Introduction to Machine Learning

Kernel Support Vector Machines

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Outline

Support Vector Machines
- SVM Learning
- Kernel SVM

Support Vector Machines

- A hyperplane based classifier defined by $\mathbf{w}$ and b
- Like perceptron
- Find hyperplane with *maximum separation margin* on the training data
- Assume that data is linearly separable (will relax this later)
  - Zero training error (loss)

SVM Prediction Rule

$$y = sign(\mathbf{w}^\top \mathbf{x} + b)$$

SVM Learning

- **Input**: Training data $\{(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \ldots, (\mathbf{x}_N, y_N)\}$
- **Objective**: Learn $\mathbf{w}$ and b that maximizes the margin

SVM Learning

- SVM learning task as an optimization problem
- Find $\mathbf{w}$ and b that gives zero training error
- Maximizes the margin ($= \frac{2}{\|w\|}$)
- Same as minimizing $\|\mathbf{w}\|$

Optimization Formulation

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

- **Optimization** with N linear inequality constraint

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, $\alpha_n,\ n = 1, \ldots, N$

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

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

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

- Substituting in L_P to get the dual L_D

Solving the Lagrangian

- Set gradient of L_P to 0

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

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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)

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

- 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

Concluding Remarks on SVM

- Training time for SVM training is $O(N^3)$
- Many *faster* but approximate approaches exist
  - Approximate QP solvers
  - Online training
- SVMs can be extended in different ways
  1. Non-linear boundaries (**kernel trick**)
  2. Multi-class classification
  3. Probabilistic output
  4. Regression (Support Vector Regression)

References