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** $w = \vec{0}$.
- **For** each $(x, y) \in S$:
  - **If** $f_w(x) \neq y$, **then**:
    - **Update**: $w := w + yx$
  - **Return** $w$

If $y\langle w_*, x \rangle \geq 1$ for all $(x, y) \in S$, and $R := \max_{(x, y) \in S} \|x\|_2$, then Online Perceptron makes at most $R^2 \|w_*\|_2^2$ mistakes (and updates).
Example run of Online Perceptron
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Example run of Online Perceptron
Example run of Online Perceptron

\[ w = x_1 - x_7 \]
What if data is not linearly separable?

Noise: even Bayes classifier not perfect

Bayes classifier not (approx.) linear
Adding new features

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

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**:
    \[1\{\text{aardvark} \in \text{doc}\}, 1\{\text{abacus} \in \text{doc}\}, \ldots, 1\{\text{zygote} \in \text{doc}\}\]
  • **Bi-gram features**:
    \[1\{\text{bank deposit} \in \text{doc}\}, 1\{\text{river bank} \in \text{doc}\}, \ldots\]
  • **Tri-gram features**:
    \[1\{\text{new york city} \in \text{doc}\}, 1\{\text{wherefore art thou} \in \text{doc}\}, \ldots\]

• **Example**: new features from old features \(x \in \mathbb{R}^d\)
  • Pairwise interactions:
    \[(x_1 x_2, x_1 x_3, \ldots, x_1 x_d, x_2 x_3, \ldots, x_{d-1} x_d) \in \mathbb{R}^{(d)}\]
All degree $\leq 2$ interaction features
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 $f_w: \mathbb{R}^D \rightarrow \{\pm 1\}$ (i.e., weight vector $w \in \mathbb{R}^D$) using data with expanded features: $((\phi(x_1), y_1), (\phi(x_2), y_2), ...)$

• 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

$\phi: \mathbb{R}^d \rightarrow \mathbb{R}^{1+2d+\binom{d}{2}}$

$\phi(x) := (1, \sqrt{2}x_1, \sqrt{2}x_2, \ldots, \sqrt{2}x_d, x_1^2, x_2^2, \ldots, x_d^2, \sqrt{2}x_1x_2, \sqrt{2}x_1x_3, \ldots, \sqrt{2}x_1x_d, \sqrt{2}x_2x_3, \ldots, \sqrt{2}x_{d-1}x_d)$

(Don’t mind the $\sqrt{2}$'s)

Computation of $\langle \phi(x), \phi(x') \rangle$ in $O(d)$ time:

$(1 + \langle x, x' \rangle)^2 = \langle \phi(x), \phi(x') \rangle$
Products of all feature subsets

\[ \phi: \mathbb{R}^d \to \mathbb{R}^{2^d} \]

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

**Computation of \( \langle \phi(x), \phi(x') \rangle \) in \( O(d) \) 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** $K: \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ 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 $\phi: \mathbb{R}^d \to \mathbb{H}$ 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)

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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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<td>0.039</td>
<td>0.038</td>
<td>0.038</td>
<td>0.038</td>
<td>0.037</td>
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<tr>
<td>Test error (degree 2)</td>
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<td>0.012</td>
<td>0.010</td>
<td>0.010</td>
<td>0.009</td>
<td>0.009</td>
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<tr>
<td>Test error (degree 4)</td>
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<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 $z: \mathbb{R}^d \to \mathbb{R}^m$ 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