Features and kernels

Online Perceptron

Online Perceptron

input Labeled examples $\{(\boldsymbol{x}_i, y_i)\}_{i=1}^{n}$ from $\mathbb{R}^d \times \{-1,+1\}$.

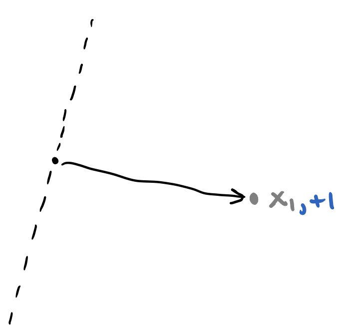
initialize $\hat{\boldsymbol{w}}_1 := \boldsymbol{0}$.
for $t = 1, 2, \dots, n$ **do**
    if $y_t \langle \hat{\boldsymbol{w}}_t, \boldsymbol{x}_t \rangle \leq 0$ **then**
        $\hat{\boldsymbol{w}}_{t+1} := \hat{\boldsymbol{w}}_t + y_t \boldsymbol{x}_t$.
    else
        $\hat{\boldsymbol{w}}_{t+1} := \hat{\boldsymbol{w}}_t$
    end if
end for
return $\hat{\boldsymbol{w}}_{n+1}$.

Theorem: If $R := \max_{t \in \{1,\dots,n\}} \|\boldsymbol{x}_t\|_2$, and $\boldsymbol{w}_\star \in \mathbb{R}^d$ satisfies

$$y \langle \boldsymbol{w}_\star, \boldsymbol{x}_t \rangle \; \geq \; 1 \quad \text{for all } (\boldsymbol{x}_t, y_t),$$

then Online Perceptron makes at most $\|\boldsymbol{w}_\star\|_2^2 \cdot R^2$ mistakes (and updates).

Example run of Online Perceptron



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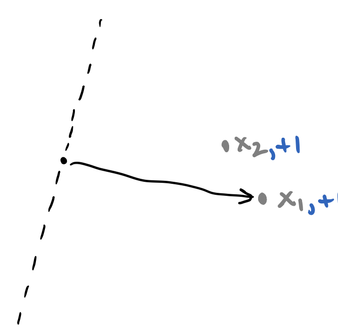

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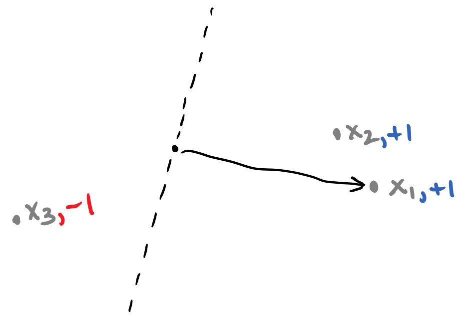

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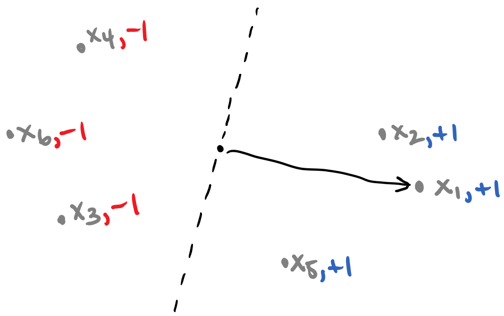

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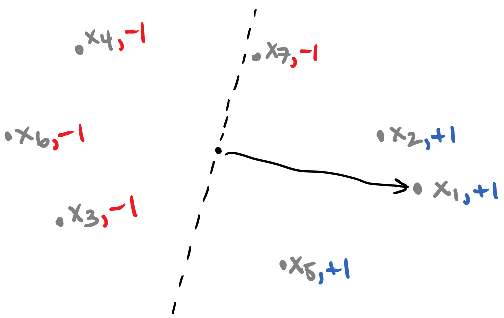

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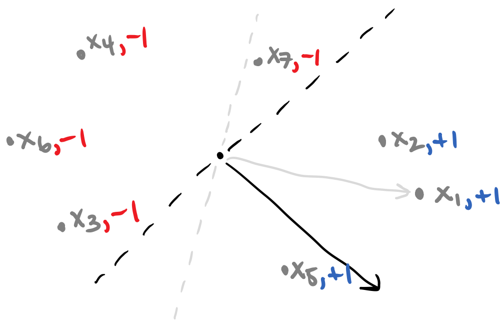

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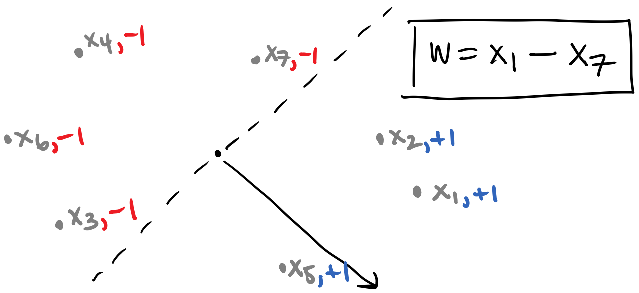
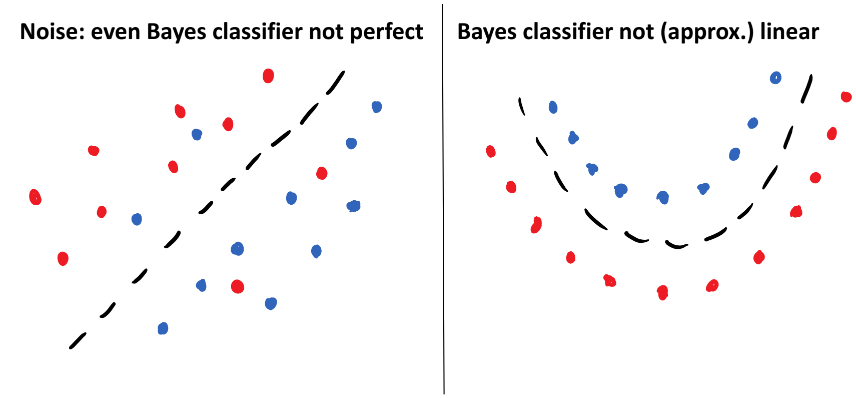
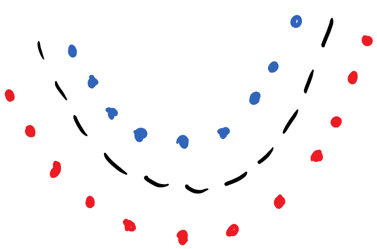


What to do if data is not linearly separable



Adding new features

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



Decision boundary is non-linear in $\boldsymbol{x}$, but is linear in $\boldsymbol{\phi}(\boldsymbol{x})$.

Getting the most out of linear classifiers

Often, with a "good" set of features, a linear classifier can 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**:

$$\mathbb{1}\{\text{“aardvark” appears}\}, \mathbb{1}\{\text{“abacus” appears}\}, \dots, \mathbb{1}\{\text{“zygote” appears}\}$$

- **Bi-gram features**:

$$\mathbb{1}\{\text{“bank deposit” appears}\}, \mathbb{1}\{\text{“river bank” appears}\}, \dots$$

- **Tri-gram features**:

$$\mathbb{1}\{\text{“New York City” appears}\}, \mathbb{1}\{\text{“wherefore art though” appears}\}, \dots$$

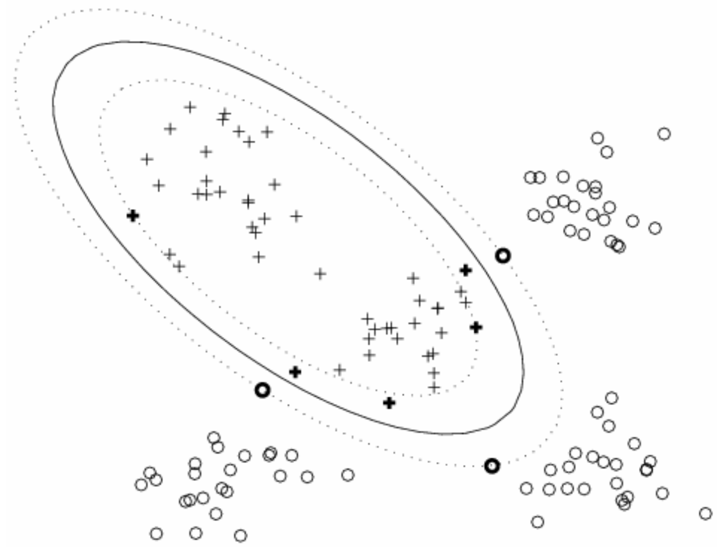
Example: new features from old features $\boldsymbol{x} \in \mathbb{R}^d$

- **Pairwise interactions**:

$$(x_1 x_2,\ x_1 x_3,\ \dots,\ x_1 x_d,\ x_2 x_3,\ \dots,\ x_{d-1} x_d) \ \in\ \mathbb{R}^{\binom{d}{2}}$$

- Etc.

All degree ≤ 2 interaction features



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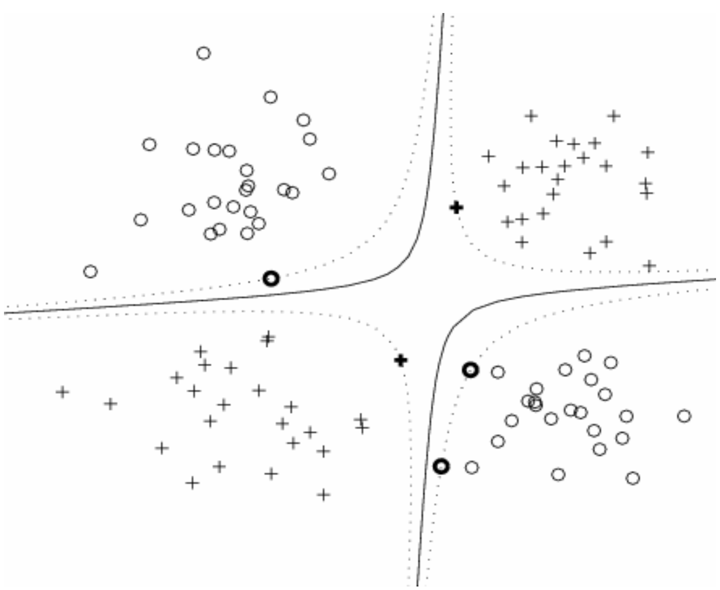


Learning with the kitchen sink of features

- Let $\boldsymbol{\phi} \colon \mathbb{R}^d \to \mathbb{R}^D$ be the mapping to the expanded feature space (e.g., all original features and all deg. 2 interactions, so $D = \Omega(d^2)$).
- Learn linear classifier $f_{\boldsymbol{w}} \colon \mathbb{R}^D \to \{\pm 1\}$ (i.e., learn a weight vector $\boldsymbol{w} \in \mathbb{R}^D$) using data with expanded features $\{(\boldsymbol{\phi}(\boldsymbol{x}_i), y_i)\}_{i=1}^n$.
- **Caveat**: can be computationally expensive to do this directly if D is large. Naïvely: takes $\Omega(D)$ time to even make a prediction.

Kernel trick

- **Recall**: Online Perceptron weight vector (using expanded features) is

$$\boldsymbol{w} \;=\; \sum_{(\boldsymbol{x},y)\in\mathcal{M}} y\boldsymbol{\phi}(\boldsymbol{x})$$

where $\mathcal{M}$ is the subset of labeled examples where Online Perceptron made a mistake during training.

- **Prediction** using Online Perceptron weight vector on new point $\boldsymbol{z} \in \mathbb{R}^d$:

$$\langle \boldsymbol{w}, \boldsymbol{\phi}(\boldsymbol{z})\rangle \;=\; \sum_{(\boldsymbol{x},y)\in\mathcal{M}} y\langle \boldsymbol{\phi}(\boldsymbol{x}), \boldsymbol{\phi}(\boldsymbol{z})\rangle\,.$$

Computational cost: $|\mathcal{M}|\times$ time to compute inner product $\langle \boldsymbol{\phi}(\boldsymbol{x}), \boldsymbol{\phi}(\boldsymbol{z})\rangle$.
Sometimes this can be faster than $O(D)$.

Degree ≤ 2 interaction features

- $\boldsymbol{\phi}\colon \mathbb{R}^d \to \mathbb{R}^{1+2d+\binom{d}{2}}$, where

$$\boldsymbol{\phi}(\boldsymbol{x}) \;=\; \Big(1,\, \sqrt{2}x_1,\, \dots,\, \sqrt{2}x_d,\, x_1^2,\, \dots,\, x_d^2,\, \sqrt{2}x_1x_2,\, \dots,\, \sqrt{2}x_1x_d,\, \dots,\, \sqrt{2}x_{d-1}x_d\Big)$$

(Don't mind the $\sqrt{2}$'s.)

- **Computing** $\langle \boldsymbol{\phi}(\boldsymbol{x}), \boldsymbol{\phi}(\boldsymbol{x}')\rangle$ **in** $O(d)$ **time**:

$$\langle \boldsymbol{\phi}(\boldsymbol{x}), \boldsymbol{\phi}(\boldsymbol{x}')\rangle \;=\; (1 + \langle \boldsymbol{x}, \boldsymbol{x}'\rangle)^2\,.$$

- Much better than $\Omega(d^2)$.

Products of all feature subsets

- $\boldsymbol{\phi}\colon \mathbb{R}^d \to \mathbb{R}^{2^d}$, where

$$\boldsymbol{\phi}(\boldsymbol{x}) \;=\; \left(\prod_{i\in S} x_i \;:\; S \subseteq \{1,2,\dots,d\}\right)$$

- **Computing** $\langle \boldsymbol{\phi}(\boldsymbol{x}), \boldsymbol{\phi}(\boldsymbol{x}')\rangle$ **in** $O(d)$ **time**:

$$\langle \boldsymbol{\phi}(\boldsymbol{x}), \boldsymbol{\phi}(\boldsymbol{x}')\rangle \;=\; \prod_{i=1}^{d}(1 + x_i x_i')\,.$$

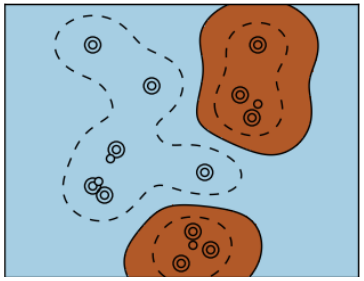
- Much better than $\Omega(2^d)$.

Infinite dimensional feature expansion

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

$$\langle \boldsymbol{\phi}(\boldsymbol{x}), \boldsymbol{\phi}(\boldsymbol{x}')\rangle \;=\; \exp\left(-\frac{\|\boldsymbol{x}-\boldsymbol{x}'\|_2^2}{2\sigma^2}\right),$$

which can be computed in $O(d)$ time.



(This is called the **Gaussian kernel** with bandwidth σ.)

Kernels

A **kernel function** $K\colon \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is a symmetric function with the following property:

For any $\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_n \in \mathcal{X}$, the $n \times n$ matrix whose (i,j)-th entry is $K(\boldsymbol{x}_i, \boldsymbol{x}_j)$ is positive semidefinite.

For any kernel K, there is a feature mapping $\boldsymbol{\phi}\colon \mathcal{X} \to \mathbb{H}$ such that

$$\langle \boldsymbol{\phi}(\boldsymbol{x}), \boldsymbol{\phi}(\boldsymbol{x}') \rangle \;=\; K(\boldsymbol{x}, \boldsymbol{x}'),$$

($\mathbb{H}$ is a Hilbert space—i.e., a special kind of inner product space—called the *Reproducing Kernel Hilbert Space corresponding to* K.)

String kernels

- $\boldsymbol{\phi}$: Strings $\to \mathbb{N}^{\text{Strings}}$, where

$$\boldsymbol{\phi}(\boldsymbol{x}) \;=\; (\text{number of times } \boldsymbol{s} \text{ appears in } \boldsymbol{x} \;:\; \boldsymbol{s} \in \text{Strings})$$

$$K(\boldsymbol{x}, \boldsymbol{x}') \;=\; \langle \boldsymbol{\phi}(\boldsymbol{x}), \boldsymbol{\phi}(\boldsymbol{x}') \rangle \;=\; \text{measure of similarity between strings}\,.$$

- **Computing** $K(\boldsymbol{x}, \boldsymbol{x}')$:
  For each substring $\boldsymbol{s}$ of $\boldsymbol{x}$, count how many times $\boldsymbol{s}$ appears in $\boldsymbol{x}'$ and add to total.

  Dynamic programming in time $O(\text{length}(\boldsymbol{x}) \times \text{length}(\boldsymbol{x}'))$.

Implicit representation of weight vector

- **Implicit representation**:

$$\boldsymbol{w} \;=\; \sum_{(\boldsymbol{x},y) \in \mathcal{M}} y \boldsymbol{\phi}(\boldsymbol{x})$$

- Never explicitly form weight vector $\boldsymbol{w}$.
- Instead, store all labeled examples in $\mathcal{M}$.
- Whenever need to compute $\langle \boldsymbol{w}, \boldsymbol{\phi}(\boldsymbol{z}) \rangle$ for new point $\boldsymbol{z}$, iterate over examples in $\mathcal{M}$ to compute

$$\langle \boldsymbol{w}, \boldsymbol{\phi}(\boldsymbol{z}) \rangle \;=\; \sum_{(\boldsymbol{x},y) \in \mathcal{M}} y \langle \boldsymbol{\phi}(\boldsymbol{x}), \boldsymbol{\phi}(\boldsymbol{z}) \rangle \;=\; \sum_{(\boldsymbol{x},y) \in \mathcal{M}} y K(\boldsymbol{x}, \boldsymbol{z})\,.$$

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 / have been “kernelized” (like Perceptron).

Experimental results on OCR

- OCR digits data, binary classification problem: distinguish "9" from other digits.
- # training examples: 60000 (about 6000 are from class "9").
- Test error rates using Kernelized Averaged Perceptron (similar to Voted Perceptron).

# passes	0.1	1	2	3	4	10
Linear kernel	0.045	0.039	0.038	0.038	0.038	0.037
Degree 2	0.024	0.012	0.010	0.010	0.009	0.009
Degree 4	0.020	0.009	0.008	0.007	0.007	0.006

More computational issues

- **Implicit representation**:

$$\boldsymbol{w} = \sum_{(\boldsymbol{x},y)\in\mathcal{M}} y\boldsymbol{\phi}(\boldsymbol{x})$$

- Number of mistakes $|\mathcal{M}|$ could be $\Omega(n)$.
- Computing predictions as expensive as brute-force NN search.
- Training algorithms quite slow (e.g., $\Omega(n^2)$).

Kernel approximations

Many ways to try to speed-up kernel methods using approximations.

- Limit number of examples used to represent weight vector.
  "Nystrom approximation"
  "Budgeted Perceptron"
- Use *explicit* feature maps $\boldsymbol{z}\colon \mathbb{R}^d \to \mathbb{R}^m$ such that

$$\langle \boldsymbol{z}(\boldsymbol{x}), \boldsymbol{z}(\boldsymbol{x}')\rangle \approx K(\boldsymbol{x},\boldsymbol{x}')\,.$$

  "Random projections / feature hashing"
  "Random kitchen sinks"

Experimental results on e-mail data

- Spam data set (4601 e-mail messages, 39.4% are spam).
- $\mathcal{Y} = \{$spam, not spam$\}$, $\mathcal{X} = \mathbb{R}^{57}$ (message features)
- # training examples: 3065, # test examples: 1536
- Test error rates
  - **Decision tree learning**: 9.3%
  - **Averaged Perceptron** (128 passes): 8.27%
  - **Random Kitchen Sink Averaged Perceptron** (64 passes): 6.12% (approximates Gaussian kernel)

Key takeaways

1. Linear classifiers only as good as given feature representation.
2. Explicit feature expansion (sometimes okay!)
3. Kernel trick: sometimes never need $\boldsymbol{\phi}(\boldsymbol{x})$ directly, but only via $\langle \boldsymbol{\phi}(\boldsymbol{x}), \boldsymbol{\phi}(\boldsymbol{x}') \rangle$, computed quickly as $K(\boldsymbol{x}, \boldsymbol{x}')$.
4. Kernel approach: "similarity engineering" rather than "feature engineering"
5. High-level idea of using kernel approximations.