COMS 4721: Machine Learning for Data Science
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Maximum likelihood

Approaches to data modeling

Our approaches to modeling data thus far have been either probabilistic or non-probabilistic in motivation.

- Probabilistic models: Probability distributions defined on data, e.g.,
  1. Bayes classifiers
  2. Logistic regression
  3. Least squares and ridge regression (using ML and MAP interpretation)
  4. Bayesian linear regression
- Non-probabilistic models: No probability distributions involved, e.g.,
  1. Perceptron
  2. Support vector machine
  3. Decision trees
  4. K-means

In *every* case, we have some objective function we are trying to optimize (greedily vs non-greedily, locally vs globally).

MAXIMUM LIKELIHOOD

As we've seen, one *probabilistic* objective function is maximum likelihood.

Setup: In the most basic scenario, we start with

1. some set of model parameters θ
2. a set of data $\{x_1, \dots, x_n\}$
3. a probability distribution $p(x|\theta)$
4. an i.i.d. assumption, $x_i \overset{iid}{\sim} p(x|\theta)$

Maximum likelihood seeks the θ that maximizes the likelihood

$$\theta_{\text{ML}} = \arg\max_{\theta}\ p(x_1, \dots, x_n|\theta) \ \overset{(a)}{=}\ \arg\max_{\theta} \prod_{i=1}^{n} p(x_i|\theta) \ \overset{(b)}{=}\ \arg\max_{\theta} \sum_{i=1}^{n} \ln p(x_i|\theta)$$

(a) follows from i.i.d. assumption.
(b) follows since $f(y) > f(x) \ \Rightarrow\ \ln f(y) > \ln f(x)$.

MAXIMUM LIKELIHOOD

We've discussed maximum likelihood for a few models, e.g., least squares linear regression and the Bayes classifier.

Both of these models were "nice" because we could find their respective θ_{ML} analytically by writing an equation and plugging in data to solve.

Gaussian with unknown mean and covariance

In the first lecture, we saw if $x_i \overset{iid}{\sim} N(\mu, \Sigma)$, where $\theta = \{\mu, \Sigma\}$, then

$$\nabla_\theta \ln \prod_{i=1}^{n} p(x_i|\theta) = 0$$

gives the following maximum likelihood values for μ and Σ:

$$\mu_{\text{ML}} = \frac{1}{n}\sum_{i=1}^{n} x_i, \qquad \Sigma_{\text{ML}} = \frac{1}{n}\sum_{i=1}^{n}(x_i - \mu_{\text{ML}})(x_i - \mu_{\text{ML}})^T$$

Coordinate ascent and maximum likelihood

In more complicated models, we might split the parameters into groups θ_1, θ_2 and try to maximize the likelihood over both of these,

$$\theta_{1,\text{ML}}, \theta_{2,\text{ML}} \;=\; \arg\max_{\theta_1,\theta_2} \; \sum_{i=1}^{n} \ln p(x_i|\theta_1, \theta_2),$$

Although we can solve one *given* the other, we can't solve it *simultaneously*.

Coordinate ascent (probabilistic version)

We saw how K-means presented a similar situation, and that we could optimize using coordinate ascent. This technique is generalizable.

Algorithm: For iteration $t = 1, 2, \ldots,$

1. Optimize $\theta_1^{(t)} = \arg\max_{\theta_1} \; \sum_{i=1}^{n} \ln p(x_i|\theta_1, \theta_2^{(t-1)})$
2. Optimize $\theta_2^{(t)} = \arg\max_{\theta_2} \; \sum_{i=1}^{n} \ln p(x_i|\theta_1^{(t)}, \theta_2)$

Coordinate ascent and maximum likelihood

There is a third (subtly) different situation, where we really want to find

$$\theta_{1,\text{ML}} = \arg\max_{\theta_1} \sum_{i=1}^{n} \ln p(x_i|\theta_1).$$

Except this function is "tricky" to optimize directly. However, we figure out that we can add a second variable θ_2 such that

$$\sum_{i=1}^{n} \ln p(x_i, \theta_2|\theta_1) \qquad \text{(Function 2)}$$

is easier to work with. We'll make this clearer later.

- Notice in this second case that θ_2 is on the *left* side of the conditioning bar. This implies a prior on θ_2, (whatever "θ_2" turns out to be).
- We will next discuss a fundamental technique called the EM algorithm for finding $\theta_{1,\text{ML}}$ by using Function 2 instead.

Expectation-Maximization Algorithm

A MOTIVATING EXAMPLE

Let $x_i \in \mathbb{R}^d$, be a vector with *missing data*. Split this vector into two parts:

1. x_i^o – observed portion (the sub-vector of x_i that is measured)
2. x_i^m – missing portion (the sub-vector of x_i that is still unknown)
3. The missing dimensions can be different for different x_i.

We assume that $x_i \overset{iid}{\sim} N(\mu, \Sigma)$, and want to solve

$$\mu_{\text{ML}}, \Sigma_{\text{ML}} = \arg\max_{\mu,\Sigma} \sum_{i=1}^{n} \ln p(x_i^o|\mu, \Sigma).$$

This is tricky. However, if we knew x_i^m (and therefore x_i), then

$$\mu_{\text{ML}}, \Sigma_{\text{ML}} = \arg\max_{\mu,\Sigma} \sum_{i=1}^{n} \ln \underbrace{p(x_i^o, x_i^m|\mu, \Sigma)}_{= p(x_i|\mu,\Sigma)}$$

is very easy to optimize (we just did it on a previous slide).

CONNECTING TO A MORE GENERAL SETUP

We will discuss a method for optimizing $\sum_{i=1}^{n} \ln p(x_i^o|\mu, \Sigma)$ and imputing its missing values $\{x_1^m, \ldots, x_n^m\}$. This is a very general technique.

General setup

Imagine we have two parameter sets θ_1, θ_2, where

$$p(x|\theta_1) = \int p(x, \theta_2|\theta_1)\, d\theta_2 \qquad \text{(marginal distribution)}$$

Example: For the previous example we can show that

$$p(x_i^o|\mu, \Sigma) = \int p(x_i^o, x_i^m|\mu, \Sigma)\, dx_i^m = N(\mu_i^o, \Sigma_i^o),$$

where μ_i^o and Σ_i^o are the sub-vector/sub-matrix of μ and Σ defined by x_i^o.

The EM objective function

We need to define a general *objective function* that gives us what we want:

1. It lets us optimize the marginal $p(x|\theta_1)$ over θ_1,
2. It uses $p(x, \theta_2|\theta_1)$ in doing so purely for computational convenience.

The EM objective function

Before picking it apart, we claim that this objective function is

$$\ln p(x|\theta_1) = \int q(\theta_2) \ln \frac{p(x, \theta_2|\theta_1)}{q(\theta_2)} \, d\theta_2 \; + \; \int q(\theta_2) \ln \frac{q(\theta_2)}{p(\theta_2|x, \theta_1)} \, d\theta_2$$

Some immediate comments:

- $q(\theta_2)$ is *any* probability distribution (assumed continuous for now)
- We assume we know $p(\theta_2|x, \theta_1)$. That is, given the data x and fixed values for θ_1, we can solve the conditional posterior distribution of θ_2.

DERIVING THE EM OBJECTIVE FUNCTION

Let's show that this equality is actually true

$$\begin{aligned}\ln p(x|\theta_1) &= \int q(\theta_2) \ln \frac{p(x, \theta_2|\theta_1)}{q(\theta_2)} \, d\theta_2 \; + \int q(\theta_2) \ln \frac{q(\theta_2)}{p(\theta_2|x, \theta_1)} \, d\theta_2 \\ &= \int q(\theta_2) \ln \frac{p(x, \theta_2|\theta_1) q(\theta_2)}{p(\theta_2|x, \theta_1) q(\theta_2)} \, d\theta_2\end{aligned}$$

Remember some rules of probability:

$$p(a, b|c) = p(a|b, c) p(b|c) \quad \Rightarrow \quad p(b|c) = \frac{p(a, b|c)}{p(a|b, c)}.$$

Letting $a = \theta_1$, $b = x$ and $c = \theta_1$, we conclude

$$\begin{aligned}\ln p(x|\theta_1) &= \int q(\theta_2) \ln p(x|\theta_1) \, d\theta_2 \\ &= \ln p(x|\theta_1)\end{aligned}$$

THE EM OBJECTIVE FUNCTION

The EM objective function splits our desired objective into two terms:

$$\ln p(x|\theta_1) = \underbrace{\int q(\theta_2) \ln \frac{p(x, \theta_2|\theta_1)}{q(\theta_2)} \, d\theta_2}_{\text{A function only of } \theta_1 \text{, we'll call it } \mathcal{L}} + \underbrace{\int q(\theta_2) \ln \frac{q(\theta_2)}{p(\theta_2|x, \theta_1)} \, d\theta_2}_{\text{Kullback-Leibler divergence}}$$

Some more observations about the right hand side:

1. The **KL diverence** is always ≥ 0 and only $= 0$ when $q = p$.
2. We are assuming that the integral in $\mathcal{L}$ can be calculated, leaving a function only of θ_1 (for a particular setting of the distribution q).

BIGGER PICTURE

Q: What does it mean to iteratively optimize $\ln p(x|\theta_1)$ w.r.t. θ_1?

A: One way to think about it is that we want a method for generating:

1. A sequence of values for θ_1 such that $\ln p(x|\theta_1^{(t)}) \geq \ln p(x|\theta_1^{(t-1)})$.
2. We want $\theta_1^{(t)}$ to converge to a local maximum of $\ln p(x|\theta_1)$.

It doesn't matter how we generate the sequence $\theta_1^{(1)}, \theta_1^{(2)}, \theta_1^{(3)}, \ldots$

We will show how EM generates #1 and just mention that EM satisfies #2.

THE EM ALGORITHM

The EM objective function

$$\ln p(x|\theta_1) = \underbrace{\int q(\theta_2) \ln \frac{p(x, \theta_2|\theta_1)}{q(\theta_2)}\, d\theta_2}_{\text{define this to be } \mathcal{L}(x,\theta_1)} + \underbrace{\int q(\theta_2) \ln \frac{q(\theta_2)}{p(\theta_2|x, \theta_1)}\, d\theta_2}_{\text{Kullback-Leibler divergence}}$$

Definition: The EM algorithm

Given the value $\theta_1^{(t)}$, **find** the value $\theta_1^{(t+1)}$ as follows:

E-step: Set $q_t(\theta_2) = p(\theta_2|x, \theta_1^{(t)})$ and calculate

$$\mathcal{L}_{q_t}(x, \theta_1) = \int q_t(\theta_2) \ln p(x, \theta_2|\theta_1)\, d\theta_2 \;-\; \underbrace{\int q_t(\theta_2) \ln q_t(\theta_2)\, d\theta_2}_{\text{can ignore this term}}.$$

M-step: Set $\theta_1^{(t+1)} = \arg\max_{\theta_1} \; \mathcal{L}_{q_t}(x, \theta_1)$.

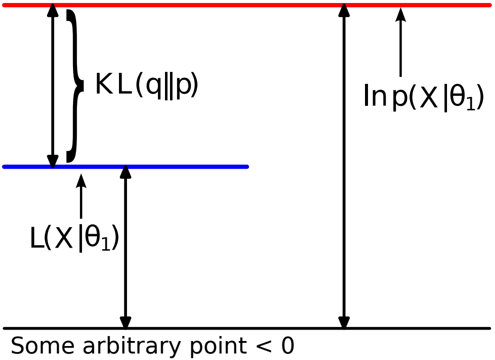
PROOF OF MONOTONIC IMPROVEMENT

Once we're comfortable with the moving parts, the proof that the sequence $\theta_1^{(t)}$ monotonically improves $\ln p(x|\theta_1)$ just requires *analysis*:

$$
\begin{aligned}
\ln p(x|\theta_1^{(t)}) &= \mathcal{L}(x,\theta_1^{(t)}) + \underbrace{KL\left(q(\theta_2)\,\|\,p(\theta_2|x_1,\theta_1^{(t)})\right)}_{=\,0 \text{ by setting } q\,=\,p} \\
&= \mathcal{L}_{q_t}(x,\theta_1^{(t)}) \qquad \leftarrow \text{E-step} \\
&\leq \mathcal{L}_{q_t}(x,\theta_1^{(t+1)}) \qquad \leftarrow \text{M-step} \\
&\leq \mathcal{L}_{q_t}(x,\theta_1^{(t+1)}) + \underbrace{KL\left(q_t(\theta_2)\,\|\,p(\theta_2|x_1,\theta_1^{(t+1)})\right)}_{>\,0 \text{ because } q \neq p} \\
&= \mathcal{L}(x,\theta_1^{(t+1)}) + KL\left(q(\theta_2)\,\|\,p(\theta_2|x_1,\theta_1^{(t+1)})\right) \\
&= \ln p(x|\theta_1^{(t+1)})
\end{aligned}
$$

ONE ITERATION OF EM

Start: Current setting of θ_1 and $q(\theta_2)$



For reference:

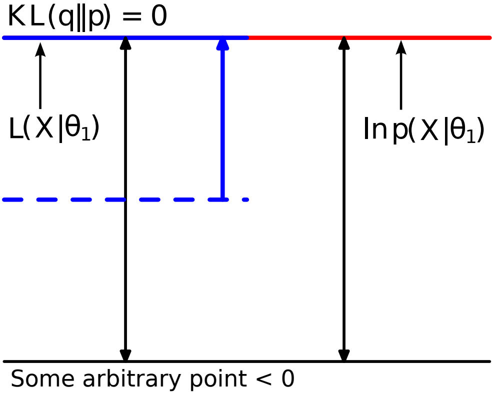
$$\ln p(x|\theta_1) = \mathcal{L} + KL$$

$$\mathcal{L} = \int q(\theta_2) \ln \frac{p(x, \theta_2|\theta_1)}{q(\theta_2)} \, d\theta_2$$

$$KL = \int q(\theta_2) \ln \frac{q(\theta_2)}{p(\theta_2|x, \theta_1)} \, d\theta_2$$

One iteration of EM

E-step: Set $q(\theta_2) = p(\theta_2|x, \theta_1)$ and update $\mathcal{L}$.



For reference:

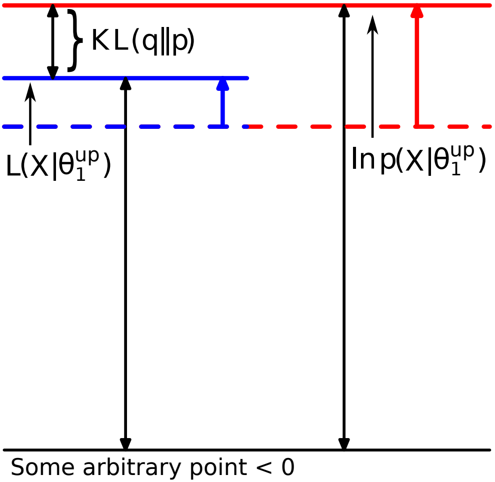
$$\ln p(x|\theta_1) = \mathcal{L} + KL$$

$$\mathcal{L} = \int q(\theta_2) \ln \frac{p(x, \theta_2|\theta_1)}{q(\theta_2)} \, d\theta_2$$

$$KL = \int q(\theta_2) \ln \frac{q(\theta_2)}{p(\theta_2|x, \theta_1)} \, d\theta_2$$

One iteration of EM

M-step: Maximize $\mathcal{L}$ wrt θ_1. Now $q \neq p$.



For reference:

$\ln p(x|\theta_1) = \mathcal{L} + KL$

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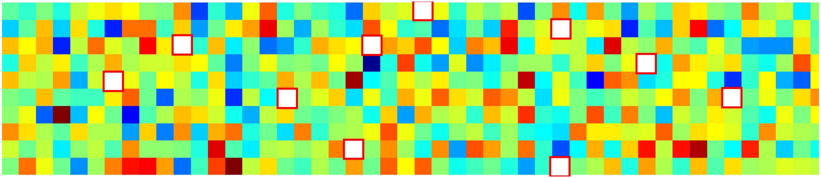
$$KL = \int q(\theta_2) \ln \frac{q(\theta_2)}{p(\theta_2|x, \theta_1)} \, d\theta_2$$

EM FOR MISSING DATA

THE PROBLEM



We have a data matrix with missing entries. We model the columns as

$$x_i \stackrel{iid}{\sim} N(\mu, \Sigma).$$

Our goal could be to

1. Learn μ and Σ using maximum likelihood
2. Fill in the missing values "intelligently" (e.g., using a model)
3. Both

We will see how to achieve both of these goals using the EM algorithm.

EM FOR SINGLE GAUSSIAN MODEL WITH MISSING DATA

The original, generic EM objective is

$$\ln p(x|\theta_1) = \int q(\theta_2) \ln \frac{p(x, \theta_2|\theta_1)}{q(\theta_2)} \, d\theta_2 \; + \; \int q(\theta_2) \ln \frac{q(\theta_2)}{p(\theta_2|x, \theta_1)} \, d\theta_2$$

The EM objective for this specific problem and notation is

$$\begin{aligned} \sum_{i=1}^{n} \ln p(x_i^o|\mu, \Sigma) \quad &= \quad \sum_{i=1}^{n} \int q(x_i^m) \ln \frac{p(x_i^o, x_i^m|\mu, \Sigma)}{q(x_i^m)} \, dx_i^m \quad + \\ & \quad\quad \sum_{i=1}^{n} \int q(x_i^m) \ln \frac{q(x_i^m)}{p(x_i^m|x_i^o, \mu, \Sigma)} \, dx_i^m \end{aligned}$$

We can calculate everything required to do this.

E-STEP (PART ONE)

Set $q(x_i^m) = p(x_i^m | x_i^o, \mu, \Sigma)$ using current μ, Σ

Let x_i^o and x_i^m represent the observed and missing dimensions of x_i. For notational convenience, think

$$x_i = \left[\begin{array}{c} x_i^o \\ x_i^m \end{array} \right] \sim N\left(\left[\begin{array}{c} \mu_i^o \\ \mu_i^m \end{array} \right], \left[\begin{array}{cc} \Sigma_i^{oo} & \Sigma_i^{om} \\ \Sigma_i^{mo} & \Sigma_i^{mm} \end{array} \right] \right)$$

Then we can show that $p(x_i^m | x_i^o, \mu, \Sigma) = N(\widehat{\mu}_i, \widehat{\Sigma}_i)$, where

$$\widehat{\mu}_i = \mu_i^m + \Sigma_i^{mo} (\Sigma_i^{oo})^{-1} (x_i^o - \mu_i^o), \quad \widehat{\Sigma}_i = \Sigma_i^{mm} - \Sigma_i^{mo} (\Sigma_i^{oo})^{-1} \Sigma_i^{om}.$$

It doesn't look nice, but these are just functions of sub-vectors of μ and sub-matrices of Σ using the relevant dimensions defined by x_i.

E-STEP (PART TWO)

E-step: $\mathbb{E}_{q(x_i^m)}[\ln p(x_i^o, x_i^m | \mu, \Sigma)]$

For each i we will need to calculate the following term,

$$\begin{aligned}\mathbb{E}_q[(x_i - \mu)^T \Sigma^{-1} (x_i - \mu)] &= \mathbb{E}_q[\text{trace}\{\Sigma^{-1}(x_i - \mu)(x_i - \mu)^T\}] \\ &= \text{trace}\{\Sigma^{-1}\mathbb{E}_q[(x_i - \mu)(x_i - \mu)^T]\}\end{aligned}$$

The expectation is calculated using $q(x_i^m) = p(x_i^m | x_i^o, \mu, \Sigma)$. So only the x_i^m portion of x_i will be integrated.

To this end, recall $q(x_i^m) = N(\widehat{\mu}_i, \widehat{\Sigma}_i)$. We define

1. $\widehat{x}_i$: A vector where we replace the missing values in x_i with $\widehat{\mu}_i$.
2. $\widehat{V}_i$: A matrix of 0's, plus sub-matrix $\widehat{\Sigma}_i$ in the missing dimensions.

M-STEP

M-step: Maximize $\sum_{i=1}^{n} \mathbb{E}_q[\ln p(x_i^o, x_i^m | \mu, \Sigma)]$

We'll omit the derivation, but the expectation can now be solved and

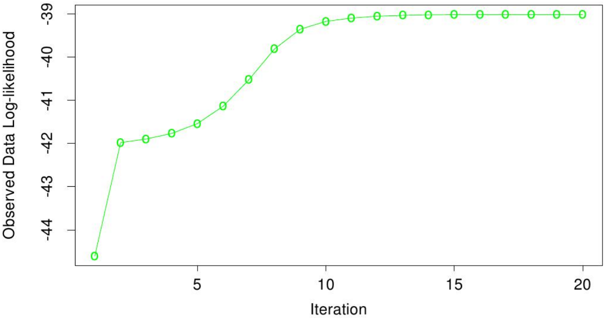
$$\mu_{\text{up}}, \Sigma_{\text{up}} = \arg\max_{\mu,\Sigma} \sum_{i=1}^{n} \mathbb{E}_q[\ln p(x_i^o, x_i^m | \mu, \Sigma)]$$

can be found. Recalling the $\widehat{\ }$ notation,

$$\begin{aligned} \mu_{\text{up}} &= \frac{1}{n} \sum_{i=1}^{n} \widehat{x}_i, \\ \Sigma_{\text{up}} &= \frac{1}{n} \sum_{i=1}^{n} \{(\widehat{x}_i - \mu_{\text{up}})(\widehat{x}_i - \mu_{\text{up}})^T + \widehat{V}_i\} \end{aligned}$$

Then return to the E-step to calculate the new $p(x_i^m | x_i^o, \mu_{\text{up}}, \Sigma_{\text{up}})$.

Implementation details



We need to initialize μ and Σ, for example, by setting missing values to zero and calculating μ_{ML} and Σ_{ML}. (We can also use random initialization.)

The EM objective function is then calculated after each update to μ and Σ and will look like the figure above. Stop when the change is "small."

The output is μ_{ML}, Σ_{ML} and $q(x_i^m)$ for all missing entries.