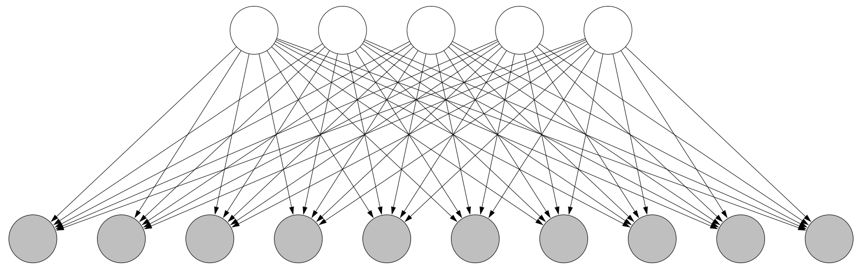
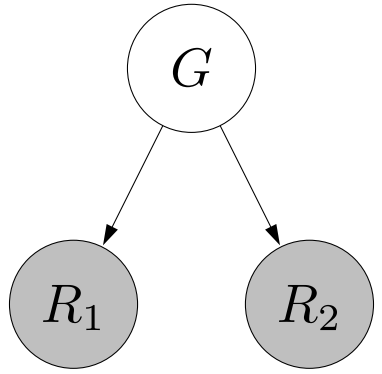
Bayesian networks: EM algorithm



- In this module, I'll introduce the EM algorithm for learning Bayesian networks when we have unobserved variables in our training data.

Motivation



Genre $G \in \{\text{drama}, \text{comedy}\}$

Jim's rating $R_1 \in \{1, 2, 3, 4, 5\}$

Martha's rating $R_2 \in \{1, 2, 3, 4, 5\}$

If observe all the variables: maximum likelihood $=$ count and normalize

$$\mathcal{D}_{\text{train}} = \{(\text{d}, 4, 5), (\text{d}, 4, 4), (\text{d}, 5, 3), (\text{c}, 1, 2), (\text{c}, 5, 4)\}$$

What if we **don't observe** some of the variables?

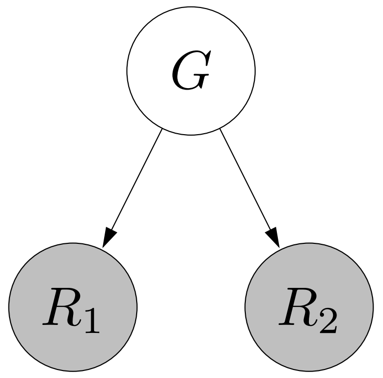
$$\mathcal{D}_{\text{train}} = \{(?, 4, 5), (?, 4, 4), (?, 5, 3), (?, 1, 2), (?, 5, 4)\}$$

- Let's start with our familiar movie rating example, where we have genre G, Jim's rating R_1, and Martha's rating R_2.
- If we observe all the variables in each training example, then we saw how we can do maximum likelihood estimation (a.k.a. count + normalize).
- Data collection is hard, and often we don't observe the value of every single variable. Maybe we only see the ratings (R_1, R_2), but not the genre G. Can we learn in this setting, which is clearly more difficult?
- Intuitively, it might seem hopeless. After all, how can we ever learn anything about the relationship between G and R_1 if we never observe G at all?
- The magic of EM (or unsupervised learning in general) is that you can in many (but certainly not all) cases.

Maximum marginal likelihood

Variables: H is hidden, $E = e$ is observed

Example:



$H = G \qquad E = (R_1, R_2) \qquad e = (1, 2)$

$\theta = (p_G, p_R)$

Maximum marginal likelihood objective:

$$\max_\theta \prod_{e \in \mathcal{D}_{\text{train}}} \mathbb{P}(E = e; \theta)$$

$$= \max_\theta \prod_{e \in \mathcal{D}_{\text{train}}} \sum_h \mathbb{P}(H = h, E = e; \theta)$$

- Let's try to solve this problem top-down — what do we want, mathematically?
- Formally we have a set of hidden variables H, observed variables E, and parameters θ, which define all the local conditional distributions. We observe $E = e$, but we don't know H or θ.
- If there were no hidden variables, then we would just use maximum likelihood: $\max_\theta \prod_{(h,e) \in \mathcal{D}_{\text{train}}} \mathbb{P}(H = h, E = e; \theta)$. But since H is unobserved, we can simply replace the joint probability $\mathbb{P}(H = h, E = e; \theta)$ with the marginal probability $\mathbb{P}(E = e; \theta)$, which is just a sum over values h that the hidden variables H could take on.

Expectation Maximization (EM)

Intuition: generalization of the K-means algorithm

cluster centroids $=$ parameters θ cluster assignments $=$ hidden variables H

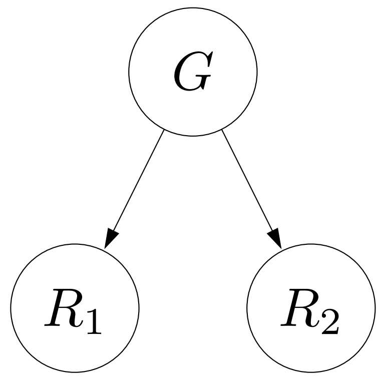
Variables: H is hidden, $E = e$ is observed

Algorithm: Expectation Maximization (EM)

```
Initialize $\theta$ randomly
Repeat until convergence:
    E-step:
        Compute $q(h) = \mathbb{P}(H = h \mid E = e; \theta)$ for each $h$ (probabilistic inference)
        Create fully-observed weighted examples: $(h, e)$ with weight $q(h)$
    M-step:
        Maximum likelihood (count and normalize) on weighted examples to get $\theta$
```

- Expectation Maximization (EM), which was developed in statistics in the 1970s, is an algorithm that attempts to maximize the marginal likelihood, although special cases had been developed earlier (e.g., for HMMs).
- To get intuition for EM, consider K-means, which turns out to be a special case of EM (for Gaussian mixture models with variance tending to 0). In K-means, we had to somehow estimate the cluster centers, but we didn't know which points were assigned to which clusters. And in that setting, we took an alternating optimization approach: find the best cluster assignment given the current cluster centers, find the best cluster centers given the assignments, etc.
- The EM algorithm works analogously. EM consists of alternating between two steps, the E-step and the M-step. In the E-step, we don't know what the hidden variables are, so we compute the posterior distribution over them given our current parameters ($\mathbb{P}(H \mid E = e; \theta)$). This can be done using any probabilistic inference algorithm. If H takes on a few values, then we can enumerate over all of them. If $\mathbb{P}(H, E)$ is defined by an HMM, we can use the forward-backward algorithm. These posterior distributions provide a weight $q(h)$ (which is a temporary variable in the EM algorithm) to every value h that H could take on. Conceptually, the E-step then generates a set of weighted full assignments (h, e) with weight $q(h)$. (In implementation, we don't need to create the data points explicitly, since we can just add counts directly.)
- In the M-step, we take in our set of full assignments (h, e) with weights, and we just do maximum likelihood estimation, which can be done in closed form — just counting and normalizing (perhaps with smoothing if you want)!
- If we repeat the E-step and the M-step over and over again, we are guaranteed to converge to a **local optima**. Just like the K-means algorithm, we might need to run the algorithm from different random initializations of θ and take the best one.

Example: one iteration of EM



$$\mathcal{D}_{\text{train}} = \{(?, 2, 2), (?, 1, 2)\}$$

θ:

g	$p_G(g)$
c	0.5
d	0.5

g	r	$p_R(r \mid g)$
c	1	0.4
c	2	0.6
d	1	0.6
d	2	0.4

E-step

(r_1, r_2)	g	$\mathbb{P}(G = g, R_1 = r_1, R_2 = r_2)$	$q(g)$
(2, 2)	c	$0.5 \cdot 0.6 \cdot 0.6 = 0.18$	$\frac{0.18}{0.18+0.08} = 0.69$
(2, 2)	d	$0.5 \cdot 0.4 \cdot 0.4 = 0.08$	$\frac{0.08}{0.18+0.08} = 0.31$
(1, 2)	c	$0.5 \cdot 0.4 \cdot 0.6 = 0.12$	$\frac{0.12}{0.12+0.12} = 0.5$
(1, 2)	d	$0.5 \cdot 0.6 \cdot 0.4 = 0.12$	$\frac{0.12}{0.12+0.12} = 0.5$

M-step

θ:

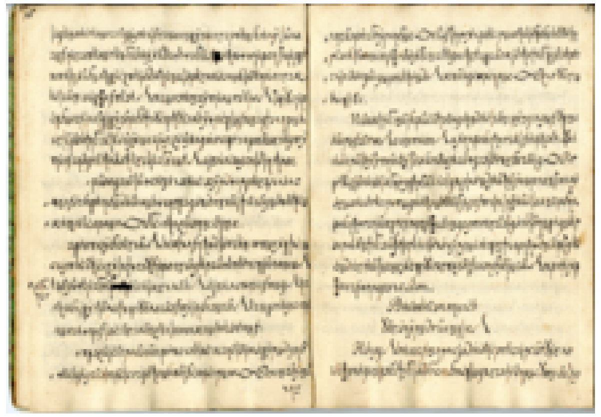
g	count	$p_G(g)$
c	0.69 + 0.5	0.59
d	0.31 + 0.5	0.41

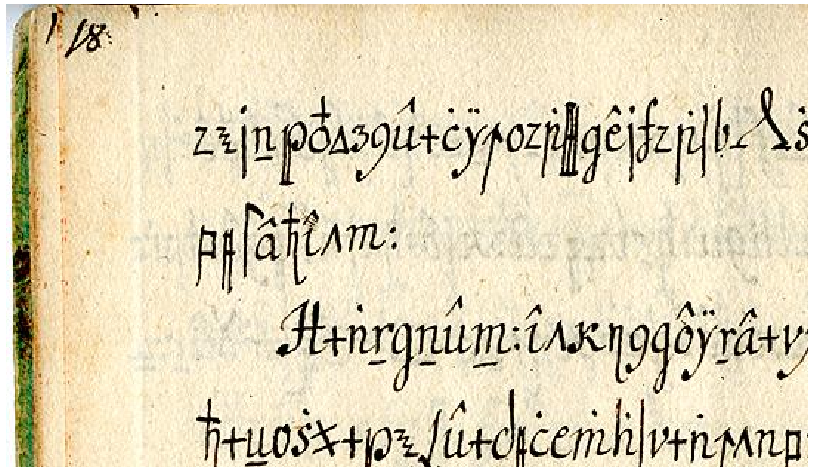
g	r	count	$p_R(r \mid g)$
c	1	0.5	0.21
c	2	0.5 + 0.69 + 0.69	0.79
d	1	0.5	0.31
d	2	0.5 + 0.31 + 0.31	0.69

- In the E-step, we are presented with the current set of parameters θ. We go through all the examples (in this case $(2,2)$ and $(1,2)$). For each example (r_1, r_2), we will consider all possible values of g (c or d), and compute the posterior distribution $q(g) = \mathbb{P}(G = g \mid R_1 = r_1, R_2 = r_2)$.
- The easiest way to do this is to write down the joint probability $\mathbb{P}(G = g, R_1 = r_1, R_2 = r_2)$ because this is just simply a product of the parameters. For example, the first line is the product of $p_G(\text{c}) = 0.5$, $p_R(2 \mid \text{c}) = 0.6$ for $r_1 = 2$, and $p_R(2 \mid \text{c}) = 0.6$ for $r_2 = 2$. For each example (r_1, r_2), we normalize these joint probability to get $q(g)$.
- Now each row consists of a fictitious data point with g filled in, but appropriately weighted according to the corresponding $q(g)$, which is based on what we currently believe about g.
- In the M-step, for each of the parameters (e.g., $p_G(\text{c})$), we simply add up the weighted number of times that parameter was used in the data (e.g., 0.69 for (c, 2, 2) and 0.5 for (c, 1, 2)). Then we normalize these counts to get probabilities.
- If we compare the old parameters and new parameters after one round of EM, you'll notice that parameters tend to sharpen (though not always): probabilities tend to move towards 0 or 1.

Application: decipherment

Copiale cipher (105-page encrypted volume from 1730s):





Cracked in 2011 with the help of EM!

- Let's now look at an interesting application of EM (or Bayesian networks in general): decipherment. Given a ciphertext (a string), how can we decipher it?
- The Copiale cipher was deciphered in 2011 (it turned out to be the handbook of a German secret society), largely with the help of Kevin Knight, an NLP researcher.
- Real ciphers are a bit too complex, so we will focus on the simple case of substitution ciphers.

Substitution ciphers

Letter substitution table (unknown):

Plain:	`abcdefghijklmnopqrstuvwxyz`
Cipher:	`plokmijnuhbygvtfcrdxeszaqw`

Plaintext (unknown): `hello world`

Ciphertext (known): `nmyyt ztryk`

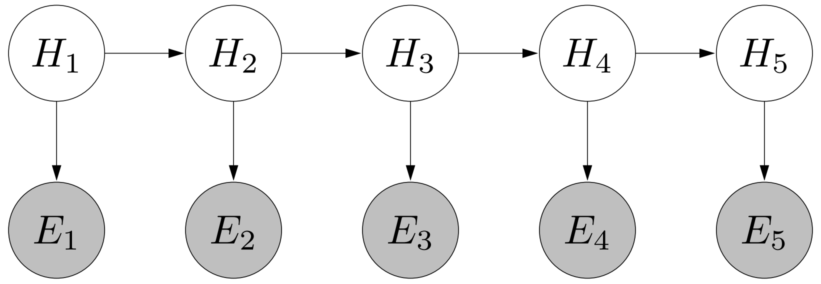
Challenge: Give ciphertext, recover the plaintext

- The input to decipherment is a ciphertext. Let's put our modeling hats on and think about how this ciphertext came to be.
- In a simple substitution cipher, someone comes up with a permutation of the letters (e.g., "a" maps to "p"). You can think about these as the unknown parameters of the model.
- Then they think of something to say — the plaintext (e.g., "hello world"). Finally, they apply the substitution table to generate the ciphertext (deterministically).

Application: decipherment as an HMM

Variables:

- $H_1, \dots, H_n$ (e.g., characters of plaintext)
- $E_1, \dots, E_n$ (e.g., characters of ciphertext)

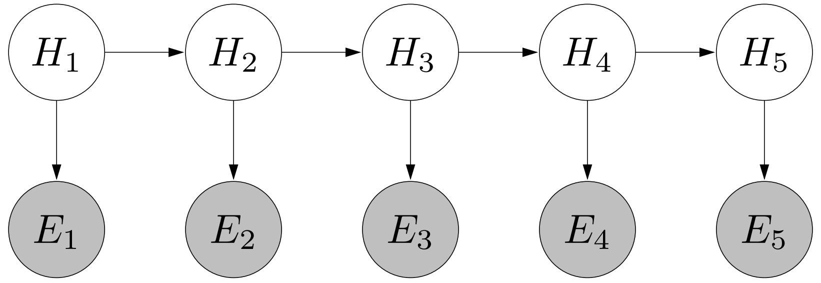


$$\mathbb{P}(H = h, E = e) = p_{\text{start}}(h_1) \prod_{i=2}^{n} p_{\text{trans}}(h_i \mid h_{i-1}) \prod_{i=1}^{n} p_{\text{emit}}(e_i \mid h_i)$$

Parameters: $\theta = (p_{\text{start}}, p_{\text{trans}}, p_{\text{emit}})$

- We can formalize this process as an HMM as follows. The hidden variables are the plaintext and the observations are the ciphertext. Each character of the plaintext is related to the corresponding character in the ciphertext based on the cipher, and the transitions encode the fact that the characters in English are highly dependent on each other. For simplicity, we use a character-level bigram model (though n-gram models would yield better results).

Application: decipherment as an HMM



Strategy:

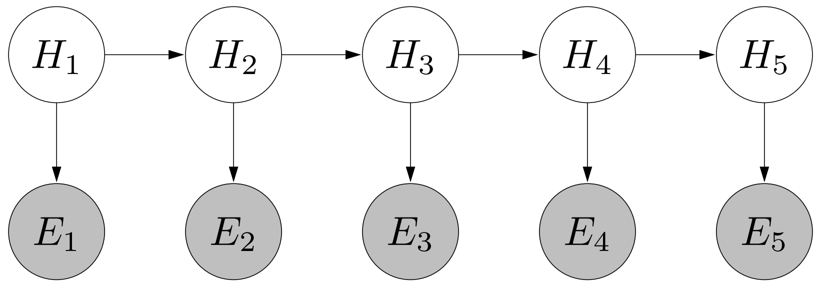
- p_{start}: set to uniform
- p_{trans}: estimate on tons of English text
- p_{emit}: **substitution table**, estimated from EM

Intuitions:

- p_{trans} to favor plaintexts h that look like English
- p_{emit} favors consistent characters substitutions

- We need to specify how we estimate the starting probabilities p_{start} the transition probabilities p_{trans}, and the emission probabilities p_{emit}.
- The **starting probabilities** we won't care about so much and just set to a uniform distribution.
- The **transition probabilities** specify how someone might have generated the plaintext. We can estimate p_{trans} on a large corpora of English text. Note we need not use the same data to estimate all the parameters of the model. Indeed, there is generally much more English plaintext lying around than ciphertext. This is one of the other nice things about Bayesian networks, is that estimation can sometimes be done in a modular way.
- The **emission probabilities** encode the substitution table. Here, we know that the substitution table is deterministic, but we let the parameters be general distributions, which can certainly encode deterministic functions (e.g., $p_{\text{emit}}(\text{p} \mid \text{a}) = 1$). We use EM to only estimate the emission probabilities.
- We emphasize that the principal difficulty here is that we neither know the plaintext nor the parameters! But why might this work? The intuition is that the transitions p_{trans} (which are known, so it's a bit easier than standard EM) will favor plaintexts h that look like English (e.g., $h_{i-1} = \text{t}$ to $h_i = \text{a}$ rather than to $h_i = \text{b}$). The emissions p_{emit} will favor character substitutions that are consistent (so all occurrences of a should be mapped to the same character).

Application: decipherment as an HMM



E-step: forward-backward computes for each position i and character h

$$q_i(h) \overset{\text{def}}{=} \mathbb{P}(H_i = h \mid E_1 = e_1, \dots E_n = e_n)$$

M-step: count (fractional) and normalize for all characters e, h

$$\text{count}_{\text{emit}}(h, e) = \textstyle\sum_{i : e_i = e} q_i(h)$$

$$p_{\text{emit}}(e \mid h) \propto \text{count}_{\text{emit}}(h, e)$$

- Let's focus on the EM algorithm for estimating the emission probabilities. In the E-step, we can use the forward-backward algorithm to compute the posterior distribution over hidden assignments $\mathbb{P}(H \mid E = e)$. More precisely, the algorithm returns $q_i(h) \overset{\text{def}}{=} \mathbb{P}(H_i = h \mid E = e)$ for each position $i = 1, \dots, n$ and possible hidden state h.
- We can use $q_i(h)$ as fractional counts of each H_i. To compute the counts $\text{count}_{\text{emit}}(h, e)$, we loop over all the positions algorithm i where $E_i = e$ and add the fractional count $q_i(h)$.

Decipherment in Python

[code]

- In the code, we first estimate the Markov model p_{trans} on some plain text. Then we run EM to estimate the p_{emit}, where we leave p_{start} and p_{trans} alone.
- As you can see from the demo, the result isn't perfect, but not bad given the difficulty of the problem and the simplicity of the approach.

Summary

$$\begin{tikzcd}
H_1 \arrow[r] \arrow[d] & H_2 \arrow[r] \arrow[d] & H_3 \arrow[r] \arrow[d] & H_4 \arrow[r] \arrow[d] & H_5 \arrow[d] \\
E_1 & E_2 & E_3 & E_4 & E_5
\end{tikzcd}$$

Maximum marginal likelihood:

$$\max_\theta \prod_{e \in \mathcal{D}_{\text{train}}} \mathbb{P}(E = e; \theta)$$

EM algorithm:

$\Leftarrow$ probabilistic inference (E-step)

hidden variables $q(h)$

parameters θ

count and normalize (M-step) $\Rightarrow$

Applications: decipherment, phylogenetic reconstruction, crowdsourcing

- In summary, we introduced the EM algorithm for estimating the parameters of a Bayesian network when there are unobserved variables.
- The principle we follow is maximum marginal likelihood. The algorithm that optimizes this is the EM algorithm, which is very intuitive. Ultimately, like in k-means, we have a chicken-and-egg problem, where we don't know the hidden variables and we also don't know the parameters.
- But we can update each conditioned on the other: In the E-step, we use probabilistic inference to compute a distribution over hidden variables conditioned on the evidence. In the M-step, we have a weighted set of fully-observable examples, and we simply count and normalize. This procedure is guaranteed to converge to a local optimum of the marginal likelihood objective.
- Finally, after you have learned the parameters of your Bayesian network, you can go off and perform inference to answer all sorts of questions, which could be on the unobserved variables on new test examples or completely other variables. This highlights the flexibility of Bayesian networks in dealing with heterogenous data between training and test time.
- There are many applications of the EM algorithm. We looked at a simple form of decipherment, where we try to infer the plaintext form the ciphertext. EM can also be used to reconstruct the phylogenetic tree given the DNA of modern organisms. It can also be used to infer the unknown label of a data point, where the observations are the possibly noisy labels provided by crowdworkers.
- EM is the most canonical version of a broader class of variational inference approaches, which include things like variational autoencoders (VAEs), where the q distribution (encoder) is given by a neural network, and the Bayesian network is the decoder. I'd encourage you to go explore this connection in more detail.