Semi-Supervised Learning

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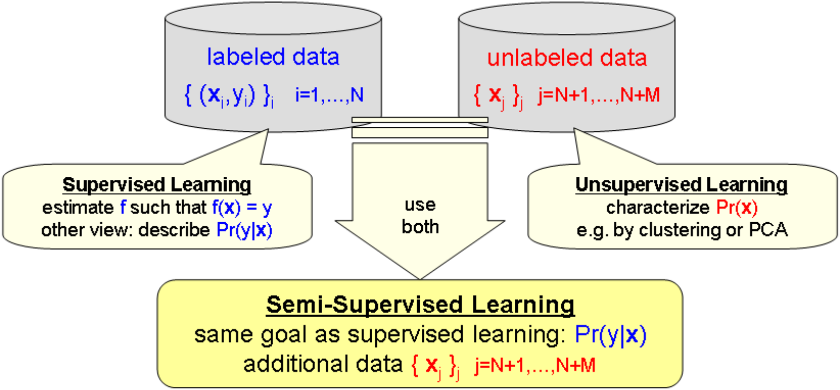
of the Max Planck Society

FIRST

Outline



In this lecture: SSL = semi-supervised *classification*.

Why Semi-Supervised Learning (SSL)?

- **labeled data**: labeling usually
  - ... requires experts
  - ... costs time
  - ... is boring
  - ... requires measurements and devices
  - ... costs money

  $\Rightarrow$ scarce, expensive

- **unlabeled data**: can often be
  - ... measured automatically
  - ... found on the web
  - ... retrieved from databases and collections

  $\Rightarrow$ abundant, cheap ... "for free"

Web page / image classification

labeled:

- someone has to read the text
- labels may come from huge ontologies
- hence has to be done conscientiously

unlabeled:

- billions available at no cost

Protein function prediction from sequence

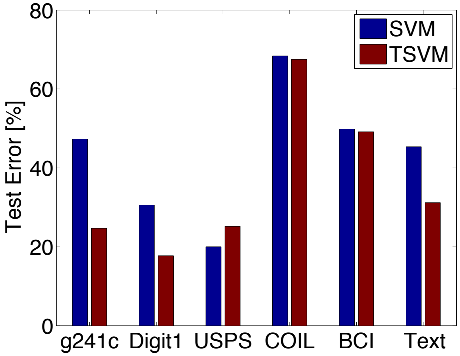
labeled:

- measurement requires human ingenuity
- can take years for a single label!

unlabeled:

- protein sequences can be predicted from DNA
- DNA sequencing now industrialized
- $\Rightarrow$ millions available

Can unlabeled data aid in classification?



10 labeled points
∼1400 unlabeled points

SVM: supervised
TSVM: semi-supervised

Yes.

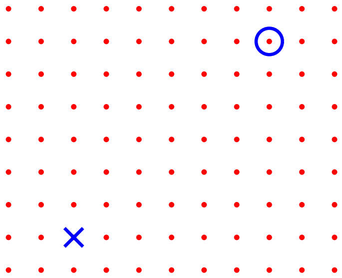
Outline

1. Why Semi-Supervised Learning?

2. Why and How Does SSL Work?
   - Generative Models
   - The Semi-Supervised SVM (S^3VM)
   - Graph-Based Methods
   - Further Approaches (incl. Co-Training, Transduction)

3. Summary and Outlook

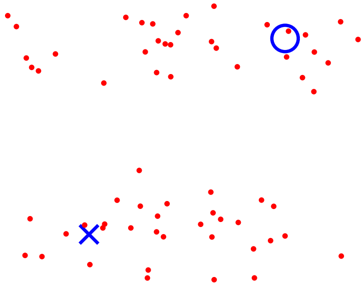
Why would unlabeled data be useful at all?



- Uniformly distributed data do not help.
- Must use properties of $Pr(\mathbf{x})$.

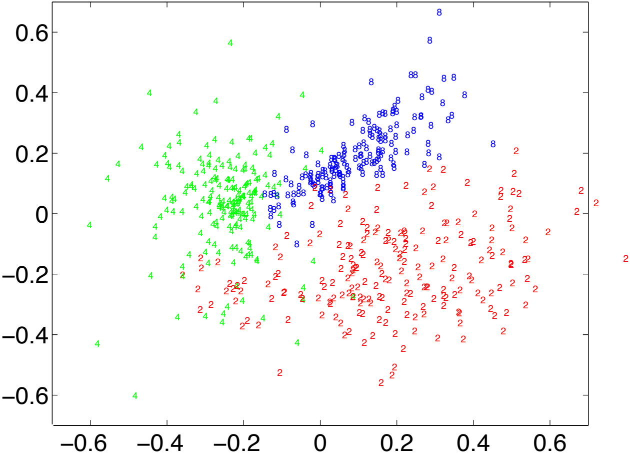
Cluster Assumption

1. The data form clusters.
2. Points in the **same cluster** are likely to be of the **same class**.



Don't confuse with the standard **Supervised Learning Assumption**: similar (ie nearby) points tend to have similar labels.

Example: 2D view on **handwritten digits 2, 4, 8**



[non-linear 2D-embedding with "Stochastic Neighbor Embedding"]

- The cluster assumption seems to hold for many real data sets.
- Many SSL algorithms (implicitly) make use of it.

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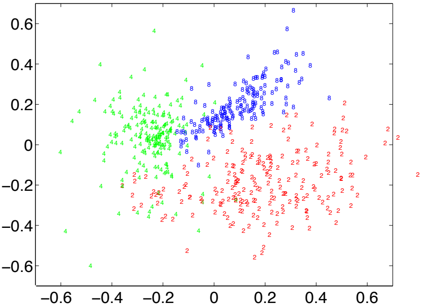
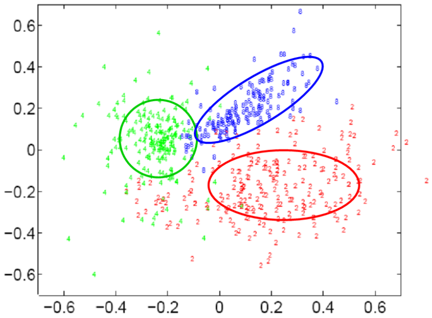
Generative model: $Pr(\mathbf{x}, y)$

Gaussian mixture model:

- one Gaussian cluster for each class
- $Pr(\mathbf{x}, y) \;=\; Pr(\mathbf{x}\,|y)\,Pr(y) \;=\; \mathcal{N}(\mathbf{x}|\mu_y, \mathbf{\Sigma}_y)\,Pr(y)$



Does this model match our cluster assumption?



This generative model is much stronger:

- Exactly one cluster for each class.
- Clusters have Gaussian shape.

Likelihood (assuming independently drawn data points)

$$\begin{aligned} Pr\,(data\,|\theta\,) &= \prod_i Pr\,(\mathbf{x}_i, y_i\,|\theta\,) \prod_j Pr\,(\mathbf{x}_j\,|\theta\,) \\ &= \prod_i Pr\,(\mathbf{x}_i, y_i\,|\theta\,) \prod_j \sum_y Pr\,(\mathbf{x}_j, y\,|\theta\,) \end{aligned}$$

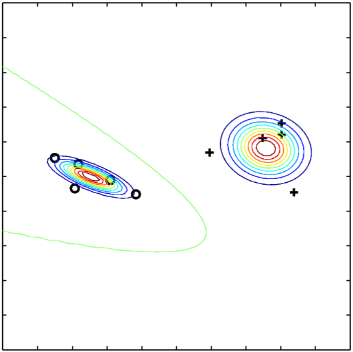
Minimize negative log likelihood:

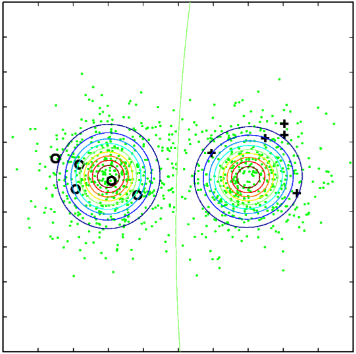
$$-\log \mathcal{L}\,(\theta) = \underbrace{-\sum_i \log Pr\,(\mathbf{x}_i, y_i\,|\theta\,)}_{\textit{typically convex}} \underbrace{-\sum_j \log\left(\sum_y Pr\,(\mathbf{x}_j, y\,|\theta\,)\right)}_{\textit{typically non-convex}}$$

Standard tool for optimization (=training):
Expectation-Maximization (EM) algorithm

only labeled data

with unlabeled data





from [Semi-Supervised Learning, ICML 2007 Tutorial; Xiaojin Zhu]

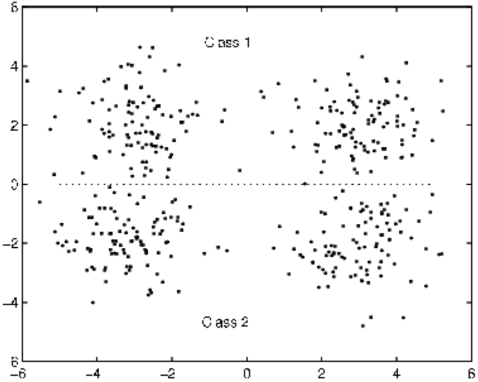
Disadvantages of Generative Models

- non-convex optimization
  $\Rightarrow$ may pick bad local minima

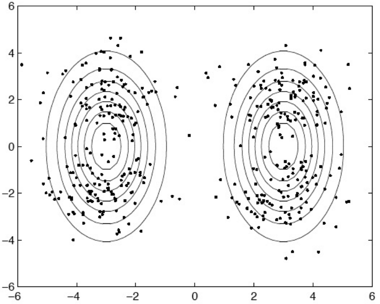
- often discriminative methods are more accurate
  - generative model: $Pr\left(\mathbf{x}, y\right)$
  - discriminative model: $Pr\left(y\left|\mathbf{x}\right.\right)$
    less modelling assumtions (about $Pr\left(\mathbf{x}\right)$)

- with mis-specified models, unlabeled data can hurt!

Unlabeled data can be misleading...



from [Semi-Supervised Learning, ICML 2007 Tutorial; Xiaojin Zhu] high likelihood wrong | low likelihood correct



from [Semi-Supervised Learning, ICML 2007 Tutorial; Xiaojin Zhu]

it is important to use a “correct” model

Discriminative model: $Pr\left(y\,|\mathbf{x}\right)$

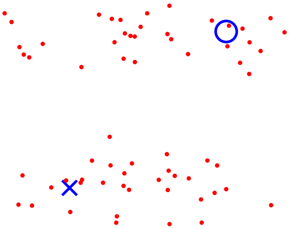
$$\mathcal{L}\left(\theta\right) \quad = \quad \prod_i Pr\left(y_i\,|\mathbf{x}_i, \theta\right)$$

Problem!

Density of $\mathbf{x}$ does not help to estimate conditional $Pr\left(y\,|\mathbf{x}\right)$!

Cluster Assumption

Points in the **same cluster** are likely to be of the **same class**.



Equivalent assumption:

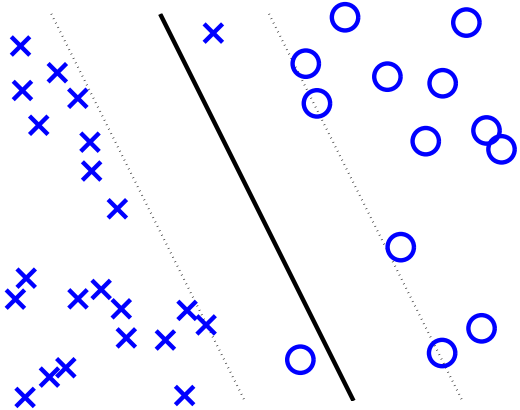
Low Density Separation Assumption

The decision boundary lies in a low density region.

$\Rightarrow$ Algorithmic idea: **Low Density Separation**

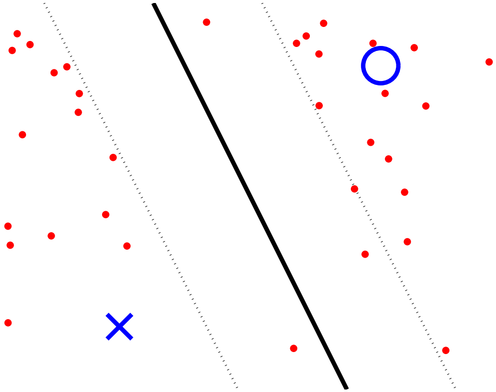
Outline

soft margin
SVM



$$\min_{\mathbf{w},b,(\xi_k)} \quad \begin{array}{c}\frac{1}{2}\langle \mathbf{w}, \mathbf{w}\rangle \\ +C\sum_i \xi_i\end{array} \quad s.t. \quad \begin{array}{c}\xi_i \geq 0 \\ y_i(\langle \mathbf{w}, \mathbf{x}_i\rangle + b) \geq 1 - \xi_i\end{array}$$

soft margin
S^{3}VM



$$\min_{\mathbf{w},b,(y_j),(\xi_k)} \quad \begin{array}{c} \frac{1}{2}\langle \mathbf{w},\mathbf{w}\rangle \\ +C\sum_i \xi_i \\ +C^*\sum_j \xi_j \end{array} \quad s.t. \quad \begin{array}{c} \xi_i \geq 0 \quad \xi_j \geq 0 \\ y_i(\langle \mathbf{w},\mathbf{x}_i\rangle + b) \geq 1-\xi_i \\ y_j(\langle \mathbf{w},\mathbf{x}_j\rangle + b) \geq 1-\xi_j \end{array}$$

Supervised Support Vector Machine (SVM)

$$\min_{\mathbf{w},b,(\xi_k)} \quad \begin{array}{c} \frac{1}{2}\langle\mathbf{w},\mathbf{w}\rangle \\ +C\sum_i \xi_i \end{array} \quad s.t. \quad \begin{array}{c} \xi_i \geq 0 \\ y_i(\langle\mathbf{w},\mathbf{x}_i\rangle + b) \geq 1 - \xi_i \end{array}$$

- maximize margin on (labeled) points
- convex optimization problem (QP, quadratic programming)

Semi-Supervised Support Vector Machine (S^{3}VM)

$$\min_{\mathbf{w},b,(y_j),(\xi_k)} \quad \begin{array}{c} \frac{1}{2}\langle\mathbf{w},\mathbf{w}\rangle \\ +C\sum_i \xi_i \\ +C^*\sum_j \xi_j \end{array} \quad s.t. \quad \begin{array}{c} \xi_i \geq 0 \quad \xi_j \geq 0 \\ y_i(\langle\mathbf{w},\mathbf{x}_i\rangle + b) \geq 1 - \xi_i \\ y_j(\langle\mathbf{w},\mathbf{x}_j\rangle + b) \geq 1 - \xi_j \end{array}$$

- maximize margin on labeled and unlabeled points
- also QP?

$$\min_{\mathbf{w},b,(y_j),(\xi_k)} \quad \frac{1}{2}\langle \mathbf{w},\mathbf{w}\rangle + C\sum_i \xi_i + C^*\sum_j \xi_j$$

$$s.t. \quad \begin{array}{ll} y_i(\langle \mathbf{w},\mathbf{x}_i\rangle + b) \geq 1-\xi_i & \xi_i \geq 0 \\ y_j(\langle \mathbf{w},\mathbf{x}_j\rangle + b) \geq 1-\xi_j & \xi_j \geq 0 \end{array}$$

Problem!

- y_j **are discrete!**
- **Combinatorial** task.
- **NP-hard!**

Optimization methods used for S^{3}VM training

exact:

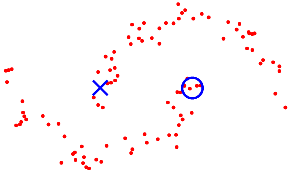
- Mixed Integer Programming [Bennett, Demiriz; NIPS 1998]
- Branch & Bound [Chapelle, Sindhwani, Keerthi; NIPS 2006]

approximative:

- self-labeling heuristic S^{3}VM^{light} [T. Joachims; ICML 1999]
- gradient descent [Chapelle, Zien; AISTATS 2005]
- CCCP-S^{3}VM [R. Collobert et al.; ICML 2006]
- contS^{3}VM [Chapelle et al.; ICML 2006]

"Two Moons" toy data

- easy for human (0% error)
- hard for S^{3}VMs!



S^{3}VM optimization method		test error	objective value
global min.	{Branch & Bound	0.0%	7.81
find local minima	CCCP	64.0%	39.55
	S^{3}VM^{light}	66.2%	20.94
	∇S^{3}VM	59.3%	13.64
	cS^{3}VM	45.7%	13.25

- **S^{3}VM objective function is good for SSL**
- exact optimization: only possible for small datasets
- approximate optimization: **method matters!**

Self-Labeling aka "Self-Training"

iterative wrapper around any supervised base-learner:

1. train base-learner on labeled (incl. self-labeled) points
2. predict on unlabeled points
3. assign most confident predictions as labels

problem: early mistakes may reinforce themselves

self-labeling approach with SVMs $\Rightarrow$ heuristic for S^{3}VMs

variant used in S^{3}VM^{light}:

1. use predictions on all unlabeled data
2. given them initially low, then increasing weight in base-learner

$$\min_{\mathbf{w},b,({\color{red}y_j}),(\xi_k)} \quad \frac{1}{2}\langle \mathbf{w},\mathbf{w}\rangle + C\sum_i \xi_i + C^*\sum_j \xi_j$$

$$s.t. \quad \begin{array}{ll} {\color{blue}y_i}(\langle \mathbf{w}, {\color{blue}\mathbf{x}_i}\rangle + b) \geq 1 - \xi_i & \xi_i \geq 0 \\ {\color{red}y_j}(\langle \mathbf{w}, {\color{red}\mathbf{x}_j}\rangle + b) \geq 1 - \xi_j & \xi_j \geq 0 \end{array}$$

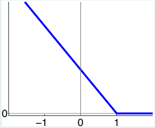
Effective Loss Functions

$$\xi_i = \max\left\{1 - {\color{blue}y_i}(\langle \mathbf{w}, {\color{blue}\mathbf{x}_i}\rangle + b), 0\right\}$$

$$\xi_j = \max_{{\color{red}y_j}\in\{+1,-1\}}\left\{1 - {\color{red}y_j}(\langle \mathbf{w}, {\color{red}\mathbf{x}_j}\rangle + b), 0\right\}$$

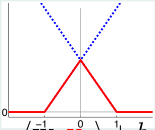
loss functions

ξ_i



${\color{blue}y_i}(\langle \mathbf{w}, {\color{blue}\mathbf{x}_i}\rangle + b)$

ξ_j



$\langle \mathbf{w}, {\color{red}\mathbf{x}_j}\rangle + b$

$$\min_{\mathbf{w},b,(y_j),(\xi_k)} \quad \frac{1}{2}\langle \mathbf{w},\mathbf{w}\rangle + C\sum_i \xi_i + C^*\sum_j \xi_j$$

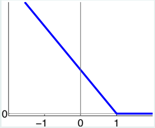
$$s.t. \quad \begin{array}{ll} y_i(\langle \mathbf{w},\mathbf{x}_i\rangle + b) \geq 1-\xi_i & \xi_i \geq 0 \\ y_j(\langle \mathbf{w},\mathbf{x}_j\rangle + b) \geq 1-\xi_j & \xi_j \geq 0 \end{array}$$

Resolving the Constraints

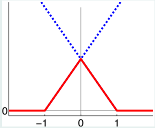
$$\frac{1}{2}\langle \mathbf{w},\mathbf{w}\rangle + C\sum_i \ell_l\left(y_i(\langle \mathbf{w},\mathbf{x}_i\rangle + b)\right) + C^*\sum_j \ell_u\left(\langle \mathbf{w},\mathbf{x}_j\rangle + b\right)$$

loss functions

ℓ_l



ℓ_u

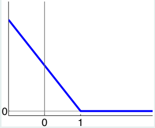


$$\frac{1}{2}\langle \mathbf{w}, \mathbf{w} \rangle + C \sum_i \ell_l \left(y_i(\langle \mathbf{w}, \mathbf{x}_i \rangle + b) \right) + C^* \sum_j \ell_u \left(\langle \mathbf{w}, \mathbf{x}_j \rangle + b \right)$$

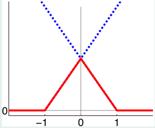
S^{3}VM as Unconstrained Differentiable Optimization Problem

original loss functions

ℓ_l

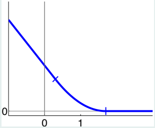


ℓ_u

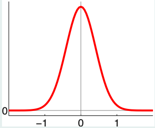


smooth loss functions

ℓ_l



ℓ_u



$$\frac{1}{2}\langle \mathbf{w}, \mathbf{w} \rangle + C \sum_i \ell_l\left(y_i(\langle \mathbf{w}, \mathbf{x}_i \rangle + b)\right) + C^* \sum_j \ell_u\left(\langle \mathbf{w}, \mathbf{x}_j \rangle + b\right)$$

∇S^{3}VM [Chapelle, Zien; AISTATS 2005]

- simply do gradient descent!
- thereby stepwise increase C^*

contS^{3}VM [Chapelle et al.; ICML 2006]

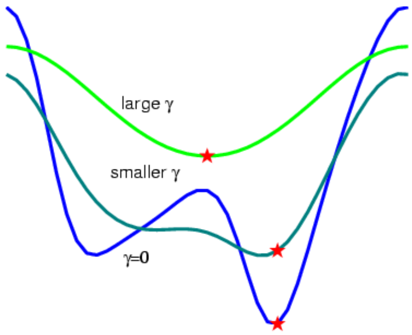
next slide...

The Continuation Method in a Nutshell

Procedure

1. smooth function until convex
2. find minimum
3. track minimum while decreasing amount of smoothing

Illustration

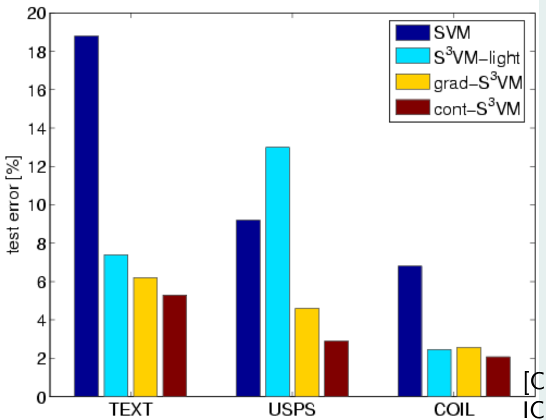


Comparison of S^{3}VM Optimizers on Real World Data

Three tasks ($N = 100$ labeled, $M \approx 2000$ unlabeled points each)

- TEXT
  - do newsgroup texts refert to mac or to windows?
    $\Rightarrow$ binary classification
  - bag of words representation: $\sim$7500 dimensions, sparse
- USPS
  - recognize handwritten digits
  - 10 classes $\Rightarrow$ 45 one-vs-one binary tasks
  - 16×16 pixel image as input (256 dimensions)
- COIL
  - recognize 20 objects in images: 20 classes
  - 32×32 pixel image as input (1024 dimensions)

Comparison of S^{3}VM Optimization Methods



- averaged over splits (and pairs of classes)
- fixed hyperparams (close to hard margin)
- similar results for other hyperparameter settings

[Chapelle, Chi, Zien; ICML 2006]

⇒ **Optimization matters**

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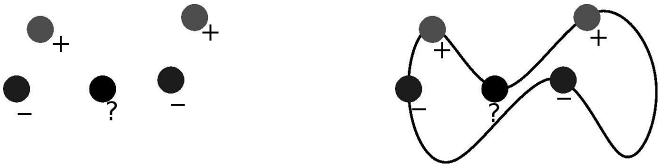
Manifold Assumption

1. The data lie on (or close to) a low-dimensional manifold.
2. Its intrinsic distance is relevant for classification.



[images from "The Geometric Basis of Semi-Supervised Learning", Sindhwani, Belkin, Niyogi in "Semi-Supervised Learning" Chapelle, Schölkopf, Zien]

Algorithmic idea: use **Nearest-Neighbor Graph**

Graph Construction

- nodes: data points $\mathbf{x}_k$, labeled and unlabeled
- edges: every edge $(\mathbf{x}_k, \mathbf{x}_l)$ weighted with $a_{kl} \geq 0$
- weights: represent similarity, eg $a_{kl} = \exp(-\gamma \|\mathbf{x}_k - \mathbf{x}_l\|)$
- adjacency matrix $\mathbf{A} \in \mathbb{R}^{(N+M)\times(N+M)}$

approximate manifold / achieve sparsity – two choices:

1. k nearest neighbor graph (usually prefered)
2. ϵ distance graph

Learning on the Graph

estimation of a function on the nodes, ie $f : V \rightarrow \{-1, +1\}$
[recall: for SVMs, $f : \mathcal{X} \rightarrow \{-1, +1\}$, $\mathbf{x} \mapsto sign(\langle \mathbf{w}, \mathbf{x} \rangle + b)$]

Regularization on a Graph – penalize change along edges

$$\min_{(y_j)} g(\mathbf{y}) \quad \text{with} \quad g(\mathbf{y}) := \frac{1}{2} \sum_{k}^{N+M} \sum_{l}^{N+M} a_{kl}(y_k - y_l)^2$$

$$\begin{aligned} g(\mathbf{y}) &= \frac{1}{2}\left(\sum_k \sum_l a_{kl} y_k^2 + \sum_k \sum_l a_{kl} y_l^2\right) - \sum_k \sum_l a_{kl} y_k y_l \\ &= \sum_k y_k^2 \sum_l a_{kl} - \sum_k \sum_l y_k a_{kl} y_l \\ &= \mathbf{y}^\top \mathbf{D} \mathbf{y} - \mathbf{y}^\top \mathbf{A} \mathbf{y} \quad = \quad \mathbf{y}^\top \mathbf{L} \mathbf{y} \end{aligned}$$

where $\mathbf{D}$ is the diagonal degree matrix with $d_{kl} = \sum_k a_{kl}$
and $\mathbf{L} := \mathbf{D} - \mathbf{A} \in \mathbb{R}^{(N+M)\times(N+M)}$ is called the *graph Laplacian*

with constraints $y_j \in \{-1, +1\}$ essentially yields min-cut problem

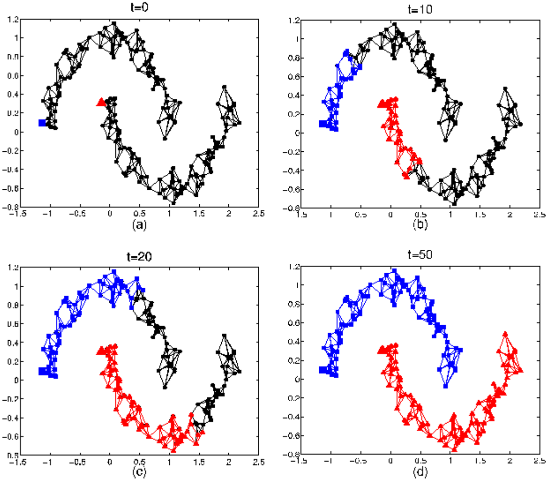
"Label Propagation" Method

relax: instead of $y_j \in \{-1, +1\}$, optimize free f_j
$\Rightarrow$ fix $\mathbf{f}_l = (f_i) = (y_i)$, solve for $\mathbf{f}_u = (f_j)$, predict $y_j = sign(f_j)$
$\Rightarrow$ convex QP ($\mathbf{L}$ is positive semi-definite)

$$
\begin{aligned}
0 &= \frac{\partial}{\partial \mathbf{f}_u} \begin{pmatrix} \mathbf{f}_l \\ \mathbf{f}_u \end{pmatrix}^\top \begin{pmatrix} \mathbf{L}_{ll} \mathbf{L}_{ul}^\top \\ \mathbf{L}_{ul} \mathbf{L}_{uu} \end{pmatrix} \begin{pmatrix} \mathbf{f}_l \\ \mathbf{f}_u \end{pmatrix} \\
&= \frac{\partial}{\partial \mathbf{f}_u} \left(\mathbf{f}_u{}^\top \mathbf{L}_{ul} \mathbf{f}_l + \mathbf{f}_l{}^\top \mathbf{L}_{ul}^\top \mathbf{f}_u + \mathbf{f}_u{}^\top \mathbf{L}_{uu}^\top \mathbf{f}_u \right) \\
&= 2\mathbf{f}_l{}^\top \mathbf{L}_{ul}^\top + 2\mathbf{f}_u{}^\top \mathbf{L}_{uu}^\top
\end{aligned}
$$

- $\Rightarrow$ solve linear system $\quad \mathbf{L}_{uu} \mathbf{f}_u = -\mathbf{L}_{lu}^\top \mathbf{f}_l \quad (\mathbf{f}_u = -\mathbf{L}_{uu}^{-1} \mathbf{L}_{lu}^\top \mathbf{f}_l)$
- easy to do in $\mathcal{O}(n^3)$ time; faster for sparse graphs
- solution can be shown to satisfy $f_j \in [-1, +1]$

Called **Label Propagation**, as the same solution is achieved by iteratively propagating labels along edges until convergence



Note: here
color $\triangleq$ classes

[images from "Label Propagation Through Linear Neighborhoods", Wang, Zhang, ICML 2006]

"Beyond the Point Cloud" [Sindhwani, Niyogi, Belkin]

Idea:

- model output f_j as linear function of the node value $\mathbf{x}_j$
  $f_k = \mathbf{w}^\top \mathbf{x}_k$ (with kernels: $f_k = \sum_l \alpha_l k(\mathbf{x}_l, \mathbf{x}_k)$)
- add graph regularizer to SVM cost function
  $R_g(\mathbf{w}) = \frac{1}{2} \sum_k \sum_l a_{kl}(f_k - f_l)^2 = \mathbf{f}^\top \mathbf{L} \mathbf{f}$

$$\min_{\mathbf{w}} \quad \underbrace{\sum_i \ell(y_i(\mathbf{w}^\top \mathbf{x}_i))}_{\text{data fitting}} + \underbrace{\lambda \|\mathbf{w}\|^2 + \gamma R_g(\mathbf{w})}_{\text{regularizers}}$$

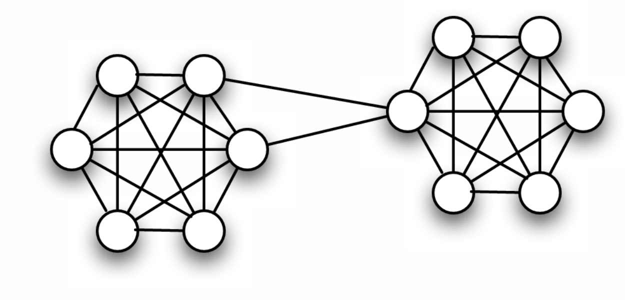
- linear ($\mathbf{f} = \mathbf{X}\mathbf{w}$): $\Rightarrow \quad \lambda \mathbf{w}^\top \mathbf{w} + \gamma \mathbf{w}^\top \mathbf{X}^\top \mathbf{L} \mathbf{X} \mathbf{w}$
- w. kernel ($\mathbf{f} = \mathbf{K}\alpha$): $\Rightarrow \quad \lambda \alpha^\top \mathbf{K} \alpha + \gamma \alpha^\top \mathbf{K} \mathbf{L} \mathbf{K} \alpha$

“Deep Learning via Semi-Supervised Embedding”

[J. Weston, F. Ratle, R. Collobert; ICML 2008]

- add graph-regularizer etc to some layers of deep net
- alternate gradient step wrt . . .
  - . . . a labeled point
  - . . . an unlabeled point
- learn low-dim. representation of data along with classification
- very good results!

Graph Methods



Observation

graphs model **density** on manifold
$\Rightarrow$ graph methods also implement cluster assumption

Cluster Assumption

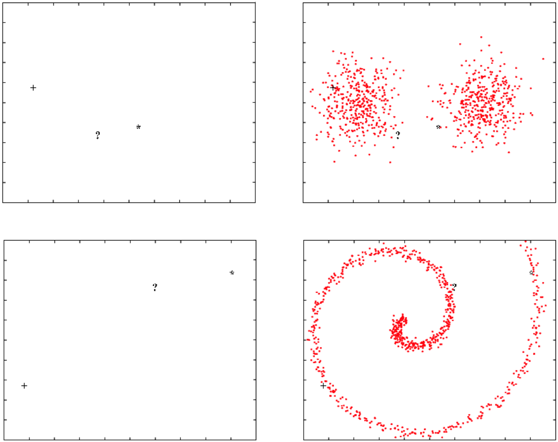
1. The data form clusters.
2. Points in the **same cluster** are likely to be of the **same class**.

Manifold Assumption

1. The data lie on (or close to) a low-dimensional manifold.
2. Its intrinsic distance is relevant for classification.

Semi-Supervised Smoothness Assumption

1. The density is non-uniform.
2. If two points are close in a high density region ($\Rightarrow$ connected by a high density path), their outputs are similar.



Semi-Supervised Smoothness Assumption

If two points are close in a high density region ($\Rightarrow$ connected by a high density path), their outputs are similar.

Outline

Change of Representation

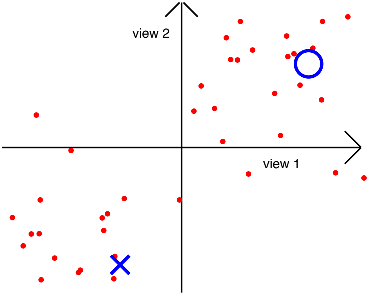
1. do **unsupervised** learning on all data (discarding the labels)
2. derive **new representation** (eg distance measure) of data
3. perform **supervised** learning with labeled data only,
   but unsing the new representation

- can implement *Semi-Supervised Smoothness Assumption*:
  assign small distances in high density areas
- generalizes graph methods:
  graph construction is crude unsupervised step
- currently hot paradigm: **Deep Belief Networks**
  [Hinton et al.; Neural Comp, 2006]
  (but mind [J. Weston, F. Ratle, R. Collobert; ICML 2008])

Assumption: Independent Views Exist

There exist **subsets of features, called views,** each of which

- is **independent** of the others given the class;
- is **sufficient** for classification.



Algorithmic idea: **Co-Training**

Co-Training with SVM

use multiple views v on the input data

$$\min_{\mathbf{w}^v,(y_j),\xi_k} \quad \sum_v \left(\frac{1}{2} \|\mathbf{w}_v\|^2 + C \sum_i \xi_{iv} + C^* \sum_j \xi_{jv} \right)$$

$$s.t. \quad \begin{array}{l} \forall_v : \; y_i \left(\langle \mathbf{w}_v, \Phi_v(\mathbf{x}_i) \rangle + b \right) \; \geq \; 1 - \xi_{iv}, \quad \xi_{iv} \geq 0 \\ \forall_v : \; y_j \left(\langle \mathbf{w}_v, \Phi_v(\mathbf{x}_j) \rangle + b \right) \; \geq \; 1 - \xi_{jv}, \quad \xi_{jv} \geq 0 \end{array}$$

- even a co-training S^3VM (large margin on unlabeled points)
- again, combinatorial optimization
- $\Rightarrow$ after continuous relaxation, non-convex

Transduction

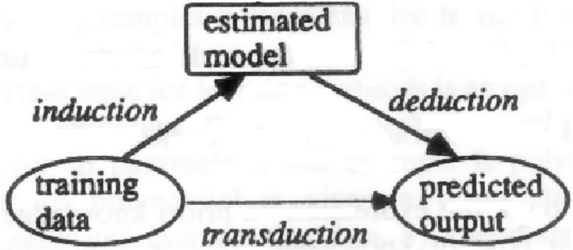


image from [Learning from Data: Concepts, Theory and Methods. V. Cherkassky, F. Mulier. Wiley, 1998.]

- concept introduced by Vladimir Vapnik
- philosophy: solve simpler task
- S^3VM originally called "Transductive SVM" (TSVM)

SSL vs Transduction

- Any SSL algorithm can be run in "transductive setting": use test data as unlabeled data.
- The "Transductive SVM" (S^3VM) is inductive.
- Some graph algorithms are transductive: prediction only available for nodes.
- Which assumption does transduction implement?

Outline

SSL Approaches

Assumption	Approach	Example Algorithm
Cluster Assumption	Low Density Separation	S^3VM (and many others)
Manifold Assumption	Graph-based Methods	• build weighted graph (w_{kl}) • $\min\limits_{(y_j)} \sum\limits_k \sum\limits_l w_{kl}(y_k - y_l)^2$
Independent Views	Co-Training	• train two predictors $y_j^{(1)}$, $y_j^{(2)}$ • couple objectives by adding $\sum_j \left(y_j^{(1)} - y_j^{(2)}\right)^2$

SSL Benchmark

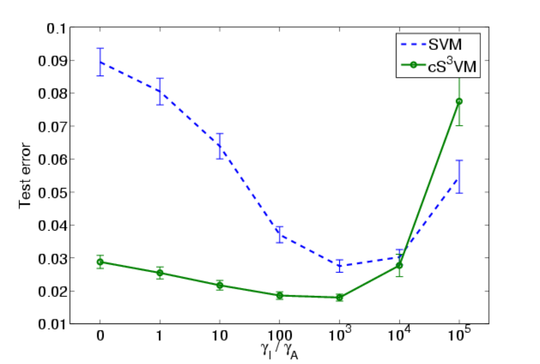
average error [%] on N=100 labeled and $M \approx 1400$ unlabeled points

Method	g241c	g241d	Digit1	USPS	COIL	BCI	Text
1-NN	43.93	42.45	3.89	5.81	17.35	48.67	30.11
SVM	23.11	24.64	5.53	9.75	22.93	34.31	26.45
MVU + 1-NN	43.01	38.20	2.83	6.50	28.71	47.89	32.83
LEM + 1-NN	40.28	37.49	6.12	7.64	23.27	44.83	30.77
Label-Prop.	22.05	28.20	3.15	6.36	10.03	46.22	25.71
Discrete Reg.	43.65	41.65	2.77	4.68	9.61	47.67	24.00
S^{3}SVM	18.46	22.42	6.15	9.77	25.80	33.25	24.52
SGT	17.41	9.11	2.61	6.80	–	45.03	23.09
Cluster-Kernel	13.49	4.95	3.79	9.68	21.99	35.17	24.38
Data-Dep. Reg.	20.31	32.82	2.44	5.10	11.46	47.47	–
LDS	18.04	23.74	3.46	4.96	13.72	43.97	23.15
Graph-Reg.	24.36	26.46	2.92	4.68	*11.92*	31.36	23.57
CHM (normed)	24.82	25.67	3.79	7.65	–	36.03	–

[Semi-Supervised Learning. Chapelle, Schölkopf, Zien. MIT Press, 2006.]

Combining S^{3}VM with Graph-based Regularizer

- apply SVM and S^{3}VM with graph regularizer
- x-axis: strength of graph regularizer
- MNIST digit classification data, "3" vs "5"



[A Continuation Method for S^{3}VM; Chapelle, Chi, Zien; ICML 2006]

SSL for Domain Adaptation

- domain adaptation: training data and test data from different distributions
- example: spam filtering for emails (topics change over time)
- S^3VM would have done very well in spam filtering competition
    - would have been **second** on "task B"
    - would have been **best** on "task A"

(ECML 2006 discovery challenge, `http://www.ecmlpkdd2006.org/challenge.html`)

SSL for Regression

- The **cluster** assumption does not make sense for regression.
- The **manifold** assumption might make sense for regression.
  - but hard to implement well without cluster assumption
  - not yet well explored and investigated
- The **independent-views** assumption (co-training) seems to make sense for regression [Zhou, Li; IJCAI 2005].
  - for regression, it's even convex
- A few more approaches exist (which I don't understand in terms of their assumptions, and thus don't put faith in).

The Three Great Challenges of SSL

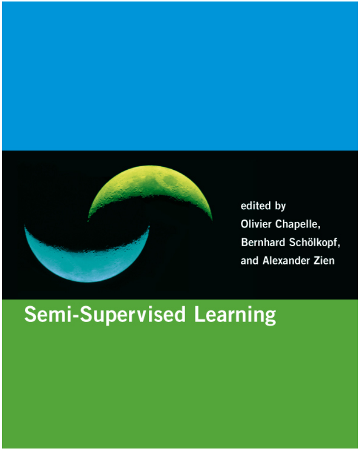
1. scalability
2. scalability
3. scalability

ok, there is also: SSL for structured outputs

Why scalability?

- many methods are **cubic** in $N + M$
- unlabeled data are most useful in large amounts $M \to +\infty$
- even quadratic is too costly for such applications
- but there is hope, eg [M. Karlen et al.; ICML 2008]

- **SSL Book.** `http://www.kyb.tuebingen.mpg.de/ssl-book/`



- MIT Press, Sept. 2006
- edited by B. Schölkopf, O. Chapelle, A. Zien
- contains many state-of-art algorithms by top researchers
- extensive SSL benchmark
- online material:
  - sample chapters
  - benchmark data
  - more information

- Xiaojin Zhu. Semi-Supervised Learning Literature Survey. TR 1530, U. Wisconsin.

Summary

- unlabeled data can improve classification
  (at present, most useful if few labeled data available)
- verify whether assumptions hold!
- two ways to use unlabeled data:
  - in the loss function (S^{3}VM, co-training)
    non-convex – optimization method matters!
  - in the regularizer (graph methods)
    convex, but graph construction matters
- combination seems to work best

Questions?