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

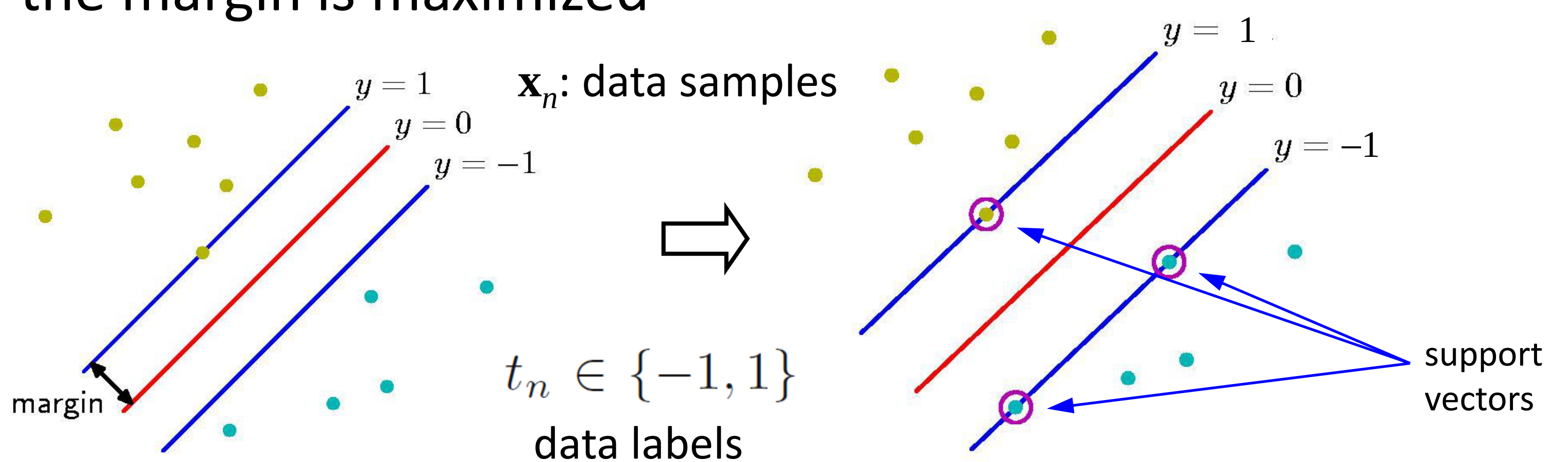
- Support Vector Machines
- SVMs and Logistic Regression
- SVMs for Regression
- Relevance Vector Machines
- RVMs for Regression
- RVMs for Classification

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

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

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

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

where S is the set of support vectors.

Maximum Margin Classifier

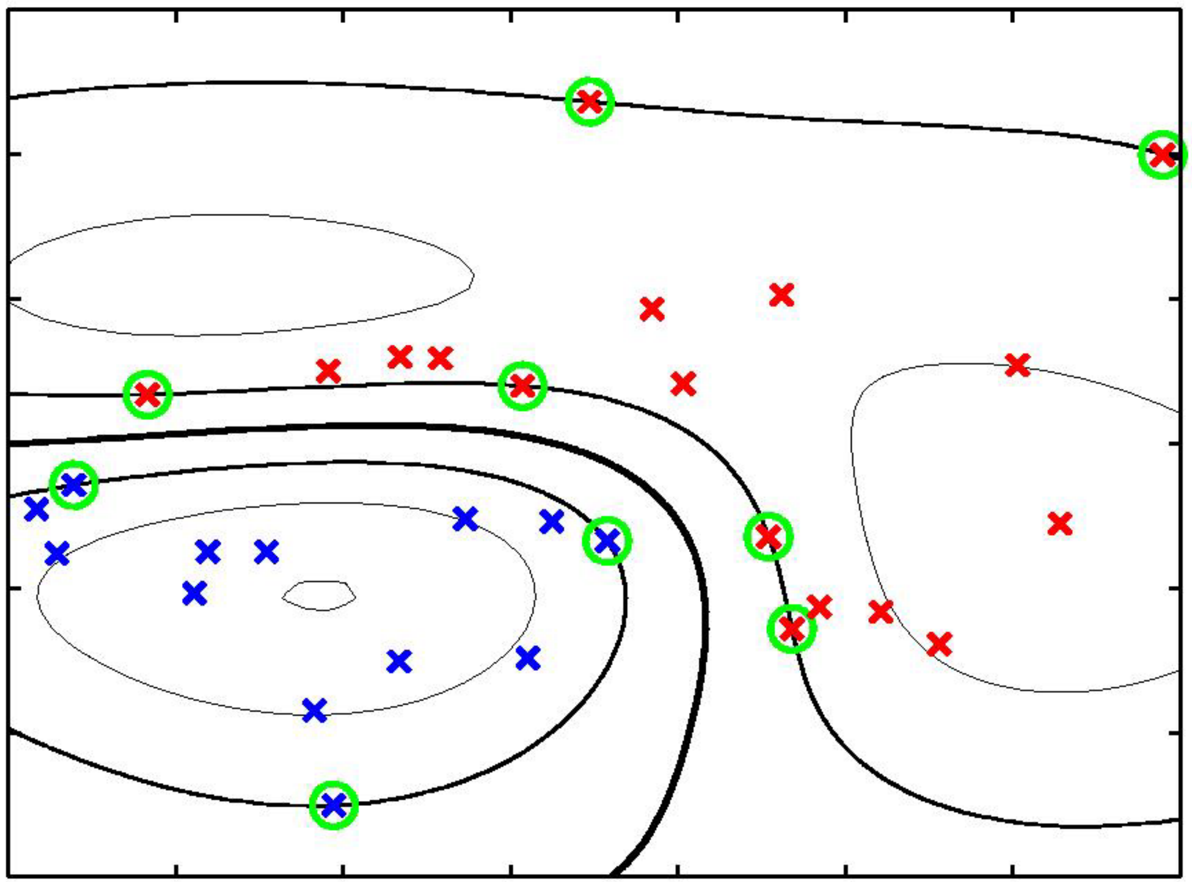
- Training maximum margin classifiers can be generalized as

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

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

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

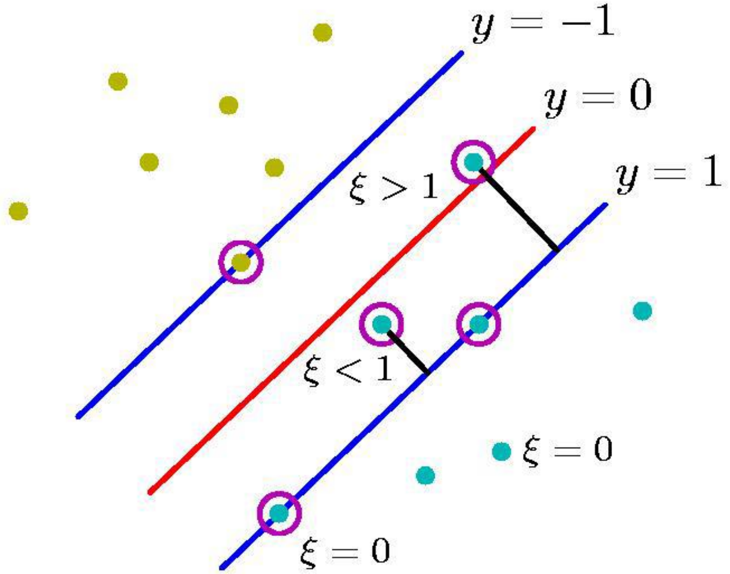
Example of Separable Data Classification



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

ν-SVM (Schölkopf *et al.*, 2000)

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

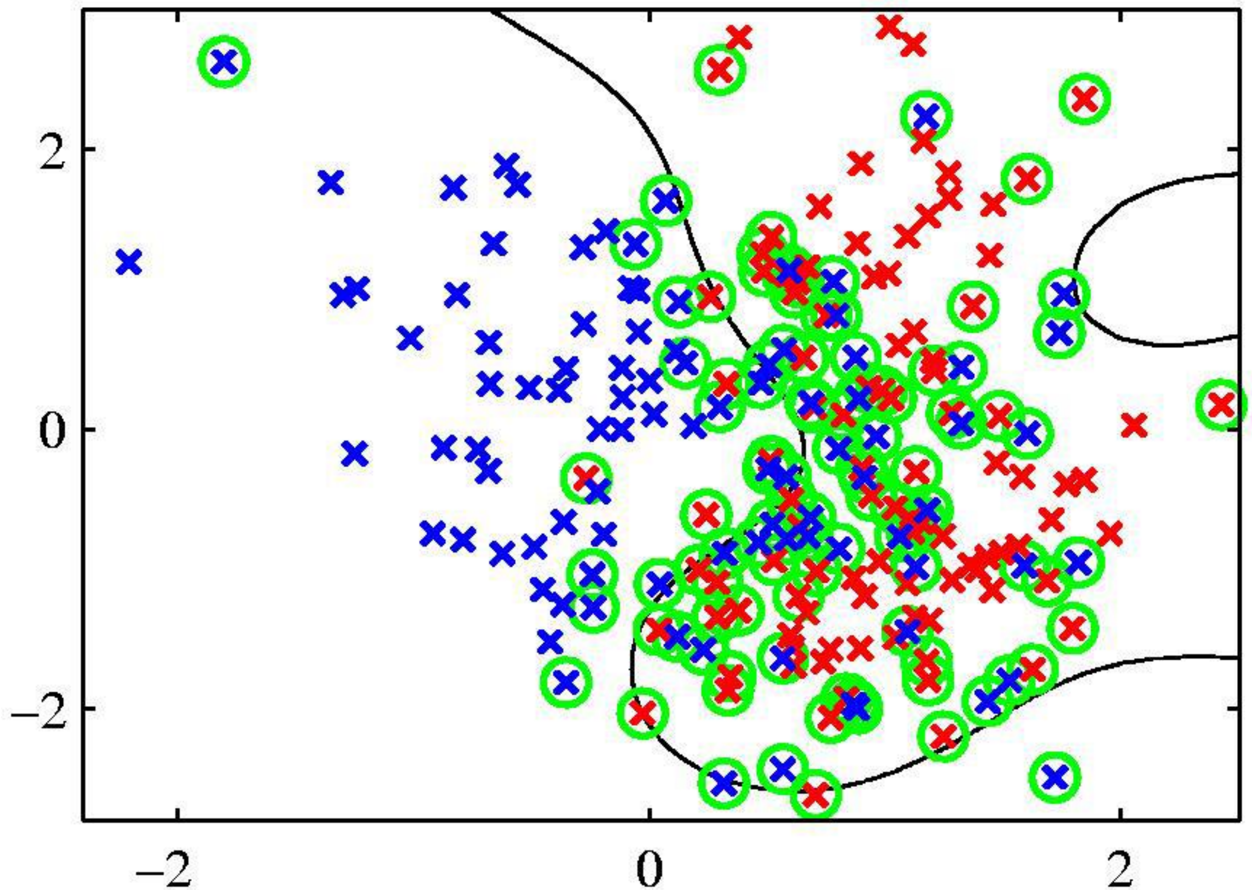
subject to $0 \le a_n \le 1/N$

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

$$\sum_{\mathrm{n}=1}^{\mathrm{N}} a_n \ge \nu$$

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

Relation to Logistic Regression III

b: Bernoulli parameter

y: natural parameter

- Cross-Entropy

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

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

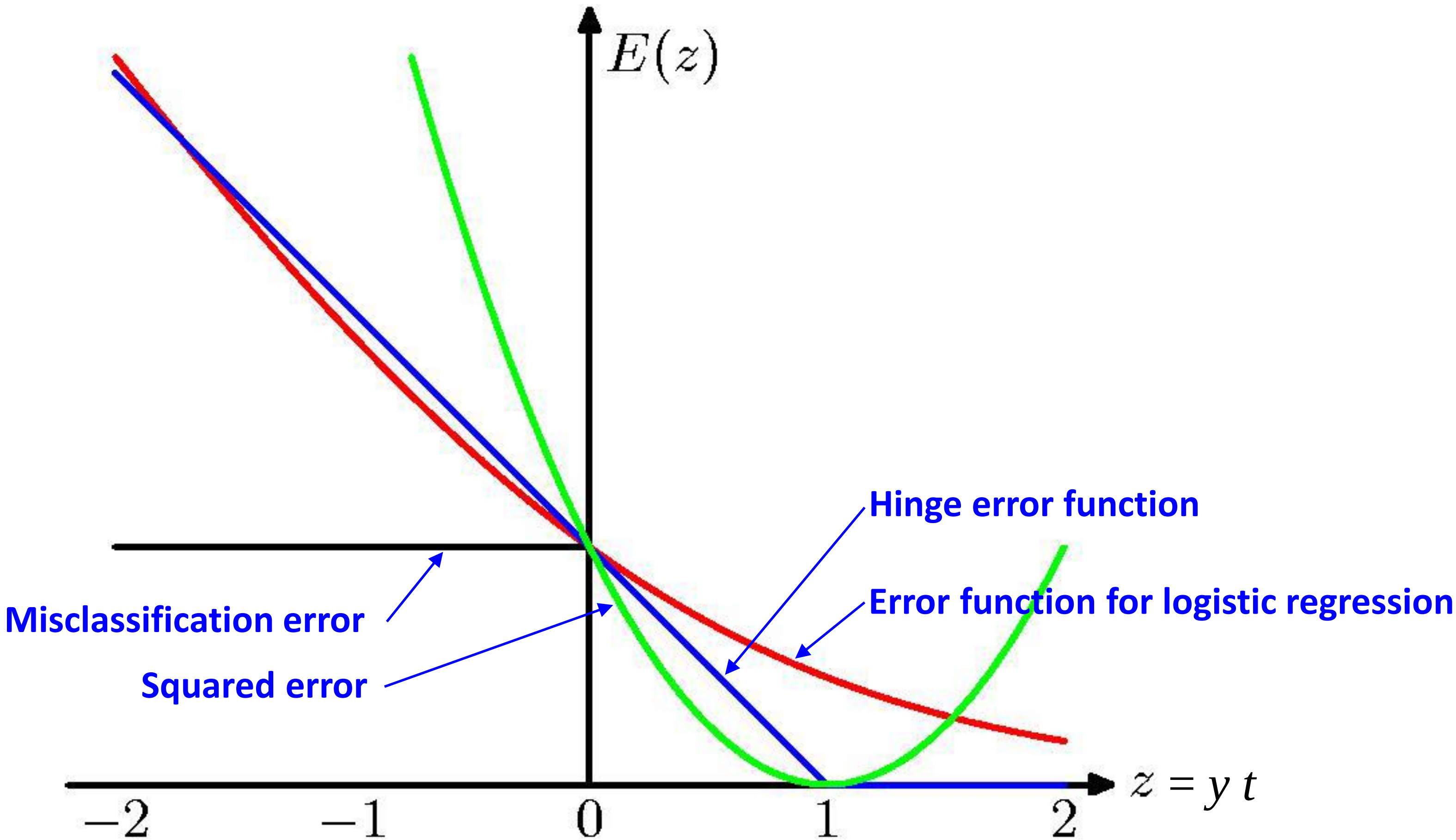
- Cross-Entropy with prior

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

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

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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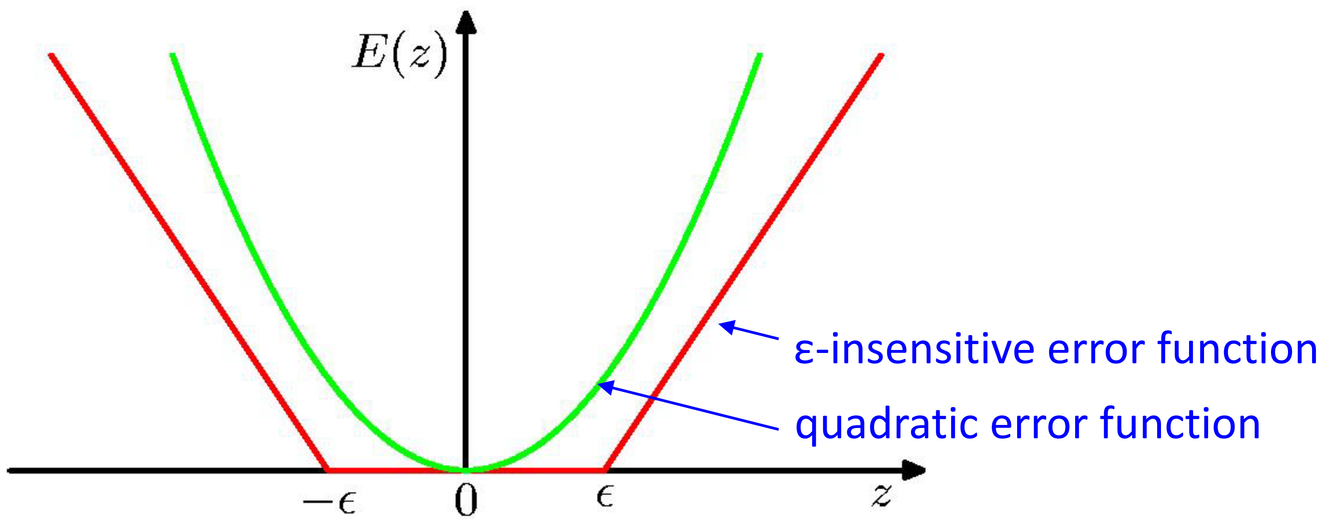
SVMs for Regression I

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

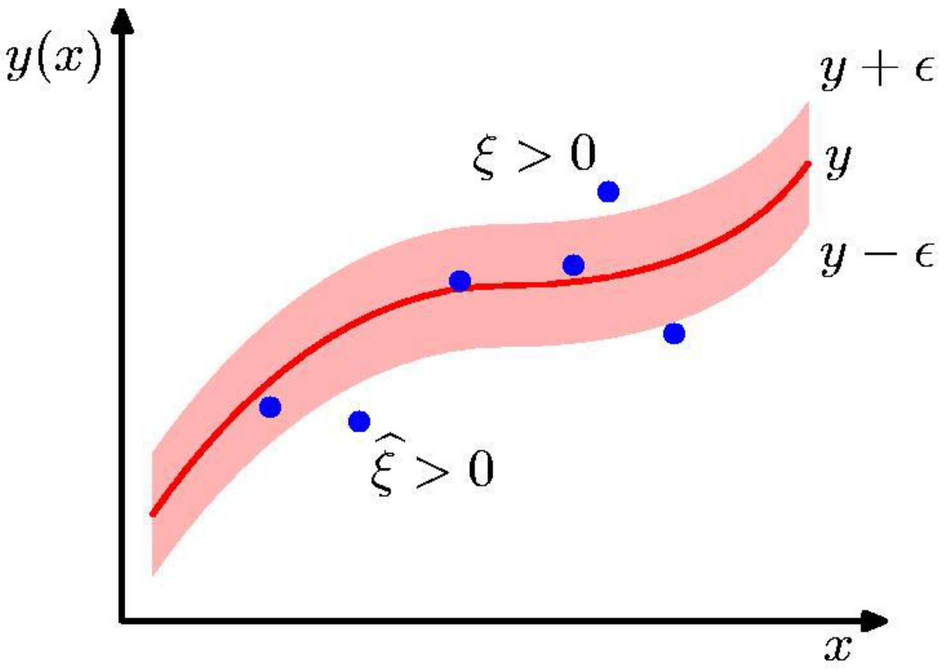
$$C\sum_{n=1}^{N} E_{\varepsilon}\left(y(\mathbf{x}_n)-t_n\right)+\frac{1}{2}\|\mathbf{w}\|^2$$

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

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:

$$a_n \left(\underline{\varepsilon + \xi_n + y_n - t_n} \right) = 0$$

$$\hat{a}_n \left(\underline{\varepsilon + \hat{\xi}_n - y_n + t_n} \right) = 0$$

$$(C - a_n) \xi_n = 0$$

$$(C - \hat{a}_n) \hat{\xi}_n = 0$$

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

Alternative Formulation

v-SVM (Schölkopf *et al.*, 2000)

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

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

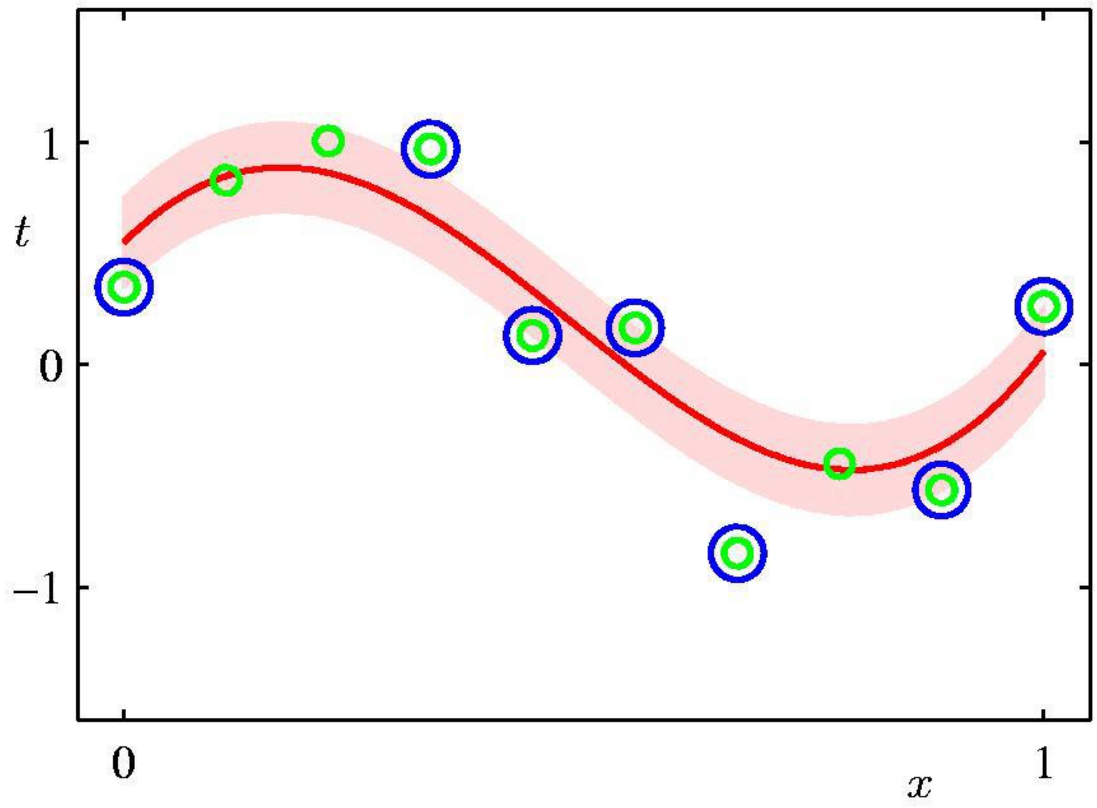
subject to $0 \leq a_n, \hat{a}_n \leq C/N$

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

$$\sum_{\mathrm{n}=1}^{\mathrm{N}}\left(a_n + \hat{a}_n\right) \leq \nu C$$

fraction of points lying outside the tube

Example of ν-SVM Regression



Outlines

- Support Vector Machines
- SVM and Logistic Regression
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Relevance Vector Machines

- SVM
  - Outputs are decisions rather than posterior probabilities
  - The extension to K>2 classes is problematic
  - There is a complexity parameter
  - Kernel functions are centered on training data points and required to be positive definite
- RVM
  - Bayesian regression and classification frameworks
  - Bayesian sparse kernel technique
  - Much sparser models
  - Faster performance on test data

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RVM for Regression I

- RVM is a linear form with a modified prior

$$p(t \mid \mathbf{x}, \mathbf{w}, \beta) = N(t \mid y(\mathbf{x}), \beta^{-1})$$

where $y(\mathbf{x}) = \sum_{i=1}^{M} w_i \phi_i(\mathbf{x}) = \mathbf{w}^T \phi(\mathbf{x}) \Rightarrow y(\mathbf{x}) = \sum_{i=1}^{N} w_n k(\mathbf{x}, \mathbf{x}_n) + b$

$$\beta = \sigma^{-2}$$

$$p(\mathbf{t}|\mathbf{X}, \mathbf{w}, \beta) = \prod_{n=1}^{N} p(t_n|\mathbf{x}_n, \mathbf{w}, \beta^{-1})$$

$$p(\mathbf{w}|\boldsymbol{\alpha}) = \prod_{i=1}^{N} \mathcal{N}(w_i|0, \alpha_i^{-1})$$

Each data sample has a weight

RVM for Regression II

$$p(\mathbf{w} \mid \mathbf{t}, \mathbf{X}, \boldsymbol{\alpha}, \beta) = N(\mathbf{w} \mid \mathbf{m}, \Sigma)$$

From the result (3.49) for linear regression models

where $\mathbf{m} = \beta \Sigma \boldsymbol{\Phi}^T \mathbf{t}$

$$\Sigma = \left(\mathbf{A} + \beta \boldsymbol{\Phi}^T \boldsymbol{\Phi}\right)^{-1}$$

where $\boldsymbol{\Phi} : N \times M$ matrix with elements $\Phi_{ni} = \phi_i(\mathbf{x}_n)$

$$\mathbf{A} = diag(\alpha_i)$$

<u>α and β are determined using *evidence approximation*</u>

$$p(\mathbf{t} \mid \mathbf{X}, \boldsymbol{\alpha}, \beta) = \int p(\mathbf{t} \mid \mathbf{X}, \mathbf{w}, \beta) p(\mathbf{w} \mid \boldsymbol{\alpha}) d\mathbf{w}$$

Prior Predictive Distribution

$$\ln p(\mathbf{t} \mid \mathbf{X}, \boldsymbol{\alpha}, \beta) = \ln N(\mathbf{t} \mid \mathbf{0}, \mathbf{C})$$

$$= -\frac{1}{2}\left\{N \ln(2\pi) + \ln|\mathbf{C}| + \mathbf{t}^T \mathbf{C}^{-1} \mathbf{t}\right\} \Rightarrow$$ **Maximize**

where $\mathbf{t} = (t_1, \ldots, t_N)^T$, $\mathbf{C} = \beta^{-1}\mathbf{I} + \boldsymbol{\Phi}\mathbf{A}^{-1}\boldsymbol{\Phi}^T$

RVM for Regression III

Two steps

① From derivatives of the marginal likelihood, we have

$$\alpha_i^{new} = \frac{\gamma_i}{m_i^2}, \quad \left(\beta^{new}\right)^{-1} = \frac{\|\mathbf{t} - \boldsymbol{\Phi}\mathbf{m}\|^2}{N - \sum_i \gamma_i}$$

where $\gamma_i = 1 - \alpha_i \Sigma_{ii}$

Σ_{ii} : i^{th} diagonal element of Σ

② Predictive distribution

Posterior Predictive Distribution

$$p(t \mid \mathbf{x}, \mathbf{X}, \mathbf{t}, \boldsymbol{\alpha}^*, \beta^*) = \int p(t \mid \mathbf{x}, \mathbf{w}, \beta^*) \, p(\mathbf{w} \mid \mathbf{x}, \mathbf{X}, \mathbf{t}, \boldsymbol{\alpha}^*, \beta^*) d\mathbf{w}$$

$$= N\left(t \mid \mathbf{m}^T \phi(\mathbf{x}), \sigma^2(\mathbf{x})\right)$$

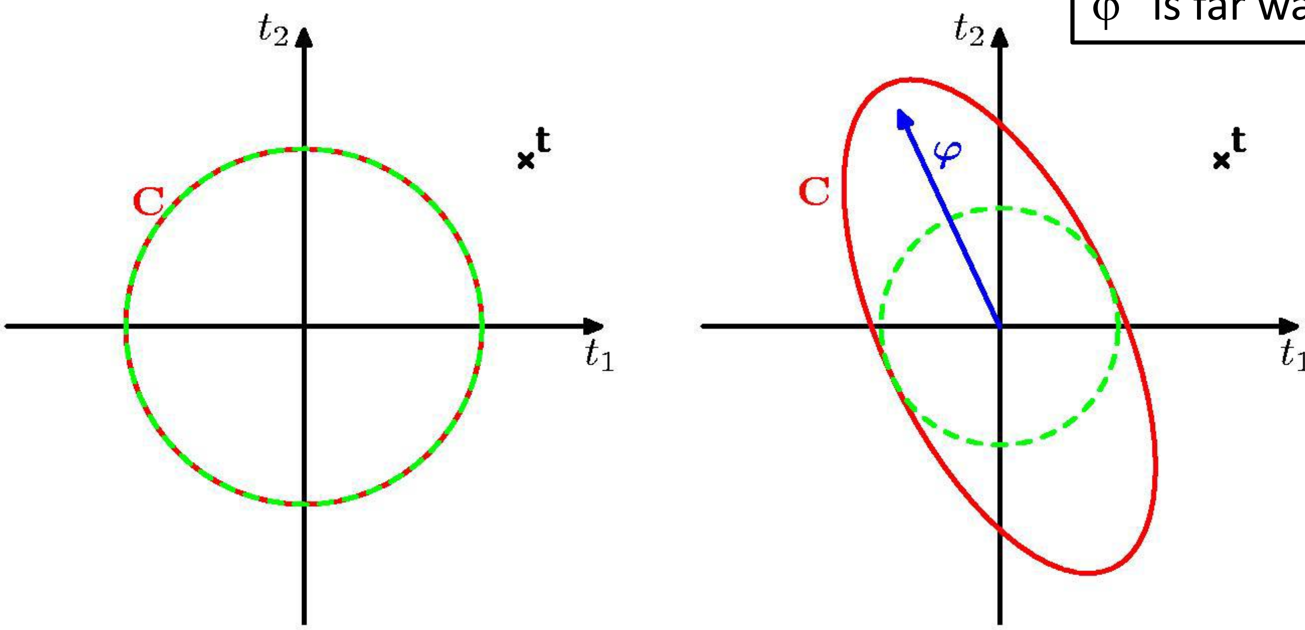
where $\sigma^2(\mathbf{x}) = \left(\beta^*\right)^{-1} + \phi(\mathbf{x})^T \Sigma \phi(\mathbf{x})$

Mechanism for Sparsity

$$p(\mathbf{t}\,|\,\alpha,\beta) = N(\mathbf{t}\,|\,\mathbf{0},\mathbf{C})$$

where $\mathbf{t} = (t_1, t_2)^T$, $\mathbf{C} = \beta^{-1}\mathbf{I} + \alpha^{-1}\varphi\varphi^T$

φ is far way from x^t

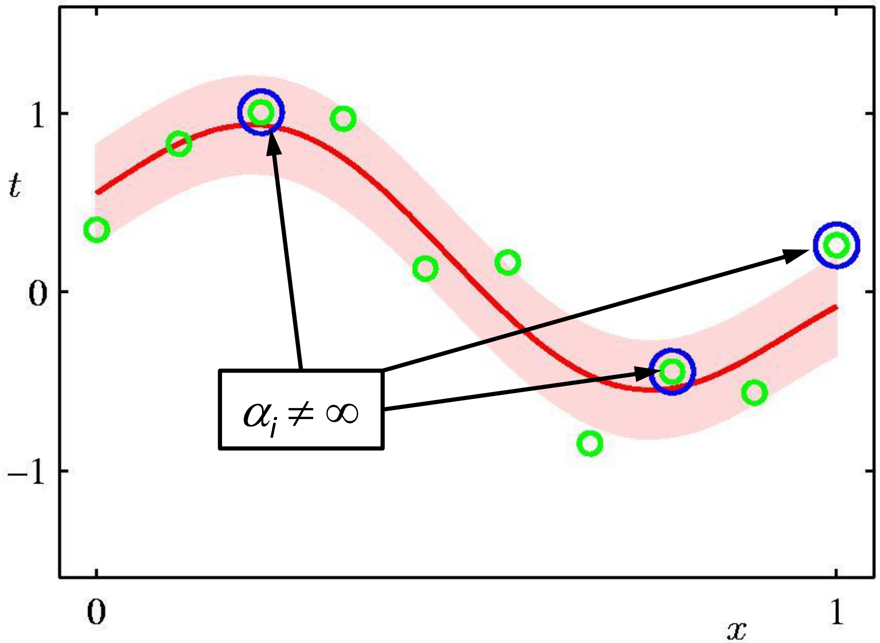


only isotropic noise, α = ∞

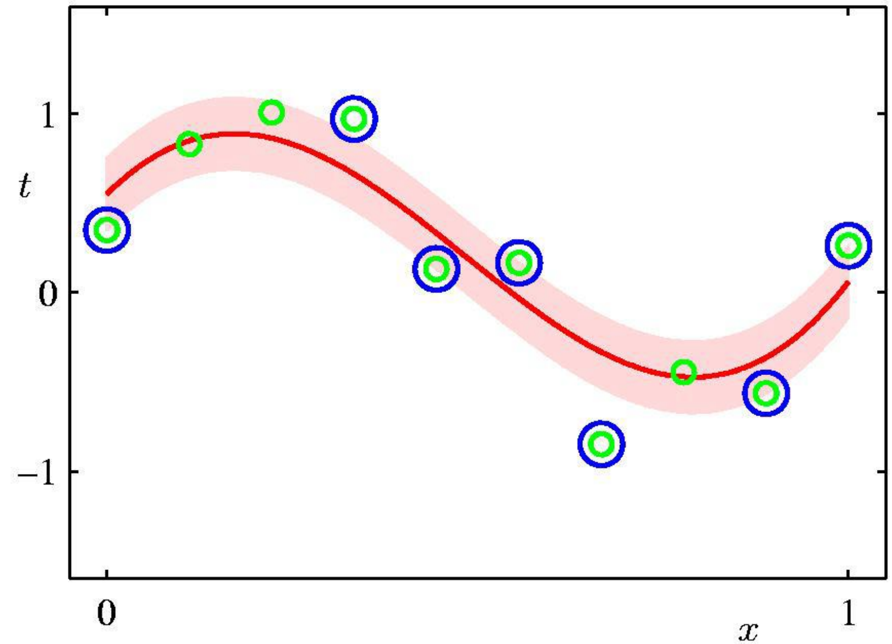
a finite value of α

Examples of RVM Regression

RVM regression



v-SVM regression



More compact than SVM (3 relevance vectors v.s. 7 support vectors)

Parameters are determined automatically

Require more training time than SVM

Sparse Solution I

Pull out the contribution from α_i in

$$\mathbf{C} = \beta^{-1}\mathbf{I} + \mathbf{\Phi}\mathbf{A}^{-1}\mathbf{\Phi}^T$$

$$\mathbf{C} = \beta^{-1}\mathbf{I} + \sum_{j \neq i} \alpha_j^{-1}\varphi_j\varphi_j^T + \alpha_i^{-1}\varphi_i\varphi_i^T$$

where φ_i : ith column of $\mathbf{\Phi}$

$$= \mathbf{C}_{-i} + \alpha_i^{-1}\varphi_i\varphi_i^T$$

$$|\mathbf{C}| = |\mathbf{C}_{-i}||1 + \alpha_i^{-1}\varphi_i^T\mathbf{C}_{-i}^{-1}\varphi_i|$$

Using (C.7), (C.15) in Appendix C

$$\mathbf{C}^{-1} = \mathbf{C}_{-i}^{-1} - \frac{\mathbf{C}_{-i}^{-1}\varphi_i\varphi_i^T\mathbf{C}_{-i}^{-1}}{\alpha_i + \varphi_i^T\mathbf{C}_{-i}^{-1}\varphi_i}$$

Sparse Solution II

- Then log marginal likelihood function L becomes,

$$L(\boldsymbol{\alpha}) = L(\boldsymbol{\alpha}_{-i}) + \lambda(\alpha_i)$$

$L(\boldsymbol{\alpha}_{-i})$: omitting α_i

$$\lambda(\alpha_i) = \frac{1}{2}\left[\ln \alpha_i - \ln(\alpha_i + s_i) + \frac{q_i^2}{\alpha_i + s_i}\right]$$

$$\text{where } s_i = \varphi_i^T \mathbf{C}_{-i}^{-1} \varphi_i$$

$$q_i = \varphi_i^T \mathbf{C}_{-i}^{-1} \mathbf{t}$$

Sparsity: measures the extent to which φ_i overlaps with the other basis vectors

Quality of φ_i : represents a measure of the alignment of the basis vector with the error between **t** and $\mathbf{y}_{-i}$

- Stationary points of the marginal likelihood w.r.t. α_i

$$\Rightarrow \frac{d\lambda(\alpha_i)}{d\alpha_i} = \frac{\alpha_i^{-1} s_i^2 - (q_i^2 - s_i)}{2(\alpha_i + s_i)^2} = 0$$

Sequential Sparse Bayesian Learning

1. Initialize β
2. Initialize using φ_1, with $\alpha_1 = s_1^2 / \left(q_1^2 - s_1\right)$, with the remaining $\alpha_{j(j \neq i)} = \infty$
3. Evaluate Σ and $\mathbf{m}$ for all basis functions
4. Select a candidate φ_i
5. If $q_i^2 > s_i$, $\alpha_i < \infty$ (φ_i is already in the model), update $\alpha_i = s_i^2 / \left(q_i^2 - s_i\right)$
6. If $q_i^2 > s_i$, $\alpha_i = \infty$, add φ_i to the model, and evaluate $\alpha_i = s_i^2 / \left(q_i^2 - s_i\right)$
7. If $q_i^2 \leq s_i$, $\alpha_i < \infty$, remove φ_i from the model, and set $\alpha_i = \infty$
8. Update β
9. Go to 3 until converged

Outlines

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

RVM for Classification

- Probabilistic linear classification model with Gaussian prior

$$y(\mathbf{x}, \mathbf{w}) = \sigma\left(\mathbf{w}^T \phi(\mathbf{x})\right) \qquad p(\mathbf{w} \mid \boldsymbol{\alpha}) = \prod_{n=1}^{N} N(w_i \mid 0, \alpha_i^{-1})$$

- Initialize $\boldsymbol{\alpha}$
- Build a Gaussian approximation to the posterior distribution
- Obtain an approximation to the marginal likelihood
- Maximize the marginal likelihood (re-estimate $\boldsymbol{\alpha}$) until converged

RVM for Classification (Cont'd)

- The posterior distribution is obtained by maximizing

$$\ln p(\mathbf{w}|\mathbf{t},\boldsymbol{\alpha}) = \ln\{p(\mathbf{t}|\mathbf{w})\,p(\mathbf{w}|\boldsymbol{\alpha})\} - \ln p(\mathbf{t}|\boldsymbol{\alpha})$$

$$= \sum_{n=1}^{N}\{t_n \ln y_n + (1-t_n)\ln(1-y_n)\} - \frac{1}{2}\mathbf{w}^T\mathbf{A}\mathbf{w} + \text{const}$$

where $\mathbf{A} = diag(\alpha_i)$

⇨ Iterative reweighted least squares (IRLS)

$$\nabla \ln p(\mathbf{w}|\mathbf{t},\boldsymbol{\alpha}) = \boldsymbol{\Phi}^T(\mathbf{t}-\mathbf{y}) - \mathbf{A}\mathbf{w}$$

$$\nabla\nabla \ln p(\mathbf{w}|\mathbf{t},\boldsymbol{\alpha}) = -\left(\boldsymbol{\Phi}^T\mathbf{B}\boldsymbol{\Phi} + \mathbf{A}\right)$$

where $\mathbf{B}: N \times N$ diagonal matrix, $b_n = y_n(1-y_n)$,

$\boldsymbol{\Phi}$: design matrix, $\Phi_{ni} = \phi_i(\mathbf{x}_n)$

⇨ Resulting Gaussian approximation to the posterior distribution

$$\mathbf{w}^* = \mathbf{A}^{-1}\boldsymbol{\Phi}^T(\mathbf{t}-\mathbf{y}),\ \Sigma = \left(\boldsymbol{\Phi}^T\mathbf{B}\boldsymbol{\Phi} + \mathbf{A}\right)^{-1} \quad \Leftarrow \quad \nabla \ln p(\mathbf{w}|\mathbf{t},\alpha) = 0$$

RVM for Classification (Cont'd)

- Marginal likelihood using Laplace approximation

$$p(\mathbf{t}\,|\,\boldsymbol{\alpha}) = \int p(\mathbf{t}\,|\,\mathbf{w})p(\mathbf{w}\,|\,\boldsymbol{\alpha})d\mathbf{w}$$

$$= p(\mathbf{t}\,|\,\mathbf{w}^*)\,p(\mathbf{w}^*\,|\,\boldsymbol{\alpha})(2\pi)^{M/2}|\Sigma|^{1/2}$$

- Set the derivative of the marginal likelihood equal to zero, and rearranging then gives

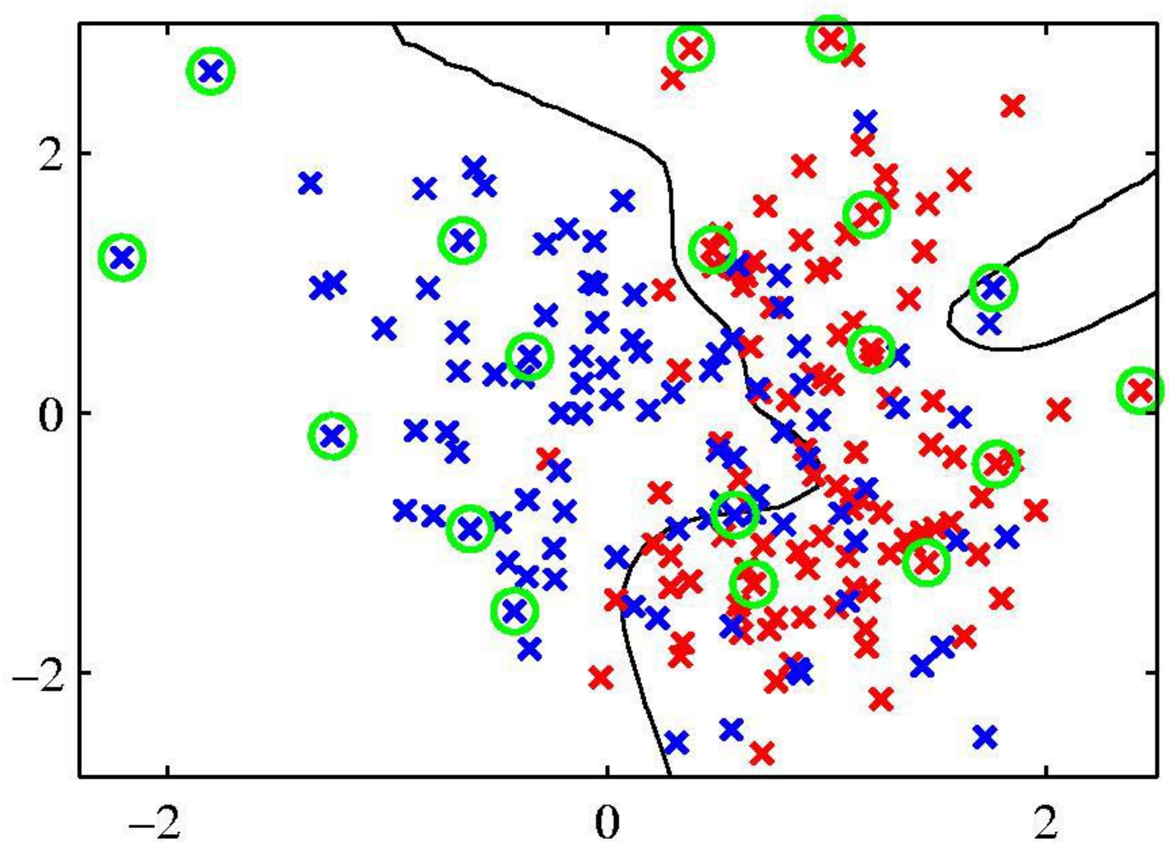
$$\alpha_i^{new} = \frac{\gamma_i}{(w_i^*)^2} \quad \text{where} \quad \gamma_i = 1 - \alpha_i \Sigma_{ii}$$

If we define $\hat{\mathbf{t}} = \mathbf{\Phi}\mathbf{w}^* + \mathbf{B}^{-1}(\mathbf{t} - \mathbf{y})$

$$\ln p(\mathbf{t}\,|\,\boldsymbol{\alpha},\beta) = -\frac{1}{2}\left\{N\ln(2\pi) + \ln|\mathbf{C}| + (\hat{\mathbf{t}})^T\mathbf{C}^{-1}\hat{\mathbf{t}}\right\} \Rightarrow$$ **Same in the regression case**

where $\mathbf{C} = \mathbf{B} + \mathbf{\Phi}\mathbf{A}\mathbf{\Phi}^T$

Example of RVM Classification



Summary

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