

# Introduction to Machine Learning

## Maximum A Posteriori (MAP)

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# Outline

## 1 Introduction

- Beyond Likelihood
- Maximum Likelihood Vs Maximum A Posteriori
- Properties of the MAP

## 2 A Classic Application, The EM-Algorithm

- Introduction
- Using the Expected Value
- Analogy
- Hidden Features
  - Proving Concavity
- Using the Concave Functions for Approximation
- From The Concave Function to the EM
- The Final Algorithm
- Notes and Convergence of EM

## 3 Example of Application of MAP and EM

- Example
- Linear Regression
- The Gaussian Noise
- Regression with a Laplacian Prior
- A Hierarchical-Bayes View of the Laplacian Prior
- Sparse Regression via EM
- Jeffrey's Prior



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# Big Problem

We have that we depend on the distribution we choose

- When using the Likelihood... Can do better?

Actually, yes

- Something that comes from the Bayesian idea...



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# Introduction

We go back to the Bayesian Rule

$$p(\Theta|\mathcal{X}) = \frac{p(\mathcal{X}|\Theta)p(\Theta)}{p(\mathcal{X})} \quad (1)$$

We now seek that value for  $\Theta$ , called  $\Theta_{MAP}$ .

It allows to maximize the posterior  $p(\Theta|\mathcal{X})$



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# Development of the solution

We look to maximize  $\hat{\Theta}_{MAP}$

$$\begin{aligned}\hat{\Theta}_{MAP} &= \underset{\Theta}{\operatorname{argmax}} p(\Theta|\mathcal{X}) \\ &= \underset{\Theta}{\operatorname{argmax}} \frac{p(\mathcal{X}|\Theta) p(\Theta)}{P(\mathcal{X})} \\ &\approx \underset{\Theta}{\operatorname{argmax}} p(\mathcal{X}|\Theta) p(\Theta) \\ &= \underset{\Theta}{\operatorname{argmax}} \prod_{x_i \in \mathcal{X}} p(x_i|\Theta) p(\Theta)\end{aligned}$$

$P(\mathcal{X})$  can be removed because it has no functional relation with  $\Theta$ .



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We can make this easier

Use logarithms

$$\hat{\Theta}_{MAP} = \operatorname{argmax}_{\Theta} \left[ \sum_{x_i \in \mathcal{X}} \log p(x_i | \Theta) + \log p(\Theta) \right] \quad (2)$$



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# What Does the MAP Estimate Get?

## Something Notable

The MAP estimate allows us to inject into the estimation calculation our prior beliefs regarding the parameters values in  $\Theta$ .

For example:

Let's conduct  $N$  independent trials of the following Bernoulli experiment with  $\theta$  parameter:

- We will ask each individual we run into in the hallway whether they will vote PRI or PAN in the next presidential election.

With probability  $\theta$  to vote PRI.

Where the values of  $x_i$  is either PRI or PAN.



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# First the Maximum Likelihood Estimate

## Samples

$$\mathcal{X} = \left\{ x_i = \begin{cases} PAN \\ PRI \end{cases} \quad i = 1, \dots, N \right\} \quad (3)$$

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Where  $n_{PRI}$  are the numbers of individuals who are planning to vote PRI this fall

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## We use our classic tricks

By setting

$$\mathcal{L} = \log p(\mathcal{X}|q) \quad (4)$$

We have that

$$\frac{\partial \mathcal{L}}{\partial q} = 0 \quad (5)$$

Thus

$$\frac{n_{PRI}}{q} - \frac{(N - n_{PRI})}{(1 - q)} = 0 \quad (6)$$





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# Final Solution of ML

We get

$$\hat{q}_{PRI} = \frac{n_{PRI}}{N} \quad (7)$$

Thus

If we say that  $N = 20$  and if 12 are going to vote PRI, we get  $\hat{q}_{PRI} = 0.6$ .



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# Building the MAP estimate

Obviously we need a prior belief distribution

We have the following constraints:

- The prior for  $q$  must be zero outside the  $[0, 1]$  interval.
- Within the  $[0, 1]$  interval, we are free to specify our beliefs in any way we wish.
- In most cases, we would want to choose a distribution for the prior beliefs that peaks somewhere in the  $[0, 1]$  interval.

We assume the following

- The state of Colima has traditionally voted PRI in presidential elections.
- However, on account of the prevailing economic conditions, the voters are more likely to vote PAN in the election in question.

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## What prior distribution can we use?

We could use a Beta distribution being parametrized by two values  $\alpha$  and  $\beta$

$$p(q) = \frac{1}{B(\alpha, \beta)} q^{\alpha-1} (1-q)^{\beta-1}. \quad (8)$$

Where

We have  $B(\alpha, \beta) = \frac{\Gamma(\alpha)\Gamma(\beta)}{\Gamma(\alpha+\beta)}$  is the beta function where  $\Gamma$  is the generalization of the notion of factorial in the case of the real numbers.

Properties

When both the  $\alpha, \beta > 0$  then the beta distribution has its mode (Maximum value) at

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# We then do the following

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We can choose  $\alpha = \beta$  so the beta prior peaks at 0.5.

As a further expression of our belief

We make the following choice  $\alpha = \beta = 5$ .

What? Look at the variance of the beta distribution

$$\frac{\alpha\beta}{(\alpha+\beta)^2(\alpha+\beta+1)}. \quad (10)$$



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Thus, we have the following nice properties

We have a variance with  $\alpha = \beta = 5$

$$\text{Var}(q) \approx 0.025$$

Thus, the standard deviation

$sd \approx 0.16$  which is a nice dispersion at the peak point!!!



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Now, our MAP estimate for  $\hat{p}_{MAP}$ ...

We have then

$$\hat{p}_{MAP} = \underset{\Theta}{\operatorname{argmax}} \left[ \sum_{x_i \in \mathcal{X}} \log p(x_i|q) + \log p(q) \right] \quad (11)$$

Plugging back the ML

$$\hat{p}_{MAP} = \underset{\Theta}{\operatorname{argmax}} [n_{PRI} \log q + (N - n_{PRI}) \log (1 - q) + \log p(q)] \quad (12)$$

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# The log of $p(q)$

We have that

$$\log p(q) = (\alpha - 1) \log q + (\beta - 1) \log (1 - q) - \log B(\alpha, \beta) \quad (14)$$

Now taking the derivative with respect to  $q$ , we get

$$\frac{n_{PRI}}{q} - \frac{(N - n_{PRI})}{(1 - q)} - \frac{\beta - 1}{1 - q} + \frac{\alpha - 1}{q} = 0 \quad (15)$$

Thus

$$\hat{q}_{MAP} = \frac{n_{PRI} + \alpha - 1}{N + \alpha + \beta - 2} \quad (16)$$



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Now

With  $N = 20$  with  $n_{PRI} = 12$  and  $\alpha = \beta = 5$

$$\hat{q}_{MAP} = 0.571$$



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# Properties

## First

**MAP** estimation “pulls” the estimate toward the prior.

## Second

The more focused our prior belief, the larger the pull toward the prior.

## Example

If  $\alpha = \beta$  = equal to large value

- It will make the MAP estimate to move closer to the prior.



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## Third

In the expression we derived for  $\hat{q}_{MAP}$ , the parameters  $\alpha$  and  $\beta$  play a “smoothing” role vis-a-vis the measurement  $n_{PRI}$ .

## Fourth

Since we referred to  $q$  as the parameter to be estimated, we can refer to  $\alpha$  and  $\beta$  as the hyper-parameters in the estimation calculations.



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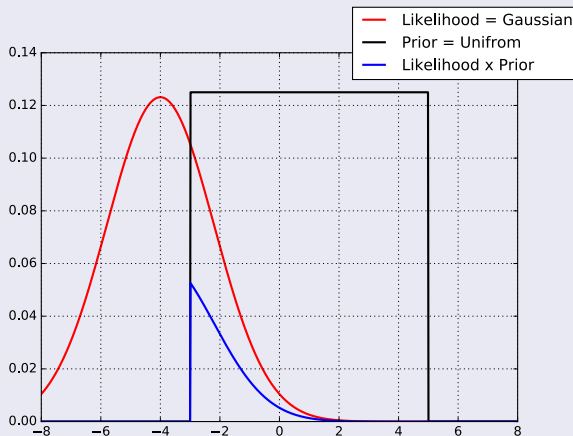
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# Basically the MAP

It is using the power of Likelihood  $\times$  Prior to obtain more information from the data



# Beyond simple derivation

## In the previous technique

We took an logarithm of the **likelihood**  $\times$  **the prior** to obtain a function that can be derived in order to obtain each of the parameters to be estimated.

What if we cannot derive the likelihood  $\times$  the prior?

For example when we have something like  $\{\theta_i\}$ .

We can try the following:

EM + MAP to be able to estimate the sought parameters.



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# Incomplete Data

We assume the following

Two parts of data

- $\mathcal{X}$  = observed data or incomplete data
- $\mathcal{Y}$  = unobserved data

Thus

$$Z = (\mathcal{X}, \mathcal{Y}) = \text{Complete Data} \quad (17)$$

Thus, we have the following probability:

$$p(z|\Theta) = p(x, y|\Theta) = p(y|x, \Theta) p(x|\Theta) \quad (18)$$



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# New Likelihood Function

## The New Likelihood Function

$$\mathcal{L}(\Theta|\mathcal{Z}) = \mathcal{L}(\Theta|\mathcal{X}, \mathcal{Y}) = p(\mathcal{X}, \mathcal{Y}|\Theta) \quad (19)$$

**Note:** The complete data likelihood.

Thus, we have

$$\mathcal{L}(\Theta|\mathcal{X}, \mathcal{Y}) = p(\mathcal{X}, \mathcal{Y}|\Theta) = p(\mathcal{Y}|\mathcal{X}, \Theta) p(\mathcal{X}|\Theta) \quad (20)$$

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## Did you notice?

- $p(\mathcal{X}|\Theta)$  is the likelihood of the observed data.
- $p(\mathcal{Y}|\mathcal{X}, \Theta)$  is the likelihood of the no-observed data under the observed data!!!

# Rewriting

This can be rewritten as

$$\mathcal{L}(\Theta|\mathcal{X},\mathcal{Y}) = h_{\mathcal{X},\Theta}(\mathcal{Y}) \quad (21)$$

This basically signify that  $\mathcal{X}, \Theta$  are constant and the only random part is  $\mathcal{Y}$ .

In addition

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Thus

We can connect both incomplete-complete data equations by doing the following

$$\begin{aligned}\mathcal{L}(\Theta|\mathcal{X}) &= p(\mathcal{X}|\Theta) \\ &= \sum_{\mathcal{Y}} p(\mathcal{X}, \mathcal{Y}|\Theta) \\ &= \sum_{\mathcal{Y}} p(\mathcal{Y}|\mathcal{X}, \Theta) p(\mathcal{X}|\Theta) \\ &= \sum_{\mathcal{Y}} \left( \prod_{i=1}^N p(x_i|\Theta) \right) p(\mathcal{Y}|\mathcal{X}, \Theta)\end{aligned}$$



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## Problems

Normally, it is almost impossible to obtain a closed analytical solution for the previous equation.

## However

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# The function we would like to have

## The Q function

We want an estimation of the complete-data log-likelihood

$$\log p(\mathcal{X}, \mathcal{Y} | \Theta) \quad (23)$$

Based in the info provided by  $\mathcal{X}$ ,  $\Theta_{n-1}$  where  $\Theta_{n-1}$  is a previously estimated set of parameters at step  $n$ .

Think about the following, if we want to remove  $\mathcal{Y}$

$$\int [\log p(\mathcal{X}, \mathcal{Y} | \Theta)] p(\mathcal{Y} | \mathcal{X}, \Theta_{n-1}) d\mathcal{Y} \quad (24)$$

**Remark:** We integrate out  $\mathcal{Y}$  - Actually, this is the expected value of  $\log p(\mathcal{X}, \mathcal{Y} | \Theta)$ .



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## Use the Expected Value

Then, we want an iterative method to guess  $\Theta$  from  $\Theta_{n-1}$

$$Q(\Theta, \Theta_{n-1}) = E[\log p(\mathcal{X}, \mathcal{Y}|\Theta) | \mathcal{X}, \Theta_{n-1}] \quad (25)$$

Take in account that

- $\mathcal{X}, \Theta_{n-1}$  are taken as constants.
- $\Theta$  is a normal variable that we wish to adjust.
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## Another Interpretation

Given the previous information

$$E[\log p(\mathcal{X}, \mathcal{Y}|\Theta) | \mathcal{X}, \Theta_{n-1}] = \int_{\mathcal{Y} \in \mathbb{Y}} \log p(\mathcal{X}, \mathcal{Y}|\Theta) p(\mathcal{Y}|\mathcal{X}, \Theta_{n-1}) d\mathcal{Y}$$

Something Notable

- In the best of cases, this marginal distribution is a simple analytical expression of the assumed parameter  $\Theta_{n-1}$ .
- In the worst of cases, this density might be very hard to obtain.

Actually, we use

$$p(\mathcal{Y}, \mathcal{X}|\Theta_{n-1}) = p(\mathcal{Y}|\mathcal{X}, \Theta_{n-1}) p(\mathcal{X}|\Theta_{n-1}) \quad (26)$$

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# Back to the $Q$ function

## The intuition

We have the following analogy:

- Consider  $h(\theta, Y)$  a function
  - ▶  $\theta$  a constant
  - ▶  $Y \sim p_Y(y)$ , a random variable with distribution  $p_Y(y)$ .

Thus, if  $Y$  is a discrete random variable

$$q(\theta) = E_Y[h(\theta, Y)] = \sum_y h(\theta, y) p_Y(y) \quad (27)$$





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# Why E-step!!!

From here the name

This is basically the E-step

The second step

It tries to maximize the  $Q$  function

$$\Theta_n = \operatorname{argmax}_{\Theta} Q(\Theta, \Theta_{n-1}) \quad (28)$$



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# The EM-Algorithm

The likelihood function we are going to use

Let  $\mathcal{X}$  be a random vector which results from a parametrized family:

$$\mathcal{L}(\Theta) = \ln \mathcal{P}(\mathcal{X}|\Theta) \quad (29)$$

**Note:**  $\ln(x)$  is a strictly increasing function.

We wish to compute  $\Theta$

Based on an estimate  $\Theta_n$  (After the  $n^{th}$ ) such that  $\mathcal{L}(\Theta) > \mathcal{L}(\Theta_n)$

Or the maximization of this difference

$$\mathcal{L}(\Theta) - \mathcal{L}(\Theta_n) = \ln \mathcal{P}(\mathcal{X}|\Theta) - \ln \mathcal{P}(\mathcal{X}|\Theta_n) \quad (30)$$





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# Introducing the Hidden Features

Given that the hidden random vector  $\mathcal{Y}$  exists with  $y$  values

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# Here, we introduce some concepts of convexity

## For Convexity

### Theorem (Jensen's inequality)

Let  $f$  be a convex function defined on an interval  $I$ . If  $x_1, x_2, \dots, x_n \in I$  and  $\lambda_1, \lambda_2, \dots, \lambda_n \geq 0$  with  $\sum_{i=1}^n \lambda_i = 1$ , then

$$f\left(\sum_{i=1}^n \lambda_i x_i\right) \leq \sum_{i=1}^n \lambda_i f(x_i) \quad (33)$$



# Proof:

For  $n = 1$

We have the trivial case

For  $n = 2$

The convexity definition.

Now, the inductive hypothesis

We assume that the theorem is true for some  $n$ .



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Now, we have

The following linear combination for  $\lambda_i$

$$\begin{aligned} f\left(\sum_{i=1}^{n+1} \lambda_i x_i\right) &= f\left(\lambda_{n+1} x_{n+1} + \sum_{i=1}^n \lambda_i x_i\right) \\ &= f\left(\lambda_{n+1} x_{n+1} + \frac{(1 - \lambda_{n+1})}{(1 - \lambda_{n+1})} \sum_{i=1}^n \lambda_i x_i\right) \\ &\leq \lambda_{n+1} f(x_{n+1}) + (1 - \lambda_{n+1}) f\left(\frac{1}{(1 - \lambda_{n+1})} \sum_{i=1}^n \lambda_i x_i\right) \end{aligned}$$



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Did you notice?

## Something Notable

$$\sum_{i=1}^{n+1} \lambda_i = 1$$

Thus

$$\sum_{i=1}^n \lambda_i = 1 - \lambda_{n+1}$$

Finally

$$\frac{1}{(1 - \lambda_{n+1})} \sum_{i=1}^n \lambda_i = 1$$



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We have that

$$f\left(\sum_{i=1}^{n+1} \lambda_i x_i\right) \leq \lambda_{n+1} f(x_{n+1}) + (1 - \lambda_{n+1}) f\left(\frac{1}{(1 - \lambda_{n+1})} \sum_{i=1}^n \lambda_i x_i\right)$$

$$\leq \lambda_{n+1} f(x_{n+1}) + (1 - \lambda_{n+1}) \frac{1}{(1 - \lambda_{n+1})} \sum_{i=1}^n \lambda_i f(x_i)$$

$$\leq \lambda_{n+1} f(x_{n+1}) + \sum_{i=1}^n \lambda_i f(x_i) \quad \text{Q.E.D.}$$



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Now

We have that

$$\begin{aligned} f\left(\sum_{i=1}^{n+1} \lambda_i x_i\right) &\leq \lambda_{n+1} f(x_{n+1}) + (1 - \lambda_{n+1}) f\left(\frac{1}{(1 - \lambda_{n+1})} \sum_{i=1}^n \lambda_i x_i\right) \\ &\leq \lambda_{n+1} f(x_{n+1}) + (1 - \lambda_{n+1}) \frac{1}{(1 - \lambda_{n+1})} \sum_{i=1}^n \lambda_i f(x_i) \\ &\leq \lambda_{n+1} f(x_{n+1}) + \sum_{i=1}^n \lambda_i f(x_i) \quad \text{Q.E.D.} \end{aligned}$$



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Thus, for concave functions

It is possible to show that

Given  $\ln(x)$  a concave function:

$$\ln \left[ \sum_{i=1}^n \lambda_i x_i \right] \geq \sum_{i=1}^n \lambda_i \ln(x_i)$$

If we take in consideration

Assume that the  $\lambda_i = \mathcal{P}(y|\mathcal{X}, \Theta_n)$ . We know that

- $\mathcal{P}(y|\mathcal{X}, \Theta_n) \geq 0$
- $\sum_y \mathcal{P}(y|\mathcal{X}, \Theta_n) = 1$



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## First

$$\begin{aligned}\mathcal{L}(\Theta) - \mathcal{L}(\Theta_n) &= \ln \left( \sum_y \mathcal{P}(\mathcal{X}|y, \Theta) \mathcal{P}(y|\Theta) \right) - \ln \mathcal{P}(\mathcal{X}|\Theta_n) \\&= \ln \left( \sum_y \mathcal{P}(\mathcal{X}|y, \Theta) \mathcal{P}(y|\Theta) \frac{\mathcal{P}(y|\mathcal{X}, \Theta_n)}{\mathcal{P}(y|\mathcal{X}, \Theta_n)} \right) - \ln \mathcal{P}(\mathcal{X}|\Theta_n) \\&= \ln \left( \sum_y \mathcal{P}(y|\mathcal{X}, \Theta_n) \frac{\mathcal{P}(\mathcal{X}|y, \Theta) \mathcal{P}(y|\Theta)}{\mathcal{P}(y|\mathcal{X}, \Theta_n)} \right) - \ln \mathcal{P}(\mathcal{X}|\Theta_n) \\&\geq \sum_y \mathcal{P}(y|\mathcal{X}, \Theta_n) \ln \left( \frac{\mathcal{P}(\mathcal{X}|y, \Theta) \mathcal{P}(y|\Theta)}{\mathcal{P}(y|\mathcal{X}, \Theta_n)} \right) - \dots \\&\quad \sum_y \mathcal{P}(y|\mathcal{X}, \Theta_n) \ln \mathcal{P}(\mathcal{X}|\Theta_n) \text{ Why this?}\end{aligned}$$

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Because

$$\sum_y \mathcal{P}(y|\mathcal{X}, \Theta_n) = 1$$

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Then, we have

Then, we have proved that

$$\mathcal{L}(\Theta) \geq \mathcal{L}(\Theta_n) + \Delta(\Theta|\Theta_n) \quad (34)$$

Then, we define a new function

$$l(\Theta|\Theta_n) = \mathcal{L}(\Theta_n) + \Delta(\Theta|\Theta_n) \quad (35)$$

Thus  $l(\Theta|\Theta_n)$

It is bounded from above by  $\mathcal{L}(\Theta)$  i.e  $l(\Theta|\Theta_n) \leq \mathcal{L}(\Theta)$



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We evaluate in  $\Theta_n$

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This means that

For  $\Theta = \Theta_n$ , functions  $\mathcal{L}(\Theta)$  and  $l(\Theta|\Theta_n)$  are equal



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# Therefore

The function  $l(\Theta|\Theta_n)$  has the following properties

① It is bounded from above by  $\mathcal{L}(\Theta)$  i.e  $l(\Theta|\Theta_n) \leq \mathcal{L}(\Theta)$ .

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## 1 Introduction

- Beyond Likelihood
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- Properties of the MAP

## 2 A Classic Application, The EM-Algorithm

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- Using the Expected Value
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- **Hidden Features**
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- Using the Concave Functions for Approximation
- From The Concave Function to the EM
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## 3 Example of Application of MAP and EM

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# First

We have the value  $\mathcal{L}(\Theta_n)$

We know that  $\mathcal{L}(\Theta_n)$  is constant i.e. an offset value

What about  $\Delta(\Theta|\Theta_n)$

$$\sum_y \mathcal{P}(y|\mathcal{X}, \Theta_n) \ln \left( \frac{\mathcal{P}(\mathcal{X}|y, \Theta) \mathcal{P}(y|\Theta)}{\mathcal{P}(y|\mathcal{X}, \Theta_n) \mathcal{P}(\mathcal{X}|\Theta_n)} \right)$$

We have that the  $\ln$  is a concave function

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Each element is concave

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# Given the Concave Function

Thus, we have that

- 1 We can select  $\Theta_n$  such that  $l(\Theta|\Theta_n)$  is maximized.

Thus, given a  $\Theta_n$ , we can generate  $\Theta_{n+1}$ .

The process can be seen in the following graph



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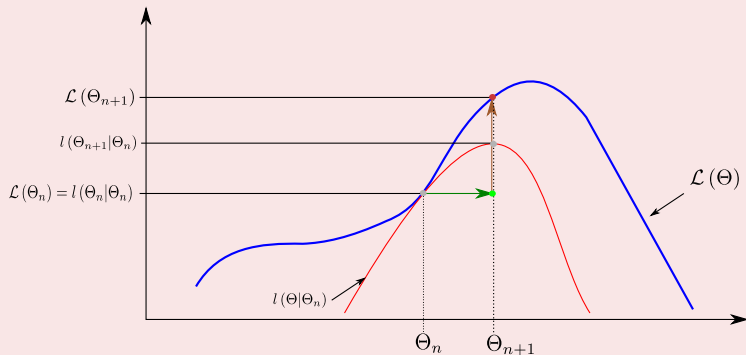
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## The following

$$\Theta_{n+1} = \operatorname{argmax}_{\Theta} \{l(\Theta|\Theta_n)\}$$

$$= \operatorname{argmax}_{\Theta} \left\{ \mathcal{L}(\Theta_n) + \sum_y \mathcal{P}(y|\mathcal{X}, \Theta_n) \ln \left( \frac{\mathcal{P}(\mathcal{X}|y, \Theta) \mathcal{P}(y|\Theta)}{\mathcal{P}(y|\mathcal{X}, \Theta_n) \mathcal{P}(\mathcal{X}|\Theta_n)} \right) \right\}$$

The terms with  $\Theta_n$  are constants.

$$\approx \operatorname{argmax}_{\Theta} \left\{ \sum_y \mathcal{P}(y|\mathcal{X}, \Theta_n) \ln (\mathcal{P}(\mathcal{X}|y, \Theta) \mathcal{P}(y|\Theta)) \right\}$$

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- Beyond Likelihood
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## 2 A Classic Application, The EM-Algorithm

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- Hidden Features
  - Proving Concavity
- Using the Concave Functions for Approximation
- From The Concave Function to the EM
- **The Final Algorithm**
- Notes and Convergence of EM

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# The EM-Algorithm

## Steps of EM

➊ Expectation under hidden variables.

➋ Maximization of the resulting formula.

### E-Step

Determine the conditional expectation,  $E_{y|x, \Theta_n} [\ln (\mathcal{P}(\mathcal{X}, y|\Theta))]$ .

### M-Step

Maximize this expression with respect to  $\Theta$ .



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# Notes and Convergence of EM

## Gains between $\mathcal{L}(\Theta)$ and $l(\Theta|\Theta_n)$

Using the hidden variables it is possible to simplify the optimization of  $\mathcal{L}(\Theta)$  through  $l(\Theta|\Theta_n)$ .

## Convergence

- Remember that  $\Theta_{n+1}$  is the estimate for  $\Theta$  which maximizes the difference  $\Delta(\Theta|\Theta_n)$ .



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Therefore

Then, we have

Given the initial estimate of  $\Theta$  by  $\Theta_n$

$$\Delta(\Theta_n|\Theta_n) = 0$$

Now,

If we choose  $\Theta_{n+1}$  to maximize the  $\Delta(\Theta|\Theta_n)$ , then

$$\Delta(\Theta_{n+1}|\Theta_n) \geq \Delta(\Theta_n|\Theta_n) = 0$$

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The Likelihood  $\mathcal{L}(\Theta)$  is not a decreasing function with respect to  $\Theta$ .



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# Notes and Convergence of EM

## Properties

When the algorithm reaches a fixed point for some  $\Theta_n$ , the value maximizes  $l(\Theta|\Theta_n)$ .

## Definition

A fixed point of a function is an element on domain that is mapped to itself by the function:

$$f(x) = x$$

Essentially the EM algorithm does the following

$$EM[\Theta^*] = \Theta^*$$



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# At this moment

We have that

The algorithm reaches a fixed point for some  $\Theta_n$ , the value  $\Theta^*$  maximizes  $l(\Theta|\Theta_n)$ .

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- It reaches a fixed point for some  $\Theta_n$  the value maximizes  $l(\Theta|\Theta_n)$ .
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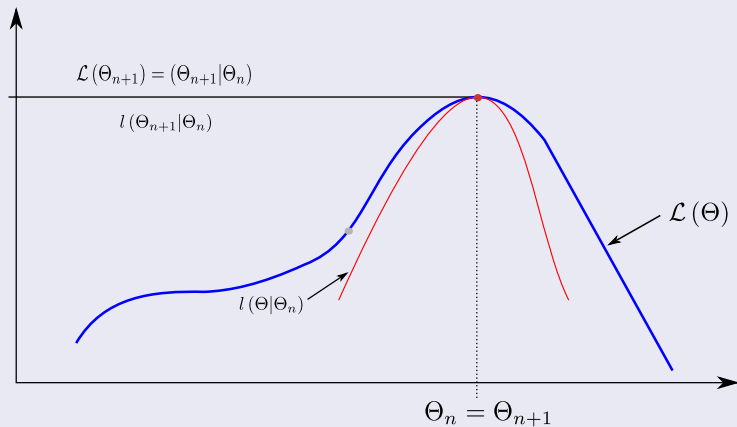
- It reaches a fixed point for some  $\Theta_n$  the value maximizes  $l(\Theta|\Theta_n)$ .
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Therefore

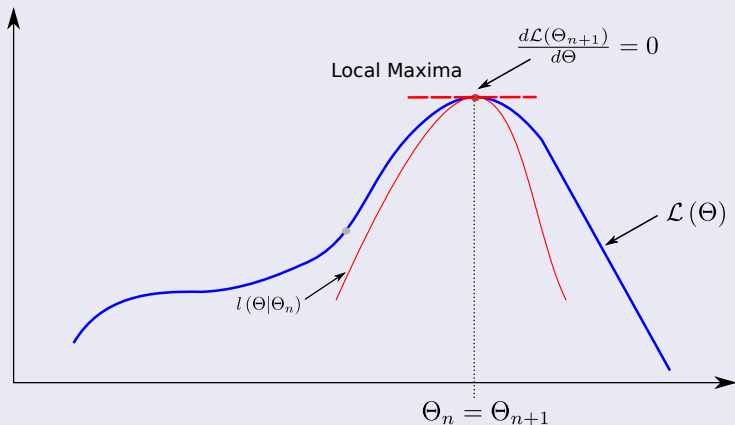
We have



# Then

If  $\mathcal{L}$  and  $l$  are differentiable at  $\Theta_n$

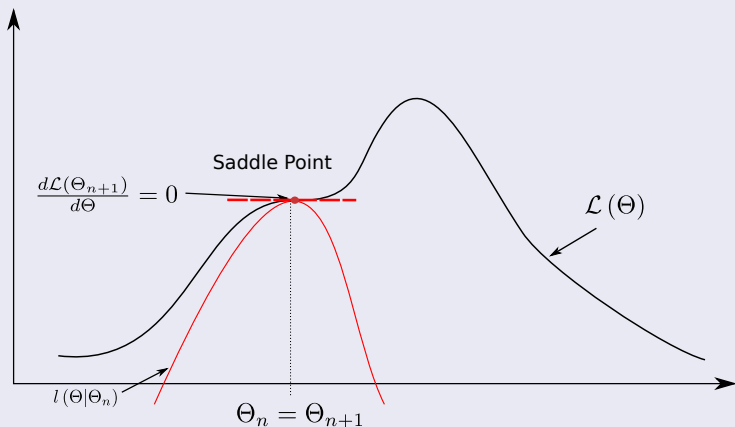
- Since  $\mathcal{L}$  and  $l$  are equal at  $\Theta_n$ 
  - ▶ Then,  $\Theta_n$  is a stationary point of  $\mathcal{L}$  i.e. the derivative of  $\mathcal{L}$  vanishes at that point.





However

You could finish with the following case, no local maxima



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For more on the subject

Please take a look to

Geoffrey McLachlan and Thriyambakam Krishnan, "*The EM Algorithm and Extensions*," John Wiley & Sons, New York, 1996.



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# Example

This application comes from

“Adaptive Sparseness for Supervised Learning” by Mário A.T. Figueiredo

In

IEEE TRANSACTIONS ON PATTERN ANALYSIS AND MACHINE  
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# Linear Regression with Gaussian Prior

We consider regression functions that are linear with respect to the parameter vector  $\beta$

$$f(\mathbf{x}, \mathbf{w}) = \sum_{i=1}^k w_i h(\mathbf{x}) = \mathbf{w}^T \mathbf{h}(\mathbf{x})$$

Where

$\mathbf{h}(\mathbf{x}) = [h_1(\mathbf{x}), \dots, h_k(\mathbf{x})]^T$  is a vector of  $k$  fixed function of the input, often called features.



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Actually, it can be...

## Linear Regression

Linear regression, in which  $\mathbf{h}(\mathbf{x}) = [1, x_1, \dots, x_d]^T$  i; in this case,  $k = d + 1$ .

## Non-Linear Regression

Here, you have a fixed basis function where

$\mathbf{h}(\mathbf{x}) = [\phi_1(\mathbf{x}), \phi_2(\mathbf{x}), \dots, \phi_l(\mathbf{x})]^T$  with  $\phi_1(\mathbf{x}) = 1$ .

## Kernel Regression

Here  $\mathbf{h}(\mathbf{x}) = [1, K(\mathbf{x}, \mathbf{x}_1), K(\mathbf{x}, \mathbf{x}_2), \dots, K(\mathbf{x}, \mathbf{x}_n)]^T$  where  $K(\mathbf{x}, \mathbf{x}_i)$  is some kernel function.



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# Gaussian Noise

We assume that the training set is contaminated by additive white Gaussian Noise

$$y_i = f(\mathbf{x}_i, \mathbf{w}) + \omega_i = \mathbf{w}^T \mathbf{x}_i + \omega_i \quad (36)$$

for  $i = 1, \dots, N$  where  $[\omega_1, \dots, \omega_N]$  is a set of independent zero-mean Gaussian samples with variance  $\sigma^2$

With this,  $\omega_i \sim \mathcal{N}(0, \sigma^2)$

Thus, for  $\mathbf{y} = [y_1, \dots, y_N]^T$ , we have the following likelihood

$$p(\omega_1, \omega_2, \dots, \omega_N) = \prod_{i=1}^N p(\omega_i | 0, \sigma^2)$$

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# Something Interesting

We have that

$$\begin{aligned}\prod_{i=1}^N p(\omega_i | 0, \sigma^2) &= \frac{1}{(2\pi)^{\frac{N}{2}} \sigma^N} \prod_{i=1}^N \exp \left\{ -\frac{\omega_i^2}{2\sigma^2} \right\} \\ &= \frac{1}{(2\pi)^{\frac{N}{2}} \sigma^N} \prod_{i=1}^N \exp \left\{ -\frac{(y_i - w^T x_i)^2}{2\sigma^2} \right\}\end{aligned}$$

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Then

We can rewrite this in vector form

$$p(\mathbf{y} | X\mathbf{w}, \sigma^2 I) \approx \exp \left\{ -(\mathbf{y} - X\mathbf{w})^T \frac{1}{\sigma'^2} I (\mathbf{y} - X\mathbf{w}) \right\}$$

- With  $\sigma' = \sqrt{2}\sigma$

Thus, for  $\mathbf{y} \sim \mathcal{N}(\mathbf{y} | X\mathbf{w}, \sigma^2 I)$ , we have the following likelihood

$$p(\mathbf{y} | \mathbf{w}) = \mathcal{N}(\mathbf{y} | X\mathbf{w}, \sigma'^2 I) \quad (37)$$



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Thus, for  $[y_1, \dots, y_N]$ , we have the following likelihood

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# Gaussian Noise

What if we assume a prior zero mean Gaussian for  $w$

$$p(w|0, A) = N(0, A)$$

The posterior looks like

$$p(w|y) \approx \exp \left\{ - (y - Xw)^T \frac{1}{\sigma^2} I (y - Xw) \right\} \exp \left\{ - w^T A^{-1} w \right\} \quad (38)$$

We have the following

$$\log p(w|y) \approx - (y - Xw)^T \frac{1}{\sigma^2} I (y - Xw) - w^T A^{-1} w$$



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Therefore

The posterior  $p(\mathbf{w}|\mathbf{y})$  is still Gaussian and the mode/maximal estimation is given by

$$\hat{\mathbf{w}} = \left( \sigma^2 \mathbf{A}^{-1} + \mathbf{X}^T \mathbf{X} \right)^{-1} \mathbf{X}^T \mathbf{y} \quad (39)$$

Remark: The Ridge regression.



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# Regression with a Laplacian Prior

Thus, the MAP estimate of  $\mathbf{w}$  look like

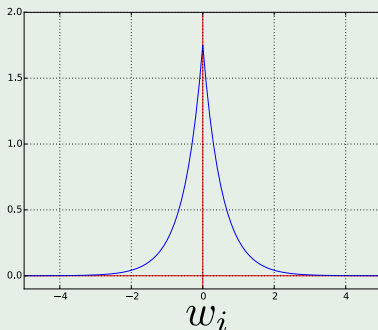
$$\hat{\mathbf{w}} = \underset{\mathbf{w}}{\operatorname{argmin}} \left\{ \|\mathbf{X}\mathbf{w} - \mathbf{y}\|_2^2 + 2\sigma^2\alpha \|\mathbf{w}\|_1 \right\} \quad (40)$$



# Regression with a Laplacian Prior

In order to favor sparse estimate, we can adopt priors

$$p(\mathbf{w}|\alpha) = \prod_{i=1}^d \frac{\alpha}{2} \exp\{-\alpha |w_i|\} = \left(\frac{\alpha}{2}\right)^d \exp\{-\alpha \|\mathbf{w}\|_1\} \quad (41)$$



## Regression with a Laplacian Prior

Thus, the Maximum A Posterior (MAP) estimate of  $\mathbf{w}$  look like

$$\hat{\mathbf{w}} = \underset{\mathbf{w}}{\operatorname{argmin}} \left\{ \|\mathbf{X}\mathbf{w} - \mathbf{y}\|_2^2 + 2\sigma^2\alpha \|\mathbf{w}\|_1 \right\} \quad (42)$$



## Remark

This criterion is known

- As the **Least Absolute Shrinkage and Selection Operator** (LASSO)
- This norm  $l_1$  induces sparsity in the weight terms.

$$\|w\|_1 = \sum_{i=1}^d |w_i|$$

How?

- For example,  $\|[1, 0]^T\|_2 = \|[1/\sqrt{2}, 1/\sqrt{2}]^T\|_2 = 1$ .
- In the other case,  $\|[1, 0]^T\|_1 = 1 < \|[1/\sqrt{2}, 1/\sqrt{2}]^T\|_1 = \sqrt{2}$ .



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## An example

What if  $\mathbf{X}$  is a orthogonal matrix

In this case  $\mathbf{X}^T \mathbf{X} = \mathbf{I}$

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We can solve this last part as follow

We can group for each  $w_i$

$$w_i^2 - 2w_i \left( \mathbf{X}^T \mathbf{y} \right)_i + 2\sigma^2 \alpha |w_i| + y_i^2 \quad (43)$$

If we can minimize each group we will be able to get the solution

$$\hat{w}_i = \underset{w_i}{\operatorname{argmin}} \left\{ w_i^2 - 2w_i \left( \mathbf{X}^T \mathbf{y} \right)_i + 2\sigma^2 \alpha |w_i| \right\} \quad (44)$$

We have two cases

- $w_i > 0$
- $w_i < 0$



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If  $w_i > 0$

We then derive with respect to  $w_i$

$$\frac{\partial \left( w_i^2 - 2w_i \left( \mathbf{X}^T \mathbf{y} \right)_i + 2\sigma^2 \alpha_i w_i \right)}{\partial w_i} = 2w_i - 2 \left( \mathbf{X}^T \mathbf{y} \right)_i + 2\sigma^2 \alpha$$

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If  $w_i < 0$

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The value of  $(\mathbf{X}^T \mathbf{y})_i$

We have that

We have that:

- if  $w_i > 0$  then  $(\mathbf{X}^T \mathbf{y})_i > \sigma^2 \alpha$
- if  $w_i < 0$  then  $(\mathbf{X}^T \mathbf{y})_i < -\sigma^2 \alpha$



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# We can put all this together

## A compact Version

$$\hat{w}_i = \text{sgn} \left( \left( \mathbf{X}^T \mathbf{y} \right)_i \right) \left( \left| \left( \mathbf{X}^T \mathbf{y} \right)_i \right| - \sigma^2 \alpha \right)_+ \quad (47)$$

With

$$(a)_+ = \begin{cases} a & \text{if } a \geq 0 \\ 0 & \text{if } a < 0 \end{cases}$$

- Where  $(a)_+$  is the sign function.

This rule is known as the

- The soft threshold!!!



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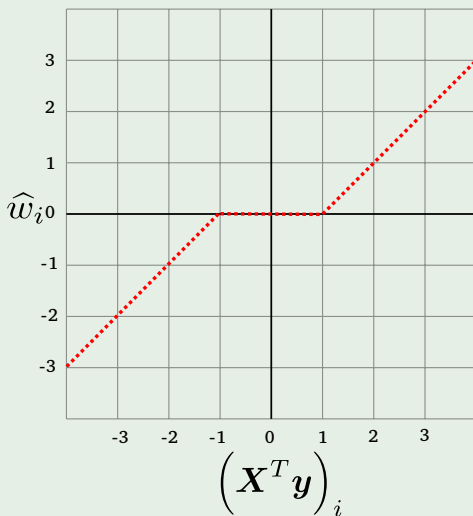
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## Example

We have the dotted  $\cdots$  line as the soft threshold



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Now, we need an estimate of each  $w_i$

Given that each  $w_i$  has a zero-mean Gaussian prior

$$p(w_i|\tau_i) = \mathcal{N}(w_i|0, \tau_i) \quad (48)$$

Where  $\tau_i$  has the following exponential hyper-prior

$$p(\tau_i|\gamma) = \frac{\gamma}{2} \exp\left\{-\frac{\gamma}{2}\tau_i\right\} \text{ for } \tau_i \geq 0 \quad (49)$$

This is a tough property – so we take it by heart

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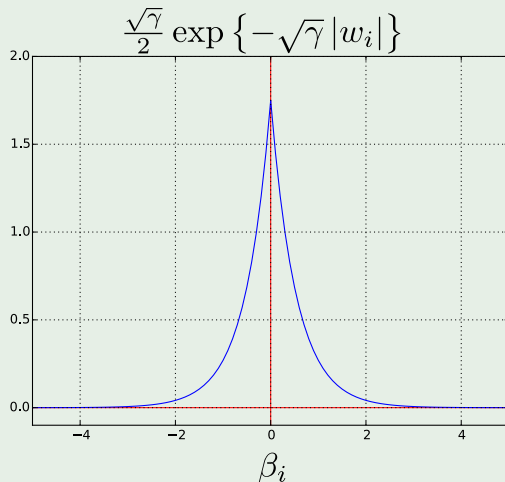
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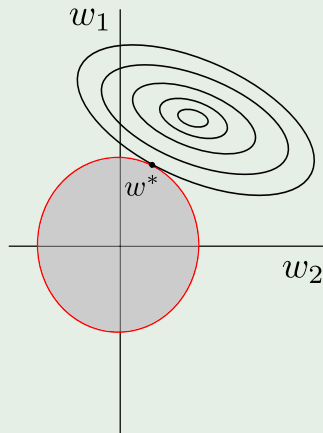
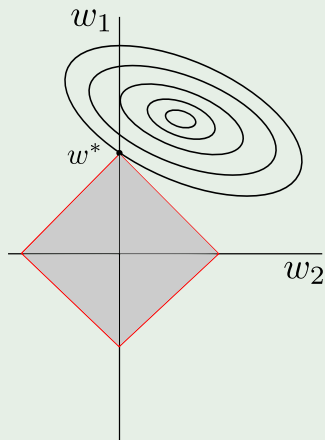
# Example

## The double exponential



This is equivalent to the use of the  $L_1$ -norm for regularization

$L_1$ (Left) is better for sparsity promotion than  $L_2$ (Right)



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# The EM trick

## How do we do this?

This is done by regarding  $\tau = [\tau_1, \dots, \tau_d]$  as the hidden/missing data

Then, if we could observe  $\tau$ , complete log-posterior  $\log p(w, \sigma^2 | y, \tau)$  can be easily calculated

$$p(w, \sigma^2 | y, \tau) \propto p(y | w, \sigma^2) p(w | \tau) p(\sigma^2) \quad (51)$$

Then, we would want to maximize



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Where

- $p(\mathbf{y} | \mathbf{w}, \sigma^2) \sim \mathcal{N}(\mathbf{X}\mathbf{w}, \sigma^2 \mathbf{I})$

- $p(\mathbf{w} | \tau) \sim \mathcal{N}(\mathbf{w} | \tau)$



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- $p(\mathbf{y} | \mathbf{w}, \sigma^2) \sim \mathcal{N}(\mathbf{X}\mathbf{w}, \sigma^2 I)$
- $p(\mathbf{w} | 0, \tau) \sim \prod_{i=1}^k \mathcal{N}(w_i | 0, \tau_i) = \mathcal{N}\left(0, \text{diag}\left(\tau_1^{-1}, \dots, \tau_d^{-1}\right)\right)$



# What about $p(\sigma^2)$ ?

We select

$p(\sigma^2)$  as a constant

However:

We can adopt a conjugate inverse Gamma prior for  $\sigma^2$ , but for large number of samples the prior on the estimate of  $\sigma^2$  is very small.

In the constant case:

We can use the MAP idea, however we have hidden parameters so we resort to the EM



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## E-step

Computes the expected value of the complete log-posterior

$$Q\left(\mathbf{w}, \sigma^2 | \hat{\mathbf{w}}_{(t)}, \hat{\sigma}^2_{(t)}\right) = \int \log p\left(\mathbf{w}, \sigma^2 | \mathbf{y}, \tau\right) p\left(\tau | \hat{\mathbf{w}}_{(t)}, \hat{\sigma}^2_{(t)}, \mathbf{y}\right) d\tau \quad (52)$$



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## M-step

Updates the parameter estimates by maximizing the  $Q$ -function

$$\left(\hat{\boldsymbol{w}}_{(t+1)}, \hat{\sigma}^2_{(t+1)}\right) = \operatorname{argmax}_{\boldsymbol{w}, \sigma^2} Q\left(\boldsymbol{w}, \sigma^2 \mid \hat{\boldsymbol{w}}_{(t)}, \hat{\sigma}^2_{(t)}\right) \quad (53)$$





## Remark

### First

The EM algorithm converges to a local maximum of the a posteriori probability density function

$$p(\mathbf{w}, \sigma^2 | \mathbf{y}) \propto p(\mathbf{y} | \mathbf{w}, \sigma^2) p(\mathbf{w} | \gamma) \quad (54)$$

Without using the marginal prior  $p(\mathbf{w})$  which is not Gaussian.  
Instead we use a conditional Gaussian prior  $p(\mathbf{w} | \gamma)$ .



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# The Final Model

We have

$$p(\mathbf{y}|\mathbf{w}, \sigma^2) = \mathcal{N}(\mathbf{X}\mathbf{w}, \sigma^2 I)$$

$$p(\sigma^2) \propto \text{"constant"}$$

$$p(\mathbf{w}|\tau) = \prod_{i=1}^d \mathcal{N}(w_i|0, \tau_i) = \mathcal{N}(\mathbf{w}|0, (\mathcal{Y}(\tau))^{-1})$$

$$p(\tau|\gamma) = \left(\frac{\gamma}{2}\right)^d \prod_{i=1}^d \exp\left\{-\frac{\gamma}{2}\tau_i\right\}$$

With  $\mathcal{Y}(\tau) = \text{diag}(\tau_1^{-1}, \dots, \tau_d^{-1})$  is the diagonal matrix with the inverse variances of all the  $w_i$ 's.



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Now, we find the  $Q$  function

First

$$\begin{aligned}\log p(\mathbf{w}, \sigma^2 | \mathbf{y}, \tau) &\propto \log p(\mathbf{y} | \mathbf{w}, \sigma^2) + \log p(\mathbf{w} | \tau) \\ &\propto -n \log \sigma^2 - \frac{\|\mathbf{y} - \mathbf{X}\mathbf{w}\|_2^2}{\sigma^2} - \mathbf{w}^T \Upsilon(\tau) \mathbf{w}\end{aligned}$$

How can we get this?

Remember

$$\mathcal{N}(\mathbf{y} | \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{\frac{n}{2}} |\boldsymbol{\Sigma}|^{\frac{1}{2}}} \exp \left\{ -\frac{1}{2} (\mathbf{y} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\mathbf{y} - \boldsymbol{\mu}) \right\} \quad (55)$$

Volunteers?

Please to the blackboard.



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## Second

Did you notice that the term  $\mathbf{w}^T \Upsilon(\tau) \mathbf{w}$  is linear with respect to  $\Upsilon(\tau)$  and the other terms do not depend on  $\tau$ ?

Thus, the E-step is reduced to the computation of  $\Upsilon(\tau)$ .



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$$\mathbf{V}_{(t)} = E \left( \Upsilon(\tau) \mid \mathbf{y}, \hat{\mathbf{w}}_{(t)}, \hat{\sigma}^2_{(t)} \right) \\ = \text{diag} \left( E \left[ \tau_1^{-1} \mid \mathbf{y}, \hat{\mathbf{w}}_{(t)}, \hat{\sigma}^2_{(t)} \right], \dots, E \left[ \tau_d^{-1} \mid \mathbf{y}, \hat{\mathbf{w}}_{(t)}, \hat{\sigma}^2_{(t)} \right] \right)$$

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Now

What do we need to calculate each of this expectations?

$$p\left(\tau_i|\mathbf{y}, \widehat{\mathbf{w}}_{(t)}, \widehat{\sigma}^2_{(t)}\right) = p\left(\tau_i|\mathbf{y}, \widehat{w}_{i,(t)}, \widehat{\sigma}^2_{i,(t)}\right) \quad (56)$$

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## Here is the interesting part

We have the following probability density

$$p\left(\tau_i | \mathbf{y}, \hat{\beta}_{i,(t)}, \hat{\sigma}_{i,(t)}^2\right) = \frac{\mathcal{N}\left(\beta_{i,(t)} | 0, \tau_i\right) \frac{\gamma}{2} \exp\left\{-\frac{\gamma}{2}\tau_i\right\}}{\int_0^\infty \mathcal{N}\left(\beta_{i,(t)} | 0, \tau_i\right) \frac{\gamma}{2} \exp\left\{-\frac{\gamma}{2}\tau_i\right\} d\tau_i} \quad (57)$$

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$$E \left[ \tau_i^{-1} | \mathbf{y}, \hat{w}_{i,(t)}, \hat{\sigma}^2_{(t)} \right] = \frac{\gamma}{|\hat{w}_{i,(t)}|} \quad (59)$$

Finally

$$\mathbf{V}_{(t)} = \gamma \text{diag} \left( |\hat{w}_{1,(t)}|^{-1}, \dots, |\hat{w}_{d,(t)}|^{-1} \right) \quad (60)$$



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# The Final $Q$ function

## Something Notable

$$\begin{aligned} Q\left(\boldsymbol{w}, \sigma^2 | \hat{\boldsymbol{w}}_{(t)}, \hat{\sigma}^2_{(t)}\right) &= \int \log p\left(\boldsymbol{w}, \sigma^2 | \boldsymbol{y}, \tau\right) p\left(\tau | \hat{\boldsymbol{w}}_{(t)}, \hat{\sigma}^2_{(t)}, \boldsymbol{y}\right) d\tau \\ &= \int \left[-n \log \sigma^2 - \frac{\|\boldsymbol{y} - \boldsymbol{X} \boldsymbol{w}\|_2^2}{\sigma^2} - \boldsymbol{w}^T \boldsymbol{\Gamma}(\tau) \boldsymbol{w}\right] p\left(\tau | \hat{\boldsymbol{w}}_{(t)}, \hat{\sigma}^2_{(t)}, \boldsymbol{y}\right) d\tau \\ &= -n \log \sigma^2 - \frac{\|\boldsymbol{y} - \boldsymbol{X} \boldsymbol{w}\|_2^2}{\sigma^2} - \boldsymbol{w}^T \left[\int \boldsymbol{\Gamma}(\tau) p\left(\tau | \hat{\boldsymbol{w}}_{(t)}, \hat{\sigma}^2_{(t)}, \boldsymbol{y}\right) d\tau\right] \boldsymbol{w} \\ &= -n \log \sigma^2 - \frac{\|\boldsymbol{y} - \boldsymbol{X} \boldsymbol{w}\|_2^2}{\sigma^2} - \boldsymbol{w}^T \boldsymbol{V}_{(t)} \boldsymbol{w} \end{aligned}$$



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# Finally, the M-step

First

$$\begin{aligned}\widehat{\sigma^2}_{(t+1)} &= \operatorname{argmax}_{\sigma^2} \left\{ -n \log \sigma^2 - \frac{\|\mathbf{y} - \mathbf{X}\mathbf{w}\|_2^2}{\sigma^2} \right\} \\ &= \frac{\|\mathbf{y} - \mathbf{X}\mathbf{w}\|_2^2}{n}\end{aligned}$$

Second

$$\begin{aligned}\widehat{\mathbf{w}}_{(t+1)} &= \operatorname{argmax}_{\mathbf{w}} \left\{ -\frac{\|\mathbf{y} - \mathbf{X}\mathbf{w}\|_2^2}{\sigma^2} - \mathbf{w}^T \mathbf{V}_{(t)} \mathbf{w} \right\} \\ &= \left( \widehat{\sigma^2}_{(t+1)} \mathbf{V}_{(t)} + \mathbf{X}^T \mathbf{X} \right)^{-1} \mathbf{X}^T \mathbf{y}\end{aligned}$$

This also I leave to you.

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It can come in the test.

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# Outline

## 1 Introduction

- Beyond Likelihood
- Maximum Likelihood Vs Maximum A Posteriori
- Properties of the MAP

## 2 A Classic Application, The EM-Algorithm

- Introduction
- Using the Expected Value
- Analogy
- Hidden Features
  - Proving Concavity
- Using the Concave Functions for Approximation
- From The Concave Function to the EM
- The Final Algorithm
- Notes and Convergence of EM

## 3 Example of Application of MAP and EM

- Example
- Linear Regression
- The Gaussian Noise
- Regression with a Laplacian Prior
- A Hierarchical-Bayes View of the Laplacian Prior
- Sparse Regression via EM
- Jeffrey's Prior



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However

We need to deal in some way with the  $\gamma$  term

It controls the degree of sparseness!!!

We can do assuming a Jeffrey's Prior

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# Properties of the Jeffrey's Prior

## Important

This prior expresses ignorance with respect to scale and is parameter free

## Why scale invariant

Imagine, we change the scale of  $\tau$  by  $\tau' = K\tau$  where  $K$  is a constant expressing that change

Thus, we have that

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This prior is known as an improper prior.

In addition

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## Introducing this prior into the equations

Matrix  $V_{(t)}$  is now

$$V_{(t)} = \text{diag} \left( |\hat{w}_{1,(t)}|^{-2}, \dots, |\hat{w}_{d,(t)}|^{-2} \right) \quad (63)$$

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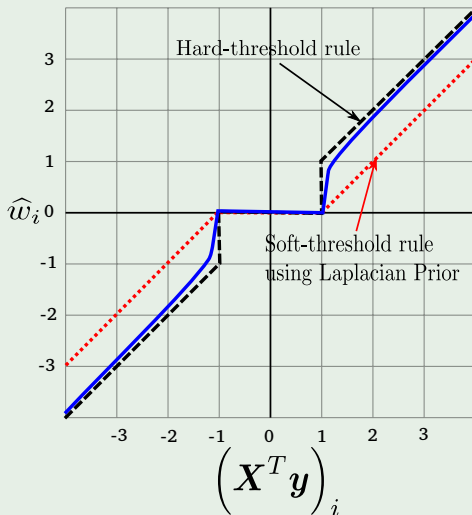
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Here, we can see the new threshold

Blue solid line - estimation rule using EM and Jeffrey's Hyperprior



# Observations

## The new rule is between

- The soft threshold rule.
- The hard threshold rule.

## Something Notable

With large values of  $(X^T y)_i$ , the new rule approaches the hard threshold.

Once  $(X^T y)_i$  gets smaller

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## Finally, an implementation detail

Since several elements of  $\widehat{\mathbf{w}}$  will go to zero

$\mathbf{V}_{(t)} = \text{diag} \left( \left| \widehat{w}_{1,(t)} \right|^{-2}, \dots, \left| \widehat{w}_{d,(t)} \right|^{-2} \right)$  will have several elements going to large numbers

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# Advantages!!!

## Quite Important

We avoid the inversion of the elements of  $\hat{\mathbf{w}}_{(t)}$ .

We can avoid getting the inverse matrix

We simply solve the corresponding linear system whose dimension is only the number of nonzero elements in  $\mathbf{U}_{(t)}$ . Why?

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