CSE 250A. Principles of AI

Probabilistic Reasoning and Decision-Making

Lecture 8 – Learning from Complete Data

Lawrence Saul
Department of Computer Science and Engineering
University of California, San Diego

Fall 2021

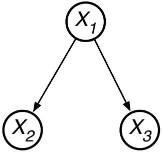
Outline

1. Maximum likelihood
2. Markov models
3. Naive Bayes models
4. Preview

Learning in BNs (review)

ASSUMPTIONS

- Discrete random variables $\{X_1, X_2, \ldots, X_n\}$
- DAG is specified, assumed to be known and fixed.
- CPTs enumerate $P\left(X_i = x | \mathrm{pa}_i = \pi\right)$.
- IID data $\left\{\left(x_1^{(t)}, x_2^{(t)}, \ldots, x_n^{(t)}\right)\right\}_{t=1}^{T}$



example	x_1	x_2	x_3
1	1	4	5
2	3	2	4
3	2	1	3
⋮	⋮	⋮	⋮
T	1	3	2

Each example gives a **complete** instantiation of the nodes in the belief network.

Computing the log-likelihood

$$\begin{aligned}
\mathcal{L} &= \log P(\mathrm{data}) \\
&= \log \prod_{t=1}^{T} P\left(x_1^{(t)}, x_2^{(t)}, \ldots, x_n^{(t)}\right) && \boxed{\textbf{IID data}} \\
&= \log \prod_{t=1}^{T} \prod_{i=1}^{n} P\left(x_i^{(t)} \middle| \mathrm{pa}_i^{(t)}\right) && \boxed{\textbf{product rule in BN}} \\
&= \sum_{i=1}^{n} \sum_{t=1}^{T} \log P\left(x_i^{(t)} \middle| \mathrm{pa}_i^{(t)}\right) && \boxed{\textbf{unweighted sum over examples}} \\
&= \sum_{i=1}^{n} \sum_{x} \sum_{\pi} \mathrm{count}(X_i = x, \mathrm{pa}_i = \pi) \log P(X_i = x | \mathrm{pa}_i = \pi)
\end{aligned}$$

$$\boxed{\textbf{weighted sum over co-occurrences}}$$

Interpreting the log-likelihood

$$\mathcal{L} = \sum_i \sum_x \sum_\pi \overbrace{\mathrm{count}(X_i\!=\!x, \mathrm{pa}_i\!=\!\pi)}^{\textbf{constants of the data}} \underbrace{\log P(X_i\!=\!x|\mathrm{pa}_i\!=\!\pi)}_{\textbf{CPTs to optimize}}$$

- **The log-likelihood for complete data is a triple sum over**

  i — the nodes in the BN
  x — the values of each node X_i
  π — the values π of the parents of X_i

- **How to optimize?**

  Intuitively, the larger the $\mathrm{count}(X_i\!=\!x, \mathrm{pa}_i\!=\!\pi)$,
  the larger we should choose $P(X_i\!=\!x|\mathrm{pa}_i\!=\!\pi)$.

Decomposing the log-likelihood

- **Log-likelihood for BN**

$$\mathcal{L} = \sum_{i} \sum_{\pi} \sum_{x} \mathrm{count}(X_i = x, \mathrm{pa}_i = \pi) \log P(X_i = x | \mathrm{pa}_i = \pi)$$

- **Contribution from row π of i^{th} node's CPT**

$$\mathcal{L}_{i\pi} = \sum_{x} \mathrm{count}(X_i = x, \mathrm{pa}_i = \pi) \log P(X_i = x | \mathrm{pa}_i = \pi)$$

- **Divide and conquer**

  The overall optimization over $\mathcal{L}$ reduces to many simpler and smaller optimizations over each $\mathcal{L}_{i\pi}$.

This is a special property of ML estimation for **complete** *data.*

ML Estimation

- **Problem**

  For each node X_i in the BN, and for each row π of its CPT, our goal is to maximize

$$\mathcal{L}_{i\pi} \;=\; \sum_x \mathrm{count}(X_i\!=\!x, \mathrm{pa}_i\!=\!\pi)\ \log P(X_i\!=\!x|\mathrm{pa}_i\!=\!\pi)$$

  subject to two constraints:

  1. $\sum_x P(X_i\!=\!x|\mathrm{pa}_i\!=\!\pi) = 1$ *(normalized)*
  2. $P(X_i\!=\!x|\mathrm{pa}_i\!=\!\pi) \geq 0$ *(nonnegative)*

- **Shorthand**

$$\begin{array}{rcl} C_\alpha & = & \mathrm{count}(X_i\!=\!\alpha, \mathrm{pa}_i\!=\!\pi) \\ p_\alpha & = & P(X_i\!=\!\alpha|\mathrm{pa}_i\!=\!\pi) \end{array} \quad \Longrightarrow$$

How to maximize $\sum_\alpha C_\alpha \log p_\alpha$ such that $\sum_\alpha p_\alpha = 1$ and $p_\alpha \geq 0$?

Maximizing the likelihood

- **Compute the normalized counts:**

  Define $q_\alpha = \frac{C_\alpha}{\sum_\beta C_\beta}$ so that $\sum_\alpha q_\alpha = 1$.

  Note that q_α is itself a distribution.

- **All these problems have the same solution:**

  Maximize $\sum_\alpha C_\alpha \log p_\alpha$ such that $\sum_\alpha p_\alpha = 1,\ p_\alpha \geq 0.$

  Minimize $\sum_\alpha C_\alpha \log \frac{1}{p_\alpha}$ such that $\sum_\alpha p_\alpha = 1,\ p_\alpha \geq 0.$

  Minimize $\sum_\alpha C_\alpha \log \frac{C_\alpha}{p_\alpha}$ such that $\sum_\alpha p_\alpha = 1,\ p_\alpha \geq 0.$

  Minimize $\underbrace{\sum_\alpha q_\alpha \log \frac{q_\alpha}{p_\alpha}}_{\mathrm{KL}(q,p)}$ such that $\sum_\alpha p_\alpha = 1,\ p_\alpha \geq 0.$

  $\mathrm{KL}(q,p)$ ← $\boxed{\textbf{KL distance from HW 1}}$

  $\boxed{\textbf{Solution: } p_\alpha = q_\alpha}$

ML solution from normalized counts

$$\boxed{P_{\text{ML}}(X_i\!=\!x|\text{pa}_i\!=\!\pi) \;=\; \frac{\text{count}(X_i\!=\!x, \text{pa}_i\!=\!\pi)}{\sum_{x'} \text{count}(X_i\!=\!x', \text{pa}_i\!=\!\pi)}}$$

- **For nodes with parents:**

$$P_{\text{ML}}(X_i\!=\!x|\text{pa}_i\!=\!\pi) \;=\; \frac{\text{count}(X_i\!=\!x, \text{pa}_i\!=\!\pi)}{\text{count}(\text{pa}_i\!=\!\pi)}$$

- **For root nodes:**

$$P_{\text{ML}}(X_i\!=\!x) \;=\; \frac{\text{count}(X_i\!=\!x)}{T}$$

Properties of ML solution

- **Asymptotically correct:**

  The more data you have, the better your estimates.
  If $P(x_1, x_2, \ldots, x_n) > 0$, then

$$\lim_{T\to\infty} P_{\mathrm{ML}}(x_1, x_2, \ldots, x_n) \;=\; P(x_1, x_2, \ldots, x_n)$$

- **But problematic for sparse data:**

$$P_{\mathrm{ML}}(X_i\!=\!x|\mathrm{pa}_i\!=\!\pi) \;=\; \frac{\mathrm{count}(X_i\!=\!x, \mathrm{pa}_i\!=\!\pi)}{\mathrm{count}(\mathrm{pa}_i\!=\!\pi)}$$

  This is **undefined** when $\mathrm{count}(\mathrm{pa}_i\!=\!\pi) = 0$.
  Otherwise it is **zero** when $\mathrm{count}(X_i\!=\!x, \mathrm{pa}_i\!=\!\pi) = 0$.

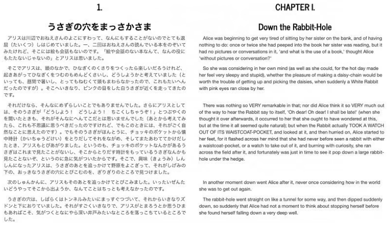
Outline

1. **Maximum likelihood estimation**
2. **Markov models**
3. **Naive Bayes models**
4. **Preview**

Statistical language modeling

Let w_ℓ denote the ℓ^{th} word in a sentence (or text).
How to model $P(w_1, w_2, \ldots, w_L)$?

What can I help you with?



1.

うさぎの穴をまっさかさま

アリスは川辺でおねえさんのよこにすわって、なんにもすることがないのでとても退屈（たいくつ）しはじめていました。一、二回はおねえさんの読んでいる本をのぞいてみたけれど、そこには絵も会話もないのです。「絵や会話のない本なんて、なんの役にもたたないじゃないの」とアリスは思いました。

そこでアリスは、頭のなかで、ひなぎくのくさりをつくったら楽しいだろうけれど、起きあがってひなぎくをつむのもめんどくさいし、どうしようかと考えていました（といっても、昼間で暑いし、とってもねむくて頭もまわらなかったので、これもたいへんだったのですが）。そこへいきなり、ピンクの目をした白うさぎが近くを走ってきたのです。

それだけなら、そんなにめずらしいことでもありませんでした。さらにアリスとしては、そのうさぎが「どうしよう！　どうしよう！　ちこくしちゃうぞ！」とつぶやくのを聞いたときも、それがそんなにへんてこだとは思いませんでした（あとから考えてみたら、これも不思議に思うべきだったのですけれど、でもこのときには、それがごく自然なことに思えたのです）。でもそのうさぎがほんとうに、チョッキのポケットから懐中時計（かいちゅうどけい）をとりだしてそれをながめ、そしてまたあわててかけだしたとき、アリスもとびあがりました。というのも、チョッキのポケットなんかがあるうさぎはこれまで見たことがないし、そこからとりだす時計をもっているうさぎなんかも見たことないぞ、というのに急に気がついたからです。そこで、興味（きょうみ）しんしんになったアリスは、うさぎのあとを追っかけて野原をよこぎって、それがしげみの下の、おっきなうさぎの穴にとびこむのを、ぎりぎりのところで見つけました。

次のしゅんかんに、アリスもそのあとを追っかけてとびこみました。いったいぜんたいどうやってそこから出ようか、なんてことはちっとも考えなかったのです。

うさぎの穴は、しばらくはトンネルみたいにまっすぐつづいて、それからいきなりズドンと下におりていました。それがすごくいきなりで、アリスがとまろうとか思うひまもあればこそ、気がつくとなにやら深い井戸みたいなところを落っこちているところでした。

CHAPTER I.

Down the Rabbit-Hole

Alice was beginning to get very tired of sitting by her sister on the bank, and of having nothing to do: once or twice she had peeped into the book her sister was reading, but it had no pictures or conversations in it, 'and what is the use of a book,' thought Alice 'without pictures or conversation?'

So she was considering in her own mind (as well as she could, for the hot day made her feel very sleepy and stupid), whether the pleasure of making a daisy-chain would be worth the trouble of getting up and picking the daisies, when suddenly a White Rabbit with pink eyes ran close by her.

There was nothing so VERY remarkable in that; nor did Alice think it so VERY much out of the way to hear the Rabbit say to itself, 'Oh dear! Oh dear! I shall be late!' (when she thought it over afterwards, it occurred to her that she ought to have wondered at this, but at the time it all seemed quite natural); but when the Rabbit actually TOOK A WATCH OUT OF ITS WAISTCOAT-POCKET, and looked at it, and then hurried on, Alice started to her feet, for it flashed across her mind that she had never before seen a rabbit with either a waistcoat-pocket, or a watch to take out of it, and burning with curiosity, she ran across the field after it, and fortunately was just in time to see it pop down a large rabbit-hole under the hedge.

In another moment down went Alice after it, never once considering how in the world she was to get out again.

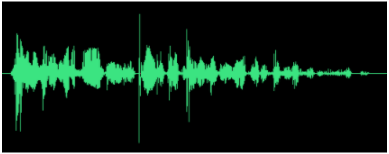
The rabbit-hole went straight on like a tunnel for some way, and then dipped suddenly down, so suddenly that Alice had not a moment to think about stopping herself before she found herself falling down a very deep well.

automatic speech recognition

machine translation

Context and expectations in language

"It's hard to wreck a nice beach."



"It's hard to recognize speech."

Simplifying assumptions

1. **Finite context**

   To predict the ℓ^{th} word, it is sufficient to consider a *finite* number of words that precede it:

   $$P(w_\ell | w_1, w_2, \ldots, w_{\ell-1}) \;=\; P(w_\ell | \underbrace{w_{\ell-(n-1)}, \ldots, w_{\ell-1}}_{n-1 \textbf{ previous words}})$$

2. **Position invariance**

   Predictions should not depend on where the context occurs in the sentence or text:

   $$P(W_\ell = w' | w_{\ell-(n-1)}, \ldots, w_{\ell-1})$$

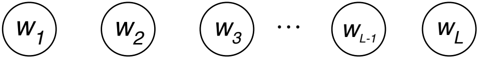
   $$= \quad P(W_{s+\ell} = w' | W_{s+\ell-(n-1)} = w_{\ell-(n-1)}, \ldots, W_{s+\ell-1} = w_{\ell-1})$$

Markov models

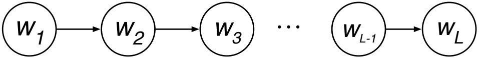
$$
\begin{aligned}
P(w_1, w_2, \ldots, w_L) & \\
&= \prod_{\ell} P(w_\ell | w_1, w_2, \ldots, w_{\ell-1}) \qquad \boxed{\textbf{product rule}} \\
&= \prod_{\ell} P(w_\ell | w_{\ell-(n-1)}, \ldots, w_{\ell-1}) \qquad \boxed{\textbf{conditional independence}}
\end{aligned}
$$

$\boxed{\textbf{Models of different orders}}$

$n = 1$ **unigram**



$n = 2$ **bigram**



$n = 3$ **trigram**

Markov models

$$P(w_1, w_2, \ldots, w_L)$$

$$= \prod_{\ell} P(w_\ell | w_1, w_2, \ldots, w_{\ell-1}) \qquad \boxed{\textbf{product rule}}$$

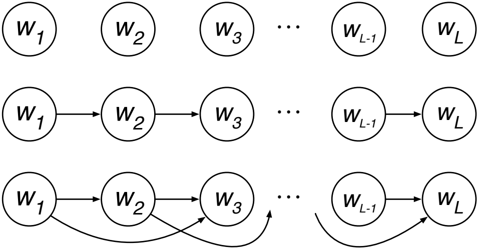
$$= \prod_{\ell} P(w_\ell | w_{\ell-({\color{red}n}-1)}, \ldots, w_{\ell-1}) \qquad \boxed{\textbf{conditional independence}}$$

Models of different orders

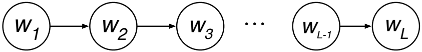
$n = 1$ **unigram**

$n = 2$ **bigram**

$n = 3$ **trigram**



Bigram models



Note that the same CPT for $P(w_\ell = w' | w_{\ell-1} = w)$ is used at each node (for $\ell > 1$).

How to learn?

Collect a large corpus of text with a well-defined vocabulary.

Count how often word w is followed by the word w'.
Count how often word w is followed by any word.

Estimate from empirical frequencies:

$$P_{\mathrm{ML}}(w_\ell = w' | w_{\ell-1} = w) \;=\; \frac{\mathrm{count}(w \to w')}{\mathrm{count}(w \to *)} \;=\; \frac{\mathrm{count}(w \to w')}{\sum_{w''} \mathrm{count}(w \to w'')}$$

Problems with ML estimates

1. **No generalization to unseen *n*-grams:**

   ML estimates assign **zero** probability to *n*-grams that do not appear in the training corpus.

2. **The larger *n*, the worse the problem:**

   n-gram counts become increasingly sparse as *n* increases. Many possible (but improbable) *n*-grams are not observed.

You will explore this problem further in HW 4.

Outline

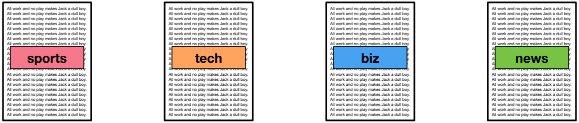
1. Maximum likelihood estimation

2. Markov models

3. Naive Bayes models

4. Preview

Document classification



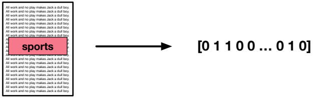
- **Setup**

  Each document can be labeled by one of m topics.
  Each document consists of words from a finite vocabulary.

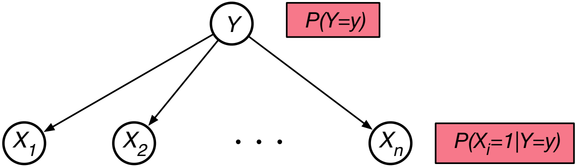
- **Random variables**

  Let $Y \in \{1, 2, \ldots, m\}$ denote the label.
  Let $X_i \in \{0, 1\}$ denote whether the i^{th} word appears.

This representation maps each document to a sparse binary vector of fixed length.



Belief network

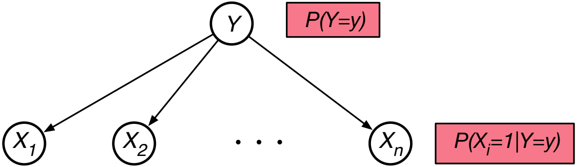


This DAG makes a fairly drastic assumption of conditional independence:

$$P(X_1, \ldots, X_n | Y) \; = \; \prod_{i=1}^{n} P(X_i | Y)$$

For this reason it is called a **Naive Bayes** model.

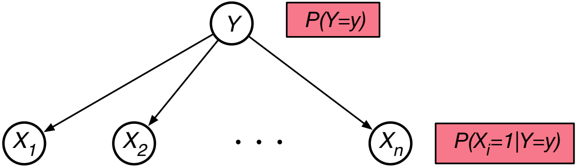
Naive Bayes model



Suppose this DAG is given, but the CPTs are not specified.
How to learn the CPTs from data?

- **Collect** a large corpus of documents.
- **Label** each document by a topic.
- **Estimate** the CPTs by maximizing the likelihood.

ML estimation



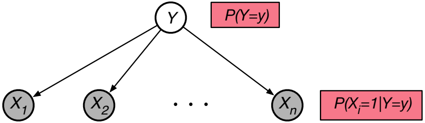
$$P_{\mathrm{ML}}(Y=y) \quad = \quad \text{fraction of documents with label } y \text{ in the corpus}$$

$$P_{\mathrm{ML}}(X_i=1|Y=y) \quad = \quad \text{fraction of documents with label } y \text{ that contain the } i^{\mathrm{th}} \text{ word in the vocabulary}$$

Once the model is learned, what is it good for?

Inference

How to classify an unlabeled document?



$$P(Y=y|X_1,X_2,\ldots,X_n)$$

$$= \frac{P(X_1,X_2,\ldots,X_n|Y=y)\,P(Y=y)}{P(X_1,X_2,\ldots,X_n)}$$

Bayes rule

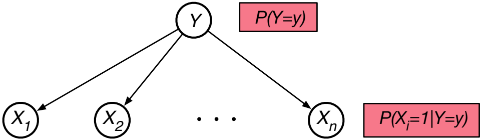
$$= \frac{P(Y=y)\prod_{i=1}^{n} P(X_i|Y=y)}{P(X_1,X_2,\ldots,X_n)}$$

conditional independence

$$= \frac{P(Y=y)\prod_{i=1}^{n} P(X_i|Y=y)}{\sum_{y'} P(Y=y')\prod_{i=1}^{n} P(X_i|Y=y')}$$

normalization

Strengths and weaknesses



Strengths

- Easy to learn from data.
- Easy to classify unlabeled documents.

Weaknesses

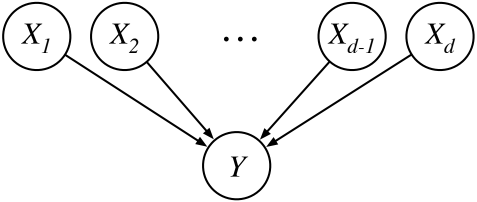
- Naive Bayes assumption of conditional independence
- No information about word ordering
- Binarization of word counts
- Etc ...

Outline

1. Maximum likelihood estimation
2. Markov models
3. Naive Bayes models
4. Preview

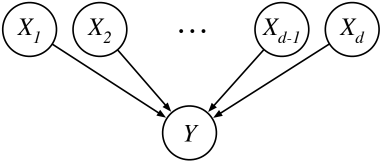
Parametric models

If the parent nodes are real-valued, then it is no longer possible to enumerate a conditional probability table.



How to predict Y from real-valued parents $\vec{X} \in \mathbb{R}^d$?

Gaussian model

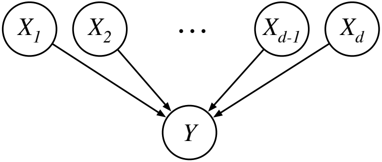


Suppose $Y \in \mathbb{R}$ is a real-valued random variable.
Then we can use a **Gaussian conditional distribution**:

$$P(y|\vec{x}) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left\{-\frac{(y - \vec{w} \cdot \vec{x})^2}{2\sigma^2}\right\}$$

How to learn the parameters σ^2 and $\vec{w} = (w_1, w_2, \ldots, w_d)$?
This is the problem of **linear regression**.

Sigmoid model



Suppose $Y \in \{0,1\}$ is a binary random variable.
Then we can use a **sigmoid conditional distribution**:

$$P\,(Y\!=\!1|\vec{x}) \;=\; \sigma(\vec{w}\cdot\vec{x}) \;=\; \frac{1}{1+e^{-\vec{w}\cdot\vec{x}}}$$

How to learn the parameter $\vec{w} \in \mathbb{R}^d$?
This is the problem of **logistic regression**.

Before next lecture ...

Now would be a good time to review your linear algebra:

- dot products
- matrix-vector multiplication
- systems of linear equations

And also your multivariable calculus:

- functions of several real variables
- partial derivatives
- gradients and Hessians