Introduction to Machine Learning

Kernel Methods

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Some slides are modified from S.-J. Wang and H.-T. Chen

Outline

- Dual representations
- Constructing kernels
- Support vector machines for classification
- Support vector machines for regression

Outline

- Dual representations
- Constructing kernels
- Support vector machines for classification
- Support vector machines for regression

Parametric vs. non-parametric model

- Parametric methods
  - A linear model for regression
  - We learn a model $y(\mathbf{x}, \mathbf{w})$ that maps input $\mathbf{x}$ to output $y(\mathbf{x}, \mathbf{w})$
  - Training data are thrown away after training
- Non-parametric methods
  - Nearest neighbor classifier
  - We predict a test data by searching its nearest neighbor
  - Training data are kept
- Kernel methods derive non-parametric models
  - Support vector machines, Gaussian processes, kernel PCA, …
  - Predictions are based on linear combinations of a kernel function evaluated at the training data points

Dual representations: Problem statement

- Consider a linear regression model whose parameters are determined by minimizing a regularized sum-of-squares error function given by

$$J(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\left\{\mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}_n) - t_n\right\}^2 + \frac{\lambda}{2}\mathbf{w}^{\mathrm{T}}\mathbf{w} \qquad \text{where } \lambda \geq 0$$

  - Data are nonlinearly transformed via functions

- Setting the derivative of $J(\mathbf{w})$ w.r.t. $\mathbf{w}$ to zero, the optimal solution takes the form of

$$\mathbf{w} = -\frac{1}{\lambda}\sum_{n=1}^{N}\left\{\mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}_n) - t_n\right\}\phi(\mathbf{x}_n)$$

Dual representations of a linear model

- The optimal solution is a linear combination of training data

$$\mathbf{w} = -\frac{1}{\lambda}\sum_{n=1}^{N}\{\mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}_n) - t_n\}\phi(\mathbf{x}_n)$$
$$= \sum_{n=1}^{N} a_n \phi(\mathbf{x}_n) = \mathbf{\Phi}^{\mathrm{T}}\mathbf{a}\,.$$

  - where $a_n = -\frac{1}{\lambda}\{\mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}_n) - t_n\}$

$$\mathbf{\Phi} : \begin{bmatrix} \vdots \\ \phi(\mathbf{x}_n)^{\mathrm{T}} \\ \vdots \end{bmatrix} \qquad \mathbf{a} = (a_1, \ldots, a_N)^{\mathrm{T}}$$

Dual representations: Gram matrix

- Instead of working with parameter vector $\mathbf{w}$, we can reformulate the least squares algorithms w.r.t. parameter vector $\mathbf{a}$, giving rise to a dual representation
- If we substitute $\mathbf{w} = \Phi^{\mathrm{T}}\mathbf{a}$ into $J(\mathbf{w})$, we obtain

$$J(\mathbf{a}) = \frac{1}{2}\mathbf{a}^{\mathrm{T}}\mathbf{\Phi}\mathbf{\Phi}^{\mathrm{T}}\mathbf{\Phi}\mathbf{\Phi}^{\mathrm{T}}\mathbf{a} - \mathbf{a}^{\mathrm{T}}\mathbf{\Phi}\mathbf{\Phi}^{\mathrm{T}}\mathbf{t} + \frac{1}{2}\mathbf{t}^{\mathrm{T}}\mathbf{t} + \frac{\lambda}{2}\mathbf{a}^{\mathrm{T}}\mathbf{\Phi}\mathbf{\Phi}^{\mathrm{T}}\mathbf{a}$$

  - Where $\mathbf{t} = (t_1, \ldots, t_N)^{\mathrm{T}}$

- We define the Gram (Kernel) matrix $\mathbf{K} = \mathbf{\Phi}\mathbf{\Phi}^{\mathrm{T}}$, which is an $N \times N$ symmetric matrix

$$K_{nm} = \phi(\mathbf{x}_n)^{\mathrm{T}}\phi(\mathbf{x}_m) = k(\mathbf{x}_n, \mathbf{x}_m)$$

  - where $k(\mathbf{x}_n, \mathbf{x}_m)$ is the kernel function

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Dual representations: Solution and inference

- In terms of the Gram matrix, the regularized sum-of-squares error function can be written as

$$J(\mathbf{a}) = \frac{1}{2}\mathbf{a}^{\mathrm{T}}\mathbf{K}\mathbf{K}\mathbf{a} - \mathbf{a}^{\mathrm{T}}\mathbf{K}\mathbf{t} + \frac{1}{2}\mathbf{t}^{\mathrm{T}}\mathbf{t} + \frac{\lambda}{2}\mathbf{a}^{\mathrm{T}}\mathbf{K}\mathbf{a}$$

- Setting the derivative of $J(\mathbf{a})$ w.r.t. $\mathbf{a}$ to zero, the optimal solution is

$$\mathbf{a} = (\mathbf{K} + \lambda \mathbf{I}_N)^{-1}\mathbf{t}.$$

- After getting the solution, we make the prediction for input $\mathbf{x}$

$$y(\mathbf{x}) = \mathbf{w}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}) = \mathbf{a}^{\mathrm{T}}\boldsymbol{\Phi}\boldsymbol{\phi}(\mathbf{x}) = \mathbf{k}(\mathbf{x})^{\mathrm{T}}(\mathbf{K} + \lambda \mathbf{I}_N)^{-1}\mathbf{t}$$

  - where $\mathbf{k}(\mathbf{x})$ is with elements $k_n(\mathbf{x}) = k(\mathbf{x}_n, \mathbf{x})$

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Predictions are based on linear combinations of a kernel function evaluated at the training data points

Dual representations: Analysis

- There are M (data dimensionality) optimization variables in $\mathbf{w}$
- There are N (data number) optimization variables in its dual representation $\mathbf{\Phi}^{\mathrm{T}}\mathbf{a}$
- In the cases where $N > M$
  - Dual representations are less efficient
  - Dual representations are not parametric
  - Dual representations can be sparse
  - Dual representations can be expressed entirely in terms of kernel functions -> It can avoid explicit introduction of the features $\phi(\mathbf{x})$, which allows us to implicitly use feature spaces of very high, even infinite, dimensionality

Outline

- Dual representations
- Constructing kernels
- Support vector machines for classification
- Support vector machines for regression

How to construct a kernel function/matrix?

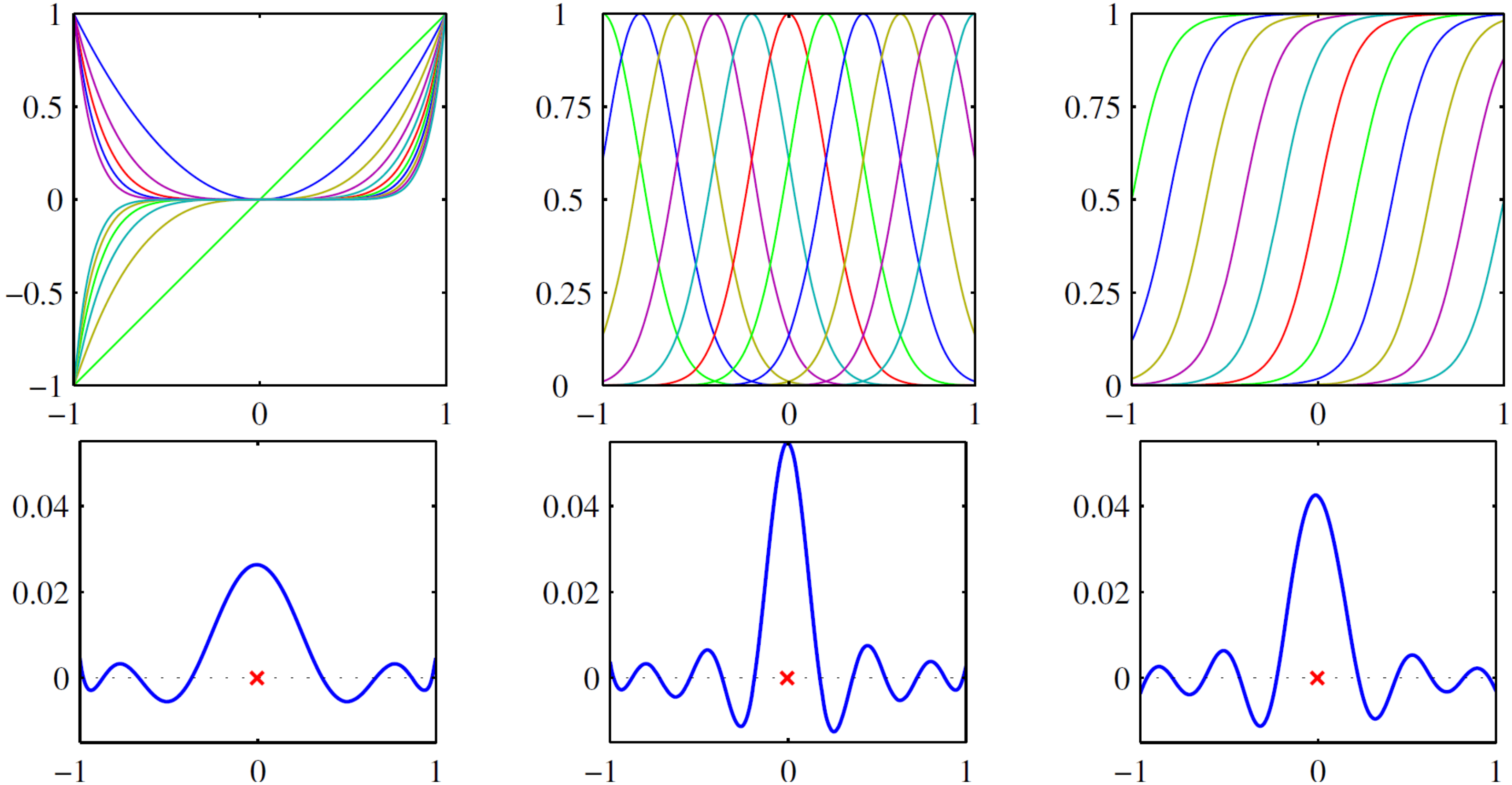
- One approach is to choose a feature space mapping and then construct the kernel

$$k(x, x') = \boldsymbol{\phi}(x)^{\mathrm{T}}\boldsymbol{\phi}(x') = \sum_{i=1}^{M}\phi_i(x)\phi_i(x')$$

  - where $\phi_i(x)$ is a basis function

- Another approach is to construct the kernel functions directly
- It is required that the constructed kernel is valid. Namely it corresponds to the inner product in some feature space

Examples of explicitly constructing kernels



- Upper figure: Several curves, one for each basis function
- Lower figure: kernel function $k(x, x')$ with $x' = 0$ by varying x

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Is it a valid kernel?

- Let's consider the following function. Is it a kernel function?

$$k(\mathbf{x}, \mathbf{z}) = \left(\mathbf{x}^{\mathrm{T}}\mathbf{z}\right)^2$$

- Check if there exists a space where the output value is equal to the inner product of the data points
- With the derivation

$$\begin{aligned} k(\mathbf{x}, \mathbf{z}) &= \left(\mathbf{x}^{\mathrm{T}}\mathbf{z}\right)^2 = (x_1 z_1 + x_2 z_2)^2 \\ &= x_1^2 z_1^2 + 2x_1 z_1 x_2 z_2 + x_2^2 z_2^2 \\ &= (x_1^2, \sqrt{2}x_1 x_2, x_2^2)(z_1^2, \sqrt{2}z_1 z_2, z_2^2)^{\mathrm{T}} \\ &= \phi(\mathbf{x})^{\mathrm{T}} \phi(\mathbf{z}). \end{aligned}$$

  - The feature space exists $\phi(\mathbf{x}) = (x_1^2, \sqrt{2}x_1 x_2, x_2^2)^{\mathrm{T}}$
  - Note that the kernel function is computed in the input space, but it corresponds to the inner product in some high-dimensional space

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A theory for checking if a function is a kernel function

- The necessary and sufficient condition for $k(\mathbf{x}, \mathbf{x}')$ to be a valid kernel: Gram matrix $\mathbf{K} = [k(\mathbf{x}_n, \mathbf{x}_m)]_{nm}$ should be positive semidefinite for all possible choices of the set

- A matrix is positive semidefinite means that all of its eigenvalues are non-negative

- $\mathbf{K}$ is symmetric. Thus, we have $\mathbf{K} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^{\mathrm{T}}$
  - where $\mathbf{V}$ is an orthonormal matrix $\mathbf{v}_t$ and the diagonal matrix $\mathbf{\Lambda}$ contains the eigenvalues λ_t of $\mathbf{K}$
  - If $\mathbf{K}$ is positive semidefinite, all eigenvalues are non-negative
  - Consider the feature map: $\phi : \mathbf{x}_i \mapsto (\sqrt{\lambda_t} v_{ti})_{t=1}^{n} \in \mathbb{R}^n$
  - We find that

$$\phi(\mathbf{x}_i)^{\mathrm{T}}\phi(\mathbf{x}_j) = \sum_{t=1}^{n} \lambda_t v_{ti} v_{tj} = (\mathbf{V}\mathbf{\Lambda}\mathbf{V}^{\mathrm{T}})_{ij} = K_{ij} = k(\mathbf{x}_i, \mathbf{x}_j)$$

Given valid kernels $k_1(\mathbf{x}, \mathbf{x}')$ and $k_2(\mathbf{x}, \mathbf{x}')$, the following new kernels will also be valid:

$$
\begin{aligned}
k(\mathbf{x}, \mathbf{x}') &= c k_1(\mathbf{x}, \mathbf{x}') && (6.13) \\
k(\mathbf{x}, \mathbf{x}') &= f(\mathbf{x}) k_1(\mathbf{x}, \mathbf{x}') f(\mathbf{x}') && (6.14) \\
k(\mathbf{x}, \mathbf{x}') &= q\left(k_1(\mathbf{x}, \mathbf{x}')\right) && (6.15) \\
k(\mathbf{x}, \mathbf{x}') &= \exp\left(k_1(\mathbf{x}, \mathbf{x}')\right) && (6.16) \\
k(\mathbf{x}, \mathbf{x}') &= k_1(\mathbf{x}, \mathbf{x}') + k_2(\mathbf{x}, \mathbf{x}') && (6.17) \\
k(\mathbf{x}, \mathbf{x}') &= k_1(\mathbf{x}, \mathbf{x}') k_2(\mathbf{x}, \mathbf{x}') && (6.18) \\
k(\mathbf{x}, \mathbf{x}') &= k_3\left(\boldsymbol{\phi}(\mathbf{x}), \boldsymbol{\phi}(\mathbf{x}')\right) && (6.19) \\
k(\mathbf{x}, \mathbf{x}') &= \mathbf{x}^{\mathrm{T}} \mathbf{A} \mathbf{x}' && (6.20) \\
k(\mathbf{x}, \mathbf{x}') &= k_a(\mathbf{x}_a, \mathbf{x}'_a) + k_b(\mathbf{x}_b, \mathbf{x}'_b) && (6.21) \\
k(\mathbf{x}, \mathbf{x}') &= k_a(\mathbf{x}_a, \mathbf{x}'_a) k_b(\mathbf{x}_b, \mathbf{x}'_b) && (6.22)
\end{aligned}
$$

where $c > 0$ is a constant, $f(\cdot)$ is any function, $q(\cdot)$ is a polynomial with nonnegative coefficients, $\boldsymbol{\phi}(\mathbf{x})$ is a function from $\mathbf{x}$ to $\mathbb{R}^M$, $k_3(\cdot, \cdot)$ is a valid kernel in $\mathbb{R}^M$, $\mathbf{A}$ is a symmetric positive semidefinite matrix, $\mathbf{x}_a$ and $\mathbf{x}_b$ are variables (not necessarily disjoint) with $\mathbf{x} = (\mathbf{x}_a, \mathbf{x}_b)$, and k_a and k_b are valid kernel functions over their respective spaces.

Polynomial kernel

- Polynomial kernel

$$k(\mathbf{x}, \mathbf{x}') = \left(\mathbf{x}^{\mathrm{T}}\mathbf{x}' + c\right)^{M}$$

  - where M is the degree and c is a positive constant

- Proof: Polynomial kernel is valid
  - 1. $k(\mathbf{x}, \mathbf{x}') = \left(\mathbf{x}^{\mathrm{T}}\mathbf{x}' + c\right)$ is a valid kernel with feature map $\mathbf{x} \rightarrow \begin{bmatrix} \mathbf{x} \\ \sqrt{c} \end{bmatrix}$
  - 2. According to

$$k(\mathbf{x}, \mathbf{x}') = k_1(\mathbf{x}, \mathbf{x}')k_2(\mathbf{x}, \mathbf{x}') \qquad (6.18)$$

we can find that $k(\mathbf{x}, \mathbf{x}') = \left(\mathbf{x}^{\mathrm{T}}\mathbf{x}' + c\right)^{M}$ is a valid kernel

Gaussian kernel (RBF kernel)

- Gaussian kernel

$$k(\mathbf{x}, \mathbf{x}') = \exp\left(-\|\mathbf{x} - \mathbf{x}'\|^2 / 2\sigma^2\right)$$

  - where σ^2 is a positive constant
  - The corresponding feature vector has infinite dimensionality
- Proof: Gaussian kernel is valid
  - 1. $\|\mathbf{x} - \mathbf{x}'\|^2 = \mathbf{x}^{\mathrm{T}}\mathbf{x} + (\mathbf{x}')^{\mathrm{T}}\mathbf{x}' - 2\mathbf{x}^{\mathrm{T}}\mathbf{x}'$
  - 2. $k(\mathbf{x}, \mathbf{x}') = \exp\left(-\mathbf{x}^{\mathrm{T}}\mathbf{x}/2\sigma^2\right) \exp\left(\mathbf{x}^{\mathrm{T}}\mathbf{x}'/\sigma^2\right) \exp\left(-(\mathbf{x}')^{\mathrm{T}}\mathbf{x}'/2\sigma^2\right)$
  - 3. According to

$$k(\mathbf{x}, \mathbf{x}') = \exp\left(k_1(\mathbf{x}, \mathbf{x}')\right) \tag{6.16}$$

$$k(\mathbf{x}, \mathbf{x}') = f(\mathbf{x}) k_1(\mathbf{x}, \mathbf{x}') f(\mathbf{x}') \tag{6.14}$$

Gaussian kernel is valid

Sigmoidal kernel

- Sigmoidal kernel

$$k(\mathbf{x}, \mathbf{x}') = \tanh\left(a\mathbf{x}^{\mathrm{T}}\mathbf{x}' + b\right)$$

  - where a and b are two constants

- The Gram matrix of this function in general is not positive semidefinite
  - No corresponding feature mapping

- However, this form of kernel has been used in practice

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- Support vector machines for classification
  - Maximum margin classifier
  - Overlapping class distributions
  - Multi-class SVMs
  - SVMs vs. logistic regression
- Support vector machines for regression

Linearly separable, binary-class classification

- Training data:
  - N training data points: $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N$
  - The corresponding target label: $t_1, t_2, \ldots, t_N$, where $t_n \in \{-1,1\}$
- The decision function of SVMs

$$y(\mathbf{x}) = \mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}) + b$$

  - $\phi(\mathbf{x})$ denotes a fixed feature-space transformation
  - $\mathbf{w}$ is the weight vector and b is the bias parameter
  - Binary classification: $\mathrm{sign}(y(\mathbf{x}))$
- Linearly separable case
  - Correctly classify a positive data: $y(\mathbf{x}) > 0$
  - Correctly classify a negative data: $y(\mathbf{x}) < 0$
  - We can achieve $t_n y(\mathbf{x}_n) > 0$ for all training data points

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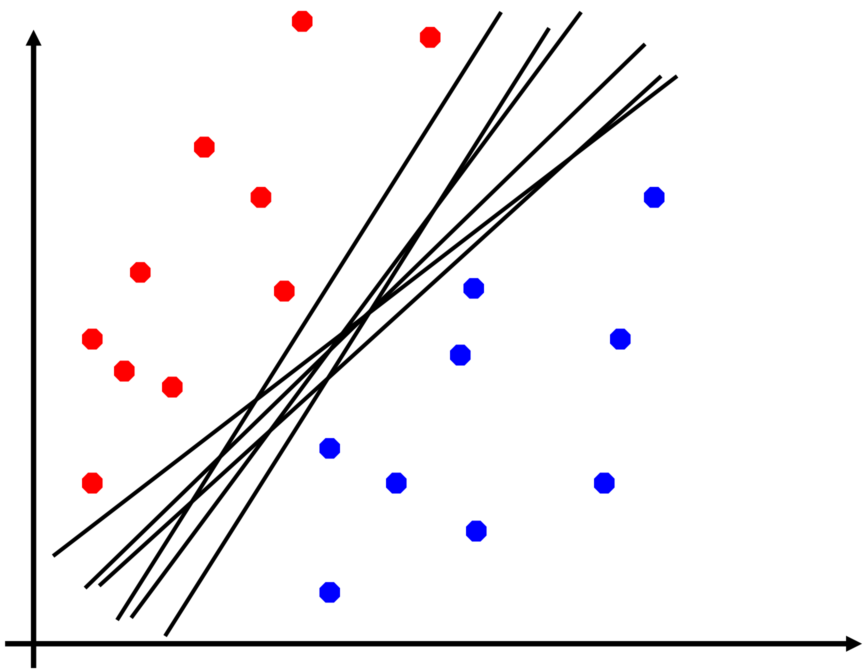
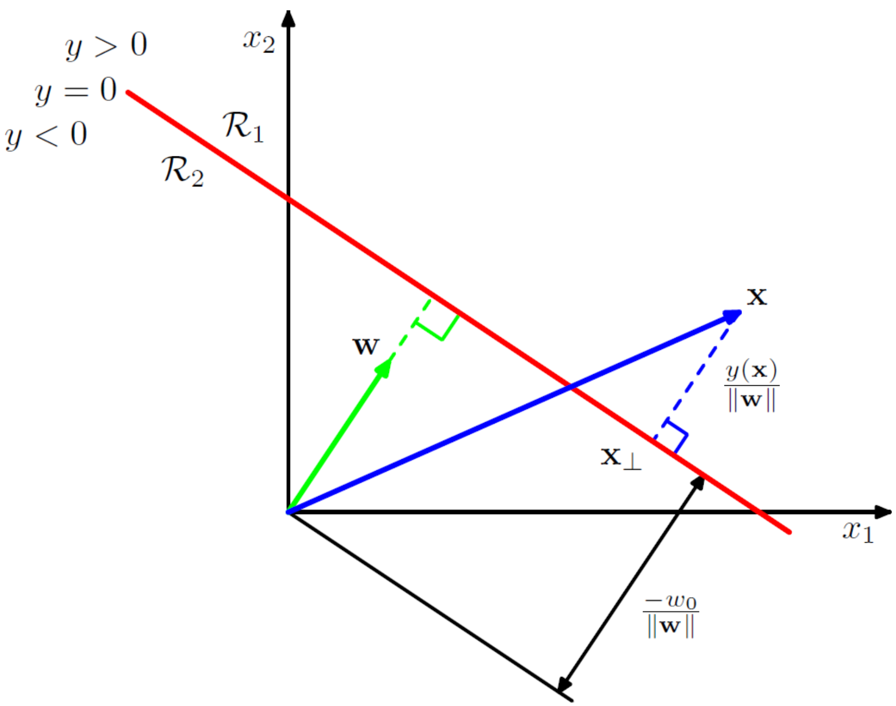
An example of a linearly separable training set

- For a linearly separable (in the feature space) data set, we may have many models that correctly classify all training data
- Which of these classifiers is optimal?



Distance from a data point to decision boundary

- How to compute the distance between a positive point $\mathbf{x}$ and the decision boundary $y = 0$?



$$\mathbf{x} = \mathbf{x}_\perp + r\frac{\mathbf{w}}{\|\mathbf{w}\|}$$

$$\begin{cases} y(\mathbf{x}) = \mathbf{w}^{\mathrm{T}}\mathbf{x} + w_0 \\ y(\mathbf{x}_\perp) = \mathbf{w}^{\mathrm{T}}\mathbf{x}_\perp + w_0 = 0 \end{cases}$$

$$y(\mathbf{x}) = \mathbf{w}^{\mathrm{T}}\mathbf{x} + w_0 = \mathbf{w}^{\mathrm{T}}\mathbf{x}_\perp + w_0 + r\frac{\mathbf{w}^{\mathrm{T}}\mathbf{w}}{\|\mathbf{w}\|}$$

$$r = \frac{y(\mathbf{x})}{\|\mathbf{w}\|}$$

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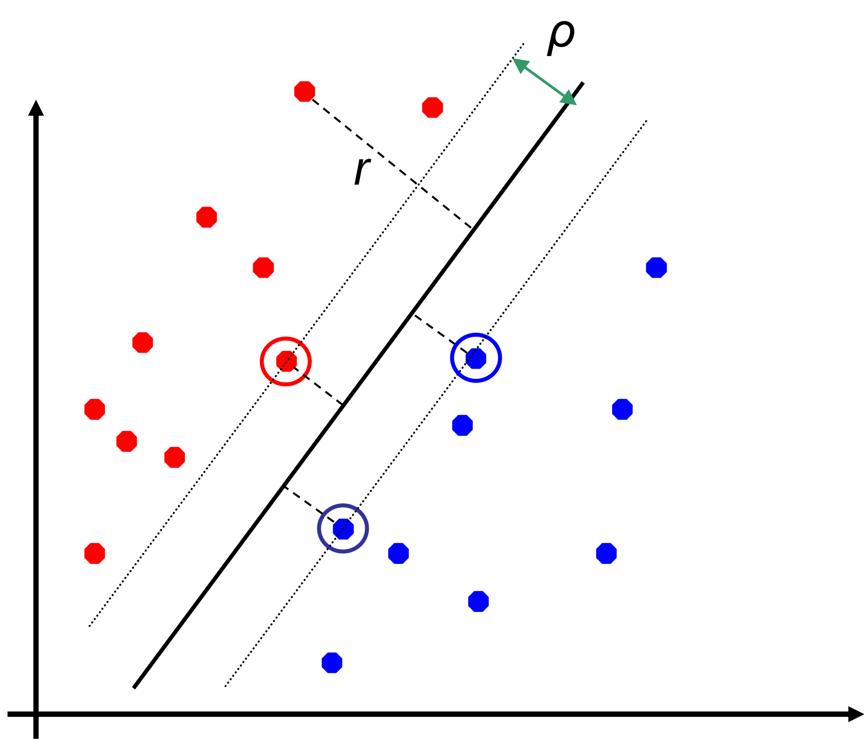
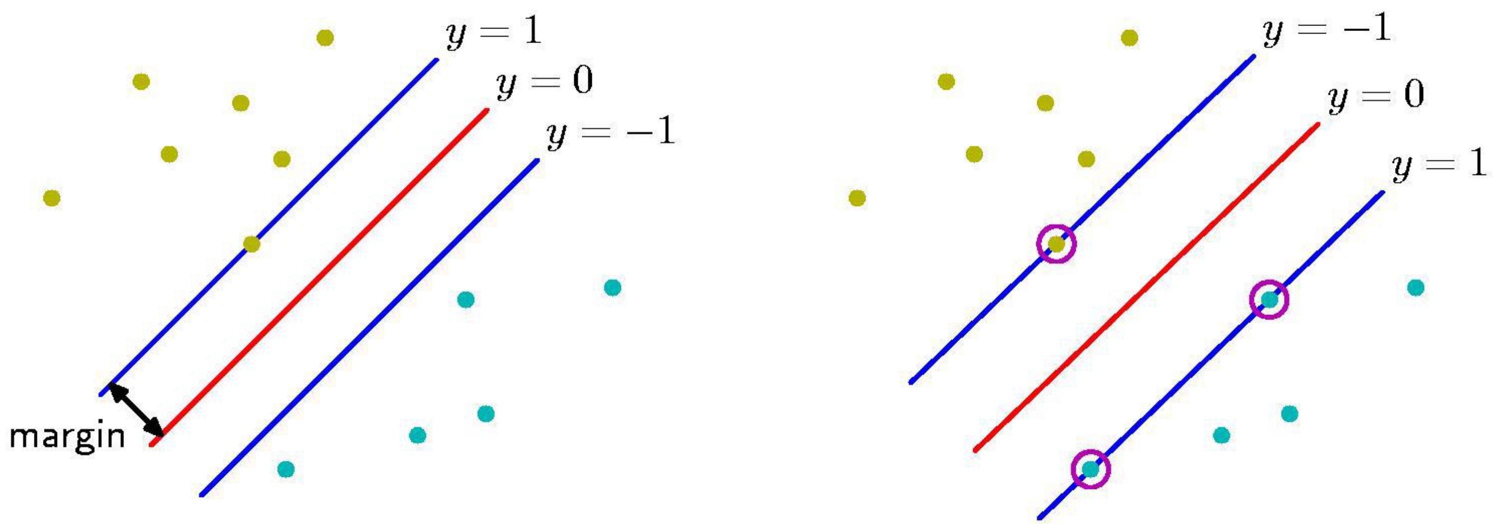
Margin

- The margin of an SVM classifier is the smallest distance between the decision boundary and any of the training points
- When multiple classifiers correctly all training data, we choose the one with the maximum margin



Maximum margin classifier

- Margin is the perpendicular distance between the decision boundary and the closest point



- Maximizing the margin leads to particular choice of the classifier

Margin maximization

- The perpendicular distance of a point $\mathbf{x_n}$ from a hyperplane $y(\mathbf{x}) = 0$ is given by

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

- The objective function of the maximum margin solution is found by solving

$$\arg\max_{\mathbf{w},b} \left\{ \frac{1}{\|\mathbf{w}\|} \min_n \left[t_n \left(\mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}_n) + b \right) \right] \right\}$$

  - Directly optimizing this objective function is very complex!

An equivalent optimization problem

- Recall the distance $\frac{t_n(\mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}_n)+b)}{\|\mathbf{w}\|}$
- If we make the rescaling $\mathbf{w} \to \kappa\mathbf{w}$ and $b \to \kappa b$, the distance from any point $\mathbf{x}_n$ to the decision surface is unchanged.
- We rescale $\mathbf{w}$ and b, which sets

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

  for the point that is closest to the surface
- In this case, all training data will stratify the following constraints

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

An equivalent optimization problem

- Original optimization problem

$$\arg\max_{\mathbf{w},b} \left\{ \frac{1}{\|\mathbf{w}\|} \min_n \left[t_n \left(\mathbf{w}^{\mathrm{T}} \phi(\mathbf{x}_n) + b \right) \right] \right\}$$

- An equivalent optimization problem

$$\arg\min_{\mathbf{w},b} \frac{1}{2} \|\mathbf{w}\|^2$$

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

- Quadratic programming
  - Quadratic objective function with linear constraints
  - Computational complexity is $O(M^3)$, where M is the number of optimization variables (number of data dimensionality)

Optimization using Lagrange multipliers

- The constrained optimization

$$\arg\min_{\mathbf{w},b} \frac{1}{2}\|\mathbf{w}\|^2$$

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

- We introduce Lagrange multipliers $\{a_n \geq 0\}$, with one multiplier a_n for each constraint $t_n\left(\mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}_n)+b\right) \geqslant 1$

- The Lagrangian function

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

Optimization using Lagrange multipliers

- The Lagrangian function

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

- Several constraints
  - Lagrange multiples are non-negative $a_n \geq 0$
  - $$\frac{\partial L(\mathbf{w}, b, \mathbf{a})}{\partial \mathbf{w}} = 0 \quad \Rightarrow \quad \boxed{\mathbf{w} = \sum_{n=1}^{N} a_n t_n \phi(\mathbf{x}_n)}$$
  - $$\frac{\partial L(\mathbf{w}, b, \mathbf{a})}{\partial b} = 0 \quad \Rightarrow \quad 0 = \sum_{n=1}^{N} a_n t_n$$

dual representation

Dual form of the optimization problem

- By eliminating $\mathbf{w}$ and b from $\mathrm{L}(\mathbf{w}, \mathrm{b}, \mathbf{a})$, we get the dual representation of the maximum margin problem in which we maximize

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

subject to
$$a_n \geqslant 0, \qquad n = 1, \ldots, N,$$
$$\sum_{n=1}^{N} a_n t_n = 0$$

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

- It can be solved by using quadratic programming with complexity $O(N^3)$, where N is the number of training data

Testing phase

- Decision function of SVMs

$$y(\mathbf{x}) = \mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}) + b$$

- Dual representation of SVMs

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

- For a test point $\mathbf{x}$, we classify it using a kernel function

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

- How to determine the value of b?

KKT conditions

- KKT (Karush-Kuhn-Tucker) conditions
- The solution to the problem of maximizing $f(\mathbf{x})$ subject to $g(\mathbf{x}) \geqslant 0$ obtained by optimizing the Lagrangian function $L(\mathbf{x}, \lambda) \equiv f(\mathbf{x}) + \lambda g(\mathbf{x})$ w.r.t. optimization variables $\mathbf{x}$ and Lagrange multiplier λ subject to the conditions

$$\begin{aligned} g(\mathbf{x}) &\geqslant 0 \\ \lambda &\geqslant 0 \\ \lambda g(\mathbf{x}) &= 0 \end{aligned}$$

KKT conditions in SVM optimization

- Karush-Kuhn-Tucker (KKT) conditions in SVMs:

$$\begin{aligned} a_n &\geqslant 0 \\ t_n y(\mathbf{x}_n) - 1 &\geqslant 0 \\ a_n \{t_n y(\mathbf{x}_n) - 1\} &= 0. \end{aligned}$$

- For every data point $\mathbf{x}_n$, either $a_n = 0$ or $t_n y(\mathbf{x}_n) = 1$
  - $a_n = 0$: This data point plays no role in making predictions for new data points in the decision function

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

  - $t_n y(\mathbf{x}_n) = 1$: This data point is called a support vector and lies on the maximum margin hyperplane in feature space
  - Only the support vectors retain, while the rest can be discarded

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How to determine the value of b

- For a test point $\mathbf{x}$, we classify it using the decision function

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

- For any support vector $\mathbf{x}_n$, we have $t_n y(\mathbf{x}_n) = 1$, i.e.,

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

- The threshold b can be determined by calculating

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

  - S: index set of support vectors; $|S|$: number of support vectors

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How to determine the value of b

- For any support vector $\mathbf{x}_n$, we have

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

- Derivation

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

$$\Rightarrow \sum_{m \in \mathcal{S}} a_m t_m k(\mathbf{x}_n, \mathbf{x}_m) + b = t_n$$

$$\Rightarrow \sum_{n \in \mathcal{S}} \left\{ \sum_{m \in \mathcal{S}} a_m t_m k(\mathbf{x}_n, \mathbf{x}_m) \right\} + |\mathcal{S}| b = \sum_{n \in \mathcal{S}} t_n$$

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

Testing

- The decision function has been determined

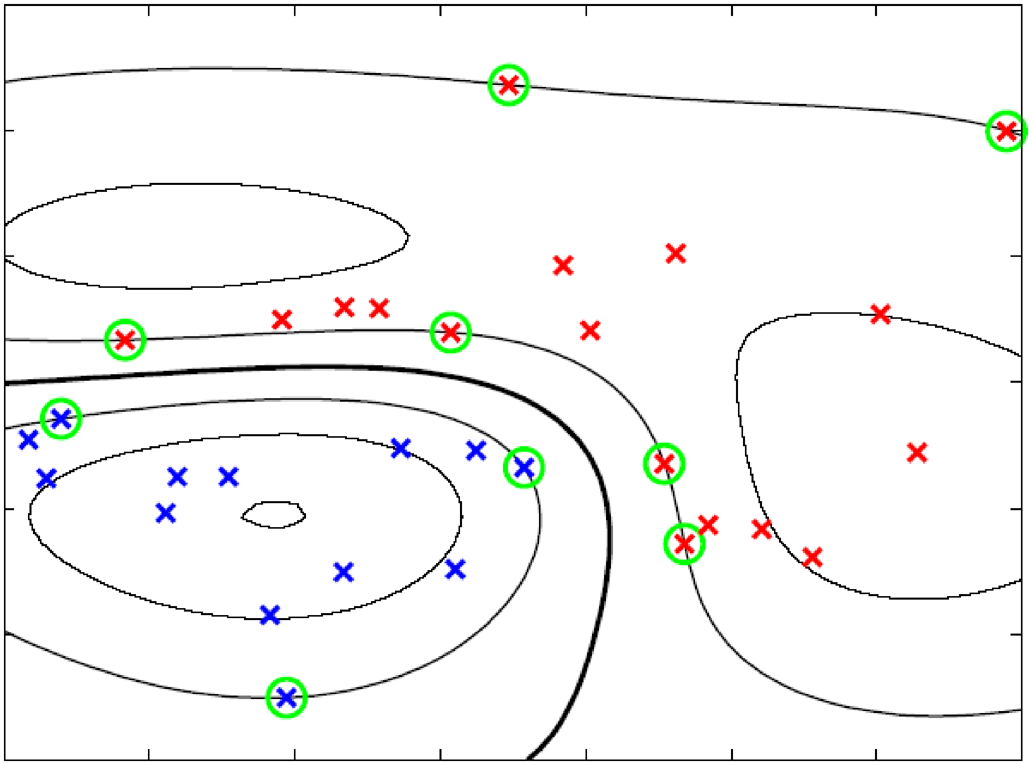
$$y(\mathbf{x}) = \sum_{n=1}^{N} a_n t_n k(\mathbf{x}, \mathbf{x}_n) + b$$

- Given a new input $\mathbf{x}$, we can use $y(\mathbf{x})$ to predict the class of $\mathbf{x}$ according to $\text{sign}(y(\mathbf{x}))$

- So far we assume the training data are linearly separable. What if the data are not linearly separable?

An example

- Two-class synthetic data in a two-dimensional input space
- Gaussian kernel function
- Decision boundary, margin boundaries, and support vectors



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  - Maximum margin classifier
  - Overlapping class distributions
  - Multi-class SVMs
  - SVMs vs. logistic regression
- Support vector machines for regression

Overlapping class distributions

- In practice, the class-conditional distributions may overlap
  - Not linearly separable in the feature space
- We need a way to modify SVMs where misclassifying some training data is allowed
- Introduce a slack variable $\xi_n \geq 0$ for each training data $\mathbf{x}_n$
  - Linearly separable case: $t_n y(\mathbf{x}_n) \geq 1$, i.e.,

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

  - Not linearly separable case: $t_n y(\mathbf{x}_n) \geq 1 - \xi_n$
  - Soft margin, which allows some training data to be misclassified

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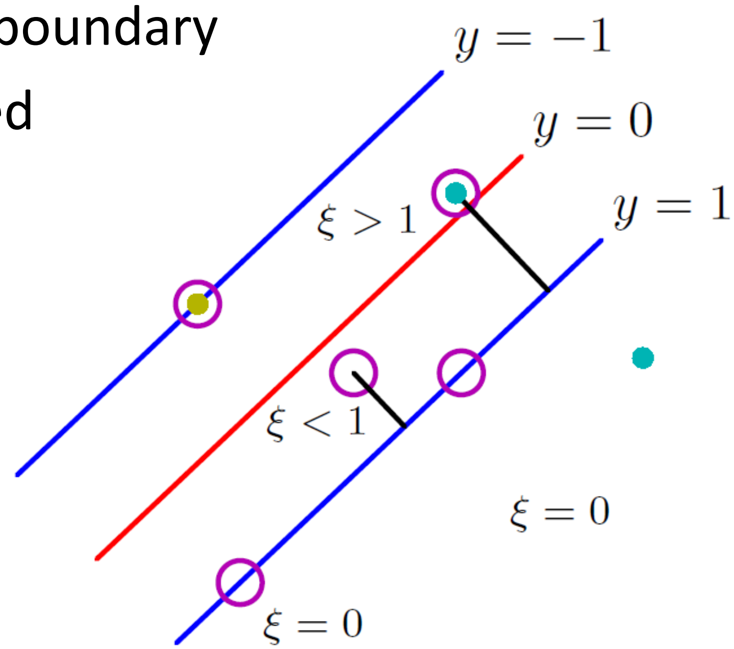
Slack variable

- Introduce slack variables, $\xi_n \geq 0$ where n = 1, . . . , N
  - New constraint: $t_n y(\mathbf{x}_n) \geq 1 - \xi_n$
  - ξ_n = 0 for data point $\mathbf{x}_n$ on or inside the correct margin boundary
  - $0 < \xi_n < 1$ for data point $\mathbf{x}_n$ inside the margin, but on the correct side of the decision boundary
  - $\xi_n = 1$ if $\mathbf{x}_n$ is on the decision boundary
  - $\xi_n > 1$ if $\mathbf{x}_n$ is wrongly classified
- The value of ξ_n indicates the degree of misclassification



Soft margin optimization: Primal form

- Hard margin optimization for linearly separable cases

$$\arg\min_{\mathbf{w},b} \frac{1}{2}\|\mathbf{w}\|^2$$

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

- Soft margin optimization for general cases

$$\arg\min_{\mathbf{w},\, b,\, \{\xi_n\}} \quad C\sum_{n=1}^{N}\xi_n + \frac{1}{2}\|\mathbf{w}\|^2$$

$$\begin{aligned} \text{subject to} \quad & t_n y(\mathbf{x}_n) \geqslant 1-\xi_n && n=1,\ldots,N \\ & \xi_n \geqslant 0 && n=1,\ldots,N \end{aligned}$$

  - where C is a positive constant

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Lagrangian function

- Primal form

$$\underset{\mathbf{w},\, b,\, \{\xi_n\}}{\arg\min} \quad C\sum_{n=1}^{N}\xi_n + \frac{1}{2}\|\mathbf{w}\|^2$$

$$\text{subject to} \quad t_n y(\mathbf{x}_n) \geqslant 1 - \xi_n \qquad n = 1, \ldots, N$$

$$\xi_n \geqslant 0 \qquad n = 1, \ldots, N$$

- Lagrangian function with Lagrange multipliers $\{a_n\}$ and $\{\mu_n\}$

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

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Lagrangian function

- Lagrangian function

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

- Some constraints

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

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

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

Soft margin optimization: Dual form

- Dual form

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

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

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

- This optimization problem can be solved by quadratic programming

Optimizing b via KKT conditions

- KKT conditions:

$$
\begin{aligned}
a_n &\geqslant 0 \\
t_n y(\mathbf{x}_n) - 1 + \xi_n &\geqslant 0 \\
\boxed{a_n \left(t_n y(\mathbf{x}_n) - 1 + \xi_n\right) = 0} \\
\mu_n &\geqslant 0 \\
\xi_n &\geqslant 0 \\
\boxed{\mu_n \xi_n = 0}
\end{aligned}
$$

- Consider a training data point $\mathbf{x}_n$ with $0 < a_n < C$.
  - $t_n y(\mathbf{x}_n) = 1 - \xi_n$
  - $\xi_n = 0$
  - $t_n y(\mathbf{x}_n) = 1$

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

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Optimizing b via KKT conditions

- Consider a training data point $\mathbf{x}_n$ with $0 < a_n < C$
  - $t_n y(\mathbf{x}_n) = 1$, i.e.,

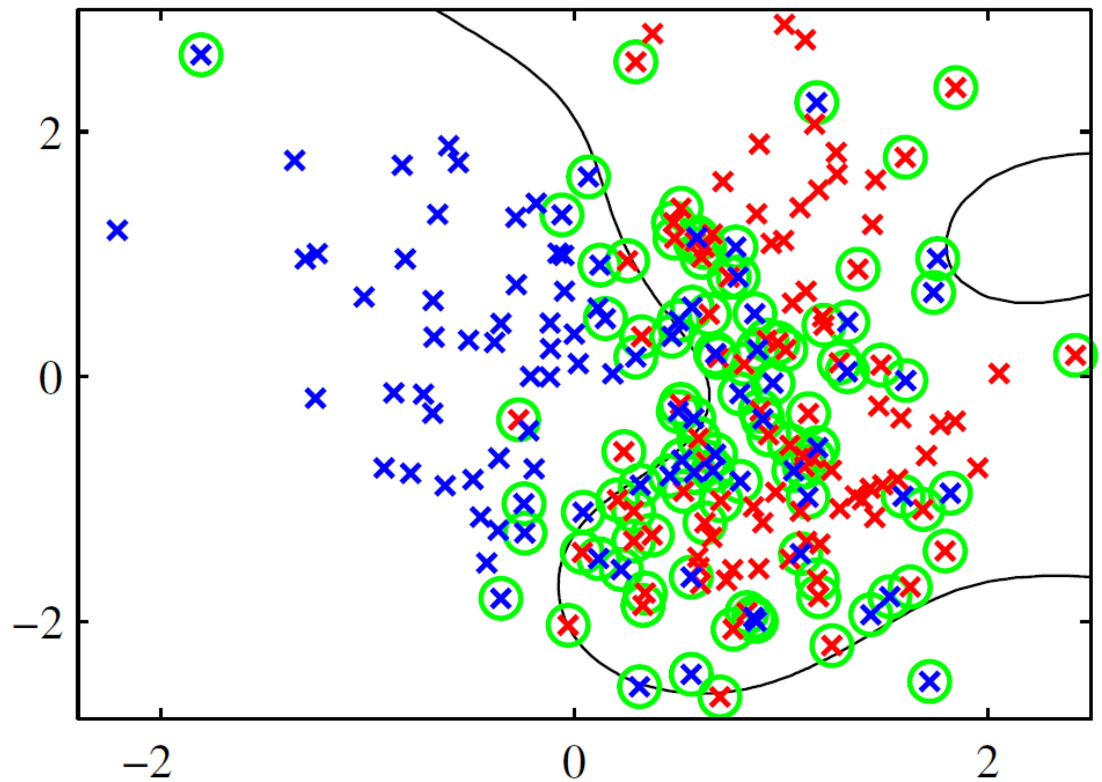
$$t_n \left(\sum_{m \in \mathcal{S}} a_m t_m k(\mathbf{x}_n, \mathbf{x}_m) + b \right) = 1$$

- A numerically stable solution

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

  - M: the set of indices of data points having $0 < a_n < C$
  - S: the set of indices of the support vectors

An example



Optimization solvers for SVMs

- Quadratic programming
  - Many off-the-shelf solvers
  - Often infeasible due to the demanding computations and memory requirement
- Chunking (Vapnik, 1982) & protected conjugate gradients (Burges, 1998)
  - Try to remove the rows and columns of the kernel matrix that correspond to zero-valued Lagrange multipliers
- Decomposition methods (Osuna et al., 1996)
  - Solve a series of smaller quadratic programming problems
- Sequential minimal optimization (SMO) (Platt, 1999)
  - Consider two Lagrange multipliers at a time
  - Iterative processing: At each iteration, choose a pair of Lagrange multipliers and update their values

Summary of SVMs

- A linear model for classification or regression

$$J(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\left\{\mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}_n) - t_n\right\}^2 + \frac{\lambda}{2}\mathbf{w}^{\mathrm{T}}\mathbf{w} \qquad \text{where } \lambda \geq 0$$

- The dual representation of the linear model: a linear combination of training data

$$\mathbf{w} = \sum_{n=1}^{N} a_n \phi(\mathbf{x}_n) = \mathbf{\Phi}^{\mathrm{T}}\mathbf{a}$$

- The optimization variables change from $\mathbf{w}$ to $\mathbf{a}$

Summary of SVMs

- Why dual representation?
- The decision function is calculated in terms of kernel functions

$$y(\mathbf{x}) = \mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}) = \mathbf{a}^{\mathrm{T}}\boldsymbol{\Phi}\phi(\mathbf{x}) = \mathbf{k}(\mathbf{x})^{\mathrm{T}}\left(\mathbf{K} + \lambda\mathbf{I}_N\right)^{-1}\mathbf{t}$$

- A kernel function

$$K_{nm} = \phi(\mathbf{x}_n)^{\mathrm{T}}\phi(\mathbf{x}_m) = k(\mathbf{x}_n, \mathbf{x}_m)$$

  - Compute the inner product between two data points in a very high (even infinite) dimensional feature space
  - Access data points in the low-dimensional input space
  - Allow the PR or ML algorithms to work on a high dimensional feature space without explicitly computing $\phi(\mathbf{x})$

Summary of SVMs

- Polynomial kernel

$$k(\mathbf{x}, \mathbf{x}') = \left(\mathbf{x}^{\mathrm{T}}\mathbf{x}' + c\right)^{M}$$

  - where M is the degree and c is a positive constant

- Gaussian (RBF) kernel

$$k(\mathbf{x}, \mathbf{x}') = \exp\left(-\|\mathbf{x} - \mathbf{x}'\|^2 / 2\sigma^2\right)$$

  - where σ^2 is a positive constant

- Sigmoidal kernel

$$k(\mathbf{x}, \mathbf{x}') = \tanh\left(a\mathbf{x}^{\mathrm{T}}\mathbf{x}' + b\right)$$

  - where a and b are two constants

- The values of these hyperparameters are often determined by using cross-validation

Summary of SVMs

- SVMs a maximum margin classifier
- The primal form of the optimization problem

$$\arg\min_{\mathbf{w},b} \frac{1}{2}\|\mathbf{w}\|^2$$

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

- Using Lagrange multipliers, we obtain its dual form

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

kernel function

$$\text{subject to} \quad a_n \geqslant 0, \qquad n=1,\ldots,N, \qquad \sum_{n=1}^{N} a_n t_n = 0$$

Summary of SVMs

- Soft margin extension where slack variables are included
- Primal form

$$\underset{\mathbf{w},\, b,\, \{\xi_n\}}{\arg\min} \quad C\sum_{n=1}^{N}\xi_n + \frac{1}{2}\|\mathbf{w}\|^2$$

$$\text{subject to} \quad t_n y(\mathbf{x}_n) \geqslant 1 - \xi_n \qquad n = 1, \ldots, N$$

$$\xi_n \geqslant 0 \qquad n = 1, \ldots, N$$

- Dual form

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

$$\text{subject to} \quad 0 \leqslant a_n \leqslant C \qquad n = 1, \ldots, N$$

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

Summary of SVMs

- We use quadratic programming or SMO to optimize $\{a_n\}$

- We exploit KKT conditions to determine the value of b

- For a test point $\mathbf{x}$, we classify it using the decision function

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

Outline

- Dual representations
- Constructing kernels
- Support vector machines for classification
  - Maximum margin classifier
  - Overlapping class distributions
  - Multi-class SVMs
  - SVMs vs. logistic regression
- Support vector machines for regression

Multiclass SVMs

- Support vector machine is fundamentally a two-class classifier
- In practice, we often deal with multi-class ($K > 2$) classification tasks
- Additional mechanism is required to combine multiple two-class SVM classifiers to handle multi-class classification
  - One-versus-the-rest
  - One-versus-one
  - DAGSVM (directed acyclic graph SVM)
  - ECOC (error-correcting output codes)

One-versus-the-rest

- Construct K two-class SVM classifiers, where K is the number of classes
- The kth SVM classifier $y_k(\mathbf{x})$ is trained by using data from class C_k as the positive examples and the data from the remaining $K-1$ classes as the negative data, for $k = 1, 2, \dots, K$
- Make the prediction for an input data point $\mathbf{x}$ by

$$y(\mathbf{x}) = \max_k y_k(\mathbf{x})$$

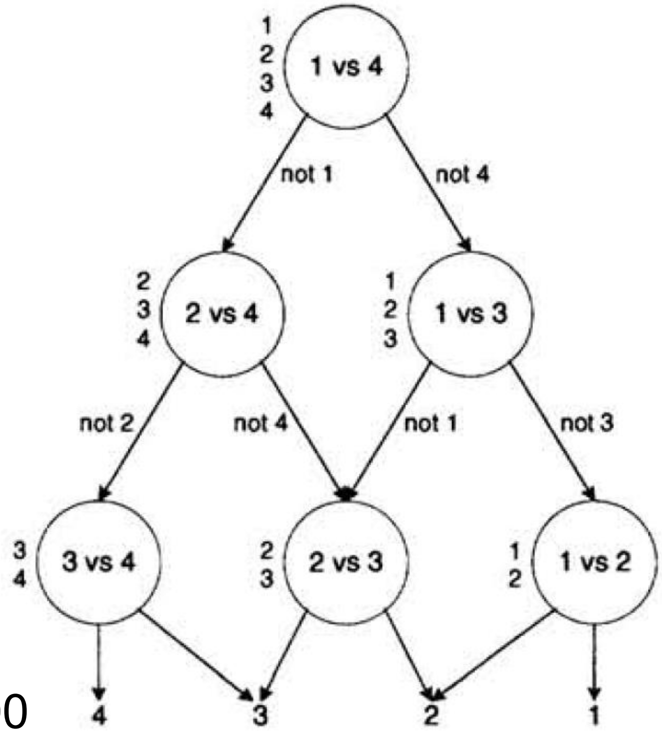
- Simple and intuitive
- Classifiers are trained separately, but comparing their decision values is used in prediction
- Imbalanced training data when training each classifier

One-versus-one

- Train an SVM classifier for each pair of classes i and j
  - Totally, $K(K-1)/2$ SVM classifiers are trained
- Classify a test point according to which class has the highest number of votes
- Simple. No issue regarding imbalanced training data
- Decision ambiguities: Two or multiple classes get the same number of votes
- Computational issue: $K(K-1)/2$ SVM classifiers

DAGSVM (directed acyclic graph SVM)

- Train an SVM classifier for each pair of classes
  - Totally, $K(K-1)/2$ SVM classifiers are trained
- Organize these classifiers into a directed acyclic graph (a tree)
- Classify a test point by going through from the root to a leaf
- DAGSVM is more efficient than one-versus-one during testing



Platt et al. NIPS'00

ECOC (error-correcting output codes)

- Multi-class classification is carried out based on error-correcting output codes
- Partition K classes into two disjoint sets. Train an SVM classifier by using data from one set as positive data and the rest as the negative data
- Repeat the above procedure n times
  - n SVM classifiers are trained
- Apply the n SVM classifiers to a test point
- Assign this test point to the class with the smallest Hamming distance

ECOC (error-correcting output codes)

- An example of $K = 5$ and $n = 15$
- A code matrix of size K by n
  - Each column represents a class partition
  - Each row is the code of the corresponding class

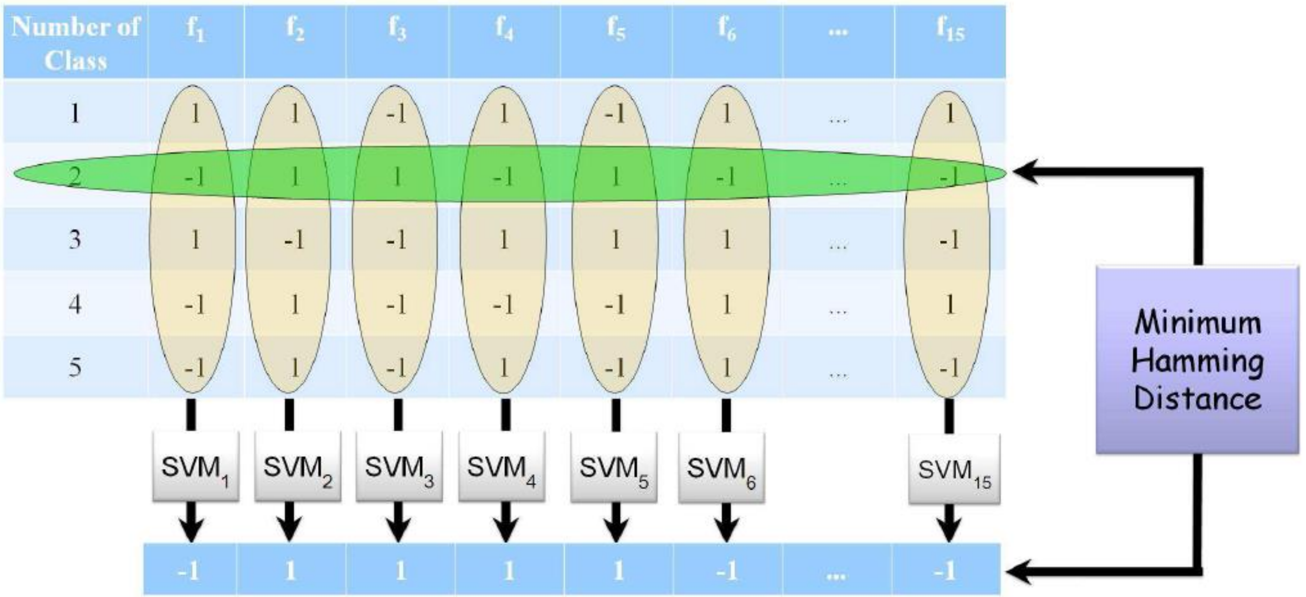


Photo credit: Ozogur et al.

Outline

- Dual representations
- Constructing kernels
- Support vector machines for classification
  - Maximum margin classifier
  - Overlapping class distributions
  - Multi-class SVMs
  - SVMs vs. logistic regression
- Support vector machines for regression

Hinge error

- The primal form of soft margin SVMs

$$\underset{\mathbf{w},\, b,\, \{\xi_n\}}{\arg\min} \quad C\sum_{n=1}^{N}\xi_n + \frac{1}{2}\|\mathbf{w}\|^2$$

$$\text{subject to} \quad t_n y(\mathbf{x}_n) \geqslant 1 - \xi_n \qquad n = 1, \ldots, N$$

$$\xi_n \geqslant 0 \qquad n = 1, \ldots, N$$

- Two cases for a training data point $\mathbf{x}_n$
  - Case 1: $t_n y(\mathbf{x}_n) \geq 1$ => $\xi_n = 0$
  - Case 2: $t_n y(\mathbf{x}_n) < 1$ => $\xi_n = 1 - t_n y(\mathbf{x}_n)$
  - For simplicity, y_n denotes $y(\mathbf{x}_n)$
- Hinge error: $E_{\mathrm{SV}}(y_n t_n) = [1 - y_n t_n]_+$
  - $[\cdot]_+$ returns the positive part

Hinge error

- The primal form of soft margin SVMs

$$\underset{\mathbf{w},\, b,\, \{\xi_n\}}{\arg\min} \quad C\sum_{n=1}^{N}\xi_n + \frac{1}{2}\|\mathbf{w}\|^2$$

$$\text{subject to} \quad t_n y(\mathbf{x}_n) \geqslant 1 - \xi_n \qquad n = 1, \dots, N$$

$$\xi_n \geqslant 0 \qquad n = 1, \dots, N$$

- An equivalent objective based on Hinge loss

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

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

Logistic regression

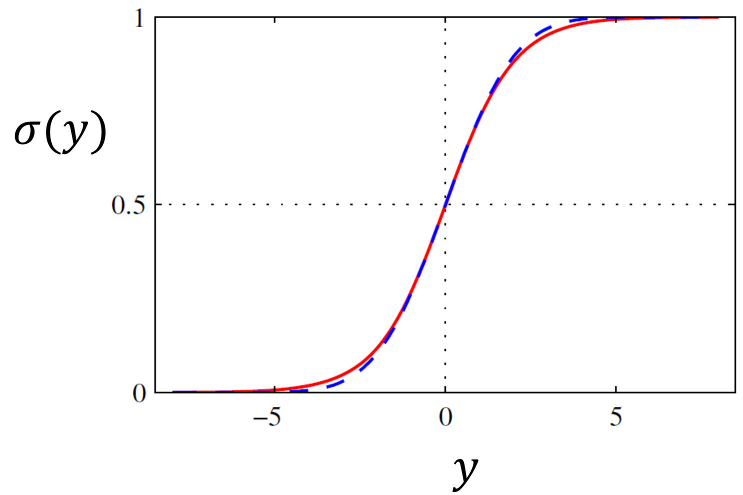
- Logistic regression estimates posterior probability for two-class classification [page 57 of slides "linear model for classification"]

$$
\begin{aligned}
p(\mathcal{C}_1|\mathbf{x}) &= \frac{p(\mathbf{x}|\mathcal{C}_1)p(\mathcal{C}_1)}{p(\mathbf{x}|\mathcal{C}_1)p(\mathcal{C}_1)+p(\mathbf{x}|\mathcal{C}_2)p(\mathcal{C}_2)} \\
&= \frac{1}{1+\exp(-y)} = \sigma(y)
\end{aligned}
$$

- where $y = \mathbf{w}^{\mathrm{T}}\phi(\mathbf{x})$
- σ is the logistic sigmoid function

$$\sigma(y) = \frac{1}{1+\exp(-y)}$$

- A property: $\sigma(-y) = 1 - \sigma(y)$



Logistic regression

- Negative log likelihood is used during training

$$-\ln \prod_{n=1}^{N} \sigma(y_n t_n) = -\sum_{n=1}^{N} \ln \sigma(y_n t_n)$$

  - Note that for comparison with SVMs, we use target labels $t \in \{-1, 1\}$

- Taking the negative log likelihood with a quadratic regularizer, gives the form

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

  - where

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

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SVMs vs. Logistic regression

- SVMs

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

  - where

$$E_{\mathrm{SV}}(y_n t_n) = [1 - y_n t_n]_+$$

- Logistic regression

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

  - where

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

SVMs vs. Logistic regression

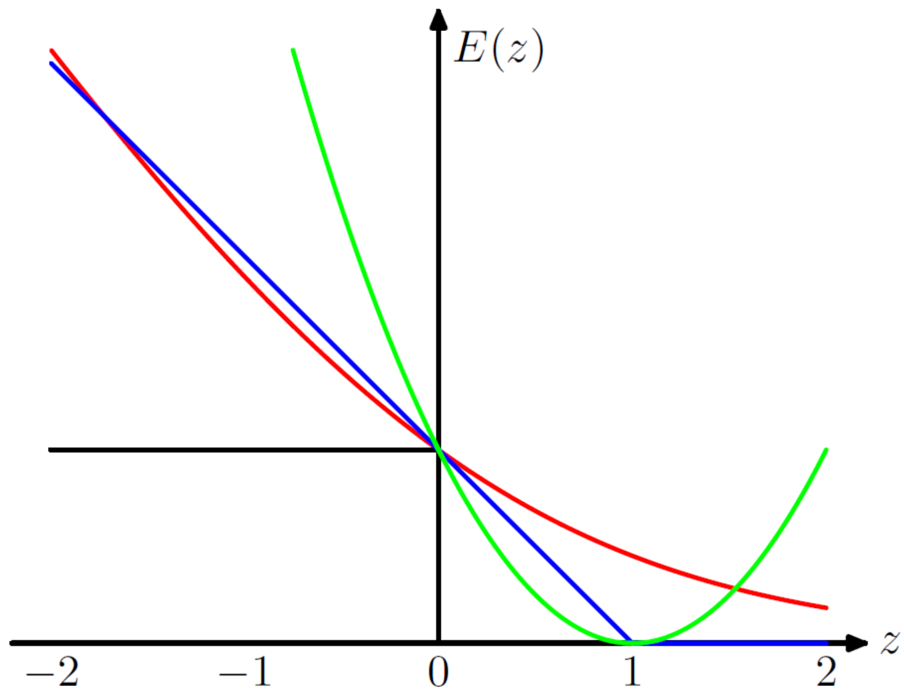
- Black curve
  - misclassification error

- Red curve
  - Logistic regression error

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

- Blue curve
  - Hinge error

$$E_{\mathrm{SV}}(y_n t_n) = [1 - y_n t_n]_+$$



$z = yt$

Outline

- Dual representations
- Constructing kernels
- Support vector machines for classification
- Support vector machines for regression

Regression

- Training data:
  - N training data points: $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N$
  - The corresponding target values: $t_1, t_2, \ldots, t_N$
- In simple linear regression, we minimize a regularized error function given by

$$\frac{1}{2}\sum_{n=1}^{N}\{y_n - t_n\}^2 + \frac{\lambda}{2}\|\mathbf{w}\|^2$$

  - Sum-of-squared error
  - A quadratic regaularizer

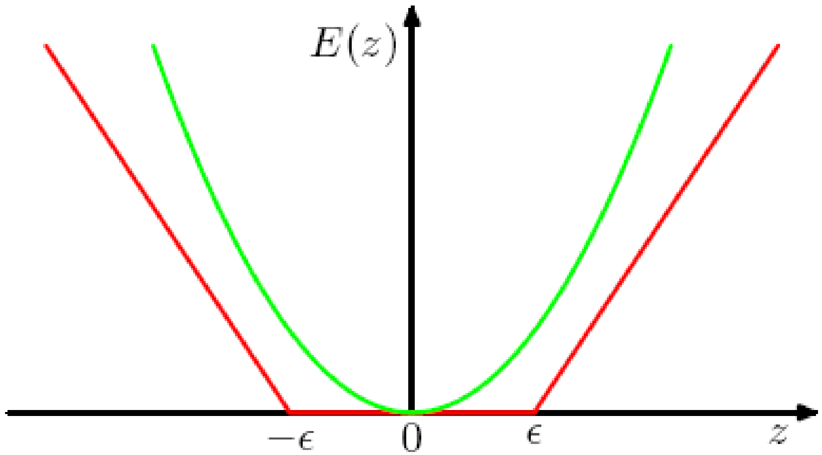
Error function in support vector regression

- In support vector regression (SVR), we define an ε-insensitive error function, which gives zero error if the absolute difference between the prediction $y(\mathbf{x})$ and the target t is less than ε where $\varepsilon > 0$

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

Green line:
quadratic error

Red line:
ε-insensitive error



Objective function for SVR

- Objective function in SVR

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

  - where decision value $y(\mathbf{x})$ is given by $y(\mathbf{x}) = \mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}) + b$
  - The first term in the objective minimizes the regression error
  - The second term is a quadratic term for regularization, which helps maximize the margin in classification
  - C is a positive constant

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How to re-express the ε-insensitive error?

- In support vector classification, a constraint is associated with a training data $\mathbf{x}_n$, and a slack variable is added for soft margin

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

- ε-insensitive error function

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

- For $\mathbf{x}_n$, removing absolute value operator yields two constraints

$$y_n - \epsilon \leqslant t_n \leqslant y_n + \epsilon$$

- Two slack variables ξ_n and $\hat{\xi}_n$ are added for soft margin

$$\begin{aligned} t_n &\leqslant y(\mathbf{x}_n) + \epsilon + \xi_n \\ t_n &\geqslant y(\mathbf{x}_n) - \epsilon - \hat{\xi}_n. \end{aligned}$$

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Optimization problem for SVR

- Original objective:

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

- Primal form of SVR

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

subject to

$$\begin{aligned} t_n &\leqslant y(\mathbf{x}_n) + \epsilon + \xi_n & n = 1, \ldots, N \\ t_n &\geqslant y(\mathbf{x}_n) - \epsilon - \widehat{\xi}_n & n = 1, \ldots, N \\ \xi_n &\geqslant 0 \quad \widehat{\xi}_n \geqslant 0 & n = 1, \ldots, N \end{aligned}$$

Lagrangian function for SVR

- Primal form

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

subject to
$$\begin{array}{llll} t_n & \leqslant & y(\mathbf{x}_n)+\epsilon+\xi_n & n=1,\ldots,N \\ t_n & \geqslant & y(\mathbf{x}_n)-\epsilon-\widehat{\xi}_n & n=1,\ldots,N \\ \xi_n \geqslant 0 & & \widehat{\xi}_n \geqslant 0 & n=1,\ldots,N \end{array}$$

- Lagrangian function with Lagrange multipliers $\{a_n\}$, $\{\hat{a}_n\}$, $\{\mu_n\}$, and $\{\widehat{\mu}_n\}$

$$\begin{aligned} L \;=\;& C\sum_{n=1}^{N}(\xi_n+\widehat{\xi}_n)+\frac{1}{2}\|\mathbf{w}\|^2-\sum_{n=1}^{N}(\mu_n\xi_n+\widehat{\mu}_n\widehat{\xi}_n) \\ & -\sum_{n=1}^{N}a_n(\epsilon+\xi_n+y_n-t_n)-\sum_{n=1}^{N}\widehat{a}_n(\epsilon+\widehat{\xi}_n-y_n+t_n) \end{aligned}$$

Lagrangian function for SVR

- Lagrangian function

$$\begin{aligned} L &= C\sum_{n=1}^{N}(\xi_n + \widehat{\xi}_n) + \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{n=1}^{N}(\mu_n\xi_n + \widehat{\mu}_n\widehat{\xi}_n) \\ &\quad - \sum_{n=1}^{N} a_n(\epsilon + \xi_n + y_n - t_n) - \sum_{n=1}^{N}\widehat{a}_n(\epsilon + \widehat{\xi}_n - y_n + t_n) \end{aligned}$$

- Some constraints

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

$$\frac{\partial L}{\partial b} = 0 \quad \Rightarrow \quad \sum_{n=1}^{N}(a_n - \widehat{a}_n) = 0$$

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

$$\frac{\partial L}{\partial \widehat{\xi}_n} = 0 \quad \Rightarrow \quad \widehat{a}_n + \widehat{\mu}_n = C$$

Dual form for SVR

- Dual form for SVR

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

subject to

$$0 \leqslant a_n \leqslant C \qquad n = 1, \ldots, N$$

$$0 \leqslant \widehat{a}_n \leqslant C \qquad n = 1, \ldots, N$$

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

- This optimization problem can be solved by quadratic programming

Decision function of SVR

- The decision function of SVR

$$y(\mathbf{x}) = \mathbf{w}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}) + b$$

- The dual representation of weight vector $\mathbf{w}$

$$\mathbf{w} = \sum_{n=1}^{N}(a_n - \widehat{a}_n)\boldsymbol{\phi}(\mathbf{x}_n)$$

- The prediction for a new test point $\mathbf{x}$

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

- How to determine the value of b?

Optimizing b via KKT conditions

- The corresponding KKT conditions of SVR

$$\begin{aligned} a_n(\epsilon + \xi_n + y_n - t_n) &= 0 \\ \widehat{a}_n(\epsilon + \widehat{\xi}_n - y_n + t_n) &= 0 \\ (C - a_n)\xi_n &= 0 \\ (C - \widehat{a}_n)\widehat{\xi}_n &= 0 \end{aligned}$$

- Consider a training data point $\mathbf{x}_n$ with $0 < a_n < C$
  - According to $(C - a_n)\xi_n = 0$, it implies $\xi_n = 0$
  - According to $a_n(\epsilon + \xi_n + y_n - t_n) = 0$, we have $\epsilon + y_n - t_n = 0$

$$\begin{aligned} b &= t_n - \epsilon - \mathbf{w}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}_n) \\ &= t_n - \epsilon - \sum_{m=1}^{N}(a_m - \widehat{a}_m)k(\mathbf{x}_n, \mathbf{x}_m) \end{aligned}$$

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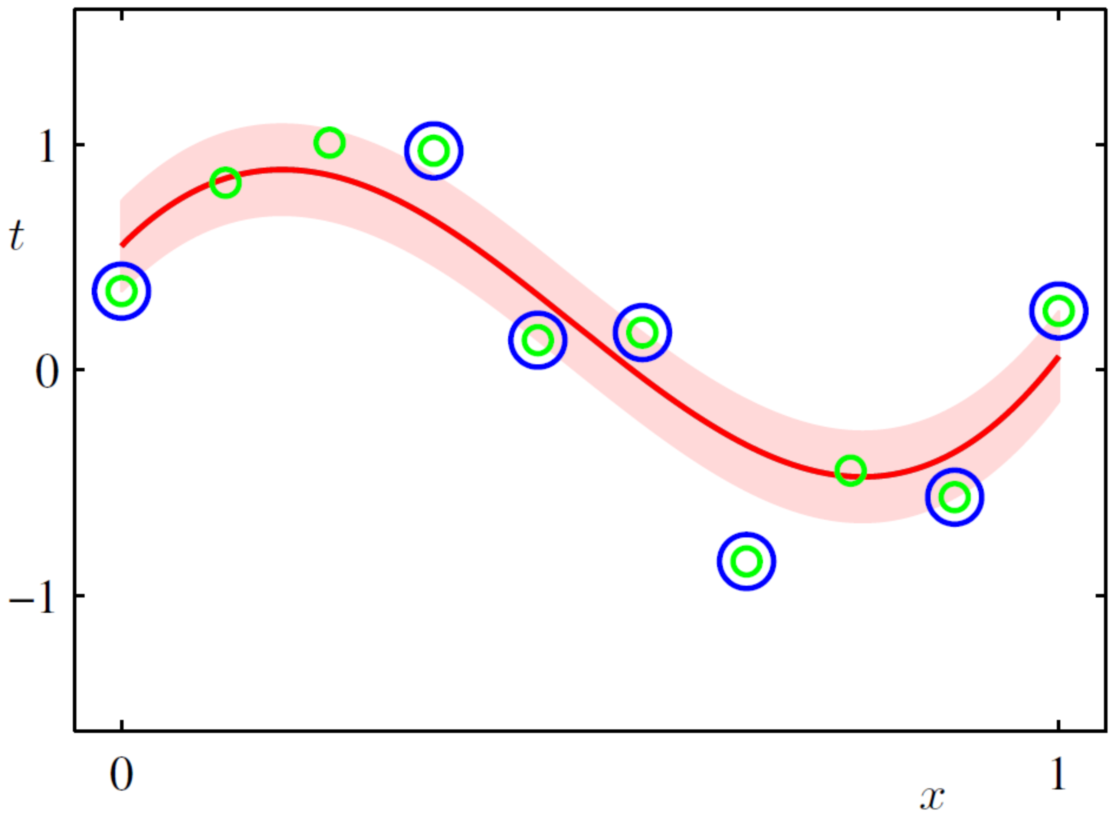
Optimizing b via KKT conditions

- For each training data $\mathbf{x}_n$ with $0 < a_n < C$ or $0 < \widehat{a}_n < C$, we can estimate the value of b

- In practice, it is better to average over all such estimates of b

An example



Summary of SVR

- 1. Choose a kernel function
- 2. Solve the Lagrange multipliers $\{a_n\}$ and $\{\hat{a}_n\}$ in the dual form of SVR by using quadratic programming or SMO

$$\begin{aligned}\widetilde{L}(\mathbf{a},\widehat{\mathbf{a}}) &= -\frac{1}{2}\sum_{n=1}^{N}\sum_{m=1}^{N}(a_n-\widehat{a}_n)(a_m-\widehat{a}_m)k(\mathbf{x}_n,\mathbf{x}_m)\\ &\quad -\epsilon\sum_{n=1}^{N}(a_n+\widehat{a}_n)+\sum_{n=1}^{N}(a_n-\widehat{a}_n)t_n\end{aligned}$$

subject to

$$0 \leqslant a_n \leqslant C \qquad n=1,\ldots,N$$

$$0 \leqslant \widehat{a}_n \leqslant C \qquad n=1,\ldots,N$$

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

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Summary of SVR

- 3. Optimize b via KKT conditions

- 4. Make a prediction for a testing data point $\mathbf{x}$ via

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

References

- Dual representations
  - Chapter 6.1 in the PRML textbook
- Constructing kernels
  - Chapter 6.2 in the PRML textbook
- Support vector machines for classification
  - Chapters 7.1, 7.1.1, 7.1.2, and 7.1.3 in the PRML textbook
- Support vector machines for regression
  - Chapter 7.1.4 in the PRML textbook
- Lagrange multipliers and KKT conditions (optional)
  - Appendix E in the PRML textbook

Thank You for Your Attention!

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