Introduction to Probabilistic Graphical Models

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Markov Networks

Markov Networks

So far: write probability as a product of conditional distributions

$$p(x_1, \ldots, x_D) = \prod_{i=1}^{D} p(x_i \mid pa(x_i))$$

- exactly one term per variable
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- normalization constant Z or partition function

$$Z = ?$$

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- convenience notation: $p(x, y, z) \propto \phi(x, y)\phi(y, z)$ "proportional to"

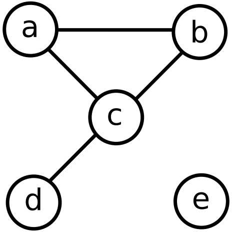
Definitions

Potential

A potential $\phi(x_1, \dots, x_D)$ is a non-negative function of the set of variables.

- special case: conditional distributions $\phi(x_1, \dots, x_D) = p(x_1 | x_2, \dots, x_D)$ as in belief networks

Markov Network



Markov Network

For a set of variables $\mathcal{X} = \{x_1, \dots, x_D\}$ a Markov network (or Markov random field) is defined as a product of potentials over the cliques $\mathcal{X}_c$ of the graph $\mathcal{G}$

$$p(x_1, \dots, x_D) = \frac{1}{Z} \prod_{c=1}^{C} \phi_c(\mathcal{X}_c)$$

For example:

$$p(a, \dots, e) \propto \phi_{abc}(a, b, c)\phi_{ab}(a, b)\phi_{cd}(c, d)\phi_c(c)\phi_e(e)$$

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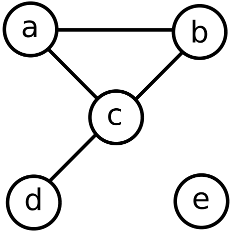

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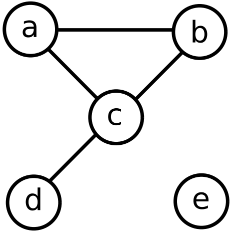

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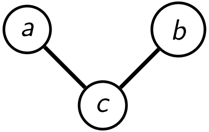
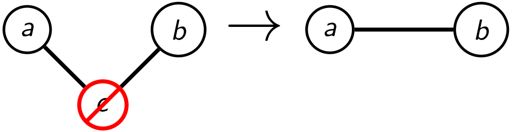
- Special case: cliques of size 2 – pairwise Markov network

Properties of Markov Networks



$$p(a, b, c) = \frac{1}{Z}\phi_{ac}(a, c)\phi_{bc}(b, c)$$



Variables are independent if they have no path between them.
Otherwise they are usually dependent.

Check (by marginalising over c): $p(a, b) \neq p(a)p(b)$.

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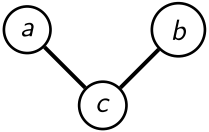

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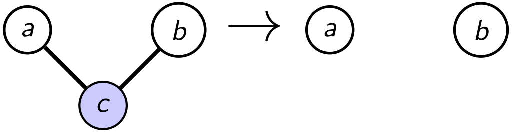


Conditioning on c makes a and b independent. Check: $p(a, b|c) = p(a|c)p(b|c)$.

Difference to directed model: there, conditioning could *introduce* dependency:

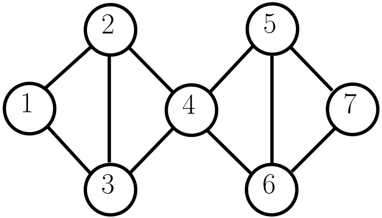
- for example, $a \rightarrow c \leftarrow b$ $\quad a \perp\!\!\!\perp b$, but $a \not\perp\!\!\!\perp b|c$

Global Markov Property

Separation

A subset $\mathcal{S}$ separates $\mathcal{A}$ from $\mathcal{B}$ if every path from a member of $\mathcal{A}$ to any member of $\mathcal{B}$ passes through $\mathcal{S}$.

Example: $\{x_4\}$ separates $\{x_1, x_2, x_3\}$ from $\{x_5, x_6, x_7\}$.



Global Markov Property

For disjoint sets of variables $(\mathcal{A}, \mathcal{B}, \mathcal{S})$ where $\mathcal{S}$ separates $\mathcal{A}$ from $\mathcal{B}$, then $\mathcal{A} \perp\!\!\!\perp \mathcal{B} \mid \mathcal{S}$

Example: $\{x_1, x_2, x_3, x_4\}$ are conditionally independent of $\{x_7\}$ conditioned on $\{x_5, x_6\}$

Gibbs Distributions

Gibbs Distribution

A probability distribution that can be written in the form $p(x) = \frac{1}{Z} e^{-E(x)}$ for a function $E : \mathcal{X} \to \mathbb{R}$ is called Gibbs distribution. E is called energy function.

In particular, a Gibbs distribution can only have strictly positive values (i.e. no zero values).

Any Markov network that has only strictly positive potentials is a Gibbs distribution:

$$p(x_1, \ldots, x_D) = \frac{1}{Z} \prod_{c=1}^{C} \phi_c(\mathcal{X}_c) = \frac{1}{Z} e^{-E(x_1, \ldots, x_D)}$$

with energy function $E(x_1, \ldots, x_D) = \sum_c E_c(\mathcal{X}_c)$ for $E_c(\mathcal{X}_c) = -\log \phi(\mathcal{X}_c)$

Gibbs distributions are often also written as

$$p(x_1, \ldots, x_D) = e^{-E(x_1, \ldots, x_D) - \log Z} = e^{-\sum_c \log \phi_c(\mathcal{X}_c) - \log Z}$$

Local Markov Property

For Markov networks that are Gibbs distributions, the so-called local Markov property holds

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$$p(x \mid \mathcal{X} \setminus \{x\}) = p(x \mid ne(x))$$

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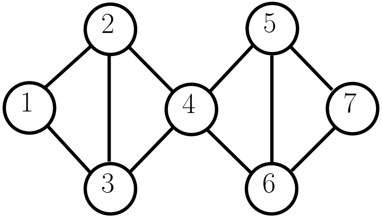
$$p(x \mid \mathcal{X} \setminus \{x\}) = p(x \mid ne(x))$$

- The set of neighboring nodes $ne(x)$ is called the Markov blanket
- This also holds for sets of variables $\Rightarrow$ simple independence check by separation

Local Markov Property – Example



- $p(x_4 \mid x_1, x_2, x_3, x_4, x_5, x_6, x_7) = p(x_4 \mid x_2, x_3, x_5, x_6)$
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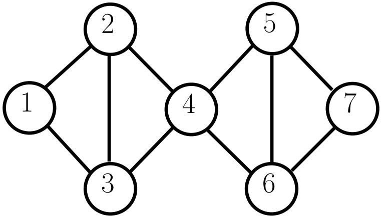

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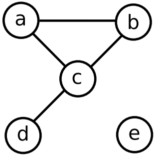
- and others

The Hammersley-Clifford Theorem

We know:



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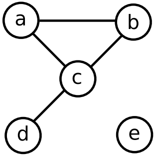

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The opposite also holds!

Hammersely-Clifford Theorem [Hammersley, Clifford, 1971]

Every positive distribution that fulfills the local Markov property with respect to a graph $\mathcal{G}$ can be written as a Markov network over $\mathcal{G}$.

Directed vs Undirected who wins?

Bayes or Markov?

- So which one is better? Directed or Undirected ?
- Both directed and undirected graphical models imply sets of conditional independences

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- Which one models more distributions? Or are they the same?

Bayes or Markov?

- So which one is better? Directed or Undirected ?
- Both directed and undirected graphical models imply sets of conditional independences
- Which one models more distributions? Or are they the same?
- First introduce “canonical” representation

Relationship directed – undirected models: maps

D Map

A graph is said to be a D map (dependency map) of a distribution if every conditional independence statement satisfied by the distribution is reflected in the graph

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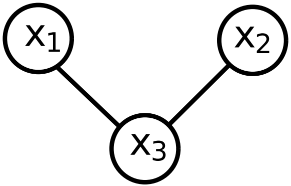

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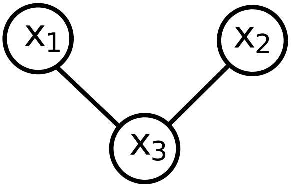

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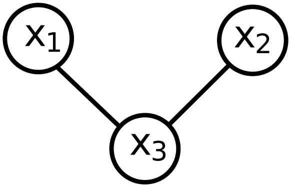
- A completely disconnected graph contains all possible independence statements for its variables
- $\Rightarrow$ it is a trivial D map for any distribution



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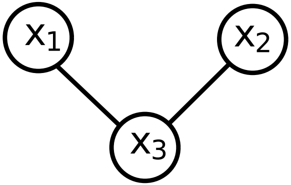

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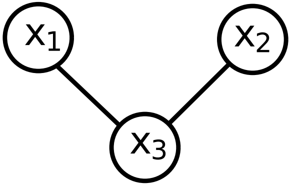

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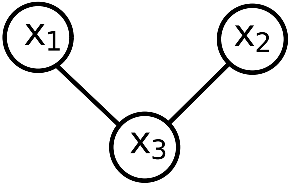
- A fully connected graph implies no independence statements
- $\Rightarrow$ it is a trivial I map for any distribution



Relationship directed – undirected models: maps

Perfect Map

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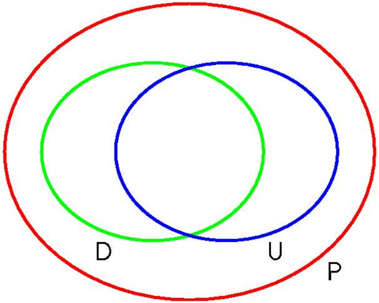
- A perfect map: Both I map and a D map of the distribution

Relationship directed – undirected GM



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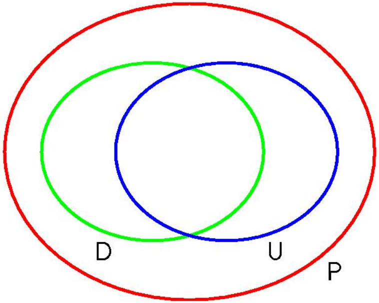
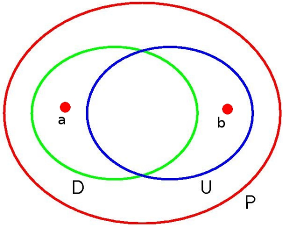
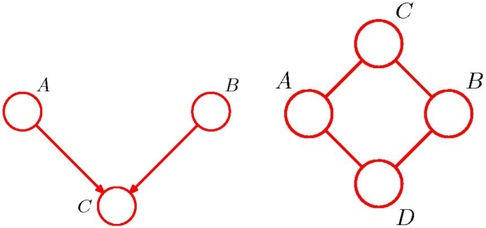


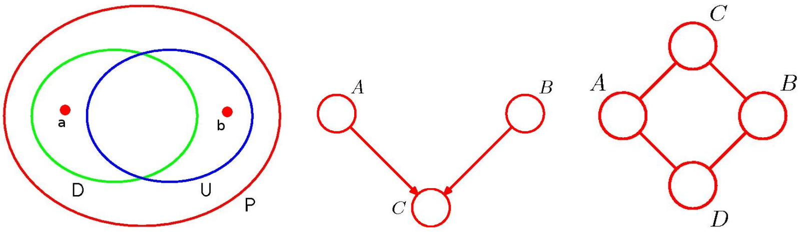
- P – set of all distributions for a given set of variables
- Distributions that can be represented as a perfect map
  - using undirected graph – U
  - using a directed graph – D





(a) (b)

- Middle: conditional independence properties cannot be expressed using an undirected graph over the same three variables



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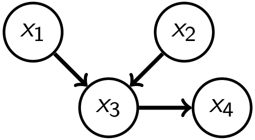
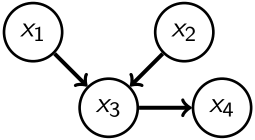
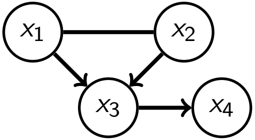
- Middle: conditional independence properties cannot be expressed using an undirected graph over the same three variables
- Right: conditional independence properties cannot be expressed using a directed graph over the same four variables

a) 

- How to form the smallest undirect model that is at least as powerful as a)?

a) 

b) 

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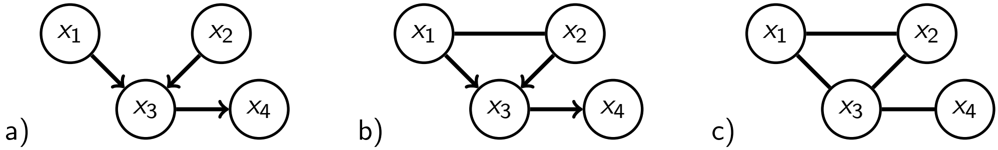

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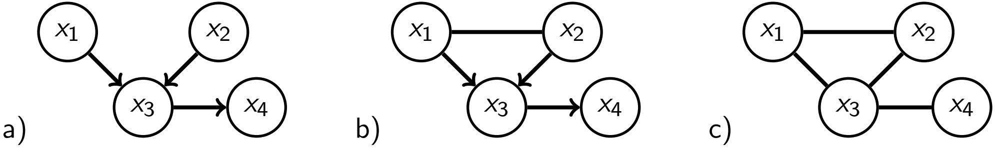

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c) is the 'smallest' undirected model that can represent all distributed that a) can. There's many others, *e.g.* fully connected.

Factor Graphs

Relationship Factorizations to Graphs

- Consider $p(a, b, c) = \phi(a, b)\phi(b, c)\phi(c, a)$

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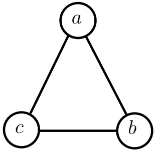
- What is the graph of the corresponding Markov network?



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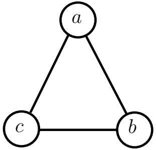

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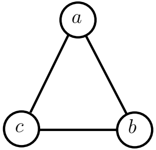

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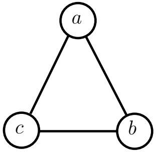

- How about this one? $p(a, b, c) = \phi(a, b, c)$
- The same!
- no one-to-one relation between the graph and the factorization of the potential functions!

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Why is this a problem?

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- $p(x_1, \ldots, x_6) = \frac{1}{Z} \prod_{i \neq j} \phi_{ij}(x_i, x_j) \qquad$ with $x_i \in \{1, \ldots, L\}$
- $\binom{6}{2} = 15$ factors of size 2 $\quad \rightarrow \quad$ distribution specified by $15L^2$ values

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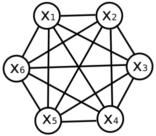

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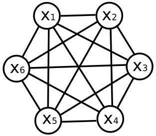

- also compatible with, *e.g.*,

$$p(x_1, \dots, x_6) = \frac{1}{Z} \phi(x_1, x_2, x_3, x_4) \phi(x_1, x_2, x_5, x_6) \phi(x_3, x_4, x_5, x_6) \quad \rightarrow \quad 3L^4 \text{ values!}$$

- or even $p(x_1, \dots, x_6) = \frac{1}{Z} \phi(x_1, \dots, x_6)$ $\rightarrow$ L^6 values!

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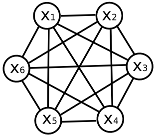

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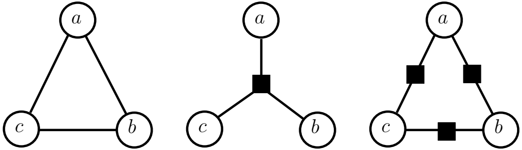
The graph alone does not tell us if the model is tractable or not. So why bother with it???

Relationship Potentials to Graphs

- We overcome his by augmenting the notation.
- We introduce an extra node (a square) for each factor in the factorization
  The square is connected to all nodes contributing to the factor.



(a) (b) (c)

- (a): Markov Network graph

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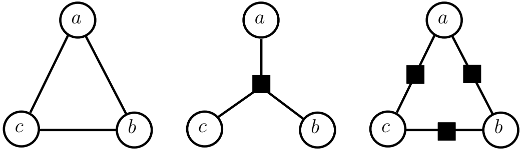

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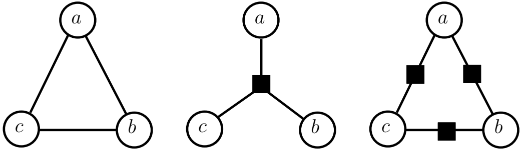

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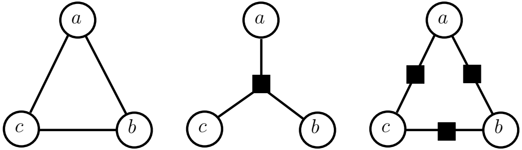

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- (a): Markov Network graph
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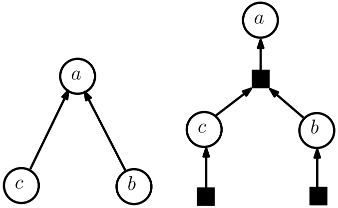
- (c): Factor graph representation of $p(a, b, c) \propto \phi(a, b)\phi(b, c)\phi(c, a)$
- Different factor graphs can have the same Markov network (b,c)⇒(a)

Directed Factor Graphs

- This also works for directed graph / belief network.
- The structure of the factorization is retained:



- But doesn't add much information, so typically not used.

Factor Graph Definition

Factor Graph

Given a function

$$f(x_1, \ldots, x_n) = \prod_i \psi_i(\mathcal{X}_i),$$

the **factor graph** (FG) has a node (represented by a square) for each factor $\psi_i(\mathcal{X}_i)$ and a variable node (represented by a circle) for each variable x_j.

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the factor graph (FG) has a node (represented by a square) for each factor $\psi_i(\mathcal{X}_i)$ and a variable node (represented by a circle) for each variable x_j. When used to represent a distribution

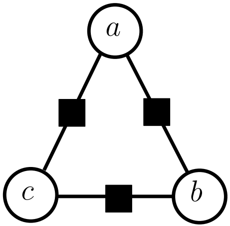
$$p(x_1, \ldots, x_n) = \frac{1}{Z} \prod_i \psi_i(\mathcal{X}_i),$$

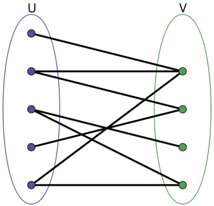
a normalization constant is assumed.

Bipartite graph

Bipartite

A bipartite graph is a graph whose vertices can be divided into two disjoint sets U and V such that every edge connects a vertex in U to one in V

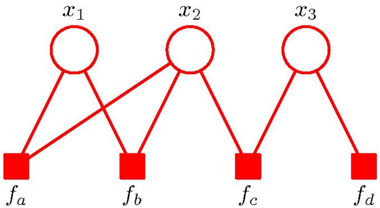




- Factor graphs are bipartite graphs. Edge are always between a *variables node* (circle) and a *factor node* (square).

Factor graph: example 1

- Question: which distribution ?



- Answer:

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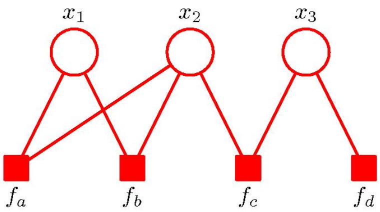


- Answer:

$$p(x) = \frac{1}{Z} f_a(x_1, x_2) f_b(x_1, x_2) f_c(x_2, x_3) f_d(x_3)$$

Factor graph: example 2

- Question: Which factor graph ?

$$p(x_1, x_2, x_3) = p(x_1)p(x_2)p(x_3 \mid x_1, x_2)$$

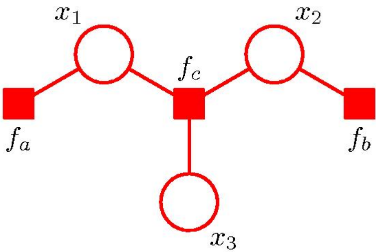
- Answer:

Factor graph: example 2

- Question: Which factor graph ?

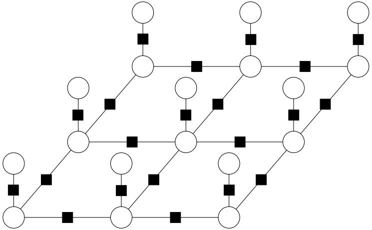
$$p(x_1, x_2, x_3) = p(x_1)p(x_2)p(x_3 \mid x_1, x_2)$$

- Answer:



Example: A Factor Graph and Energy Function for Image Denoising

$\mathcal{X}$:  $\mathcal{Y}$: 

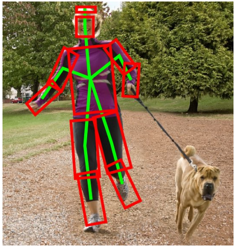


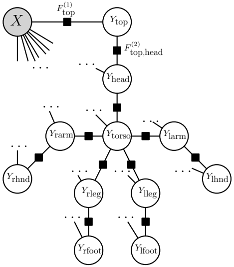
$$p(x,y) = \frac{1}{Z} e^{-E(x,y)} \qquad E(x,y) = \sum_{i \in \{\text{pixels}\}} E_i(x_i, y_i) + \sum_{(i,j) \in \{\text{edges}\}} E_{ij}(y_i, y_j)$$

Pairwise Markov Random Field (MRF):

- $E_i(x_i, y_i) = \alpha(x_i - y_i)^2$ outputs are likely similar to inputs
- $E_{ij}(y_i, y_j) = \beta|y_i - y_j|$ neighboring outputs are likely similar to each other $\rightarrow$ smooth output
- $\alpha \in \mathbb{R}$ and $\beta \in \mathbb{R}$ can be adjusted per image

Example: A Factor Graph and Energy Function for Human Pose Estimation





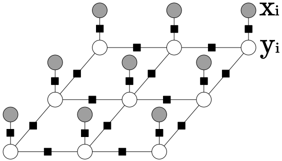
$$p(y|x) = \frac{1}{Z} e^{-E(y;x)} \qquad E(y;x) = \sum_{i \in \{\text{head}, \text{torso}, \dots\}} E_i(y_i; x_i) + \sum_{(i,j)} E_{ij}(y_i, y_j)$$

- unary factors (depend on one label): appearance
  - *e.g.* $E_{\text{head}}(y;x)$ *"Does location y in image x look like a head?"*
- pairwise factors (depend on two labels): geometry
  - *e.g.* $E_{\text{head-torso}}(y_{\text{head}}, y_{\text{torso}})$ *"Is location y_{head} above location y_{torso}?"*

Example: A Factor Graph and Energy Function for Image Segmentation

$\mathcal{X}$: 

$\mathcal{Y}$: 



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Energy function components ("Ising" model):

- $E_i(y_i = 1, x_i) = \begin{cases} \text{low} & \text{if } x_i \text{ is the right color, e.g. } \texttt{brown} \\ \text{high} & \text{otherwise} \end{cases}$ $\qquad E_i(y_i = 0, x_i) = -E_i(y_i = 1, x_i)$
- $E_i(y_i, y_j) = \begin{cases} \text{low} & \text{if } y_i = y_j \\ \text{high} & \text{otherwise} \end{cases}$ higher probability if neighbors have same labels $\rightarrow$ smooth labelings

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The graphs of graphical models represent families of probability distributions graphically:

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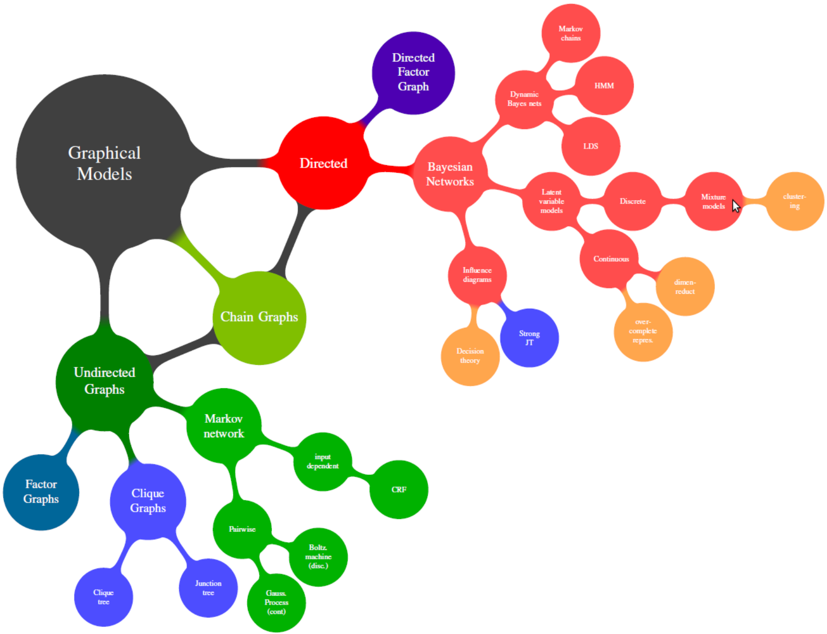
To specify an actual distribution, we also have to provide:

- for directed models: the conditional tables
- for undirected models: the potentials

Often, these are learned from training data (while the graph structure is fixed manually).



Graphical Models
Directed
Directed Factor Graph
Bayesian Networks
Dynamic Bayes nets
Markov chains
HMM
LDS
Latent variable models
Discrete
Mixture models
cluster-ing
Continuous
dimen-reduct
over-complete repres.
Influence diagrams
Decision theory
Strong JT
Chain Graphs
Undirected Graphs
Markov network
input dependent
CRF
Pairwise
Boltz. machine (disc.)
Gauss. Process (cont)
Factor Graphs
Clique Graphs
Clique tree
Junction tree