CPSC 440: Advanced Machine Learning

Learning Graphical Models

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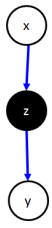
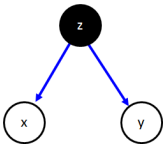
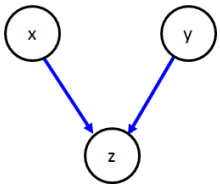
Last Time: D-Separation

- D-separation can be used to "read" conditional independence from graph.
  - Can be derived by considering DAG as "inheritance of genes".
- 3 Cases that can "block" a path between nodes:

Case 1:


Case 2:


Case 3:


- Case 1: Observing a variable in a "chain" blocks a path.
- Case 2: Observing a parent in a "fork" blocks a path.
- Case 3: Not observing a child in a "v-structure" blocks a path.
  - We say that variables are "d-separated" if every path between them is blocked.

Discussion of D-Separation

- Last time we discussed equivalent graphs (same independent assumptions).
- We also discussed how extra independence assumptions may not appear in graph.

- 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 340/440.
    - Except for multivariate Gaussians, which are undirected graphical models.

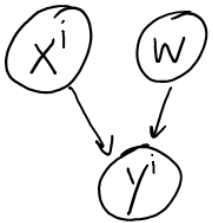
- Requires using DAGs to represent relationships between data and parameters.
  - This allows us to see and reason about their relationships.

Tilde Notation as a DAG

- When we write

$$y^i \sim \mathcal{N}(w^T x^i, 1),$$

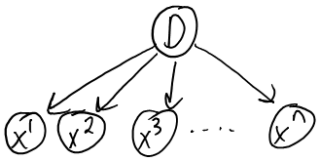
this can be interpretd as a DAG model:



- "The variables on the right of $\sim$ are the parents of the variables on the left".
  - We can see our standard $X \perp w$ assumption in the graph.
    - Common child case: w only depends on X if we know y.

IID Assumption as a DAG

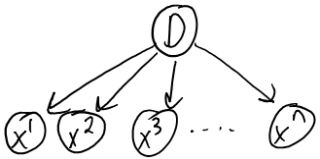
- During week 1, our first independence assumption was the IID assumption:



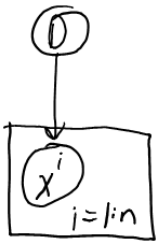
- Training/test examples come independently from data-generating process D.
- But D is unobserved, so knowing about some x^i tells us about the others.
  - This why the IID assumptions lets us learn.

Plate Notation

- Graphical representation of the IID assumption:

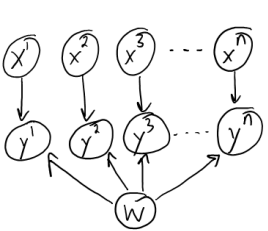


- It's common to represent repeated parts of graphs using plate notation:

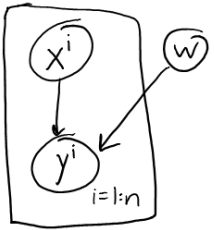


Tilde Notation as a DAG

- If the x^i are IID then we can represent linear regression as



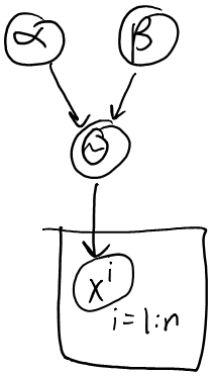
or



- From d-separation on this graph we have $p(y \mid X, w) = \prod_{i=1}^{n} p(y^i \mid x^i, w)$.
  - Our standard assumption that data is independent given parameters.
- We often omit the data-generating distribution D.
  - But if you want to learn then you should remember that it's there.
- Note that plate reflects parameter tieing: that we use same w for all i.

IID Bernoulli-Beta Model

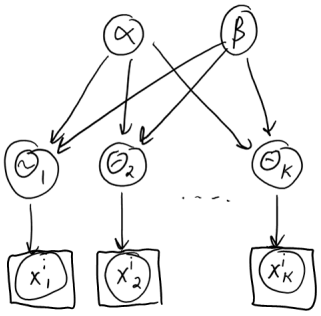
- The Bernoulli-beta model as a DAG (with parameters and hyper-parameters):



- Notice data is independent of hyper-parameters given parameters.
  - This is another of our standard independence assumptions.

Non-IID Bernoulli-Beta Model

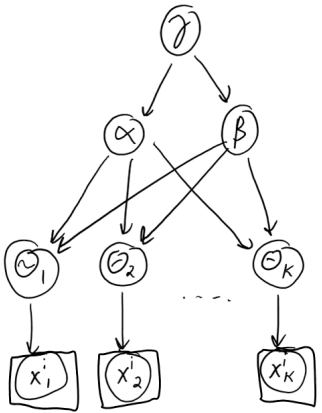
- The non-IID variant we considered with grouped data:



- DAG reflects that we do not tie parameters across all training examples.
- Notice that if you fix α and β then you can't learn across groups:
  - The θ_j are d-separated given α and β.

Non-IID Bernoulli-Beta Model

- Variant of the previous model with a hyper-hyper-parameter:



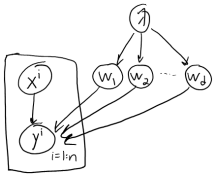
- Which is needed to avoid degeneracy.

Bayesian Linear Regression as a DAG

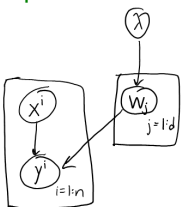
- In Bayesian linear regression we assume

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

which we can interpret it as the DAG model:



- Or introducing a second plate over parmaeters:



Outline

Density Estimators vs. Relationship Visualizers

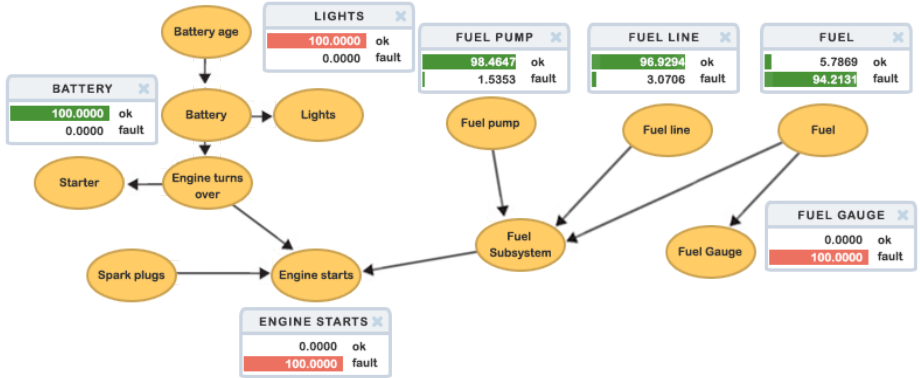
- Besides dependency visualization, we can use DAGs as density estimators.
- Recall that DAGs model joint distribution using

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

- We need to choose a parameterization for these conditional probabilities:
  - Tabular parameterization (discrete x_j): can model any joint probability.
    - Common choice, sometimes setting parameters using expert knowledge.
  - Gaussian (continuous x_j): $x_j \sim \mathcal{N}(w^T x_{\mathsf{pa}(j)}, \sigma^2)$.
    - Called a Gaussian belief net. Jointdistribution becomes a multivariate Gaussian.
  - Sigmoid (binary $x_j \in \{-1, +1\}$): $p(x_j \mid x_{j-1}, w) = 1/1 + \exp(-x_j w^T x_{\mathsf{pa}(j)})$.
    - Called a sigmoid belief net.
  - Could use softmax, probabilistic random forest, neural network, and so on.
    - Our tricks for probabilistic supervised learning can be used for unsuperivsed learning.

Tabular Parameterization Example

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



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

DAG Learning and Sampling

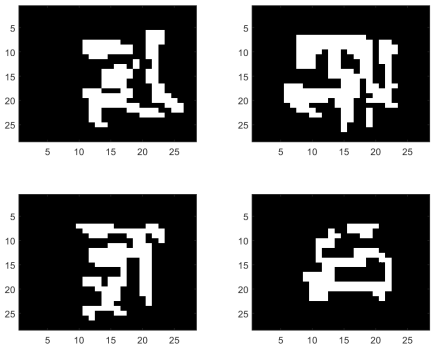
- For $j = 1 : d$:
  1. Set $\bar{y}^i = x_j^i$ and $\bar{x}^i = x_{\mathsf{pa}(j)}^i$.
  2. Solve a supervised learning problem using $\{\bar{X}, \bar{y}\}$.
     - Gives you a model of $p(x_j \mid x_{\mathsf{pa}(j)})$.

- Can sample from DAGs using ancestral sampling:
  - Sample x_1 from $p(x_1)$.
  - Sample x_2 from $p(x_2 \mid x_{\mathsf{pa}(2)})$.
  - Sample x_3 from $p(x_3 \mid x_{\mathsf{pa}(3)})$.
  - Until we have sampled x_d.

- This allows us to do inference with Monte Carlo methods.
  - Conditional sampling can be hard, may need rejection sampling for conditionals.

MNIST Digits with Tabular DAG Model

- Recall our latest MNIST model using a tabular DAG:

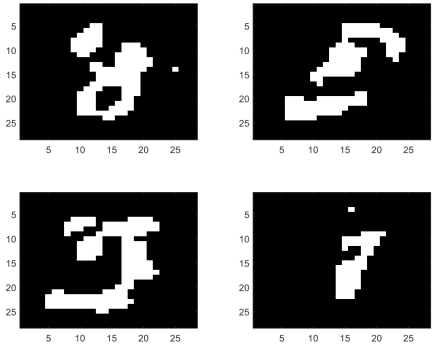


- This model is pretty bad because you only see 8 parents.

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).

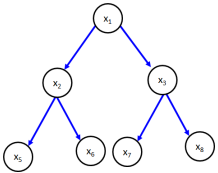
- Models long-range dependencies but has a linear assumption.

Exact Inference in DAGs?

- Can we do exact inference in DAGs like in Markov chains?
- Continuous-state Gaussian DAGs:
  - Special case of multvariate Gaussian, so inference is tractable.
    - Most operations are $O(d)$ or $O(d^3)$.
- Continuous-state non-Gaussian DAGs:
  - Inference usually not closed-form, so need Monte Carlo or variational inference.
  - If parents are conjugate, then Gibbs sampling is easy to implement.
- Discrete-state DAGs (whether tabular or sigmoid or other):
  - Inference takes exponential-time in the "treewidth" of the graph.
  - Exact inference is cheap in trees and forests, which have a treewidth of 1.
    - Low-treewidth graphs allow efficient exact inference, otherwise need approximations.

Inference in Forest DAGs ("Belief Propagation")

- Graphs with at most one parent per node are called trees (connected).



  - Also called "singly-connected" or forests (if disconnected).
- We can generalize the CK equations to trees/forests:

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

- Trees/forests allow efficient dynamic programming methods as in Markov chains.
  - In particular, decoding and univariate marginals/conditionals in $O(dk^2)$.
  - Forward-backward applied to tree-structured graphs is called belief propagation.
  - It also possible to find optimal tree given data ("structure learning").

Undirected Graphical Models (UGMs)

- Undirected graphical models (UGMs) are another popular graphical model class.
  - UGMs are also known as Markov random fields.
- UGMs define joint distribution in terms of non-negative potential functions,

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

- Define potential ϕ_c for each set c where we want to model a direct relationship.
- The most common choice is a pairwise UGM,

$$p(x_1, x_2, \ldots, x_d) \propto \left(\prod_{j=1}^{d} \phi_j(x_j) \right) \left(\prod_{(i,j) \in \mathcal{E}} \psi_{ij}(x_i, x_j) \right).$$

  which only has potentials on single variables (ϕ) and pairs of variables (ψ).
  - The "edge potentials" ψ are defined on edge of an undirected graph $\mathcal{E}$.

Pairwise Undirected Graphical Models

- Pairwise undirected graphical models factorize probability using

$$p(x_1, x_2, \ldots, x_d) \propto \left(\prod_{j=1}^{d} \phi_j(x_j) \right) \left(\prod_{(i,j) \in \mathcal{E}} \psi_{ij}(x_i, x_j) \right).$$

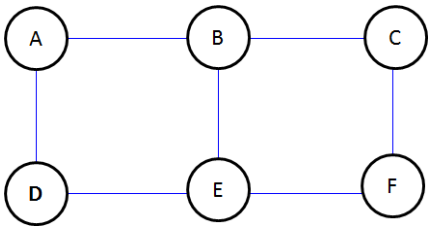
- Special cases:
  - Markov chains are the special case $\mathcal{E}$ only has edges between adjacent nodes.
  - Multivaiate Gaussian corresponds to specific choice of the ϕ and ψ functions.
    - Gaussians AKA "Gaussian graphical models" or "Gaussian Markov random fields".
  - Ising model for binary x_j uses

$$\phi_j(x_j) = \exp(x_i w_i), \quad \phi_{ij}(x_i, x_j) = \exp(x_i x_j w_{ij}),$$

    where w_i is the node weight and w_{ij} is the edge weight.
    - If $w_{ij} > 0$ it encourages neighbours to have same value ("attractive").
    - If $w_{ij} < 0$ it encourages neighbours to have different values ("repulsive").

Conditional Independence in UGMs

- UGM independence properties described by an undirected graph.
  - For pairwise UGMs, the edges are given by the set of edges $\mathcal{E}$.



- Constructing graph when you may have 3-variable or higher-order potentials:
  - Graph has edge (i, j) if i and j are together in at least one c.
- So these two factorizations have the same graph:

$$p(x_1.x_2, x_3) \propto \phi_{12}(x_1, x_2)\phi_{13}(x_1, x_3)\phi_{23}(x_2, x_3), \quad p(x_1, x_2, x_3) \propto \phi_{123}(x_1, x_3, x_3).$$

- UGM implies $A \perp B \mid C$ if C separates all nodes in A from all nodes in B.
  - Same rule as a Gaussians.

DAGs vs. UGMs

- Neither DAGs or UGMs are "more powerful" than the other.
  - Any distribution can be re-written as a DAG or UGM.
  - But may need to use a highly-connected graph.

- Set of independences in DAG cannot always be written as UGM (and vice versa).
  - UGMs cannot reflect independences in common child graph: $(x) \rightarrow (y) \leftarrow (z)$.
  - DAGs cannot reflect independences in 4-node loop: (x) - (y) - (z) - (x).
  - Independences representable as both DAGs and UGMs are called decomposable.
    - An example is Markov chains: independences are same in DAG and UGM graphs.

- DAGs are often used when it makes sense to work with conditionals, or we have an idea of causal directions.

- UGMs are often used when there are no obvious directions (like MNIST), and are more-often used when we want to add features to do supervised learning.

Tractability of UGMs

- Without using $\propto$, a UGM probability would be

$$p(x) = \frac{1}{Z} \prod_{c \in \mathcal{C}} \phi_c(x_c),$$

where Z is the constant that makes the probabilites sum up to 1.

$$Z = \sum_{x_1} \sum_{x_2} \cdots \sum_{x_d} \prod_{c \in \mathcal{C}} \phi_c(x_c) \quad \text{or} \quad Z = \int_{x_1} \int_{x_2} \cdots \int_{x_d} \prod_{c \in \mathcal{C}} \phi_c(x_c) dx_d dx_{d-1} \ldots dx_1.$$

- Whether you can compute Z (and do inference) depends on the choice of the ϕ_c:
  - Gaussian case: $O(d^3)$ in general, but $O(d)$ for forests (no loops).
  - Continuous non-Gaussian: usually requires approximate inference.
  - Discrete case: #P-hard in general, but $O(dk^2)$ for forests (no loops).

Discrete DAGs vs. Discrete UGMs

- Common inference tasks in graphical models:
  1. Compute $p(x)$ for an assignment to the variables x.
  2. Generate a sample x from the distribution.
  3. Compute univariate marginals $p(x_j)$.
  4. Compute decoding $\text{argmax}_x\, p(x)$.
  5. Compute univariate conditional $p(x_j \mid x_{j'})$.

- With discrete x_i, all of the above are easy in tree-structured graphs.
  - For DAGs, a tree-structured graph has at most one parent.
  - For UGMs, a tree-structured graph has no cycles.

- With discrete x_i, the above may be harder for general graphs:
  - In DAGs the first two are easy, the others are NP-hard.
  - In UGMs all of these are NP-hard.

Bonus Slides on Inference in UGMs

- I am not planning to go into details on inference in graphical models.
- I put all my slides on the topic available here:
  - `https://www.cs.ubc.ca/~schmidtm/Courses/440-W22/L31.5.pdf`
- Covers topics such as:
  - Inference in non-tree DAGs/UGMs.
  - Learning the graph structure.
  - Writing Gaussians as pairwise UGMs.
  - Treewidth of graphs, and efficient inference with low treewidth.
  - Exact decoding for binary attractive models using graph cuts.
  - ICM and alpha-expansion algorithms for approximate decoding.
  - Block Gibbs sampling in UGMs (UGMs are what Gibbs sampling was invented for).

Summary

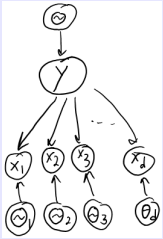
- Independence assumptions about data and parameters can be written as DAGs.
- Plate Notation lets us compactly draw graphs with repeated patterns.
  - There are fancier versions of plate notation called "probabilistic programming".
- Parameter learning in DAGs:
  - Can fit each $p(x_j \mid x_{\text{pa}(j)})$ independently.
  - Tabular parameterization, or treat as supervised learning.
- Sampling in DAGs is easy (ancestral sampling).
- Exact inference in discrete DAGs is easy for trees.
  - But becomes exponential in "treewidth" of graph.
- Undirected graphical models factorize probability into non-negative potentials.
  - Gaussians are a special case, but can place potentials on any subset of variables.
  - Inference is again exponential in "treewidth" of graph.

- Next time: adding graphical models to neural networks.

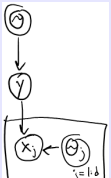
Naive Bayes with DAGs/Plates

- For naive Bayes we have

$$y^i \sim \text{Cat}(\theta), \quad x^i \mid y^i = c \sim Cat(\theta_c).$$



- Or in plate notation as

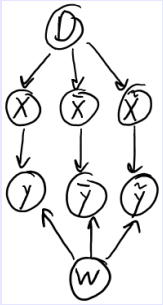


Does Semi-Supervised Learning Make Sense?

- Should unlabeled examples always help supervised learning?
  - No!
- Consider choosing unlabeled features $\bar{x}^i$ uniformly at random.
  - Unlabeled examples collected in this way will not help.
  - By construction, distribution of $\bar{x}^i$ says nothing about $\bar{y}^i$.
- Example where SSL is not possible:
  - Try to detect food allergy by trying random combinations of food:
    - The actual random process isn't important, as long as it isn't affected by labels.
    - You can sample an infinite number of $\bar{x}^i$ values, but they says nothing about labels.
- Example where SSL is possible:
  - Trying to classify images as "cat" vs. "dog.":
    - Unlabeled data would need to be images of cats or dogs (not random images).
    - Unlabeled data contains information about what images of cats and dogs look like.
    - For example, there could be clusters or manifolds in the unlabeled images.

Does Semi-Supervised Learning Make Sense?

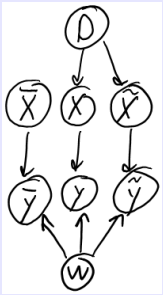
- Let's assume our semi-supervised learning model is represented by this DAG:



- Assume we observe $\{X, y, \tilde{X}\}$ and are interested in test labels $\tilde{y}$:
  - There is a dependency between y and $\tilde{y}$ because of path through w.
    - Parameter w is tied between training and test distributions.
  - There is a dependency between X and $\tilde{y}$ because of path through w (given y).
    - But note that there is also a second path through D and $\tilde{X}$.
  - There is a dependency between $\tilde{X}$ and $\tilde{y}$ because of path through D and $\tilde{X}$.
    - Unlabeled data helps because it tells us about data-generating distribution D.

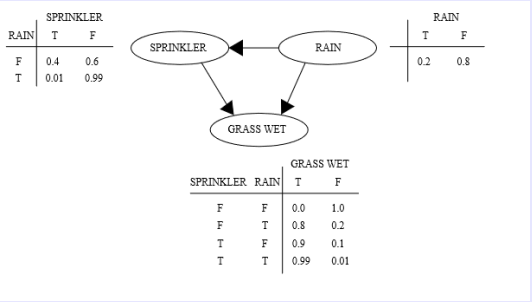
Does Semi-Supervised Learning Make Sense?

- Now consider generating $\bar{X}$ independent of D:



- Assume we observe $\{X, y, \bar{X}\}$ and are interested in test labels $\tilde{y}$:
  - Knowing X and y are useful for the same reasons as before.
  - But knowing $\bar{X}$ is not useful:
    - Without knowing $\bar{y}$, $\bar{X}$ is d-separated from $\tilde{y}$ (no dependence).

Tabular Parameterization Example



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

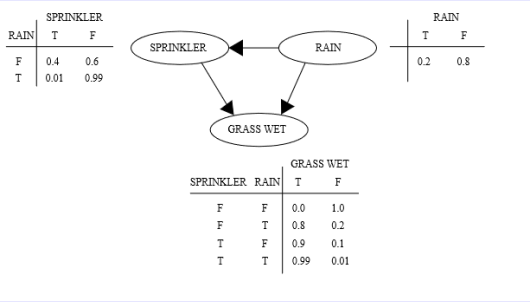
Some quantities can be directly read from the tables:

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

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

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

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

Can calculate any probabilities using marginalization/product-rule/Bayes-rule, for example:

$$p(G=1 \mid R=1) = p(G=1, S=0 \mid R=1) + p(G=1, S=1 \mid R=1) \quad \left(p(a \mid c) = \sum_b p(a, b \mid c) \right)$$
$$= p(G=1 \mid S=0, R=1) p(S=0 \mid R=1) + p(G=1 \mid S=1, R=1) p(S=1 \mid R=1)$$
$$= 0.8(0.99) + 0.99(0.01) = 0.81.$$

Dynamic Bayesian Networks

- Dynamic Bayesian networks combine ideas from DAGs and Markov chains:
  - At each time, we have a set of variables x^t.
  - The initial x^0 comes from an "initial" DAG.
  - Given x^{t-1}, we generate x^t from a "transition" DAG.

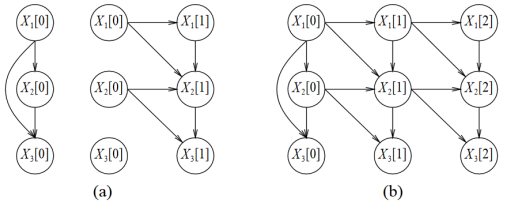


Figure 1: (a) A prior network and transition network defining a DPN for the attributes X_1, X_2, X_3. (b) The corresponding "unrolled" network.

https://www.cs.ubc.ca/~murphyk/Papers/dbnsem_uai98.pdf

- Can be used to model multiple variables over time.
  - Unconditional sampling is easy but inference may be hard.