Machine Learning
Semisupervised Learning

Prof. Matthias Hein

Machine Learning Group
Department of Mathematics and Computer Science
Saarland University, Saarbrücken, Germany

Lecture 19, 17.01.2014

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,

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 !

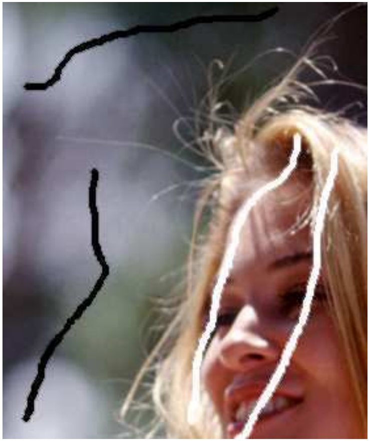
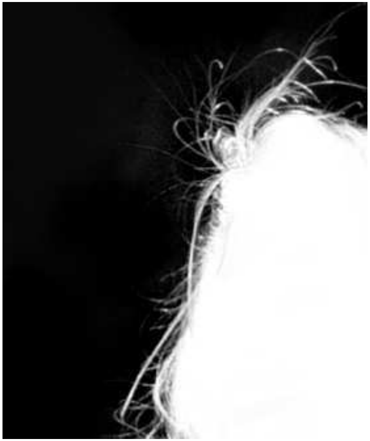
Because:

- 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 from an unexpected side: spectral matting (Levin et al. 2006) a kind of user-interactive 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

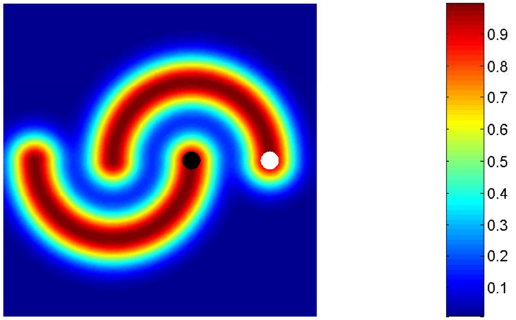
Other more principled approaches to SSL:

- 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).

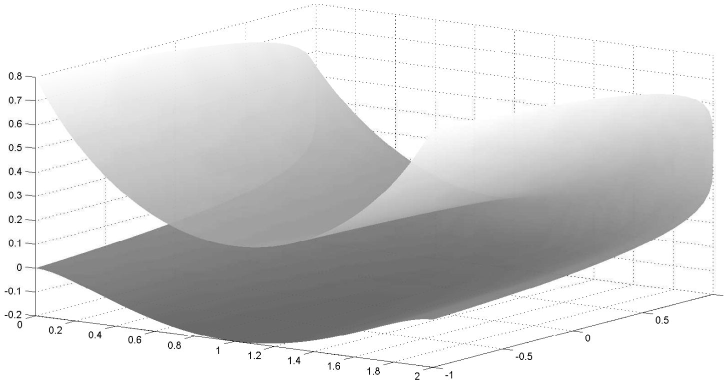
The cluster assumption

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



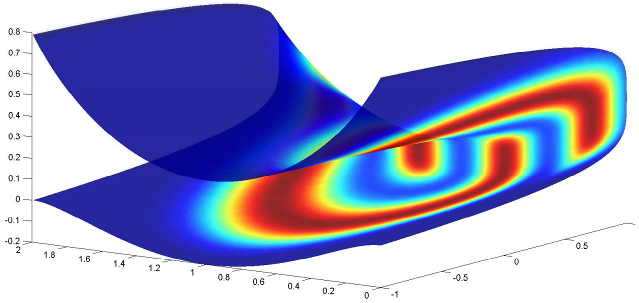
The manifold-assumption

Manifold assumption: each class lies on a separate manifold.



The cluster/manifold-assumption

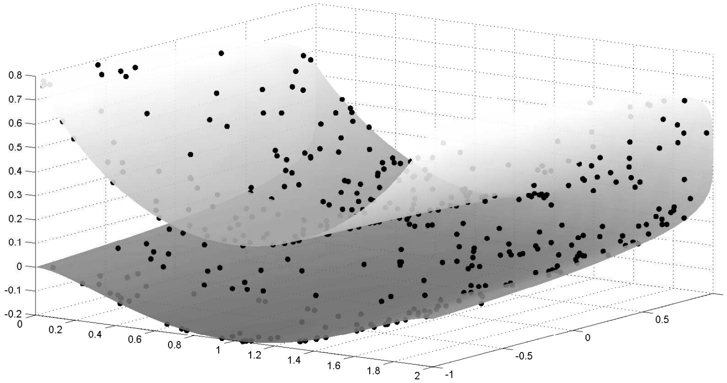
Cluster/Manifold assumption: points which can be connected via a path through high density regions on the data manifold are likely to have the same label.



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

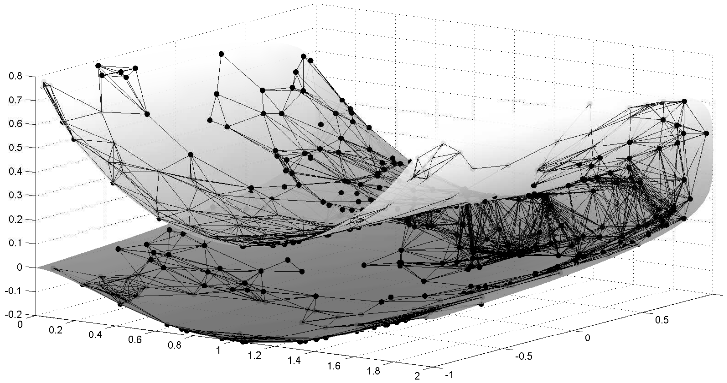
The cluster/manifold-assumption II

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):

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

Belkin and Niyogi (2003):

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

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

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

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

Regularized least squares

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

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

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

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 $|\alpha| \, \|S\| \leq 1$.

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

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,

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

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 $i \in U$,

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

Do you trust all your labels ?

Relaxed version of the approach of Belkin et al:

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

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

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

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

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.