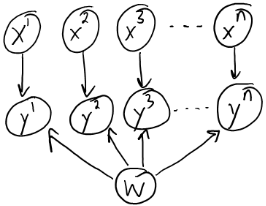
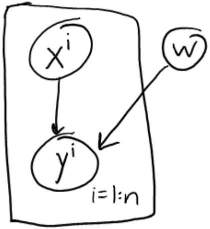


- If the x^i are IID then we can represent supervised learning as



or



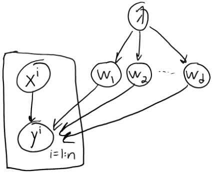
- From d-separation on this graph we have $p(y|X, w) = \prod_{i=1}^{n} p(y^i|x^i, w)$.

Tilde Notation in DAG and Plate Notation

- When we do MAP estimation under the assumptions

$$y^i \sim \mathcal{N}(w^T x^i, 1), \quad w_j \sim \mathcal{N}(0, 1/\lambda),$$

we can interpret it as the DAG model:



Tilde Notation in DAG and Plate Notation

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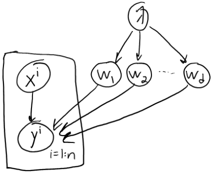
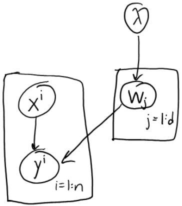


- Or introducing a second plate using:



Other Models in DAG/Plate Notation

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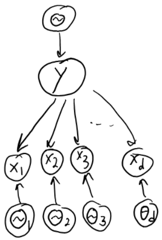
$$y^i \sim \mathrm{Cat}(\theta), \quad x^i | y^i = c \sim D(\theta_c).$$



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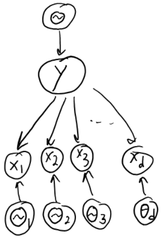
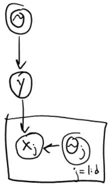


- Or in plate notation as



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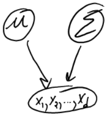

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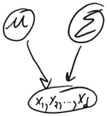
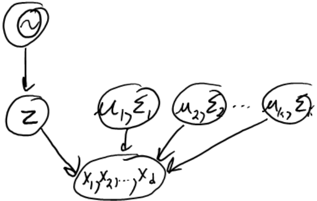
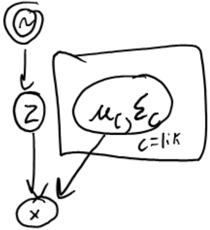


- For mixture of Gaussians we have

$$z^i \sim \text{Cat}(\theta), \quad x^i | z^i = c \sim \mathcal{N}(\mu_c, \Sigma_c).$$



or



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  - Joint distribution of models we've discussed can be written as DAG models.
- D-separation allows us to test conditional independences based on graph.
- Plate Notation lets compactly draw graphs with repeated patterns.
  - There are fancier versions of plate notation called "probabilistic programming".

- Next time: undirected graphical models and how we use graphical models.