Summary Pattern Analysis
Sommersemester 2017

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Density Estimation

The task of density estimation is to obtain a continous representation of the underlying pdf from a set of discrete samples (massumants). Note: that if we have the pdf we can do statistical analysis.

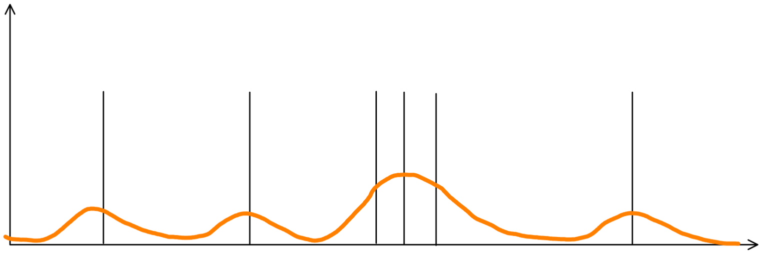


Figure 1: A PDF describing the distribution of measurements

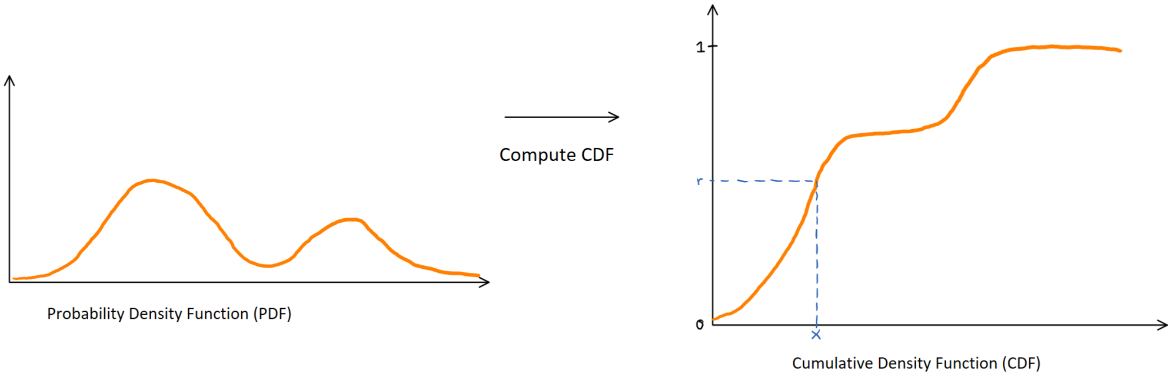
Let $p(\vec{x})$ denote a probability density function pdf then:

1. $p(\vec{x}) \geq 0$
2. $\int_{-\infty}^{\infty} p(\vec{x})\, d\vec{x} = 1$
3. $p(\vec{a} \leq \vec{x} \leq \vec{b}) = \int_{\vec{a}}^{\vec{b}} p(\vec{x})\, d\vec{x}$

Parametric density estimation (mostly Pattern Recognition)
Make an assumption about the underlying distribution (e.g. Gausian, GMM) and determine the best fitting distribution parameters from the data. (ML estimation, MAP estimation)

Non-parametric density estimation We make no assumption of the underlying Model. (Example Parzen-Rosenblatt estimator)

Sampling from a pdf Sampling provides a princeple way of generating new / more data that behaves / looks similary to the observations.


Probability Density Function (PDF)
Compute CDF
1
r
0
Cumulative Density Function (CDF)

Compute through discretisation of the pdf $cdf[i] = cdf[i-1] + pdf[i]$. Then draw a uniformly distributed number (r) between 0 and 1. The sampled value is x where $cdf[x] = r$.

Parzen-Window estimator

Idea: Quantify the number of samples with a appropriate kernel/window function. In other words we interpolate the pdf from the observations in the neighbourhood of a position $\vec{x}$.

Derivation: We can express p_R, the probability that $\vec{x}$ lies within a region R, in terms of the volume V_R of this region[1], when $p(\vec{x})$ is approximately constant in R.

$$p_R = \int_R p(\vec{x})\,d\vec{x} \;\approx\; p(\vec{x})\int_R d\vec{x} = p(\vec{x})V_R$$

We determine $p_R = \frac{k_R}{N}$ the probability of making observations in region R (also "relative frequency") by counting the samples in R ($= k_R$) and dividing by the total number of samples.

$$p(\vec{x}) = \frac{p_R}{V_R} = \frac{k_R}{V_R N}$$

Let's write the parzen window estimator as a function of a kernel $k(\vec{x};\vec{x_i})$. If R is a d-dimensional hypercube with side length h, then its volume is h^d.

$$\boxed{p(\vec{x}) = \frac{1}{h^d N}\sum_{i=1}^{N} k(\vec{x};\vec{x_i})}$$

where we can choose a suitable kernel function $k(\vec{x};\vec{x_i})$. E.g. binary decision[2] or a (multivariate) gaussian kernel[3]:

$$k(\vec{x};\vec{x_i}) = \begin{cases} 1 & \text{when } \frac{|x_{i,k} - x_k|}{h} \leq \frac{1}{2} \\ 0 & \text{otherwise} \end{cases} \qquad\qquad k(\vec{x};\vec{x_i}) = \frac{1}{(2\pi)^d|\Sigma|} e^{-(\vec{x}-\vec{x_i})^T\Sigma^{-1}(\vec{x}-\vec{x_i})}$$

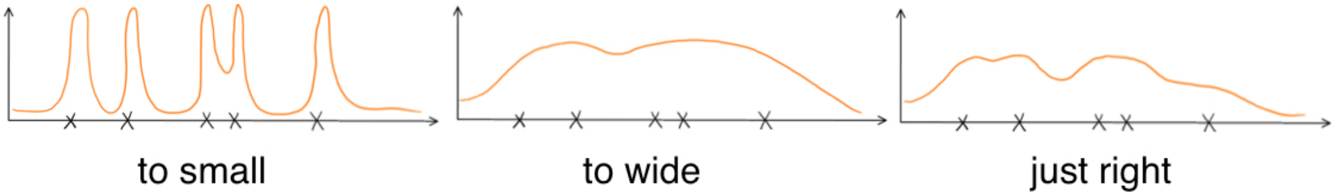


Figure 2: Effects of the window / kernel size

How can we determine a good window / kernel size $\hat{h}$?
Let's do ML est. with a cross-validation (cv) e.g. leave-one-sample-out cv. Estimate the pdf from all samples except $\vec{x_j}$, which will be used to evaluate the quality of the pdf using window size h.

$$p^j_{h,N-1}(\vec{x}) = \frac{1}{h^d N}\sum_{i=1(i\neq j)}^{N} k(\vec{x};\vec{x_i})$$

$$\hat{h} = \arg\max_h L(h) = \arg\max_h \prod_{j=1}^{N} p^j_{h,N-1}(\vec{x_j}) = \arg\max_h \sum_{j=1}^{N} \log p^j_{h,N-1}(\vec{x_j})$$

The position of the maximum does not change (when using log-likelihood), because the logarithm is a strictly monotonic function.

[1] $\int_R d\vec{x}$ is just the volume of R, we also write V_R for the volume
[2] $\vec{x_i}$ and $\vec{x}$ are not father apart then $0.5h$ in any dimension k
[3] Omit h^d if the kernel is gaussian

Clustering [4]

Grouping or segmenting a samples into clusters, such that those within each cluster are more closely related to one another[5]. All clustering methods depend on the distance metric (dissimilarity measure) used (e.g. squared distance $d(\vec{x_i}, \vec{x_j}) = ||\vec{x_i} - \vec{x_j}||^2$). Specifying an appropriate dissimilarity measure is far more important in obtaining success with clustering than choice of clustering algorithm.

Types of Clustering Algorithms

- **Mode seeking(”bump hunting”):** takes a nonparametric perspective, attempting to directly estimate distinct modes of the pdf. Observations ”closest” to each respective mode then define the individual clusters (Mean Shift).
- **Combinatorial:** work directly on the observed data with no direct reference to an unterlying probability model (k-means and flavors).
- **Mixture modeling:** assumes an underlying distribution, usually Gaussians. The pdf describing the data is characterized by a mixture of parameterized distributions (Gaussians). Each component density describes one of the clusters (Dirichlet process, GMM, CRP).

[4] For clustering see section 14 of “The Elements of Statistical Learning” (Hastie, Tibshirani, Friedman - 2009). Section 14.3 “Cluster Analysis” introduces different flavours of k-means.

[5] Sometimes the goal also is to arrange the clusters into a natural hierarchy.

Mean Shift Algorithm

Idea: Find maxima in pdf without actually performing a full density estimation [6]. Maxima can be found, where the gradient of the pdf is zero.

Assume that we have a full density estimation

$$p(\vec{x}) = \frac{1}{N}\sum_{i=1}^{N} k_h(\vec{x};\vec{x_i})$$

denotes the multivariate kernel density estimation, where we assume k_h to be a radially symmetric kernel, i.e. $k(\vec{x};\vec{x_i}) = k_h(||\vec{x_i}-\vec{x}||^2)$. A local maximum of the pdf can be assumed where the gradient vanishes

$$\nabla p(\vec{x}) = \frac{1}{N}\sum_{i=1}^{N} \nabla k(\vec{x};\vec{x_i}) \doteq \vec{0}$$

$$\nabla p(\vec{x}) = \frac{1}{N}\sum_{i=1}^{N} k_h'(||\vec{x_i}-\vec{x}||^2)\cdot(-2(\vec{x_i}-\vec{x})) \doteq \vec{0}$$

All constants can be dropped, then we multiply the kernel with it's derivative

$$\sum_{i=1}^{N} k_h'(||\vec{x_i}-\vec{x}||^2)\vec{x_i} - \sum_{i=1}^{N} k_h'(||\vec{x_i}-\vec{x}||^2)\vec{x} \doteq \vec{0}$$

Then we get the mean shift vector

$$\boxed{\Rightarrow m(\vec{x}) = \frac{\sum_{i=1}^{N} k_h'(||\vec{x_i}-\vec{x}||^2)\vec{x_i}}{\sum_{i=1}^{N} k_h'(||\vec{x_i}-\vec{x}||^2)} - \vec{x} \doteq \vec{0}}$$

To perform a gradient ascent, compute the gradient, walk one step, re-compute the gradient, walk a step, ...

Mean Shift Algorithm

1. Compute the mean shift vector $m(\vec{x}^{(t)})$
2. Update $\vec{x}$: $\vec{x}^{(t+1)} = \vec{x}^{(t)} + m(\vec{x}^{(t)}) = \vec{x}^{(t)} + \frac{\sum_{i=1}^{N} k_h'(||\vec{x_i}-\vec{x}||^2)\vec{x_i}}{\sum_{i=1}^{N} k_h'(||\vec{x_i}-\vec{x}||^2)} - \vec{x}^{(t)} = \frac{\sum_{i=1}^{N} k_h'(||\vec{x_i}-\vec{x}||^2)\vec{x_i}}{\sum_{i=1}^{N} k_h'(||\vec{x_i}-\vec{x}||^2)}$

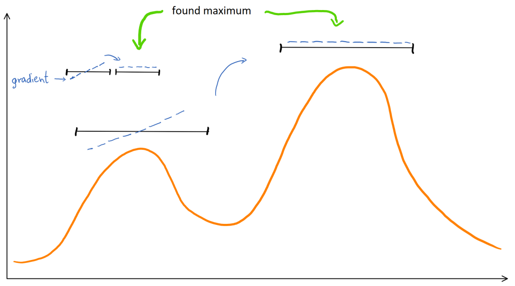


Figure 3: The kernel size h indirectly controls the number of indentified maxima

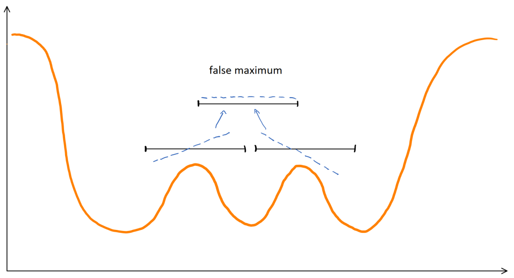


Figure 4: One of the issues is, the case when a zero gradient is just between two finer maxima

[6] This applies only in some cases, e.g. quickly finding clusters through particle tracing or with a downsampled PDF

Epanechnikov kernel If we use the Epanechnikov kernel as k_h, then the computation breaks down to the mean of the samples in a circular (hyper-spherical) around $\vec{x}^{(t)}$

$$k_E(\vec{x}) = \begin{cases} c \cdot (1 - \vec{x}^T\vec{x}) & \text{when } \vec{x}^T\vec{x} \leq 1 \\ 0 & \text{otherwise} \end{cases}$$

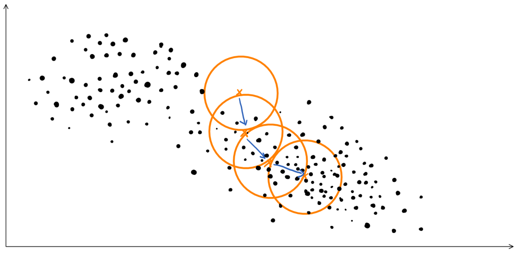


Figure 5: Mean Shift iterations with an Epanechnikov kernel

Application:

- (Color) quantization: Note, the RGB colorspace is not perceptually uniform (Lab or Luv are used in practice)
- (Color) segmentation
  - Similar in result to a super pixel segmentation: operates locally in the image
  - Incorporate the position of each pixel
  - Properly scale each feature dimension, such that distances are comparable (e.g. $\vec{x}$ =(x,y,r,g,b))

Remarks on the found maxima:

- Different trajectories typically coverage only to **almost** the same peak, thus, we will have to post process the peaks and somehow reduce them.
- We don't have a guarantee to sit on top of a maximum when reaching a 0-gradient. This is due to the finite window size and the discrete representation of our density (see figure 4).
- If the amount of data is large, then it may become extremly costly to iteratively evaluate the "neighbourhood finder". In that case we have to help ourself, either with a smart data structure (oct-tree or a generalisation for many dimensions) or locality sensitve hashing (LSH).

K-means

- **Initialization:** randomly assign k mean vectors as cluster centers
- **Repeat:**
  - Assign each observation to the closest cluster mean
  - For a given cluster assignment C, compute each clusters mean
- **Stopping criterium:** no more change between iterations or number of iterations exceeded.

Each iteration reduces the value of the criterion, so that convergence is assured, but the solution may be local minimum depending on the initial (random) assignment[7]. In addition, on should start the algorithm with many different random choices for the starting means, and choose the solution having smallest value of the objective function.
As a quality measure we use the within-cluster scatter, which can be written as

$$W(C) = \sum_{k=1}^{K} N_k \sum_{C(i)=k} ||x_i - \mu_k||^2$$

where μ_k is the mean vector associated with the kth cluster, and N_k is the number of observations assigned to a cluster. K must be chosen beforehand. Thus, the criterion is minimized by assigning the N observations to the K clusters in such a way that within each cluster the average dissimilarity of the observations from the cluster mean, as defined by the points in that cluster, is minimized.

Vector Quantization

The K-means clustering algorithm represents a key tool in the apparently unrelated area of image and signal compression, particular in *vector quantization* or *VQ*(Gersho and Gray, 1992).
Algorithm:

1. Convert to grayscale
2. Break image into small blocks, e.g. 2×2 blocks of pixels
3. Each block is regarded as a vector in $\mathcal{R}^4$
4. Apply K-means
5. Each of the blocks is approximated by its closest cluster centroid, known as codeword. The clustering process is called the *encoding* step, and the collection of centroids is called the *codebook*.

K-medioids

$K-$means stuggels with outliers, because using *squared* Euclidean distance places the highest influence on the larger distances.
Instead of taking means as cluster center, one can identify the sample inside each cluster, which is nearest to all other samples inside it. One then assigns this sample to be the new cluster center.
The downside is that K-medioids is far more computationally intensive.

[7] practical approach: apply k-means multiple times (with random initialization) and choose best result.

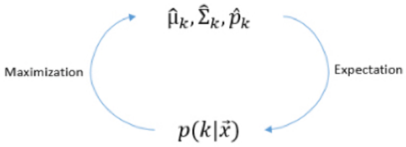
Spectral clustering

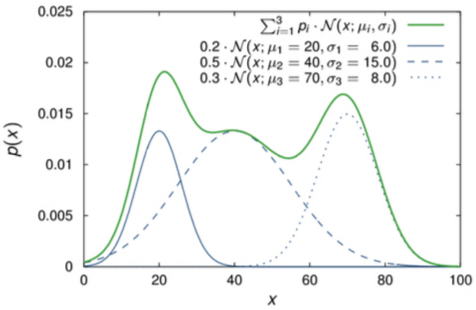
This is essentially executing Laplacian Eigenmaps + k-Means on the lower dimensional space.
How to choose a appropriate d'? The distribution of the eigenvalues gives an indication about the intrinsic dimensionality of the data. If there is a certain gap between eigenvalue, this is a good indication. We don't have this available when using LLE.

Gaussian Mixtures as Soft K-means Clustering

The K-means clustering procedure is closely related to the EM algorithm for estimating a certain Gaussian mixture model. Suppose we specify K mixture components, each with a Gaussian density having a scalar covariance matrix $\sigma^2 I$. Then the relative density under each mixture component is a monotone function of the Euclidean distance between the data point and the mixture center. Hence in this setup EM is a "soft" version of K-means clustering, making probabilistic assignments of points to cluster centers. As the variance $\sigma^2 \to 0$, these probabilities become 0 and 1, and the two methods coincide (responsibility of mixture component $i : \frac{g_i(x)}{\sum_m g_m(x)}$).

Short reminder: Gaussian mixture models Start with random initialization, expectation (how much does each component contribute to each point), maximization (update component parameters), repeat until convergence





From a more abstract perspective, EM performs two tasks simultaneously: segmentation/clustering assignment, and model parameters estimation/fitting

Practical Issues

In order to use K-means or -medioids one must select the number of clusters K^* as initialization. A choice for the number of clusters K depends on the goal. For data segmentation K is usually defined a part of the problem.
Data-based methods for estimating K^* typically examine the within cluster dissimilarity W_k as a function of the number of clusters K. Seperate solutions are obtained for $K \in \{1, 2, \ldots, K_{max}\}$. The corresponding values generally decrease with increasing K.

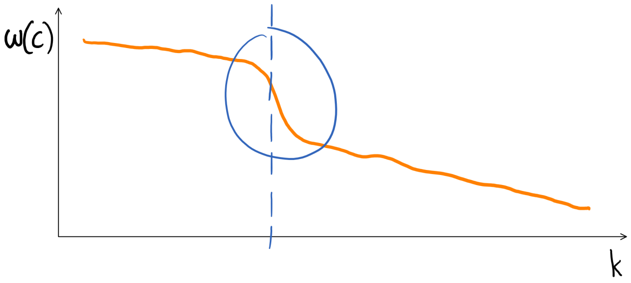


Figure 6: Approach 1: Track the rate of change of a quality metric (like $w(c)$). Proposed in “Pattern Classification” (Duda, Hart, Stork).

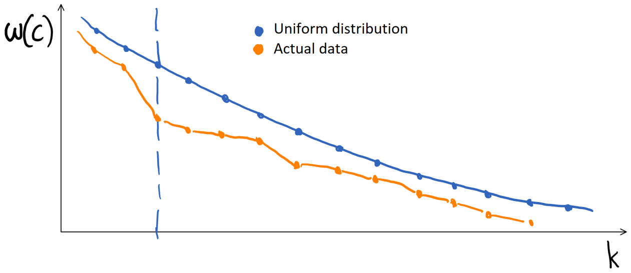
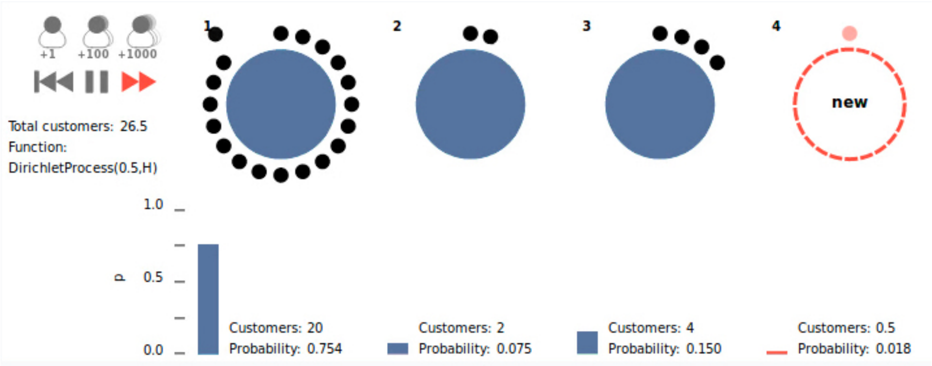


Figure 7: Approach 2: Relate change of $w(c)$ to change of $w'(c)$. Optimal K is where the gap between the two curves is largest (Proposed in TEoSL).

Note: We have several options for clustering data. K-means and its variants are straight forward and easy to understand, but if the proper number of clusters is part of the unknowns, it may be a suboptimal choice. One alternative is mean shift clustering. Here is the number of clusters determined implicitly by the kernel type and size plus the type of bump post process.

Dirichlet Process

Idea The Dirichlet Process is the idea of drawing a GMM from a meta-distribution, which can model infinite gaussian mixtures.
We need a fitting algorithm (**Gibbs sampling**) that fits a GMM to the data independent of the number of components. This is based on the **Chinese restaurant process**, which provides a constructive way of sampling from a dirichlet process.



Total customers: 26.5
Function:
DirichletProcess(0.5,H)

This CRP extends a "normal" GMM:

1. If a customer prefers to sit at a new table, this is possible we can add arbitrary many tables
2. The more people sit on a table the more attractive it is to the new customers (rich get richer)

Gibbs sampling: A straight forward (probailistic[8]) clustering algorithm based on the CRP

1. Init: assign each sample to a cluster (e.g. randomly, or do $k-$means)
2. Randomly select a sample x_i from the data
3. Compute a affinity of x_i to each table: $t_i = \frac{N_i}{N+\alpha}\mathcal{N}(x_i, \mu_i, \Sigma_i)$ (Gaussian distance of x_i to (μ_i, Σ_i)), where N_i is the number of customers on the table (number of samples assigned to $\mathcal{N}(\mu_i, \Sigma_i)$ and N is the total number of samples, α is an "expansion parameter"
4. Compute affinity to a new table $t_0 = \frac{\alpha}{N+\alpha} \cdot \mathcal{N}(x_i, \mu_0, \Sigma_0)$
5. Collect all affinities $t_0, \ldots, t_T$ in a list, normalize sum to one
6. Sample from that list a table assignment (all affinities are interpreted as a PDF from which we sample)
7. Recompute μ_i, Σ_i for the assigned table
8. Goto 2, stop after certain number of iterations

Back to the top-down view: Using the CRP, we are effectivly drawing a GMM using a dirichlet process. Implicitly, the mixture weights β_i match a $Beta(\alpha)$ distribution and the normal distributions are drawn from a hyper-distribution, i.e. $\vartheta_i \sim H(\lambda)$

[8] because we sample from the list

Stick breaking process: (check the wiki-page)

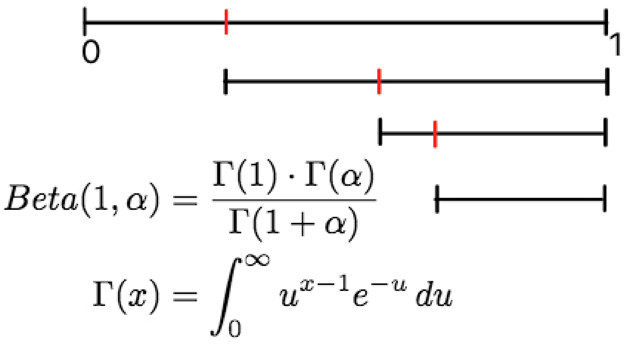

0
1
$Beta(1,\alpha) = \frac{\Gamma(1)\cdot\Gamma(\alpha)}{\Gamma(1+\alpha)}$
$\Gamma(x) = \int_0^\infty u^{x-1}e^{-u}\,du$

Figure 8: Illustration of a *Beta* distribution

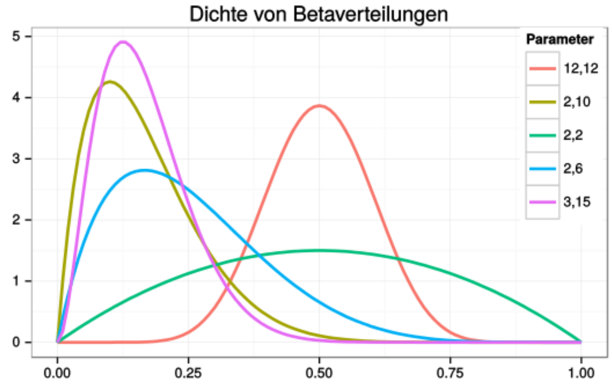


Figure 9: Qualitatively, this is what the *Beta* distribution looks like

The expansion parameter α is a prior that influences the number of clusters that will be created.

Observation 1: The larger the expansion parameter α is, the more likely it is to draw a number that is close to 0 form $Beta(1, \alpha)$
The number that has been drawn form $Beta(1, \alpha)$ is used in the stick breaking process to determine the weight of the i-th mixture component β_i

Observation 2: The number that has been drawn from $Beta(1, \alpha)$ is used in the stick breaking process to determine the weight of the i-th mixture component β_i.

Stick breaking process (formalised):

$$b_i \sim Beta(1, \alpha)$$

$$\beta_i = b_i \prod_{i=l}^{i-1} (1 - b_l) = b_i(1 - \sum_{l=1}^{i-1} \beta_l)$$

Manifold Learning

Principal idea: Reduce the dimensions of the Data, but preserve the structure of the data / underling manifold.

Curse of Dimensionality

"Human intuition breaks in high dimensional spaces" - (Bellman, 1961)

Let's illustrate this: Consider a d-dimensional feature vector $\vec{x_1}, \vec{x_2}, \dots, \vec{x_N} \in \mathbb{R}^d$ where $0 \leq x_i \leq 1$ uniformly distributed in a d-dimensional hyperspace of volume 1. Let's say we would like to cover enough volume of the cube to collect 1% of the data. Let's say we also use a cube for this task. What is the required edge length s of the cube to obtain that 1% of space?

Example for a 10 dimensional hypercube $V = s^d \Rightarrow s = V^{\frac{1}{d}} = 0,01^{\frac{1}{10}} = 0.63$

Another way of thinking about this is, that in a very high dimensional space, virtually every feature point is located at the boundary of the feature space[9]. This leads to the effect, that common distance measures loose their effectivity. E.g. the *median* distance for the nearest neighbour to the origin.

Example applications: ("Notorious" examples for high dimensional data)

- hyper-spectral remote sensing image classification
- satellite image: perform e.g. agricultural monitoring classify type of vegetation from hyper-spectral (many color channels) image.

In such classification pipelines, dimensionality reduction is often one integral component.

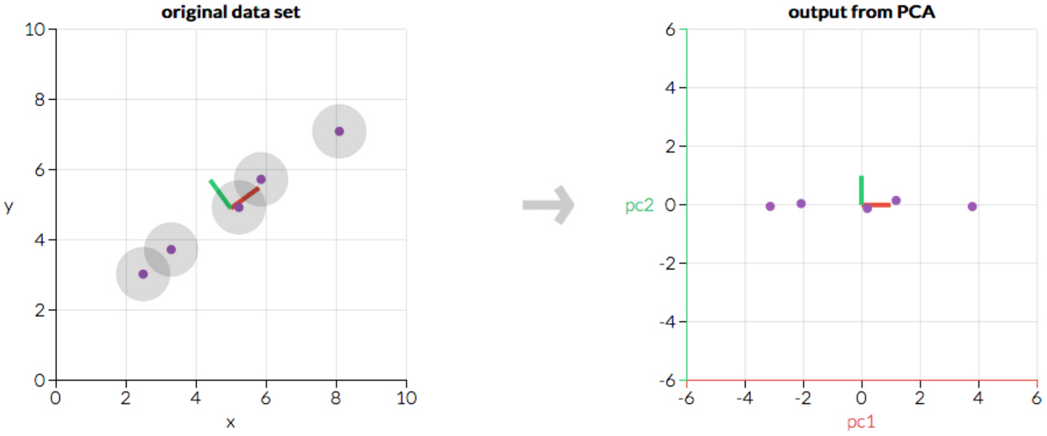
Additional notes

- Manifold learning algorithms are based on the idea that the dimensionality of many data sets is only artificially high. Although the data points may consist of thousands of features, they may be described as a function of only a few underlying parameters. That is, the data points are actually sampled from a low-dimensional manifold that is embedded in a high dimensional space. Manifold learning algorithms attempt to uncover these parameters in order to find a low-dimensional representation of the data.
- Finding optimal dimensionality: Look at residual variance (or error) (depending on d) and search for "elbow" at which the curve ceases to decrease significanlty with added dimensions. (PCA/MDS tend to overestimate dimensionality)
- PCA and MDS are guaranteed, given sufficient data, to recover the true structure of linear manifolds
- Possible problems:
  - If k for k-NN is to large, or noise in the data moves the points slightly off the manifold, ISOMAP is vulnerable to "short-circuiut error", where even single errors can alter the low-dim embedding drastically
  - If k is to small, the neighborhood graph may become too sparse to approximate geodesic paths accuratly

[9] Because in at least one dimension, we draw a very low of very high value

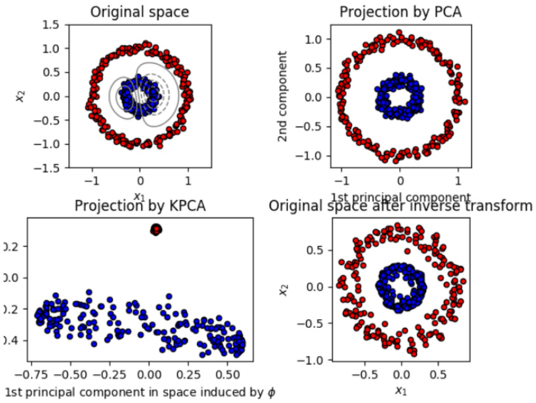
(k)PCA

Our known approch is the principle component analysis (PCA).



Orthogonal basis that is aligned with the "maximum spread" (w.r.t. the covariance) of the data. It is a global unsupervised method[10]. Consider that PCA as a linear method.

$$\sum_{i}^{N} (\vec{n}^T \vec{x_i})(\vec{n}^T \vec{x_i}) + \lambda(\vec{n}^T \vec{n} - 1)$$



The Kernel PCA performs a non-linear mapping of the data, then perform a standard (linear) PCA on the result. With the kernel-trick we can do that in one step. The Objective function: (the non-linear mapping is part of ϕ)

$$\delta = \sum_{i,j=1}^{N} (\phi(\vec{x_i}) - \phi(\vec{x_j}))^T (\phi(\vec{x_i}) - \phi(\vec{x_j})) + \lambda(\phi^T \phi - 1)$$

Some offsprings of the Kernel PCA idea are:

1. Perform some preprocessing / mapping that operates non-linearly
2. The dimensionality reduction itself is an operation that operates linearly.

[10] Operating on all data points, no labels, find one global optimal solution

Multi Dimensional Scaling (MDS)

Idea: Reconstruct a set of points (potentially in a lower dimension) from their differences.[11]

- Let X denote a matrix consisting of all samples, $X = [\vec{x_1}, \ldots, \vec{x_N}] \in \mathbb{R}^{d \times N}$
- Let $D^2 = [d^2_{ij}]_{i,j \in \{1,\ldots,N\}}$, where $d^2_{ij} = (\vec{x_i} - \vec{x_j})^T(\vec{x_i} - \vec{x_j})$
- We assume that $\vec{x_1}, \ldots, \vec{x_N}$ have zero mean i.e. $\sum_{i=1}^N \vec{x_i} = \vec{0}$
- Goal: Given D^2, compute X

Let us consider the distances in terms of $\vec{x}$

$$d^2_{ij} = (\vec{x_i} - \vec{x_j})^T(\vec{x_i} - \vec{x_j}) = \vec{x_i}^T\vec{x_i} - 2\vec{x_i}^T\vec{x_j} + \vec{x_j}^T\vec{x_j}$$

In matrix notation,[12]

$$D^2 = diag(X^TX) \cdot \vec{1}^T - 2X^TX + \vec{1} \cdot diag(X^TX)^T$$

Multiply D^2 from left and right with a centering matrix $C = (I - \frac{1}{N}\vec{1}\ \vec{1}^T)$, and weight the result by $-\frac{1}{2}$

$$\begin{aligned} -\frac{1}{2}CD^2C &= -\frac{1}{2}(I - \frac{1}{N}\vec{1}\ \vec{1}^T)(diag(X^TX) \cdot \vec{1}^T - 2X^TX + \vec{1} \cdot diag(X^TX)^T)(I - \frac{1}{N}\vec{1}\ \vec{1}^T) \\ &= \ldots \text{(because of the zero mean assumtion this breaks down to)} \\ &= X^TX \end{aligned}$$

Obtaining X is a matrix factorization problem, which we can solve by computing the eigenvector-eigenvalue decomposition[13] of X^TX. Therefore MDS breaks down to:

$$\boxed{SVD(-\frac{1}{2}CD^2C) = U\Sigma U^T}$$

$$\Rightarrow X = \Sigma^{\frac{1}{2}}U^T$$

We can reduce the dimensionality of our data by:

- Determining the d largest eigennvalues and their corresponding eigenvectors
- Dropping the remaining eigenvalue and eigennvectors inside the multiplication

MDS is essentially the same thing as PCA, but it operates on distances.

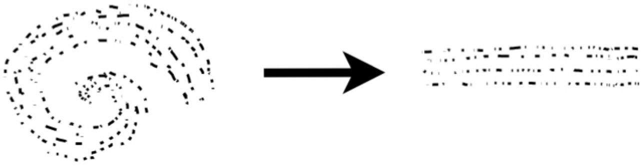
[11] MDS computes the "best" (in a least square sense) coordinates up to rotation, translation and mirroring (axis reversal).

[12] where $diag(A)$ denotes a vector diagonal entries of A, i.e. $diag(A) = (a_{11}, a_{22}, \ldots, a_{NN})^2$

[13] we can do this because its an square matrix

Isometric Feature Mapping (ISOMAP)

A non-linearity "patch" to MDS



Idea: Nearby points have their "usual" euclidian distance. If a pair of points are not within a local neigbourhood, then the distance between these points is a **graph distance**[14]. Then run MDS on the resulting distance Matrix. ISOMAP operates on geodesic distances (like a distance on earths surface/distances on the manifold).

- ISOMAP is guaranteed asymptotically to recover the true dimensionality and geometric structure of a strictly larger class of nonlinear manifolds, which intrinsic geometry is that of a convex region of Euclidean space
- ISOMAP is a polynomial time, noniterative procedure which guarantees global optimality

[14] Compute the all pairs shortest path (Dejkstra, A*, DFS, Floyd–Warshall, ...)

Locally Linear Embedding (LLE)

Idea: Describe each point $\vec{x_i}$ as linear combination of its local neighborhood [15].

$$\vec{x_i} = \sum_{j \in N(\vec{x_i}), j \neq i} w_{ij}\vec{x_j} \qquad \text{subject to} \sum_j w_{ij} = 1$$

This way we maintain the weights inside the local neighborhood. In the lower dimension we can then linearly interpolate a point $\vec{x_i'}$ from its neighbors weights. $\vec{x_i}' = \sum_{j \in N(\vec{x_i}')} w_{ij}\vec{x_j}'$

Algorithm:

1. Define the neighborhood (k-nearest neighbors, distance thresholding)
2. Solve for w_{ij} in the high dimensional space (Modified version)[16]

$$min \sum_i ||\vec{x_i} - \sum_{j \in N(\vec{x_i})} w_{ij}\vec{x_j}||_2^2 \qquad \text{subject to} \sum_{j \in N(\vec{x_i})} w_{ij}^2 = 1$$

Note the objective function is invariant to translation, therefore we can move each point $\vec{x_i}$ and its neigborhood to the origin

$$= min \sum_i || - \sum_j w_{ij}(\vec{x_j} - \vec{x_i})||_2^2$$

$$= min \sum_i ||M_i\vec{w_i}||_2^2$$

where $M_i = \begin{pmatrix} \vec{x_1} - \vec{x_i} & \vec{x_2} - \vec{x_i} & \dots & \vec{x_N} - \vec{x_i} \end{pmatrix}$[17]

$$\Rightarrow min \sum_i (M_i\vec{w_i})^T(M_i\vec{w_i}) + \lambda(1 - w_i^T\vec{w_i})$$

where the latter is the constraint that the squared weights should sum up to one. If we would compute the derivative of $\lambda(1 - w_i)$, the constraint would vanish to 0.

Compute

$$\frac{\partial}{\partial \vec{w_i}}(\vec{w_i}^T M_i^T M_i\vec{w_i} + \lambda(1 - w_i^T\vec{w_i}) = 2 \cdot M_i^T M_i\vec{w_i} - 2\lambda \cdot \vec{w_i} = 0$$

$$\Rightarrow \boxed{M_i^T M_i\vec{w_i} = \lambda\vec{w_i}}$$

This is an eigenvector eigenvalue problem.

3. Reconstruct the lower dimensional embedding by solving for $\vec{x_i}' \in \mathbb{R}^{d'} (d' \ll d)$:

$$min \sum_i ||\vec{x_i}' - \sum_{j \in N(\vec{x_i})} w_{ij}\vec{x_j}'||_2^2 \qquad \text{subject to} \ \frac{1}{N}\sum_i \vec{x_i}'\vec{x_i}'^T = I, \sum_i \vec{x_i}' = \vec{0}$$

The first constraint says that the covariance is the identity. Which basically fixes the volume. The second one centers the samples. This again boils down to an eigenvector eigenvalue problem, where $M = (I - W)^T(I - W)$

$$\Rightarrow \boxed{M\vec{x_i} = \lambda\vec{x_i}}$$

[15] This makes the mapping an overall non-linear mapping consisting of small linear patches

[16] The original formulation (s. t. $w_{ij} = 1$) is sometimes unstable if applied on real data.

[17] differences $\vec{x_j} - \vec{x_i} = 0$ for $\vec{x_j}$ outside the neighborhood of $\vec{x_i}$

Laplacian Eigenmaps

Idea: TODO: add short description from lecture

1. Build an adjacency graph on the set of feature points $S = \{\vec{x_1}, \dots, \vec{x_n}\}$. We use the **Graph Laplacian** [18] L.

$$L = (D - W)$$

where D is a diagonal matrix which is there for normalization[19] and W is the adjacency matrix.

$$d_{ij} = \begin{cases} \sum_{k=1}^{N} w_{ik} & if\ i = j \\ 0 & if\ i \neq j \end{cases} \qquad w_{ij} = \begin{cases} \text{weight between nodes i and j} & if\ i \neq j \\ 0 & if\ i = j \end{cases}$$

2. Compute affinities as weights w_{ij} for the edges of the graph, such that closer point pairs have higher weights. One common choice for the weights is the so-called heat kernel or just binary affinity.

$$w_{ij} = \begin{cases} e^{-||\vec{x_i} - \vec{x_j}||_2^2} & if\ i \neq j \\ 0 & if\ i = j \end{cases} \qquad w_{ij} = \begin{cases} 1 & if\ ||x - \vec{x_j}||_2^2 \leq t \\ 0 & otherwise \end{cases}$$

3. Perform eigendecomposition of the graph Laplacian

$$\Rightarrow \boxed{D^{-1}L\vec{x_i'} = \lambda\vec{x_i'}}$$

4. Obtain low-dimensional embedding by selecting a ordered subset of eigenvectors from the decomposition.
   - Discard the eigenvalue/eigenvector pair for the lowest eigenvalues[20] (the 0 eigenvalue)
   - The d' next smallest eigenvalue/eigenvector pairs form the lower dimensional embedding: ith row of $E = (\vec{e_1}, \vec{e_2}, \dots, \vec{e_{d'}})$ equals $\vec{x_i}'^T$ which represents the lower dimensioanl embedding of $\vec{x_i}^T$.

Relationship of the objective function to the graph Laplacian L:

$$min\sum_{i=1}^{N}\sum_{j=1}^{N}||\vec{x_i}' - \vec{x_j}'||_2^2 w_{ij} \qquad \text{subject to[21]}\ x'^T D x' = 1$$

where $x' \in \mathbb{R}^{d'}, d' \ll d$.

$$= \sum_{i,j}(\vec{x_i}'^T\vec{x_i}' - 2\vec{x_i}'^T\vec{x_j}' + \vec{x_j}'^T\vec{x_j}')w_{ij} = 2 \cdot x'^T(D - W)x'$$

$$min\ x'^T L x' \qquad \text{subject to } x'^T D x' = 1$$

$$\frac{\partial}{\partial x'}(x'^T L x + \lambda(1 - x'^T D x')) = \vec{0}$$

$$2Lx' - \lambda D x' = \vec{0}$$

$$Lx' = \lambda D x'$$

$$\Rightarrow \boxed{D^{-1}L\vec{x'} = \lambda\vec{x'}}$$

[18] Matrix representation of a graph

[19] row sums up to zero 0 ($\sum_{k=1}^{N} l_{ik} = 0$)

[20] The number of eigenvalues depends on the connected components in the graph

Random Forest

Is a learing based approach for analysing the feature space, with an ensemble of decision trees. A decision tree is a binary tree with a "decision"[22] at every internal and the root node. It's a learning based approach, because good decision functions at the internal nodes are the result of training.

Training: of a single tree in a forest of size T

1. Select a number of splitting functions (e.g. hyperplanes or conics, ...)[23]
2. Evaluate the information gain $I = H_{\text{before}} - H_{\text{after-l, weighted}} - H_{\text{after-r, weighted}}$ for each splitting function [24]

$$I = H(S_j) - \sum_{i \in \{L,R\}} \frac{|S_j^i|}{|S_j|} H(S_j^i)$$

3. Set the one with maximum information gain as the current nodes' decision function
4. Recursively repeat for the child nodes, until max tree depth (or other stopping criteria[25]) is reached

If we have a trained decision tree, we can test it by evaluating the function at the root node.

$$h(\vec{x}, \vec{\vartheta}_j) : \mathbb{R}^d \times \underset{\text{tree parameters}}{\mathcal{T}} \rightarrow \{0, 1\}$$

Depending on the result (0 or 1) we evaluate the test function at either the left successor or the right successor of the root node, and continue down the tree recursively until a terminal/leaf node is reached. This "binary tree paradigm" essentially performs a partitioning of the feature space, where the incoming samples are subdivided into two parts by each internal node. The leaf node performs an application-specific action. For example, if the task is to perform classification, it assigns a label to the sample. Applications differ only in the computation of the information gain (objective function) and the "action" in the leaf node.

Design parameters are:

- the tree height/depth[26]
- the number of splitting functions at each internal node
- number of trees

Why an ensemble of trees? Experience showed that it is complicated to train a single, highly accurate decision tree. The idea of random forests is therefore to train a large number of individually less accurate trees in a randomized fashion. Because of this randomization, each tree splits at a slightly different location, and thus the discontinuities are "averaged out" in the forest.

Randomization parameters:

- The candidate functions, out of which the best on is chosen are randomly drawn
- if also linear projection of the data shall be drawn (e.g. consider only dimensions $\{d_{i_1}, d_{i_2}, \ldots, d_{i_n}\}$
- how the splitting parameters are sampled [27]
- (how many candidate functions are drawn)

[22] "Is this sample on the right side of a hyperplane?"

[23] simpler functions are typically prefered. Simplest function: "axis aligned split"

[24] where S_j is the data that flows into the node, $S_j^L S_j^R$ is the data that flows to the left/right and $H()$ denotes the entropy.

[25] minimum number of samples for a split

[26] trade-off: deeper trees tend to overfit, can be complemented with increased number of trees

[27] a sparser sampling leads to more "noise"/less optimal results (might be desired, e.g. prevents overfitting).

Classification Forests

Goal: Use the random forest model to train a classifier, which can be used to predict class labels.

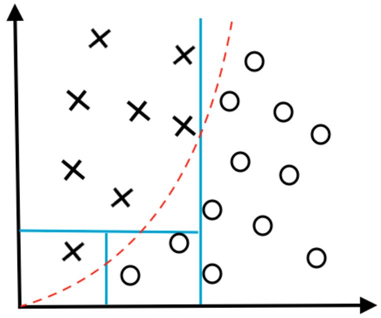


Figure 10: Possible space partitioning of one tree

The entropy in the classification case is defined as

$$H(S_j) = -\sum_{c \in C} p(c) \cdot log(p(c))$$

where c denotes the class label, and $p(c)$ the empirical distribution computed from S_j.

$$\Rightarrow I = H(S_j) - \sum_{i \in \{L,R\}} \frac{|S_j^i|}{|S_j|} H(S_j^i)$$

Training: basically the same as in the general case, but with the different objective function.

- Possible stopping criterion if e.g. 99% of features in a node belong to one class
- Leaf nodes, report the relative frequencies of the class labels in that node (e.g., 15%: class 1, 85% class 2)

The final classifier combines all trees by averaging the individual tree outputs. If a single discrete label is required, decide for the class with maximum probability.

Regression Forests

Goal: Use the random forest model to predict a <u>continous</u> label $p(y|\vec{x})$.
(Remark: choice of the model complexity is related to the bias/variance trade off)
"Leaf prediction model": a base function that is fitted to the samples. The leaf prediction model could be constant (maximise the bias), linear, polynomial, ...
To faithfully represent all of the data with a single function, it would certainly make sense to use a polynomial model, or something even more complex. However, the random idea implies to subdivide/partition the space, and to fit simpler models to the individual partitions.

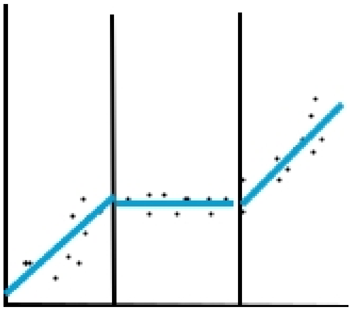


Figure 11: (Linear) regression split

The decision criterion for the splitting function works analogously to the classification case. The only difference is that we need to define the entropy on continuous values:

$$H(S_j) = -\frac{1}{|S_j|} \cdot \sum_{\vec{x}\in S_j} \int_y p(y|x) \cdot log(y|x)dy$$

where $p(y|x)$ can, e.g. be chosen as a Gaussian distribution $p(y|x) = \mathcal{N}(y; \overline{y}(x), \sigma_y^2(x))$, where $\overline{y}(x)$ is a linear function and $\sigma_y(x)$ is the conditional variance computed from a linear fit.

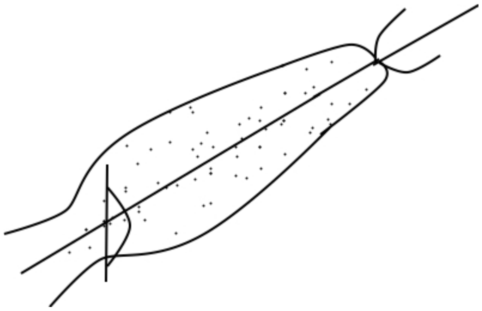


Figure 12: Probabilistic linear fit (left Gaussian, right constraint)

Combining the expression for $p(y|x)$ into $H(S_j)$ yields

$$H(S_j) = \frac{1}{|S_j|} \cdot \sum_{\vec{x}\in S_j} \frac{1}{2} \cdot log((2\pi e)^2 \sigma_y^2(\vec{x}))$$

$$\Rightarrow I(S_j, \vartheta) = \sum_{\vec{x}\in S_j} log(\sigma_y(\vec{x})) - \sum_{i\in\{L,R\}} (\sum_{x\in S_j^i} log(\sigma_y(\vec{x})))$$

Density Forests

Very same idea, adapted to unlabeled data ⇒ learning-based density estimator.
Each leaf node is modeled as a multivariate Gaussian distribution. The information gain metric can again be reused, but let us choose $H(S_j)$ defined by $|\Lambda|$ [28]

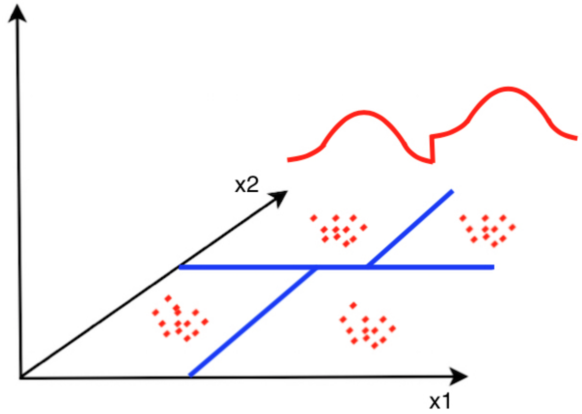
$$H(S_j) = \frac{1}{2} \cdot log((2\pi e)^d |\Lambda S_j|)$$

Motivation: Determinant of covariance matrix is a function of the volume of the ellipsoid corresponding to that cluster. Maximizing the information gain tends to split the data into a number of compact clusters. The centers of those clusters tend to be placed in areas of high data density, while the separating surfaces are placed along regions of low density.

Plugging $H(S_j)$ back into $I(S_j, \vartheta)$ yields

$$I(S_j, \vartheta) = log(|\Sigma(S_j)|) - \sum_{i \in \{L,R\}} \frac{|S_j^i|}{|S_j|} \cdot log(|\Lambda(S_j^i)|)$$

In each leaf, fit a multivariate Gaussian distribution to the data in that leaf using, e.g. MLE.



Note that the fitted densities have discontinuities at the splitting boundaries (this is the same type of discontinuity that we observed for regression forests or classification forests).

Sampling from this generative model

1. Draw uniformly a random tree index $t \in \{1, T\}$ to select a single tree in the forest
2. Descend the tree
   - Starting at the root node, for each split node randomly generate the child index with probability proportional to the number of training points in edge (proportional to edge thickness)
   - Repeat step 2 until a leaf is reached
3. At the leaf draw a random sample from the *domain bounded* Gaussian stored at that leaf

[28] Λ is the associated $d \times d$ covariance matrix of the data, $|\Lambda|$ can be seen as the "volume of a cluster"

Manifold Forest (Manifold Learning with Random Forests)

Idea: Learn a partitioning of the feature space by training a density forest.[29] These partitions define a local neighborhood of the samples, which can be used to compute affinities[30], and then to apply e.g. Laplacian Eigenmaps on them.

Task Define affinities on a readily trained density forest.
Let $w_{ij} = e^{-Q(x_i, x_j)}$ denote the affinity between samples x_i, x_j, where $Q(x_i, x_j)$ denotes a distance function.
The "speciaility" of a Manifold Forest (in contrast, e.g. to standard Laplacian Eigenmaps) is that these distances are defined w.r.t. the leafs of the trees (i.e. the partitions).

Example choices of Q: Let $d_{ij} = x_i - x_j$, then

$$\text{Mahalanobis: } Q(x_i, x_j) = \begin{cases} d_{ij}^T (\Lambda_{l(x_i)})^{-1} d_{ij} & \text{if in the same leaf } l(x_i) \\ \infty & otherwise \end{cases}$$

$$\text{Binary: } Q(x_i, x_j) = \begin{cases} 0 & \text{if in the same leaf} \\ \infty & otherwise \end{cases}$$

Gaussian:...

In a single tree, only the samples within the same leaf-node have a non-zero affinity. Thus, a single tree produces a number of disconnected neighborhoods. However if the affinities are averaged over the whole forest, all points become connected.

- ⇒ We have a full adjacency matrix $A = \frac{1}{T} \sum_{t=1}^{T} w_i j^t$, where T denotes the total number of trees.
- ⇒ Compute LE on A.

Note that the graph Laplacian in Criminisi/Shotton are differently normalized, but it is the same algorithm:

$$L = I - \Gamma^{-\frac{1}{2}} A \Gamma^{-\frac{1}{2}}$$

where $\Gamma = D = \sum_{i,j} A_{ij}$ denotes the sum of the weights for sample x_i.[31]

⇒: analogous to LE eigenvalue decomposition, arrange d' eigenvectors that are associated with the lowest eigenvalues in a matrix E.

$$E = (\vec{e_1}, \vec{e_2}, \ldots, \vec{e_{d'}})$$

The projection of x_i onto a d' dimensional space just corresponds to the i-th row of E. (note: drop the first eigenvector, where the eigenvalue is 0)

Advantages:

1. Automatic selection of discriminative features via information-based energy optimization
2. Automatic estimation of the optimal dimensionality of the target space
3. Being part of a more general forest model and, in turn code re-usability

[29] Note that we don't explicitly use the density
[30] Affinity intuition: Decreases with increasing distance
[31] just for normalization

Hidden Markov Models HMM

Motivation: We want to model dependencies between features in a sequence. A HMM is a generative probabilistic approach to describing sequential data (e.g. speech data).

Let $S_1, \ldots, S_N$ denote N hidden states
Let $o_1, \ldots, o_M$ denote M features (or observations, e.g. preprocessed speech data). These usually form a sequence.

A HMM models the joint probability (generative!) of hidden states and a sequence of observations:

$$p(< o_1, \ldots, o_M >, < S_1, \ldots, S_M >)$$

HMM Definition: $\lambda = (A, B, \vec{\pi})$

- A is a matrix of state transition probabilities $a_{ij} = P[q_{t+1} = S_j | q_t = S_i]$
- B is a matrix of production probabilities $b_j(v_k) = P[v_k at state S_j]$, where $V = v_1, \ldots, v_{|V|}$ is the set of possible observations.
- Values in each row of the matrices A and B sum up to 1.
- $\vec{\pi}$ is a vector of starting probabilities for each state.

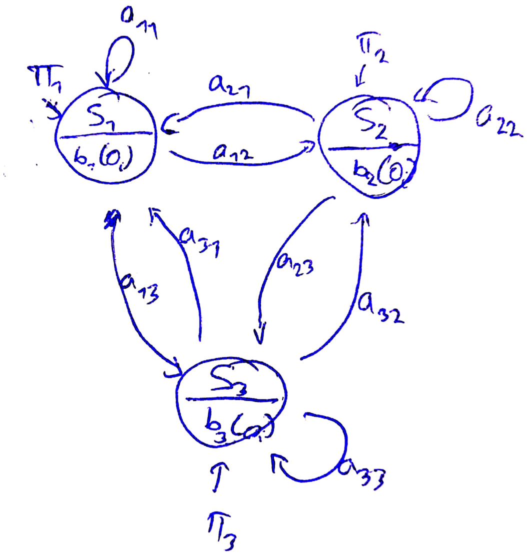


Figure 13: We can represent a HMM as a graphical model similar to a state machine.

Questions we can ask with an HMM

1. Given a model λ, what is $p(< o_1, \ldots, o_M > | \lambda)$, the probability of making an observation $< o_1, \ldots, o_M >$ given λ?
2. Given a model λ and an observation sequence $< o_1, \ldots, o_M >$, what is the most likely sequence of states $< S_1, \ldots, S_M >$ that generated it?
3. How can we obtain the model parameters λ in a fully automated way (training)?

Question (1), probability of an observation: *Forward-/Backward-Algorithm*

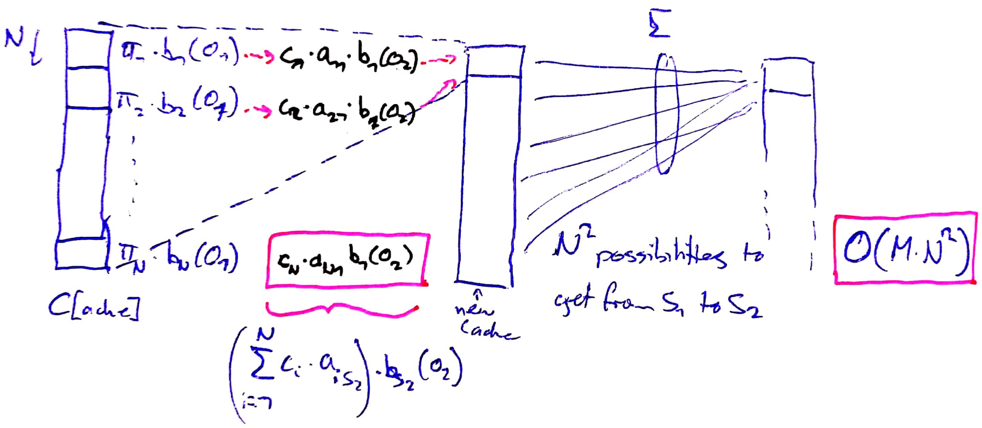
Marginalize over all state sequences [32]:

$$p(< o_1, \ldots, o_M >= \sum_{S_1=1}^{N} \sum_{S_2=1}^{N} \cdots \sum_{S_M=1}^{N} \pi_{S_1} \cdot \prod_{i=1}^{M-1} a_{S_i S_{i+1}} \cdot \prod_{i=1}^{M} b_{S_i}(o_i)$$

Problems with implementation:

- Multiplying many small values will cause precision problems
- The sums will create M for loops in an implementation
- Computing cost: $O(N^M)$
- Solution: dynamic programming & Forward-/Backward Algorithm

Forward Algorithm TODO


N
$\pi_1 \cdot b_1(O_1)$
$c_1 \cdot a_{11} \cdot b_1(O_2)$
$\pi_2 \cdot b_2(O_1)$
$c_2 \cdot a_{21} \cdot b_1(O_2)$
$\pi_N \cdot b_N(O_1)$
$c_N \cdot a_{N1} b_1(O_2)$
C[ache]
$\left(\sum_{i=1}^{N} c_i \cdot a_{iS_2}\right) \cdot b_{S_2}(O_2)$
new Cache
Σ
N^2 possibilities to get from S_1 to S_2
$O(M \cdot N^2)$

Backward Algorithm TODO

0.1 Question (2), most likely state sequence: *Viterbi Algorithm*

TODO

0.2 Question (3), how to train a HMM: *Baum-Welch-Algorithm*

TODO

Remarks on HMM

3 algorithm

1. How to train the HMM (determain the parameters $\lambda(A, B, \pi)$)
2. Determine the propbaility of a symbole being produced
3. Recover the most likly state sequence

[32] The sums enumerate all possible state sequences; The products represent $p(< S_1, \ldots, S_M >) \cdot (p(< o_1, \ldots, o_M > | < S_1, \ldots, S_M >)$

- the directed edge in a HMM graph can be understood as a statistical dependency $p(S_2|S_1)$ (more section 8 in bishops book on pattern recognition)
- generative approch
- For many tasks including speach processing, we often only allow state transitions a_{ij} with $i \leq j$ (no backward links). So called "left-right-HMMs".

Markov Random Fields (MRF)

Example use cases are denoiseing, segmentation or stero matching. [33] Consider the pixel gird as a lattice of random variables. More specifically let us asume, that the image F is given by the random matrix $[f_{i,j}]$.
Assumption: limited statisical depenency (between the pixels)

$$p(f_{i,j}|f_{i-1,j}f_{i,j-1}f_{i-1,j-1})$$

where $f_{i-1,j}f_{i,j-1}f_{i-1,j-1}$ form a dependency of the neigbours to $f_{i,j}$ (This will later be our Markov property)

$$p([f_{i,j}] = \prod_{i,j} p(f_{i,j}|f_{i-1,j}f_{i,j-1}f_{i-1,j-1})$$

Definition of MRF:
Let us consider the features / observations $\vec{x}_1, \vec{x}_2, \dots, \vec{x}_N$

1. Positivity:[34] $p(\vec{x}_1, \vec{x}_2, \dots, \vec{x}_N) > 0$
2. Markokv property:[35] $p(\vec{x}_k|\vec{x}_1, \dots, \vec{x}_{k-1}, \vec{x}_{k+1}, \dots, \vec{x}_N) = p(\vec{x}_k)|\mathcal{N}(\vec{x}_k))$

Definition of the neighborhood:

1. $\vec{x}_k \notin \mathcal{N}(\vec{x}_k)$
2. $\vec{x}_i \in \mathcal{N}(\vec{x}_k) \Leftrightarrow \vec{x}_k \in \mathcal{N}(\vec{x}_i)$
3. $\mathcal{N}(\vec{x}_k) = \{x_i | 0 < dist(x_i, x_k) \leq t\}$

Example: Pixel gird

$$\mathcal{N}(\vec{x}_{i,j}) = \{x_{k,l} | (i-k)^2 + (j-l)^2 \leq c^2, \quad i \neq k; j \neq l\}$$

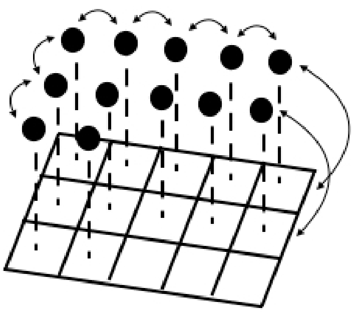


Figure 14: The idea of MRF on images the arrows indicate relations

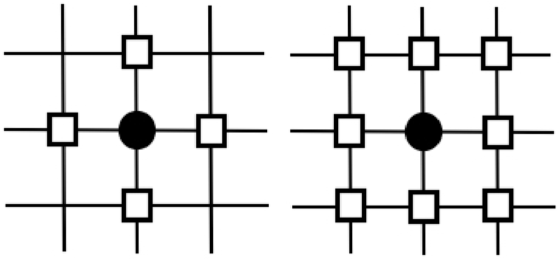


Figure 15: 4-Neighborhood ($c = 1$), 8-Neighborhood ($c = \sqrt{2}$) (and dinamic-Neighborhood)

Note: that the neibhborhoods can also be decomposed in graph Cliques (complete subgraphs) of two. Which is useul later on (factorization + there are solvers for two variables)

[33] Geman / Geman introduced MRF to image processing (1985)

[34] For a certain observation the probability is non zero

[35] where $\mathcal{N}(\vec{x}_k))$ denotes the neighborhood of $\vec{x}_k$ ($\vec{x}_k$ only depends on its neighbors)

Gibbs Random Fields (GRF): is given by the PDF ($Z = \sum_{x'} H(x')$ is called a partition function and $H(x)$ is an energy function, i.e. a sum of potential functions.)

$$p(x) = \frac{1}{Z} e^{-H(x)}$$

Remark: For a given PDF $p(x)$, the choice of the energy function $H(x)$ is not unique. Consider for example

$$H(x) = -\log p(x) - \log Z$$

$$p(x) = \frac{1}{Z} e^{-H(x)} = \frac{1}{Z} e^{\log p(x)} e^{\log Z} = p(x)$$

→ we can choose Z arbitarily

The interesting theoretical property is that GRFs and MRFs are equivalent. The proof for this is called Hammersley-Clifford Theorem.

Example: Image denoising
Given: The observed noisy image $[g_{i,j}]$
Searched: Hidden variables are the ideal (noiseless) image $[f_{i,j}]$

Assumption 1: The ideal image is spatially smooth

$$p(f_{i,j}]) = \frac{1}{Z} e^{-H([f_{i,j}])}, \quad \text{where } H([f_{i,j}]) = \sum_{i,j} ||\nabla f_{i,j}||_2^2$$

$H([f_{i,j}])$ is sum of squared gradients, computed over a neighborhood (or the sum over all clique potentials)

Assumption 2: $[g_{i,j}]$ is similar to $[f_{i,j}]$, but corrupted by additive Gaussian noise

$$p([g_{i,j}]|f_{i,j}]) = \prod_{i,j} \frac{1}{\sqrt{2\pi} G_{i,j}} \exp(-\frac{1}{2G_{i,j}^2} \cdot \underbrace{(f_{i,j} - g_{i,j})^2}_{\text{energy function } H})$$

With these two functions defined, we can solve for a MAP estimate for f:

$$\begin{aligned}
\underbrace{[\hat{f}_{i,j}]}_{\text{estimated ideal image}} &= \arg\max_{[f_{i,j}]} p([f_{i,j}]|[g_{i,j}]) \\
&= \arg\max_{[f_{i,j}]} p([g_{i,j}]|[f_{i,j}]) \cdot p([f_{i,j}]) \\
&\dots \\
&\arg\min_{[f_{i,j}]} \{\sum_{i,j} \lambda_{i,j} (f_{i,j} - g_{i,j})^2 + \sum_{i,j} ||\nabla f_{i,j}||_2^2\}
\end{aligned}$$

$||\Delta f_{i,j}||_2^2$: function of clique of size 2