Institut
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INFMDI 341 Advanced Machine Learning, Semi-supervised learning

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Outline

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Learning from unlabeled data

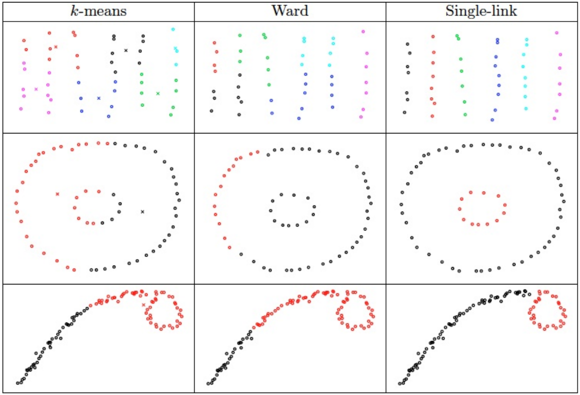
Unlabeled data

- Available data are unlabeled : documents, webpages, clients database . . .
- Labeling data is expensive and requires some expertise

Learning from unlabeled data

- Modeling probability distribution $\rightarrow$ graphical models
- Dimension reduction $\rightarrow$ pre-processing for pattern recognition
- **Clustering** : group data into homogeneous clusters $\rightarrow$ organize your data, make easier access to them, pre and post processing, application in segmentation, document retrieval, bioinformatics . . .

Different clusterings



Learning from labeled and unlabeled data

Semi-supervised learning

- Benefit from the availability of huge sets of unlabeled data
- Unlabeled data inform us about the probability distribution of the data $p(x)$
- Can we use it ? does it improve the performance of the resulting regressors/classifiers ?

Semi-supervised learning

Goal

- Labeled data : $\mathcal{S}_\ell = \{(x_1, y_1), \ldots, (x_\ell, y\ell)\}$
- Unlabeled data : $\mathcal{X}_u = \{x_{\ell+1}, \ldots, x_{\ell+u}\}$, $n = \ell + u$: available during training !
- Usually $\ell << u$
- Test data : $\mathcal{X}_{test} = \{x_{n+1}, \ldots, x_{n+m}\}$: not available during training
- **Learn a function f : $\mathcal{X} \rightarrow \mathcal{Y}$ (regression/classification) that behaves well on test data**

Outline

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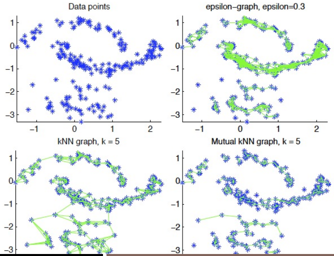
Data as nodes in a graph

- Data $x_1, \ldots, x_n$ with their similarity values $s_{ij} \geq 0$ or with their distance d_{ij} values
- Build a graph $G = (V, E)$
- vertex v_i corresponds to data x_i
- An edge w_{ij} is defined according the ϵ-graph method or the k-nn method

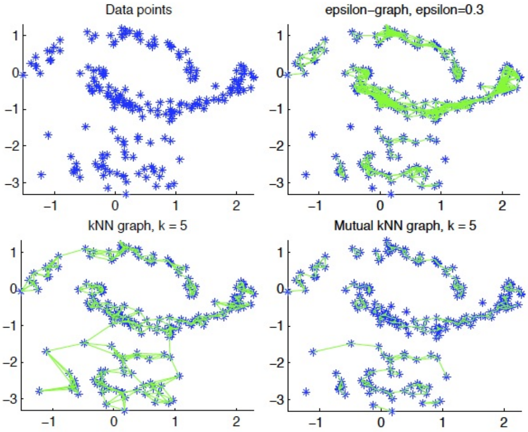
Importance of the initial graph

Several ways to construct adjacency matrix W from similarity matrix S :

- ϵ-graph : connect all points whose pairwise distance is at most ϵ (alt. whose pairwise similarity is at least ϵ
- k-nearest-neighbour-graph : connect v_i and v_j if x_i is among the k-nearest-neighbours of x_j OR x_i is among the k-nearest-neighbours of x_j

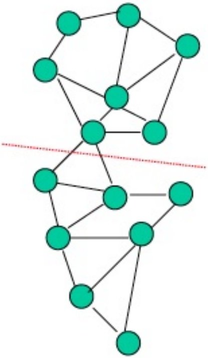


Importance of the initial graph



Clustering as a graph cut

Input of the learning algorithm : adjacency matrix W
Output : a partition into two clusters



- $Cut(A, \bar{A}) = \sum_{i \in A, j \in \bar{A}} w_{ij}$

Graph notions

Definitions

- W matrix : adjacency matrix
- Degree matrix D : $d_{ii} = \sum_j w_{ij}$, if $i \neq j$, $d_{ij} = 0$
- Graph Laplacian : L = D - W

Graph Laplacian Properties

Eigenvalues/eigenvectors

- Eigenvector u : $Lu = \lambda u$
- We notice that (D-W) 1_n = D - W.1 = 0, then the smallest eigenvalue is $\lambda_1 = 0$

Graph Laplacian Properties

Connected components

- The multiplicity of the smallest eigenvalue (0) of L is the number of connected components in the graph

$$L = \begin{pmatrix} L_1 & & & \\ & L_2 & & \\ & & \ddots & \\ & & & L_k \end{pmatrix}$$

Two-ways Spectral clustering

Clustering with Laplacian graph

- $f_i, i = 1, \ldots, n$: membership of data i to cluster 1
- $f_i = 1$ if $x_i \in Cluster1(A)$, -1 otherwise Cluster 2 ($\bar{A}$)
- Find f that minimizes $J(f)$:

$$
\begin{aligned}
J(f) &= \frac{1}{4}\sum_{i,j} w_{ij}(f_i - f_j)^2 \\
&= \frac{1}{4}\sum_{i,j} w_{ij}(f_i^2 + f_j^2 - 2f_i f_j) \\
&= \frac{1}{2} f^T (D - W) f
\end{aligned}
$$

Two-ways spectral clustering

- Avoid trivial solution : $f \perp 1_n$
- Control the complexity of f (ℓ_2 regularization) : $\sum_i f_i^2 = n$

$\min_{f \in \mathbb{R}^n} f^T L f$
subject to : $f \perp 1$, $||f|| = \sqrt{n}$

Two-ways spectral clustering

- Solve the previous relaxed problem $\rightarrow$ the vector corresponding to the second smallest eigenvalue is solution
- Threshold the values of f to get discrete values1 and -1

k-ways spectral clustering

Algorithm

- Solve the previous relaxed problem $\rightarrow$ take the k eigenvectors $(v_1, \ldots, v_k)$ corresponding to the k smallest positive eigenvalues
- Represent your data in the new space spanned by these k vectors : form the matrix V with the v_k's as column vectors
- each row of V represents an individual
- Apply k-means in the k-dimensional space

Normalized cut

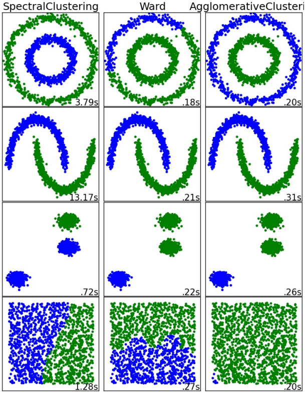
- Notations : A and B are two disjoint subsets of the nodes set V that form a partition
- $cut(A, B) = \sum_{t \in A, u \in B} w_{t,u}$
- $vol(A) = \sum_{t \in A, u \in V} w_{t,u}$
- Normalized cut (avoid isolated subset) :
  $Ncut(A, B) = \frac{cut(A,B)}{vol(A)} + \frac{cut(B,A)}{vol(B)}$

$\min_{f \in \mathbb{R}^n} \frac{f^T L f}{f^T D f}$
subject to : $f^T D1 = 0$
Solve the generalized eigenvalue problem :
$(D - W)f = \lambda D f$ which can be re-written as $D^{-\frac{1}{2}}(D - W)D^{-\frac{1}{2}} z = \lambda z$ with $z = D^{-\frac{1}{2}} f$.

Properties of spectral clustering

- Importance of the initial graph : several ways to construct it (k-neighbours)
- Able to extract clusters on a manifold
- Stability
- Model selection : eigengap

Difficult clustering tasks



- Figure from scikitkearn :
- code : spectral $=$ cluster.SpectralClustering(n$_c$*lusters* $=$ 2, *eigen$_s$olver* $='$ *arpack*$'$, *affinity* $=$ " *nearest$_n$eighbors*")

Eigengap heuristic

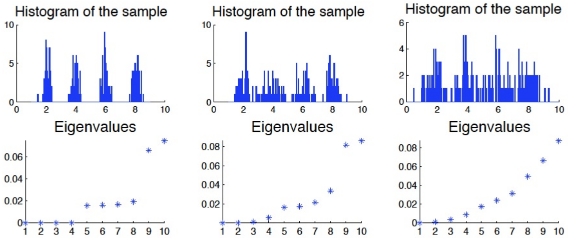


Figure 4: Three data sets, and the smallest 10 eigenvalues of L_{rw}.

- Source Tutorial U. Von Luxburg

Outline

Unsupervised and semi-supervised learning

Spectral clustering

Semi-supervised learning

References

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Semi-supervised methods

- Learn f from $\mathcal{X}$ to $\mathcal{Y}$ using $\mathcal{S}_\ell = \{(x_1, y_1), \dots, (x_\ell, y_\ell)\}$ and $\mathcal{X}_u = \{x_{\ell+1}, \dots, x_{\ell+u}\}$
- Methods
  - Self-training (including generative approaches)
  - Loss-based methods
    - Margin for unlabeled data
    - Smoothness penalty (graph-based semi-supervised learning)

Self-training

- Any classifier : f

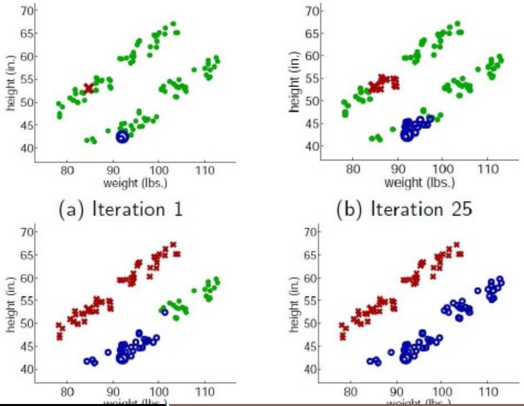
Principle

1. k=0
2. Learn f_k by training on $\mathcal{S}_k = \mathcal{S}$
3. Use f to label $\mathcal{X}_u$ and get $\mathcal{S}_{k+1}$ new set of $\ell + u$ labeled data
4. Learn f_{k+1} by training on $\mathcal{S}_{k+1}$
5. If $D(f_{k+1}, f_k)$ is small then STOP else GOTO 3

Self-training : example with k-NN (1)

- Two nice clusters without outliers [example Piyush Ray]

Base learner: KNN classifier

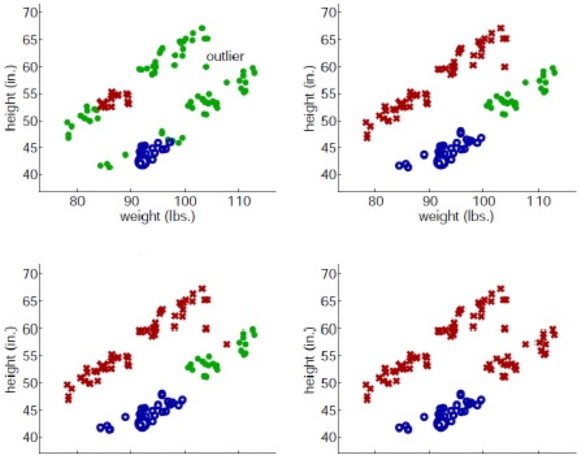


(a) Iteration 1

(b) Iteration 25

Self-training : example with k-NN (2)

- Two clusters with outliers



Semi-supervised learning with margin maximization

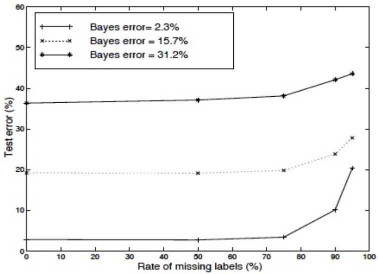
- Margin : $\rho(x, y, h) = y.h(x)$
- Which margin for unlabeled data ?
- Reinforce the confidence of the classifier
  - $\rho_2(x, h) = h(x)^2$
  - $\rho_1(x, h) = |h(x)|$
  - **Implicit assumption** : cluster assumption : data in the same cluster share the same label
- Worked for SVM, MarginBoost, ...

Semi-supervised MarginBoost

- $h_t \in \mathcal{H}$: base classifier
- Boosting model : $H_T(x) = \sum_t \alpha_t h_t(x)$
- Loss function : $J(H_t) = \sum_{i=1}^{\ell} exp(-\rho(x_i, y_i, H_t)) + \lambda \sum_{j=\ell+1}^{n} exp(-\rho_u(x_j, H_t))$

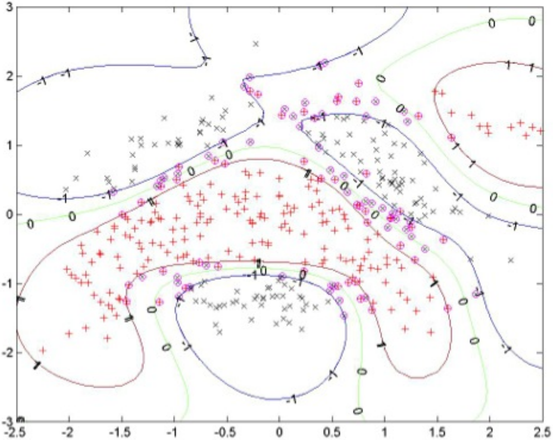
Semi-supervised MarginBoost

- Toys problems with different level of difficulty (we control Bayes error by mixing more or less the generative models)



[figure : NIPS 2001]

Data used in the previous sample



Transductive Support Vector Machine (Joachims)

In transduction, one wants to predict the outputs of the test set $y_{\ell+1}, \ldots, y_{\ell+u}$. Let us call $\mathbf{y}^* = [y_1^*, \ldots, y_u^*]$ the prediction vector. Joachims proposed a Transductive SVM with a soft margin :

TSVM

$$\underset{\mathbf{w}, y^*, b}{\text{minimize}} \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{i=1}^{\ell} \xi_i + C^* \sum_{j=1}^{u} \xi_i^*$$

under the constraints

$$y_i(\mathbf{w}^T \mathbf{x}_i + \mathrm{b}) \geq 1 - \xi_i,\ i = 1, \ldots, n$$

$$y_j^*(\mathbf{w}^T \mathbf{x}_{\ell+j} + \mathrm{b}) \geq 1 - \xi_j^*,\ i = 1, \ldots, n$$

$$y_j^* \in \{-1, +1\},\ j = 1, \ldots, u$$

Semi-supervised Support Vector Machine (S3VM)

- Bennet and Demiriz 1999, 2001
- Bennet and Demiriz proposed $\rho_1(x, h) = |h(x)|$ and an implementation of S3VM based on Mangasarian's work.
- Robust Linear Programming

Semi-supervised Support Vector Machine (S3VM) 1/2

SVM formulation :

$$\min_{w,b,\eta} C \sum_{i=1}^{t} \eta_i + \frac{1}{2}||w||^2$$
$$s.t.\ y_i[wx_i - b] + \eta_i \geqslant 1$$
$$\eta_i \geqslant 0, i = 1, \ldots, l$$

Semi-supervised Support Vector Machine (S3VM) 2/2

S3VM formulation (Bennet and Demiriz) :

$$\begin{array}{ll} \min\limits_{\mathbf{w},b,\eta,\xi,z} & C\left[\sum\limits_{i=1}^{\ell}\eta_i + \sum\limits_{j=\ell+1}^{\ell+k} min(\xi_j, z_j)\right] + \|\mathbf{w}\| \\ subject\ to & y_i(\mathbf{w}\cdot x_i + b) + \eta_i \geq 1 \quad \eta_i \geq 0 \quad i = 1,\dots,\ell \\ & \mathbf{w}\cdot x_j - b + \xi_j \geq 1 \quad \xi_j \geq 0 \quad j = \ell+1,\dots,\ell+k \\ & -(\mathbf{w}\cdot x_j - b) + z_j \geq 1 \quad z_j \geq 0 \end{array}$$

With integer variables $d_i = 0 or 1$ according it belongs to class 1 or class -1 (d has to be learned as well) :

$$\begin{array}{ll} \min\limits_{\mathbf{w},b,\eta,\xi,z,d} & C\left[\sum\limits_{i=1}^{\ell}\eta_i + \sum\limits_{j=\ell+1}^{\ell+k} (\xi_j + z_j)\right] + \|\mathbf{w}\| \\ subject\ to & y_i(\mathbf{w}\cdot x_i - b) + \eta_i \geq 1 \quad \eta_i \geq 0 \quad i = 1,\dots,\ell \\ & \mathbf{w}\cdot x_j - b + \xi_j + M(1-d_j) \geq 1 \quad \xi_j \geq 0 \quad j = \ell+1,\dots,\ell+k \\ & -(\mathbf{w}\cdot x_j - b) + z_j + Md_j \geq 1 \quad z_j \geq 0 \quad d_j = \{0,1\} \end{array}$$

Mixed integer programming.

Semi-supervised learning with a smoothness constraint

Let k be a positive definite kernel and $\mathcal{H}_k$ the unique RKHS induced by k.

Smoothness constraint / Manifold regularization 1/2

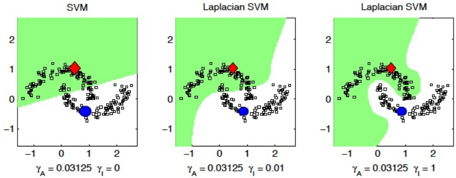
- Training data : $\mathcal{S}_\ell = \{(x_i, y_i, i =, \ldots \ell\}$ and $\mathcal{S}_u = \{x_{\ell+1}, \ldots, x_{\ell+u}\}$
- For $f \in \mathcal{H}_k$ and W a similarity matrix between data
- Impose an additional penalty that ensures smoothness of function f : for two close inputs, f takes close values
- Ref : Belkin, Nyogi and Sindwani (2006)

How to use the geometry of the marginal distribution P_x ?

The key ideas :

- We assume that a better knowledge of the marginal distribution $P_x(x)$ will give us bette knowledge of $P(Y|x)$.
- If two points x_1 and x_2 are close in the intrinsic geometry of P_x then the conditional distribution $P(y|x_1)$ and $P(y|x_2)$ will be close.

Manifold regularization



- If , the support of P_x is a submanifold $\subset \mathbb{R}^p$, then we can try to minimize the penalty :

$$||f||_I^2 = \int ||\nabla f||^2 p(x) dx$$

- ∇f is the gradient of f along the manifold
- Approximation of $||f||_I^2$:

$$||f||_I^2 \approx \sum w_{ij}(f(x_i) - f(x_j))^2,$$

Semi-supervised learning with a smoothness constraint 2/2

Let k be a positive definite kernel and $\mathcal{H}_k$ the unique RKHS induced by k.

Smoothness constraint / Manifold regularization

Minimize $J(f)$ in $\mathcal{H}_k$:

$$J(f) = \frac{1}{\ell}\sum_{i=1}^{\ell} V(x_i, y_i, f) + \lambda ||f||_k^2 + \lambda_u \sum_{ij} w_{ij}(f(x_i) - f(x_j))^2$$

Semi-supervised learning with a smoothness constraint 2/2

Let k be a positive definite kernel and $\mathcal{H}_k$ the unique RKHS induced by k.

Smoothness constraint / Manifold regularization

Minimize $J(f)$ in $\mathcal{H}_k$:

$$
\begin{aligned}
J(f) &= \frac{1}{\ell}\sum_{i=1}^{\ell} V(x_i, y_i, f) + \lambda ||f||_k^2 + \lambda_u \sum_{ij} w_{ij}(f(x_i) - f(x_j))^2 \\
&= \frac{1}{\ell}\sum_{i=1}^{\ell} V(x_i, y_i, f) + \lambda ||f||_k^2 + \lambda_u f^T L f
\end{aligned}
$$

Representer theorem

$$
\begin{aligned}
J(f) &= \frac{1}{\ell}\sum_{i=1}^{\ell} V(x_i, y_i, f) + \lambda ||f||_k^2 + \lambda_u \sum_{ij=1}^{\ell+u} w_{ij}(f(x_i) - f(x_j))^2 \\
&= \frac{1}{\ell}\sum_{i=1}^{\ell} V(x_i, y_i, f) + \lambda ||f||_k^2 + \lambda_u f^T L f
\end{aligned}
$$

Any minimizer of $J(f)$ admits a representation $\hat{f}(\cdot) = \sum_{i=1}^{\ell+u} \alpha_i k(x_i, \cdot)$

Laplacian Regularized Least Square regression

- Closed-from solution : extension of ridge regression

$$V(x_i, y_i, f) = (y_i - f(x_i))^2$$

$$\lambda_L = \frac{\lambda_u}{u+\ell}$$

$$\hat{\alpha} = (JK + \lambda\ell Id + \frac{\lambda_u \ell}{(u+\ell)^2} LK)^{-1} Y$$

K : Gram matrix for all data
J : $(\ell + u) \times (\ell + u)$ diagonal matrix with the first ℓ values equal to 1 and the remaining ones to 0.

Laplacian SVM

We choose the hinge loss functions :

$$\min_{f \in \mathcal{H}_k} \frac{1}{\ell} \sum_{i=1}^{\ell} (1 - y_i f(x_i))_+ + \lambda ||f||_k^2 + \frac{\lambda_u}{u+\ell} f^T L f$$

We benefit from the representer theorem.

Laplacian SVM

In practise, we solve :

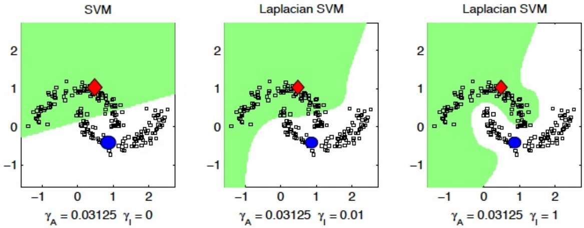
$$\min_{\alpha \in \mathbb{R}^{l+u}, \xi \in \mathbb{R}^l} \frac{1}{l} \sum_{i=1}^{l} \xi_i + \gamma_A \alpha^T K \alpha + \frac{\gamma_I}{(u+l)^2} \alpha^T K L K \alpha$$

$$\text{subject to: } y_i\left(\sum_{j=1}^{l+u} \alpha_j K(x_i, x_j) + b\right) \geq 1 - \xi_i, \quad i = 1, \ldots, l$$

$$\xi_i \geq 0 \quad i = 1, \ldots, l.$$

Laplacian SVM :results

Results : Belkin et al. 2006, JMLR.



When does semi-supervised learning work ?

- Clustering condition : if data comes from different clusters or can be easily clustered and you have one labeled data per cluster, these approaches will work
- Otherwise, and at some point (too few labeled data), it hurts

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References

- Tutorial : spectral clustering : U. Von Luxburg
- Book : Semi-supervised learning, Chapelle, Scholpkoft, Zien,MIT