CPSC 540: Machine Learning

More DAGs, Undirected Graphical Models

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Admin

- Assignment 3:
  - 2 late days to hand in today.
- Assignment 4:
  - Due March 20.
- For graduate students planning to graduate in May:
  - Send me a private message on Piazza ASAP.

Last Time: Directed Acyclic Graphical (DAG) Models

- DAG models use a factorization of the joint distribution,

$$p(x_1, x_2, \dots, x_d) = \prod_{j=1}^{d} p(x_j | x_{\text{pa}(j)}),$$

where $\text{pa}(j)$ are the parents of node j.

- This assumes a Markov property,

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

which generalizes the Markov property in Markov chains,

$$p(x_j | x_{1:j-1}) = p(x_j | x_{j-1}).$$

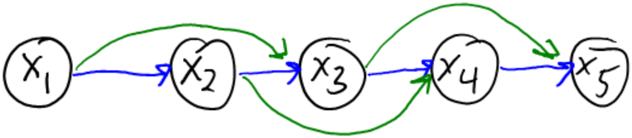
Last Time: Directed Acyclic Graphical (DAG) Models

- DAG models use a factorization of the joint distribution,

$$p(x_1, x_2, \dots, x_d) = \prod_{j=1}^{d} p(x_j | x_{\mathsf{pa}(j)}),$$

  where $\mathsf{pa}(j)$ are the parents of node j.

- We visualize the assumptions made by the model as a graph:

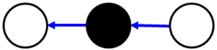


- Structure determines conditional independences and computational tractability.

Outline

D-Separation

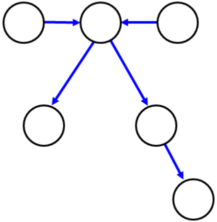
- We say that A and B are d-separated (conditionally independent) if *all paths* P from A to B are "blocked" because *at least one* of the following holds:
  1. P includes a "chain" with an observed middle node (e.g., Markov chain):

  2. P includes a "fork" with an observed parent node (e.g., mixture model):

  3. P includes a "v-structure" or "collider" (e.g., factor analysis):

  where *"child" and all its descendants* are unobserved.

Alarm Example

- Earthquake $\not\perp$ Call.
- Earthquake $\perp$ Call $|$ Alarm.
- Alarm $\not\perp$ Stuff Missing.
- Alarm $\perp$ Stuff Missing $|$ Burglary.

Alarm Example

- Earthquake $\perp$ Burglary.
- Earthquake $\not\perp$ Burglary $|$ Alarm.
  - Explaining away: Knowing Earthquake would make Burglary is less likely.
- Call $\not\perp$ Stuff Missing.
- Earthquake $\perp$ Stuff Missing.
- Earthquake $\not\perp$ Stuff Missing $|$ Call.

Discussion of D-Separation

- D-separation lets you say if conditional independence is implied by assumptions:

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

- However, there might be extra conditional independences in the distribution:
  - These would depend on specific choices of the $p(x_j | x_{\mathrm{pa}(j)})$.
  - Or some *orderings* may reveal extra independences....

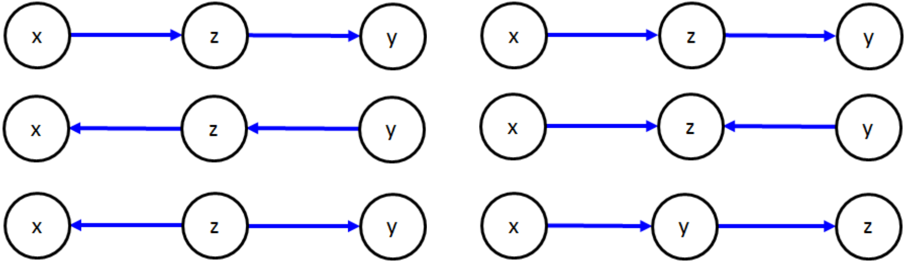
- Instead of restricting to $\{1, 2, \ldots, j-1\}$, consider general parent choices.
  - x_2 could be a parent of x_1.

- As long the graph is acyclic, there exists a valid ordering.

(all DAGs have a “topological order” of variables where parents are before children)

Non-Uniqueness of Graph and Equivalent Graphs

- Note that some graphs imply same conditional independences:
  - Equivalent graphs: same v-structures and other (undirected) edges are the same.
  - Examples of 3 *equivalent* graphs (left) and 3 non-equivalent graphs (right):

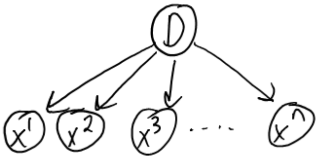


Discussion of D-Separation

- So the graph is not necessarily unique and is not the whole story.
- But, we can do a lot with d-separation:
  - Implies every independence/conditional-independence we've used in 340/540.
- Here we start blurring distinction between data/parameters/hyper-parameters...

IID Assumption as a DAG

- On Day 2, our first independence assumption was the IID assumption:



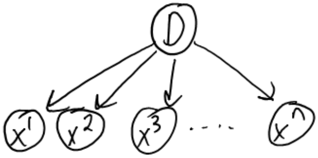
- Training/test examples come independently from data-generating process D.

- If we knew D, then there would be no need to learn.
- But D is unobserved, so knowing about some x^i tells us about the others.

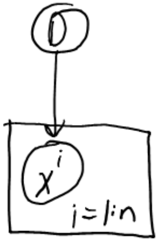
- We'll use this understanding later to relax the IID assumption.

Plate Notation

- Graphical representation of the IID assumption:

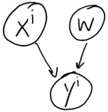


- We can concisely represent repeated parts of graphs using plate notation:

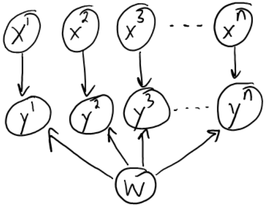


Tilde Notation as a DAG

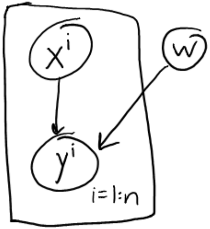
- When we write
$$y^i \sim \mathcal{N}(w^T x^i, 1),$$
  we can interpret it as the DAG model:



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



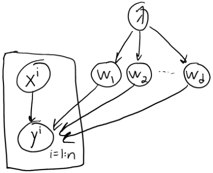
or



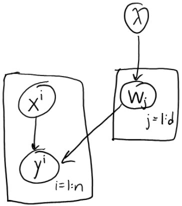
- From d-separation on this graph we have $p(y|X,w) = \prod_{i=1}^{n} p(y^i|x^i,w)$.

Tilde Notation as a DAG

- 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:



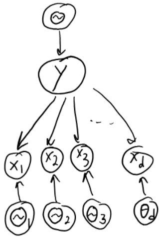
- Or introducing a second plate using:



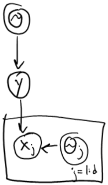
Other Models in DAG/Plate Notation

- For naive Bayes or Gaussian discriminant analysis with diagonal Σ_c we have

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



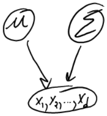
- Or in plate notation as



Other Models in DAG/Plate Notation

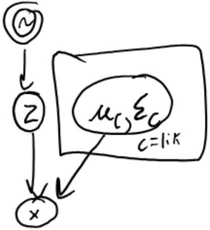
- In a full Gaussian model for a single x we have

$$x^i \sim \mathcal{N}(\mu, \Sigma).$$



- For mixture of Gaussians we have

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



Outline

Parameter Learning in General DAG Models

- The log-likelihood in DAG models is separable in the conditionals,

$$\log p(x|\Theta) = \log \prod_{j=1}^{d} p(x_j|x_{\mathsf{pa}(j)}, \Theta_j)$$
$$= \sum_{j=1}^{d} \log p(x_j|x_{\mathsf{pa}(j)}, \Theta_j)$$

- If each $p(x_j|x_{\mathsf{pa}(j)})$ has its own parameters Θ_j, we can fit them independently.
  - We've done this before: naive Bayes, Gaussian discriminant analysis, etc.

- Sometimes you want to have tied parameters $(\Theta_j = \Theta_{j'})$
  - Homogeneous Markov chains, Gaussian discriminant analysis with shared covariance.
  - Still easy, but need to fit $p(x_j|x_{\mathsf{pa}(j)}, \Theta_j)$ and $p(x_{j'}|x_{\mathsf{pa}(j')}, \Theta_j)$ together.

Tabular Parameterization in DAG Models

- To specify distribution, we need to decide on the form of $p(x_j | x_{\text{pa}(j)}, \Theta_j)$.
- For discrete data a default choice is the tabular parameterization:

$$p(x_j | x_{\text{pa}(j)}, \Theta_j) = \theta_{x_j, x_{\text{pa}(j)}},$$

  as we did for Markov chains (but now with multiple parents).

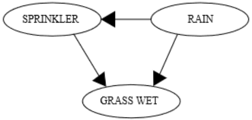
- Intuitive: just need conditional probabilities of children given parents like

$$p(\text{“wet grass”} = 1 \mid \text{“sprinkler”} = 1, \text{“rain”} = 0),$$

  and MLE is just counting.

Tabular Parameterization Example

RAIN	SPRINKLER T	SPRINKLER F
F	0.4	0.6
T	0.01	0.99



RAIN T	RAIN F
0.2	0.8

SPRINKLER	RAIN	GRASS WET T	GRASS WET F
F	F	0.0	1.0
F	T	0.8	0.2
T	F	0.9	0.1
T	T	0.99	0.01

https://en.wikipedia.org/wiki/Bayesian_network

Some quantities can be directly read from the tables:

$$p(R = 1) = 0.2.$$

$$p(G = 1 | S = 0, R = 1) = 0.8.$$

Tabular Parameterization Example

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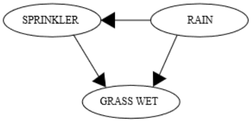

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F	F	0.0	1.0
F	T	0.8	0.2
T	F	0.9	0.1
T	T	0.99	0.01

https://en.wikipedia.org/wiki/Bayesian_network

Can calculate any probabilities using marginalization/product-rule/Bayes-rule.

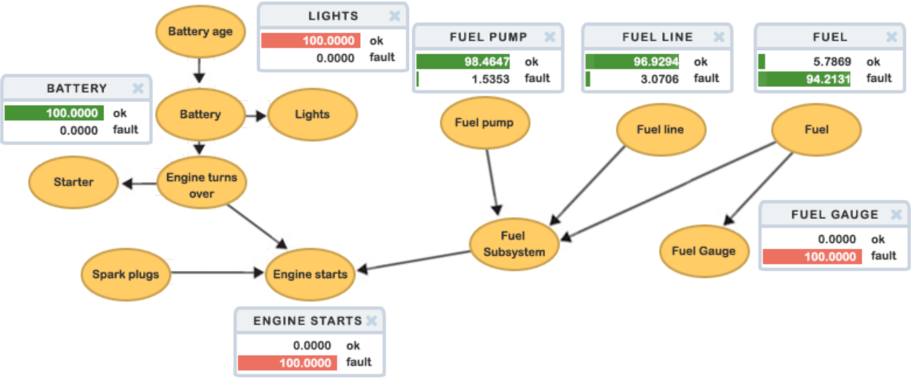
$$p(G = 1|R = 1) = p(G = 1, S = 0|R = 1) + p(G = 1, S = 1|R = 1) \quad \left(p(a|c) = \sum_b p(a, b|c)\right)$$

$$= p(G = 1|S = 0, R = 1)p(S = 0|R = 1) + p(G = 1|S = 1, R = 1)p(S = 1|R = 1)$$

$$= 0.8(0.99) + 0.99(0.01) = 0.81.$$

Tabular Parameterization Example

Some companies sell software to help companies reason using tabular DAGs:



http://www.hugin.com/index.php/technology

Fitting DAGs using Supervised Learning

- But tabular parameterization requires too many parameters:
  - With binary states and k parents, need 2^{k+1} parameters.
- One solution is letting users specify a "parsimonious" parameterization:
  - Typically have a linear number of parameters.
  - For example, the "noisy-or" model: $p(x_j|x_{\text{pa}(j)}) = 1 - \prod_{k \in \text{pa}(j)} q_k$.
- But if we have data, we can use supervised learning.
  - Write fitting $p(x_j|x_{\text{pa}(j)})$ as our usual $p(y|x)$.
  - We're predicting one column of X given the values of other columns.

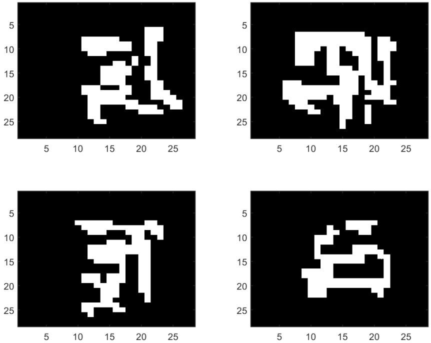
Fitting DAGs using Supervised Learning

- Fitting DAGs using supervised learning:
  - For $j = 1 : d$:
    1. Set $\tilde{y}^i = x^i_j$ and $\tilde{x}^i = x^i_{\text{pa}(j)}$.
    2. Solve a supervised learning problem using $\{\tilde{X}, \tilde{y}\}$.
  - Use the d regression/classification models as the density estimator.

- We can use our usual tricks:
  - Linear models, non-linear bases, regularization, kernel trick, random forests, etc.
  - With least squares it's called a Gaussian belief network.
  - With logistic regression it's called a sigmoid belief networks.
  - Don't need Markov assumptions to tractably fit these models.

MNIST Digits with Tabular DAG Model

- Recall our latest MNIST model using a tabular DAG:

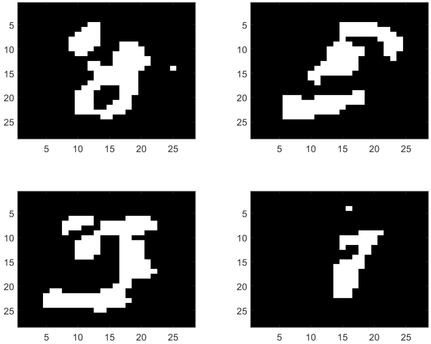


- This model is pretty bad because you only see 8 parents.

MNIST Digits with Sigmoid Belief Network

- Samples from sigmoid belief network:

(DAG with logistic regression for each variable)



where we use all previous pixels as parents (from 0 to 783 parents).

- Models long-range dependencies but has a linear assumption.

Sampling in DAGs

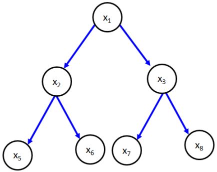
- We can use ancestral sampling to generate samples from a DAG:
  1. Sample x_1 from $p(x_1)$.
  2. If x_1 is a parent of x_2, sample x_2 from $p(x_2|x_1)$.
     - Otherwise, sample x_2 from $p(x_2)$.
  3. Go through the subsequent j in order sampling x_j from $p(x_j|x_{\text{pa}(j)})$.
- We can use these samples within Monte Carlo methods.
- How do sample from a multivariate Gaussian?
  - Write it as a Gaussian belief network, apply ancestral sampling.

Inference in Forest DAGs

- If we try to generalize the CK equations to DAGs we obtain

$$p(x_j = s) = \sum_{x_{\text{pa}(j)}} p(x_j = s, x_{\text{pa}(j)}) = \sum_{x_{\text{pa}(j)}} \underbrace{p(x_j = s | x_{\text{pa}(j)})}_{\text{given}} p(x_{\text{pa}(j)}).$$

  which works if each node has at most one parent.
  - Such graphs are called trees (connected), or forests (disconnected).
    - Also called "singly-connected".



  - Forests allow efficient message-passing methods as in Markov chains.
    - In particular, decoding and univariate marginals/conditionals in $O(dk^2)$.
    - Message passing applied to tree-structured graphs is called belief propagation.

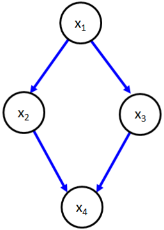
Inference in General DAGs

- If we try to generalize the CK equations to DAGs we obtain

$$p(x_j = s) = \sum_{x_{\mathsf{pa}(j)}} p(x_j = s, x_{\mathsf{pa}(j)}) = \sum_{x_{\mathsf{pa}(j)}} \underbrace{p(x_j = s | x_{\mathsf{pa}(j)})}_{\text{given}} p(x_{\mathsf{pa}(j)}).$$

- What goes wrong if nodes have multiple parents?
  - The expression $p(x_{\mathsf{pa}(j)})$ is a joint distribution and is not given recursively.

- Consider the non-tree graph:



Inference in General DAGs

- We can compute $p(x_4)$ in this non-tree using:

$$\begin{aligned} p(x_4) &= \sum_{x_3}\sum_{x_2}\sum_{x_1} p(x_1,x_2,x_3,x_4) \\ &= \sum_{x_3}\sum_{x_2}\sum_{x_1} p(x_4|x_2,x_3)p(x_3|x_1)p(x_2|x_1)p(x_1) \\ &= \sum_{x_3}\sum_{x_2} p(x_4|x_2,x_3) \underbrace{\sum_{x_1} p(x_3|x_1)p(x_2|x_1)p(x_1)}_{M_{23}(x_2,x_3)} \end{aligned}$$

- Dependencies between $\{x_1,x_2,x_3\}$ mean our message depends on two variables.

$$\begin{aligned} p(x_4) &= \sum_{x_3}\sum_{x_2} p(x_4|x_2,x_3)M_{23}(x_2,x_3) \\ &= \sum_{x_3} M_{34}(x_3,x_4), \end{aligned}$$

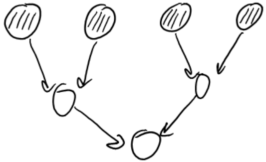
Inference in General DAGs

- With 2-variable messages, our cost increases to $O(dk^3)$.
- If we add the edge $x_1 - > x_4$, then the cost is $O(dk^4)$.

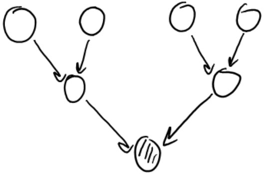
  (the same cost as enumerating all possible assignments)
- Unfortunately, cost is not as simple as counting number of parents.
  - Even if each node has 2 parents, we may need huge messages.
  - Decoding is NP-hard and marginals are $\#$P-hard in general.
  - We'll see later that maximum message is given by treewidth of a particular graph.
- In general, we'll need approximate inference methods to use general DAGs.

Conditional Sampling in DAGs

- What about conditional sampling in DAGs?
  - Could be easy or hard depending on what we condition on.
- For example, still easy if we condition on the first variables in the order:
  - Just fix these and run ancestral sampling.



- Hard to condition on the last variables in the order:
  - Conditioning on descendent makes ancestors dependent.



Outline

Directed vs. Undirected Models

- In some applications we have a natural ordering of the x_j.
  - In the "rain" data, the past affects the future.
- In some applications we don't have a natural order.
  - E.g., pixels in an image.
- In these settings we often use undirected graphical models.
  - Also known as Markov random fields and originally from statistical physics.

Undirected Graphical Models

- Undirected graphical models (UGMs) assume $p(x)$ factorizes over subsets c,

$$p(x_1, x_2, \ldots, x_d) \propto \prod_{c \in \mathcal{C}} \phi_c(x_c),$$

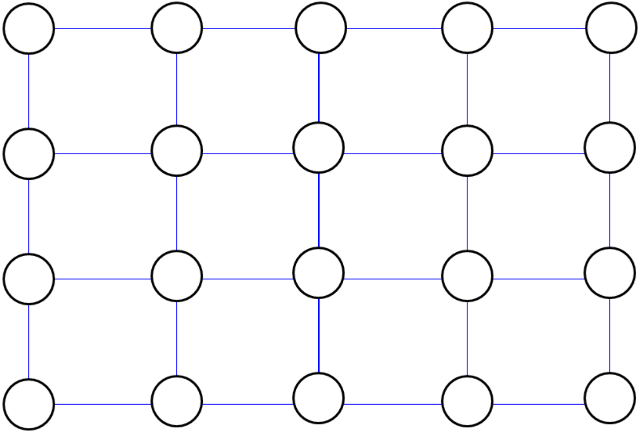
  from among a set of subsets of $\mathcal{C}$.
- The ϕ_c are called potential functions: can be any non-negative function.
  - Ordering doesn't matter: more natural for things like pixels of an image.
  - Theoretically, only need ϕ_c for maximal subsets in C.
- Important special case is pairwise undirected graphical model:

$$p(x) \propto \left(\prod_{j=1}^{d} \phi_j(x_j)\right) \left(\prod_{(i,j) \in E} \phi_{ij}(x_i, x_j)\right),$$

  where E are a set of undirected edges.

Undirected Graphical Models

- Pairwise UGMs are a classic way to model dependencies in images:



- Can model dependency between neighbouring pixels, without imposing ordering.

From Probability Factorization to Graphs

- For a pairwise UGM,

$$p(x) \propto \left(\prod_{j=1}^{d} \phi_j(x_j)\right)\left(\prod_{(i,j)\in E} \phi_{ij}(x_i, x_j)\right),$$

  we visualize independence assumptions as an undirected graph:
  - We have edge i to j if $(i, j) \in E$.

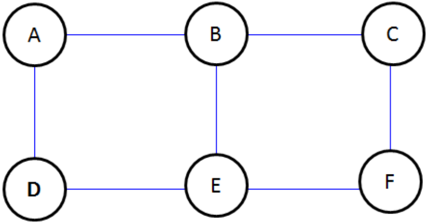
- For general UGMs,

$$p(x_1, x_2, \dots, x_d) \propto \prod_{c \in \mathcal{C}} \phi_c(x_c),$$

  we have the edge (i, j) if i and j are together in at least one c.

Conditional Independence in Undirected Graphical Models

- It's easy to check conditional independence in UGMs:
  - $A \perp B | C$ if C blocks all paths from any A to any B.
- Example:



  - $A \not\perp C$.
  - $A \not\perp C | B$.
  - $A \perp C | B, E$.
  - $A, B \not\perp F | C$
  - $A, B \perp F | C, E$.

Multivariate Gaussian and Pairwise Graphical Models

- Multivarate Gaussian is a special case of a pairwise UGM.
- Edges of the graph are (i, j) values where $\Sigma_{ij}^{-1} \neq 0$.
- Unconditional independence of (i, j) corresponds to having $\Sigma_{ij} = 0$.
  - Can be seen from block Gaussian formula.
  - Corresponds to reachability in the graph.
- We use the term Gaussian graphical model (GGM) in this context.
  - Or Gaussian Markov random field.

Digression: Gaussian Graphical Models

- Multivariate Gaussian can be written as

$$p(x) \propto \exp\left(-\frac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu)\right) \propto \exp\left(-\frac{1}{2}x^T\Sigma^{-1}x + x^T\underbrace{\Sigma^{-1}\mu}_{v}\right),$$

and from here we can see that it's a pairwise UGM:

$$\begin{aligned} p(x) &\propto \exp(\left(-\frac{1}{2}\sum_{i=1}^{d}\sum_{j=1}^{d}x_i x_j \Sigma^{-1}_{ij} + \sum_{i=1}^{d}x_i v_i\right) \\ &= \left(\prod_{i=1}^{d}\prod_{j=1}^{d}\underbrace{\exp\left(-\frac{1}{2}x_i x_j \Sigma^{-1}_{ij}\right)}_{\phi_{ij}(x_i,x_j)}\right)\left(\prod_{i=1}^{d}\underbrace{\exp\left(x_i v_i\right)}_{\phi_i(x_i)}\right)\end{aligned}$$

Independence in GGMs

- So Gaussians are pairwise UGMs with $\phi_{ij}(x_i, x_j) = \exp\left(-\frac{1}{2}x_i x_j \Theta_{ij}\right)$,
  - Where Θ_{ij} is element (i, j) of Σ^{-1}.
- Connection between precision matrix $\Theta = \Sigma^{-1}$ and conditional independence:
  - Setting $\Theta_{ij} = 0$ is equivalent to removing $\phi_{ij}(x_i, x_j)$ from the UGM.

$$\Theta_{ij} \neq 0 \Rightarrow x_i \not\perp x_j | x_{-ij}.$$

- Gaussian conditional independencies corresponds to sparsity in precision matrix.
  - Diagonal Θ gives disconnected graph: all variables are indpendent.
  - Full Θ gives fully-connected graph: there are no independences.

Independence in GGMs

- Consider Gaussian with tri-diagonal precision Θ:

$$\Sigma^{-1} = \begin{bmatrix} 32.0897 & 13.1740 & 0 & 0 & 0 \\ 13.1740 & 18.3444 & -5.2602 & 0 & 0 \\ 0 & -5.2602 & 7.7173 & 2.1597 & 0 \\ 0 & 0 & 2.1597 & 20.1232 & 1.1670 \\ 0 & 0 & 0 & 1.1670 & 3.8644 \end{bmatrix}$$

$$\Sigma = \begin{bmatrix} 0.0494 & -0.0444 & -0.0312 & 0.0034 & -0.0010 \\ -0.0444 & 0.1083 & 0.0761 & -0.0083 & 0.0025 \\ -0.0312 & 0.0761 & 0.1872 & -0.0204 & 0.0062 \\ 0.0034 & -0.0083 & -0.0204 & 0.0528 & -0.0159 \\ -0.0010 & 0.0025 & 0.0062 & -0.0159 & 0.2636 \end{bmatrix}$$

- $\Sigma_{ij} \neq 0$ so all variables are dependent: $x_1 \not\perp x_2$, $x_1 \not\perp x_5$, and so on.
- But conditional independence is described by a Markov chain:

$$p(x_1 | x_2, x_3, x_4, x_5) = p(x_1 | x_2).$$

Graphical Lasso

- Conditional independence in GGMs is described by sparsity in Θ.
- Recall fitting multivariate Gaussian with L1-regularization,

$$\underset{\Theta \succ 0}{\text{argmin}}\, \text{Tr}(S\Theta) - \log|\Theta| + \lambda\|\Theta\|_1,$$

  which is called the graphical Lasso because it encourages a sparse graph.
    - Special case of graph structure learning.
- Consider instead fitting DAG model with Gaussian probabilities:
    - DAG structure corresponds to sparsity in Cholesky of covariance.

Tractability of UGMs

- In UGMs we assume that
$$p(x) = \frac{1}{Z}\prod_{c\in\mathcal{C}}\phi_c(x_c),$$
where Z is the constant such that
$$\sum_{x_1}\sum_{x_2}\cdots\sum_{x_d} p(x) = 1 \text{ (discrete)}, \quad \int_{x_1}\int_{x_2}\cdots\int_{x_d} p(x)dx_d dx_{d-1}\dots dx_1 = 1 \text{ (cont)}.$$
- So Z is
$$Z = \sum_x \prod_{c\in\mathcal{C}}\phi_c(x_c) \text{ (discrete)}, \quad \int_x \prod_{c\in\mathcal{C}}\phi_c(x_c)dx \text{ (cont)}$$
- Whether you can compute Z depends on the choice of ϕ_c:
  - Gaussian case: $O(d^3)$ in general, but $O(d)$ for forests (no loops).
  - Discrete case: #P-hard in general, but $O(dk^2)$ for forests (no loops).
  - Continuous non-Gaussian: usually requires numerical integration.

Summary

- Plate Notation lets compactly draw graphs with repeated patterns.
  - There are fancier versions of plate notation called “probabilistic programming”.
- Parameter learning in DAGs:
  - Can fit each $p(x_j|x_{\text{pa}(j)})$ independently.
  - Tabular parameterization, or treat as supervised learning.
- Inference in DAGs:
  - Ancestral sampling and Monte Carlo methods work as faster.
  - Message-passing message sizes depend on graph structure.
- Undirected graphical models factorize probability into non-negative potentials.
  - Simple conditional independence properties.
  - Include Gaussians as special case.

- Next time: our first visit to the wild world of approximate inference.