Machine Learning
Semisupervised Learning

Paul Swoboda

Lecture 17, 17.12.2018

Roadmap

- What is semi-supervised learning (SSL) ? What is transduction ?
- The cluster/manifold assumption
- Graph-based SSL using regularized least squares
  1. Interpretation in terms of label propagation
  2. Interpretation in terms of a data-dependent kernel
- Experiments

Why semi-supervised learning ?

- Human labels can be expensive and time consuming,
- There is a lot of unlabeled data around us e.g. images and text on the web. The knowledge about the unlabeled data "should" be helpful to build better classifiers,

Distinction from weakly supervised learning

- one uses weaker information than full supervision e.g. instead of pixel-wise accurate object labels you just have bounding box containing the object.

What is semi-supervised learning ?

Input space X, Output: $\{-1, 1\}$ (binary classification):

- a small set L of labeled data (X_l, Y_l),
- a large set U of unlabeled data X_u.
- notation: n=l+u, total number of data points. T denotes the set of all points.

e.g. a small number of labeled images and a huge number of unlabeled images from the internet.

Definition:

- **Transduction:** Prediction of the labels Y_u of the unlabeled data X_u,
- **SSL:** Construction of a classifier $f : X \to \{-1, 1\}$ on the whole input space (using the unlabeled data).

Is it always helpful ?

No !

Because:

- in order to deal with a small amount of labeled data we have to make strong assumptions about the underlying joint probability measure $\mathrm{P}(X, Y)$ e.g. a relation of $\mathrm{P}(X)$ and $\mathrm{P}(Y|X)$.

But:

- empirical success of SSL methods shows that unlabeled data can improve performance.
- nice application of SSL (Levin et al. 2006) in user-guided image segmentation (foreground / background).

Matting

Left: Input Image with user labels, Right: Image segmentation

Approaches to SSL

The obvious one - Self Training

- use labeled data to build classifier,
- the unlabeled points on which the classifier is most "confident" are added to the label set,
- repeat until all points are labeled.

Problem:

- Wrongly assigned labels in the beginning can spoil the whole performance.
- How should we measure the confidence in the labels ?

Approaches to SSL II

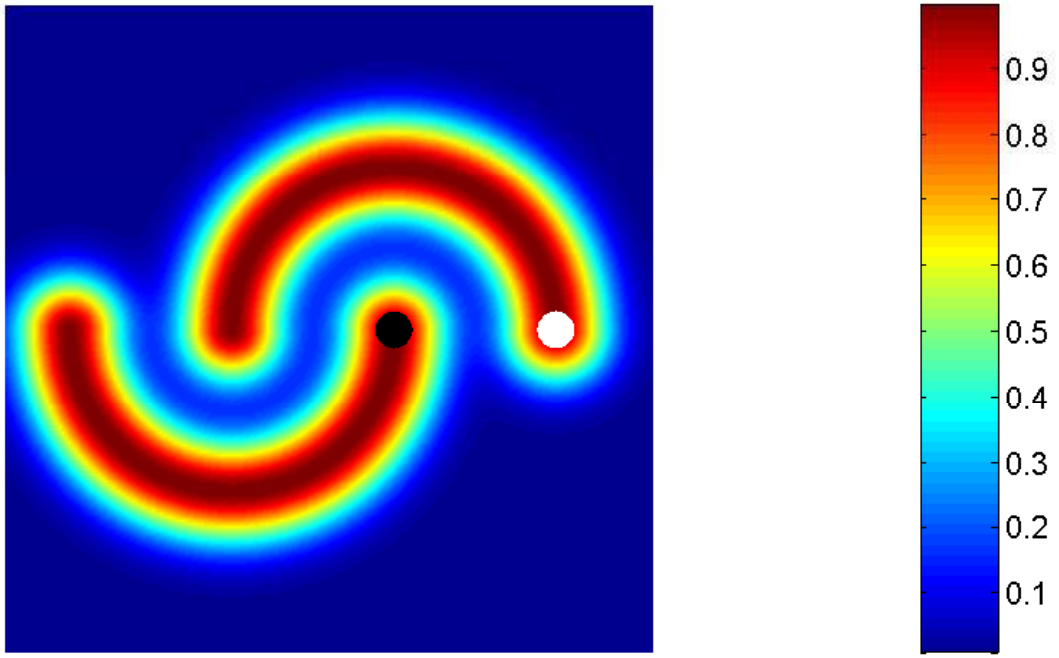
Other more principled approaches to SSL:

- Co-Training,
- Transductive SVM,
- Harmonic function,
  Regularized least squares with the graph Laplacian,
  Label Propagation
  $\Longrightarrow$ Different aspects of the same graph based method
- Low Density Separation

$\Rightarrow$ in this lecture we treat the graph-based methods using Laplacian regularization.
$\Rightarrow$ graph-based methods are very flexible (can be applied on any kind of data).

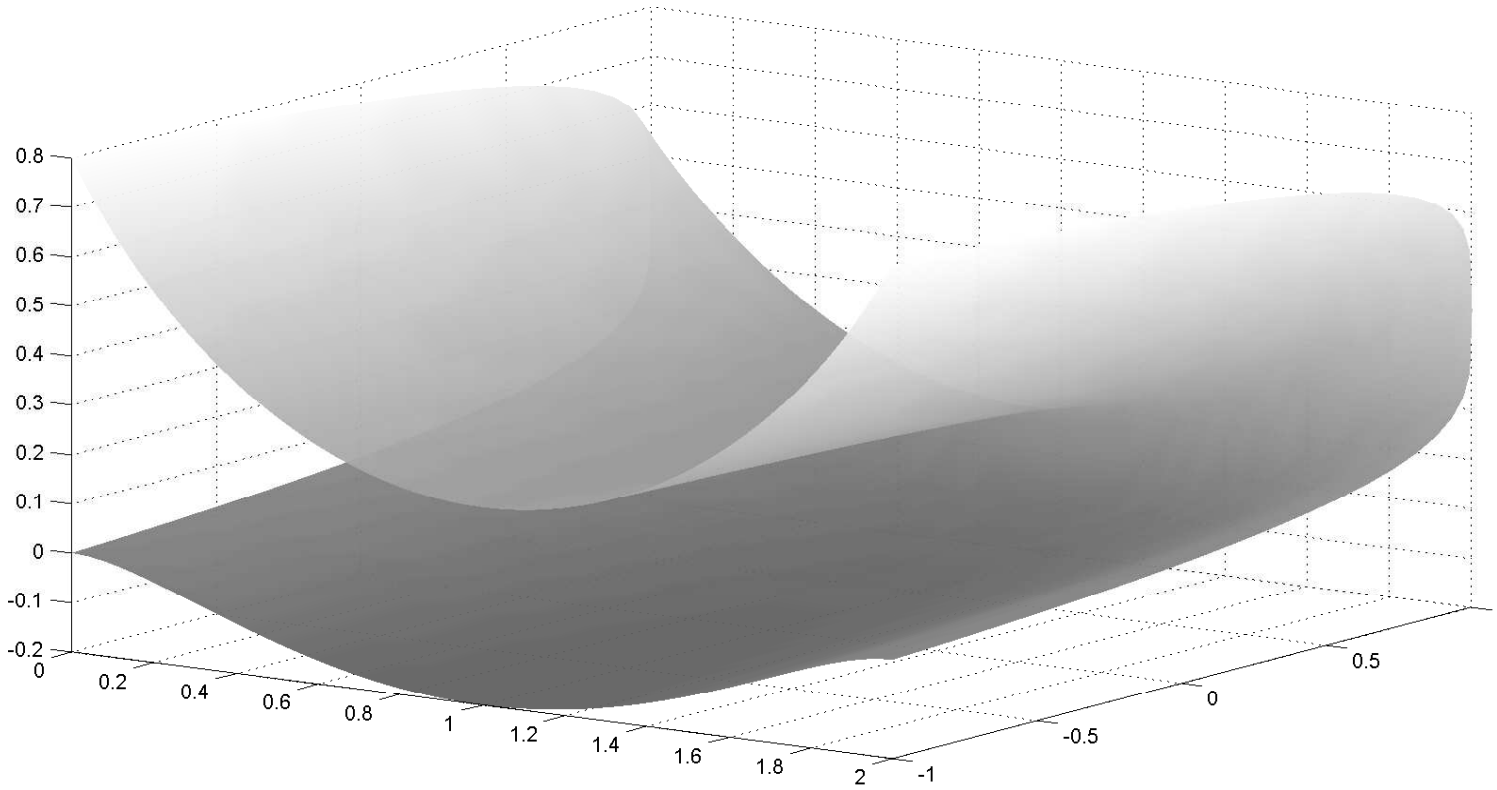
The cluster assumption

Cluster assumption: points which can be connected via (many) paths through high-density regions are likely to have the same label.



The manifold-assumption

Manifold assumption: each class lies on a separate manifold.



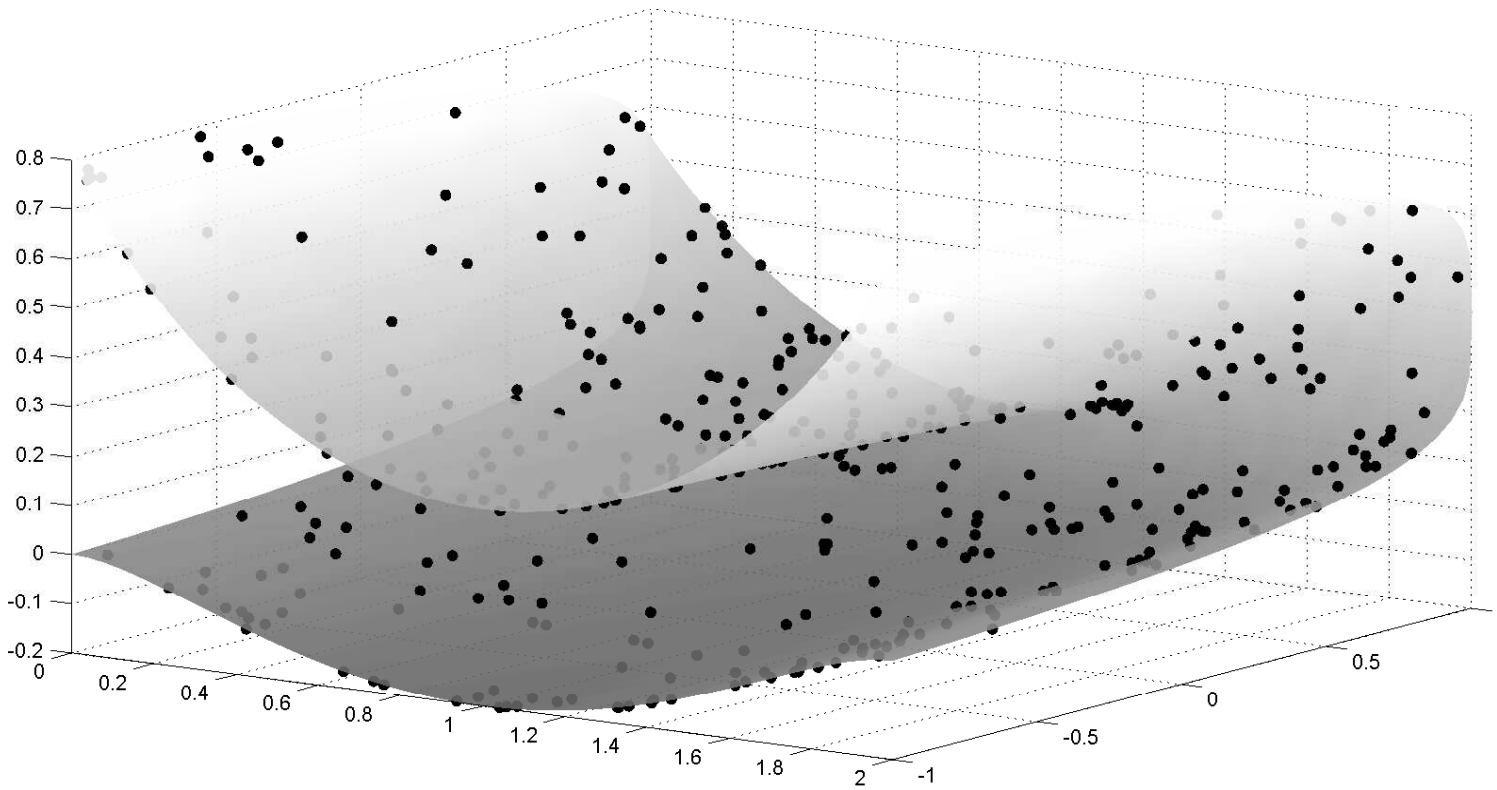
The cluster/manifold-assumption

Cluster/Manifold assumption: points which can be connected via a path through high density regions on the data manifold are likely to have the same label.

$\Longrightarrow$ Use regularizer which prefers functions which **vary smoothly along the manifold** and **do not vary in high density regions.**

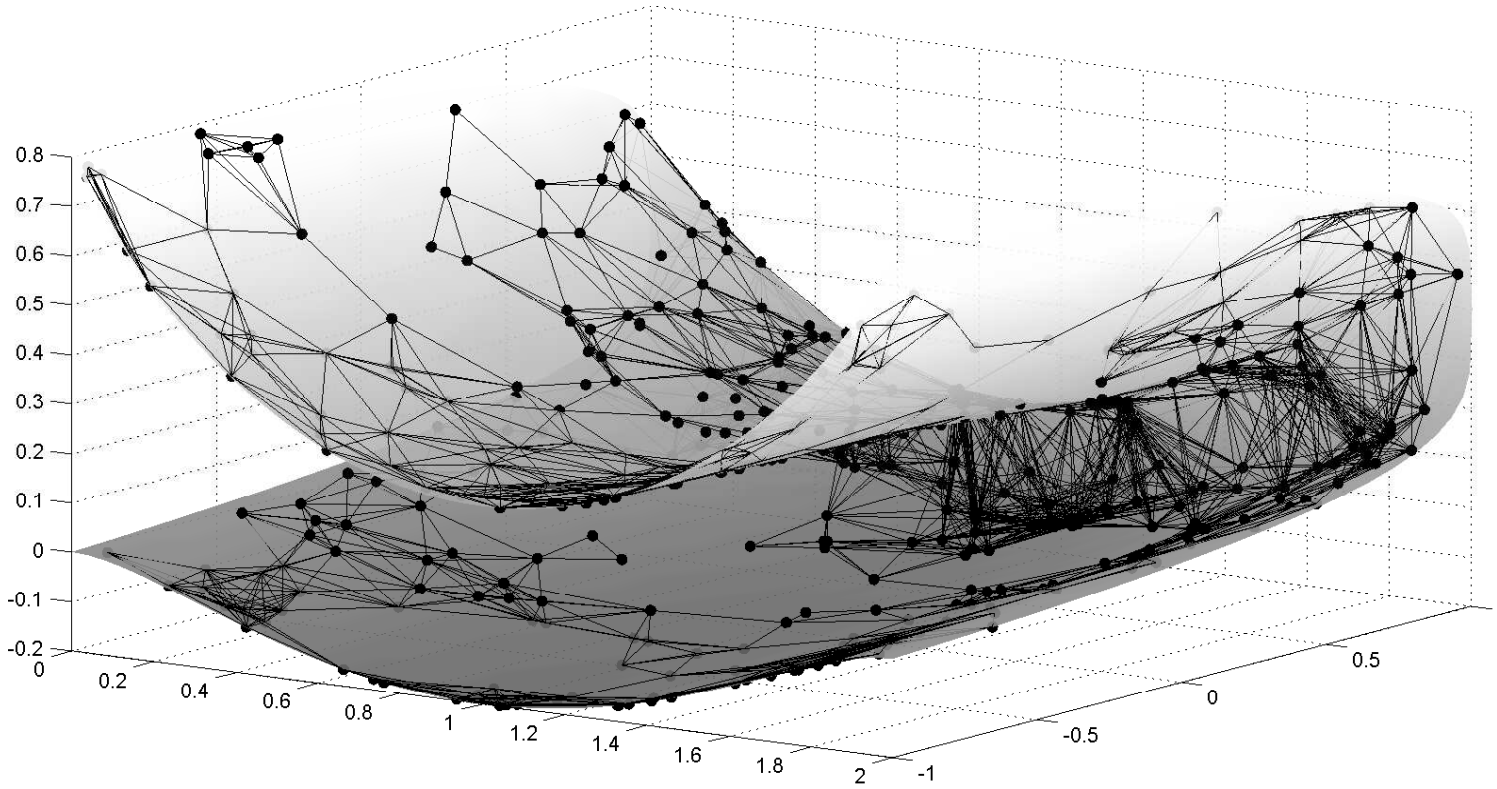
The cluster/manifold-assumption II

Problem: We have only (a lot of) unlabeled and some labeled points and no information about the density and the manifold.



The cluster/manifold-assumption III

Approach: Use a graph to approximate the manifold (and density).



How to build such graphs ?

Neighborhood graphs:

Given similarity $s : \mathcal{X} \times \mathcal{X} \to \mathbb{R}_+$ or dissimilarity measure $d : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$.
Denote by $\mathrm{kNN}(X_i)$ the k most similar or least dissimilar points.

- **k-nearest neighbor graphs:** connect points X_i to X_j if
  - $X_j \in \mathrm{knn}(X_i) \Rightarrow$ kNN-graph (directed)
  - $X_i \in \mathrm{kNN}(X_j)$ **and** $X_j \in \mathrm{kNN}(X_i)$ (mutual) $\Rightarrow$ mutual kNN-graph.
  - $X_i \in \mathrm{kNN}(X_j)$ **or** $X_j \in \mathrm{kNN}(X_i) \Rightarrow$ symmetric kNN-graph.

  The symmetric and mutual kNN-graph are undirected.
- **epsilon-graphs:** connect points X_i and X_j if
  - dissimilarity: $d(X_i, X_j) \leq \varepsilon$,
  - similarity: $s(X_i, X_j) \geq 1 - \varepsilon$,
    Assumption: $\max_{x,y} s(x, y) = \max_x s(x, x) = 1$.

  The epsilon-graph is undirected.

How to build such graphs ?

Weighted neighborhood graph:

- Gaussian weights (single scale):

$$w(X_i, X_j) = e^{-\frac{d(X_i,X_j)^2}{\sigma^2}},$$

where $\sigma^2 = \frac{1}{n(n-1)} \sum_{i \neq j} d(X_i, X_j)^2$ or chosen by cross-validation.

- Gaussian weights (adaptive scaling)

$$w(X_i, X_j) = e^{-\lambda \frac{d(X_i,X_j)^2}{\sigma_k^2}},$$

where e.g. $\sigma_k^2 = \frac{1}{2}(\mathrm{dist}_k(X_i) + \mathrm{dist}_k(X_j))$ and $\mathrm{dist}_k(X_i)$ is the distance of X_i to its k-nearest neighbor and λ is either one or chosen by cross-validation.

- Other user-defined measures...

The cluster/manifold-assumption IV

Define a regularization functional which penalizes functions which vary in high-density regions.

$$\langle f, \Delta f \rangle = \langle f, (D - W) f \rangle = \frac{1}{2} \sum_{i,j=1}^{n} w_{ij} (f_i - f_j)^2,$$

where $D = d_i \delta_{ij}$ with $d_i = \sum_{j=1}^{n} w_{ij}$ and the graph Laplacian is defined as $\Delta = D - W$.

For the ϵ-neighborhood graph one can show (Bousquet, Chapelle and H.(2003), H.(2006)) under certain technical conditions that as $\epsilon \to 0$ and $n\epsilon^m \to \infty$ (m is dimension of the manifold).

$$\lim_{n \to \infty} \frac{1}{n\epsilon^{m+2}} \sum_{i,j=1}^{n} w_{ij} (f_i - f_j)^2 \sim \int_M \|\nabla f\|^2 \, p(x)^2 dx$$

Regularized least squares

Transductive Learning via regularized least squares:

Zhu, Ghahramani, Lafferty (2002,2003):

$$\boxed{\underset{f\in\mathbb{R}^n,\, f_L=Y_L}{\arg\min} \quad \sum_{i,j\in T}^{n} w_{ij}(f_i - f_j)^2}.$$

Belkin and Niyogi (2003):

$$\boxed{\underset{f\in\mathbb{R}^n}{\arg\min} \quad \sum_{i\in L}(y_i - f_i)^2 + \frac{\lambda}{2} \sum_{i,j\in T} w_{ij}(f_i - f_j)^2}.$$

Zhou, Bousquet, Lal, Weston and Schoelkopf (2003):

$$\boxed{\underset{f\in\mathbb{R}^n}{\arg\min} \quad \sum_{i\in T}(y_i - f_i)^2 + \frac{\lambda}{2} \sum_{i,j\in T} w_{ij}\left(\frac{f_i}{\sqrt{d_i}} - \frac{f_j}{\sqrt{d_j}}\right)^2},$$

where $y_i = 0$ if $i \in U$.

Regularized least squares

$$\boxed{\underset{f\in\mathbb{R}^n}{\arg\min} \quad \sum_{i\in T}(y_i - f_i)^2 + \lambda \sum_{i,j\in T} w_{ij}\left(\frac{f_i}{\sqrt{d_i}} - \frac{f_j}{\sqrt{d_j}}\right)^2,}$$

where $y_i = 0$ if $i \in U$. Note that

$$f^T(\mathbb{1} - D^{-1/2}WD^{-1/2})f = \frac{1}{2}\sum_{i,j\in T} w_{ij}\left(\frac{f_i}{\sqrt{d_i}} - \frac{f_j}{\sqrt{d_j}}\right)^2.$$

The solution f^* can be found as:

$$\boxed{f^* = \left(\mathbb{1} + \lambda(\mathbb{1} - D^{-1/2}WD^{-1/2})\right)^{-1} Y}$$

or with $S = D^{-1/2}WD^{-1/2}$ and $\alpha = \frac{\lambda}{1+\lambda}$ $(0 < \alpha < 1)$,

$$\boxed{f^* = \frac{1}{1+\lambda}\left[\mathbb{1} - \frac{\lambda}{1+\lambda}S\right]^{-1} Y = (1-\alpha)[\mathbb{1} - \alpha S]^{-1} Y,.}$$

Label Propagation

Interpretation of the solution f^* in terms of label propagation:

$$\boxed{f^* = (1-\alpha)\Big[\mathbb{1} - \alpha S\Big]^{-1} Y}$$

One can show $[\mathbb{1} - \alpha S]^{-1} = \sum_{r=0}^{\infty} \alpha^r S^r$ if $|\alpha| \, \|S\| < 1$.

$$\boxed{f^* = (1-\alpha)\Big[\mathbb{1} - \alpha S\Big]^{-1} Y = \frac{\sum_{r=0}^{\infty} \alpha^r S^r}{\sum_{r=0}^{\infty} \alpha^r} Y}$$

Solution f^* can be interpreted as the limit $f^* = \lim_{t\to\infty} f_t$ of the iterative scheme f_t, typically $f_0 = Y$,

$$\boxed{f_{t+1} = \alpha S f_t + (1-\alpha) Y \quad \Rightarrow \quad f_{t+1} = \alpha^t S^t f_0 + (1-\alpha) \sum_{r=0}^{t} (\alpha S)^r Y,}$$

where $\lim_{t\to\infty} \alpha^t S^t f_0 = 0$.

Random walks on a graph

Given a weighted, undirected graph with n vertices we define the matrix P,

$$P = D^{-1}W,$$

P is a stochastic matrix :

- P is a $n \times n$-matrix,
- $P_{ij} \geq 0, \ \forall\, 1 \leq i, j \leq n,$
- $\sum_{j=1}^{n} P_{ij} = 1.$

Interpretation:

P_{ij} is the probability to go to vertex j when the current vertex is i.

$$P_{ij} = \mathrm{P}(X_{t+1} = j \,|\, X_t = i).$$

Random walks on a graph II

Probability measure $p_i(t) = \mathrm{P}(X_t = i)$ on the graph at time t: $\sum_{i=1}^{n} p_i(t) = 1$. **One step of the random walk:**

$$\mathrm{P}(X_{t+1} = j) = p_j(t+1) = \sum_{i=1}^{n} p_i(t) P_{ij} = \sum_{i=1}^{n} \mathrm{P}(X_{t+1} = j \,|\, X_t = i)\mathrm{P}(X_t = i).$$

This is again a probability measure,

$$\sum_{j=1}^{n} p_j(t+1) = \sum_{j=1}^{n}\sum_{i=1}^{n} p_i(t) P_{ij} = \sum_{i=1}^{n} p_i(t) \sum_{j=1}^{n} P_{ij}$$
$$= \sum_{i=1}^{n} p_i(t) = 1.$$

This is a Markov stochastic process since the probability to do the next step just depends on the current probability measure on the graph and not on previous states.

Random walks on a graph III

Stationary distribution π: A probability distribution π is stationary if

$$\pi_j = \sum_{i=1}^{n} \pi_i P_{ij}.$$

Results:

- For an undirected graph there exists a not necessarily unique stationary distribution,

$$\pi_i = \frac{d_i}{d}, \text{ where } d = \sum_{i=1}^{n} d_i,$$

  and $d_i = \sum_{j=1}^{n} w_{ij}$ (degree function).
- For an undirected graph the random walk converges to the stationary distribution if the graph is **connected** and **non-bipartite**. In this case the stationary distribution is unique.

Relation to random walks

The solution is given by

$$\boxed{f^* = (1-\alpha)\Big[\mathbb{1} - \alpha S\Big]^{-1} Y = \frac{\sum_{r=0}^{\infty} \alpha^r S^r}{\sum_{r=0}^{\infty} \alpha^r} Y}$$

Using $S = D^{-1/2} W D^{-1/2}$ we get with the stochastic matrix $P = D^{-1} W$,

$$S = D^{1/2} P D^{-1/2} \quad \text{and} \quad \boxed{S^r = D^{1/2} P^r D^{-1/2}}.$$

Plugging the expression for S^r into the equation for the solution f,

$$\boxed{f^* = D^{1/2} \frac{\sum_{r=0}^{\infty} \alpha^r P^r}{\sum_{r=0}^{\infty} \alpha^r} D^{-1/2} Y}$$

Harmonic function

Semi-supervised learning as finding a harmonic function with boundary conditions:

$$\boxed{\underset{f\in\mathbb{R}^n,\, f_L=Y_L}{\arg\min} \quad \sum_{i,j\in T}^{n} w_{ij}(f_i - f_j)^2 = \langle f, \Delta f\rangle}.$$

The solution can be found as:

$$\boxed{f_L = Y_L, \qquad \Delta f = 0.}$$

This leads to

$$\boxed{f_U = (D_{UU} - W_{UU})^{-1} W_{UL} Y_L = (\mathbb{1}_{UU} - P_{UU})^{-1} P_{UL} Y_L.}$$

where $P = D^{-1}W$ is the stochastic matrix of the random walk associated to the undirected graph.

Label Propagation

Interpretation of the solution in terms of a random walk:

$$\boxed{f_U = (D_{UU} - W_{UU})^{-1} W_{UL} Y_L = (\mathbb{1}_{UU} - P_{UU})^{-1} P_{UL} Y_L.}$$

We will use $(\mathbb{1}_{UU} - P_{UU})^{-1} = \sum_{s=0}^{\infty} (P_{UU}^s)$. Then we get for a point $i \in U$,

$$\begin{aligned}
(f_U)_i &= \sum_{k \in L} \sum_{j \in U} (\mathbb{1}_{UU} - P_{UU})^{-1}_{ij} (P_{UL})_{jk} (Y_L)_k \\
&= \sum_{k \in L} \sum_{j \in U} \sum_{s=0}^{\infty} (P_{UU}^s)_{ij} (P_{UL})_{jk} (Y_L)_k \\
&= \sum_{k \in L_+} \sum_{j \in U} \sum_{s=0}^{\infty} (P_{UU}^s)_{ij} (P_{UL})_{jk} - \sum_{k \in L_-} \sum_{j \in U} \sum_{s=0}^{\infty} (P_{UU}^s)_{ij} (P_{UL})_{jk} \\
&= \mathrm{P}(\text{hits positive points} \,|\, \text{started in } i) - \mathrm{P}(\text{hits negative points} \,|\, \text{start}
\end{aligned}$$

Do you trust all your labels ?

Relaxed version of the approach of Belkin et al:

$$\boxed{\arg\min_{f\in\mathbb{R}^n} \quad \sum_{i\in L}(y_i - f_i)^2 + \frac{\lambda}{2} \sum_{i,j\in T} w_{ij}(f_i - f_j)^2,}$$

where $\lambda > 0$ is the regularization parameter.

Extremal equations with $\Delta = D - W$:

$$(\mathbb{1} + \lambda\Delta)f = Y, \text{ on the labeled points,}$$
$$\lambda\Delta f = 0, \text{ on the unlabeled points.}$$

With $Y_i = 0$ if i-th point and $(\mathbb{1}_L)_{ij} = \begin{cases} 1 & \text{if } i = j \text{ and } i \text{ is labeled,} \\ 0 & \text{if } i \text{ is unlabeled.} \end{cases}$,

$$(\mathbb{1}_L + \lambda\Delta)f = Y.$$

Comments

- All approaches can also be interpreted as kernel machines. Let $\Delta^\dagger$ be the pseudo-inverse of the graph Laplacian. Then

$$K = \Delta^\dagger,$$

is a (data-dependent) kernel on n points. Let $f_i = \sum_{j=1}^{n} \alpha_j k(x_i, x_j)$. Then

$$f^\top \Delta f = \alpha^\top K^T \Delta K \alpha = \alpha^\top K \alpha.$$

- The structure of the graph influences significantly the result. For high-dimensional data one can improve the performance by using "Manifold Denoising" as a preprocessing method.

Experiments

- DemoSSL
- Graph structure has large influence on result (mainly unexplored area in machine learning),
- Result "can" be pretty stable with respect to the location of the labeled points,
- If cluster assumption is not valid then SSL does not help (in the worst case it yields even a worse performance).
- for a few labeled points (say 10 times the number of classes) cross validation works already pretty well.