DSSP 14 : Unsupervised Learning

December 5, 2019

Outline

Motivation

- **Marketing:** finding groups of customers with similar behavior given a large database of customer data containing their properties and past buying records;
- **Biology:** classification of plants and animals given their features;
- **Libraries:** book ordering;
- **Insurance:** identifying groups of motor insurance policy holders with a high average claim cost; identifying frauds;
- **City-planning:** identifying groups of houses according to their house type, value and geographical location;
- **Internet:** document classification; clustering weblog data to discover groups of similar access patterns.

Marketing

- **Data:** Base of customer data containing their properties and past buying records
- **Goal:** Use the customers *similarities* to find groups.
- **Two directions:**
  - **Visualization:** propose a representation of the customers so that the groups are *visible*
  - **Clustering:** propose an explicit *grouping* of the customers

Source: Unknown

Dimension Reduction

- How to view a high-dimensional dataset?
- High-dimension: dimension larger than 2!
- *Projection* in a 2D space.

Source: F. Belardi

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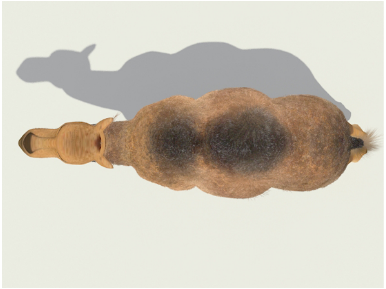
Dimension Reduction



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Dimension Reduction

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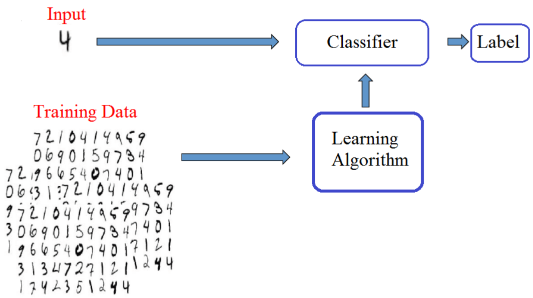
Machine Learning



A definition by Tom Mitchell (`http://www.cs.cmu.edu/~tom/`)

A computer program is said to learn from **experience E** with respect to some **class of tasks T** and **performance measure P**, if its performance at tasks in T, as measured by P, improves with experience E.

Source: Unknown

Supervised Learning

Experience, Task and Performance measure

- **Training data** : $\mathcal{D} = \{(\underline{X}_1, Y_1), \dots, (\underline{X}_n, Y_n)\}$ (i.i.d. $\sim \mathbb{P}$)
- **Predictor**: $f : \mathcal{X} \to \mathcal{Y}$ measurable
- **Cost/Loss function**: $\ell(f(\underline{X}), Y)$ measure how well $f(\underline{X})$ *predicts* Y
- **Risk**:
$$\mathcal{R}(f) = \mathbb{E}\left[\ell(Y, f(\underline{X}))\right] = \mathbb{E}_X\left[\mathbb{E}_{Y|\underline{X}}\left[\ell(Y, f(\underline{X}))\right]\right]$$

- Often $\ell(f(\underline{X}), Y) = \|f(\underline{X}) - Y\|^2$ or $\ell(f(\underline{X}), Y) = \mathbf{1}_{Y \neq f(\underline{X})}$

Goal

- Learn a rule to construct a **classifier** $\widehat{f} \in \mathcal{F}$ from the training data $\mathcal{D}_n$ s.t. **the risk** $\mathcal{R}(\widehat{f})$ is **small on average** or with high probability with respect to $\mathcal{D}_n$.

Unsupervised Learning

Experience, Task and Performance measure

- **Training data** : $\mathcal{D} = \{\underline{X}_1, \ldots, \underline{X}_n\}$ (i.i.d. $\sim \mathbb{P}$)
- **Task**: ???
- **Performance measure**: ???

- No obvious task definition!

Tasks for this lecture

- **Dimension reduction:** construct a map of the data in a **low dimensional** space without **distorting** it too much.
- **Clustering (or unsupervised classification):** construct a **grouping** of the data in **homogeneous** classes.

Dimension Reduction

- **Training data** : $\mathcal{D} = \{\underline{X}_1, \ldots, \underline{X}_n\} \in \mathcal{X}^n$ (i.i.d. $\sim \mathbb{P}$)
- Space $\mathcal{X}$ of possibly high dimension.

Dimension Reduction Map

- Construct a map Φ from the space $\mathcal{X}$ into a space $\mathcal{X}'$ of **smaller dimension**:

$$\begin{aligned} \Phi : \quad & \mathcal{X} \to \mathcal{X}' \\ & \underline{X} \mapsto \Phi(\underline{X}) \end{aligned}$$

- Map can be defined only on the dataset.

Motivations

- Visualization of the data
- Dimension reduction before further processing

Dimension Reduction

- Need to control the **distortion** between $\mathcal{D}$ and $\Phi(\mathcal{D}) = \{\Phi(\underline{X}_1), \ldots, \Phi(\underline{X}_n)\}$

Distortion(s)

- Reconstruction error:
  - Construct $\widetilde{\Phi}$ from $\mathcal{X}'$ to $\mathcal{X}$
  - Control the error between $\underline{X}$ and its reconstruction $\widetilde{\Phi}(\Phi(\underline{X}))$
- Relationship preservation:
  - Compute a *relation* $\underline{X}_i$ and $\underline{X}_j$ and a *relation* between $\Phi(\underline{X}_i)$ and $\Phi(\underline{X}_j)$
  - Control the difference between those two *relations*.

- Leads to different constructions....

Clustering

- **Training data** : $\mathcal{D} = \{\underline{X}_1, \dots, \underline{X}_n\} \in \mathcal{X}^n$ (i.i.d. $\sim \mathbb{P}$)
- Latent groups?

Clustering

- Construct a map f from $\mathcal{D}$ to $\{1, \dots, K\}$ where K is a number of classes to be fixed:

$$f : \quad \underline{X}_i \mapsto k_i$$

- Similar to classification except:
  - no ground truth (no given labels)
  - label only elements of the dataset!

Motivations

- Interpretation of the groups
- Use of the groups in further processing

Clustering

- Need to define the **quality** of the cluster.
- No obvious measure!

Clustering quality

- Inner homogeneity: samples in the same group should be similar.
- Outer inhomogeneity: samples in two different groups should be different.

- Several possible definitions of similar and different.
- Often based on the distance between the samples.
- Example based on the euclidean distance:
  - Inner homogeneity = intra class variance,
  - Outer inhomogeneity = inter class variance.
- **Beware:** choice of the number of cluster K often complex!

Outline

Dimension Reduction

- **Training data** : $\mathcal{D} = \{\underline{X}_1, \ldots, \underline{X}_n\} \in \mathcal{X}^n \quad$ (i.i.d. $\sim \mathbb{P}$)
- Space $\mathcal{X}$ of possibly high dimension.

Dimension Reduction Map

- Construct a map Φ from the space $\mathcal{X}$ into a space $\mathcal{X}'$ of **smaller dimension**:

$$\begin{aligned} \Phi : \quad \mathcal{X} &\to \mathcal{X}' \\ \underline{X} &\mapsto \Phi(\underline{X}) \end{aligned}$$

Criterion

- Reconstruction error
- Relationship preservation

Outline

Dimensionality Curse

High Dimension Geometry Curse

- Folks theorem: In high dimension, everyone is alone.
- Theorem: If $\underline{X}_1, \dots, \underline{X}_n$ in the hypercube of dimension d such that their coordinates are i.i.d then

$$d^{-1/p}\left(\max \|\underline{X}_i - \underline{X}_j\|_p - \min \|\underline{X}_i - \underline{X}_j\|_p\right) = 0 + O\left(\sqrt{\frac{\log n}{d}}\right)$$

$$\frac{\max \|\underline{X}_i - \underline{X}_j\|_p}{\min \|\underline{X}_i - \underline{X}_j\|_p} = 1 + O\left(\sqrt{\frac{\log n}{d}}\right).$$

- When d is large, all the points are almost equidistant...
- Nearest neighbors are meaningless!

Inertia

- $\underline{X}_1, \ldots, \underline{X}_n \in \mathbf{R}^d$
- $m = \frac{1}{n} \sum_{i=1}^{n} \underline{X}_i$

Two views on inertia

- Inertia:

$$\begin{aligned} I &= \frac{1}{n} \sum_{i=1}^{n} \|\underline{X}_i - m\|^2 \\ &= \frac{1}{2n^2} \sum_{i,j} \|\underline{X}_i - \underline{X}_j\|^2 \end{aligned}$$

- 2 times the mean squared distance to the mean = Mean squared distance between individual

- Heuristic: a good representation is a representation with a large inertia
- Large dispersion $\sim$ Large average separation!

Inertia and Projection

- What if we replace $\underline{X}$ by its projection $\widetilde{\underline{X}} = P(\underline{X} - m) + m$?

Two views on inertia

- Inertia:

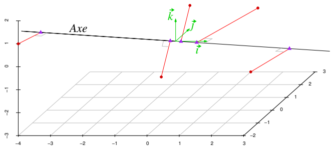
$$\begin{aligned}\widetilde{I} &= \frac{1}{n}\sum_{i=1}^{n} \|\widetilde{\underline{X}}_i - m\|^2 \\ &= \frac{1}{2n^2}\sum_{i,j} \|\widetilde{\underline{X}}_i - \widetilde{\underline{X}}_j\|^2\end{aligned}$$

- Inertia:

$$\begin{aligned}\widetilde{I} &= I - \frac{1}{n}\sum_{i=1}^{n} \|\widetilde{\underline{X}}_i - \underline{X}_i\|^2 \\ &= I - \frac{1}{2n^2}\sum_{i,j} \left(\|\underline{X}_i - \underline{X}_j\|^2 - \|\widetilde{\underline{X}}_i - \widetilde{\underline{X}}_j\|^2\right)\end{aligned}$$

- Four different way to obtain a large inertia!

First Component of the PCA



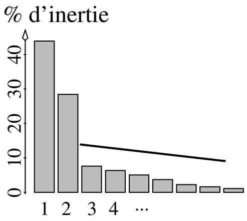
- 1D case: $\underset{\sim}{\widetilde{X}} = m + a^\top(\underline{X} - m)a$ with $\|a\| = 1$
- Inertia: $\widetilde{I} = \frac{1}{n}\sum_{i=1}^{n} a^\top(\underline{X}_i - m)(\underline{X}_i - m)^\top a$

Principal Component Analysis : optimization of the projection

- Maximization of $\widetilde{I} = \frac{1}{n}\sum_{i=1}^{n} a^\top(\underline{X}_i - m)(\underline{X}_i - m)^\top a = a^\top \Sigma a$ with $\Sigma = \frac{1}{n}\sum_{i=1}^{n}(\underline{X}_i - m)(\underline{X}_i - m)^\top$ the empirical covariance matrix.
- Explicit optimal choice given by the eigenvector of the largest eigenvalue of Σ.

Source: E. Matzner-Løber

PCA



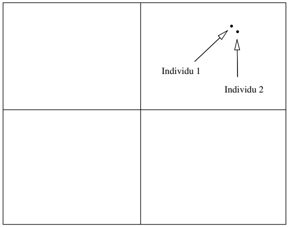
Principal Component Analysis : optimization of the projection

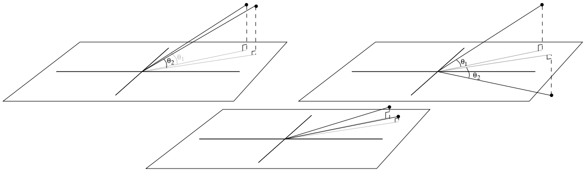
- Explicit optimal solution obtain by the projection on the eigenvectors of the largest eigenvalues of Σ.
- Projected inertia given by the sum of those eigenvalues.

- Often fast decay of the eigenvalues: some dimensions are much more important than other.
- Not exactly the curse of dimensionality setting...
- Yet a lot of *small* dimension can drive the distance!

Source: E. Matzner-Løber

PCA and Distances





Close projection doesn't mean close individuals!

- Same projections but different situations.
- Quality of the projection measured by the angle!

Source: E. Matzner-Løber

Outline

Reconstruction Error Approach

Goal

- Construct a map Φ from the space $\mathcal{X}$ into a space $\mathcal{X}'$ of **smaller dimension**:
$$\begin{aligned} \Phi : \quad & \mathcal{X} \to \mathcal{X}' \\ & \underline{X} \mapsto \Phi(\underline{X}) \end{aligned}$$
- Construct $\widetilde{\Phi}$ from $\mathcal{X}'$ to $\mathcal{X}$
- Control the error between $\underline{X}$ and its reconstruction $\widetilde{\Phi}(\Phi(\underline{X}))$

- Canonical example for $\underline{X} \in \mathbb{R}^d$: find Φ and $\widetilde{\Phi}$ in a parametric family that minimize
$$\frac{1}{n}\sum_{i=1}^{n} \|\underline{X}_i - \widetilde{\Phi}(\Phi(\underline{X}_i))\|^2$$

Principal Component Analysis

- $\mathcal{X} \in \mathbb{R}^d$ and $\mathcal{X}' = \mathbb{R}^{d'}$
- Affine model $\underline{X} \sim m + \sum_{l=1}^{d'} \underline{X}'^{(l)} V^{(l)}$ with $(V^{(l)})$ an orthonormal family.
- Equivalent to:
$$\Phi(\underline{X}) = V^\top(\underline{X} - m) \quad \text{and} \quad \widetilde{\Phi}(\underline{X}') = m + V\underline{X}'$$
- Reconstruction error criterion:
$$\frac{1}{n}\sum_{i=1}^{n} \|\underline{X}_i - (m + VV^\top(\underline{X}_i - m)\|^2$$
- **Explicit solution:** m is the empirical mean and V is any orthonormal basis of the space spanned by the d' first eigenvectors (the one with largest eigenvalues) of the empirical covariance matrix $\frac{1}{n}\sum_{i=1}^{n}(\underline{X}_i - m)(\underline{X}_i - m)^\top$.

Principal Component Analysis

PCA Algorithm

- Compute the empirical mean $m = \frac{1}{n} \sum_{i=1}^{n} \underline{X}_i$
- Compute the empirical covariance matrix $\frac{1}{n} \sum_{i=1}^{n} (\underline{X}_i - m)(\underline{X}_i - m)^\top$.
- Compute the d' first eigenvectors of this matrix: $V^{(1)}, \dots, V^{(d')}$
- Set $\Phi(\underline{X}) = V^\top(\underline{X} - m)$

- Complexity: $O(n(d + d^2) + d'd^2)$
- Interpretation:
  - $\Phi(\underline{X}) = V^\top(\underline{X} - m)$: coordinates in the restricted space.
  - $V^{(i)}$: influence of each original coordinates in the ith new one.
- **Scaling:** This method is not invariant to a scaling of the variables! It is custom to normalize the variables (at least within groups) before applying PCA.

Multiple Factor Analysis

- PCA assumes $\mathcal{X} = \mathbb{R}^d$!
- How to deal with categorical values?
- MFA = PCA with clever coding strategy for categorical values.

Categorical value code for a single variable

- Classical redundant dummy coding:
$$\underline{X} \in \{1, \ldots, V\} \mapsto P(\underline{X}) = \left(\mathbf{1}_{\underline{X}=1}, \ldots, \mathbf{1}_{\underline{X}=V}\right)^\top$$
- Compute the mean (i.e. the empirical proportions): $\overline{P} = \frac{1}{n}\sum_{i=1}^n P(\underline{X}_i)$
- *Renormalize* $P(\underline{X})$ by $1/\sqrt{(V-1)\overline{P}}$:
$$P(\underline{X}) \mapsto P^r(\underline{X})$$
$$(\mathbf{1}_{\underline{X}=1}, \ldots \mathbf{1}_{\underline{X}=V}) \mapsto \left(\frac{\mathbf{1}_{\underline{X}=1}}{\sqrt{(V-1)\overline{P}_1}}, \ldots, \frac{\mathbf{1}_{\underline{X}=V}}{\sqrt{(V-1)\overline{P}_V}}\right)$$

- χ^2 type distance!

Multiple Factor Analysis

- PCA becomes the minimization of

$$\frac{1}{n}\sum_{i=1}^{n}\|P^r(\underline{X}_i) - (m + VV^\top(P^r(\underline{X}_i) - m))\|^2$$

$$= \frac{1}{n}\sum_{i=1}^{n}\sum_{v=1}^{V} \frac{\left|\mathbf{1}_{\underline{X}_i=v} - (m' + \sum_{l=1}^{d'} V^{(l)\top}(P(\underline{X}_i) - m')V^{(l,v)})\right|^2}{(V-1)\overline{P}_v}$$

- Interpretation:
  - $m' = \overline{P}$
  - $\Phi(\underline{X}) = V^\top(P^r\underline{X} - m)$: coordinates in the restricted space.
  - $V^{(l)}$ can be interpreted s as a probability profile.
- Complexity: $O(n(V + V^2) + d'V^2)$
- Link with Correspondence Analysis (CA)

Multiple Factor Analysis

MFA Algorithm

- Redundant dummy coding of each categorical variable.
- Renormalization of each block of dummy variable.
- Classical PCA algorithm on the resulting variables

- Interpretation as a reconstruction error with a rescaled/χ^2 metric.
- Interpretation:
  - $\Phi(\underline{X}) = V^\top(P^r(\underline{X}) - m)$: coordinates in the restricted space.
  - $V^{(l)}$: influence of each modality/variable in the ith new coordinates.
- **Scaling:** This method is not invariant to a scaling of the continuous variables! It is custom to normalize the variables (at least within groups) before applying PCA.

Non Linear PCA

PCA Model

- PCA: Linear model assumption

$$\underline{X} \simeq m + \sum_{l=1}^{d'} \underline{X}^{\prime,(l)} V^{(l)} = m + V\underline{X}'$$

- with
  - $V^{(l)}$ orthonormal
  - $\underline{X}^{\prime,(l)}$ without constrains.

- Two directions of extension:
  - Other constrains on V (or the coordinates in the restricted space): ICA, NMF, Dictionary approach
  - PCA on a non linear image of $\underline{X}$: kernel-PCA
- Much more complex algorithm!

Non Linear PCA

ICA (Independent Component Analysis)

- Linear model assumption
- with
$$\underline{X} \simeq m + \sum_{l=1}^{d'} \underline{X}'^{,(l)} V^{(l)} = m + V\underline{X}'$$
  - $V^{(l)}$ without constrains.
  - $\underline{X}'^{,(l)}$ independent

NMF (Non Negative Matrix Factorization)

- (Linear) Model assumption
- with
$$\underline{X} \simeq m + \sum_{l=1}^{d'} \underline{X}'^{,(l)} V^{(l)} = m + V\underline{X}'$$
  - $V^{(l)}$ non negative
  - $\underline{X}'^{,(l)}$ non negative.

Non Linear PCA

Dictionary

- (Linear) Model assumption

$$\underline{X} \simeq m + \sum_{l=1}^{d'} \underline{X}'^{,(l)} V^{(l)} = m + V \underline{X}'$$

- with
  - $V^{(l)}$ without constrains
  - $\underline{X}'$ sparse (with a lot of 0)

kernel PCA

- Linear model assumption

$$\Psi(\underline{X} - m) \simeq \sum_{l=1}^{d'} \underline{X}'^{,(l)} V^{(l)} = V \underline{X}'$$

- with
  - $V^{(l)}$ orthonormal
  - $\underline{X}'_l$ without constrains.

Link with SVD

- Linear model assumption:

$$\underline{X} \simeq m + \sum_{l=1}^{d'} \underline{X}'^{,(l)} V^{(l)} = m + V \underline{X}'$$

- Vector rewriting

$$\underline{X}^\top \simeq m^\top + \underline{X}'^\top V^\top$$

Matrix Rewriting and Low Rank Factorization

- Matrix rewriting

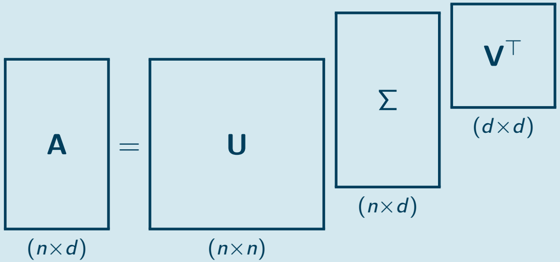
$$\underset{(n \times d)}{\boxed{\begin{array}{c} \underline{X}_1{}^\top - m^\top \\ \vdots \\ \vdots \\ \underline{X}_n{}^\top - m^\top \end{array}}} \simeq \underset{(n \times d')}{\boxed{\begin{array}{c} \underline{X}_1{}'^\top \\ \vdots \\ \vdots \\ \underline{X}_n{}'^\top \end{array}}} \underset{(d' \times d)}{\boxed{\mathbf{V}^\top}}$$

- Low rank matrix factorization! (Truncated SVD solution...)

SVD

SVD Decomposition

- Any matrix $n \times d$ matrix A can de decomposed as

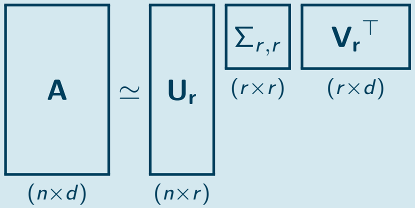


with U and V two orthononormal matrices and Σ a *diagonal* matrix with decreasing values.

SVD

Low Rank Approximation

- The best low rank approximation or rank r is obtained by restriction of the matrices to the first r dimensions:



for both the operator norm and the Frobenius norm!

- PCA: Frobenius norm, $d' = r$ and

$$\begin{pmatrix} \underline{X}_1{}^\top - m^\top \\ \vdots \\ \vdots \\ \underline{X}_n{}^\top - m^\top \end{pmatrix} \leftrightarrow A, \quad \begin{pmatrix} \underline{X}_1{}'^\top \\ \vdots \\ \vdots \\ \underline{X}_n{}'^\top \end{pmatrix} \leftrightarrow \mathbf{U_r}\Sigma_{r,r}, \quad \mathbf{V}^\top \leftrightarrow \mathbf{V_r}^\top$$

Auto Encoder

Deep Auto Encoder

- Construct a map Φ with a **NN** from the space $\mathcal{X}$ into a space $\mathcal{X}'$ of smaller dimension:

$$\begin{aligned}\Phi: \quad & \mathcal{X} \to \mathcal{X}' \\ & \underline{X} \mapsto \Phi(\underline{X})\end{aligned}$$

- Construct $\widetilde{\Phi}$ with a **NN** from $\mathcal{X}'$ to $\mathcal{X}$
- Control the error between $\underline{X}$ and its reconstruction $\widetilde{\Phi}(\Phi(\underline{X}))$:

$$\frac{1}{n}\sum_{i=1}^{n} \|\underline{X}_i - \widetilde{\Phi}(\Phi(\underline{X}_i))\|^2$$

- Optimization by gradient descent.
- NN can be replaced by another parametric function...

Outline

Pairwise Relation

- Different point of view!
- Focus on pairwise relation $\mathcal{R}(\underline{X}_i, \underline{X}_j)$.

Distance Preservation

- Construct a map Φ from the space $\mathcal{X}$ into a space $\mathcal{X}'$ of **smaller dimension**:

$$\begin{aligned} \Phi: \quad & \mathcal{X} \to \mathcal{X}' \\ & \underline{X} \mapsto \Phi(\underline{X}) = \underline{X}' \end{aligned}$$

- such that

$$\mathcal{R}(\underline{X}_i, \underline{X}_j) \sim \mathcal{R}'(\underline{X}'_i, \underline{X}'_j)$$

- Most classical version (MDS):
  - Scalar product relation: $\mathcal{R}(\underline{X}_i, \underline{X}_j) = (\underline{X}_i - m)^\top (\underline{X}_j - m)$
  - Linear mapping $\underline{X}' = \Phi(\underline{X}) = V^\top (\underline{X} - m)$.
  - Euclidean scalar product matching:

$$\frac{1}{n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} \left| (\underline{X}_i - m)^\top (\underline{X}_j - m) - (\underline{X}'_i)^\top \underline{X}'_j \right|^2$$

- Φ often defined only on $\mathcal{D}$...

MultiDimensional Scaling

MDS Heuristic

- Match the *scalar* products:
$$\frac{1}{n^2}\sum_{i=1}^{n}\sum_{j=1}^{n}\left|(\underline{X}_i - m)^\top(\underline{X}_j - m) - \underline{X}_i{'}^\top \underline{X}_j'\right|^2$$
- Linear method: $\underline{X}' = U^\top(\underline{X} - m)$ with U orthonormal

- **Beware:** $\underline{X}$ can be unknown, only the scalar products are required!
- Resulting criterion: minimization in $U^\top(\underline{X}_i - m)$ of
$$\frac{1}{n^2}\sum_{i=1}^{n}\sum_{j=1}^{n}\left|(\underline{X}_i - m)^\top(\underline{X}_j - m) - (\underline{X}_i - m)^\top UU^\top(\underline{X}_j - m)\right|^2$$
without knowing explicitly $\underline{X}$...
- Explicit solution obtained through the eigendecomposition of the know Gram matrix $(\underline{X}_i - m)^\top(\underline{X}_j - m)$ by keeping only the d' largest eigenvalues.

MultiDimensional Scaling

- In this case, MDS yields the same result than the PCA (but with different inputs, distance between observation vs correlations)!
- **Explanation:** Same SVD problem up to a transposition:
  - MDS
  $$\underline{\overline{X}}_{(n)}{}^\top \underline{\overline{X}}_{(n)} \sim \underline{\overline{X}}_{(n)}{}^\top U U^\top \underline{\overline{X}}_{(n)}$$
  - PCA
  $$\underline{\overline{X}}_{(n)} \underline{\overline{X}}_{(n)}{}^\top \sim U^\top \underline{\overline{X}}_{(n)} \underline{\overline{X}}_{(n)}{}^\top U$$
- Complexity: PCA $O((n+d')d^2)$ vs MDS $O((d+d')n^2)$...

Generalized MDS

- Preserving the scalar products amounts to preserve the euclidean distance.
- Easier **generalization** if we work in term of distance!

Generalized MDS

- Generalized MDS:
  - Distance relation: $\mathcal{R}(\underline{X}_i, \underline{X}_j) = d(\underline{X}_i, \underline{X}_j)$
  - Linear mapping $\underline{X}' = \Phi(\underline{X}) = V^\top(\underline{X} - m)$.
  - Euclidean matching:

$$\frac{1}{n^2}\sum_{i=1}^{n}\sum_{j=1}^{n}\left|d(\underline{X}_i, \underline{X}_j) - d'(\underline{X}'_i, \underline{X}'_j)\right|^2$$

- Strong connection (but no equivalence) with MDS when $d(x, y) = \|x - y\|^2$!
- **Minimization:** Simple gradient descent can be used (can be stuck in local minima).

ISOMAP

- MDS: equivalent to PCA (but more expensive) if $d(x, y) = \|x - y\|^2$!
- ISOMAP: use a *localized* distance instead to limit the influence of very far point.

ISOMAP

- For each point $\underline{X}_i$, define a neighborhood $\mathcal{N}_i$ (either by a distance or a number of points) and let

$$d_0(\underline{X}_i, \underline{X}_j) = \begin{cases} +\infty & \text{if } \underline{X}_j \notin \mathcal{N}_i \\ \|\underline{X}_i - \underline{X}_j\|^2 & \text{otherwise} \end{cases}$$

- Compute the shortest path distance for each pair.
- Use the MDS algorithm with this distance

Random Projection

Random Projection Heuristic

- Draw at random d' unit vector (direction) U_i.
- Use $\underline{X}' = U^\top(\underline{X} - m)$ with $m = \frac{1}{n}\sum_{i=1}^{n} \underline{X}_i$

- **Property:** If $\underline{X}$ lives in a space of dimension d'', then, as soon as, $d' \sim d'' \log(d'')$,
$$\|\underline{X}_i - \underline{X}_j\|^2 \sim \frac{d}{d'}\|\underline{X}'_i - \underline{X}'_j\|^2$$
- Do not really use the data!

Locally Linear Embedding

LLE Heuristic

- For each point $\underline{X}_i$, define a neighborhood $\mathcal{N}_i$ (either by a distance or a number of points).
- Compute some weights $W_{i,j}$ such that
$$W_{i,j} = 0 \quad \text{if } \underline{X}_j \notin \mathcal{N}_i$$
$$\underline{X}_i \sim \sum_j W_{i,j} \underline{X}_j$$
- Find some $\underline{X}'_i$ in a space $\mathcal{X}'$ of **smaller dimension** such that
$$\underline{X}'_i \sim \sum_j W_{i,j} \underline{X}'_j$$

- LLE: use a least square metric for the fits.

t-Stochastic Neighbor Embedding

SNE heuristic

- From $\underline{X}_i \in \mathcal{X}$, construct a set of conditional probability:
$$P_{j|i} = \frac{e^{-\|\underline{X}_i - \underline{X}_j\|^2/2\sigma_i^2}}{\sum_{k\neq i} e^{-\|\underline{X}_i - \underline{X}_j\|^2/2\sigma_i^2}} \qquad P_{i|i} = 0$$
- Find $\underline{X}'_i$ in $\mathbb{R}^{d'}$ such that the set of conditional probability:
$$Q_{j|i} = \frac{e^{-\|\underline{X}'_i - \underline{X}'_j\|^2/2\sigma_i^2}}{\sum_{k\neq i} e^{-\|\underline{X}'_i - \underline{X}'_j\|^2/2\sigma_i^2}} \qquad Q_{i|i} = 0$$
is close from P.

- **t-SNE:** use a Student-t term $(1 + \|\underline{X}'_i - \underline{X}'_j\|^2)^{-1}$ for $\underline{X}'_i$
- Minimize the Kullback-Leibler divergence $(\sum_{i,j} P_{j|i} \log \frac{P_{j|i}}{Q_{j|i}})$ by a simple gradient descent (can be stuck in local minima).
- Parameters σ_i such that $H(P_i) = -\sum_{j=1}^{n} P_{j|i} \log P_{j|i} = \text{cst}$.

UMAP

- Topological Data Analysis inspired.

Uniform Manifold Approximation and Projection

- Define a notion of asymetric scaled local proximity between neighbors:
  - Compute the k-neighborhood of $\underline{X}_i$, its diameter σ_i and the distance ρ_i between $\underline{X}_i$ and its nearest neighbor.
  - Define
    $$w_i(\underline{X}_i, \underline{X}_j) = \begin{cases} e^{-(d(\underline{X}_i,\underline{X}_j)-\rho_i)/\sigma_i} & \text{for } \underline{X}_j \text{ in the } k\text{-neighborhood} \\ 0 & \text{otherwise} \end{cases}$$
- Symmetrize into a *fuzzy* nearest neighbor criterion
  $$w(\underline{X}_i, \underline{X}_j) = w_i(\underline{X}_i, \underline{X}_j) + w_j(\underline{X}_j, \underline{X}_i) - w_i(\underline{X}_i, \underline{X}_j) w_j(\underline{X}_j, \underline{X}_i)$$
- Determine the points $\underline{X}'_i$ in a low dimensional space such that

$$\sum_{i \neq j} w(\underline{X}_i, \underline{X}_j) \log \left(\frac{w(\underline{X}_i, \underline{X}_j)}{w'(\underline{X}'_i, \underline{X}'_j)} \right) + (1 - w(\underline{X}_i, \underline{X}_j)) \log \left(\frac{(1 - w(\underline{X}_i, \underline{X}_j))}{(1 - w'(\underline{X}'_i, \underline{X}'_j))} \right)$$

- Can be performed by local gradient descent.

Graph based

Graph heuristic

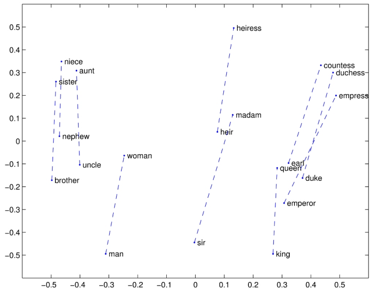
- Construct a graph with weighted edges $w_{i,j}$ measuring the *proximity* of $\underline{X}_i$ and $\underline{X}_j$ ($w_{i,j}$ large if close and 0 if there is no information).
- Find the points $\underline{X}'_i \in \mathbb{R}^{d'}$ minimizing

$$\frac{1}{n}\frac{1}{n}\sum_{i=1}^{n}\sum_{j=1}^{n} w_{i,j}\|\underline{X}'_i - \underline{X}'_j\|^2$$

- Need of a constraint on the size of $\underline{X}'_i$...
- Explicit solution through linear algebra: d' eigenvectors with smallest eigenvalues of the Laplacian of the graph $D - W$, where D is a diagonal matrix with $D_{i,i} = \sum_j w_{i,j}$.
- Variation on the definition of the Laplacian...

Outline

Word Vectors



Word Embedding

- Map from the set of words to $\mathbb{R}^d$.
- Each word is associated to a vector.
- Hope that the relationship between two vectors is related to the relationship between the corresponding words!

Source: nlp.stanford.edu

Word And Context

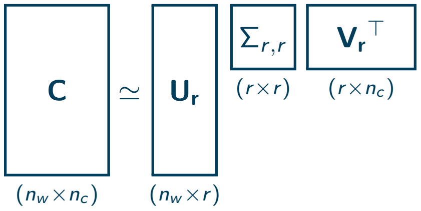
Look ! $\boxed{\text{A}}$ $\boxed{\text{single}}$ $\boxed{\textbf{word}}$ $\boxed{\text{and}}$ $\boxed{\text{its}}$ context

Word and Context

- **Idea:** characterize a word w through its relation with its context c...
- **Probabilistic description**:
  - Joint distribution: $f(w,c) = \mathbb{P}(w,c)$
  - Conditional distribution(s): $f(w,c) = \mathbb{P}(w|c)$ or $f(w,c) = \mathbb{P}(c|w)$.
  - Pointwise mutual information: $f(w,c) = \mathbb{P}(w,c)/(\mathbb{P}(w)\mathbb{P}(c))$
- Word w characterized by the vector $C_w = (f(w,c))_c$ or $C_w = (\log f(w,c))_c$.

- In practice, C is replaced by an estimate on large corpus.
- Very high dimensional model!

A (Naive) SVD Approach



Truncated SVD Approach

- Approximate the code matrix C using the truncated SVD decomposition (best low rank approximation).
- Use as a code

$$C'_w = U_{r,w}\Sigma^{\alpha}_{r,r}$$

with $\alpha \in [0, 1]$.

- Variation possible on C.
- State of the art results but computationally intensive...

A Least Square Approach

- All the previous models corresponds to
$$-log\mathbb{P}\left(w,c\right) \sim C'^t_w C''_c + \alpha_w + \beta_c$$

GloVe (Global Vectors)

- Enforce such a fit through a (weighted) least square formulation:
$$\sum_{w,c} h(\mathbb{P}\left(w,c\right)) \left\| -log\mathbb{P}\left(w,c\right) - \left(C'^t_w C''_c + \alpha_w + \beta_c\right) \right\|^2$$
with h a increasing weight.
- Minimization by alternating least square...

- Much more efficient than SVD.

A Learning Approach

Supervised Learning Formulation

- Couples (w, c) are positive examples.
- Artificially generate negative examples (w', c') (for instance by copying c and generating w' independently of c.)
- Model the probability of being positive given (w, c) as a (simple) function of the codes C'_w and C''_c

- Word2vec: logistic modeling
$$\mathbb{P}\left(1|w, c\right) = \frac{e^{C'^t_W C''_c}}{1 + e^{C'^t_W C''_c}}$$
- State of the art and efficient computation.
- Similar to a factorization of $-\log(\mathbb{P}\left(w, c\right) / (\mathbb{P}\left(w\right) \mathbb{P}\left(c\right)))$!

Outline

Clustering

- **Training data** : $\mathcal{D} = \{\underline{X}_1, \dots, \underline{X}_n\} \in \mathcal{X}^n$ (i.i.d. $\sim \mathbb{P}$)
- Latent groups?

Clustering

- Construct a map f from $\mathcal{D}$ to $\{1, \dots, K\}$ where K is a number of classes to be fixed:
$$f : \quad \underline{X}_i \mapsto k_i$$

Motivations

- Interpretation of the groups
- Use of the groups in further processing

- Several strategies possible!
- Can use dimension reduction as a preprocessing.

Outline

Partition based

Partition Heuristic

- Clustering is defined by a partition in K classes...
- that minimizes a homogeneity criterion.

K- Means

- Cluster k defined by a *center* μ_k.
- Each sample is associated to the closest center.
- Centers defined as the minimizer of $\sum_{i=1}^{n} \min_k \|\underline{X}_i - \mu_k\|^2$
- Iterative scheme (Loyd):
  - Start by a (pseudo) random choice for the centers μ_k
  - Assign each samples to its nearby center
  - Replace the center of a cluster by the mean on its assigned samples.
  - Repeat the last two steps until convergence.

Partition based

Partition based

- Other schemes:
  - McQueen: modify the mean each time a sample is assigned to a new cluster.
  - Hartigan: modify the mean by removing the considered sample, assign it to the nearby center and recompute the new mean after assignment.
- A good initialization is crucial!
  - Initialize by samples.
  - k-Mean++: try to take them as separated as possible.
  - No guarantee to converge to a global optimum: repeat and keep the best result!
- Complexity : $O(n \times K \times T)$ where T is the number of step in the algorithm.

Partition based

- k-Medoid: use a sample as a center
  - PAM: for a given cluster, use the sample that minimizes the intra distance (sum of the squared distance to the other points)
  - Approximate medoid: for a given cluster, assign the point that is the closest to the mean.
- Complexity:
  - PAM: $O(n^2 \times T)$ in the worst case!
  - Approximate medoid: $O(n \times K \times T)$ where T is the number of step in the algorithm.
- **Remark:** Any distance can be used...

Outline

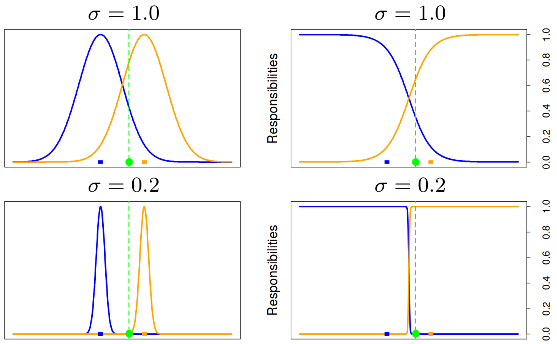
Model Based

Model Heuristic

- Use a generative model of the data:
$$\mathbb{P}\left(\underline{X}\right) = \sum_{k=1}^{K} \pi_k \mathbb{P}_{\theta_k}\left(\underline{X}|k\right)$$
where π_k are proportions and $\mathbb{P}_\theta\left(\underline{X}|k\right)$ are parametric probability models.
- Estimate those parameters (often by a ML principle).
- Assign each observations to the class maximizing the a posteriori probability (obtained by Bayes formula)
$$\frac{\widehat{\pi_k}\mathbb{P}_{\widehat{\theta_k}}\left(\underline{X}|k\right)}{\sum_{k'=1}^{K} \widehat{\pi_{k'}}\mathbb{P}_{\widehat{\theta_{k'}}}\left(\underline{X}|k'\right)}$$

- Link with Generative model in supervised classification!

Model Based



A two class example

- A mixture $\pi_1 f_1(\underline{X}) + \pi_2 f_2(\underline{X})$
- and the posterior probability $\pi_i f_i(\underline{X})/(\pi_1 f_1(\underline{X}) + \pi_2 f_2(\underline{X}))$
- Natural class assignment!

Model Based

Sub-population estimation

- A mixture $\pi_1 f_1(\underline{X}) + \pi_2 f_2(\underline{X})$
- Two populations with a parametric distribution f_i.
- Most classical choice: Gaussian distribution

Gaussian Setting

- $\underline{X}_1, \dots, \underline{X}_n$ independent
- $\underline{X}_i \sim \mathcal{N}(\mu_1, \sigma_1^2)$ with probability π_1 or $\underline{X}_i \sim \mathcal{N}(\mu_2, \sigma_2^2)$ with probability π_2
- We don't know the parameters μ_i, σ_i, π_i.
- We don't know from which distribution each $\underline{X}_i$ has been drawn.

Model Based

Maximum Likelihood

- Density: $\pi_1 \Phi(\underline{X}, \mu_1, \sigma_1^2) + \pi_2 \Phi(\underline{X}, \mu_2, \sigma_2^2)$
- log-likelihood:
$$\mathcal{L}(\theta) = \sum_{i=1}^{n} \log \left(\pi_1 \Phi(\underline{X}_i, \mu_1, \sigma_1^2) + \pi_2 \Phi(\underline{X}_i, \mu_2, \sigma_2^2) \right)$$
- No straightforward way to optimize the parameters!

What if algorithm

- Assume we know from which distribution each sample has been sampled: $Z_i = 1$ if from f_1 and $Z_i = 0$ otherwise.
- log-likelihood:
$$\sum_{i=1}^{n} Z_i \log \; \Phi(\underline{X}_i, \mu_1, \sigma_1^2) + (1 - Z_i) \log \Phi(\underline{X}_i, \mu_2, \sigma_2^2)$$
- Easy optimization
- but the Z_i are unknown...

Model Based

What if algorithm

- Assume we know from which distribution each sample has been sampled: $Z_i = 1$ if from f_1 and $Z_i = 0$ otherwise.
- log-likelihood:
$$\sum_{i=1}^{n} Z_i \log \ \Phi(\underline{X}_i, \mu_1, \sigma_1^2) + (1 - Z_i) \log \Phi(\underline{X}_i, \mu_2, \sigma_2^2)$$
- Easy optimization
- but the Z_i are unknown...

Bootstrapping Idea

- Replace Z_i by its expectaion given the current estimate.
- $\mathbb{E}\left[Z_i\right] = \mathbb{P}\left(Z_i = 1|\theta\right)$ (A posteriori probability)
- and iterate...
- Can be proved to be good idea!

Model Based

EM Algorithm

- (Random) initialization: μ_i^0, σ_i^0, π_i^0.
- Repeat:
  - Expectation (Current a posteriori probability):

$$\mathbb{E}_t\left[Z_i\right] = \mathbb{P}\left(Z_i = 1 | \theta^t\right) = \frac{\pi_1^t \Phi(\underline{X}_i, \mu_1^t, (\sigma_1^t)^2)}{\pi_1^t \Phi(\underline{X}_i, \mu_1^t, (\sigma_1^t)^2) + \pi_2^t \Phi(\underline{X}_i, \mu_2^t, (\sigma_2^t)^2)}$$

  - Maximization of

$$\sum_{i=1}^{n} \mathbb{E}_t\left[Z_i\right] \log\ \Phi(\underline{X}_i, \mu_1, \sigma_1^2) + \mathbb{E}_t\left[1 - Z_i\right] \log \Phi(\underline{X}_i, \mu_2, \sigma_2^2)$$

  to obtain μ_i^{t+1}, σ_i^{t+1}, π_i^{t+1}.

Model Based

- Large choice of parametric models.

Gaussian Mixture Model

- Use

$$\mathbb{P}_{\theta_k}\left(\underline{\vec{X}}|k\right) \sim \mathcal{N}(\mu_k, \Sigma_k)$$

with $\mathcal{N}(\mu, \Sigma)$ the Gaussian law of mean μ and covariance matrix Σ.

- Efficient optimization algorithm available (EM)
- Often some constrain on the covariance matrices: identical, with a similar structure...
- Strong connection with K-means when the covariance matrices are assumed to be the same multiple of the identity.

Model Based

Probabilistic latent semantic analysis (PLSA)

- Documents described by their word counts w
- Model:
$$\mathbb{P}\left(w\right) = \sum_{k=1}^{K} \mathbb{P}\left(k\right) \mathbb{P}_{\theta_k}\left(w|k\right)$$
with k the (hidden) topic, $\mathbb{P}\left(k\right)$ a topic probability and $\mathbb{P}\left(w|k\right)$ a multinomial law for a given topic.
- Clustering according to
$$\mathbb{P}\left(k|w\right) = \frac{\widehat{\mathbb{P}\left(k\right)}\mathbb{P}_{\widehat{\theta_k}}\left(w|k\right)}{\sum_{k'} \widehat{\mathbb{P}\left(k'\right)}\mathbb{P}_{\widehat{\theta_{k'}}}\left(w|k'\right)}$$

- Same idea than GMM!
- Bayesian variant called LDA.

Model Based

Parametric Density Estimation Principle

- Assign a probability of membership.
- Lots of theoretical studies…
- Model selection principle can be used to select K the number of class:
  - AIC / BIC /MDL penalization
  - Cross Validation is also possible!

- Complexity: $O(n \times K \times T)$

Outline

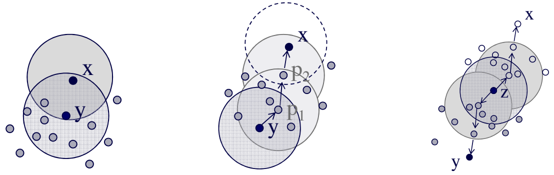
(Non Parametric) Density Based

Density Heuristic

- Cluster are connected dense zone separated by low density zone.
- Not all points belong to a cluster.

- Basic bricks:
  - Estimate the density.
  - Find points with high densities.
  - Gather those points according to the density
- Density estimation:
  - Classical kernel density estimate...
- Gathering:
  - Link points of high density and use the resulted component.
  - Move them toward top of density *hill* by following the gradient and gather all the points arriving at the same *summit*.

(Non Parametric) Density Based



- Examples:
  - DBSCAN: link point of high densities using a very simple kernel.
  - PdfCLuster: find connected zone of high density.
  - Mean-shift: move points toward top of density *hill* following an evolving kernel density estimate.
- Complexity: $O(n^2 \times T)$ in the worst case.
- Can be reduced to $O(n \log(n) T)$ if samples can be encoded in a tree structure (n-body problem type approximation).

Outline

Agglomerative Clustering

Agglomerative Clustering Heuristic

- Start with very small clusters (a sample by cluster?)
- Sequential merging of the most similar clusters...
- according to some *greedy* criterion Δ.

- Generates a hierarchy of clustering instead of a single one.
- Need to select the number of cluster afterwards.
- Several choice for the merging criterion...
- Examples:
  - Minimum Linkage: merge the closest cluster in term of the usual distance
  - Ward's criterion: merge the two clusters yielding the less inner inertia loss (k-means criterion)

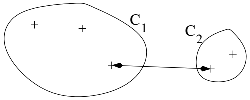
Agglomerative Clustering

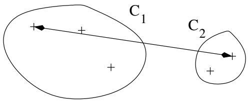
Algorithm

- Start with $(\mathcal{C}_i^{(0)}) = (\{\underline{X}_i\})$ the collection of all singletons.
- At step s, we have $n - s$ clusters $(\mathcal{C}_i^{(s)})$:
    - Find the two most similar clusters according to a criterion Δ:
      $$(i, i') = \operatorname*{argmin}_{(j,j')} \Delta(\mathcal{C}_j^{(s)}, \mathcal{C}_{j'}^{(s)})$$
    - Merge $\mathcal{C}_i^{(s)}$ and $\mathcal{C}_{i'}^{(s)}$ into $\mathcal{C}_i^{(s+1)}$
    - Keep the $n - s - 2$ other clusters $\mathcal{C}_{i''}^{(s+1)} = \mathcal{C}_{i''}^{(s)}$
- Repeat until there is only one cluster.

- Complexity: $O(n^3)$ in general.
- Can be reduced to $O(n^2)$
    - if only a bounded number of merging is possible for a given cluster,
    - for the most classical distances by maintaining a nearest neighbors list.

Agglomerative Clustering





Merging criterion based on the distance between points

- Minimum linkage:

$$\Delta(\mathcal{C}_i,\mathcal{C}_j) = \min_{\underline{X}_i\in\mathcal{C}_i}\ \min_{\underline{X}_{\in}\mathcal{C}_j} d(\underline{X}_i,\underline{X}_j)$$

- Maximum linkage:

$$\Delta(\mathcal{C}_i,\mathcal{C}_j) = \max_{\underline{X}_i\in\mathcal{C}_i}\ \max_{\underline{X}_{\in}\mathcal{C}_j} d(\underline{X}_i,\underline{X}_j)$$

- Average linkage:

$$\Delta(\mathcal{C}_i,\mathcal{C}_j) = \frac{1}{|\mathcal{C}_i||\mathcal{C}_j|}\sum_{\underline{X}_i\in\mathcal{C}_i}\ \sum_{\underline{X}_{\in}\mathcal{C}_j} d(\underline{X}_i,\underline{X}_j)$$

- Clustering based on the proximity...

Source: E. Matzner-Löber

Agglomerative Clustering

Merging criterion based on the inertia (distance to the mean)

- Ward's criterion:

$$\Delta(\mathcal{C}_i, \mathcal{C}_j) = \sum_{\underline{X}_i \in \mathcal{C}_i} \left(d^2(\underline{X}_i, \mu_{\mathcal{C}_i \cup \mathcal{C}_j}) - d^2(\underline{X}_i, \mu_{\mathcal{C}_i}) \right) + \sum_{\underline{X}_j \in \mathcal{C}_j} \left(d^2(\underline{X}_j, \mu_{\mathcal{C}_i \cup \mathcal{C}_j}) - d^2(\underline{X}_j, \mu_{\mathcal{C}_j}) \right)$$

- If d is the euclidean distance:

$$\Delta(\mathcal{C}_i, \mathcal{C}_j) = \frac{2|\mathcal{C}_i||\mathcal{C}_j|}{|\mathcal{C}_i| + |\mathcal{C}_j|} d^2(\mu_{\mathcal{C}_i}, \mu_{\mathcal{C}_j})$$

- Same criterion than in the k-means algorithm but greedy optimization.

Outline

Grid based

Grid heuristic

- Split the space in pieces
- Group those of high density according to their proximity

- Similar to density based estimate (with partition based initial clustering)
- Space splitting can be fixed or adaptive to the data.
- Examples:
  - STING (Statistical Information Grid): Hierarchical tree construction plus DBSCAN type algorithm
  - AMR (Adaptive Mesh Refinement): Adaptive tree refinement plus k-means type assignment from high density leaves.
  - CLIQUE: Tensorial grid and 1D detection.
- Linked to Divisive clustering (DIANA)

Others

Graph based

- Spectral clustering: dimension reduction + k-means.
- Message passing: iterative local algorithm.
- Graph cut: min/max flow.

- Kohonen Map,
- ...

Outline

Scalability

Large dataset issue

- When n is large, a $O(n^{\alpha} \log n)$ with $\alpha > 1$ is not acceptable!
- How to deal with such a situation?

- **Beware:** Computing all the pairwise distance requires $O(n^2)$ operations!

Ideas

- Sampling
- Online processing
- Simplification
- Parallelization

Sampling

Sampling heuristic

- Use only a subsample to construct the clustering.
- Assign the other points to the constructed clusters afterwards.

- Requires a clustering method that can assign new points (partition, model...)
- Often repetition and choice of the best clustering
- Example:
  - CLARA: K-medoid with sampling and repetition
- Two step algorithm:
  - Generate a large number n' of clusters using a fast algorithm (with $n' \ll n$)
  - Cluster the clusters with a more accurate algorithm.

Online

Online heuristic

- Modify the current clusters according to the value of a single observation.

- Requires compactly described clusters.
- Examples:
  - Add to an existing cluster (and modify it) if it is close enough and create a new cluster otherwise (k-means without reassignment)
  - Stochastic descent gradient (GMM)
- May leads to far from optimal clustering.

Simplification

Simplification heuristic

- Simplify the algorithm to be more efficient at the cost of some precision.

- Algorithm dependent!
- Examples:
  - Replace groups of observation (preliminary cluster) by the (approximate) statistics.
  - Approximate the distances by cheaper ones.
  - Use n-body type techniques.

Parallelization

Parallelization heuristic

- Split the computation on several computers.

- Algorithm dependent!
- Examples:
  - Distance computation in k-means, parameter gradient in model based clustering
  - Grid density estimation, Space splitting strategies
- Classical batch sampling not easy to perform as partitions are not easily merged...

Outline

Generative Modeling and Density Estimation

Generative Model

- Probabilistic model of the world.
- Allow to *generate* samples that mimics $\underline{X}$.
- Classical approaches are based on likelihood:
    - Parametric model,
    - Bayesian model.

Generative Algorithm

- Computational probabilistic model of the world.
- Allow to *generate* samples $G(Z)$ that mimic $\underline{X}$ from
    - a randomness source Z,
    - a computable function G.
- No explicit form of the likelihood!

- How to learn G?

A Clever Idea

$$G(Z) \sim \quad \underline{X} \; ?$$

- From estimation to...

A Clever Idea

$$\Phi(G(Z)) \sim \Phi(\underline{X})?$$

- From estimation to... discrimination

Discriminator (Goodfellow 14)

- Let
$$(\underline{\tilde{X}}, Y) = \begin{cases} (X, 1) & \text{with probability } 1/2 \\ (G(Z), 0) & \text{with probability } 1/2 \end{cases}$$
- Can we guess from $\underline{\tilde{X}}$ whether it comes from $\underline{X}$ or $G(Z)$?
- Discriminator loss = Classifier loss:

$$\mathcal{L}(D, G) = 1/2\mathbb{E}_{\underline{X}}\left[-\log D(\underline{X})\right] + 1/2\mathbb{E}_{G(Z)}\left[-\log(1 - D(G(Z)))\right]$$

Heuristic

- One can learn a discriminator from the data for a fixed G.
- The ideal generator is such that this problem is hard!

A Clever Idea

Best Discriminator

- Bayes Discriminator D^*:

$$D^*(\underline{\tilde{X}}) = \mathbb{P}\left(Y = 1 | \underline{\tilde{X}}\right) = \frac{1/2 f_{\underline{X}}(\underline{\tilde{X}})}{1/2 f_{\underline{X}}(\underline{\tilde{X}}) + 1/2 f_{G(Z)}(\underline{\tilde{X}})}$$

- Optimal loss:

$$\begin{aligned}\mathcal{L}(D^*, G) = 1/2\mathbb{E}_{\underline{X}}&\left[- \log 1/2 + - \log \frac{f_{\underline{X}}(\underline{X})}{1/2 f_{\underline{X}}(\underline{X}) + 1/2 f_{G(Z)}(\underline{X})}\right] \\ &+ 1/2\mathbb{E}_G\left[- \log 1/2 + - \log \frac{f_G(G)}{1/2 f_{\underline{X}}(G) + 1/2 f_G(G)}\right] \\ &= -1/2 KL(f_{\underline{X}}, 1/2 f_{\underline{X}} + 1/2 f_{G(Z)}) \\ &\quad - 1/2 KL(f_{G(Z)}, 1/2 f_{\underline{X}} + 1/2 f_{G(Z)}) + \log 2 \\ &= -JKL_{1/2}(f_{\underline{X}}, f_{G(Z)}) + \log 2\end{aligned}$$

- Adversarial minimization:

$$\operatorname*{argmax}_G \min_D \mathcal{L}(D, G) = \operatorname*{argmin}_G JKL_{1/2}(f_{\underline{X}}, f_{G(Z)})$$

Generative Adversarial Network

$$G^* = \underset{G}{\operatorname{argmin}} \max_{D} \left[1/2\mathbb{E}_{\underline{X}} \left[\log D(\underline{X}) \right] + 1/2\mathbb{E}_{G(Z)} \left[\log(1 - D(G(Z))) \right] \right]$$

Generative Adversarial Network

- Replace the set of all possible G and D by a set of parametric functions, for instance some deep neural networks
- Replace the expectations by some empirical means.
- Alternate a maximization on D and a minimization on G.

- Z is often $\mathcal{U}[-1,1]$ or $\mathcal{N}(0,1)$.
- Not that easy to train:
  - hard to achieve Nash equilibrium (no guaranteed convergence)
  - mode collapse (restart required)
  - support issue of KL like divergence (add noise)
  - adding feature matching helps!

GAN and f-divergence

$$D_f(P,Q) = \int f\left(\frac{p(x)}{q(x)}\right) q(x)$$
$$= sup_T \mathbb{E}_{\underline{X}\sim P}\left[T(\underline{X})\right] - \mathbb{E}_{G\sim Q}\left[f^*(T(G))\right]$$

f-divergence and dual representation

- Defines a divergence for any convex f.
- Dual representation with $f^*(x) = \sup_u \langle x, u\rangle - f(u)$

$$\min_G \sup_T \mathbb{E}_{\underline{X}\sim P}\left[T(\underline{X})\right] - \mathbb{E}_Z\left[f^*(T(G(Z)))\right]$$

f-GAN

- Replace the set of all possible G and T by a set of parametric functions, for instance some deep neural networks
- Replace the expectations by some empirical means.
- Alternate a maximization on D and a minimization on G.

Classical GAN and f-GAN

$$JKL(P,Q) = sup_T \mathbb{E}_{\underline{X}\sim P}\left[T(\underline{X})\right] - \mathbb{E}_{G\sim Q}\left[-\log(2 - exp\, T(G))\right]$$

Classical GAN as a f-GAN

- JKL-divergence is a f divergence with $f(u) = -(u+1)\log\frac{1+u}{2} + u\log u$.
- Parameterize T by $\log 2 - \log(1+e^{-T'})$ so that

$$\begin{aligned}JKL(P,Q) = &\sup_{T'} \mathbb{E}_{\underline{X}\sim P}\left[\log 2 - \log(1+e^{-T'})\right]\\ &- \mathbb{E}_{G\sim Q}\left[\log(2 - 2/(1+e^{-T'})\right]\\ = &\, 2\log 2 + \sup_{T'} \mathbb{E}_{\underline{X}\sim P}\left[\log(1/(1+e^{-T'}))\right]\\ &+ \mathbb{E}_{G\sim Q}\left[\log(1 - 1/(1+e^{-T'}))\right]\end{aligned}$$

- GAN formulation up to the parameterization of T:

$$\begin{aligned}\min_G \max_{T'} &\, \mathbb{E}_{\underline{X}}\left[\log(1/(1+e^{-T'(\underline{X})}))\right]\\ &+ \mathbb{E}_{G(Z)}\left[\log(1 - 1/(1+e^{-T'(G(Z))}))\right]\end{aligned}$$

GAN and Wasserstein

$$\begin{aligned} W(P,Q) &= \inf_{\xi\pi(P,Q)} \mathbb{E}_{(p,q)\sim\xi}\left[\|p-q\|\right] \\ &= \frac{1}{K} sup_{\|f\|_L \leq K} \mathbb{E}_{\underline{X}\sim P}\left[f(\underline{X})\right] - \mathbb{E}_{G\sim Q}\left[f(G)\right] \end{aligned}$$

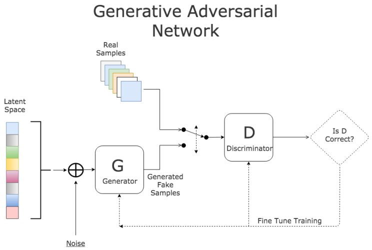
$$\min_G \sup_{\|f\|_L\leq 1} \mathbb{E}_{\underline{X}\sim P}\left[f(\underline{X})\right] - \mathbb{E}_Z\left[f(G(Z))\right]$$

WGAN

- Replace the set of all possible G and f by a set of parametric functions, for instance some deep neural networks
- Replace the expectations by some empirical means.
- Alternate a maximization on D and a minimization on G.

- Constrain on the Lipschitz norm is the most complex part:
  - clip on the network weights
  - or penalization of the gradient norm
- **Rk:** More a case of integral probability metric than optimal transport...

GAN



Generative Adversial Network

- Clever idea combined with state of the art NN architecture.
- Impressive results!

- Can it be used to perform clustering in the latent space?

Outline

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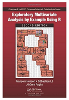
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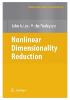
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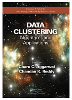
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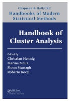
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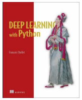
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