SVMs with Slack

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Based roughly on the slides of David Sontag

Dual SVM

$$\max_{\lambda \geq 0} -\frac{1}{2} \sum_i \sum_j \lambda_i \lambda_j y_i y_j x^{(i)^T} x^{(j)} + \sum_i \lambda_i$$

such that

$$\sum_i \lambda_i y_i = 0$$

- The dual formulation only depends on inner products between the data points
    - Same thing is true if we use feature vectors instead

Dual SVM

$$\max_{\lambda \geq 0} -\frac{1}{2}\sum_i \sum_j \lambda_i \lambda_j y_i y_j \Phi\left(x^{(i)}\right)^T \Phi\left(x^{(j)}\right) + \sum_i \lambda_i$$

such that

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- The dual formulation only depends on inner products between the data points
  - Same thing is true if we use feature vectors instead

The Kernel Trick

- For some feature vectors, we can compute the inner products quickly, even if the feature vectors are very large
- This is best illustrated by example
  - Let $\phi(x_1, x_2) = \begin{bmatrix} x_1 x_2 \\ x_2 x_1 \\ x_1^2 \\ x_2^2 \end{bmatrix}$
  - $\phi(x_1, x_2)^T \phi(z_1, z_2) = x_1^2 z_1^2 + 2x_1 x_2 z_1 z_2 + x_2^2 z_2^2$

$$= (x_1 z_1 + x_2 z_2)^2$$

$$= (x^T z)^2$$

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$$= (x_1 z_1 + x_2 z_2)^2$$

$$= (x^T z)^2$$

Reduces to a dot product in the original space

The Kernel Trick

- The same idea can be applied for the feature vector ϕ of all polynomials of degree (exactly) d
  - $\phi(x)^T \phi(z) = (x^T z)^d$
- More generally, a kernel is a function $k(x, z) = \phi(x)^T \phi(z)$ for some feature map ϕ
- Rewrite the dual objective

$$\max_{\lambda \geq 0, \sum_i \lambda_i y_i = 0} -\frac{1}{2} \sum_i \sum_j \lambda_i \lambda_j y_i y_j k(x^{(i)}, x^{(j)}) + \sum_i \lambda_i$$

Examples of Kernels

- Polynomial kernel of degree exactly d
  - $k(x, z) = (x^T z)^d$
- General polynomial kernel of degree d for some c
  - $k(x, z) = (x^T z + c)^d$
- Gaussian kernel for some σ
  - $k(x, z) = \exp\left(\frac{-\|x - z\|^2}{2\sigma^2}\right)$
  - The corresponding ϕ is infinite dimensional!
- So many more…

Gaussian Kernels

- Consider the Gaussian kernel

$$\exp\left(\frac{-\|x-z\|^2}{2\sigma^2}\right) = \exp\left(\frac{-(x-z)^T(x-z)}{2\sigma^2}\right)$$

$$= \exp\left(\frac{-\|x\|^2 + 2x^Tz - \|z\|^2}{2\sigma^2}\right)$$

$$= \exp\left(-\frac{\|x\|^2}{2\sigma^2}\right)\exp\left(-\frac{\|z\|^2}{2\sigma^2}\right)\exp\left(\frac{x^Tz}{\sigma^2}\right)$$

- Use the Taylor expansion for exp()

$$\exp\left(\frac{x^Tz}{\sigma^2}\right) = \sum_{n=0}^{\infty}\frac{(x^Tz)^n}{\sigma^{2n}n!}$$

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Polynomial kernels of every degree!

Kernels

- Bigger feature space increases the possibility of overfitting
  - Large margin solutions may still generalize reasonably well
- Alternative: add "penalties" to the objective to disincentivize complicated solutions

$$\min_{w} \frac{1}{2}\|w\|^2 + c \cdot (\#\, of\ misclassifications)$$

  - Not a quadratic program anymore (in fact, it's NP-hard)
  - Similar problem to counting the number of misclassifications, no notion of how badly the data is misclassified

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- Allow misclassification
  - Penalize misclassification linearly (just like in the perceptron algorithm)
    - Again, easier to work with than counting misclassifications
    - Objective stays convex
  - Will let us handle data that isn't linearly separable!

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$$\min_{w,b,\xi} \frac{1}{2}\|w\|^2 + c\sum_i \xi_i$$

such that

$$y_i\left(w^T x^{(i)} + b\right) \geq 1 - \xi_i, \text{for all } i$$

$$\xi_i \geq 0, \text{for all } i$$

SVMs with Slack

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such that

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$$\xi_i \geq 0, \text{for all } i$$

Potentially allows some points to be misclassified/inside the margin

SVMs with Slack

$$\min_{w,b,\xi} \frac{1}{2}\|w\|^2 + c\sum_i \xi_i$$

Constant c determines degree to which slack is penalized

such that

$$y_i(w^T x^{(i)} + b) \geq 1 - \xi_i, \text{for all } i$$

$$\xi_i \geq 0, \text{for all } i$$

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- How does this objective change with c?

SVMs with Slack

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such that

$$y_i\left(w^T x^{(i)} + b\right) \geq 1 - \xi_i, \text{for all } i$$

$$\xi_i \geq 0, \text{for all } i$$

- How does this objective change with c?
  - As $c \rightarrow \infty$, requires a perfect classifier
  - As $c \rightarrow 0$, allows arbitrary classifiers (i.e., ignores the data)

SVMs with Slack

$$\min_{w,b,\xi} \frac{1}{2}\|w\|^2 + c\sum_i \xi_i$$

such that

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- How should we pick c?

SVMs with Slack

$$\min_{w,b,\xi} \frac{1}{2}\|w\|^2 + c\sum_i \xi_i$$

such that

$$y_i\left(w^T x^{(i)} + b\right) \geq 1 - \xi_i, \text{for all } i$$

$$\xi_i \geq 0, \text{for all } i$$

- How should we pick c?
  - Divide the data into three pieces training, testing, and validation
  - Use the validation set to tune the value of the hyperparameter c

Evaluation Methodology

- General learning strategy
  - Build a classifier using the training data
  - Select hyperparameters using validation data
  - Evaluate the chosen model with the selected hyperparameters on the test data

How can we tell if we overfit the training data?

ML in Practice

- Gather Data + Labels
- Select feature vectors
- Randomly split into three groups
  - Training set
  - Validation set
  - Test set
- Experimentation cycle
  - Select a “good” hypothesis from the hypothesis space
  - Tune hyperparameters using validation set
  - Compute accuracy on test set (fraction of correctly classified instances)

SVMs with Slack

$$\min_{w,b,\xi} \frac{1}{2}\|w\|^2 + c\sum_i \xi_i$$

such that

$$y_i\left(w^T x^{(i)} + b\right) \geq 1 - \xi_i, \text{for all } i$$

$$\xi_i \geq 0, \text{for all } i$$

- What is the optimal value of ξ for fixed w and b?

SVMs with Slack

$$\min_{w,b,\xi} \frac{1}{2}\|w\|^2 + c\sum_i \xi_i$$

such that

$$y_i\left(w^T x^{(i)} + b\right) \geq 1 - \xi_i, \text{for all } i$$

$$\xi_i \geq 0, \text{for all } i$$

- What is the optimal value of ξ for fixed w and b?
  - If $y_i\left(w^T x^{(i)} + b\right) \geq 1$, then $\xi_i = 0$
  - If $y_i\left(w^T x^{(i)} + b\right) < 1$, then $\xi_i = 1 - y_i\left(w^T x^{(i)} + b\right)$

SVMs with Slack

$$\min_{w,b,\xi} \frac{1}{2}\|w\|^2 + c\sum_i \xi_i$$

such that

$$y_i\left(w^T x^{(i)} + b\right) \geq 1 - \xi_i, \text{for all } i$$

$$\xi_i \geq 0, \text{for all } i$$

- We can formulate this slightly differently
  - $\xi_i = \max\left\{0, 1 - y_i\left(w^T x^{(i)} + b\right)\right\}$
  - Does this look familiar?
  - Hinge loss provides an upper bound on Hamming loss

Hinge Loss Formulation

- Obtain a new objective by substituting in for ξ

$$\min_{w,b} \frac{1}{2}||w||^2 + c\sum_i \max\{0, 1 - y_i\left(w^T x^{(i)} + b\right)\}$$

Can minimize with gradient descent!

Hinge Loss Formulation

- Obtain a new objective by substituting in for ξ

$$\min_{w,b} \underbrace{\frac{1}{2}\|w\|^2}_{\text{Penalty to prevent overfitting}} + \underbrace{c\sum_i \max\{0, 1 - y_i\left(w^T x^{(i)} + b\right)\}}_{\text{Hinge loss}}$$

Imbalanced Data

- If the data is imbalanced (i.e., more positive examples than negative examples), may want to evenly distribute the error between the two classes

$$\min_{w,b,\xi} \frac{1}{2}\|w\|^2 + \frac{c}{N_+}\sum_{i:y_i=1} \xi_i + \frac{c}{N_-}\sum_{i:y_i=-1} \xi_i$$

such that

$$y_i\left(w^T x^{(i)} + b\right) \geq 1 - \xi_i, \text{for all } i$$

$$\xi_i \geq 0, \text{for all } i$$

Dual of Slack Formulation

$$\min_{w,b,\xi} \frac{1}{2}\|w\|^2 + c\sum_i \xi_i$$

such that

$$y_i\left(w^T x^{(i)} + b\right) \geq 1 - \xi_i, \text{for all } i$$

$$\xi_i \geq 0, \text{for all } i$$

Dual of Slack Formulation

$$L(w, b, \xi, \lambda, \mu) = \frac{1}{2} w^T w + c \sum_i \xi_i + \sum_i \lambda_i (1 - \xi_i - y_i (w^T x^{(i)} + b)) + \sum_i -\mu_i \xi_i$$

Convex in w, b, ξ, so take derivatives to form the dual

$$\frac{\partial L}{\partial w_k} = w_k + \sum_i -\lambda_i y_i x_k^{(i)} = 0$$

$$\frac{\partial L}{\partial b} = \sum_i -\lambda_i y_i = 0$$

$$\frac{\partial L}{\partial \xi_k} = c - \lambda_k - \mu_k = 0$$

Dual of Slack Formulation

$$\max_{\lambda \geq 0} -\frac{1}{2}\sum_i \sum_j \lambda_i \lambda_j y_i y_j {x^{(i)}}^T x^{(j)} + \sum_i \lambda_i$$

such that

$$\sum_i \lambda_i y_i = 0$$

$$c \geq \lambda_i \geq 0, \text{for all } i$$

Generalization

- We argued, intuitively, that SVMs generalize better than the perceptron algorithm
  - How can we make this precise?
  - Coming soon... but first...

Roadmap

- Where are we headed?
  - Other simple hypothesis spaces for supervised learning
    - k nearest neighbor
    - Decision trees
  - Learning theory
    - Generalization and PAC bounds
    - VC dimension
    - Bias/variance tradeoff