Introduction to Machine Learning

Kernel Support Vector Machines

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Outline

Support Vector Machines

- SVM Learning
- Kernel SVM

SVM Optimization

Optimization Formulation

$$\underset{\mathbf{w},b}{\text{minimize}} \quad \frac{\|\mathbf{w}\|^2}{2}$$
$$\text{subject to} \quad y_n(\mathbf{w}^\top \mathbf{x}_n + b) \geq 1, \; n = 1, \ldots, N.$$

- Introducing Lagrange Multipliers, α_n, $n = 1, \ldots, N$

Rewriting as a (primal) Lagrangian

$$\underset{\mathbf{w},b,\alpha}{\text{minimize}} \quad L_P(\mathbf{w}, b, \alpha) = \frac{\|\mathbf{w}\|^2}{2} + \sum_{n=1}^{N} \alpha_n \{1 - y_n(\mathbf{w}^\top \mathbf{x}_n + b)\}$$
$$\text{subject to} \quad \alpha_n \geq 0 \; n = 1, \ldots, N.$$

Solving the Lagrangian

- Set gradient of L_P to 0

$$\frac{\partial L_P}{\partial \mathbf{w}} = 0 \Rightarrow \mathbf{w} = \sum_{n=1}^{N} \alpha_n y_n \mathbf{x}_n$$

$$\frac{\partial L_P}{\partial b} = 0 \Rightarrow \sum_{n=1}^{N} \alpha_n y_n = 0$$

- Substituting in L_P to get the dual L_D

Solving the Lagrangian

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- Substituting in L_P to get the dual L_D

Dual Lagrangian Formulation

$$\underset{\mathbf{w},b,\alpha}{\text{maximize}} \quad L_D(\mathbf{w}, b, \alpha) = \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{m,n=1}^{N} \alpha_m \alpha_n y_m y_n (\mathbf{x}_m^\top \mathbf{x}_n)$$

$$\text{subject to} \quad \sum_{n=1}^{N} \alpha_n y_n = 0, \alpha_n \geq 0 \; n = 1, \ldots, N.$$

A Key Observation from Dual Formulation

Dot Product Formulation

- All training examples ($\mathbf{x}_n$'s) occur in *dot/inner products*
- Also recall the prediction using SVMs

$$
\begin{aligned}
y^* &= sign(\mathbf{w}^\top \mathbf{x}^* + b) \\
&= sign((\sum_{n=1}^{N} \alpha_n y_n \mathbf{x}_n)^\top \mathbf{x}^* + b) \\
&= sign(\sum_{n=1}^{N} \alpha_n y_n (\mathbf{x}_n^\top \mathbf{x}^*) + b)
\end{aligned}
$$

- Replace the dot products with kernel functions
  - Kernel or non-linear SVM

Widely used variant of SVM

- Kernel SVM with radial basis function kernel (RBF)

$$k(\mathbf{x}_i, \mathbf{x}_j) = exp\left(-\frac{1}{2\gamma^2}||\mathbf{x}_i - \mathbf{x}_j||^2\right)$$

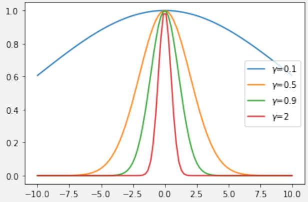
Setting γ and C

- C is the regularization parameter

$$L(\mathbf{w}, b) = \|\mathbf{w}\|^2 + C\sum_{i=1}^{N}\xi_i \quad \text{subject to constraints}$$

- For the role of γ, consider the following two aspects:

$$y^* = sign(\sum_{n=1}^{N}\alpha_n y_n (\mathbf{x}_n^\top \mathbf{x}^*) + b)$$



What should γ and C be?

- γ determines the influence of a training example - inverse of the radius of influence of support vectors
- C determines the trade-off between the total slack (errors on training data) and the size of the margin (regularization)
- Setting γ too large makes the decision boundary too complex, C will not prevent overfitting
- Setting γ very small makes the decision boundary simple (linear)
- Usually a grid search is performed to identify optimal C and γ

References