PATTERN RECOGNITION AND MACHINE LEARNING

CHAPTER 7: SPARSE KERNEL MACHINES

Learning Objectives

1、What are support vector machines?

2、What are maximum (soft) margin classifiers?

3、What the relation between SVMs and logistic regression?

4、How to use SVMs for regression?

5、What are relevance vector machines?

6、How to use RVMs for regression?

7、How to use RVMs for classification?

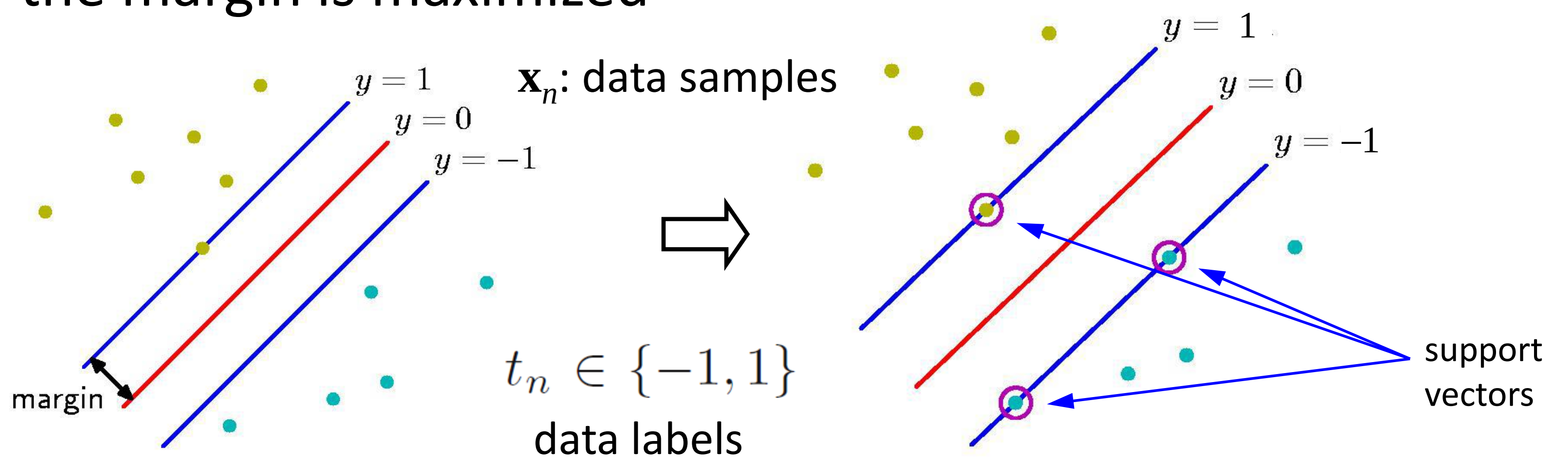
8、What is the mechanism for RVMs to have sparse solutions?

Outlines

- Support Vector Machines
- SVMs and Logistic Regression
- SVMs for Regression
- Relevance Vector Machines
- RVMs for Regression
- RVMs for Classification

Support Vector Machines

- Problem settings $$y(\mathbf{x}) = \mathbf{w}^T \phi(\mathbf{x}) + b$$
  - ✓ Two-class classification using linear models
  - ✓ Assume that training data set is linearly separable
- Support vector machine approaches
  - ✓ The decision boundary is chosen to be the one for which the margin is maximized



Maximum Margin Classifier I

For all data points, $t_n y(\mathbf{x}_n) > 0$

The distance of a point to the decision surface

$$\frac{t_n y(\mathbf{x}_n)}{\|\mathbf{w}\|} = \frac{t_n(\mathbf{w}^T\phi(\mathbf{x}_n) + b)}{\|\mathbf{w}\|}$$

The maximum margin solution

$$\arg\max_{\mathbf{w},b}\left\{\frac{1}{\|\mathbf{w}\|}\underbrace{\min_n\left[t_n(\mathbf{w}^T\phi(\mathbf{x}_n) + b)\right]}_{\boxed{\text{support vectors}}}\right\}$$

A difficult problem !

Maximum Margin Classifier II

- After rescaling w and b, the point closest to the surface becomes

$$t_n\left(\mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}_n)+b\right)=1$$

- The constraints for all points become

$$t_n\left(\mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}_n)+b\right)\geqslant 1, \qquad n=1,\ldots,N$$

“=“ means active constraints, “>” means inactive constraints

$$\Rightarrow \boxed{\arg\min_{\mathbf{w},b}\frac{1}{2}\|\mathbf{w}\|^2 \text{ subject to } t_n(\mathbf{w}^T\phi(\mathbf{x}_n)+b)\geq 1,\ n=1,\ldots,N}$$

An easier problem !

Lagrange Method

- Minimize an object function $s.\,t.$ constraints of inequality

$$\min_x f(x) \quad s.t. \quad g(x) \geq 0$$

- By Introducing a Lagrange multiplier $\lambda \geq 0$, then we will have

$$\min_x \max_{\lambda \geq 0} \{\mathcal{L}(x,\lambda) = f(x) - \lambda g(x)\}$$

- When certain conditions are satisfied, its dual problem is

$$\max_{\lambda \geq 0} \min_x \{\mathcal{L}(x,\lambda) = f(x) - \lambda g(x)\}$$

- By setting derivatives of $\mathcal{L}$ w.r.t. x equal to 0, we will have

$x = h(\lambda)$, and then the problem becomes $\lambda^* = \max_{\lambda \geq 0} Q(\lambda)$

- Finally, $x^* = h(\lambda^*)$ is the solution

Dual Representation I

- Introducing Lagrange multipliers $a_n \geqslant 0$, then we will have

$$L(\mathbf{w}, b, \mathbf{a}) = \frac{1}{2}\|\mathbf{w}\|^2 \underbrace{- \sum_{n=1}^{N} a_n \left\{ \overbrace{t_n(\mathbf{w}^T \phi(\mathbf{x}_n) + b) - 1}^{\geq 0} \right\}}_{\leq 0}$$

which minimizes the first part and maximizes the second part:
either $a_n = 0$ or $a_n \neq 0 \;\cap\; t_n\left(\mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}_n) + b\right) = 1$

inactive constraint | active constraint : support vectors

- By setting derivatives of *L* w.r.t. **w** and *b* equal 0, we will have

$$\mathbf{w} = \sum_{n=1}^{N} a_n t_n \phi(\mathbf{x}_n), \quad 0 = \sum_{n=1}^{N} a_n t_n$$

Dual Representation II

- Eliminating **w** and *b* with $\mathbf{w} = \sum_{n=1}^{N} a_n t_n \phi(\mathbf{x}_n), \quad 0 = \sum_{n=1}^{N} a_n t_n$ from *L*, we will have the dual representation

$$\widetilde{L}(\mathbf{a}) = \sum_{n=1}^{N} a_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} a_n a_m t_n t_m k(\mathbf{x}_n, \mathbf{x}_m)$$

subject to $a_n \geq 0, \; n = 1, \ldots, N$

$$\sum_{n=1}^{N} a_n t_n = 0$$

quadratic programming

$\Rightarrow$ solving a_n

$a_n \neq 0$: support vectors

where

$$k(\mathbf{x}, \mathbf{x}') = \phi(\mathbf{x})^{\mathrm{T}} \phi(\mathbf{x}')$$

Classifier Parameters

- The classifier can be rewritten as

$$y(\mathbf{x}) = \mathbf{w}^T \phi(\mathbf{x}) + b \;\Rightarrow\; y(\mathbf{x}) = \sum_{n=1}^{N} a_n t_n k(\mathbf{x}, \mathbf{x}_n) + b$$

$\mathbf{x}_n$: support vectors

- After finding *a* by solving the quadratic programming problem, we need to estimate *b*. For support vectors, $a_n \neq 0$, we will have

$$t_n \underbrace{\left(\sum_{m \in \mathcal{S}} a_m t_m k(\mathbf{x}_n, \mathbf{x}_m) + b \right)}_{y(\mathbf{x}_n)} = 1 \qquad t_n^2 = 1$$

$$b = \frac{1}{N_S} \sum_{n \in S} \left(t_n - \sum_{m \in S} a_m t_m k(\mathbf{x}_n, \mathbf{x}_m) \right)$$

where S is the set of support vectors.

Maximum Margin Classifier

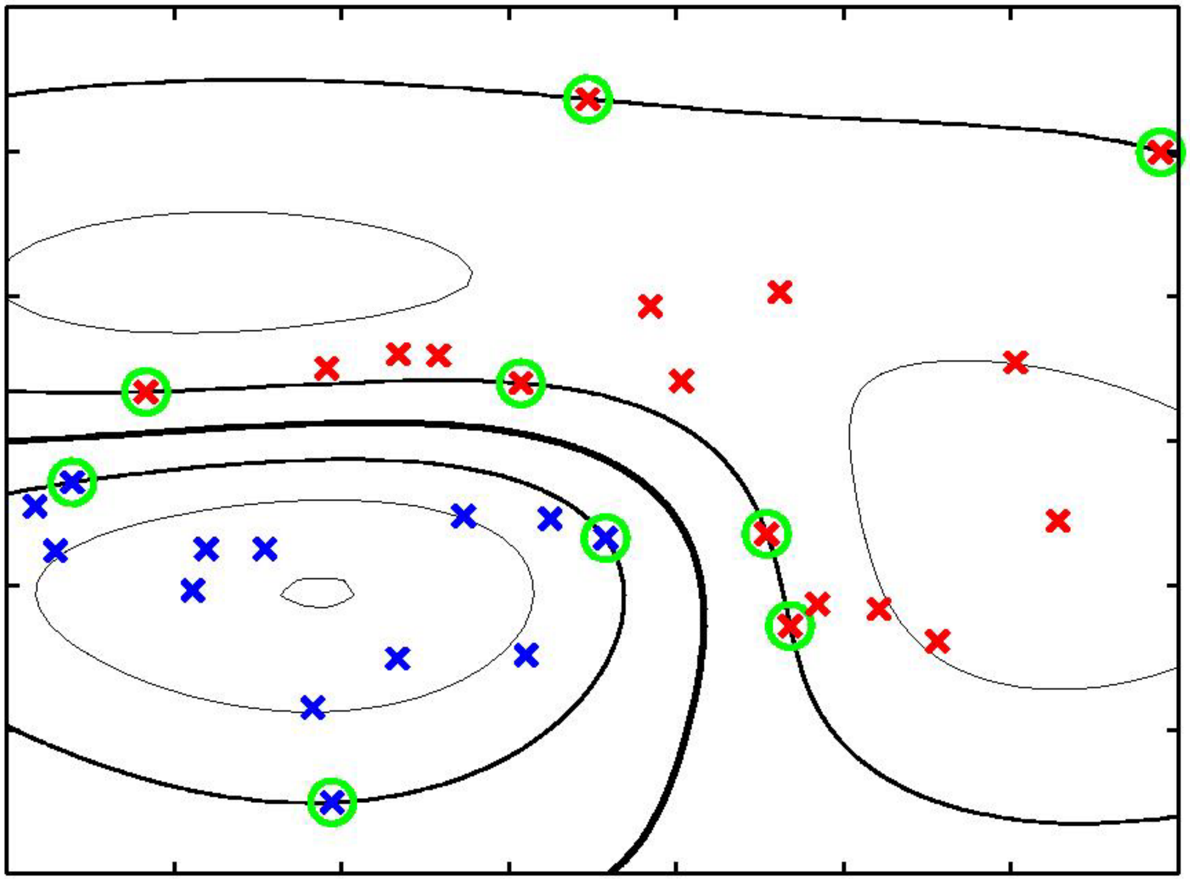
- Training maximum margin classifiers can be generalized as

$$\arg\min_{\mathbf{w},b} \sum_{n=1}^{N} E_{\infty}(y(\mathbf{x}_n)t_n - 1) + \lambda||\mathbf{w}||^2 \qquad \lambda > 0$$

where $E_{\infty}(z)$ is a function that is zero if z >=0 and ∞ otherwise.

- Such that only support vectors will be selected to optimize model parameters

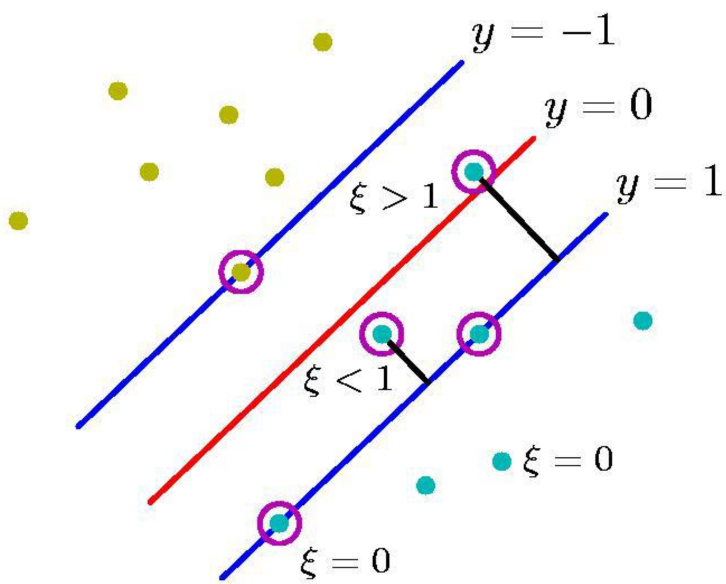
Example of Separable Data Classification



Overlapping Class Distributions

Allow some misclassified examples → soft margin

Introduce slack variables $\xi_n \geq 0,\ n = 1, \ldots, N$



$$t_n y(\mathbf{x}_n) = t_n(\mathbf{w}^T \phi(\mathbf{x}_n) + b) \geq 1 \;\Rightarrow\; t_n y(\mathbf{x}_n) \geq 1 - \xi_n$$

Soft Margin Classifier

Minimize $$C\sum_{n=1}^{N}\xi_n+\frac{1}{2}\|\mathbf{w}\|^2$$

$C>0$: **trade-off between minimizing training errors and controlling model complexity**

$$L(\mathbf{w},b,\mathbf{a})=\frac{1}{2}\|\mathbf{w}\|^2+C\sum_{n=1}^{N}\xi_n-\sum_{n=1}^{N}a_n\{t_n y(\mathbf{x}_n)-1+\xi_n\}-\sum_{n=1}^{N}\mu_n\xi_n$$

KKT conditions:

$$a_n\geq 0$$

$$t_n y(\mathbf{x}_n)-1+\xi_n\geq 0$$

$$a_n\left(t_n y(\mathbf{x}_n)-1+\xi_n\right)=0$$

: support vectors

$$\mu_n\geq 0$$

$$\xi_n\geq 0$$

$$\mu_n\xi_n=0$$

$\boxed{a_n=0}$

or

$\boxed{t_n y(\mathbf{x}_n)=1-\xi_n}$

Dual Representation

- By setting derivatives of *L* w.r.t. **w**, *b*, and $\{\xi_n\}$ equal 0, we will have

$$\frac{\partial L}{\partial \mathbf{w}} = 0 \quad \Rightarrow \quad \mathbf{w} = \sum_{n=1}^{N} a_n t_n \boldsymbol{\phi}(\mathbf{x}_n)$$

$$\frac{\partial L}{\partial b} = 0 \quad \Rightarrow \quad \sum_{n=1}^{N} a_n t_n = 0$$

$$\frac{\partial L}{\partial \xi_n} = 0 \quad \Rightarrow \quad a_n = C - \mu_n.$$

Dual Representation

- Dual representation

$$\widetilde{L}(\mathbf{a}) = \sum_{n=1}^{N} a_n - \frac{1}{2}\sum_{n=1}^{N}\sum_{m=1}^{N} a_n a_m t_n t_m k(\mathbf{x}_n, \mathbf{x}_m)$$

subject to $0 \le a_n \le C,\ n = 1,\ldots,N$

$$\sum_{\mathrm{n}=1}^{\mathrm{N}} a_n t_n = 0$$

- Estimating *b*

(➔ same as hard maximum margin classifiers)

Alternative Formulation

v-SVM (Schölkopf *et al*., 2000)

$$\widetilde{L}(\mathbf{a}) = -\frac{1}{2}\sum_{n=1}^{N}\sum_{m=1}^{N} a_n a_m t_n t_m k(\mathbf{x}_n, \mathbf{x}_m)$$

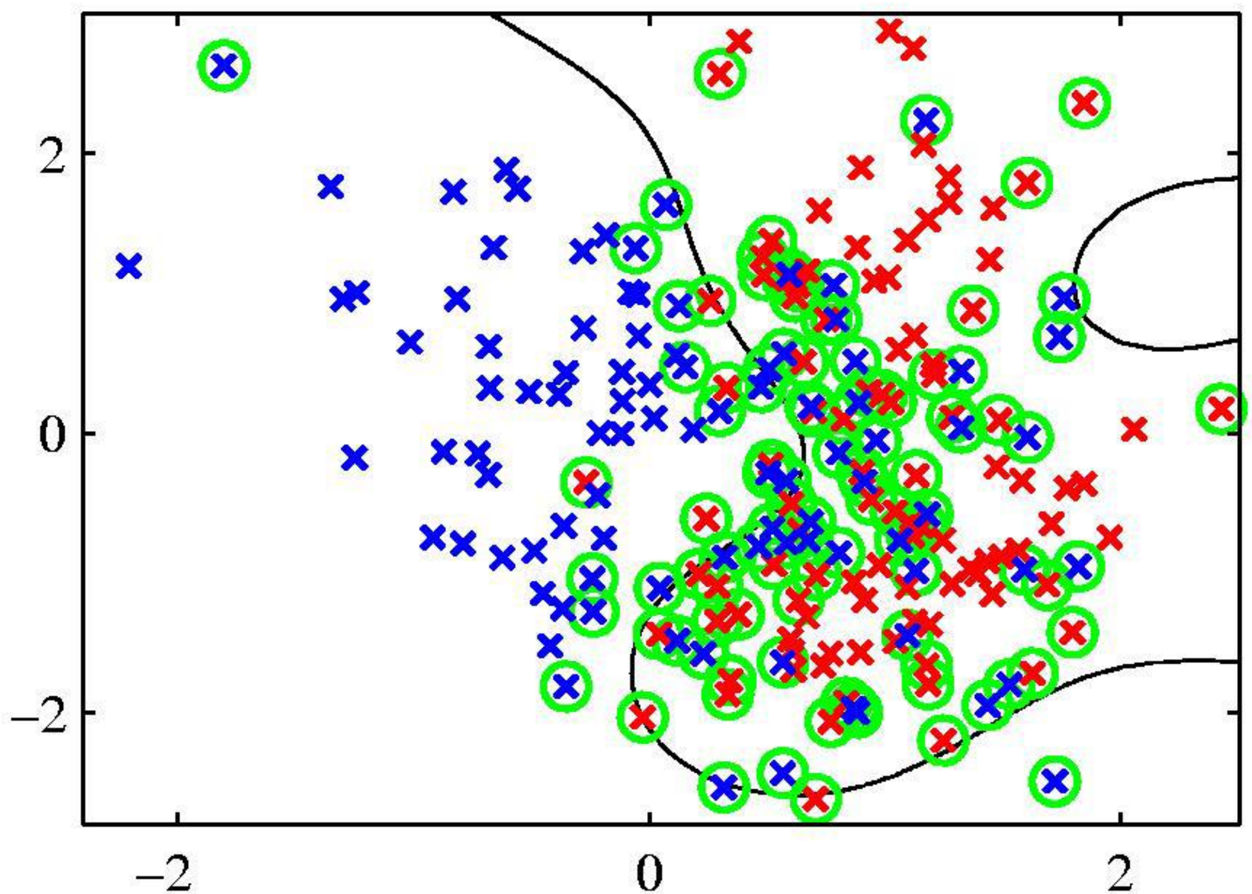
subject to $0 \leq a_n \leq 1/N$

$$\sum_{\mathrm{n}=1}^{\mathrm{N}} a_n t_n = 0$$

$$\sum_{\mathrm{n}=1}^{\mathrm{N}} a_n \geq \underline{v}$$

- Upper bound on the fraction of margin errors
- Lower bound on the fraction of support vectors

Nonseparable Data Classification (ν-SVM)



Solutions of the QP Problem

- Chunking (Vapnik, 1982)

  Idea: the value of Lagrangian is unchanged if we remove the rows and columns of the kernel matrix corresponding to Lagrange multipliers that have value zero
- Decomposition methods (Osuna *et al.*, 1996)
- Protected conjugate gradients (Burges, 1998)
- Sequential minimal optimization (Platt, 1999)

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Relation to Logistic Regression I

For data points on the correct side, $\xi = 0$

For the remaining points, $\xi = 1 - y_n t_n$

$$C \sum_{n=1}^{N} \xi_n + \frac{1}{2} \|\mathbf{w}\|^2 \Rightarrow \sum_{n=1}^{N} E_{SV}(y_n, t_n) + \lambda \|\mathbf{w}\|^2$$

where $\lambda = (2C)^{-1}$

$E_{SV}(y_n, t_n) = [1 - y_n t_n]_+$: **hinge error function**

where $[\cdot]_+$ denotes the positive part

Relation to Logistic Regression II

- From maximum likelihood logistic regression

$$p(t=1\mid y)=\sigma(y)$$

$$p(t=-1\mid y)=1-\sigma(y)=\sigma(-y)$$

$$\Rightarrow\ p(t\mid y)=\sigma(yt)$$

- Error function with quadratic regularization

$$\sum_{n=1}^{N} E_{LR}(y_n t_n)+\lambda\|\mathbf{w}\|^2$$

where $E_{LR}(yt)=\ln\left(1+\exp\left(-yt\right)\right)$

Relation to Logistic Regression III

b: Bernoulli parameter

y: natural parameter

- Cross-Entropy

$$-\ln p(t|b) = -t \ln b - (1-t)\ln(1-b)$$

$$-\ln p(t|y) = -\ln \sigma(yt) = \ln(1+e^{-yt}) \qquad b = \sigma(y)$$

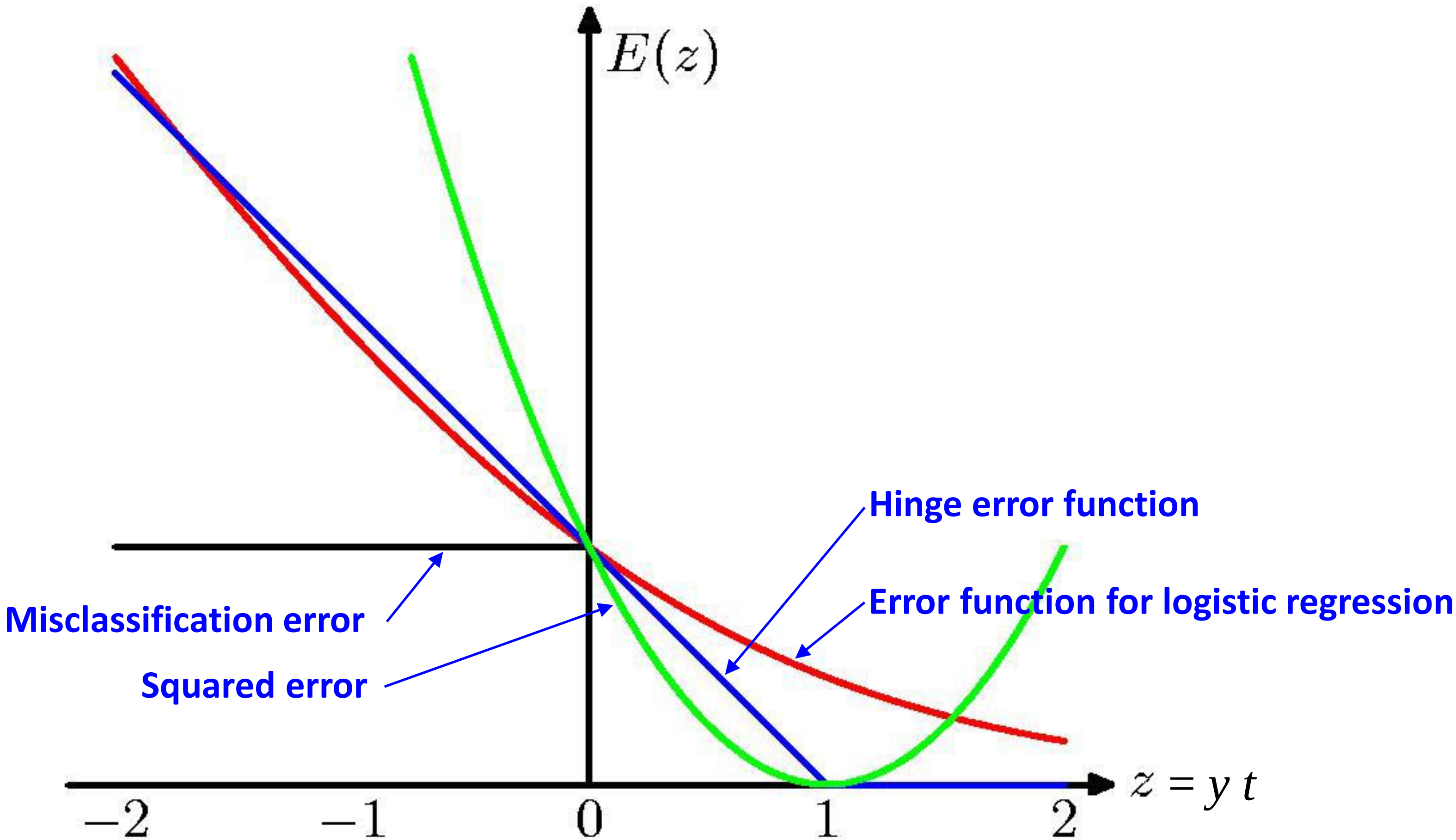
- Cross-Entropy with prior

$$-\ln p(t|b) + \alpha^{-1}\mathbf{w}^T\mathbf{w} = -t \ln b - (1-t)\ln(1-b) + \alpha^{-1}\mathbf{w}^T\mathbf{w}$$

$$-\ln p(t|y) + \alpha^{-1}\mathbf{w}^T\mathbf{w} = \ln(1+e^{-yt}) + \alpha^{-1}\mathbf{w}^T\mathbf{w}$$

softplus: $\boxed{\ln(1+e^{-x})}$

Comparison of Error Functions



Multiclass SVMs

- *One-versus-the-rest*: K separate SVMs
  - Can lead inconsistent results (Figure 4.2)
  - Imbalanced training sets
    - Positive class: +1, negative class: $-1/(K-1)$
- An objective function for training all SVMs simultaneously
- *One-versus-one*: $K(K-1)/2$ SVMs
- Error-correcting output codes
  - Generalization of the voting scheme of the *one-versus-one*

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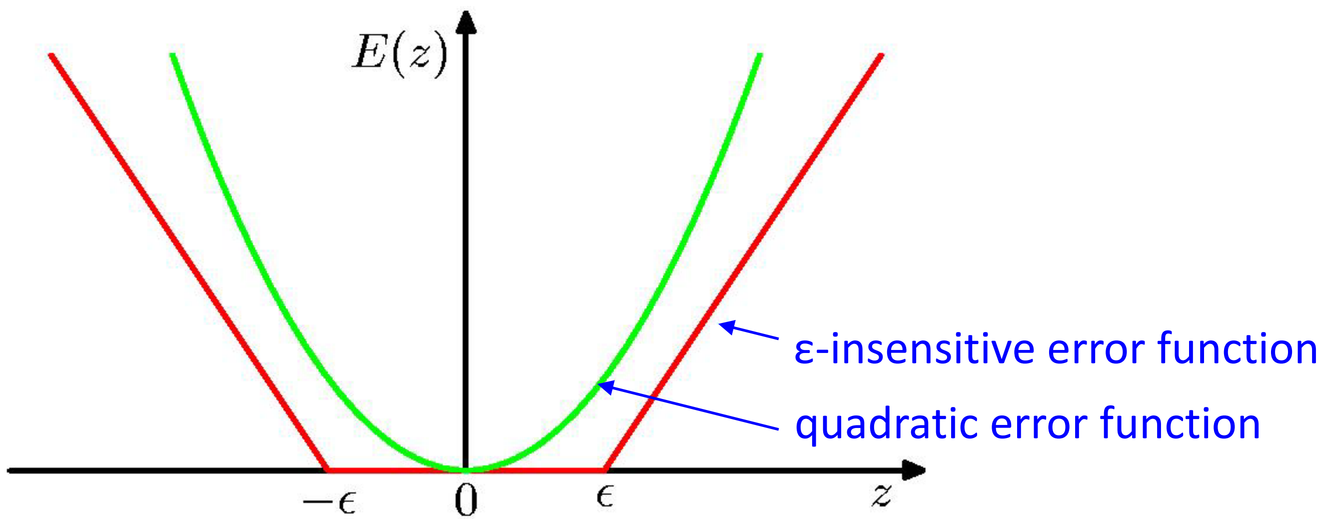
SVMs for Regression I

Simple linear regression: minimize $\frac{1}{2}\sum_{n=1}^{N}\boxed{\{y_n - t_n\}^2} + \frac{\lambda}{2}\|\mathbf{w}\|^2$

ε-insensitive error function

$$E_\varepsilon\left(y(\mathbf{x})-t\right)=\begin{cases}0, & \text{if } \left|y(\mathbf{x})-t\right|<\varepsilon\\ \left|y(\mathbf{x})-t\right|-\varepsilon, & \text{otherwise}\end{cases}$$



SVMs for Regression II

Minimize

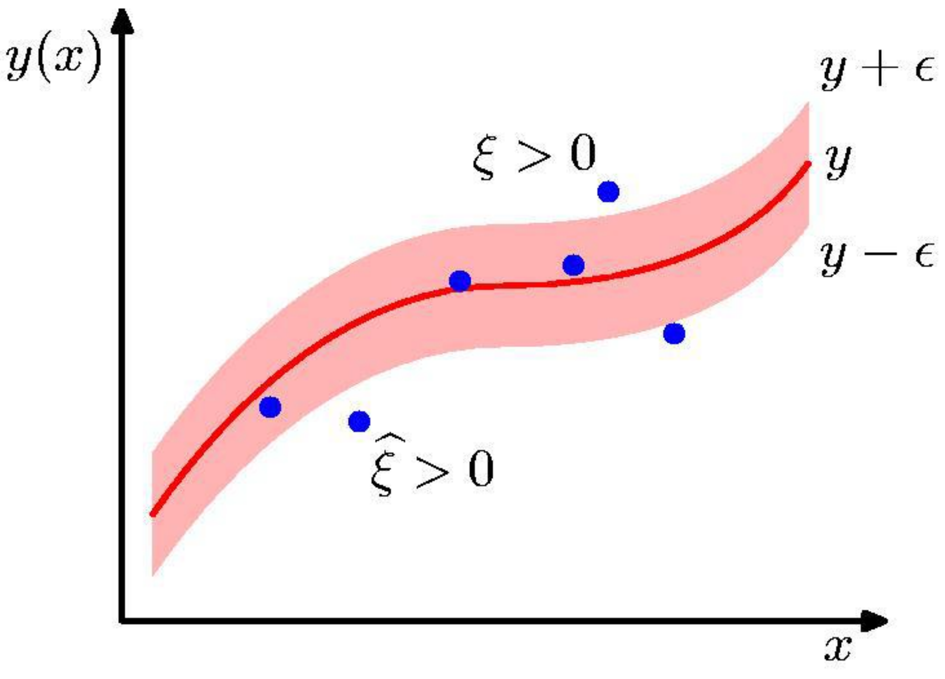
$$C\sum_{n=1}^{N} E_{\varepsilon}\left(y(\mathbf{x}_n)-t_n\right)+\frac{1}{2}\|\mathbf{w}\|^2$$

$$C\sum_{n=1}^{N}\left(\xi_n+\hat{\xi}_n\right)+\frac{1}{2}\|\mathbf{w}\|^2$$

where $t_n \le y(\mathbf{x}_n)+\varepsilon+\xi_n$

$$t_n \ge y(\mathbf{x}_n)-\varepsilon-\hat{\xi}_n$$

$$\xi_n \ge 0,\ \hat{\xi}_n \ge 0$$



Dual Problem

$$L = C\sum_{n=1}^{N}\left(\xi_n + \hat{\xi}_n\right) + \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{n=1}^{N}\left(\mu_n\xi_n + \hat{\mu}_n\hat{\xi}_n\right)$$

$$-\sum_{n=1}^{N} a_n(\varepsilon + \xi_n + y_n - t_n) - \sum_{n=1}^{N}\hat{a}_n\left(\varepsilon + \hat{\xi}_n - y_n + t_n\right)$$

$$\widetilde{L}(\mathbf{a}, \hat{\mathbf{a}}) = -\frac{1}{2}\sum_{n=1}^{N}\sum_{m=1}^{N}(a_n - \hat{a}_n)(a_m - \hat{a}_m)k(\mathbf{x}_n, \mathbf{x}_m)$$

$$-\varepsilon\sum_{n=1}^{N}(a_n + \hat{a}_n) + \sum_{n=1}^{N}(a_n - \hat{a}_n)t_n$$

subject to $0 \le a_n, \hat{a}_n \le C$

$$\sum_{\mathrm{n}=1}^{\mathrm{N}}\left(a_n - \hat{a}_n\right) = 0$$

Predictions

$$\mathbf{w} = \sum_{n=1}^{N} (a_n - \hat{a}_n)\phi(\mathbf{x}_n)$$ **(from derivatives of the Lagrangian cost equal 0)**

$$y(\mathbf{x}) = \sum_{n=1}^{N} (a_n - \hat{a}_n) k(\mathbf{x}, \mathbf{x}_n) + b$$

KKT conditions:

$$\begin{aligned} a_n\left(\underline{\varepsilon + \xi_n + y_n - t_n}\right) &= 0 \\ \hat{a}_n\left(\underline{\varepsilon + \hat{\xi}_n - y_n + t_n}\right) &= 0 \\ (C - a_n)\xi_n &= 0 \\ (C - \hat{a}_n)\hat{\xi}_n &= 0 \end{aligned}$$

$$b = t_n - \varepsilon - \mathbf{w}^T\phi(\mathbf{x}_n) = t_n - \varepsilon - \sum_{m=1}^{N} (a_m - \hat{a}_m) k(\mathbf{x}_n, \mathbf{x}_m)$$

Alternative Formulation

v-SVM (Schölkopf *et al.*, 2000)

$$\widetilde{L}(\mathbf{a},\hat{\mathbf{a}}) = -\frac{1}{2}\sum_{n=1}^{N}\sum_{m=1}^{N}(a_n - \hat{a}_n)(a_m - \hat{a}_m)k(\mathbf{x}_n,\mathbf{x}_m) + \sum_{n=1}^{N}(a_n - \hat{a}_n)t_n$$

subject to $0 \le a_n, \hat{a}_n \le C/N$

$$\sum_{n=1}^{N}\left(a_n - \hat{a}_n\right) = 0$$

$$\sum_{n=1}^{N}\left(a_n + \hat{a}_n\right) \le \underline{v}C$$

fraction of points lying outside the tube

Example of ν-SVM Regression