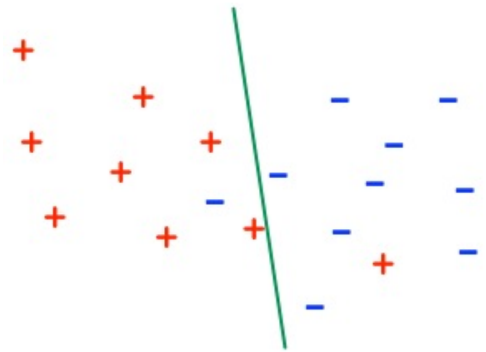
Kernel methods

CSE 250B

Deviations from linear separability

Noise



Find a separator that minimizes a convex loss function related to the number of mistakes.

e.g. SVM, logistic regression.

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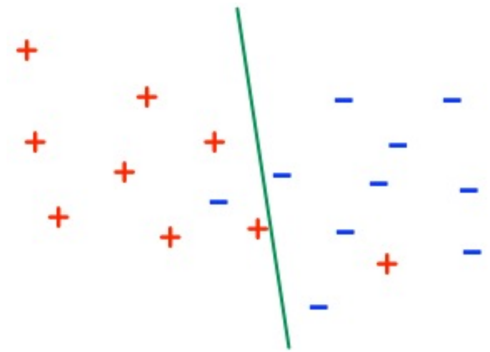

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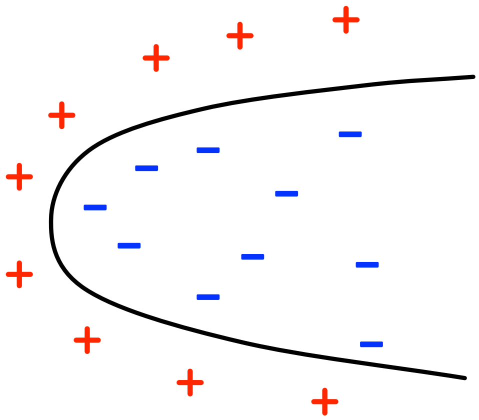
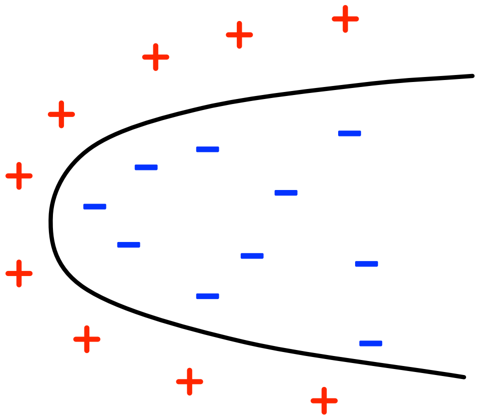
Systematic deviation



What to do with this?

Adding new features



Actual boundary is something like $x_1 = x_2^2 + 5$.

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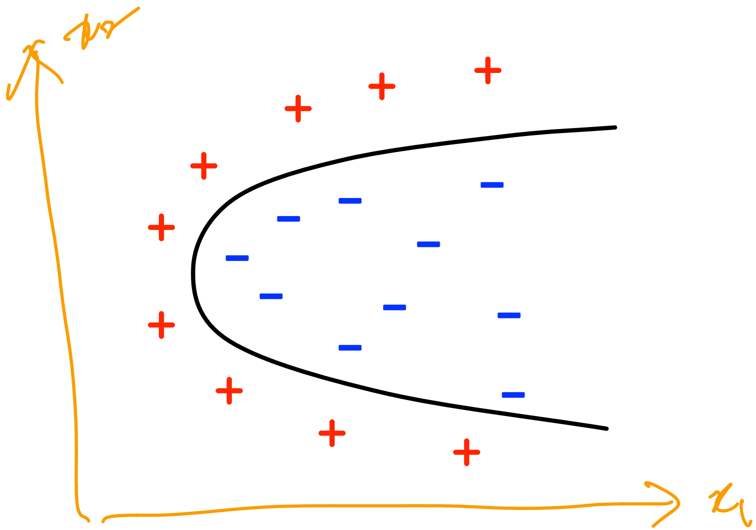


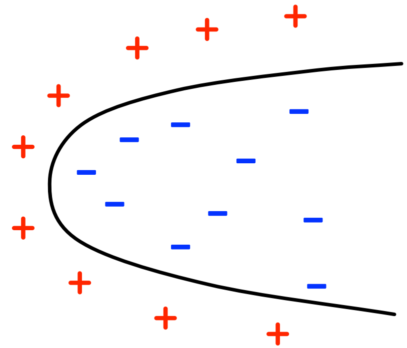
Actual boundary is something like $x_1 = x_2^2 + 5$.

- This is quadratic in $x = (x_1, x_2)$
- But it is linear in $\Phi(x) = (x_1, x_2, x_1^2, x_2^2, x_1 x_2)$

Basis expansion: embed data in higher-dimensional feature space. Then we can use a linear classifier!

Basis expansion for quadratic boundaries

How to deal with a **quadratic** boundary?



Idea: augment the regular features $x = (x_1, x_2, \ldots, x_d)$ with

$$x_1^2,\ x_2^2,\ \ldots,\ x_d^2$$

$$x_1x_2,\ x_1x_3,\ \ldots,\ x_{d-1}x_d \rightarrow \binom{d}{2} \text{ terms}$$

Enhanced data vectors of the form:

$$\Phi(x) = (\underbrace{x_1, \ldots, x_d}_{d}, \underbrace{x_1^2, \ldots, x_d^2}_{d}, \underbrace{x_1x_2, \ldots, x_{d-1}x_d}_{\binom{d}{2} = \frac{d(d-1)}{2}}) \rightarrow O(d^2) \text{ terms.}$$

Quick question

Suppose $x = (x_1, x_2, x_3)$. What is the dimension of $\Phi(x)$?

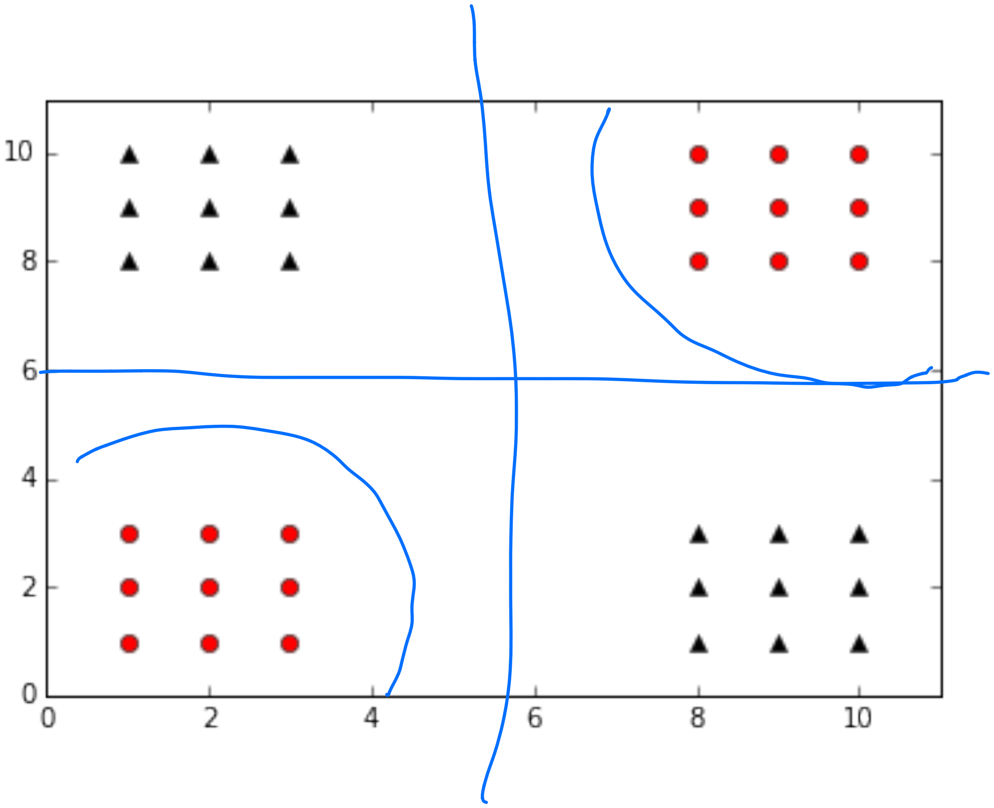
Suppose $x = (x_1, \ldots, x_d)$. What is the dimension of $\Phi(x)$?

Perceptron revisited

Learning in the higher-dimensional feature space:

- $w = 0$ and $b = 0$
- while some $y(w \cdot \Phi(x) + b) \leq 0$:
  - $w = w + y\,\Phi(x)$
  - $b = b + y$

Perceptron with basis expansion: examples



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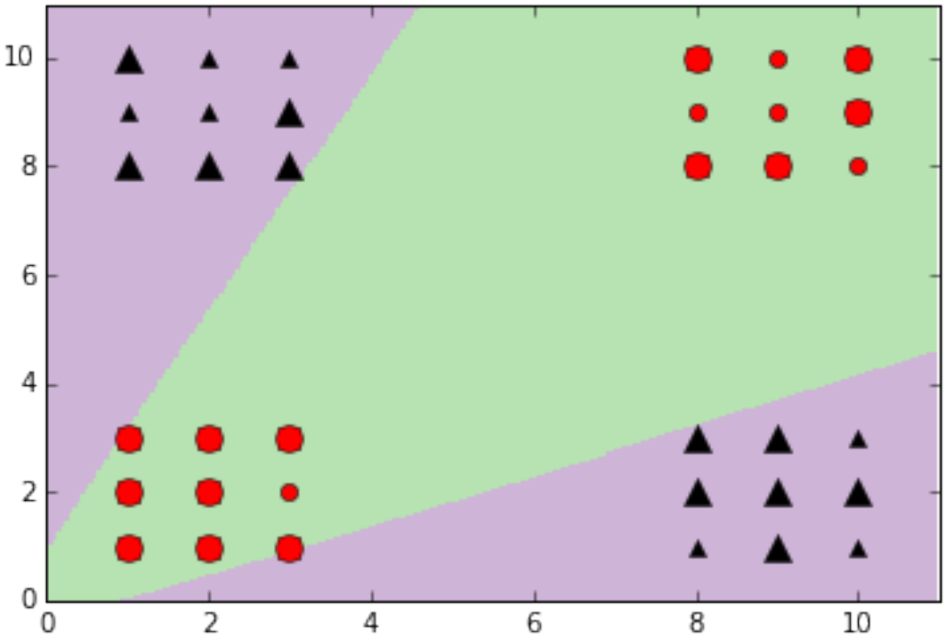

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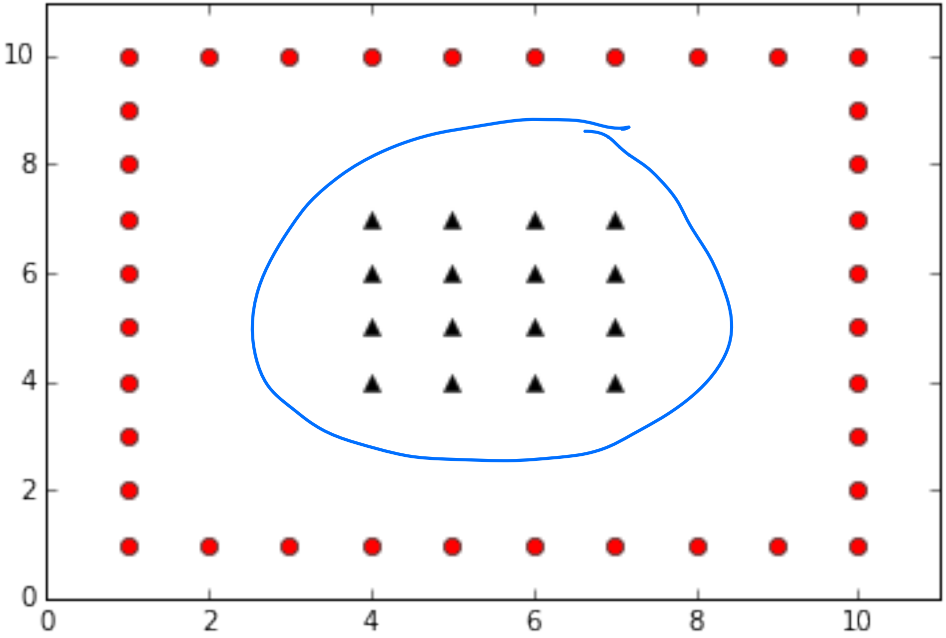

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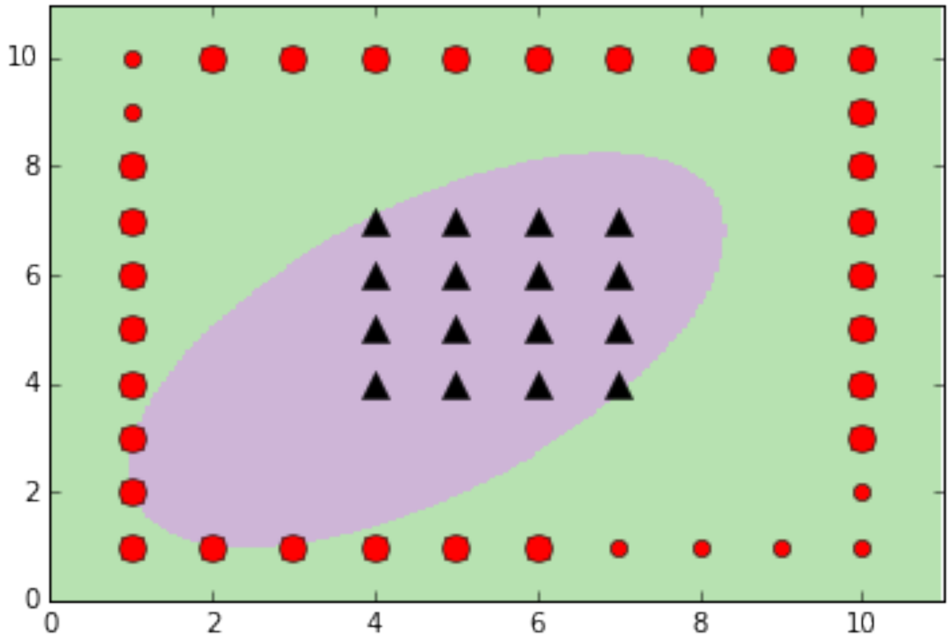

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Problem: number of features has now increased dramatically.
For MNIST, with quadratic boundary: from 784 to 308504.

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Problem: number of features has now increased dramatically. For MNIST, with quadratic boundary: from 784 to 308504.

The kernel trick: implement this without ever writing down a vector in the higher-dimensional space!

The kernel trick

- $w = 0$ and $b = 0$
- while some $y^{(i)}(w \cdot \Phi(x^{(i)}) + b) \leq 0$:
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1. Represent w in **dual** form: $\alpha = (\alpha_1, \ldots, \alpha_n)$.

$$w = \sum_{j=1}^{n} \alpha_j y^{(j)} \Phi(x^{(j)})$$

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$$w \cdot \Phi(x) = \sum_{j=1}^{n} \alpha_j y^{(j)} (\Phi(x^{(j)}) \cdot \Phi(x))$$

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3. Compute $\Phi(x) \cdot \Phi(z)$ without ever writing out $\Phi(x)$ or $\Phi(z)$.

Computing dot products

First, in 2-d.
Suppose $x = (x_1, x_2)$ and $\Phi'(x) = (x_1, x_2, x_1^2, x_2^2, x_1 x_2)$.

Actually, tweak a little: $\Phi(x) = (1, \sqrt{2}x_1, \sqrt{2}x_2, x_1^2, x_2^2, \sqrt{2}x_1 x_2)$

What is $\Phi(x) \cdot \Phi(z)$? $\phi(z) = (1, \sqrt{2}z_1, \sqrt{2}z_2, z_1^2, z_2^2, \sqrt{2}z_1 z_2)$

$\langle \phi(x), \phi(z) \rangle$

$= 1 + 2x_1 z_1 + 2x_2 z_2 + x_1^2 z_1^2 + x_2^2 z_2^2 + 2x_1 z_1 x_2 z_2$

$= (1 + x_1 z_1 + x_2 z_2)^2 = (1 + \langle x, z \rangle)^2$

$\langle \phi'(x), \phi'(z) \rangle = x_1 z_1 + x_2 z_2 + x_1^2 z_1^2 + x_2^2 z_2^2$

$+ x_1 x_2 z_1 z_2$

Computing dot products

Suppose $x = (x_1, x_2, \ldots, x_d)$ and

$$\Phi(x) = (1, \sqrt{2}x_1, \ldots, \sqrt{2}x_d, x_1^2, \ldots, x_d^2, \sqrt{2}x_1x_2, \ldots, \sqrt{2}x_{d-1}x_d)$$

$$\boxed{\Phi(x) \cdot \Phi(z)}$$

$$= (1, \sqrt{2}x_1, \ldots, \sqrt{2}x_d, x_1^2, \ldots, x_d^2, \sqrt{2}x_1x_2, \ldots, \sqrt{2}x_{d-1}x_d) \cdot$$
$$(1, \sqrt{2}z_1, \ldots, \sqrt{2}z_d, z_1^2, \ldots, z_d^2, \sqrt{2}z_1z_2, \ldots, \sqrt{2}z_{d-1}z_d)$$

$$= 1 + 2\sum_i x_i z_i + \sum_i x_i^2 z_i^2 + 2\sum_{i \neq j} x_i x_j z_i z_j$$

$$= (1 + x_1z_1 + \cdots + x_dz_d)^2 \quad = \quad (1 + \underbrace{x \cdot z}_{O(d)})^2$$

O(d), rest is constant time

For MNIST:
We are computing dot products in 308504-dimensional space.
But it takes time proportional to 784, the original dimension!

Kernel Perceptron

Learning from data $(x^{(1)}, y^{(1)}), \ldots, (x^{(n)}, y^{(n)}) \in \mathcal{X} \times \{-1, 1\}$

Primal form:

- $w = 0$ and $b = 0$
- while there is some i with $y^{(i)}(w \cdot \Phi(x^{(i)}) + b) \leq 0$:
    - $w = w + y^{(i)}\,\Phi(x^{(i)})$
    - $b = b + y^{(i)}$

$w = w + y^{i} \phi(x^{(i)})$

Dual form: $w = \sum_j \alpha_j y^{(j)} \Phi(x^{(j)})$, where $\alpha \in \mathbb{R}^n$

- $\alpha = 0$ and $b = 0$
- while some i has $y^{(i)} \left(\sum_j \alpha_j y^{(j)} \Phi(x^{(j)}) \cdot \Phi(x^{(i)}) + b \right) \leq 0$:
    - $\alpha_i = \alpha_i + 1$
    - $b = b + y^{(i)}$

To classify a new point x: sign $\left(\sum_j \alpha_j y^{(j)} \Phi(x^{(j)}) \cdot \Phi(x) + b \right)$.

Does this work with SVMs?

$$\text{(PRIMAL)} \qquad \min_{w\in\mathbb{R}^d, b\in\mathbb{R}, \xi\in\mathbb{R}^n} \quad \|w\|^2 + C\sum_{i=1}^n \xi_i$$

$$\text{s.t.:} \quad y^{(i)}(w\cdot x^{(i)} + b) \geq 1 - \xi_i \quad \text{for all } i = 1, 2, \ldots, n$$

$$\xi \geq 0$$

$$\text{(DUAL)} \qquad \max_{\alpha\in\mathbb{R}^n} \quad \sum_{i=1}^n \alpha_i - \sum_{i,j=1}^n \alpha_i\alpha_j y^{(i)} y^{(j)} (x^{(i)}\cdot x^{(j)})$$

$$\text{s.t.:} \quad \sum_{i=1}^n \alpha_i y^{(i)} = 0$$

$$0 \leq \alpha_i \leq C$$

Solution: $w = \sum_i \alpha_i y^{(i)} x^{(i)}$.

Kernel SVM

1. **Basis expansion.** Mapping $x \mapsto \Phi(x)$.
2. **Learning.** Solve the dual problem:

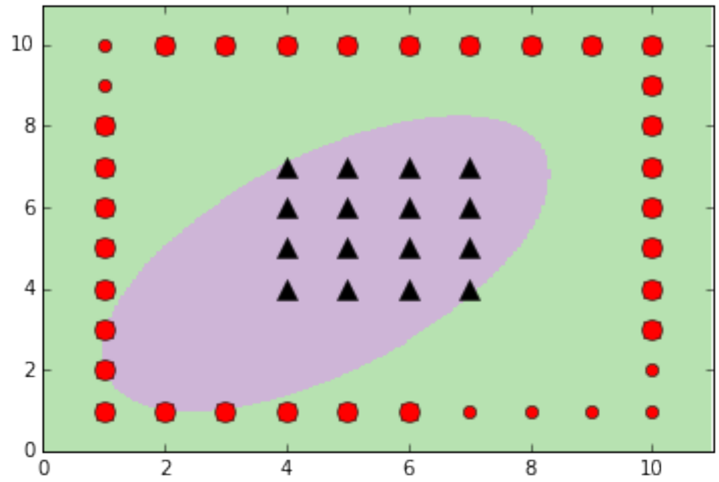
$$\boxed{\begin{aligned} \max_{\alpha \in \mathbb{R}^n} \quad & \sum_{i=1}^{n} \alpha_i - \sum_{i,j=1}^{n} \alpha_i \alpha_j y^{(i)} y^{(j)} (\Phi(x^{(i)}) \cdot \Phi(x^{(j)})) \\ \text{s.t.:} \quad & \sum_{i=1}^{n} \alpha_i y^{(i)} = 0 \\ & 0 \leq \alpha_i \leq C \end{aligned}}$$

   This yields $w = \sum_i \alpha_i y^{(i)} \Phi(x^{(i)})$. Offset b also follows.
3. **Classification.** Given a new point x, classify as

$$\operatorname{sign}\left(\sum_i \alpha_i y^{(i)} (\Phi(x^{(i)}) \cdot \Phi(x)) + b \right).$$

Kernel Perceptron vs. Kernel SVM: examples

Perceptron:



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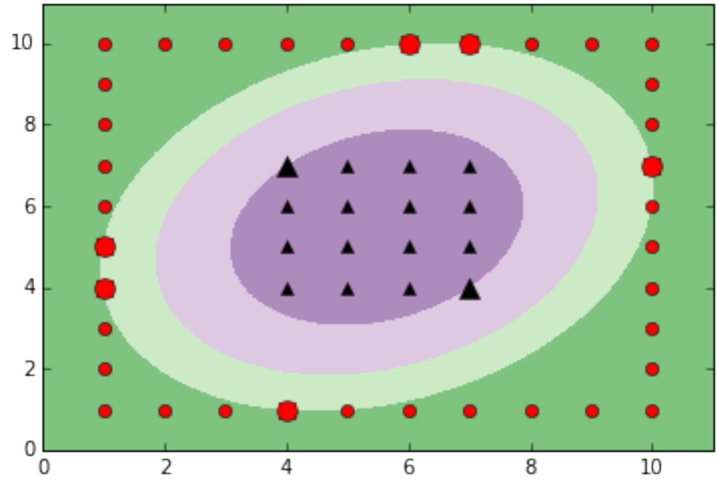

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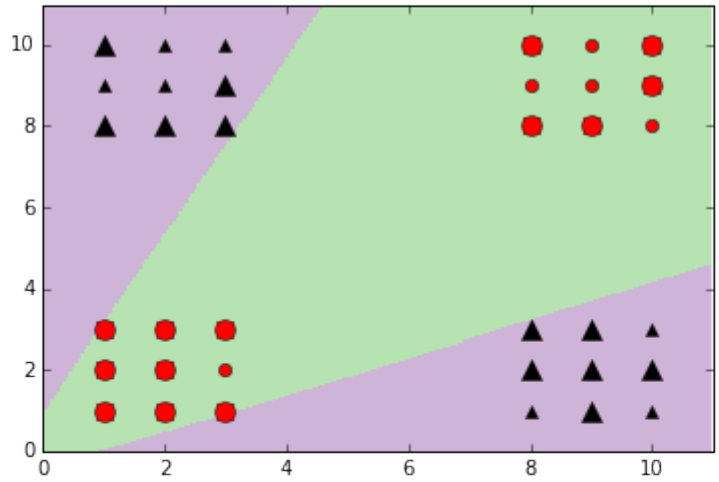

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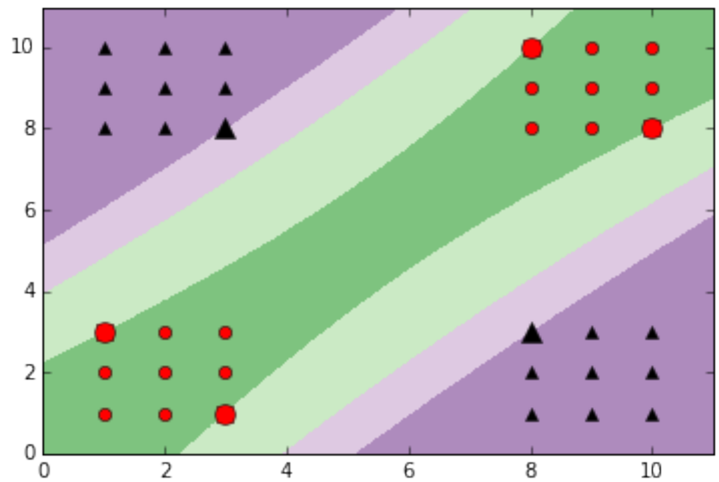
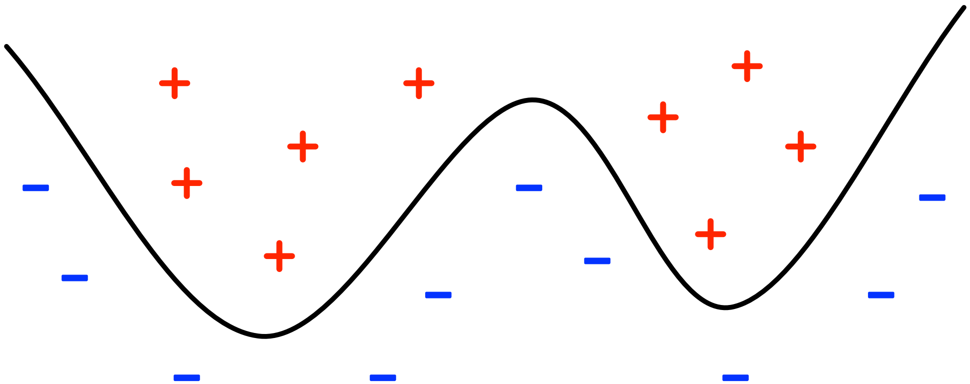


Polynomial decision boundaries

When decision surface is a polynomial of order p:



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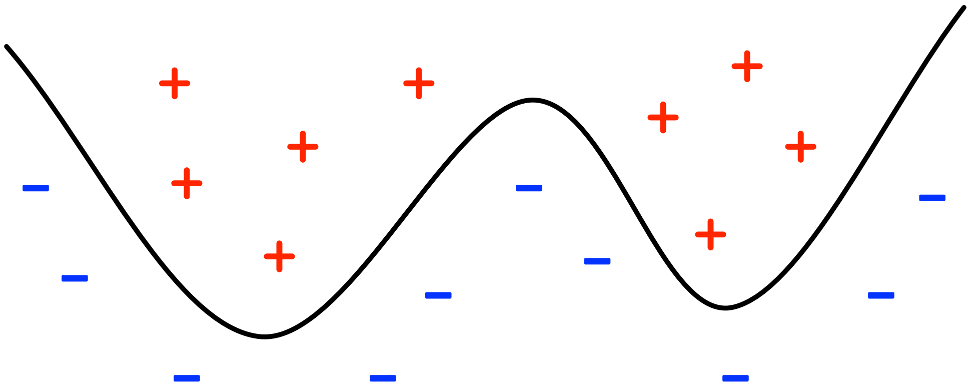

- Let $\Phi(x)$ consist of all terms of order $\leq p$, such as $x_1 x_2^2 x_3^{p-3}$.
  (How many such terms are there, roughly?)

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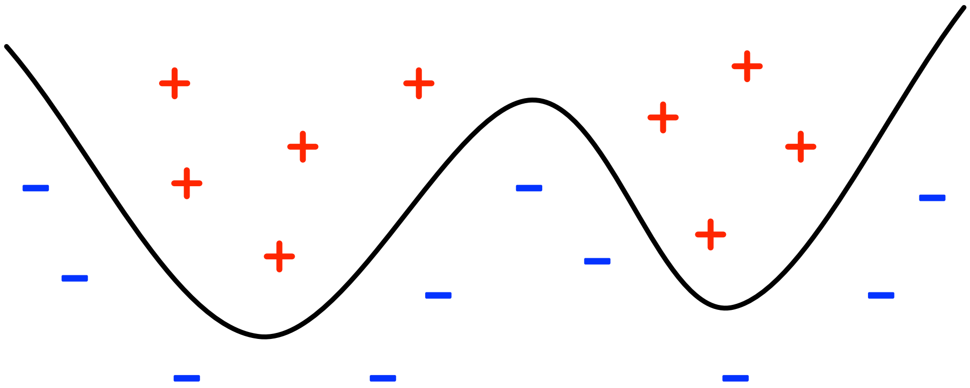

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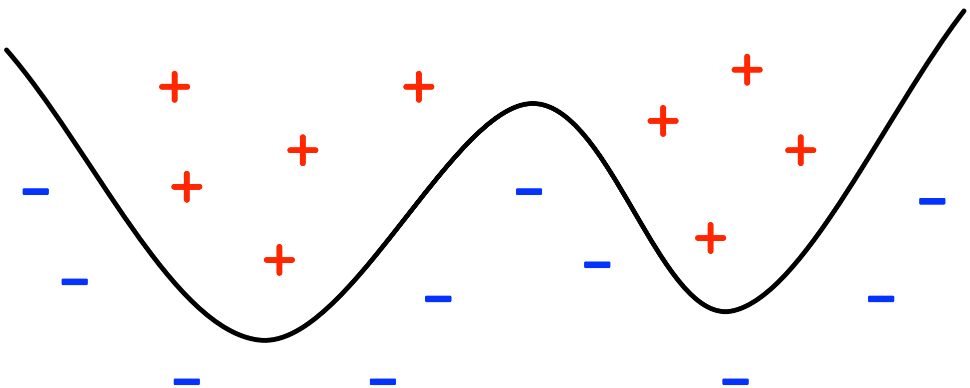

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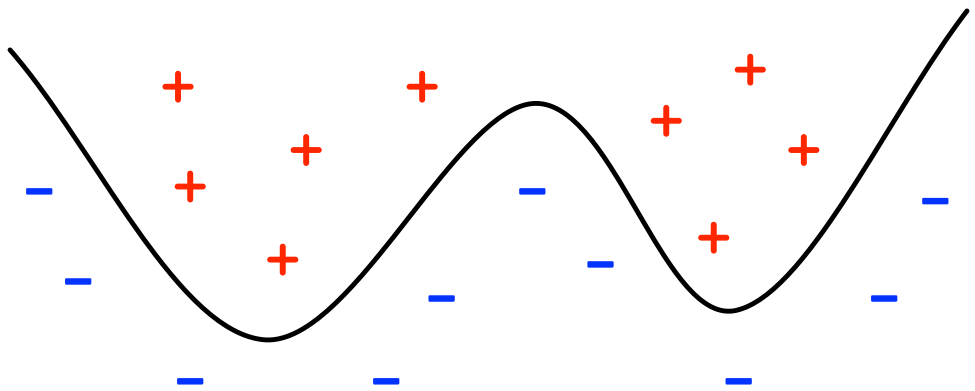

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- Same trick works: $\Phi(x) \cdot \Phi(z) = (1 + x \cdot z)^p$.
- **Kernel function:** $k(x, z) = (1 + x \cdot z)^p$.

String kernels

Sequence data:

- text documents
- speech signals
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What kind of embedding $\Phi(x)$ is suitable for variable-length sequences x?

We will use an infinite-dimensional embedding!

String kernels, cont'd

For each substring s, define *feature*:

$$\Phi_s(x) = \# \text{ of times substring } s \text{ appears in } x$$

and let $\Phi(x)$ be a vector with one coordinate for each string:

$$\Phi(x) = (\Phi_s(x) : \text{all strings } s).$$

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Example: the embedding of "aardvark" includes features

$$\Phi_{\mathrm{ar}}(\mathrm{aardvark}) = 2, \;\; \Phi_{\mathrm{th}}(\mathrm{aardvark}) = 0, \ldots$$

Linear classifier based on such features is very expressive.

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To compute $k(x, z) = \Phi(x) \cdot \Phi(z)$:

for each substring s of x: count how often s appears in z

String kernels, cont'd

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Using dynamic programming, this takes time $O(|x| \cdot |z|)$.

The kernel function

We never explicitly construct the embedding $\Phi(x)$.

- What we actually use: **kernel function** $k(x, z) = \Phi(x) \cdot \Phi(z)$.
- Think of $k(x, z)$ as a **measure of similarity** between x and z.
- Rewrite learning algorithm and final classifier in terms of k.

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Kernel Perceptron:

- $\alpha = 0$ and $b = 0$
- while some i has $y^{(i)} \left(\sum_j \alpha_j y^{(j)} k(x^{(j)}, x^{(i)}) + b \right) \leq 0$:
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To classify a new point x: $\text{sign} \left(\sum_j \alpha_j y^{(j)} k(x^{(j)}, x) + b \right)$.

Kernel SVM, revisited

1. **Kernel function.** Define a similarity function $k(x, z)$.
2. **Learning.** Solve the dual problem:

$$\boxed{\begin{aligned} \max_{\alpha \in \mathbb{R}^n} \quad & \sum_{i=1}^{n} \alpha_i - \sum_{i,j=1}^{n} \alpha_i \alpha_j y^{(i)} y^{(j)} k(x^{(i)}, x^{(j)}) \\ \text{s.t.:} \quad & \sum_{i=1}^{n} \alpha_i y^{(i)} = 0 \\ & 0 \leq \alpha_i \leq C \end{aligned}}$$

   This yields α. Offset b also follows.
3. **Classification.** Given a new point x, classify as

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Choosing the kernel function

The final classifier is a **similarity-weighted vote**,

$$F(x) = \alpha_1 y^{(1)} k(x^{(1)}, x) + \cdots + \alpha_n y^{(n)} k(x^{(n)}, x)$$

(plus an offset term, b).

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- Not quite: need $k(x, z) = \Phi(x) \cdot \Phi(z)$ for *some* embedding Φ.
- **Mercer's condition**: same as requiring that for any finite set of points $x^{(1)}, \ldots, x^{(m)}$, the $m \times m$ similarity matrix K given by
$$K_{ij} = k(x^{(i)}, x^{(j)})$$
is positive semidefinite.

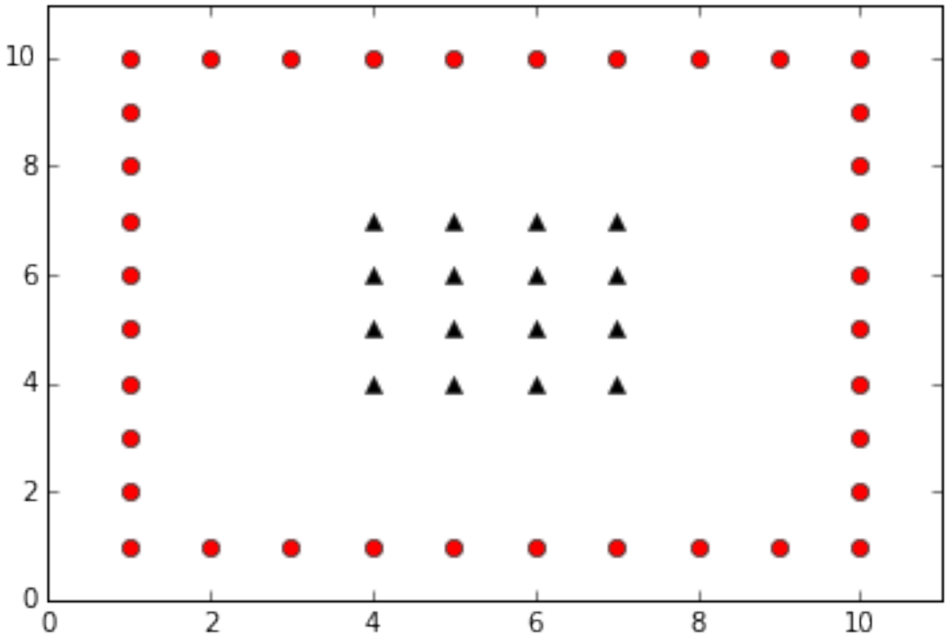
The RBF kernel

A popular similarity function: the **Gaussian kernel** or **RBF kernel**

$$k(x, z) = e^{-\|x-z\|^2/s^2},$$

where s is an adjustable scale parameter.

RBF kernel: examples



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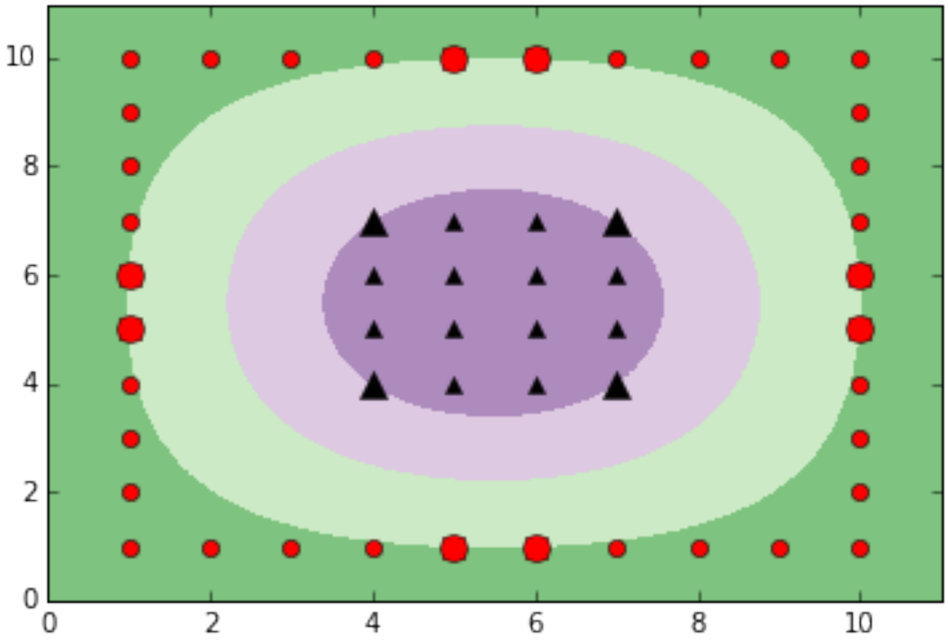

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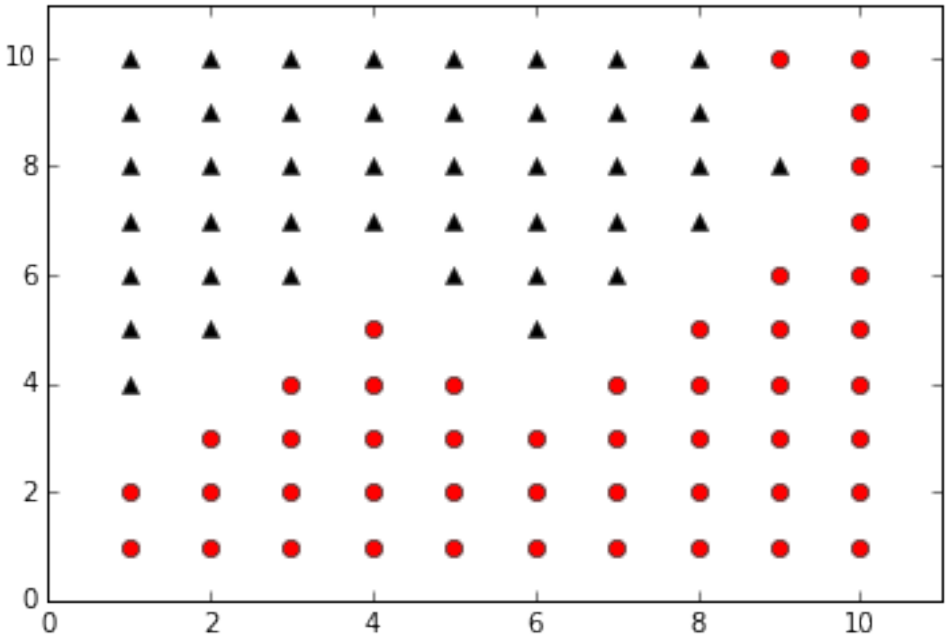
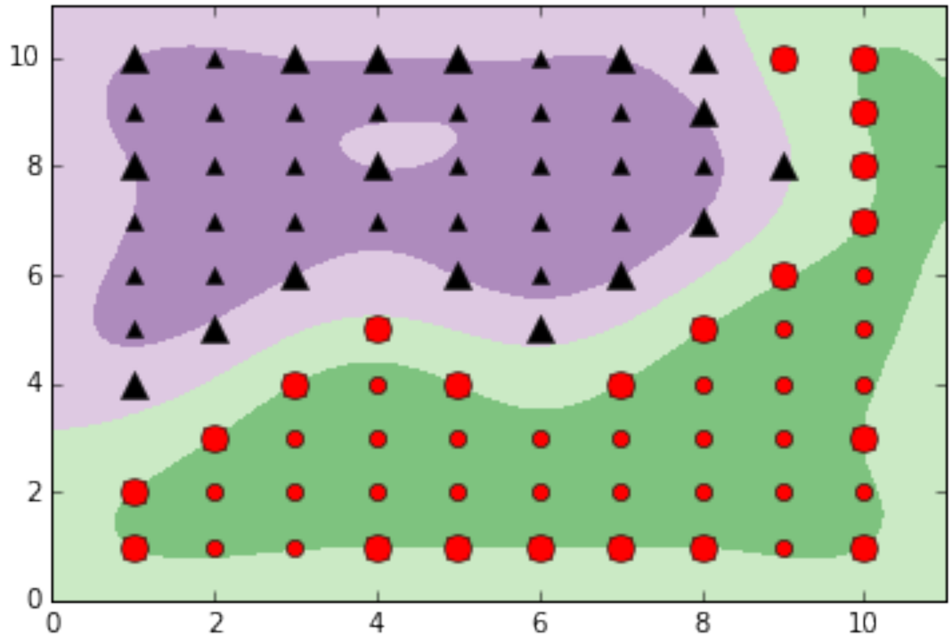


RBF kernel: examples



The scale parameter

Recall prediction function:
$F(x) = \alpha_1 y^{(1)} k(x^{(1)}, x) + \cdots + \alpha_n y^{(n)} k(x^{(n)}, x)$.

For the RBF kernel, $k(x, z) = e^{-\|x-z\|^2/s^2}$,

1. How does this function behave as $s \uparrow \infty$?
2. How does this function behave as $s \downarrow 0$?
3. As we get more data, should we increase or decrease s?

Kernels: postscript

1. Customized kernels
   - For different domains (NLP, biology, speech, ...)
   - Over different structures (sequences, sets, graphs, ...)

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   Given a set of plausible kernels, find a linear combination of them that works well.
3. Speeding up learning and prediction

   The $n \times n$ kernel matrix $k(x^{(i)}, x^{(j)})$ is a bottleneck for large n. One idea:
   - Go back to the primal space!
   - Replace the embedding Φ by a low-dimensional mapping $\widetilde{\Phi}$ such that

   $$\widetilde{\Phi}(x) \cdot \widetilde{\Phi}(z) \;\approx\; \Phi(x) \cdot \Phi(z).$$

   This can be done, for instance, by writing Φ in the Fourier basis and then randomly sampling features.