

# COMS 4721: Machine Learning for Data Science

## Lecture 15, 3/18/2021

Prof. John Paisley

Department of Electrical Engineering

Columbia University

# 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  $\theta$
2. a set of data  $\{x_1, \dots, x_n\}$
3. a probability distribution  $p(x|\theta)$
4. an i.i.d. assumption,  $x_i \stackrel{iid}{\sim} p(x|\theta)$

Maximum likelihood seeks the  $\theta$  that maximizes the likelihood

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

(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  $\theta_{\text{ML}}$  analytically by writing an equation and plugging in data to solve.

## Gaussian with unknown mean and covariance

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

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

gives the following maximum likelihood values for  $\mu$  and  $\Sigma$ :

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

# COORDINATE ASCENT AND MAXIMUM LIKELIHOOD

In more complicated models, we might split the parameters into groups  $\theta_1, \theta_2$  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 this method. This technique is generalizable.

**Algorithm:** For iteration  $t = 1, 2, \dots$ ,

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  $\theta_2$  to the model such that

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

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

- ▶ Notice in this second case that  $\theta_2$  is on the *left* side of the conditioning bar. This implies a prior on  $\theta_2$ , (whatever “ $\theta_2$ ” 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  $x_i \stackrel{iid}{\sim} N(\mu, \Sigma)$ , 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

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

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  $\{x_1^m, \dots, x_n^m\}$ . This is a very general technique.

## General setup

Imagine we have two parameter sets  $\theta_1, \theta_2$ , where

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

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  $\mu_i^o$  and  $\Sigma_i^o$  are the sub-vector/sub-matrix of  $\mu$  and  $\Sigma$  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  $\theta_1$ ,
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  $\theta_1$ , we can solve the conditional posterior distribution of  $\theta_2$ .

# 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  $a = \theta_2$ ,  $b = x$  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 divergence** is always  $\geq 0$  and only  $= 0$  when  $q = p$ .
2. We are assuming that the integral in  $\mathcal{L}$  can be calculated, leaving a function only of  $\theta_1$  (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.  $\theta_1$ ?

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

1. A sequence of values for  $\theta_1$  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  $\theta_1^{(1)}, \theta_1^{(2)}, \theta_1^{(3)}, \dots$

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*:

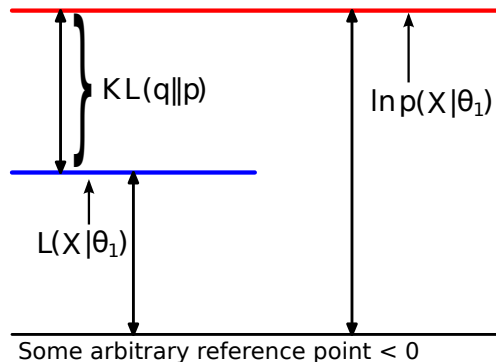
$$\begin{aligned}\ln p(x|\theta_1^{(t)}) &= \mathcal{L}(x, \theta_1^{(t)}) + \underbrace{KL\left(q(\theta_2) \parallel p(\theta_2|x_1, \theta_1^{(t)})\right)}_{= 0 \text{ by setting } q = p} \\ &= \mathcal{L}_{q_t}(x, \theta_1^{(t)}) \quad \leftarrow \text{E-step} \\ &\leq \mathcal{L}_{q_t}(x, \theta_1^{(t+1)})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

$$\begin{aligned}\text{generalize to any } q \rightarrow &= \mathcal{L}(x, \theta_1^{(t+1)}) + KL\left(q(\theta_2) \parallel p(\theta_2|x_1, \theta_1^{(t+1)})\right) \\ &= \ln p(x|\theta_1^{(t+1)})\end{aligned}$$



# ONE ITERATION OF EM

**Start:** Current setting of  $\theta_1$  and  $q(\theta_2)$



**For reference:**

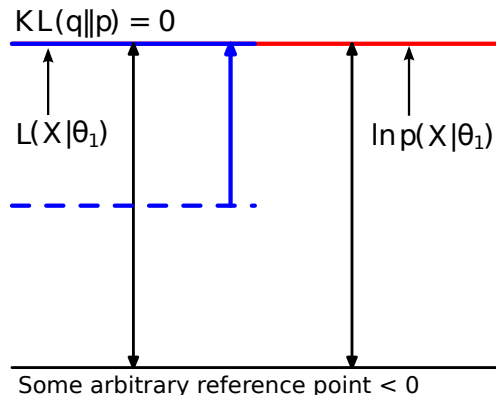
$$\ln p(x|\theta_1) = \mathcal{L} + KL$$

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

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

# ONE ITERATION OF EM

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



**For reference:**

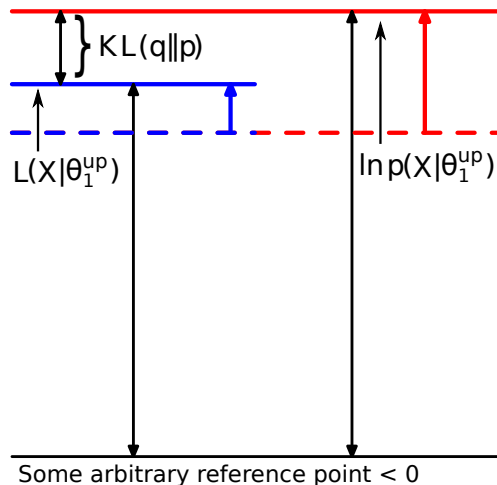
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$$KL = \int q(\theta_2) \ln \frac{q(\theta_2)}{p(\theta_2|x, \theta_1)} d\theta_2$$

# ONE ITERATION OF EM

**M-step:** Maximize  $\mathcal{L}$  wrt  $\theta_1$ . Now  $q \neq p$ .



**For reference:**

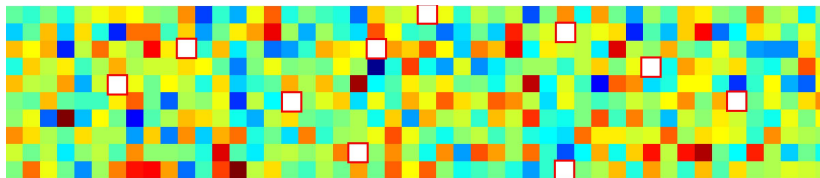
$$\ln p(x|\theta_1) = \mathcal{L} + KL$$

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

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

# 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  $\mu$  and  $\Sigma$  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

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

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  $\mu, \Sigma$

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

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

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

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

It doesn't look nice, but these are just functions of sub-vectors of  $\mu$  and sub-matrices of  $\Sigma$  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 missing  $x_i^m$  portion of  $x_i$  will be integrated over.

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

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

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

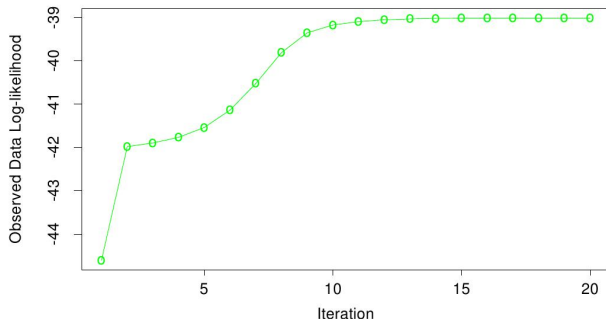
can be found. Recalling the  $\hat{\phantom{x}}$  notation,

$$\mu_{\text{up}} = \frac{1}{n} \sum_{i=1}^n \hat{x}_i,$$

$$\Sigma_{\text{up}} = \frac{1}{n} \sum_{i=1}^n \{(\hat{x}_i - \mu_{\text{up}})(\hat{x}_i - \mu_{\text{up}})^T + \hat{V}_i\}$$

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  $\mu$  and  $\Sigma$ , for example, by setting missing values to zero and calculating  $\mu_{\text{ML}}$  and  $\Sigma_{\text{ML}}$ . (We can also use random initialization.)

The EM objective function is then calculated after each update to  $\mu$  and  $\Sigma$  and will look like the figure above. Stop when the change is “small.”

The output is  $\mu_{\text{ML}}$ ,  $\Sigma_{\text{ML}}$  and  $q(x_i^m)$  for all missing entries.