Computational Statistics
Unsupervised Learning

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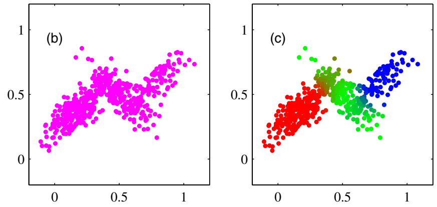
Trieste, Winter Semester 2016/2017

UNSUPERVISED LEARNING - OVERVIEW

Unsupervised learning: No labels are given to the learning algorithm (input only), leaving it on its own to find structure in its input.



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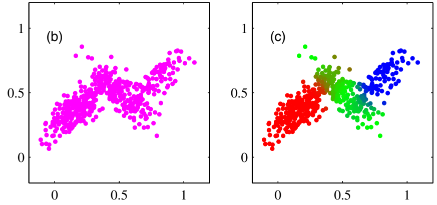


- Clustering: discover groups of similar examples within the data.
- Density estimation: determine the distribution of data within the input space.
- Dimensionality reduction: project the data from a high-dimensional space to a lower dimension space. Often down to two or three dimensions for the purpose of visualization.

Outline

Density estimation

Given input data $\mathbf{x_1}, \ldots, \mathbf{x_N}$, sampled by an unknown distribution $p(X)$, estimate p.

- One way to solve this problem is to fix a parametric family of distributions $p(X|\theta)$ and then estimate parameters θ according to ML, MAP, or with a fully Bayesian treatment. The drawback is that a bad choice of the family of distributions can result in a poor fit of data.
- Non-parametric methods try to construct an estimate from data only, avoiding the pitfalls involved in choosing the correct family of models.

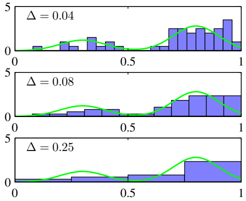
HISTOGRAM DENSITY

- (1D) Partition input space in bins (intervals) $B_1, \ldots, B_k$,s each of size Δ_i, and count how many input points n_j fall inside each bin j. Define the density $p(x)$ as p_i if $x \in B_i$, where

$$p_i = \frac{n_i}{N\Delta_i}$$

- The resulting density is discontinuous, and the quality of the fit depends on the bin size.
- Curse of dimensionality: the number of bins grows exponentially with the dimension d of $\mathbf{x}$.

An illustration of the histogram approach to density estimation, in which a data set of 50 data points is generated from the distribution shown by the green curve. Histogram density estimates, based on (2.241), with a common bin width Δ are shown for various values of Δ.



Rules for number of bins

- $k = \sqrt{N}$: simple but often used
- Scott's normal ref rule: $k = \frac{N^{1/3}}{3.5\hat{\sigma}}$
- Freedman–Diaconis' rule: $k = \frac{N^{1/3}}{2IQR}$

Data-based Estimator

- Histogram estimation at a point x uses information only from few data points close to x, those lying in the same bin. But bins are rigid and result in discontinuous densities.
- We can do better "placing a (hard/ soft) box" in each point x.
- Consider now a little box B containing point $\mathbf{x}$, with volume V, and let P be the probability that a sampled point is in B, i.e. $P = \int_B p(\mathbf{x}) d\mathbf{x}$. The probability P can be estimated as $P = K/N$, for sufficiently large K and N (law of large numbers for Binomial), where K is the number of points falling into B. Furthermore, if B is sufficiently small, we can approximate P as $p(\mathbf{x})V$. It then follows that

$$p(\mathbf{x}) = \frac{K}{NV}$$

  for $\mathbf{x} \in B$.
- We can now either fix K and estimate V from data (K-nearest-neighbour) or fix V and estimate K from data (kernel-based or Parzen estimators)

PARZEN ESTIMATOR

- Consider the function (Parzen window)

$$k(\mathbf{u}) = \begin{cases} 1, & \|\mathbf{u}\|_\infty \leq \frac{1}{2} \\ 0, & \text{otherwise} \end{cases}$$

- Then a data point $\mathbf{x}_n$ is inside the cube of edge length h centred in $\mathbf{x}$ if and only if

$$k\left(\frac{\mathbf{x} - \mathbf{x}_n}{h}\right) = 1,$$

  so that the number of data points in the cube is

$$K = \sum_n k\left(\frac{\mathbf{x} - \mathbf{x}_n}{h}\right).$$

- Then the estimate for the density p (in d dimensions) becomes:

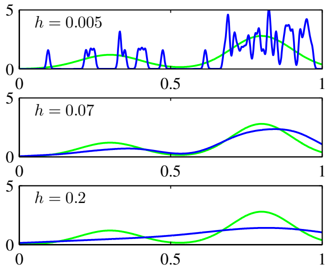
$$p(\mathbf{x}) = \frac{1}{Nh^d} \sum_n k\left(\frac{\mathbf{x} - \mathbf{x}_n}{h}\right).$$

PARZEN ESTIMATOR

- The Parzen window is still discontinuous. An alternative approach is to use a smooth function, i.e. a kernel satisfying $k(\mathbf{x}) \geq 0$ and $\int k(\mathbf{x}) d\mathbf{x} = 1$.
- a common choice is the Gaussian kernel, giving the estimate:

$$p(\mathbf{x}) = \frac{1}{N} \sum_n \frac{1}{(2\pi h^2)^{1/2}} \exp\left(\frac{\|\mathbf{x} - \mathbf{x}_n\|^2}{h^2} \right)$$

Illustration of the kernel density model (2.250) applied to the same data set used to demonstrate the histogram approach in Figure 2.24. We see that h acts as a smoothing parameter and that if it is set too small (top panel), the result is a very noisy density model, whereas if it is set too large (bottom panel), then the bimodal nature of the underlying distribution from which the data is generated (shown by the green curve) is washed out. The best density model is obtained for some intermediate value of h (middle panel).



K-NEAREST NEIGHBOUR ESTIMATOR

- It may be more convenient to have h depending on the local density of observations, to avoid over or under-smoothing.
- K-nearest neighbour solves this problem by setting the radius of the sphere/ box for Parzen estimation such that it exactly contains K points, i.e. equal to the distance of the K-th closest point to $\mathbf{x}$. Then $p(\mathbf{x})$ is estimated as $K/V(\mathbf{x})N$, where $V(\mathbf{x})$ is the volume of the sphere/box.
- K-NN can be used also for classification, by assigning to class C_k class-conditional probability in $\mathbf{x}$ equal to K_k/K, where K_k is the number of points of class K.

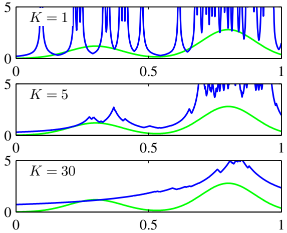


Illustration of K-nearest-neighbour density estimation using the same data set as in Figures 2.25 and 2.24. We see that the parameter K governs the degree of smoothing, so that a small value of K leads to a very noisy density model (top panel), whereas a large value (bottom panel) smoothes out the bimodal nature of the true distribution (shown by the green curve) from which the data set was generated.

Outline

CLUSTERING: AN OVERVIEW

Given input data $\mathbf{x_1}, \dots, \mathbf{x_N}$, group data into K separate groups, such that points in each group are as similar as possible and points in different groups are as different as possible.

- We need a notion of dissimilarity between input points. Different measures can produce different clusters.
- Clustering can be defined as a (hard) combinatorial optimisation problem. Clustering algorithms implement different approximate search strategies.
- Some methods require to fix a priori the number of clusters (k-means, k-medoids).
- Other methods produce a tree of possible clusters (hierarchical clustering).
- Soft clustering returns a probabilistic assignment of each point to each cluster.

DISSIMILARITY MEASURES

- There are many different ways of constructing a dissimilarity between input points, depending on the nature of the data (e.g. categorical, ordinal, numerical). The choice is usually data and application oriented.
- Typically, each input point can be seen as a vector of attributes $\mathbf{x_i} = x_{i1}, \dots, x_{in}$.
- On numerical data ($\mathbf{x} \in \mathbb{R}^n$) one usually uses a p-norm, like the (squared) Euclidean norm, or the 1-norm.
- On categorical data, one can start from a dissimilarity between single attributes and then combine it by adding the dissimilarities of single attributes in a vector of attributes, possible weighted:

$$d(\mathbf{x}, \mathbf{y}) = \sum_k w_k d(x_i, y_i)$$

- On ordinal data, one can take the distance of the (normalised) rank.

DISSIMILARITY MEASURES

- A K-clustering can be seen as a map $C : \{1, \ldots, N\} \to \{1, \ldots, K\}$, assigning each input point to a cluster.
- There are two important quantities associated with a a clustering. The within cluster distance is

$$W(C) = \frac{1}{2} \sum_{k=1}^{K} \sum_{C(i)=k} \sum_{C(j)=k} d(\mathbf{x_i}, \mathbf{x_j})$$

while the between-cluster distance is

$$B(C) = \frac{1}{2} \sum_{k=1}^{K} \sum_{C(i)=k} \sum_{C(j)\neq k} d(\mathbf{x_i}, \mathbf{x_j})$$

- It holds that $W(C) + B(C) = T = \frac{1}{2} \sum_i \sum_{j\neq i} d(\mathbf{x_i}, \mathbf{x_j})$ where T is the total distance.
- Clustering algorithms try to solve (approximatively) the NP-hard combinatorial optimisation problem:

$$\mathrm{argmax}_C B(C) = \mathrm{argmin}_C W(C)$$

HIERARCHICAL CLUSTERING

- Hierarchial clustering combines (or divide) the dataset pairwise, producing a tree of successive groupings, called dendrogram.
- The dissimilarity measure can be used to assign a length to the edges of the dendrogram.

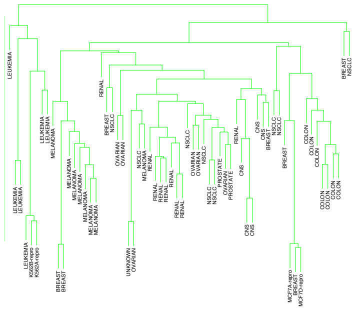


FIGURE 14.12. *Dendrogram from agglomerative hierarchical clustering with average linkage to the human tumor microarray data.*

- Agglomerative HC combines pairwise clusters (initially single data points), until they are all merged. The sequence of combinations produces the dendrogram.
- Divisive HC starts from a single cluster and splits it in two iteratively.

Agglomerative Hierarchical Clustering

- Agglomerative HC keeps a list with the current clusters, and at each step combines the two clusters G, H that are closer to each other. Different ways of measure the cluster dissimilarity give rise to different dendrograms.

- Single Linkage:

$$d_{SL}(G,H) = \min_{i\in G, j\in H} d(\mathbf{x}_i, \mathbf{x}_j)$$

- Complete Linkage:

$$d_{CL}(G,H) = \max_{i\in G, j\in H} d(\mathbf{x}_i, \mathbf{x}_j)$$

- Group Average:

$$d_{GA}(G,H) = \frac{1}{N_G N_H} \sum_{i\in G, j\in H} d(\mathbf{x}_i, \mathbf{x}_j)$$

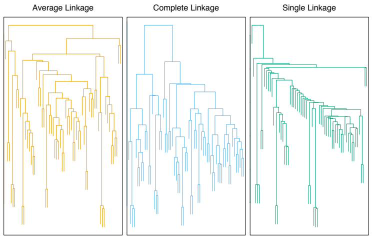


FIGURE 14.13. *Dendrograms from agglomerative hierarchical clustering of human tumor microarray data.*

k-MEANS

- The number of clusters k is fixed. The algorithm assumes numerical vectors and works with the euclidean distance.
- Each cluster is represented by its centroid $\mathbf{y}_j$. The assignment of input points $\mathbf{x}_n$ to clusters is obtained by a 1-of-k scheme (one-hot encoding), with boolean variables r_{nj} equal to one iff point $\mathbf{x}_n$ is assigned to cluster j.
- The algorithm tries to minimise the following distortion measure, related to the inter-cluster distance:

$$J = \sum_{j=1}^{k} \sum_{n=1}^{N} r_{nj} \|\mathbf{x}_n - \mathbf{y}_j\|^2$$

k-MEANS

- Minimisation of J follows a greedy strategy, and alternates between two steps:
- Minimise J w.r.t. r_{nj} holding $\mathbf{y}_j$ fixed. This is achieved by assigning each point $\mathbf{x}_n$ to the closest centroid (ties broken arbitrarily).
- Minimise J w.r.t. $\mathbf{y}_j$. The derivative in this case is

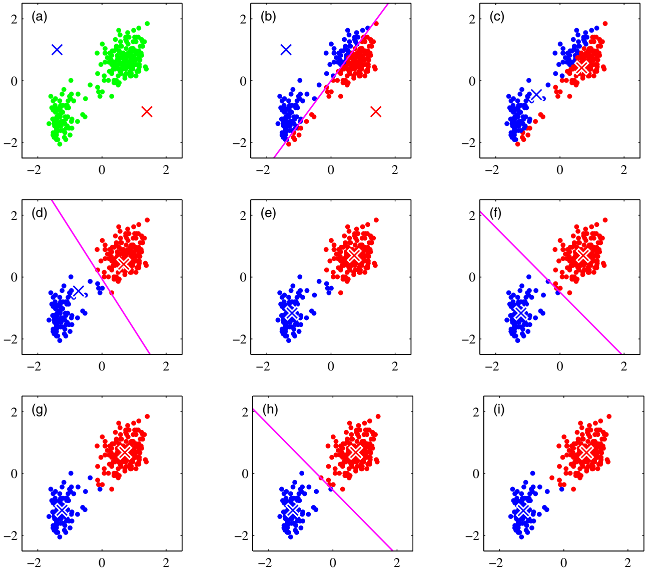
  $$2\sum_n r_{nj}(\mathbf{x}_n - \mathbf{y}_j)$$

  leading to the solution:

  $$\mathbf{y}_j = \frac{\sum_n r_{nj}\mathbf{x}_n}{\sum_n r_{nj}}$$

  i.e. each $\mathbf{y}_j$ is reassigned to the current cluster center.
- The algorithm iterates until convergence. Initially, centroids can be initialised randomly or to random data points (preferrable).

k-MEANS



k-medoids

- Works similarly to k-means, with two major differences:
- The distance between two points $\mathbf{x}$ and $\mathbf{x}'$ is given by a generic function $D(\mathbf{x}, \mathbf{x}')$.
- Centroids are restricted to be selected among data points.
- restricting centroids to datapoints makes the algorithm more robust to outliers.

MIXTURES OF GAUSSIANS

- This is a soft clustering technique: each point will have a certain probability of being assigned to any of the classes.
- It is a generative approach, assuming data is generated by a mixture of Gaussians of the form

$$p(\mathbf{x}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\mu_k, \Sigma_k)$$

- We can then learn from the input data the parameters of the mixtures, and compute the probability of assigning each point $\mathbf{x}$ to a class k.
- This learning problem is best solved by introducing latent variables $\mathbf{z}$ for the class of each point $\mathbf{x}$, and the using the Expectation-Maximisation algorithm maximise the likelihood.

MIXTURES OF GAUSSIANS

- Let us introduce latent variables $\mathbf{z} = (z_1, \ldots, z_K)$, such that z_k is one iff a point belongs to the k-th Gaussian in the mixture.
- Latent variables are not observed, but we can assume the full input would consist of pairs $(\mathbf{x}_n, \mathbf{z}_n)$.
- Then $p(\mathbf{x})$ is the marginal distribution

$$p(\mathbf{x}) = \sum_{\mathbf{z}} p(\mathbf{x}, \mathbf{z}) = \sum_{\mathbf{z}} p(\mathbf{x}|\mathbf{z}) p(\mathbf{z}),$$

where

$$p(\mathbf{z}) = \prod_k \pi_k^{z_k} \qquad \text{and} \qquad p(\mathbf{x}|\mathbf{z}) = \prod_k \mathcal{N}(\mathbf{x}|\mu_k, \Sigma_k)^{z_k}$$

- An important quantity is the responsibility $\gamma(z_k)$ (i.e. the probability of assigning $\mathbf{x}$ to class k):

$$\gamma(z_k) = p(z_k = 1|\mathbf{x}) = \frac{\pi_k \mathcal{N}(\mathbf{x}|\mu_k, \Sigma_k)}{\sum_k \pi_k \mathcal{N}(\mathbf{x}|\mu_k, \Sigma_k)}$$

Outline

LATENT VARIABLES

- Expectation-Maximisation (EP) is a general algorithm to maximise likelihood for models with observed variables $\mathbf{X} = \mathbf{x}_1, \ldots, \mathbf{x}_N$ and latent (non-observed) variables $\mathbf{Z} = \mathbf{z}_1, \ldots, \mathbf{z}_N$.
- We assume family of models parameterised by θ. The log-likelihood we have to optimise is

$$\log p(\mathbf{X}|\theta) = \log \sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z}|\theta)$$

- With some work, one can prove that the following decomposition holds (where $q(\mathbf{Z})$ is a generic distribution on $\mathbf{Z}$):

$$\log p(\mathbf{X}|\theta) = \mathcal{L}(q, \theta) + KL(q||p)$$

$$\mathcal{L}(q, \theta) = \sum_{\mathbf{Z}} q(\mathbf{Z}) \log \frac{p(\mathbf{X}, \mathbf{Z}|\theta)}{q(\mathbf{Z})}$$

$$KL(q||p) = -\sum_{\mathbf{Z}} q(\mathbf{Z}) \log \frac{p(\mathbf{Z}|\mathbf{X}, \theta)}{q(\mathbf{Z})}$$

Likelihood Decomposition

- Let's prove: $\log p(\mathbf{X}|\theta) = \mathcal{L}(q,\theta) + KL(q||p)$, with

$$\mathcal{L}(q,\theta) = \sum_{\mathbf{Z}} q(\mathbf{Z}) \log \frac{p(\mathbf{X},\mathbf{Z}|\theta)}{q(\mathbf{Z})} \quad KL(q||p) = -\sum_{\mathbf{Z}} q(\mathbf{Z}) \log \frac{p(\mathbf{Z}|\mathbf{X},\theta)}{q(\mathbf{Z})}$$

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- (Use $\log p(\mathbf{X}|\theta) = \sum_{\mathbf{Z}} q(\mathbf{Z}) \log p(\mathbf{X}|\theta)$, add and subtract to the log factor $\log p(\mathbf{Z}|\mathbf{X},\theta)$, then use $\log p(\mathbf{X}|\theta) + \log p(\mathbf{Z}|\mathbf{X},\theta) = \log p(\mathbf{X},\mathbf{Z}|\theta)$, finally add and remove $\sum_{\mathbf{Z}} q(\mathbf{Z}) \log q(\mathbf{Z})$.)

LIKELIHOOD DECOMPOSITION AND EM

- $\mathcal{L}(q, \theta)$ is a functional of q (it is a distribution on the latent variables Z) and a function of the parameters θ.
- As $KL(q||p) \geq 0$, with equality iff $q = p(\mathbf{Z}|\mathbf{X}, \theta)$, it follows that

$$\mathcal{L}(q, \theta) \leq \log p(\mathbf{X}|\theta)$$

  i.e. $\mathcal{L}(q, \theta)$ is a lower bound on the log likelihood of interest.
- Expectation-Maximisation is an optimisation algorithm which optimises the lower bound $\mathcal{L}(q, \theta)$ alternating two phases: one in which $\mathcal{L}$ is optimised w.r.t. q (E step) and one in which it is optimised w.r.t. θ (M step).
- It is guaranteed to converge to a local optimum of $\log p(\mathbf{X}|\theta)$.

EXPECTATION STEP

- In the E step, $\mathcal{L}(q, \theta)$ is optimised w.r.t. $q(\mathbf{Z})$, holding the current value θ_{old} of θ fixed.
- To find the solution, consider the decomposition $\log p(\mathbf{X}|\theta_{old}) = \mathcal{L}(q, \theta_{old}) + KL(q||p)$, and note that $\log p(\mathbf{X}|\theta_{old})$ does not depend on q, hence the value of $\mathcal{L}(q, \theta_{old})$ can never exceed $\log p(\mathbf{X}|\theta_{old})$.
- Furthermore, it attains this value when $KL(q||p) = 0$, i.e. for

$$q(\mathbf{Z}) = p(\mathbf{Z}|\mathbf{X}, \theta_{old})$$

- When observations $\mathbf{X}_n$ are i.i.d., with corresponding latent variables $\mathbf{z}_n$, then $p(\mathbf{Z}|\mathbf{X}, \theta)$ factorises w.r.t. observations:

$$p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\theta}) = \frac{p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\theta})}{\sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\theta})} = \frac{\prod_{n=1}^{N} p(\mathbf{x}_n, \mathbf{z}_n|\boldsymbol{\theta})}{\sum_{\mathbf{Z}} \prod_{n=1}^{N} p(\mathbf{x}_n, \mathbf{z}_n|\boldsymbol{\theta})} = \prod_{n=1}^{N} p(\mathbf{z}_n|\mathbf{x}_n, \boldsymbol{\theta}) \quad (9.75)$$

MAXIMISATION STEP

- In the M step, the distribution $q(\mathbf{Z})$ is held fixed, and the lower bound $\mathcal{L}(q, \theta)$ is optimised w.r.t. θ, obtaining a novel point θ_{new}.
- For the new value θ_{new}, $\mathcal{L}(q, \theta_{new})$ does not necessarily coincide with $\log p(\mathbf{X}|\theta_{new})$, i.e. the KL-divergence is generally non-zero.
- In particular, as we are optimising, this implies that both (a) the value of $\mathcal{L}(q, \theta)$ and (b) the value of $\log p(\mathbf{X}|\theta)$ are increased in the M step.
- By plugging $q(\mathbf{Z}) = p(\mathbf{Z}|\mathbf{X}, \theta_{old})$ into $\mathcal{L}(q, \theta)$, we see that we are optimising

$$\mathcal{L}(q, \boldsymbol{\theta}) = \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\theta}^{\text{old}}) \ln p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\theta}) - \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\theta}^{\text{old}}) \ln p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\theta}^{\text{old}})$$

which can be rewritten as

$$\mathcal{L}(q, \theta) = \mathbb{E}_{\mathbf{Z}|\mathbf{X}, \theta_{old}}[\log p(\mathbf{X}, \mathbf{Z}|\theta)] + H(\mathbf{Z}|\mathbf{X}, \theta_{old})$$

EM VISUALLY

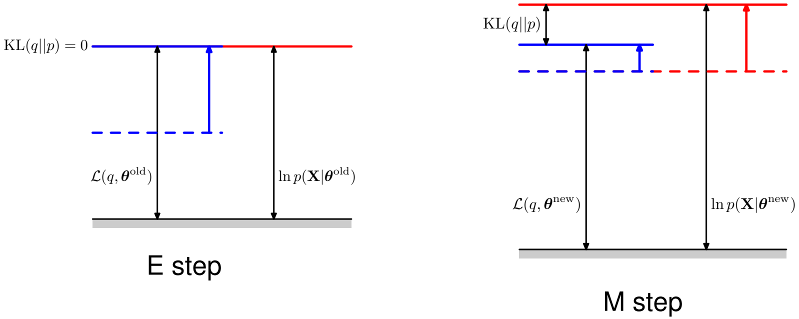
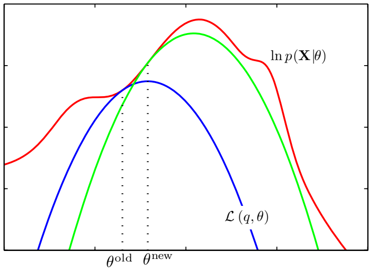

$\mathrm{KL}(q||p) = 0$
$\mathcal{L}(q, \boldsymbol{\theta}^{\text{old}})$
$\ln p(\mathbf{X}|\boldsymbol{\theta}^{\text{old}})$
E step
$\mathrm{KL}(q||p)$
$\mathcal{L}(q, \boldsymbol{\theta}^{\text{new}})$
$\ln p(\mathbf{X}|\boldsymbol{\theta}^{\text{new}})$
M step

Figure 9.14 The EM algorithm involves alternately computing a lower bound on the log likelihood for the current parameter values and then maximizing this bound to obtain the new parameter values. See the text for a full discussion.



EM: miscellanea

- In the EM algorithm, both the E and the M steps increase the lower bound, and a complete cycle increases the full log-likelihood. Hence, the algorithm will eventually converge to a (local) maximum of the full log-likelihood.
- A similar approach can be used to maximise the log-posterior distribution $\log p(\theta|\mathbf{X}) = \log p(\theta, \mathbf{X}) - \log p(\mathbf{X})$:

$$\begin{aligned} \ln p(\boldsymbol{\theta}|\mathbf{X}) &= \mathcal{L}(q, \boldsymbol{\theta}) + \mathrm{KL}(q\|p) + \ln p(\boldsymbol{\theta}) - \ln p(\mathbf{X}) \\ &\geqslant \mathcal{L}(q, \boldsymbol{\theta}) + \ln p(\boldsymbol{\theta}) - \ln p(\mathbf{X}). \end{aligned} \tag{9.77}$$

  Here the E step is the same ($\log p(\theta)$) does not depend on q, while the M step is required to maximise $\mathcal{L}(q, \theta) + \log p(\theta)$.
- There are several Generalised EM (GEM) algorithms that try to overcome a hard E or M step. E.g. the M step can be replaced by some steps increasing $\mathcal{L}(q, \theta)$ without reaching an optimum.

EM FOR THE MIXTURE OF GAUSSIANS

- Remember that for a mixture of K gaussians, we have

$$p(\mathbf{Z}) = \prod_n \pi_k^{z_{nk}}$$

and

$$p(\mathbf{X}|\mathbf{Z}) = \prod_n \prod_k \mathcal{N}(\mathbf{x}_n|\mu_k, \Sigma_k)^{z_{nk}}$$

hence the log-likelihood of the joint distribution is

$$\ln p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\pi}) = \sum_{n=1}^{N} \sum_{k=1}^{K} z_{nk} \left\{ \ln \pi_k + \ln \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \right\}. \tag{9.36}$$

EM FOR THE MIXTURE OF GAUSSIANS

- In the E step, we need to compute $p(\mathbf{Z}|\mathbf{X}, \mu\Sigma, \pi)$, which is given by

$$p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\pi}) \propto \prod_{n=1}^{N} \prod_{k=1}^{K} \left[\pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)\right]^{z_{nk}} . \qquad (9.38)$$

where the expectations of the z_{nk} are

$$\begin{aligned} \mathbb{E}[z_{nk}] &= \frac{\sum_{z_{nk}} z_{nk} \left[\pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)\right]^{z_{nk}}}{\sum_{z_{nj}} \left[\pi_j \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)\right]^{z_{nj}}} \\ &= \frac{\pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)} = \gamma(z_{nk}) \qquad (9.39) \end{aligned}$$

EM FOR THE MIXTURE OF GAUSSIANS

- In the M step, we first compute the expectation w.r.t. $p(\mathbf{Z}|\mathbf{X}, \mu, \Sigma, \pi)$, of the complete data log-likelihood

$$\mathbb{E}_{\mathbf{Z}}[\ln p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\pi})] = \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma(z_{nk}) \left\{ \ln \pi_k + \ln \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \right\}. \qquad (9.40)$$

- Then we maximise this expression w.r.t. the parameters (with $N_k = \sum_n \gamma(z_{nk})$), obtaining

$$\boldsymbol{\mu}_k^{\text{new}} = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk}) \mathbf{x}_n \qquad (9.24)$$

$$\boldsymbol{\Sigma}_k^{\text{new}} = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk}) \left(\mathbf{x}_n - \boldsymbol{\mu}_k^{\text{new}} \right) \left(\mathbf{x}_n - \boldsymbol{\mu}_k^{\text{new}} \right)^{\mathrm{T}} \qquad (9.25)$$

$$\pi_k^{\text{new}} = \frac{N_k}{N} \qquad (9.26)$$

EM FOR THE MIXTURE OF GAUSSIANS

- The algorithm is initialised by choosing μ_k, Σ_k, π_k. Typically, one runs a k-means clustering, and initialised the parameters as the result of the clustering:
  ⋄ μ_k, Σ_k: sample mean and variances in cluster k;
  ⋄ π_k: fraction of data points in cluster k.
- Each loop the EM algorithm thus compute the responsibilities and the new mean, variance and mixture probabilities.
- Computation is iterated until convergence is met, i.e. the change in parameters, or in the log-likelihood

$$\ln p(\mathbf{X}|\boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\pi}) = \sum_{n=1}^{N} \ln \left\{ \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \right\} \tag{9.28}$$

becomes smaller than a prescribed error.

MIXTURE OF GAUSSIANS AND *k*-MEANS

- *k*-means and mixtures of Gaussians are related: the latter is a soft version of *k*-means: each data point is assigned to each cluster with a given probability.
- Suppose we run EM on a gaussian mixture, by fixing the covariance to be equal to ϵI, where ϵ is held fixed. The responsibilities are now estimated as

$$\gamma(z_{nk}) = \frac{\pi_k \exp\left\{-\|\mathbf{x}_n - \boldsymbol{\mu}_k\|^2/2\epsilon\right\}}{\sum_j \pi_j \exp\left\{-\|\mathbf{x}_n - \boldsymbol{\mu}_j\|^2/2\epsilon\right\}}. \quad (9.42)$$

- In the limit $\epsilon \to 0$, this converges to 1 for the component minimising $\|\mathbf{x}_n - \mu_k\|$ (as in *k*-means). Means also converge to the same expression for *k*-means. Furthermore, the data log-likelihood in this limit is

$$\mathbb{E}_{\mathbf{Z}}[\ln p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\pi})] \to -\frac{1}{2}\sum_{n=1}^{N}\sum_{k=1}^{K} r_{nk}\|\mathbf{x}_n - \boldsymbol{\mu}_k\|^2 + \text{const.} \quad (9.43)$$

  i.e. EM and *k*-means minimise the same score function.

Outline

Principal Component Analysis

- PCA is a widely used method for dimensionality reduction, feature extraction, lossy compression, and visualisation.
- The starting point is a dataset $\mathbf{X}$ of d-dimensional input data $\mathbf{x}_1, \ldots, \mathbf{x}_N$.
- It is a linear projection technique. The idea is to project a d-dimensional dataset into an m-dimensional one, $m < d$, such that either (a) the total sum of square error is minimised or (b) the variance of the projected data is maximised.
- Both methods lead to the same result.
- The so obtained linear subspace is known as principal subspace, and its axes as principal components.
- There exist a probabilistic formulation of PCA, which assumes a linear Gaussian generative model for the data and learns its parameters by maximum likelihood, possibly exploiting an EM algorithm.

PCA: MAXIMUM VARIANCE FORMULATION

- Consider a dataset $\mathbf{X}$, and assume $\mathbf{u}_1, \dots, \mathbf{u}_m$ is an orthonormal basis of the m-dimensional space we are looking for. Arrange them column-wise in a matrix U.
- The projection of a point $\mathbf{x}_n$ in the subspace spanned by U is given by $U^T \mathbf{x}_j$.
- The mean of the projected data is thus $U^T \bar{\mathbf{x}}$, where $\bar{\mathbf{x}} = \frac{1}{N} \sum_n \mathbf{x}_n$.
- The variance of the projected data instead is

$$\frac{1}{N} \sum_n [U^T \mathbf{x}_n - U^T \bar{\mathbf{x}}][U^T \mathbf{x}_n - U^T \bar{\mathbf{x}}]^T = U^T S U$$

  where

$$S = \frac{1}{N} \sum_n (\mathbf{x}_n - \bar{\mathbf{x}})(\mathbf{x}_n - \bar{\mathbf{x}})^T$$

  is the data-covariance matrix

PCA: MAXIMUM VARIANCE FORMULATION

- Consider the case $m = 1$, for simplicity. We maximise the variance, subject to the constraint that $\mathbf{u}_1$ is normalised (otherwise the optimal solution is to take it to infinity). For this we introduce a Langrange multiplier λ_1, and maximise the Lagrangian:

$$\mathbf{u}_1^T S \mathbf{u}_1 + \lambda_1(1 - \mathbf{u}_1^T \mathbf{u}_1)$$

- Deriving w.r.t. $\mathbf{u}_1$ and setting to zero we get

$$S\mathbf{u}_1 = \lambda_1 \mathbf{u}_1$$

hence λ_1 is an eigenvalue of S and $\mathbf{u}_1$ an eigenvector.

- Multiplying both sides for $\mathbf{u}_1^T$ and using $\mathbf{u}_1^T \mathbf{u}_1 = 1$, we get

$$\mathbf{u}_1^T S \mathbf{u}_1 = \lambda_1$$

which shows that the variance is maximised by taking the eigenvector of the largest eigenvalue of S.

PCA: Maximum Variance Formulation

- In the general case of $m > 1$, one can inductively show that the optimal choice is to the the eigenvectors $\mathbf{u}_1, \dots, \mathbf{u}_m$ associated to the largest m eigenvalues $\lambda_1, \dots, \lambda_m$.
- The cost of finding all eigenvalues/ eigenvectors of S is $O(d^3)$ (plus the cost of computing S, which is $O(Nd^2)$. If we are only interested in m eigenvectors, we can use specialised algorithms that cost $O(md^2)$.

PCA: minimum-error formulation

- Here we take a complementary approach to variance maximisation. We fix an orthonormal basis $\mathbf{u}_j$, and express the data points in this new basis, as

$$\mathbf{x}_n = \sum_j (\mathbf{x}_n^T \mathbf{u}_j) \mathbf{u}_j$$

- The goal is to best approximate these points using only m dimensions, i.e. with points of the form

$$\tilde{\mathbf{x}}_n = \sum_{j=1}^{m} z_{nj} \mathbf{u}_j + \sum_{j=m+1}^{d} b_j \mathbf{u}_j$$

  where $z_{nj} = \mathbf{x}_n^T \mathbf{u}_j$ and $b_j = \bar{\mathbf{x}}^T \mathbf{u}_j$.

PCA: MINIMUM-ERROR FORMULATION

- By taking the mean sum of square error,

$$J = \frac{1}{N} \sum_{n} \|\mathbf{x}_n - \tilde{\mathbf{x}}_n\|^2$$

and inserting the expression for $\tilde{\mathbf{x}}_n$, we get

$$J = \sum_{j=m+1}^{d} \mathbf{u}_j^T S \mathbf{u}_j$$

- From this expression, using lagrange multipliers like for the max variance case, we see immediately that the minimum is obtained by taking the *m* principal components as the eigenvectors of the *m* largest eigenvalues, so that *J* is the sum of the $d - m$ smallest eigenvalues.

PCA APPLICATIONS

- Dimensionality reduction: run PCA for the m largest eigenvalues explaining α% of the data variance.
- Data compression: reduce coordinates of points by PCA and reconstruct them by using $\tilde{\mathbf{x}}_n = \sum_{j=1}^{m} z_{nj}\mathbf{u}_j + \sum_{j=m+1}^{d} b_j\mathbf{u}_j$. Example: handwritten digits

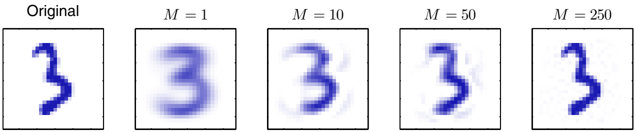


Figure 12.5 An original example from the off-line digits data set together with its PCA reconstructions obtained by retaining M principal components for various values of M. As M increases the reconstruction becomes more accurate and would become perfect when $M = D = 28 \times 28 = 784$.

PCA applications

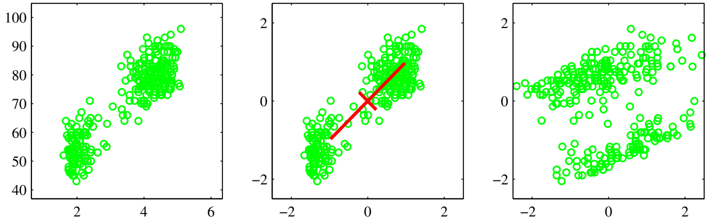
- A third common application is data renormalisation, a technique usually known as withening or sphering.
- The idea is to do a PCA with $m = d$, in order to make the data have zero mean and unit covariance.
- Consider the full eigenvalue equation $SU = UL$, where L is the diagonal matrix with eigenvalues. After solving it, we renormalise data as

$$\mathbf{y}_n = L^{-1/2} U^T (\mathbf{x}_n - \bar{\mathbf{x}})$$

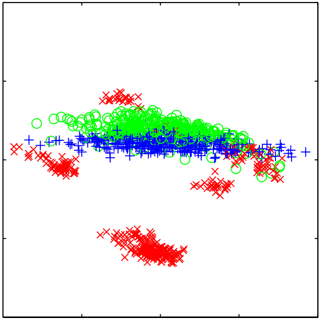
- These new points have unit covariance:

$$\begin{aligned}\frac{1}{N}\sum_{n=1}^{N}\mathbf{y}_n\mathbf{y}_n^{\mathrm{T}} &= \frac{1}{N}\sum_{n=1}^{N}\mathbf{L}^{-1/2}\mathbf{U}^{\mathrm{T}}(\mathbf{x}_n-\overline{\mathbf{x}})(\mathbf{x}_n-\overline{\mathbf{x}})^{\mathrm{T}}\mathbf{U}\mathbf{L}^{-1/2} \\ &= \mathbf{L}^{-1/2}\mathbf{U}^{\mathrm{T}}\mathbf{S}\mathbf{U}\mathbf{L}^{-1/2} = \mathbf{L}^{-1/2}\mathbf{L}\mathbf{L}^{-1/2} = \mathbf{I}. \qquad (12.25)\end{aligned}$$

PCA APPLICATIONS



- An example of withering above.
- Finally, PCA can be used for data visualisation, by projecting data on a 2D space.



PCA in high dimensions

- By defining the matrix X with rows $(\mathbf{x}_n - \bar{\mathbf{x}})^T$, we have that $S = N^{-1}X^TX$, hence the eigenvector equation is $N^{-1}X^TX\mathbf{u}_i = \lambda_i\mathbf{u}_i$.
- By multiplying both sides by X, and calling $X\mathbf{u}_i = \mathbf{v}_i$, we have that the equation $N^{-1}XX^T\mathbf{v}_i = \lambda_i\mathbf{v}_i$ holds for the same eigenvalues.
- We can solve it for $\mathbf{v}_i$ and obtain $\mathbf{u}_i$ back by setting

$$\mathbf{u}_i = \frac{1}{(N\lambda_i)^{1/2}}X^T\mathbf{v}_i$$

- The matrix XX^T is $N \times N$, while X^TX is $d \times d$, hence if $N << d$, this second formulation is more convenient (notice: X^TX will have at most $N - 1$ non null eigenvalues).

PROBABILISTIC PCA

- Probabilistic PCA rephrases PCA in a probabilistic framework by defining a generative model for the data. Assume $\mathbf{z}$ is a vector in $\mathbb{R}^m$, with distribution $\mathcal{N}(\mathbf{z}|\mathbf{0}, I)$. The generative model for $\mathbf{x}$ is

$$\mathbf{x} = W\mathbf{z} + \mu + \epsilon$$

  with $\epsilon = \mathcal{N}(0, \sigma^2 I)$.

- Hence Probabilstic PCA learns a map (i.e. W, μ, σ^2) from the low dimensional space to the high dimensional one, by maximum likelihood.
- Solution is $\mu = \bar{\mathbf{x}}$, $W = U(L - \sigma^2 I)^{1/2} R$, $\sigma^2 = 1/(d-m) \sum_{j=m+1}^{d} \lambda_j$; where U is the matrix with columns given by the m largest eigenvectors of S, L is the diagonal matrix with the m largest eigenvalues, and R is an arbitrary rotation matrix.
- The projection of a point $\mathbf{x}$ is given by $\mathbb{E}[\mathbf{z}|\mathbf{x}] = MW^T(\mathbf{x} - \bar{\mathbf{x}})$, with $M = W^T W + \sigma^2 I$ ($\mathbf{z}$ is pushed closer to $\mathbf{0}$ than with PCA).
- For $\sigma^2 \to 0$, we obtain back the classic PCA solution.

Other dimensionality reduction methods

- There are many dimensionality reduction techniques, that try to circumvent the limitations of PCA, mainly the linearity of the manifold we project into.
- We list a few here: kernel PCA, using a dual formulation in terms of kernels, principal curves and surfaces, working with non-linear manifolds, autoassociative neural networks, for which the projection is expressed as a NN, Indipendent component analysis, which uses a probabilistic formulation with a non-gaussian, but factorised distribution over the reduced variables $\mathbf{z}$.