Feature spaces and kernels

Homogeneous linear classifiers

• Homogeneous linear classifier: \( w \in \mathbb{R}^d \) (weight vector)

\[
f_w(x) = f_{w,0}(x) = \begin{cases} 
+1, & \langle x, w \rangle > 0 \\
-1, & \langle x, w \rangle \leq 0 
\end{cases}
\]

Online Perceptron

Input: training data \( S \) as an input stream.

• Let \( w = 0 \).

• For each \((x, y) \in S:\)
  • If \( f_w(x) \neq y \), then:
    • Update: \( w := w + yx \)
  • Return \( w \)

If \( y(w_x, x) \geq 1 \) for all \((x, y) \in S\), and \( R := \max_{(x,y)\in S} \|x\|_2 \),
then Online Perceptron makes at most \( R^2 \|w_x\|_2^2 \) mistakes (and updates).

Example run of Online Perceptron
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What if data is not linearly separable?

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Adding new features

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Original feature vector: \( x = (1, x_1, x_2) \)

New feature vector: \( \phi(x) = \left(1, \sqrt{2}x_1, \sqrt{2}x_2, x_1^2, \sqrt{2}x_1x_2, x_2^2\right) \)

Decision boundary non-linear in \( x \), but is linear in \( \phi(x) \).
Getting the most out of linear classifiers

Often, with the “correct” set of features, a linear classifier can very well-approximate the Bayes classifier.

Two approaches:
1. Think very hard and carefully about which features to use.
2. Use all features that come to mind.

The kitchen sink of features

• Example: document classification
  - Word features:
    1{aardvark ∈ doc}, 1{abacus ∈ doc}, ..., 1{zygote ∈ doc}
  - Bi-gram features:
    1{bank deposit ∈ doc}, 1{river bank ∈ doc}, ...
  - Tri-gram features:
    1{new york city ∈ doc}, 1{wherefore art thou ∈ doc}, ...

• Example: new features from old features \( x \in \mathbb{R}^d \)
  - Pairwise interactions:
    \( (x_1 x_2, x_1 x_3, ..., x_1 x_d, x_2 x_3, ..., x_{d-1} x_d) \in \mathbb{R}^{\binom{d}{2}} \)

All degree \( \leq 2 \) interaction features
Learning with the kitchen sink of features

• Let \( \phi: \mathbb{R}^d \rightarrow \mathbb{R}^D \) be the expanded feature mapping
  (e.g., throw in all quadratic interaction features, so \( D = \Omega(d^2) \))
  so \( \phi(x) \in \mathbb{R}^D \) is the feature vector we actually want to use

• Learn linear classifier \( f: \mathbb{R}^D \rightarrow \{\pm 1\} \) (i.e., weight vector \( w \in \mathbb{R}^D \))
  using data with expanded features: \( \phi(x), y \)

• Can be computationally expensive to do this directly when \( D \) is large
  (naively: \( \Omega(D) \) time to make a prediction)

The kernel trick

• Perceptron weight vector (using expanded features):
  \[ w = \sum_{(x,y) \in \mathcal{M}} y \phi(x) \]
  where \( \mathcal{M} \subseteq S \) are examples where Online Perceptron makes update.

• Perceptron prediction: on new point \( z \),
  \[ \langle \phi(z), w \rangle = \sum_{(x,y) \in \mathcal{M}} y \langle \phi(x), \phi(z) \rangle \]

  Computational cost: \( |\mathcal{M}| \times \text{time to compute inner product } \langle \phi(x), \phi(z) \rangle \)

All degree \( \leq 2 \) interaction features

\[ \phi: \mathbb{R}^d \rightarrow \mathbb{R}^{1+2d+\binom{d}{2}} \]
\[ \phi(x) := (1, \sqrt{2} x_1, \sqrt{2} x_2, ..., \sqrt{2} x_d, x_1^2, x_2^2, ..., x_d^2, \sqrt{2} x_1 x_2, \sqrt{2} x_1 x_3, ..., \sqrt{2} x_1 x_d, \sqrt{2} x_2 x_3, ..., \sqrt{2} x_{d-1} x_d) \]
(Don’t mind the \( \sqrt{2}'s \))

Computation of \( \langle \phi(x), \phi(x') \rangle \) in \( \mathcal{O}(d) \) time:
\[ (1 + \langle x, x' \rangle)^2 = \langle \phi(x), \phi(x') \rangle \]

Products of all feature subsets

\[ \phi: \mathbb{R}^d \rightarrow \mathbb{R}^{2^d} \]
\[ \phi(x) := \left( \prod_{i \in S} x_i : S \subseteq [d] \right) \]

Computation of \( \langle \phi(x), \phi(x') \rangle \) in \( \mathcal{O}(d) \) time:
\[ \prod_{i=1}^{d} (1 + x_i x'_i) = \sum_{S \subseteq [d]} \prod_{i \in S} (x_i x'_i) = \langle \phi(x), \phi(x') \rangle \]
An infinite dimensional feature expansion

For any \( \sigma > 0 \), there is an infinite feature expansion \( \phi: \mathbb{R}^d \rightarrow \mathbb{R}^\infty \) (involving Hermite polynomials of all orders) such that

\[
\langle \phi(x), \phi(x') \rangle = \exp \left( - \frac{\|x - x'\|^2}{2 \sigma^2} \right)
\]

This can be computed in \( O(d) \) time.

This inner product is called the Gaussian kernel with bandwidth \( \sigma \).

Kernels

A (positive definite) kernel function \( K: \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R} \) is a symmetric function with the following property:

For any \( x_1, x_2, \ldots, x_n \in \mathbb{R}^d \), the \( n \times n \) matrix whose \( (i, j) \)-th entry is \( K(x_i, x_j) \), is positive-semidefinite (all of its eigenvalues are \( \geq 0 \)).

For any kernel \( K \), there is a feature mapping \( \phi: \mathbb{R}^d \rightarrow \mathbb{H} \) such that

\[
\langle \phi(x), \phi(x') \rangle = K(x, x')
\]

(\( \mathbb{H} \) is a Hilbert space [a special kind of inner product space], called the Reproducing Kernel Hilbert Space corresponding to the kernel \( K \).)

String kernels

\[
\phi: \text{Strings} \rightarrow \mathbb{N}^\text{Strings}
\]

\[
\phi(x) = \text{(number of times } s \text{ appears in } x : s \in \text{ Strings)}
\]

\[
K(x, x') = \langle \phi(x), \phi(x') \rangle = \text{measure of similarity between strings}
\]

For each substring \( s \) in \( x \):

Count how often \( s \) appears in \( x' \) and add to total.

Dynamic programming: \( O(\text{length}(x) \cdot \text{length}(x')) \) time

The kernel approach

- Focus on designing good kernels (rather than feature maps), which means designing good similarity functions.
- Lots of ways to construct kernels (e.g., combine existing kernels).
- Lots of algorithms can be “kernelized” (whole industry around this).
Experimental results

• Using OCR digits data, binary classification problem of distinguishing “9” from other digits.
• # training examples: 60000 (about 6000 are from class “9”).
• Using Kernelized Averaged Perceptron (similar to Voted Perceptron)

<table>
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<th># passes</th>
<th>0.1</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>10</th>
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</thead>
<tbody>
<tr>
<td>Test error (linear)</td>
<td>0.045</td>
<td>0.039</td>
<td>0.038</td>
<td>0.038</td>
<td>0.038</td>
<td>0.037</td>
</tr>
<tr>
<td>Test error (degree 2)</td>
<td>0.024</td>
<td>0.012</td>
<td>0.010</td>
<td>0.010</td>
<td>0.009</td>
<td>0.009</td>
</tr>
<tr>
<td>Test error (degree 4)</td>
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<td>0.009</td>
<td>0.008</td>
<td>0.007</td>
<td>0.007</td>
<td>0.006</td>
</tr>
</tbody>
</table>

Computational issues with Kernel methods

• Recall representation of Perceptron weight vector:
  \[ w = \sum_{(x,y) \in \mathcal{M}} y \phi(x) = \sum_{(x,y) \in \mathcal{M}} y K(\cdot,x) \]
• Number of mistakes |\mathcal{M}| could be \( \Omega(n) \)!
  • Computing predictions as expensive as brute-force NN search.
  • Training can also be quite slow.

Kernel approximations

• Many ways to try to speed-up kernel methods using approximations.
• Some possibilities:
  • Limit number of examples used to represent weight vector.
    • “Nystrom approximation”
    • “Budgeted Perceptron”
  • Explicit feature maps \( z: \mathbb{R}^d \rightarrow \mathbb{R}^m \) such that
    \[ \langle z(x), z(x') \rangle \approx K(x,x') \]
    • “Random projections / feature hashing”
    • “Random kitchen sinks”

Experimental results

• Recall “Spam” data set (4601 e-mail messages, 39.4% are spam)
• \( \mathcal{Y} = \{ \text{spam, not spam} \} \)
• \( \mathcal{X} = \mathbb{R}^{57} \), features based on content of e-mail message
• # training examples: 3065, # test examples: 1536

• Decision tree learning: 9.3% test error rate
• Averaged Perceptron (128 passes): 8.27%
• Random Kitchen Sink Averaged Perceptron (64 passes): 6.12%
Recap and final remarks

- **Linear classifiers** only as good as the given feature representation
- **Sometimes explicit feature expansion is okay** (e.g., when $x$ is sparse)
- **Kernel trick**: sometimes never need $\phi(x)$ directly, but only $\langle \phi(x), \phi(x') \rangle$, which is computed quickly as $K(x, x')$
- **Kernel approach**: switch from designing good features to designing good kernels (similarity functions)
- **Computational issues**: sometimes alleviated with approximations