Principal Components Analysis
MLE, EM and MAP

CMSC 828D

Fundamentals of Computer Vision

Fall 2000

Outline

- Lagrange Multipliers
- Principal Components Analysis
- Review of parameter estimation.
- Notation and Problem Definition
- Maximum Likelihood Estimation
- Difficulties
- Bayesian view
- Maximum A Posteriori Estimation
- Algorithms: Expectation Maximization

Lagrange Multipliers

- Find stationary points of a function $f(\mathbf{x})$ subject to one or more constraints $g(\mathbf{x}) = 0$
- Consider the surface $g(\mathbf{x}) = 0$
  - The direction of increase of f is ∇f
  - However moving this direction may take us away from the constraint surface
  - **Idea**: move along component of ∇f *along the surface.*
  - Denote this component as $\nabla_g f$
  - At the extremum point this function will be stationary

$$\nabla_g f = 0$$

  - How to get $\nabla_g f$?
  - Take ∇f and subtract from it that part $\mathbf{a}$ which takes it out of the surface g

$$\nabla_g f = \nabla f - \mathbf{a}$$

Finding the component of ∇f along g

- Now let us move by a distance δ along the surface $\mathbf{g}$
  - $g(\mathbf{x}+\boldsymbol{\delta})=g(\mathbf{x})+(\boldsymbol{\delta}\,.\nabla\mathbf{g})$
  - But this still lies on the surface -- so $g(\mathbf{x}+\boldsymbol{\delta})=0$
  - So $\boldsymbol{\delta}\,.\nabla g=0$
  - $\Rightarrow \nabla g$ is perpendicular to motions along the surface
- But we wanted to remove any piece of ∇f that was perpendicular to $g(\mathbf{x})=0$
- This will be a vector of the form

$$\nabla_g f=\nabla f+\lambda\nabla g$$

(For some λ)

Lagrangian

- Consider the Lagrangian function

$$L(\mathbf{x}, \lambda) = f + \lambda g$$

$$\frac{\partial}{\partial \mathbf{x}} L(\mathbf{x}, \lambda) = \nabla f + \lambda \nabla g, \qquad \frac{\partial}{\partial \lambda} L(\mathbf{x}, \lambda) = g$$

- Extremize the Lagrangian

$$\frac{\partial}{\partial \mathbf{x}} L(\mathbf{x}, \lambda) = \nabla f + \lambda \nabla g = 0, \qquad \frac{\partial}{\partial \lambda} L(\mathbf{x}, \lambda) = g(\mathbf{x}) = 0$$

- So this gives us **both the constraint equation** and **the way to optimize the function on the surface**.

Principal Components Analysis

Key technique in dealing with data

- Data Reduction
  - Experimental measurements produce lots of data
  - Scientists postulate lots of hypotheses as to what factors affect data. Create overly complex models
  - Goal: find factors that affect data most and create small models
- Knowledge discovery
  - Collect lots of data
  - Are there patterns hidden in the collected data that can help us develop a model and understanding?
  - Can we use this understanding to classify a new piece of data?
- Applications: Almost all computer vision
  - Especially face recognition, tracking, pattern recognition… etc.

Basics

- Record data
- d dimensional data vector $\mathbf{x}$
- Record N observations
- Mean $\bar{\mathbf{x}} = \frac{1}{N}\sum_{i=1}^{N}\mathbf{x}_i$
- Covariance $\boldsymbol{\Sigma} = \frac{1}{N}\sum_{i=1}^{N}(\mathbf{x}_i - \bar{\mathbf{x}})'(\mathbf{x}_i - \bar{\mathbf{x}})$
- Problem: d can be very large
  - *"megapixel camera"* d>1 million (values of the intensity at the pixels)
  - Image is a point in a d dimensional space
- Need a way to capture the information in the data but using very few "coordinates"

Principal Components Analysis

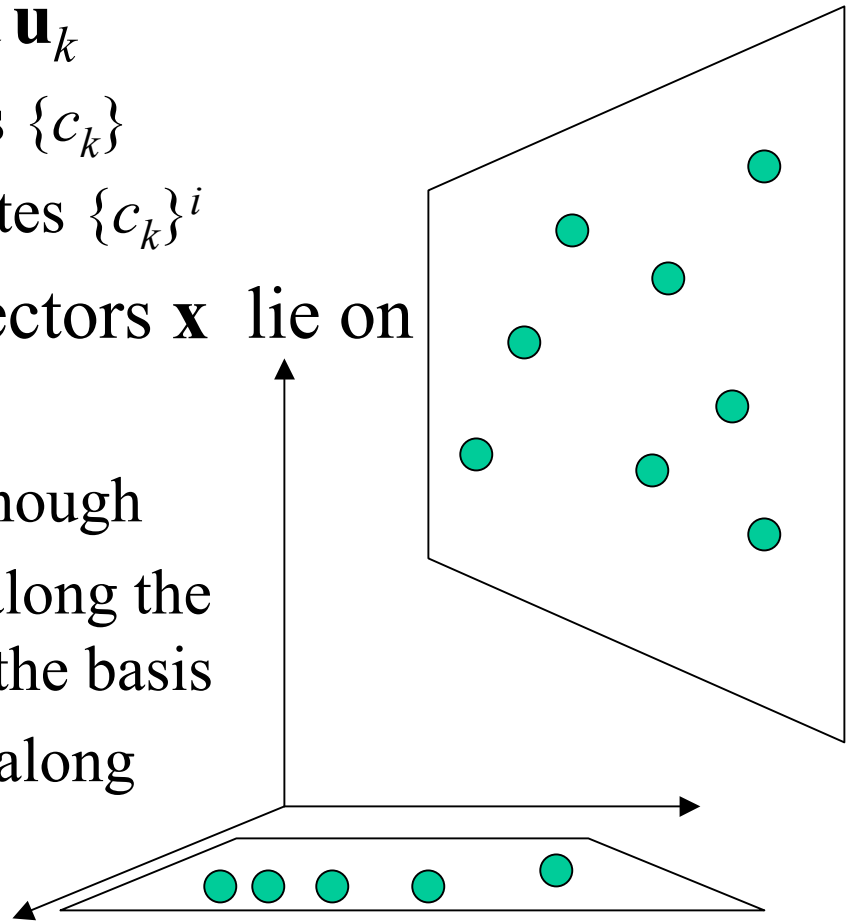
- Consider a vector $\mathbf{x}$ that lies in a d dimensional linear space.
- Let vectors $\mathbf{u}_k$, $k=1,\ldots,d$ define a basis in the space

$$\mathbf{x}=\sum c_k \mathbf{u}_k$$

$\mathbf{x}$ is characterized by d coordinates $\{c_k\}$

Different $\mathbf{x}_i$ have different coordinates $\{c_k\}^i$

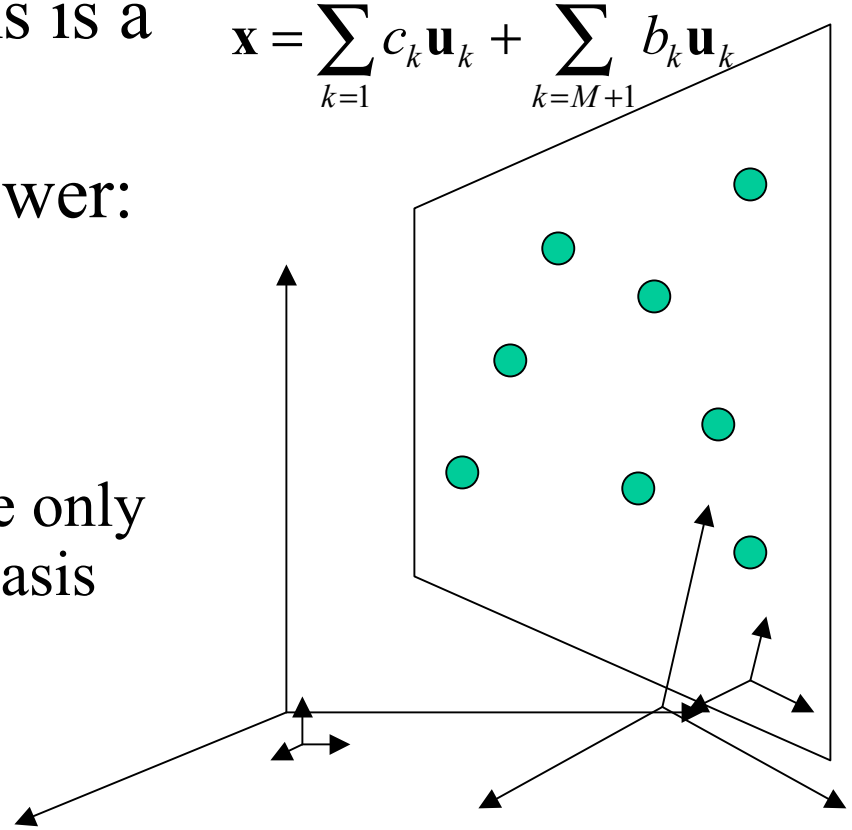
- Now consider a case that the vectors $\mathbf{x}$ lie on a lower dimensional manifold
  - Smaller number of coordinates enough
  - For small d, if points are spread along the axes it may be easy to recognize the basis
  - For larger d and if points are not along axes it is harder
  - Need mathematical tools



Dimension Reduction

- Expressing the points using the basis vectors along the axes, we still need all the coordinates to describe the $\mathbf{x}_i$
- However if we had an alternate basis we need only two variables and a constant to describe the points.
- Complexity of most algorithms is a power of *d*
- Mathematical questions to answer:
  - **Best Basis**: How to find out the basis that is best lined up with the data?
  - **Approximation question**: If we only wanted the best *k* dimensional basis how do we select it?
  - How do we account for noise?

$$\mathbf{x} = \sum_{k=1}^{M} c_k \mathbf{u}_k + \sum_{k=M+1}^{d} b_k \mathbf{u}_k$$



Approximation

- Given a dataset $\{\mathbf{x}^i\}$ with N members
- Write each vector in a basis $\{\mathbf{u}_k\}$
- Coefficients $c_k = \mathbf{x}' \mathbf{u}_k$
- Approximate each $\mathbf{x}^i$ as sum of a variable part and a constant part and

$$\mathbf{x}^i = \sum_{k=1}^{d} c_k^i \mathbf{u}_k \simeq \sum_{k=1}^{M} c_k^i \mathbf{u}_k + \sum_{k=M+1}^{d} b_k \mathbf{u}_k$$

- Dimension of variable part is M
- Error in approximting a particular vector

$$\boldsymbol{\varepsilon}_i = \mathbf{x}^i - \sum_{k=1}^{M} c_k^i \mathbf{u}_k - \sum_{k=M+1}^{d} b_k \mathbf{u}_k = \mathbf{x}^i - \sum_{k=1}^{M} c_k^i \mathbf{u}_k - \sum_{k=M+1}^{d} b_k \mathbf{u}_k = \sum_{k=M+1}^{d} \left(c_k^i - b_k \right) \mathbf{u}_k$$

- Define sum of squares error function C

$$C(b_k) = \sum_{i=1}^{N} \left[\sum_{k=M+1}^{d} \left(c_k^i - b_k \right) \mathbf{u}_k \right]^2$$

Getting the parameters b_k and $\mathbf{u}_k$

- Evaluate b_k by setting $\partial C / \partial b_k = 0$

$$b_k = \frac{1}{N}\sum_{i=1}^{N} c_k^i = \mathbf{u}'_k\,\bar{\mathbf{x}}$$

- To get best basis vectors $\mathbf{u}_k$ define cost function

$$E_M = \sum_{i=1}^{N}\sum_{k=M+1}^{d}\left[\left(\mathbf{x}^i - \bar{\mathbf{x}}\right)\cdot\mathbf{u}_k\right]^2$$

$$= \sum_{k=M+1}^{d}\mathbf{u}_k'\left[\sum_{i=1}^{N}\left[\left(\mathbf{x}^i - \bar{\mathbf{x}}\right)\left(\mathbf{x}^i - \bar{\mathbf{x}}\right)\right]\right]\mathbf{u}_k$$

$$= \sum_{k=M+1}^{d}\mathbf{u}_k'\boldsymbol{\Sigma}\mathbf{u}_k$$

- Minimize E with respect to $\mathbf{u}_k$
- However the expression is homogeneous in $\mathbf{u}_k$
  - Obvious solution is $\mathbf{u}_k = 0$

Finding the best basis

- To avoid the trivial solution we need a constraint
- Basis vectors have unit magnitude $||\mathbf{u}_k||=1$, $\mathbf{u}_j \cdot \mathbf{u}_k=\delta_{jk}$
- How do we optimize subject to constraints?
  - Lagrange Multipliers! Cost function with constraints:

$$E_M = \sum_{k=M+1}^{d} \mathbf{u}_k{}'\boldsymbol{\Sigma}\mathbf{u}_k - \sum_{j=M+1}^{N}\sum_{k=M+1}^{N} \mu_{jk}\left(\mathbf{u}_j{}'\mathbf{u}_k - \delta_{jk}\right)$$

Can be written in the form:

$$E_M = Tr\left\{\mathbf{U}'\boldsymbol{\Sigma}\mathbf{U}\right\} - Tr\left\{\mathbf{M}\left(\mathbf{U}'\mathbf{U}-\mathbf{I}\right)\right\}$$

$$\mathbf{U}=\left[\mathbf{u}_{M+1}\,|\,\mathbf{u}_{M+2}\,|\cdots|\,\mathbf{u}_d\right] \qquad \mathbf{M}=\left[\mu_{jk}\right]$$

- Minimizing with respect to $\mathbf{u}_k$

$$\left(\boldsymbol{\Sigma}+\boldsymbol{\Sigma}'\right)\mathbf{U}-\mathbf{U}\left(\mathbf{M}+\mathbf{M}'\right)=0 \quad \Rightarrow \quad \boldsymbol{\Sigma}\mathbf{U}=\mathbf{U}\mathbf{M}$$

- $\mathbf{U}$ is an orthonormal vector with columns as basis vectors
- So any set of $\mathbf{U}s$ and $\mathbf{M}s$ that satisfy $\mathbf{U}^t\boldsymbol{\Sigma}\mathbf{U}=\mathbf{M}$

PCA

- Choose the simplest solution
  - **U** vectors in the eigenbasis of **Σ**
  - **M** is the diagonal matrix of eigenvalues.
- Algorithm
  1. Compute the mean of the data

$$\mathbf{x}^- = (\sum_i \mathbf{x}_i)/N$$

  2. Compute the covariance of the data,

$$\mathbf{\Sigma} = \sum_i (\mathbf{x}^i - \mathbf{x}^-)(\mathbf{x}^i - \mathbf{x}^-)'$$

  3. Compute eigenvectors, $\mathbf{u}_i$ and corresponding eigenvalues λ_i of **Σ** sorted according to the magnitude of λ_i
  4. For a desired approximation dimension M, $\mathbf{x}^i$ can be written as

$$\mathbf{x}^i \simeq \sum_{k=1}^{M} c_k^i \mathbf{u}_k + \sum_{k=M+1}^{d} \overline{\mathbf{x}}_k$$

Selecting the approximation dimension *M*?

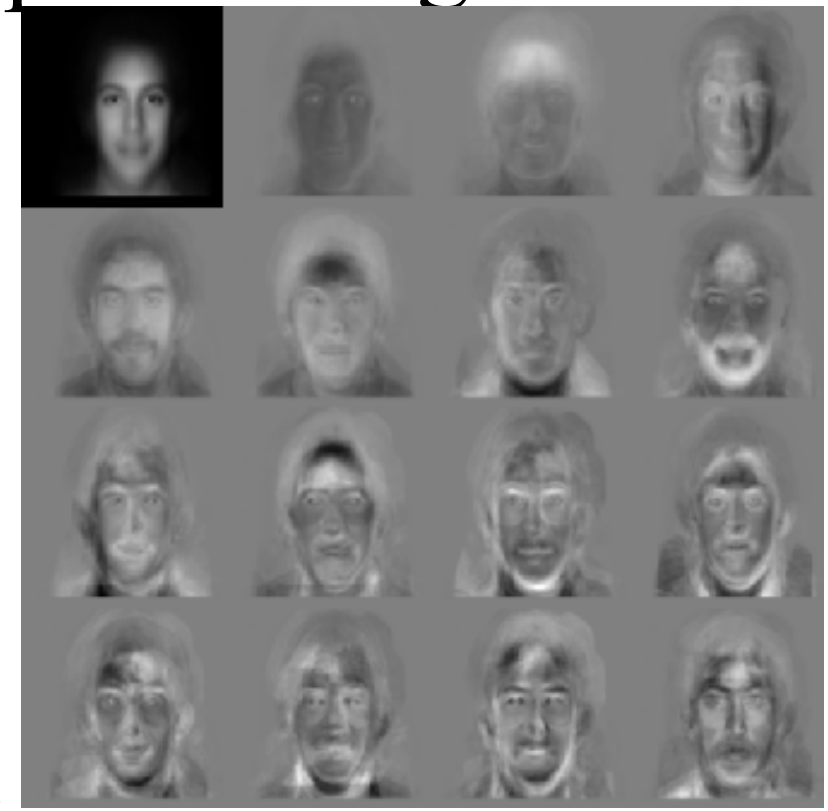
- The proportion of variance in the data captured when we truncate at a given *M* is

$$\text{Proportion of variance captured} = \frac{\sum_{i=1}^{M} \lambda_i}{\sum_{i=1}^{d} \lambda_i}$$

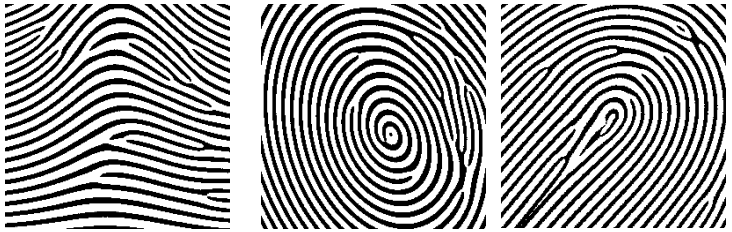
- Two strategies:
  - 1st: Specify the desired threshold e.g. 99%
  - 2nd: Look at the magnitudes of $\lambda_i / \lambda_{i+1}$
    - In some problems it will exhibit a sharp value at some value of *i*
    - *"Intrinsic dimension"* of the problem

Application: Face/fingerprint recognition

- 128 faces at 64x64 resolution for training
  - $d = 4096$
  - Perform PCA choosing 1st 20 modes (16 shown beside)
  - Approximate new faces using these
  - Greater than 95% accuracy claimed on a database of 7000 faces

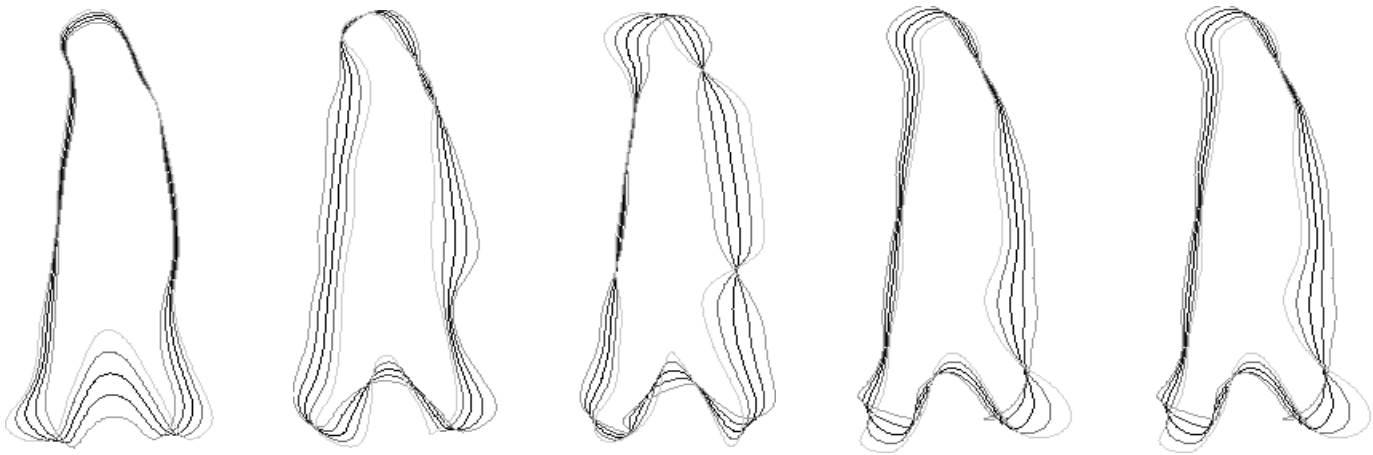


- Also used for fingerprint storage and recognition
- If interested check http://c3iwww.epfl.ch/projects_activities/jmv/fingerprint_identification.html



Pedestrian shapes from PCA modes

- Problem: track moving pedestrians from a moving camera.
- Solution: generate PCA modes (“eigenvectors”) from Pedestrian shapes
- Track pedestrian shapes in new images by searching for variations in PCA modes



Movie

- From Philomin et al 2000

Summary

Principal Components Analysis (PCA) exploits the redundancy in multivariate data. Allows one to:

- Determine (relationships) in the variables
- Reduce the dimensionality of the data set without a significant loss of information

Parameter Estimation
MLE and MAP

Problem Introduction

- Model characterized by values of a parameter vector θ
- Have several observations of a process that we think follows this model
- Using this observation set as "training data" we want to find the most probable values of the parameters
- Observations have errors and are assumed to follow a probability distribution
- **Two Approaches:**
  - ***Maximum Likelihood Estimation (MLE)***
    - ***Expectation Maximization Algorithm***
  - ***Maximum A Priori Estimation (MAP)***
    - ***"Bayesian approach"***
- Talk will only touch on a vast field, but hopefully will make you familiar with the jargon.

Notation

- parameter vector being estimated θ
- **a** test value to be compared
- *E.g., if* $N(\mu, \sigma)$ 1-D normal distribution

$$N(\mu,\sigma) = \frac{1}{\sqrt{2\pi\sigma}} \exp\left(-\frac{1}{2}\left(\frac{x-\mu}{\sigma} \right)^2 \right)$$

- Parameters to be estimated μ, σ
- d dimensional data with mean $\boldsymbol{\mu}$ and covariance matrix $\boldsymbol{\Sigma}$

$$N(\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{\sqrt{(2\pi)^d \, |\boldsymbol{\Sigma}|}} \exp\left(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})' \boldsymbol{\Sigma}^{-1} (\mathbf{x}-\boldsymbol{\mu}) \right)$$

- Parameters to be estimated $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$
- Data set on which the estimation is based $\mathcal{D}$

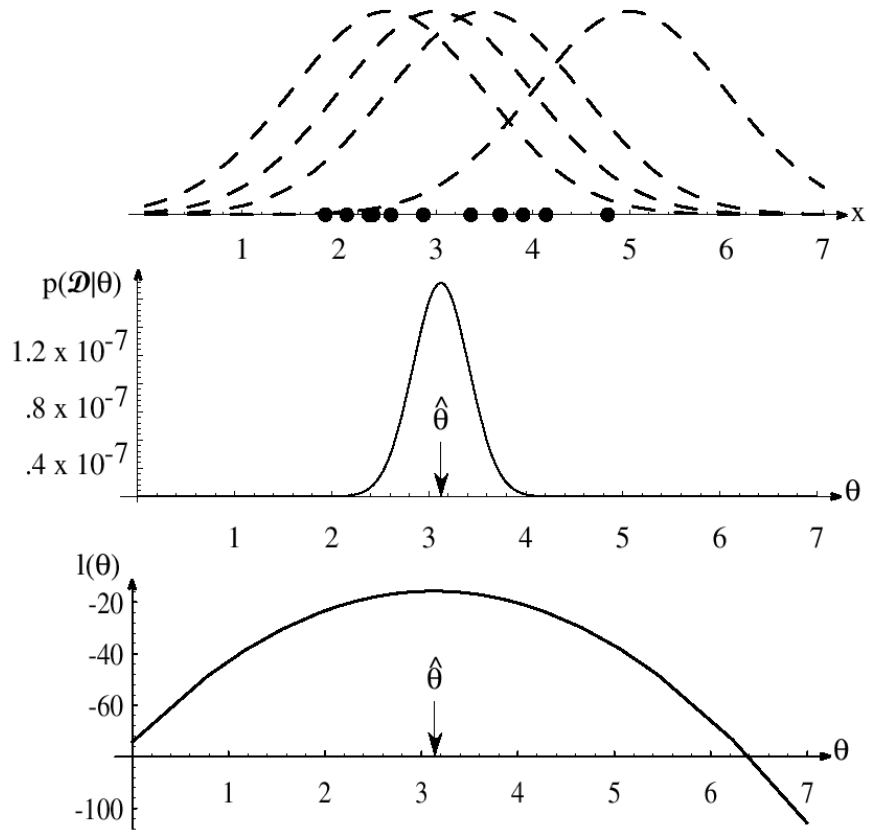
Maximum Likelihood Estimation

- Use a set of N data points $\mathbf{x}^i$ belonging to a training set $\mathcal{D}$, and assumed to be drawn independently from the probability density $p(\mathbf{x}|\boldsymbol{\theta})$ to estimate $\boldsymbol{\theta}$
- Because observations are independent $$p(\mathcal{D}|\boldsymbol{\theta}) = \prod_{i=1}^{N} p(\mathbf{x}_i|\boldsymbol{\theta})$$
- Likelihood of $\boldsymbol{\theta}$ with respect to the samples in $\mathcal{D}$, is $p(\mathcal{D}|\boldsymbol{\theta})$
  - probability that the set of observations in the dataset would have occurred, given the parameters $\boldsymbol{\theta}$
- Maximum likelihood estimate, $\hat{\boldsymbol{\theta}}$ is the value of $\boldsymbol{\theta}$ that maximizes this probability.
- Estimation problem: treat $p(\mathcal{D}|\boldsymbol{\theta})$ as a function of $\boldsymbol{\theta}$ and find value that maximizes it.

Log Likelihood Function

- Probabilities are positive.
- Logarithm is a monotonic increasing function
- So, maxima of the likelihood function will occur at the same values as its logarithm
- Easier to work with
  - Converts products to sums
  - Shrinks big numbers and small numbers to *O(1)*
  - Easier to differentiate resulting cost function
- Denoted $l(\theta)$

$$l(\theta) = \ln p(\mathcal{D}\,|\,\theta) = \sum_{k=1}^{N} \ln p(x_k\,|\,\theta)$$



$$\hat{\theta} = \arg\max_{\theta} l(\theta)$$

$$\nabla_\theta \ln p(\mathcal{D}\,|\,\theta) = \sum_{k=1}^{N} \nabla_\theta \ln p(x_k\,|\,\theta) = 0$$

Estimate can be a local minimum or a global minimum

Maximum Likelihood Estimation

- Summary
  - Given a dataset whose elements are assumed to be distributed according to a probability distribution $p(\mathbf{x}|\theta)$
  - Create the likelihood function for the data set that shows the probability that the data set could have come out of the assumed probability distribution with given parameters θ.
  - If observations in the dataset are independent the likelihood function is $p(\mathcal{D}|\theta) = \prod_{i=1}^{N} p(\mathbf{x}_i|\theta)$
  - Using the log of the likelihood function is often more convenient.
  - Parameter estimated by maximizing the likelihood or the log with respect to θ

Expectation Maximization

- Algorithm for approximate maximum likelihood parameter estimation when features are missing
- Situation:
  - Given a set of N data points $\mathbf{x}^i$ belonging to a training set Δ
  - Data is d dimensional
  - Some of the data points is missing features, or has poorly measurec values
  - Good data point $\mathbf{x}_g = \{x_1, x_2, \ldots, x_N\}$
  - Bad data point $\mathbf{x}_b = \{x_1, x_2, \ldots, x_k, \ldots, x_N\}$
- Separate features into a good set $\mathcal{D}_\mathrm{g}$ and a bad set $\mathcal{D}_\mathrm{b}$
- Using a guess $\boldsymbol{\theta}$, fix some of the parameters, and form a likelihood function over the unknown features

$$Q\left(\theta;\theta^i\right) = \varepsilon\left[\ln p\left(D_g, D_b;\theta \mid D_g;\theta^i\right)\right]$$

Maximize Q with respect to the unfixed values.
Fix the found values
Repeat for the previously fixed values

Algorithm 1 (Expectation-Maximization)

1 **begin** **initialize** $\boldsymbol{\theta}^0, T, i = 0$
2 **do** $i \leftarrow i + 1$
3 **E step** : compute $Q(\boldsymbol{\theta};\ \boldsymbol{\theta}^i)$
5 **M step** : $\boldsymbol{\theta}^{i+1} \leftarrow \arg\max_{\theta} Q(\boldsymbol{\theta};\ \boldsymbol{\theta}^i)$
6 **until** $Q(\boldsymbol{\theta}^{i+1};\ \boldsymbol{\theta}^i) - Q(\boldsymbol{\theta}^i;\ \boldsymbol{\theta}^{i-1}) \leq T$
7 **return** $\hat{\boldsymbol{\theta}} \leftarrow \boldsymbol{\theta}^{i+1}$
8 **end**

- Sometimes we prefer to apply the EM, even when there are no missing features
- *Q* may be simpler to optimize
- Get an approx. MLE solution

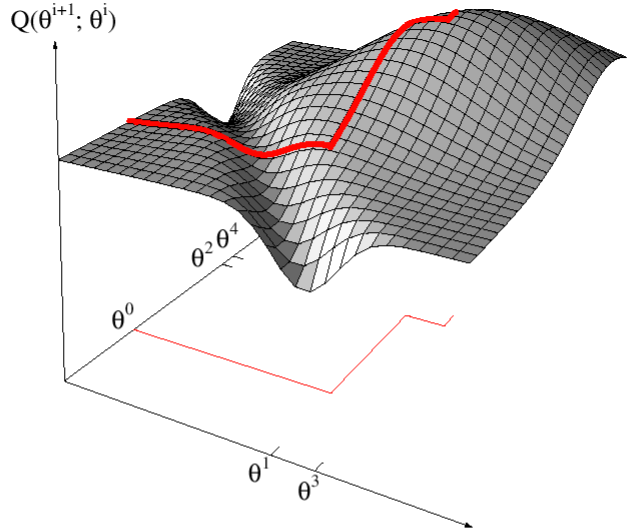


Figure 3.5: The search for the best model via the EM algorithm starts with some initial value of the model parameters, θ^0. Then, via the **M step** the optimal θ^1 is found. Next, θ^1 is held constant and the value θ^2 found which optimizes $Q(\cdot, \cdot)$. This process iterates until no value of θ can be found that will increase $Q(\cdot, \cdot)$. Note in particular that this is different from a gradient search. For example here θ^1 is the global optimum (given fixed θ^0), and would not necessarily have been found via gradient search. (In this illustration, $Q(\cdot, \cdot)$ is shown symmetric in its arguments; this need not be the case in general, however.)

Maximum A Posteriori Estimation

- In MLE the estimated value of the parameter vector $\hat{\theta}$ is not taken to be a random variable.
- This is against the philosophy of "Bayesian" methods
- Everything is random
- We have an estimate of a "prior" probability
- We make a measurement
- Based on this measurement we convert/update the prior probability to a "posterior" one.
- Thus we are given a prior probability for the parameters, $p(\theta)$
- In MAP methods instead of maximizing $l(\theta)$ we maximize $l(\theta)p(\theta)$
- In this context MLE can be viewed as finding the most likely values of θ, assuming all values are equally likely

MAP methods

- The form of the density $p(\mathbf{x}|\boldsymbol{\theta})$ is assumed to be known, but the value of the parameter vector $\boldsymbol{\theta}$ is not known exactly.
- Our initial knowledge about $\boldsymbol{\theta}$ is assumed to be contained in a known a priori density $p(\boldsymbol{\theta})$.
- The rest of our knowledge about $\boldsymbol{\theta}$ is contained in a set $\mathcal{D}$ of n samples $\mathbf{x}_1, ..., \mathbf{x}_n$ drawn independently according to the unknown probability density $p(\mathbf{x})$.

- Goal: knowing a priori estimate $p(\boldsymbol{\theta})$ compute the posterior estimate $p(\boldsymbol{\theta}|\mathcal{D})$

$$p(\mathbf{x}|\mathcal{D}) = \int p(\mathbf{x}, \boldsymbol{\theta}|\mathcal{D})\, d\boldsymbol{\theta}, \; = \int p(\mathbf{x}|\boldsymbol{\theta}) p(\boldsymbol{\theta}|\mathcal{D})\, d\boldsymbol{\theta}.$$

By Bayes' formula we have

$$p(\boldsymbol{\theta}|\mathcal{D}) = \frac{p(\mathcal{D}|\boldsymbol{\theta}) p(\boldsymbol{\theta})}{\int p(\mathcal{D}|\boldsymbol{\theta}) p(\boldsymbol{\theta})\, d\boldsymbol{\theta}},$$

and by the independence assumption

$$p(\mathcal{D}|\boldsymbol{\theta}) = \prod_{k=1}^{n} p(\mathbf{x}_k|\boldsymbol{\theta}).$$

Sources

- Christopher Bishop, “Neural Networks for Pattern Recognition”, Clarendon Press, 1995.
- R.O. Duda, Hart (and D. Stork), 1973 (new edition expected in 2000.)
  - A classic, but a bit heavy
- Numerical Recipes
  - For general discussion of MLE
- The web