SVMs with Slack

Nicholas Ruozzi
University of Texas at Dallas

Based roughly on the slides of David Sontag
Primal SVM

\[
\begin{align*}
\min_{w,b} \quad & \frac{1}{2} \|w\|^2 \\
\text{such that} \quad & y_i(w^T x^{(i)} + b) \geq 1, \text{ for all } i
\end{align*}
\]

- Note that Slater’s condition holds as long as the data is linearly separable
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
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 $\phi(x_1, x_2) = \begin{bmatrix} x_1 x_2 \\ x_2 x_1 \\ x_1^2 \\ x_2^2 \end{bmatrix}$

- $\phi(x_1, x_2)^T \phi(z_1, z_2) = x_1^2 z_1^2 + 2x_1 x_2 z_1 z_2 + x_2^2 z_2^2$

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

  $= (x^T z)^2$
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

  \[ \phi(x_1, x_2) = \begin{bmatrix} x_1 x_2 \\ x_2 x_1 \\ x_1^2 \\ x_2^2 \end{bmatrix} \]

  \[ \phi(x_1, x_2)^T \phi(z_1, z_2) = x_1^2 z_1^2 + 2x_1 x_2 z_1 z_2 + x_2^2 z_2^2 \]

  \[ = (x_1 z_1 + x_2 z_2)^2 \]

  \[ = (x^T z)^2 \]

  Reduces to a dot product in the original space
The Kernel Trick

• The same idea can be applied for the feature vector $\phi$ 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 $\phi$

• 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 $\sigma$
  
  $k(x, z) = \exp \left( \frac{-\|x-z\|^2}{2\sigma^2} \right)$
  
  – The corresponding $\phi$ is infinite dimensional!

• So many more...
Gaussian Kernels

- Consider the Gaussian kernel

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

- Use the Taylor expansion for \(\exp()\)

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

• Consider the Gaussian kernel

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

\[
= \exp\left(-\|x\|^2 + 2x^Tz - \|z\|^2\right)
\]

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

• Use the Taylor expansion for \(\exp()\)

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

Polynomial kernels of every degree!
Kernels

• Bigger feature space increases the possibility of overfitting
  – Large margin solutions should still generalize reasonably well

• Alternative: add “penalties” to the objective to disincentivize complicated solutions

\[
\min_w \frac{1}{2} ||w||^2 + c \cdot (\# \text{ of misclassifications})
\]

  – Not a quadratic program anymore (in fact, it’s NP-hard)

  – Similar problem to Hamming loss, 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 the Hamming loss
    - 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

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

\[\xi_i \geq 0, \text{ for all } i\]
SVMs with Slack

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

such that

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

\[
\xi_i \geq 0, \text{ for all } i
\]

Potentially allows some points to be misclassified/inside the margin
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\[
\min_{w, b, \xi} \frac{1}{2} \|w\|^2 + c \sum_i \xi_i
\]

such that

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

\[
\xi_i \geq 0, \text{ for all } i
\]

Constant c determines degree to which slack is penalized
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\[
\min_{w,b,\xi} \frac{1}{2} ||w||^2 + c \sum_{i} \xi_i
\]

such that

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

\[
\xi_i \geq 0, \text{ for all } i
\]

- How does this objective change with \( c \)?
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\min_{w, b, \xi} \frac{1}{2} \|w\|^2 + c \sum_i \xi_i
\]

such that

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

\[
\xi_i \geq 0, \text{ for all } i
\]

• How does this objective change with \(c\)?

  – As \(c \to \infty\), requires a perfect classifier
  – As \(c \to 0\), allows arbitrary classifiers (i.e., ignores the data)
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\[
\min_{w, b, \xi} \frac{1}{2} \|w\|^2 + c \sum_i \xi_i
\]

such that

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

\[\xi_i \geq 0, \text{ for all } i\]

• How should we pick \(c\)?
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\[
\min_{w,b,\xi} \frac{1}{2} \|w\|^2 + c \sum_i \xi_i
\]

such that

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

\[
\xi_i \geq 0, \text{ for all } i
\]

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

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

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

• Obtain a new objective by substituting in for $\xi$

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

Can minimize with gradient descent!
Hinge Loss Formulation

• Obtain a new objective by substituting in for $\xi$

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

Penalty to prevent overfitting

Hinge loss
Hinge Loss Formulation

- Obtain a new objective by substituting in for $\xi$

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

$\lambda$ controls the amount of regularization

How should we pick $\lambda$?
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

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

\[
\xi_i \geq 0, \text{ for all } i
\]
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 \( w, b, \xi \), 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

$$\sum_i \lambda_i y_i = 0$$

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

• Gather Data + Labels
  – Randomly split into three groups
    • Training set
    • Validation set
    • Test set

• Construct features vectors

• 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)
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 types of hypothesis spaces for supervised learning
    • k nearest neighbor
    • Decision trees
  – Learning theory
    • Generalization and PAC bounds
    • VC dimension
    • Bias/variance tradeoff