CSC 411: Lecture 16: Kernels

Raquel Urtasun & Rich Zemel

University of Toronto

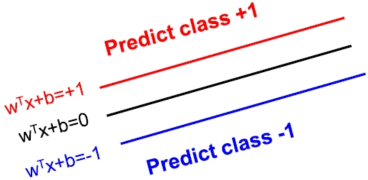
Nov 16, 2015

Today

- Support vectors
- Soft-margin
- Kernel trick

Learning a Margin-Based Classifier

- We can search for the optimal parameters ($\mathbf{w}$ and b) by finding a solution that:
  1. Correctly classifies the training examples: $\{(\mathbf{x}^{(i)}, t^{(i)})\}_{i=1}^{N}$
  2. Maximizes the margin (same as minimizing $\mathbf{w}^T\mathbf{w}$)



$$\min_{\mathbf{w},b} \frac{1}{2}||\mathbf{w}||^2$$
$$s.t. \forall i \quad (\mathbf{w}^T\mathbf{x}^{(i)} + b)t^{(i)} \geq 1,$$

- This is call the primal formulation of Support Vector Machine (SVM)
- Can optimize via projective gradient descent, etc.
- Apply Lagrange multipliers: formulate equivalent problem

Learning a Linear SVM

- Convert the constrained minimization to an unconstrained optimization problem: represent constraints as penalty terms:

$$\min_{\mathbf{w},b} \frac{1}{2}||\mathbf{w}||^2 + \text{penalty} - \text{term}$$

- For data $\{(\mathbf{x}^{(i)}, t^{(i)})\}_{i=1}^N$, use the following penalty

$$\max_{\alpha_i \geq 0} \quad \alpha_i[1 - (\mathbf{w}^T\mathbf{x}^{(i)} + b)t^{(i)}] = \begin{cases} 0 & \text{if} \quad (\mathbf{w}^T\mathbf{x}^{(i)} + b)t^{(i)} \geq 1 \\ \infty & \text{otherwise} \end{cases}$$

- Rewrite the minimization problem

$$\min_{\mathbf{w},b} \{\frac{1}{2}||\mathbf{w}||^2 + \sum_{i=1}^N \max_{\alpha_i \geq 0} \alpha_i[1 - (\mathbf{w}^T\mathbf{x}^{(i)} + b)t^{(i)}]\}$$

where α_i are the Lagrange multipliers

$$= \min_{\mathbf{w},b} \max_{\alpha_i \geq 0} \{\frac{1}{2}||\mathbf{w}||^2 + \sum_{i=1}^N \alpha_i[1 - (\mathbf{w}^T\mathbf{x}^{(i)} + b)t^{(i)}]\}$$

Solution to Linear SVM

- Swap the "max" and "min": This is a lower bound

$$\max_{\alpha_i \geq 0} \min_{\mathbf{w},b} \{ \frac{1}{2}||\mathbf{w}||^2 + \sum_{i=1}^{N} \alpha_i [1 - (\mathbf{w}^T \mathbf{x}^{(i)} + b) t^{(i)}] \} = \max_{\alpha_i \geq 0} \min_{\mathbf{w},b} J(\mathbf{w}, b; \alpha)$$

- First minimize $J()$ w.r.t. $\mathbf{w}$, b for fixed Lagrange multipliers:

$$\frac{\partial J(\mathbf{w}, b; \alpha)}{\partial \mathbf{w}} = \mathbf{w} - \sum_{i=1}^{N} \alpha_i \mathbf{x}^{(i)} t^{(i)} = 0$$

$$\frac{\partial J(\mathbf{w}, b; \alpha)}{\partial b} = -\sum_{i=1}^{N} \alpha_i t^{(i)} = 0$$

- We obtain

$$\mathbf{w} = \sum_{i=1}^{N} \alpha_i t^{(i)} \mathbf{x}^{(i)}$$

- Then substitute back to get final optimization:

$$L = \max_{\alpha_i \geq 0} \{ \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{N} t^{(i)} t^{(j)} \alpha_i \alpha_j ({\mathbf{x}^{(i)}}^T \cdot \mathbf{x}^{(j)}) \}$$

Summary of Linear SVM

- Binary and linear separable classification
- Linear classifier with maximal margin
- Training SVM by maximizing

$$\max_{\alpha_i \geq 0} \{ \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{N} t^{(i)} t^{(j)} \alpha_i \alpha_j (\mathbf{x}^{(i)^T} \cdot \mathbf{x}^{(j)}) \}$$

$$\text{subject to} \quad \alpha_i \geq 0; \quad \sum_{i=1}^{N} \alpha_i t^{(i)} = 0$$

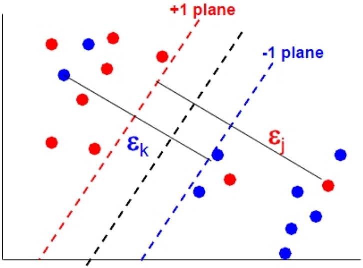
- The weights are

$$\mathbf{w} = \sum_{i=1}^{N} \alpha_i t^{(i)} \mathbf{x}^{(i)}$$

- Only a small subset of α_i's will be nonzero, and the corresponding $\mathbf{x}^{(i)}$'s are the support vectors **S**
- Prediction on a new example:

$$y = \text{sign}[b + \mathbf{x} \cdot (\sum_{i=1}^{N} \alpha_i t^{(i)} \mathbf{x}^{(i)})] = \text{sign}[b + \mathbf{x} \cdot (\sum_{i \in \mathbf{S}} \alpha_i t^{(i)} \mathbf{x}^{(i)})]$$

What if data is not linearly separable?



- Introduce slack variables ξ_i

$$\min \frac{1}{2}||\mathbf{w}||^2 + \lambda \sum_{i=1}^{N} \xi_i$$

$$\text{s.t} \quad \xi_i \geq 0; \quad \forall i \quad t^{(i)}(\mathbf{w}^T\mathbf{x}^{(i)}) \geq 1 - \xi_i = 0$$

- Example lies on wrong side of hyperplane $\xi_i > 1$
- Therefore $\sum_i \xi_i$ upper bounds the number of training errors
- λ trades off training error vs model complexity
- This is known as the soft-margin extension

Non-linear decision boundaries

- Note that both the learning objective and the decision function depend only on dot products between patterns

$$\ell = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{N} t^{(i)} t^{(j)} \alpha_i \alpha_j (\mathbf{x}^{(i)^T} \cdot \mathbf{x}^{(j)})$$

$$y = \text{sign}[b + \mathbf{x} \cdot (\sum_{i=1}^{N} \alpha_i t^{(i)} \mathbf{x}^{(i)})]$$

- How to form non-linear decision boundaries in input space?
  1. Map data into feature space $\mathbf{x} \to \phi(\mathbf{x})$
  2. Replace dot products between inputs with feature points

  $$\mathbf{x}^{(i)^T} \mathbf{x}^{(j)} \to \phi(\mathbf{x}^{(i)})^T \phi(\mathbf{x}^{(j)})$$

  3. Find linear decision boundary in feature space
- Problem: what is a good feature function $\phi(\mathbf{x})$?

Kernel Trick

- Kernel trick: dot-products in feature space can be computed as a kernel function
$$K(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}) = \phi(\mathbf{x}^{(i)})^T \phi(\mathbf{x}^{(j)})$$

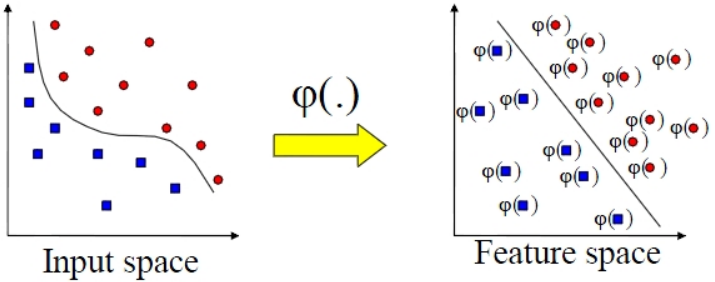
- Idea: work directly on $\mathbf{x}$, avoid having to compute $\phi(\mathbf{x})$
- Example:

$$\begin{aligned}
K(\mathbf{a}, \mathbf{b}) &= (\mathbf{a}^T \mathbf{b})^3 = ((a_1, a_2)^T (b_1, b_2))^3 \\
&= (a_1 b_1 + a_2 b_2)^3 \\
&= a_1^3 b_1^3 + 3 a_1^2 b_1^2 a_2 b_2 + 3 a_1 b_1 a_2^2 b_2^2 + a_2^3 b_2^3 \\
&= (a_1^3, \sqrt{3} a_1^2 a_2, \sqrt{3} a_1 a_2^2, a_2^3)^T (b_1^3, \sqrt{3} b_1^2 b_2, \sqrt{3} b_1 b_2^2, b_2^3) \\
&= \phi(\mathbf{a}) \cdot \phi(\mathbf{b})
\end{aligned}$$

Kernels

- Examples of kernels: kernels measure similarity
  1. Polynomial
  $$K(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}) = (\mathbf{x}^{(i)^T}\mathbf{x}^{(j)} + 1)^2$$
  2. Gaussian
  $$K(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}) = \exp(-\frac{||\mathbf{x}^{(i)} - \mathbf{x}^{(j)}||^2}{2\sigma^2})$$
  3. Sigmoid
  $$K(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}) = \tanh(\beta(\mathbf{x}^{(i)^T}\mathbf{x}^{(j)}) + a)$$
- Each kernel computation corresponds to dot product
  - calculation for particular mapping $\phi(\mathbf{x})$ implicitly maps to high-dimensional space
- Why is this useful?
  1. Rewrite training examples using more complex features
  2. Dataset not linearly separable in original space may be linearly separable in higher dimensional space

Input transformation



- Mapping to a feature space can produce problems:
  - High computational burden due to high dimensionality
  - Many more parameters
- SVM solves these two issues simultaneously
  - Kernel trick produces efficient classification
  - Dual formulation only assigns parameters to samples, not features

Classification with non-linear SVMs

- Non-linear SVM using kernel function $K()$:

$$\ell = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{N} t^{(i)} t^{(j)} \alpha_i \alpha_j K(\mathbf{x}^{(i)}, \mathbf{x}^{(j)})$$

- Maximize ℓ w.r.t. $\{\alpha\}$ under constraints $\forall i, \alpha_i \geq 0$
- Unlike linear SVM, cannot express **w** as linear combination of support vectors
  - now must retain the support vectors to classify new examples
- Final decision function:

$$y = \text{sign}[b + \sum_{i=1}^{N} t^{(i)} \alpha_i K(\mathbf{x}, \mathbf{x}^{(i)})]$$

Kernel Functions

- Mercer's Theorem (1909): any reasonable kernel corresponds to some feature space
- Reasonable means that the Gram matrix is positive definite

$$K_{ij} = K(\mathbf{x}, \mathbf{x}^{(i)})$$

- Feature space can be very large
  - polynomial kernel $(1 + \mathbf{x}^{(i)} + \mathbf{x}^{(j)})^d$ corresponds to feature space exponential in d
  - Gaussian kernel has infinitely dimensional features
- Linear separators in these super high-dim spaces correspond to highly nonlinear decision boundaries in input space

Summary

- Advantages:
  - Kernels allow very flexible hypotheses
  - Poly-time exact optimization methods rather than approximate methods
  - Soft-margin extension permits mis-classified examples
  - Variable-sized hypothesis space
  - Excellent results (1.1% error rate on handwritten digits vs. LeNet's 0.9%)
- Disadvantages:
  - Must choose kernel parameters
  - Very large problems computationally intractable
  - Batch algorithm

More Summary

- Software:
  - A list of SVM implementations can be found at `http://www.kernel-machines.org/software.html`
  - Some implementations (such as LIBSVM) can handle multi-class classification
  - SVMLight is among the earliest implementations
  - Several Matlab toolboxes for SVM are also available
- Key points:
  - Difference between logistic regression and SVMs
  - Maximum margin principle
  - Target function for SVMs
  - Slack variables for mis-classified points
  - Kernel trick allows non-linear generalizations