Classification / Regression

Support Vector Machines
Support vector machines

• Topics
  – SVM classifiers for linearly separable classes
  – SVM classifiers for non-linearly separable classes
  – SVM classifiers for nonlinear decision boundaries
    ◆ kernel functions
  – Other applications of SVMs
  – Software
Support vector machines

Linearly separable classes

Goal: find a linear decision boundary (hyperplane) that separates the classes
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One possible solution
Support vector machines

Another possible solution
Support vector machines

Other possible solutions
Support vector machines

Which one is better? B1 or B2? How do you define better?
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Hyperplane that maximizes the margin will have better generalization

=> B1 is better than B2
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Hyperplane that maximizes the margin will have better generalization
⇒ B1 is better than B2
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Hyperplane that **maximizes** the margin will have better generalization

=> B1 is better than B2
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\[ \mathbf{w} \cdot \mathbf{x} + b = 0 \]

\[ \mathbf{w} \cdot \mathbf{x} + b = -1 \]

\[ \mathbf{w} \cdot \mathbf{x} + b = +1 \]

\[ y_i = f(\mathbf{x}) = \begin{cases} +1 & \text{if } \mathbf{w} \cdot \mathbf{x} + b \geq 1 \\ -1 & \text{if } \mathbf{w} \cdot \mathbf{x} + b \leq -1 \end{cases} \]

\[ \text{margin} = \frac{2}{\| \mathbf{w} \|} \]
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- We want to maximize: \[ \text{margin} = \frac{2}{\| \mathbf{w} \|} \]

- Which is equivalent to minimizing: \[ L(\mathbf{w}) = \frac{\| \mathbf{w} \|^2}{2} \]

- But subject to the following constraints:

\[ y_i = f(\mathbf{x}) = \begin{cases} +1 & \text{if } \mathbf{w} \cdot \mathbf{x} + b \geq 1 \\ -1 & \text{if } \mathbf{w} \cdot \mathbf{x} + b \leq -1 \end{cases} \]

- This is a constrained convex optimization problem
- Solve with numerical approaches, e.g. quadratic programming
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Solving for $\mathbf{w}$ that gives maximum margin:

1. Combine objective function and constraints into new objective function, using Lagrange multipliers $\lambda_i$

$$L_{primal} = \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{i=1}^{N} \lambda_i (y_i (\mathbf{w} \cdot \mathbf{x}_i + b) - 1)$$

2. To minimize this Lagrangian, we take derivatives of $\mathbf{w}$ and $b$ and set them to 0:

$$\frac{\partial L_p}{\partial \mathbf{w}} = 0 \implies \mathbf{w} = \sum_{i=1}^{N} \lambda_i y_i \mathbf{x}_i$$

$$\frac{\partial L_p}{\partial b} = 0 \implies \sum_{i=1}^{N} \lambda_i y_i = 0$$
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Solving for $\mathbf{w}$ that gives maximum margin:

3. Substituting and rearranging gives the dual of the Lagrangian:

$$L_{\text{dual}} = \sum_{i=1}^{N} \lambda_i - \frac{1}{2} \sum_{i,j} \lambda_i \lambda_j y_i y_j \mathbf{x}_i \cdot \mathbf{x}_j$$

which we try to maximize (not minimize).

4. Once we have the $\lambda_i$, we can substitute into previous equations to get $\mathbf{w}$ and $b$.

5. This defines $\mathbf{w}$ and $b$ as linear combinations of the training data.
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- Optimizing the dual is easier.
  - Function of \( \lambda_i \) only, not \( \lambda_i \) and \( w \).

- Convex optimization \( \Rightarrow \) guaranteed to find global optimum.

- Most of the \( \lambda_i \) go to zero.
  - The \( x_i \) for which \( \lambda_i \neq 0 \) are called the support vectors. These “support” (lie on) the margin boundaries.
  - The \( x_i \) for which \( \lambda_i = 0 \) lie away from the margin boundaries. They are not required for defining the maximum margin hyperplane.
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Example of solving for maximum margin hyperplane

\[-6.64 \times 1 - 9.32 \times 2 + 7.93 = 0\]

<table>
<thead>
<tr>
<th>$x_1$</th>
<th>$x_2$</th>
<th>$y$</th>
<th>Lagrange Multiplier</th>
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<tr>
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</tr>
<tr>
<td>0.2146</td>
<td>0.0099</td>
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<td>0</td>
</tr>
</tbody>
</table>
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What if the classes are not linearly separable?
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Now which one is better? B1 or B2? How do you define better?
What if the problem is not linearly separable?

Solution: introduce slack variables

Need to minimize:

\[
L(w) = \frac{\|w\|^2}{2} + C \left( \sum_{i=1}^{N} \xi_i \right)
\]

Subject to:

\[
y_i = f(x) = \begin{cases} 
+1 & \text{if } w \cdot x + b \geq 1 + \xi_i \\
-1 & \text{if } w \cdot x + b \leq -1 + \xi_i 
\end{cases}
\]

\(C\) is an important hyperparameter, whose value is usually optimized by cross-validation.
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Slack variables for nonseparable data
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What if decision boundary is not linear?
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Solution: nonlinear transform of attributes

\[ \Phi : [x_1, x_2] \rightarrow [x_1, (x_1 + x_2)^4] \]
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Solution: nonlinear transform of attributes

\[ \Phi : [x_1, x_2] \rightarrow [(x_1^2 - x_1), (x_2^2 - x_2)] \]

(a) Decision boundary in the original two-dimensional space.

(b) Decision boundary in the transformed space.

Figure 5.28. Classifying data with a nonlinear decision boundary.
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- Issues with finding useful nonlinear transforms
  - Not feasible to do manually as number of attributes grows (i.e. any real world problem)
  - Usually involves transformation to higher dimensional space
    - increases computational burden of SVM optimization
    - curse of dimensionality

- With SVMs, can circumvent all the above via the kernel trick
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- **Kernel trick**
  - Don’t need to specify the attribute transform $\Phi(\mathbf{x})$
  - Only need to know how to calculate the dot product of any two transformed samples:

  $$k(\mathbf{x}_1, \mathbf{x}_2) = \Phi(\mathbf{x}_1) \cdot \Phi(\mathbf{x}_2)$$

  - The kernel function $k$ is substituted into the dual of the Lagrangian, allowing determination of a maximum margin hyperplane in the (implicitly) transformed space $\Phi(\mathbf{x})$
  - All subsequent calculations, including predictions on test samples, are done using the kernel in place of $\Phi(\mathbf{x}_1) \cdot \Phi(\mathbf{x}_2)$
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- Common kernel functions for SVM
  - linear
    \[ k(x_1, x_2) = x_1 \cdot x_2 \]
  - polynomial
    \[ k(x_1, x_2) = (\gamma x_1 \cdot x_2 + c)^d \]
  - Gaussian or radial basis
    \[ k(x_1, x_2) = \exp(-\gamma \|x_1 - x_2\|^2) \]
  - sigmoid
    \[ k(x_1, x_2) = \tanh(\gamma x_1 \cdot x_2 + c) \]
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- For some kernels (e.g. Gaussian) the implicit transform $\Phi(\mathbf{x})$ is infinite-dimensional!
  - But calculations with kernel are done in original space, so computational burden and curse of dimensionality aren’t a problem.
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Figure 5.29. Decision boundary produced by a nonlinear SVM with polynomial kernel.
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- Applications of SVMs to machine learning
  - Classification
    - binary
    - multiclass
    - one-class
  - Regression
  - Transduction (semi-supervised learning)
  - Ranking
  - Clustering
  - Structured labels
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- Software

  - SVM\textsuperscript{light}
    - \url{http://svmlight joachims.org/}

  - libSVM
    - \url{http://www.csie.ntu.edu.tw/~cjlin/libsvm/}
    - includes MATLAB / Octave interface