MSA101/MVE187 2021 Lecture 12
Some Information Theory
The EM algorithm

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Overview

- Some information theory.
- The EM algorithm.
- A toy example.
- The Baum-Welsh algorithm as an example of EM.

The information of an event

We assume given a probability mass function $\pi(x)$ on a finite set S.

- We want to define the "information" $h(U)$ in an event $U \subseteq S$. Requirements:
  - An event with probability 1 should have zero information.
  - The information should increase with decreasing probability $\pi(U)$.
  - If $S = S_1 \times S_2$ and $\pi(x_1, x_2) = \pi(x_1)\pi(x_2)$ on this set, then we want $h(x_1, x_2) = h(x_1) + h(x_2)$.
- We define $h(x) = -\log(\pi(x))$ for $x \in S$.
- When using the base 2 logarithm $\log_2$, information is measured in "bits". We however use the natural logarithm.

Expected information: Entropy

- Define the entropy $H[X]$ of the discrete random variable X as the expected information:

$$H[X] = \sum_x h(x)\pi(x) = -\sum_x \pi(x)\log(\pi(x))$$

- Note: $H[X]$ is always non-negative.
- Example: A uniform distribution on n values has entropy $\log n$. This is the largest entropy possible for a distribution on n values.
- Shannon's coding theorem: The entropy (using $\log_2$) is a lower bound on the expected number of bits needed to transfer the information from X.

(Differential) entropy for continuous distributions

- For any random variable X, its (differential) entropy is defined as

$$H[X] = \mathrm{E}\left[-\log(\pi(x))\right] = -\int_x \log(\pi(x))\pi(x)\,dx$$

- $H[X]$ may now be negative.
- Example: Assume $X \sim \mathrm{Normal}(\mu, \sigma^2)$. Then

$$\begin{aligned} \mathrm{E}\left[-\log(\pi(x))\right] &= \mathrm{E}\left[-\log\left(\frac{1}{\sqrt{2\pi\sigma^2}}\right) + \frac{1}{2\sigma^2}(x-\mu)^2\right] \\ &= \frac{1}{2}\log(2\pi\sigma^2) + \frac{1}{2\sigma^2}\,\mathrm{E}\left[(x-\mu)^2\right] = \frac{1}{2}\log(2\pi\sigma^2) + \frac{1}{2}. \end{aligned}$$

- In fact, among all random variables X with $\mathrm{E}[X] = \mu$ and $\mathrm{Var}[X] = \sigma^2$, the normal has the largest entropy.

Conditional entropy and mutual information

- The conditional entropy is defined as

$$H[Y|X] = \int \left[\int \pi(y \mid x)(-\log(\pi(y \mid x)))\, dy \right] \pi(x)\, dx$$

- Show that

$$H[X, Y] = H[Y|X] + H[X].$$

- The mutual information is defined as

$$I[X, Y] = -\int \int \pi(x, y) \log \left(\frac{\pi(x)\pi(y)}{\pi(x, y)} \right) dx\, dy$$

- Show that

$$I[X, Y] = H[X] + H[Y] - H[X, Y]$$

The Kullback-Leibler divergence (relative entropy)

- For a density $p(x)$ and a positive-valued function $q(x)$ we define

$$\mathrm{KL}[p||q] = -\int p(x) \log\left(\frac{q(x)}{p(x)}\right) dx$$

- When $q(x)$ is a density, this is the **Kullback-Leibler** divergence from p to q. (But notation is useful even when q is not a density).
- Note that $\mathrm{KL}[p||q]$ is generally different from $\mathrm{KL}[q||p]$.
- When q is a density, we always have $\mathrm{KL}[p||q] \geq 0$ while $\mathrm{KL}[p||q] = 0$ if and only if $p = q$.
- The standard proof uses *Jensen's inequality*.
- Jensen's inequality: If a function ψ is *convex*, then $\psi(\mathrm{E}[X]) \leq \mathrm{E}[\psi(X)]$.

The KL divergence

- Note that
$$\mathrm{KL}\left(\pi(x,y)||\pi(x)\pi(y)\right) = I[X,Y]$$
- Note that
$$\mathrm{KL}[p||q] = \mathrm{E}_p\left[-\log(q(x))\right] - H_p[X]$$
where X is a random variable with density $p(x)$.
- EXAMPLE: Assume $X \sim \mathrm{Normal}(\mu_X, \sigma_X^2)$ and $Y \sim \mathrm{Normal}(\mu_Y, \sigma_Y^2)$.
Show by direct computation that
$$\mathrm{KL}\left[\pi_X||\pi_Y\right] = \frac{1}{2}\log(2\pi\sigma_Y^2) + \frac{\sigma_X^2}{2\sigma_Y^2} + \frac{1}{2\sigma_Y^2}(\mu_X - \mu_Y)^2 - \frac{1}{2}\log(2\pi\sigma_X^2) - \frac{1}{2}.$$
We see how the result is zero when the two distributions are identical.
We see how $\mathrm{KL}\left[\pi_X||\pi_Y\right] \neq \mathrm{KL}\left[\pi_Y||\pi_X\right]$ in general.

Start of part 2: Maximum posterior (MAP)

- The Maximal APosteriori (MAP): The value $\hat{\theta}$ that maximizes the posterior $\pi(\theta \mid \text{data})$.
- When the prior is flat, $\pi(\theta) \propto 1$, this corresponds to finding the maximum likelihood (ML) estimate for θ.
- Recall the advantages and disadvantages of using a single estimate instead of the full posterior.
- The MAP should be easy to compute when θ consists of all unknown variables: Just differentiate $\log(\pi(\theta \mid \text{data}))$, i.e. differentiate $\log(\pi(\text{data} \mid \theta)\pi(\theta))$.
- Much harder if the model also contains other unknown variables Z: Then $\pi(\theta \mid \text{data})$ is the marginal of $\pi(\theta, Z \mid \text{data})$ and much harder to maximize.
- The Expectation-Maximization (EM) algorithm comes to the rescue...

The EM algorithm

- We want to find the θ maximizing the posterior $\pi(\theta \mid x)$; i.e., maximizing

$$\log\left(\pi(x \mid \theta)\pi(\theta)\right) = \log(\pi(x \mid \theta)) + \log(\pi(\theta))$$

- Assume we have a joint model $\pi(x, z \mid \theta)$ which includes augmented data z, and consider the marginal $\pi_z(z \mid x, \theta)$. We may then write, for any density $q(z)$,

$$\log(\pi(x \mid \theta)) + \log(\pi(\theta)) = \mathrm{KL}(q || \pi_z) + \mathcal{L}(q, \theta) + \log(\pi(\theta)) \quad (1)$$

  where

$$\mathcal{L}(q, \theta) = \int q(z) \log\left(\frac{\pi(x, z \mid \theta)}{q(z)}\right) dz$$

  and

$$\mathrm{KL}(q || \pi_z) = -\int q(z) \log\left(\frac{\pi_z(z \mid x, \theta)}{q(z)}\right) dz$$

The EM algorithm, cont.

- Fix $q(z) = \pi_z(z \mid x, \theta^{old})$ for some value θ^{old}.
- With this $q(z)$, $\text{KL}(q||\pi_z)$ will be zero when $\theta = \theta^{old}$ and positive for other θ's. THUS: If we find θ^{new} maximizing $\mathcal{L}(q, \theta) + \log(\pi(\theta))$, so that $\mathcal{L}(q, \theta^{new}) + \log(\pi(\theta^{new})) > \mathcal{L}(q, \theta^{old}) + \log(\pi(\theta^{old}))$, replacing θ^{old} with θ^{new} will increase the right side of Equation 1, and thus also the left side.
- Set θ^{old} to the value θ^{new} and start again from the first step above. Continue until convergence.
- Note that maximizing $\mathcal{L}(q, \theta) + \log(\pi(\theta))$ is the same as maximizing

  $$\int q(z) \log\left(\pi(x, z \mid \theta)\right) \, dz + \log(\pi(\theta))$$

  where the left term is the expected full loglikelihood, taking the expectation over the density $q(z) = \pi_z(z \mid x, \theta^{old})$.
- E-step: Computing the expectation above. M-step: Maximizing.

The EM algorithm, summary

A model with parameters θ, data x, and augmented variables z is specified using $\pi(\theta)$ and $\pi(x, z \mid \theta)$. Write $\pi_z(z \mid x, \theta)$ for conditional density for z.
Find θ maximizing $\pi(\theta \mid x) \propto_\theta \pi(x \mid \theta)\pi(\theta)$ as follows: Start with some $\theta^{(0)}$, and iteratively compute θ^{new} from θ^{old} as follows:

- **E-step**: Compute as a function of θ

$$\mathrm{E}_{z \mid \theta^{old}}\left[\log \pi(x, z \mid \theta)\right]$$

  where you take the expectation over $\pi_z(z \mid x, \theta^{old})$.
- **M-step**: Maximize the sum of this function of θ and $\log(\pi(\theta))$ to find θ^{new}.

A toy example

We have data $x_1, \ldots, x_n$, where we assume the following model, with a single parameter μ: With probability 0.5, $x_i \sim \text{Normal}(0, 1)$ and with probability 0.5, $x_i \sim \text{Normal}(\mu, 1)$. We assume a flat prior on μ.

- The likelihood can be written as

$$\pi(x_1, \ldots, x_n \mid \mu) = \prod_{i=1}^{n} \left(0.5 \cdot \text{Normal}(x_i; 0, 1) + 0.5 \cdot \text{Normal}(x_i; \mu, 1)\right)$$

- We now introduce *augmented* data $z_1, \ldots, z_n$, where each z_i has value 0 or 1, so that $z_i \sim \text{Bernoulli}(0.5)$ and $x_i \mid z_i \sim \text{Normal}(\mu z_i, 1)$. The full joint density may be written as

$$\pi(x_1, \ldots, x_n, z_1, \ldots, z_n, \mu) \propto \prod_{i=1}^{n} \pi(x_i \mid z_i, \mu) = \prod_{i=1}^{n} \text{Normal}(x_i; \mu z_i, 1)$$

- One way to use this model is for finding the μ maximizing the posterior using the EM-algorithm.

A toy example: Using the EM algorithm

- First, find the complete data logposterior (which in our case is the same as the loglikelihood). It is (up to a constant)

$$\log \pi(x_1, \ldots, x_n, z_1, \ldots, z_n \mid \mu)) = \sum_{i=1}^{n} -\frac{1}{2}(x_i - \mu z_i)^2$$

- Then, for a fixed value $\mu = \mu^{old}$, find the distribution $z_i \mid x_i, \mu^{old}$:

$$\pi(x_1, \ldots, x_n, \ldots z_i, \cdots \mid \mu^{old}) \propto_{z_i} \text{Normal}(x_i; \mu^{old} z_i, 1)$$

  Normalizing the probabilities for the two values $z_i = 0$ and $z_i = 1$:

$$\begin{aligned} z_i \mid x_i, \mu^{old} \quad &\sim \quad \text{Bernoulli}(p_i)\,, \text{ where} \\ p_i \quad &= \quad \frac{\text{Normal}(x_i; \mu^{old}, 1)}{\text{Normal}(x_i; 0, 1) + \text{Normal}(x_i; \mu^{old}, 1)} \end{aligned}$$

- E step: Compute $\text{E}_{z \mid \mu^{old}}[\log \pi(x, z \mid \mu)]$. M step: Set μ^{new} as the parameter maximizing this function.

A toy example continued

- The E step becomes

$$\begin{aligned}
\mathrm{E}_{z\mid\mu^{old}}[\log\pi(x,z\mid\mu)] &= \mathrm{E}_{z\mid\mu^{old}}\left[\sum_{i=1}^{n}-\frac{1}{2}(x_i-z_i\mu)^2\right] \\
&= \mathrm{E}_{z\mid\mu^{old}}\left[-\frac{1}{2}\sum_{i=1}^{n}x_i^2-2x_iz_i\mu+z_i^2\mu^2\right] \\
&= -\frac{1}{2}\sum_{i=1}^{n}x_i^2-2x_i\,\mathrm{E}_{z\mid\mu^{old}}[z_i]\mu+\mathrm{E}_{z\mid\mu^{old}}[z_i^2]\mu^2 \\
&= -\frac{1}{2}\sum_{i=1}^{n}x_i^2-2x_ip_i\mu+p_i\mu^2
\end{aligned}$$

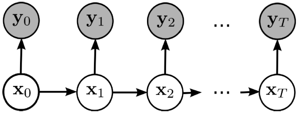
- The M step becomes

$$\frac{\partial}{\partial\mu}\mathrm{E}_{z\mid\mu^{old}}[\log\pi(x,z\mid\mu)] = -\frac{1}{2}\sum_{i=1}^{n}(-2x_ip_i+2p_i\mu) = \sum_{i=1}^{n}x_ip_i-\mu\sum_{i=1}^{n}p_i.$$

Setting this to zero results in $\mu^{new}=\left(\sum_{i=1}^{n}x_ip_i\right)/\left(\sum_{i=1}^{n}p_i\right)$.

Example: Applying EM to an HMM

We consider an HMM where all the x_i have a finite state spaces



but where some of the parameters of the distributions $\pi(X_0)$, $\pi(X_i \mid X_{i-1})$, and $\pi(Y_i \mid X_i)$ are unknown. Objective: Given fixed values for the y_i, find maximum likelihood estimates for the parameters in the model.

- Note: If assuming flat priors the problem becomes that of computing the parameters maximizing the posterior, i.e., finding the MAP.
- Idea: Use the EM algorithm, with the values of the x_i as the augmented data.
- The E step of the EM algorithm is computed using the Forward-Backward algorithm (see below).

Example: Applying EM to an HMM

For simplicity we assume each X_i can have values $1, \ldots, M$. As a first try, we assume all HMM parameters are unknown:

$$\theta = (q, p) = ((q_1, \ldots, q_M), (p_{11}, \ldots, p_{MM}))$$

be the parameters we want to estimate, where

$$\begin{aligned} q_j &= \Pr(X_0 = j) \\ p_{jk} &= \Pr(X_i = k \mid X_{i-1} = j) \end{aligned}$$

The full loglikelihood given θ becomes

$$\begin{aligned} & \log\left(\pi(x_0, \ldots, x_T, y_0, \ldots, y_T \mid \theta)\right) \\ = \; & \log\left(\pi(x_0 \mid \theta) \prod_{i=1}^{T} \pi(x_i \mid x_{i-1}, \theta) \prod_{i=0}^{T} \pi(y_i \mid x_i)\right) \\ = \; & \log \pi(x_0 \mid \theta) + \sum_{i=1}^{T} \log \pi(x_i \mid x_{i-1}, \theta) + \sum_{i=0}^{T} \log \pi(y_i \mid x_i) \\ = \; & C + \sum_{j=1}^{M} I(x_0 = j) \log q_j + \sum_{i=1}^{T} \sum_{j=1}^{M} \sum_{k=1}^{M} I(x_{i-1} = j) I(x_i = k) \log p_{jk} \end{aligned}$$

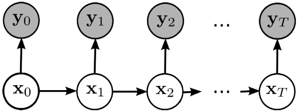
Example: Applying EM to an HMM

- In the E step, we would like to compute the expectation of the full loglikelihood under the distribution $\pi(x_0, \ldots, x_T \mid y_0, \ldots, y_T, \theta^{old})$ for some set of parameters θ^{old}.
- Thus we need to compute the expectations $\mathrm{E}\left[I(x_0 = j)\right]$ and $\mathrm{E}\left[I(x_{i-1} = j) I(x_i = k)\right]$ under this distribution.
- Fixing θ^{old}, we can use the Forward-Backward algorithm (see next overhead) to compute the densities $\pi(x_i \mid y_0, \ldots, y_i)$ and $\pi(y_{i+1}, \ldots, y_T \mid x_i)$. Further we have that

$$\begin{array}{rl} & \pi(x_i, x_{i+1} \mid y_0, \ldots, y_T) \\ \propto & \pi(y_{i+1}, \ldots, y_T \mid x_i, x_{i+1}) \pi(x_i, x_{i+1} \mid y_0, \ldots, y_i) \\ \propto & \pi(y_{i+2}, \ldots, y_T \mid x_{i+1}) \pi(y_{i+1} \mid x_{i+1}) \pi(x_{i+1} \mid x_i) \pi(x_i \mid y_0, \ldots, y_i) \end{array}$$

  making it possible to compute the joint posterior for x_i and x_{i+1} from these densities.

The Forward-Backward algorithm



Objective: Compute the marginal posterior distribution of every x_i given data $y_0, \ldots, y_T$: Use $\pi(x_i \mid y_0 \ldots, y_T) \propto_{x_i} \pi(y_{i+1}, \ldots, y_T \mid x_i)\pi(x_i \mid y_0, \ldots, y_i)$ and

1. Forward: For $i = 0, \ldots, T$ compute $\pi(x_i \mid y_0, \ldots, y_i)$ using

$$\begin{aligned}\pi(x_i \mid y_0, \ldots, y_i) &\propto_{x_i} \pi(y_i \mid x_i)\pi(x_i \mid y_0, \ldots, y_{i-1}) \\ &= \pi(y_i \mid x_i) \int \pi(x_i \mid x_{i-1})\pi(x_{i-1} \mid y_0, \ldots, y_{i-1})\, dx_{i-1}\end{aligned}$$

2. Backward: For $i = T-1, \ldots, 0$ compute $\pi(y_{i+1}, \ldots, y_T \mid x_i)$ using

$$\pi(y_{i+1}, \ldots, y_T \mid x_i) = \int \pi(y_{i+2}, \ldots, y_T \mid x_{i+1})\pi(y_{i+1} \mid x_{i+1})\pi(x_{i+1} \mid x_i)\, dx_{i+1}$$

Example: Applying EM to an HMM

The algorithm can now be summed up as

- Choose starting parameters θ^{old}.
- Run the Forward-Backward algorithm on the Markov model with parameters θ^{old} to compute the numbers $\mathrm{E}\left[I(x_0 = j)\right]$ and $\mathrm{E}\left[I(x_{i-1} = j)I(x_i = k)\right]$.
- Find the θ maximizing the expected loglikelihood

$$\sum_{j=1}^{M} \mathrm{E}\left[I(x_0 = j)\right] \log q_j + \sum_{i=1}^{T} \sum_{j=1}^{M} \sum_{k=1}^{M} \mathrm{E}\left[I(x_{i-1} = j)I(x_i = k)\right] \log p_{jk}$$

  In fact, we get

$$\hat{q}_j = \mathrm{E}\left[I(x_0 = j)\right] \text{ and } \hat{p}_{jk} = \frac{\sum_{i=1}^{T} \mathrm{E}\left[I(x_{i-1} = j)I(x_i = k)\right]}{\sum_{k=1}^{M} \sum_{i=1}^{T} \mathrm{E}\left[I(x_{i-1} = j)I(x_i = k)\right]}$$

- Set $\theta^{old} = ((\hat{q}_1, \ldots, \hat{q}_M), (\hat{p}_{11}, \ldots, \hat{p}_{MM}))$ and iterate until convergence.

Some results from an implementation

- If the observations $\pi(y_i \mid x_i)$ are noisy, the data is not very large, and θ consists of all q_j and p_{jk}, the likelihood function seems to have multiple modes. So EM does not work well.
- In such cases, MH simulation seems to confirm that the posterior is not very concentrated for specific parameters.
- However, if we have smaller amounts of noise, very much data, or restrict θ so that we only allow transition matrices from a parametric family, the EM should work well....