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

Goal: find a linear decision boundary (hyperplane) that separates the classes

Linearly separable 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
Support vector machines

Hyperplane that **maximizes the margin** will have better generalization

=> B1 is better than B2
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\[ w \cdot x + b = 0 \]
\[ w \cdot x + b = -1 \]
\[ w \cdot x + b = +1 \]

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

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

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

- But subject to the following constraints:

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

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

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

\[
L_{primal} = \frac{1}{2} \|w\|^2 - \sum_{i=1}^{N} \lambda_i (y_i (w \cdot x_i + b) - 1)
\]

2. To minimize this Lagrangian, we take derivatives of \( w \) and \( b \) and set them to 0:

\[
\frac{\partial L_p}{\partial w} = 0 \Rightarrow w = \sum_{i=1}^{N} \lambda_i y_i x_i
\]

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

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

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

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 are not required for defining the maximum margin hyperplane.
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Example of solving for maximum margin hyperplane

\[-6.64x_1 - 9.32x_2 + 7.93 = 0\]

<table>
<thead>
<tr>
<th>$x_1$</th>
<th>$x_2$</th>
<th>$y$</th>
<th>Lagrange Multiplier</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.3858</td>
<td>0.4687</td>
<td>1</td>
<td>65.5261</td>
</tr>
<tr>
<td>0.4871</td>
<td>0.611</td>
<td>-1</td>
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<tr>
<td>0.9218</td>
<td>0.4103</td>
<td>-1</td>
<td>0</td>
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<td>0.7382</td>
<td>0.8936</td>
<td>-1</td>
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<td>0</td>
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<tr>
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<td>0.3529</td>
<td>1</td>
<td>0</td>
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<tr>
<td>0.9355</td>
<td>0.8132</td>
<td>-1</td>
<td>0</td>
</tr>
<tr>
<td>0.2146</td>
<td>0.0099</td>
<td>-1</td>
<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?
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- What if the problem is not linearly separable?
- Solution: introduce slack variables
  - Need to minimize:
    \[ L(w) = \frac{\|w\|^2}{2} + C\left(\sum_{i=1}^{N} \xi_i^k\right) \]
  - 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:
    $$k(\mathbf{x}_1, \mathbf{x}_2) = \Phi(\mathbf{x}_1) \cdot \Phi(\mathbf{x}_2)$$
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- Kernel trick (cont’d.)
  - The kernel function $k(\cdot, \cdot)$ is substituted into the dual of the Lagrangian, allowing determination of a maximum margin hyperplane in the (implicitly) transformed space $\Phi(x)$:

$$L_{dual} = \sum_{i=1}^{N} \lambda_i - \frac{1}{2} \sum_{i,j} \lambda_i \lambda_j y_i y_j \Phi(x_i) \cdot \Phi(x_j) =$$

$$\sum_{i=1}^{N} \lambda_i - \frac{1}{2} \sum_{i,j} \lambda_i \lambda_j y_i y_j k(x_i, x_j)$$

- All subsequent calculations, including predictions on test samples, are done using the kernel in place of $\Phi(x_1) \cdot \Phi(x_2)$
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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 \[ k(x_1, x_2) = \exp\left(-\gamma \|x_1 - x_2\|^2\right) \]
  - 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
  - $\text{SVM}^\text{light}$
    - [http://svmlight.joachims.org/](http://svmlight.joachims.org/)
  - libSVM
    - includes MATLAB / Octave interface
  - MATLAB svmtrain / svmclassify
    - only supports binary classification
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- Online demos
  - http://cs.stanford.edu/people/karpathy/svmjs/demo/