Semi-supervised Methods

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Outline

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Semi-supervised learning

Semi-supervised learning

semi-supervised learning is a class of machine learning techniques that make use of both labeled and unlabeled data for training - typically a small amount of labeled data with a large amount of unlabeled data.

Advantages

- save manual labor in labeling data
- improve accuracy in labeling data

Example

labeled

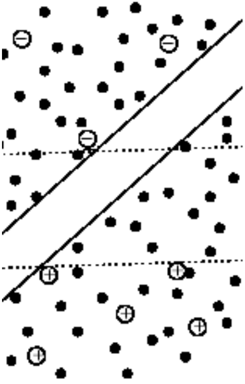

unlabeled


semi-supervised learning

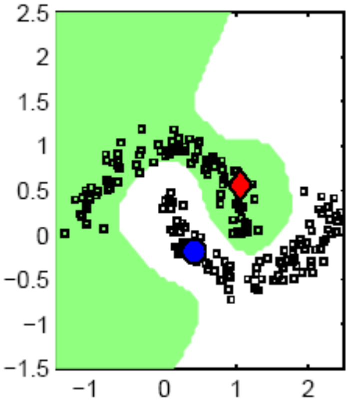
- drawn from the same distribution
- share the same label
- manifold assumption
- low density assumption
- surveys: [Zhu, 2005], [Chapelle et al., 2006]

Assumptions in semi-supervised learning

- low density assumption
- manifold assumption

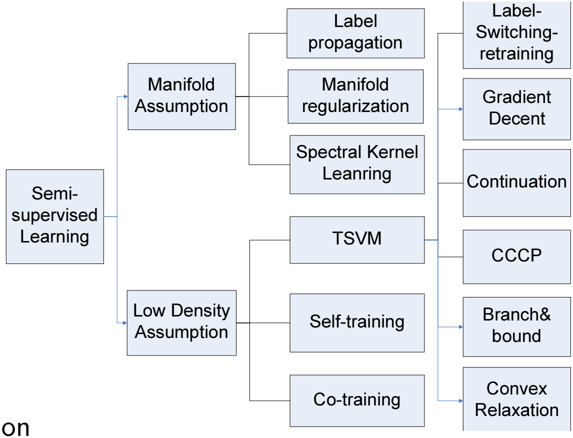


(a) Low density assumption



(b) Manifold assumption

Methods in semi-supervised learning



We will focus on

- Transductive Support Vector Machine (TSVM)

TSVM

Optimization in TSVM

- combinatorial optimization
- exponential complexity

Approximation methods for TSVM

- e.g., gradient descent optimization, label-switching-retraining, continuation method, Convex Concave Procedure, brunch and bound
- either local optima, or
- high complexity

Some challenges in semi-supervised learning

Challenges

perspectives for improving accuracy and efficiency:

- optimization technique for TSVM
- kernel for semi-supervised learning
- sparse models

Topics of this talk

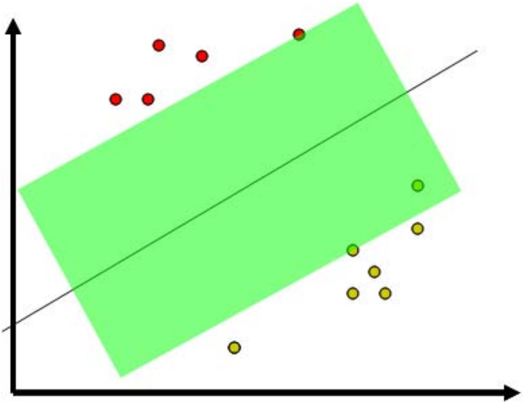
Topics

- How to learn an efficient Convex relaxation for TSVM?
- How to efficiently learn a kernel for semi-supervised learning?
- How to select features for semi-supervised learning?

Outline

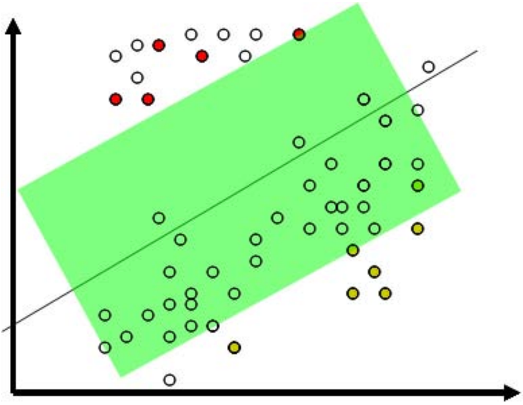
Transductive SVM

- SVM



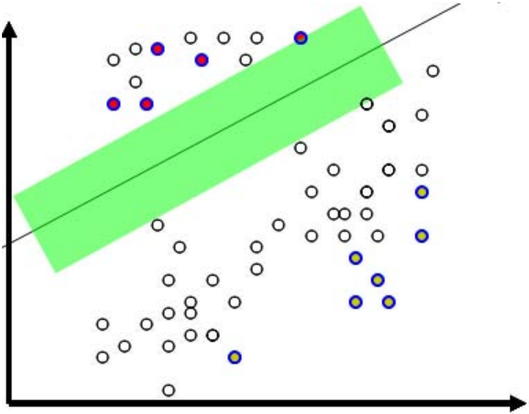
Transductive SVM

- SVM
- SVM with unlabeled data



Transductive SVM

- SVM
- SVM with unlabeled data
- Transductive SVM



Notations

- training data: $\{\mathbf{x}_i\}_{i=1}^{n}$
- kernel matrix: $\mathbf{K}$
- number of labeled examples: l
- labels of training data: $\mathbf{y}^{\ell}$
- decision function: $f = \mathbf{w}^{\top}\mathbf{x} - b$

Transductive SVM

TSVM: label **y** as a free variable

TSVM

$$\min_{\mathbf{w},b,\mathbf{y}\in\{-1,+1\}^n,\xi} \quad \|\mathbf{w}\|_2^2 + C\sum_{i=1}^{n}\xi_i \tag{1}$$

$$\text{s. t.} \quad y_i(\mathbf{w}^\top \mathbf{x}_i - b) \geq 1 - \xi_i,$$

$$\xi_i \geq 0,\ i = 1, 2, \ldots, n$$

$$y_i = y_i^\ell,\ i = 1, 2, \ldots, l,$$

- margin error: ξ
- tradeoff parameter: C

Transductive SVM

- $\circ$: element-wise product;
- $\mathbf{e}$: vector of all ones

Dual form

$$\begin{aligned} \max_{\alpha, \mathbf{y} \in \{-1,+1\}^n} \quad & \alpha^\top \mathbf{e} - \frac{1}{2}(\alpha \circ \mathbf{y})^\top \mathbf{K}(\alpha \circ \mathbf{y}) \\ \text{s. t.} \quad & 0 \leq \alpha \leq C, \\ & y_i = y_i^\ell, \ i = 1, 2, \ldots, l, \end{aligned} \tag{2}$$

problems:

- non-convex problem
- difficult to solve

Transductive SVM

Calculate the Lagrangian of (2)

$$L(\alpha, \nu, \delta, \lambda) = \alpha^\top \mathbf{e} - \frac{1}{2}(\alpha \circ \mathbf{y})^\top \mathbf{K}(\alpha \circ \mathbf{y}) + \nu^\top \alpha + \lambda \mathbf{y}^\top \alpha + \delta(C\mathbf{e} - \alpha)$$

- $\nu \in \mathbb{R}^n$: $\alpha \geq 0$
- $\delta \in \mathbb{R}^n$: $\alpha \leq C$
- λ: $\alpha^\top \mathbf{y} = 0$

Set $\frac{\partial L}{\partial \alpha} = 0$,

Dual form

$$\begin{aligned} \min_{\nu, \mathbf{y}, \lambda, \delta} \quad & \frac{1}{2}(\mathbf{e} + \nu - \delta + \lambda \mathbf{y})^\top \mathrm{D}(\mathbf{y}) \mathbf{K}^{-1} \mathrm{D}(\mathbf{y})(\mathbf{e} + \nu - \delta + \lambda \mathbf{y}) \qquad (3) \\ \text{s. t.} \quad & \nu \geq 0, \\ & y_i = y_i^\ell, \ i = 1, 2, \ldots, l, \\ & y_i^2 = 1, \ i = l+1, l+2, \ldots, n. \end{aligned}$$

Primal form of TSVM

introduce $\frac{1}{2}(\mathbf{e}+\nu-\delta+\lambda\mathbf{y})^\top \mathrm{D}(\mathbf{y})\mathbf{K}^{-1}\mathrm{D}(\mathbf{y})(\mathbf{e}+\nu-\delta+\lambda\mathbf{y}) \leq t$
According to Schur complement, (3) is equivalent to

Semi-definite programming for TSVM [Lanckriet et al., 2004]

$$\min_{\mathbf{y}\in\{-1,+1\}^n, t, \nu, \delta, \lambda} \quad t \tag{4}$$

$$\text{s. t.} \quad \begin{pmatrix} \mathbf{y}\mathbf{y}^\top \circ \mathbf{K} & \mathbf{e}+\nu-\delta+\lambda\mathbf{y} \\ (\mathbf{e}+\nu-\delta+\lambda\mathbf{y})^\top & t-2C\delta^\top\mathbf{e} \end{pmatrix} \succeq 0$$

$$\nu \geq 0,\ \delta \geq 0,\ y_i = y_i^\ell,\ i = 1, 2, \ldots, l,$$

problem:

- still non-convex for $\mathbf{y}$

Convex Relaxation of TSVM

replace $\mathbf{y}\mathbf{y}^\top$ with matrix $\mathbf{M}$ [Xu & Schuurmans, 2004]:

Convex Relaxation of TSVM

$$\begin{aligned} \min_{\mathbf{M},t,\nu,\delta,\lambda} \quad & t \\ \text{s. t.} \quad & \begin{pmatrix} \mathbf{M} \circ \mathbf{K} & \mathbf{e} + \nu - \delta \\ (\mathbf{e} + \nu - \delta)^\top & t - 2C\delta^\top \mathbf{e} \end{pmatrix} \succeq 0 \\ & \nu \geq 0, \ \delta \geq 0, \\ & \mathbf{M} \succeq 0, \ M_{i,i} = 1, \ i = 1, 2, \ldots, n, \\ & M_{ij} = y_i^\ell y_j^\ell, \ 1 \leq i,j \leq l \end{aligned} \tag{5}$$

- polynomial solution

Problems of the relaxation

1. $\mathcal{O}(n^2)$ parameters in the SDP cone
   - high worst-case computational complexity: $\mathcal{O}(n^{6.5})$
   - high storage complexity
2. drop the rank constraint of the matrix $\mathbf{y}\mathbf{y}^\top$
   - not tight approximation

Our solution

Start from the hard margin case ($\delta = 0$) of optimization problem (3),

$$\begin{aligned}
\min_{\nu,\mathbf{y},\lambda} \quad & \frac{1}{2}(\mathbf{e}+\nu+\lambda\mathbf{y})^\top \mathrm{D}(\mathbf{y})\mathbf{K}^{-1}\mathrm{D}(\mathbf{y})(\mathbf{e}+\nu+\lambda\mathbf{y}) \\
\text{s. t.} \quad & \nu \geq 0, \\
& y_i = y_i^\ell,\ i = 1, 2, \ldots, l, \\
& y_i^2 = 1,\ i = l+1, l+2, \ldots, n.
\end{aligned}$$

Our solution

- introduce $\mathbf{z} = \mathrm{D}(\mathbf{y})(\mathbf{e}+\nu) = \mathbf{y} \circ (\mathbf{e}+\nu)$
- $\mathbf{z}$ can be used as the prediction function

Hard margin TSVM

$$\begin{aligned} \min_{\mathbf{z},\lambda} \quad & \frac{1}{2}(\mathbf{z}+\lambda\mathbf{e})^\top \mathbf{K}^{-1}(\mathbf{z}+\lambda\mathbf{e}) \\ \text{s. t.} \quad & y_i^\ell z_i \geq 1,\ i = 1, 2, \ldots, l, \\ & z_i^2 \geq 1,\ i = l+1, l+2, \ldots, n. \end{aligned} \tag{6}$$

Our solution

reformulation:

- $\mathbf{w} = (\mathbf{z}, \lambda) \in \mathbb{R}^{n+1}$
- $\mathbf{P} = (\mathbf{I}_n, \mathbf{e}) \in \mathbb{R}^{n\times(n+1)}$

balance constraint (to avoid putting unlabeled examples to one side):

- $-\epsilon \leq \frac{1}{l}\sum_{i=1}^{l} w_i - \frac{1}{n-l}\sum_{i=l+1}^{n} w_i \leq \epsilon$

$$
\begin{aligned}
\min_{\mathbf{w}} \quad & \mathbf{w}^\top \mathbf{P}^\top \mathbf{K}^{-1} \mathbf{P} \mathbf{w} \\
\text{s. t.} \quad & y_i^\ell w_i \geq 1,\ i = 1, 2, \ldots, l, \\
& w_i^2 \geq 1,\ i = l+1, l+2, \ldots, n, \\
& -\epsilon \leq \frac{1}{l}\sum_{i=1}^{l} w_i - \frac{1}{n-l}\sum_{i=l+1}^{n} w_i \leq \epsilon.
\end{aligned}
\tag{7}
$$

Our solution

Lagragian of (7):

$$L = \mathbf{w}^\top \mathbf{P}^\top \mathbf{K}^{-1} \mathbf{P} \mathbf{w} + \sum_{i=1}^{l} \gamma_i (1 - y_i^\ell w_i) + \sum_{i=l+1}^{n} \gamma_i (1 - w_i^2) + \alpha(\mathbf{c}^\top \mathbf{w} - \epsilon) + \beta(-\mathbf{c}^\top \mathbf{w} - \epsilon) \quad (8)$$

Solution

$$\mathbf{w} = \frac{1}{2} \left[\mathbf{A} - \mathrm{D}(\gamma \circ \mathbf{b})\right]^{-1} (\gamma \circ \mathbf{a} - (\alpha - \beta)\mathbf{c}),$$

- $\mathbf{a} = (\mathbf{y}^l, \mathbf{0}^{n-l}, 0) \in \mathbb{R}^{n+1}$
- $\mathbf{b} = (\mathbf{0}^l, \mathbf{1}^{n-l}, 0) \in \mathbb{R}^{n+1}$
- $\mathbf{c} = (\frac{1}{l}\mathbf{1}^l, -\frac{1}{u}\mathbf{1}^{n-l}, 0) \in \mathbb{R}^{n+1}$
- $\mathbf{A} = \mathbf{P}^\top \mathbf{K}^{-1} \mathbf{P}$

Our solution

TSVM in dual

$$\max_{\gamma,t} \quad -\frac{1}{4}t + \sum_{i=1}^{n} \gamma_i - \epsilon(\alpha + \beta) \tag{9}$$

$$s.\ t. \quad \begin{pmatrix} \mathbf{A} - \mathrm{D}(\gamma \circ \mathbf{b}) & \gamma \circ \mathbf{a} - (\alpha - \beta)\mathbf{c}, \\ (\gamma \circ \mathbf{a} - (\alpha - \beta)\mathbf{c})^\top & t \end{pmatrix} \succeq 0$$

$$\alpha \geq 0,\ \beta \geq 0,\ \gamma_i \geq 0,\ i = 1, 2, \ldots, n.$$

Properties of the proposed convex relaxation model

- Lower worst-case computational complexity of $\mathcal{O}(n^{4.5})$: $\mathcal{O}(n)$ parameters and $\mathcal{O}(n)$ linear equality constraints
- Our prediction function f^* provides a tighter approximation [Hiriart et al., 1993].
- Related to the solution of [Zhu et al., 2003] :

$$\mathbf{z} = \left(\mathbf{I}_n - \sum_{i=l+1}^{n} \gamma_i \mathbf{K}\mathbf{I}_n^i\right)^{-1} \left(\sum_{i=1}^{l} \gamma_i y_i^\ell \mathbf{K}(\mathbf{x}_i, \cdot)\right) \tag{10}$$

Data sets

Table: Data sets used in the experiments, where d represents the data dimensionality, l means the number of labeled data points, and n denotes the total number of examples.

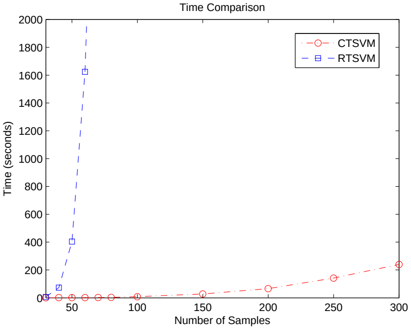
Data set	d	l	n	Data set	d	l	n
Iono	34	20	351	WinMac-m	7511	20	300
Sonar	60	20	208	IBM-m	11960	20	300
Banana	4	20	400	Course-m	1800	20	300
Breast	9	20	300	WinMac-l	7511	50	1000
IBM-s	11960	10	60	IBM-l	11960	50	1000
Course-s	1800	10	60	Course-l	1800	50	1000

Comparison algorithms

- SVM: baseline
- label-switching-retraining in SVM-light [Joachims,1999]
- Convex concave procedure [Collobert et al., 2006]
- Gradient decent (∇TSVM), [Chapelle et al., 2005]

Computation time comparison

- CTSVM: convex relaxation TSVM proposed [Xu et al., 2007]
- RTSVM: previous semi-definite relaxation TSVM [Xu & Schuurmans, 2004]



- Course, labeled 20

Accuracy comparison

Table: The classification performance of Transductive SVMs on benchmark data sets. (Note: ∇TSVM = Gradient Decent TSVM, CCCP = Concave Convex Procedure)

Data Set	SVM	SVM-light	∇TSVM	CCCP	CTSVM
IBM-s	52.75±15.01	67.60±9.29	65.80±6.56	65.62±14.83	**75.25**±7.49
Course-s	63.52±5.82	76.82±4.78	75.80±12.87	74.20±11.50	**79.75**±8.45
Iono	78.55±4.83	78.25±0.36	81.72±4.50	**82.11**±3.83	80.09±2.63
Sonar	51.76±5.05	55.26±5.88	**69.36**±4.69	56.01±6.70	67.39±6.26
Banana	58.45±7.15	-	71.54±7.28	79.33±4.22	**79.51**±3.02
Breast	96.46±1.18	95.68±1.82	97.17±0.35	96.89±0.67	**97.79**±0.23
WinMac-m	57.64±9.58	79.42±4.60	81.03±8.23	84.28±8.84	**84.82**±2.12
IBM-m	53.00±6.83	67.55±6.74	64.65±13.38	69.62±11.03	**73.17**±0.89
Course-m	80.18±1.27	**93.89**±1.49	90.35±3.59	88.78±2.87	92.92±2.28
WinMac-l	60.86±10.10	89.81±2.10	90.19±2.65	91.00±2.42	**91.25**±2.67
IBM-l	61.82±7.26	**75.40**±2.26	73.11±1.99	74.80±1.87	73.42±3.23
Course-l	83.56±3.10	92.35±3.02	93.58±2.68	91.32±4.08	**94.62**±0.97

Discussion

- More efficient than that in [Xu & Schuurmans, 2004]
- Effective prediction accuracy compared with other semi-supervised SVM algorithms
- All algorithms sensitive to data sets
- Consistent to the results in [Chapelle et al., 2008]

Outline

Semi-supervised kernels

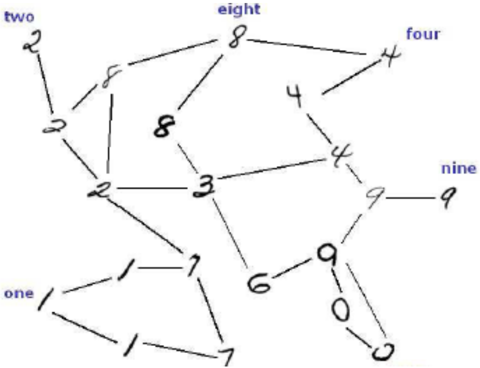
- spectral kernel learning
  - the eigenvalues are readjusted according to some principle
  - Gaussian field kernel [Zhu et. al, 2002]
  - cluster kernel [Chapelle et. al, 2003]
  - spectral kernel [Zhang & Ando, 2005]
- multiple kernel learning
  - a linear combination of a batch of base kernels [Lancriet et. al, 2004]
- graph embedding
  - embed a graph structure into the supervised kernel [Sindhwani et. al, 2005]

Graph embedding

Graph construction

- $\mathcal{G} =< \mathcal{V}, \mathcal{E} >$, where $\mathcal{V} = \{\mathbf{x}_i\}_{i=1}^{N}$
- build adjacency graph
  - ϵ-NN. $\epsilon \in \mathbb{R}^+$. Nodes $\mathbf{x}_i$ and $\mathbf{x}_j$ are connected if $\mathrm{dist}(\mathbf{x}_i, \mathbf{x}_j) \geq \epsilon$
  - k-NN. $k \in \mathbb{N}^+$. Nodes $\mathbf{x}_i$ and $\mathbf{x}_j$ are connected if $\mathbf{x}_i$ is among the k nearest neighbors of $\mathbf{x}_j$.
- graph weighting
  - Heat kernel. If $\mathbf{x}_i$ and $\mathbf{x}_j$ are connected, the weight $W_{ij} = \exp^{-\frac{dist(\mathbf{x}_i, \mathbf{x}_j)}{t}}$, where $t \in \mathbb{R}^+$.
  - Simple-minded. $W_{ij} = 1$ if $\mathbf{x}_i$ and $\mathbf{x}_j$ are connected.

Graph embedding



- $\mathcal{G} =< \mathcal{V}, \mathcal{E} >$
- W_{ij}: weights on edge $(\mathbf{x}_i, \mathbf{x}_j)$
- $D_{ii} = \sum_{j=1}^{n} W_{ij}$
- graph Laplacian: $\mathcal{L} = \mathbf{D} - \mathbf{W}$
- weighted graph Laplacian: $\mathcal{L} = \mathbf{D}^{-\frac{1}{2}}(\mathbf{D} - \mathbf{W})\mathbf{D}^{-\frac{1}{2}}$

Graph embedding

Question?

Can we define a kernel that is adapted to the geometry of the data distribution?

$\Downarrow$

Solution

Define a new RKHS to incorporate the data geometry, such that

$$\langle f, g\rangle_{\tilde{\mathcal{H}}} = \langle f, g\rangle_{\mathcal{H}} + \langle Sf, Sg\rangle_{\mathcal{V}} \tag{11}$$

- $\kappa(\mathbf{x}, \cdot)$: functional in the **Reproducing Kernel Hilbert Space** (RKHS) $\mathcal{H}$
- $\tilde{\kappa}(\mathbf{x}, \cdot)$: functional in the new RKHS $\tilde{\mathcal{H}}$
- $f(\mathbf{x}) = \langle f, \kappa(\mathbf{x}, \cdot)\rangle, \quad \kappa(\mathbf{x}, \mathbf{z}) = \langle \kappa(\mathbf{x}, \cdot), \kappa(\mathbf{x}, \cdot)\rangle_{\mathcal{H}}$
- $S : \mathcal{H} \rightarrow \mathcal{V}$: bounded linear operator

Graph embedding

Define

- $S(f) = (f(\mathbf{x}_1), \ldots, f(\mathbf{x}_n))$.
- $\|Sf\|_{\mathcal{V}}^2 = \mathbf{f}^\top \mathcal{L} \mathbf{f}$

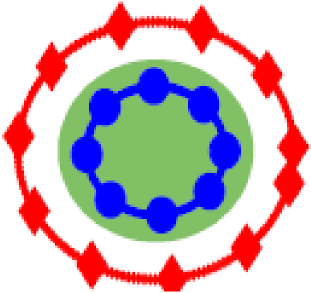
Graph embedding

According to [Sindhwani et. al, 2005], Given a kernel function $\kappa(\cdot,\cdot)$, the new kernel $\tilde{\kappa}(\cdot,\cdot)$ embedded with the graph structure is defined as

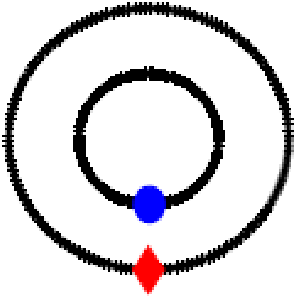
$$\tilde{\kappa}(\mathbf{x},\mathbf{z}) = \kappa(\mathbf{x},\mathbf{z}) - \mathbf{k}_{\mathbf{x}}(\mathbf{I} + \mathcal{L}\mathbf{K})^{-1}\mathcal{L}\mathbf{k}_{\mathbf{z}}. \tag{12}$$

- $\mathbf{k}_{\mathbf{x}} = (\kappa(\mathbf{x}_1,\mathbf{x}), \ldots, \kappa(\mathbf{x}_n,\mathbf{x}))^\top$

Illustration



(a) *data*

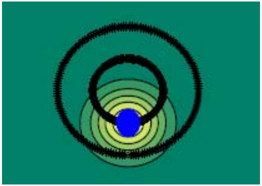


(b) *labeled data*

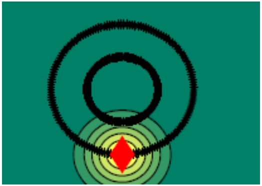
Figure: scatter plot of data

Illustration

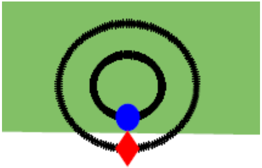
RBF kernel



(a) *Gaussian kernel centered on labeled point 1*



(b) *Gaussian kernel centered on labeled point 2*

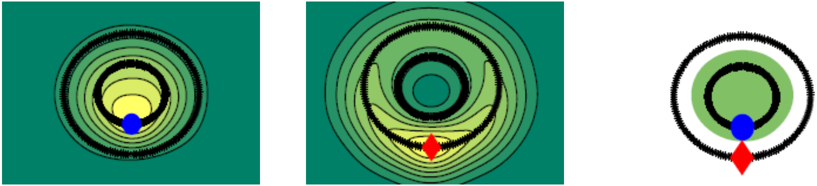


(c) *classifier learnt in the RKHS*

Figure: Gaussian kernel

Illustration

kernel embedded with the graph structure



(a) *embedded kernel centered on labeled point 1*

(b) *embedded kernel centered on labeled point 2*

(c) *classifier learnt in the deformed RKHS*

Figure: Kernel embedded with the graph structure

Challenges of graph embedding

Challenges

- the kernel function $\kappa(\cdot, \cdot)$ for embedding, and
- the graph structure that is used to calculate the graph Laplacian $\mathcal{L}$.

Solutions

- employ multiple kernel learning to select the kernel function $\kappa(\cdot, \cdot)$ and the graph structure

Multiple kernel learning (MKL)

Multiple kernel learning

Given a list of base kernel functions/matrices $\mathbf{K}_i$, $i = 1, \ldots, m$, MKL searches for a linear combination of the base kernel functions that maximizes a generalized performance measure.

Linear combination of kernels

$$\mathbf{K} = \sum_{i=1}^{m} p_i \mathbf{K}_i,\ i = 1, \ldots, m$$

where $\mathbf{p} = (p_1, \ldots, p_m)$ are combination weights in domain $\mathcal{P}$

$$\mathcal{P} = \{\mathbf{p} \in \mathbb{R}^m : \mathbf{p}^\top \mathbf{e} = 1,\ 0 \leq \mathbf{p} \leq 1\}$$

Candidate graphs for semi-supervised learning

Parameter sets when constructing the graph

- distance function: $\mathcal{D} = \{d_1, \ldots, d_r\}$
  - e.g. Euclidean distance, tangent distance
- neighborhood number: $\mathcal{K} = \{k_1, \ldots, k_s\}$
  - e.g. 2, 10, 100, ...
- heat kernel width: $\mathrm{T} = \{t_1, \ldots, t_q\}$
  - e.g. $1e^{-2}$, $1e^{-1}$, 1, 10, ...

Candidate graphs

- $u = r \times s \times q$ graphs
- $\mathcal{L}_i = \mathbf{D}_i - \mathbf{W}_i$ for $i = 1, \ldots, u$

Candidate embedded kernels for semi-supervised learning

For

- i-th ($i = 1, \ldots, u$) candidate graph
- j-th ($j = 1, \ldots, v$) base kernel

embedded kernels

$$\tilde{\kappa}_{ij}(\mathbf{x}, \mathbf{z}) = \kappa_i(\mathbf{x}, \mathbf{z}) - \mathbf{k}_\mathbf{x}(\mathbf{I} + \mathcal{L}_j \mathbf{K}_i)^{-1} \mathcal{L}_j \mathbf{k}_\mathbf{z}. \qquad (13)$$

Multiple kernel learning

- number of base kernels $m = u \times v$

Multiple kernel learning in semi-supervised setting

$$\min_{\mathbf{p}\in\mathcal{P}} \max_{\alpha\in\mathcal{Q}} f(\mathbf{p},\alpha) = \alpha^\top \mathbf{e} - \frac{1}{2}(\alpha \circ \mathbf{y})^\top \left(\sum_{i=1}^{m} p_i \tilde{\mathbf{K}}_i\right)(\alpha \circ \mathbf{y}),$$

Properties

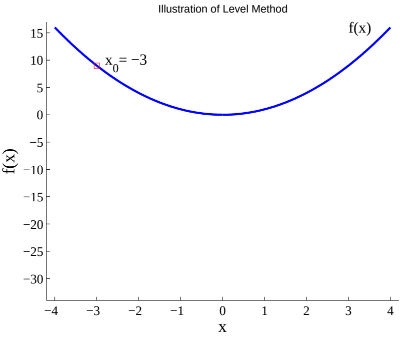
- convex-concave problem (convex in $\mathbf{p}$ and concave in α)
- saddle point $(\mathbf{p}^*, \alpha^*)$ exists and corresponds to the optimal solution

$$f(\mathbf{p},\alpha^*) \leq f(\mathbf{p}^*,\alpha^*) \leq f(\mathbf{p}^*,\alpha), \forall \mathbf{p} \in \mathcal{P}, \alpha \in \mathcal{Q}$$

Level Method

$$\min_x \{f(x) = [x]^2 : x \in \mathcal{X}, \mathcal{X} = [-4, 4]\}$$

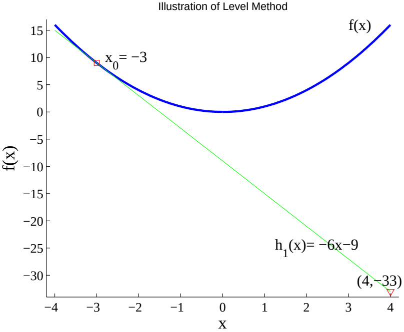
- Initialization: $x_0 = -3$, $\lambda = 0.9$



Level Method

$$\min_{x}\{f(x) = [x]^2 : x \in \mathcal{X}, \mathcal{X} = [-4, 4]\}$$

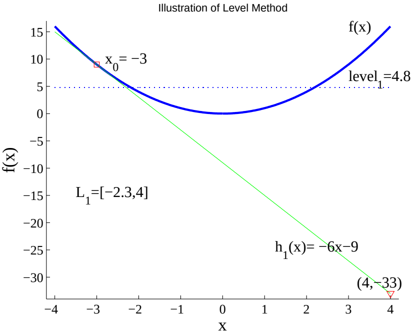
- Initialization: $x_0 = -3$, $\lambda = 0.9$
- Construct a cutting plane model $g_1(x)$



Level Method

$$\min_x \{f(x) = [x]^2 : x \in \mathcal{X}, \mathcal{X} = [-4, 4]\}$$

- Initialization: $x_0 = -3$, $\lambda = 0.9$
- Construct a cutting plane model $g_1(x)$
- Construct a level set $\mathcal{L}_1$
  $\text{level}_1 = \lambda \times f(x_0) + (1-\lambda) \times (-33)$
  $\mathcal{L}_1 = \{x \in \mathcal{X} : g_1(x) \leq \text{level}_1\}$



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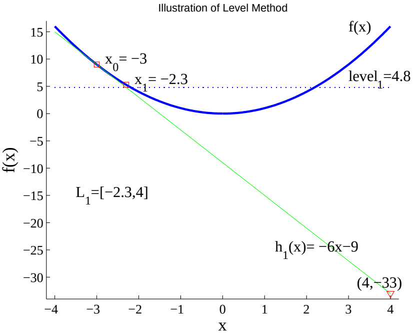
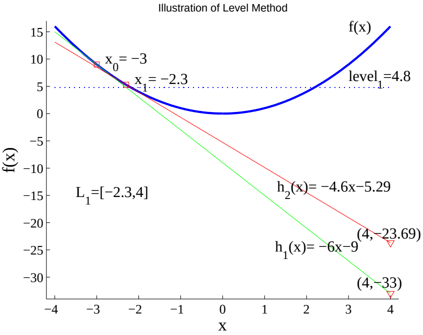
- Project x_0 to level set $\mathcal{L}_1$, i.e.,
  $x_1 = \arg\min_x \left\{\|x - x_0\|_2^2 : x \in \mathcal{L}_1\right\}$



Level method

$$\min_x \{f(x) = [x]^2 : x \in [-4, 4]\}$$

- Construct a new cutting plane model $g_2(x) = \min_x h_i(x)$



Level method

$$\min_x \{f(x) = [x]^2 : x \in [-4, 4]\}$$

- Construct a new cutting plane model $g_2(x) = \min_x h_i(x)$
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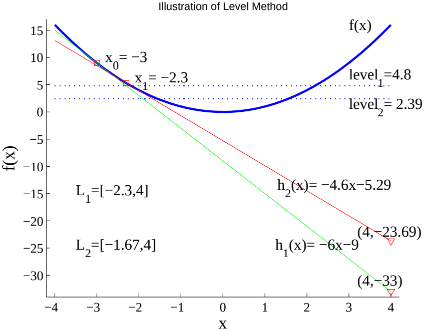

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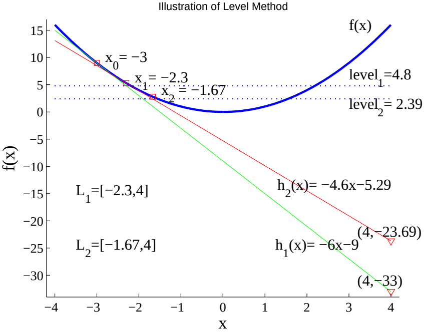
- Construct a new cutting plane model $g_2(x) = \min_x h_i(x)$
- Construct a new level set $\mathcal{L}_2$
- Project x_1 to $\mathcal{L}_2$



Cutting plane models

Cutting plane models

$$g^i(\mathbf{p}) = \max_{1 \le j \le i} f(\mathbf{p}^j, \alpha^j) + (\mathbf{p} - \mathbf{p}^j)^\top \nabla_{\mathbf{p}} f(\mathbf{p}^j, \alpha^j)$$

Properties

For any $\mathbf{p} \in \mathcal{P}$, we have

- $g^{i+1}(\mathbf{p}) \ge g^i(\mathbf{p})$, and
- $g^i(\mathbf{p}) \le \max_{\alpha \in \mathcal{Q}} f(\mathbf{p}, \alpha)$

Lower and upper bounds

Lower and upper bounds

$$\underline{f}^i = \min_{\mathbf{p}\in\mathcal{P}} g^i(\mathbf{p}), \quad \overline{f}^i = \min_{1\le j\le i} f(\mathbf{p}^j, \alpha^j)$$

Properties

$$\underline{f}^i \le f(\mathbf{p}^*, \alpha^*) \le \overline{f}^i,$$
$$\overline{f}^1 \ge \overline{f}^2 \ge \ldots \ge \overline{f}^i,$$
$$\underline{f}^1 \le \underline{f}^2 \le \ldots \le \underline{f}^i.$$

where $\mathbf{p}^*$ and α^* are the optimal solution.

Projection to level set

Level set

$$\mathcal{L}^i = \{\mathbf{p} \in \mathcal{P} : g^i(\mathbf{p}) \leq \ell^i = \lambda \overline{f}^i + (1-\lambda)\underline{f}^i\},$$

where $\lambda \in (0,1)$ is a predefined constant.

- larger $\lambda \rightarrow$ more regularization
- $\lambda = 0$: the level method becomes the cutting plane method

Projection to level set

$$\mathbf{p}^{i+1} = \arg\min_{\mathbf{p}\in\mathcal{P}} \left\{ \|\mathbf{p} - \mathbf{p}^i\|_2^2 : \mathbf{p} \in \mathcal{L}^i \right\}$$

Stopping Criterion

Define the gap Δ^i as

$$\Delta^i = \overline{f}^i - \underline{f}^i.$$

Corollary

1. $\Delta^j \geq 0, j = 1, \ldots, i$
2. $\Delta^1 \geq \Delta^2 \geq \ldots \geq \Delta^i$
3. $|f(\mathbf{p}^j, \alpha^j) - f(\mathbf{p}^*, \alpha^*)| \leq \Delta^i$

- Δ^i measures how close the current solution is from the optimal one, serving as the stopping criterion.

The level method for multiple kernel learning

Given: λ (level set) and ε (desired accuracy)

1. Initialize: $\mathbf{p}^0 = \mathbf{e}/m$, and $i = 0$

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3. Solve dual SVM with $\tilde{\mathbf{K}} = \sum_{j=1}^{m} p_j^i \tilde{\mathbf{K}}_j$ for α^i

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7. Update $i = i + 1$
8. UNTIL$\Delta^i \leq \varepsilon$

Experimental setup: semi-supervised setting

- Base kernel matrices for embedding
  - Gaussian kernels with 10 different widths ($\{2^{-3}, 2^{-2}, \ldots, 2^{6}\}$) on all features,
  - Polynomial kernels of degree 1 to 3 on all features,
- Graphs: 10 NN, cosine similarity
- heat kernel width: $\{0.5, 1, 2, 4, 8\}$
- Other settings similar to the supervised setting

Experimental setup: semi-supervised setting

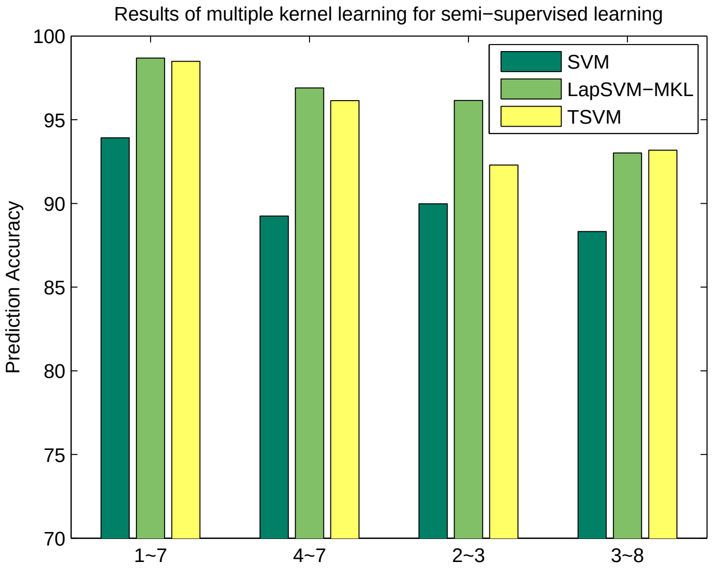
Competitive algorithms:

- baseline: SVM
- TSVM: Convex Concave Procedure (CCCP)
- LapSVM-MKL: proposed

Dataset:

- USPS (US Postal Service's handwritten digits of 400 images and 20 labelled images)

Performance comparison



Summary

Semi-supervised kernel selection

- learning graph structure and base kernels at the same time
- convex optimization
- good performance
- efficient optimization via level method

Outline

Feature selection

Feature selection

Given the number of required features, denoted by m, the goal of feature selection is to choose a subset of m features, denoted by $\mathcal{S}$, that maximizes a generalized performance criterion $\mathcal{Q}$.

Combinatorial optimization:

$$\mathcal{S}^* = \arg\max \mathcal{Q}(\mathcal{S}) \quad \text{s. t.} \quad |\mathcal{S}| = m. \tag{14}$$

How many features do we need?

The number of required features is

- dependant on learning tasks, e.g., data visualization
- dependant on computational resources, e.g., sensor networks, embedded system
- a model selection problem

We assume that an **external oracle** decides the number of selected features.

Feature selection

Feature selection criterion

- mutual information (Koller & Sahami, 1996)
- maximum margin (Weston et al., 2000; Guyon et al., 2002)
- kernel alignment (Cristianini et al., 2001; Neumann et al., 2005)
- Hilbert Schmidt independence criterion (Song et al., 2007)

Feature selection methods

SVM-based methods

Calculate weight/score **w** for each feature, and then select features with the largest weights

- L2-SVM (Vapnik, 1998; Guyon et al.,2002)
- L1-SVM (Fung & Mangasarian, 2000; Ng, 2004)
- Lasso/LARS (Tibshirani,1996; Efron et al., 2004)
- L0-SVM (Bradley & Mangasarian, 1998; Weston et al., 2003; Neumann et al., 2005; Chan et al.,2007)

Feature selection

- supervised
  - not work well when the number of labeled samples is small
- unsupervised
  - unable to identify the discriminative features
- semi-supervised
  - avoid the high cost in manually labeling data
  - exploit abundant unlabeled data

Semi-supervised feature selection

Semi-supervised feature selection based on manifold regularization

- maximum margin
  - discriminative
  - incorporating the interaction of features
- manifold regularization
  - better exploits the underlying structural information of the unlabeled data
- convex-concave optimization
  - optimality
  - efficient solver (e.g., level method)

SFS

Notations

- labeled data: $\mathbf{X}_\ell = (\mathbf{x}_1, \ldots, \mathbf{x}_l)$
- labels: $\mathbf{y} = (y_1, y_2, \ldots, y_l)$
- unlabeled examples: $\mathbf{X}_u$
- training data: $\mathbf{X} = (\mathbf{X}_\ell, \mathbf{X}_u)$
- feature indicator: $\mathbf{p} = (p_1, \ldots, p_d)^\top$ and $p_i \in \{0, 1\}$, $i = 1, \ldots, d$
- kernel matrix: $\mathbf{K}$
- kernel defined on each feature: $\mathbf{K}_i = \mathbf{x}_i \mathbf{x}_i^\top$

Semi-supervised learning

Manifold regularization

$$\|\mathbf{f}\|_I^2 = \sum_{i=1}^{n}\sum_{j=1}^{n}(f(\mathbf{x}_i) - f(\mathbf{x}_j))^2 W_{ij} = \mathbf{f}^\top \mathcal{L}\mathbf{f}, \qquad (15)$$

- W_{ij}: weights on edge $(\mathbf{x}_i, \mathbf{x}_j)$
- $D_{ii} = \sum_{j=1}^{n} W_{ij}$
- $\mathcal{L} = \mathbf{D} - \mathbf{W}$

Semi-supervised SVM based on manifold regularization

Semi-supervised SVM

$$
\begin{aligned}
\min_{\mathbf{w},b,\xi} \quad & \frac{1}{2}\|\mathbf{w}\|_2^2 + C\sum_{i=1}^{l}\xi_i + \frac{\rho}{2}\mathbf{w}^\top \mathbf{X}^\top \mathcal{L}\mathbf{X}\mathbf{w} \\
\text{s. t.} \quad & y_i(\mathbf{w}^\top \mathbf{x}_i - b) \geq 1 - \xi_i, \ i = 1, \ldots, l, \\
& \xi_i \geq 0, \ i = 1, \ldots, l,
\end{aligned}
\tag{16}
$$

- ξ: margin error
- ρ: trade-off parameter

Dual form

Semi-supervised SVM

$$\max_{\alpha \in \mathcal{Q}} \quad \alpha^\top \mathbf{e} - \frac{1}{2}(\alpha \circ \mathbf{y})^\top \mathbf{X}_\ell (\mathbf{I} + \rho \mathbf{X}^\top \mathcal{L} \mathbf{X})^{-1} \mathbf{X}_\ell^\top (\alpha \circ \mathbf{y})$$

- $\mathcal{Q} = \{\alpha \in [0, C]^l | \alpha^\top \mathbf{y} = 0\}$
- $\mathbf{I} \in \mathbb{R}^{n \times n}$: identity matrix
- $\circ$: element-wise product.

Semi-supervised feature selection

Semi-supervised feature selection

$$\min_{\mathbf{w},b,\xi,\mathbf{p}\in\mathcal{P}} \quad \frac{1}{2}\|\mathbf{w}\|_2^2 + C\sum_{i=1}^{l}\xi_i + \frac{\rho}{2}\mathbf{w}^\top \mathrm{D}(\mathbf{p})\mathbf{X}^\top \mathcal{L}\mathbf{X}\mathrm{D}(\mathbf{p})\mathbf{w} \tag{17}$$

$$\text{s. t.} \quad y_i(\mathbf{w}^\top \mathrm{D}(\mathbf{p})\mathbf{x}_i - b) \geq 1 - \xi_i,\ i = 1, \ldots, l,$$

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

- $\mathcal{P} = \{\mathbf{p} \in [0,1]^d | \mathbf{p}^\top \mathbf{e} = m\}$.
- $\mathrm{D}()$: diagonal matrix

Dual problem of semi-supervised feature selection

Semi-supervised feature selection

The dual of (17) is equivalent to the following min-max optimization problem

$$\min_{\mathbf{p}\in\mathcal{P}} \max_{\alpha\in\mathcal{Q}} \alpha^\top \mathbf{e} - \frac{1}{2}(\alpha \circ \mathbf{y})^\top \mathbf{X}_\ell \Gamma \mathbf{X}_\ell^\top (\alpha \circ \mathbf{y}) \quad (18)$$

$$\Gamma = \mathrm{D}(\mathbf{p})\left(\mathbf{I} + \rho\mathbf{Z}\right)^{-1}\mathrm{D}(\mathbf{p}) \quad (19)$$

$$\mathbf{Z} = \mathbf{X}^\top \mathcal{L} \mathbf{X} \quad (20)$$

Equivalent form

Equivalent form

$$\min_{\mathbf{p}\in\mathcal{P}} \max_{\alpha\in\mathcal{Q},\tau\in[0,1]} \alpha^\top \mathbf{e} - \frac{1}{2}(\alpha \circ \mathbf{y})^\top \mathbf{X}_\ell \mathbf{A} \mathbf{X}_\ell^\top (\alpha \circ \mathbf{y}) \quad (21)$$

- reduce the quadratic optimization of **p** to linear optimization

$$\mathbf{A} = (1-\tau)^2 \mathrm{D}(\mathbf{p}) + \frac{\tau^2}{\rho}\mathbf{Z}^{-1} \quad (22)$$

- $\mathbf{A} \succeq \Gamma$ for any $\tau \in [0, 1]$.

Connection to multiple kernel learning

Linear kernel

$$\mathbf{K} = \mathbf{X}_\ell \mathbf{X}_\ell^\top = \sum_{i=1}^{d} \mathbf{v}_i \mathbf{v}_i^\top = \sum_{i=1}^{d} \mathbf{K}_i,$$

Semi-supervised feature selection as MKL

$$\min_{\mathbf{p}\in\mathcal{P}} \max_{\alpha\in\mathcal{Q}} \quad \alpha^\top \mathbf{e} - \frac{1}{2}(\alpha \circ \mathbf{y})^\top \mathbf{M} (\alpha \circ \mathbf{y}) \tag{23}$$

- $\mathbf{M} = (1-\tau)^2 \sum_{i=1}^{d} p_i \mathbf{K}_i + \frac{\tau^2}{\rho}\mathbf{H}$.
- $\mathbf{v}_i$: i-th feature of $\mathbf{X}$
- $\mathbf{H} = \mathbf{X}_\ell^\top (\mathbf{X}^\top \mathcal{L} \mathbf{X})^{-1} \mathbf{X}_\ell$

Level method for semi-supervised feature selection

- cutting plane model

$$g^i(\mathbf{p}) = \max_{1\le j\le i} \varphi(\mathbf{p}^j, \alpha^j) + (\mathbf{p} - \mathbf{p}^j)^\top \nabla_{\mathbf{p}}(\mathbf{p}^j, \alpha^j) \tag{24}$$

- lower bound and upper bound

$$\underline{\varphi}^i = \min_{\mathbf{p}\in\mathcal{P}} g^i(\mathbf{p}), \quad \overline{\varphi}^i = \min_{1\le j\le i} \varphi(\mathbf{p}^j, \alpha^j). \tag{25}$$

- projection

$$\min_{\mathbf{p}\in\mathcal{L}^i} \|\mathbf{p} - \mathbf{p}^i\|_2^2 \tag{26}$$

- gap

$$\Delta^i = \overline{\varphi}^i - \underline{\varphi}^i. \tag{27}$$

Level method for semi-supervised feature selection

1. Initialize $\mathbf{p}^0 = \frac{m}{d}\mathbf{e}$ and $i = 0$
2. REPEAT
3. Obtain α^i by solving SVM with $\mathbf{M} = (1-\tau)^2 \mathbf{X}_\ell \mathrm{D}(\mathbf{p}^i) \mathbf{X}_\ell^\top + \frac{\tau^2}{\rho}\mathbf{H}$
4. Construct the cutting plane model $g^i(\mathbf{p})$ in (24)
5. Calculate the lower bound $\underline{\varphi}^i$ and the upper bound $\overline{\varphi}^i$ in (25), and the gap Δ^i in (27)
6. Obtain $\mathbf{p}^{i+1}$ via the projection step (26)
7. UNTIL$\Delta^i \leq \varepsilon$

Experimental setup

Comparison algorithms

- Fisher that calculates a Fisher/Correlation score for each feature (Bishop, 1995).
- L_0-appr that approximates the L_0-norm by minimizing a logarithm function (Weston et al., 2003).
- L_1-SVM that replaces L_2-norm of $\mathbf{w}$ with L_1-norm in SVM (Fung & Mangasarian, 2000).

Experimental setup

Comparison algorithms

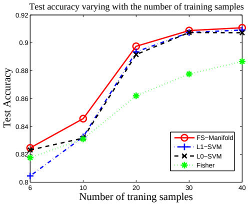
- 10% of data are employed for training
- normalize each feature to be a Gaussian distribution with zero mean and unit standard deviation, based on the training data
- C in all SVM-based feature selection methods is chosen by a 5-fold cross validation

Results on text data

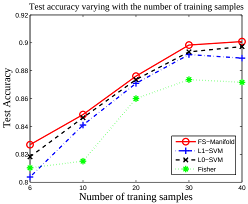
Table: The classification accuracy (%) on text data sets. The best result, and those not significantly worse than it (t-test with 95% confidence level), are highlighted.

Data	#F	FS-Manifold	L_1-SVM	L_0-SVM	Fisher
DS1	50	**82.9**±2.4	82.2±2.9	82.3±2.9	82.3±3.5
	100	**83.5**±2.2	82.9±2.6	**83.2**±2.6	**83.4**±2.6
DS2	50	**89.7**±3.9	88.7±8.6	89.1±4.9	**89.8**±6.9
	100	**91.1**±3.4	**90.9**±5.8	90.3±3.7	90.3±5.6
DS3	50	**84.2**±4.3	82.0±4.4	82.9±4.3	81.3±4.7
	100	**85.8**±3.9	84.1±4.2	85.2±4.4	84.3±4.1

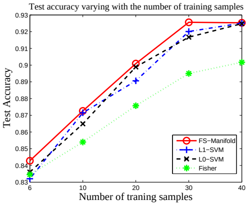
Results on USPS data



(a) *2 vs 3*



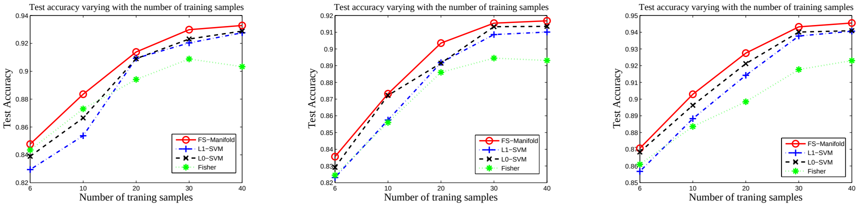
(b) *3 vs 8*



(c) *4 vs 7*

Figure: The comparison among different feature selection algorithms when the number of selected features is equal to 10.

Results on USPS data



(a) *2 vs 3* (b) *3 vs 8* (c) *4 vs 7*

Figure: The comparison among different feature selection algorithms when the number of selected features is equal to 20.

Outline

Conclusion

Presented

- a brief introduction to semi-supervised learning
- three semi-supervised methods
  - an efficient convex relaxation model for Transductive SVM
  - an effective method for semi-supervised kernel learning
  - an effective method for semi-supervised feature selection

Future topics

- when semi-supervised learning will be helpful?
- what is the connection between the low-density assumption and manifold assumption in semi-supervised learning?
- how to obtain or better approximate the optimal solution of semi-supervised models?

Recent publications of our lab in machine learning

- Conference papers
  1. Z. Xu, R. Jin, J. Ye, I. King, and M. R. Lyu. Non-monotonic feature selection, *ICML 2009*.
  2. Z. Xu, R. Jin, M. R. Lyu, and I. King. Semi-supervised Feature Selection via Manifold Regularization. *IJCAI 2009*.
  3. Z. Xu, R. Jin, I. King, and M. R. Lyu, An Extended Level Method for Multiple Kernel Learning, *NIPS 2008*.
  4. Z. Xu, R. Jin, K. Huang, I. King, and M. R. Lyu. Semi-supervised text categorization by active search, *CIKM 2008*.
  5. K. Huang, Z. Xu, I. King, and Michael R. Lyu, Semi-supervised Learning from General Unlabeled Data, *ICDM 2008*.
  6. H. Yang, I. King, and M. Lyu, Learning with Consistency between Inductive Functions and Kernels, *NIPS*, 2008
  7. Z. Xu, R. Jin, J. Zhu, I. King, and M. R. Lyu. Efficient convex relaxation for transductive support vector machine, *NIPS 2007*.

Publications of our lab in machine learning

- Journal papers
  1. Z. Xu, K. Huang, J. Zhu, I. King, and M. R. Lyu. A Novel Kernel-based Maximum A Posteriori Classification Method. *Neural Networks*, 2009.
  2. K. Huang, Z. Xu, I. King, M. R. Lyu, and Z. Zhou, A Novel Discriminative Naive Bayesian Network for Classification, in Bayesian Network Technologies: Applications and Graphical Models, 2007.
  3. Z. Xu, I. King, and M. R. Lyu, Feature Selection Based on Minimum Error Minimax Probability Machine, IJPRAI, 2007.
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Thanks for your attention!