Kernels

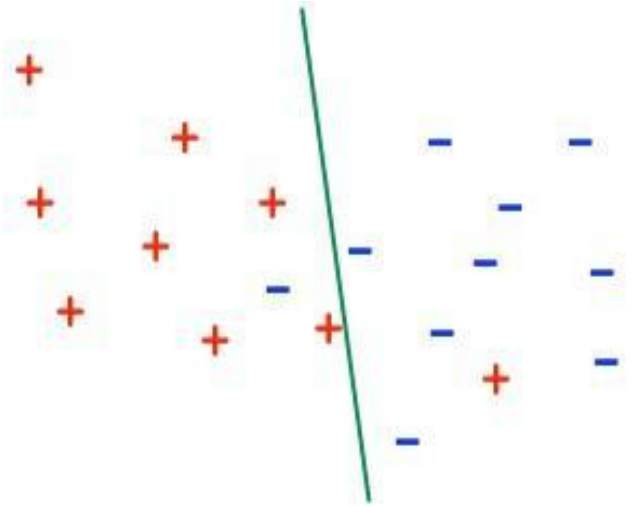
MGTF 495

Class Outline

- Parametric Methods
  - Discriminative Methods
    - Logistic Regression
      - Gradient Descent
      - Newton-Raphson
      - Hands-On
    - SVM
      - Hands-On
    - Perceptron
      - Hands-On
  - Kernels
  - Richer Output Spaces

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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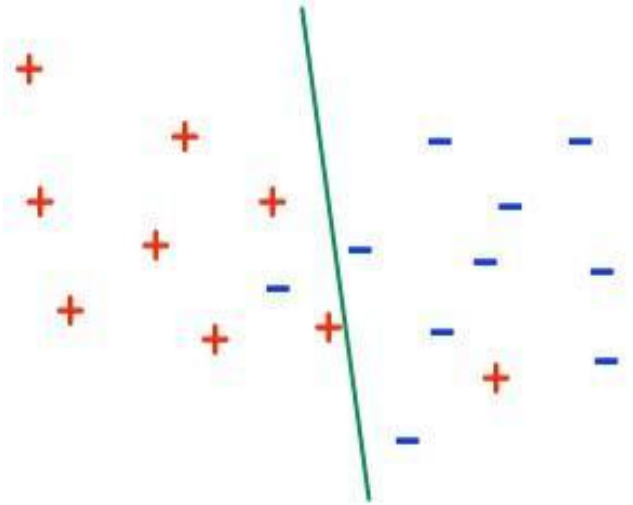

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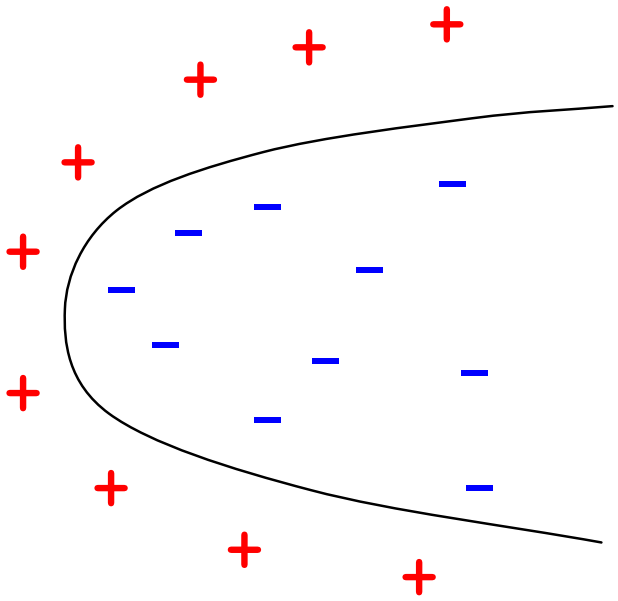
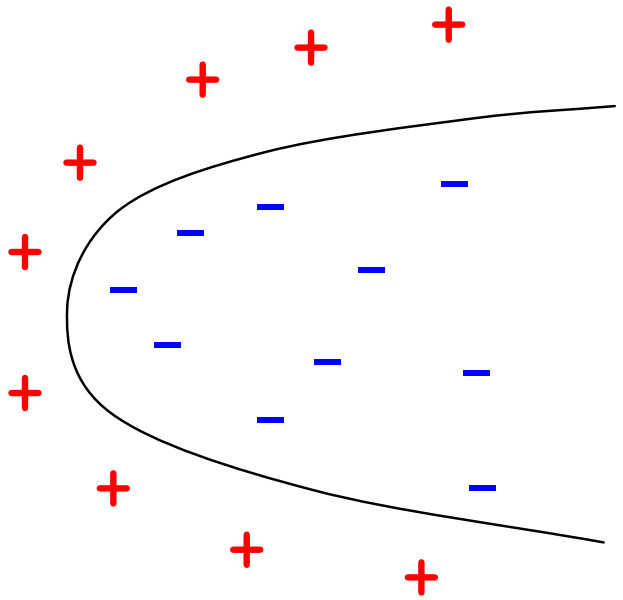
Systematic deviation



What to do with this?

Systematic inseparability

In this case, the actual boundary looks quadratic.



Quick fix: in addition to the regular features $x = (x_1, x_2, \ldots, x_p)$, add in extra features:

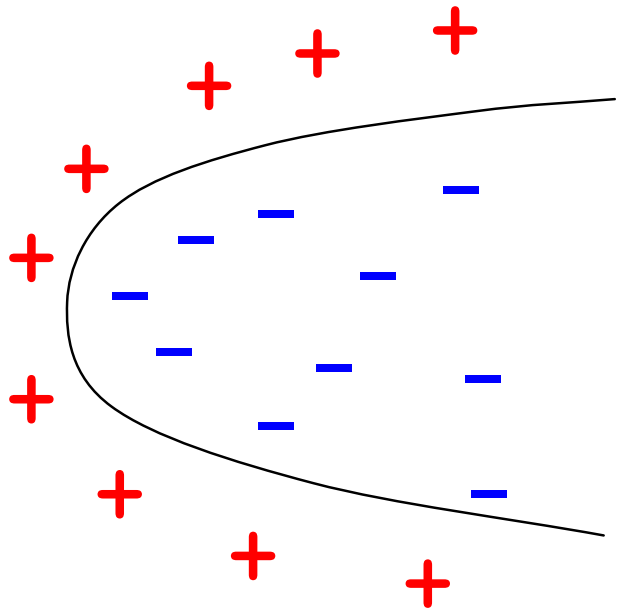
$$x_1^2,\ x_2^2,\ \ldots,\ x_p^2$$

$$x_1x_2,\ x_1x_3,\ \ldots,\ x_{p-1}x_p$$

The new, enhanced data vectors are of the form:

$$\Phi(x) = (1, \sqrt{2}x_1, \ldots, \sqrt{2}x_p, x_1^2, \ldots, x_p^2, \sqrt{2}x_1x_2, \ldots, \sqrt{2}x_{p-1}x_p).$$

Adding new features



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

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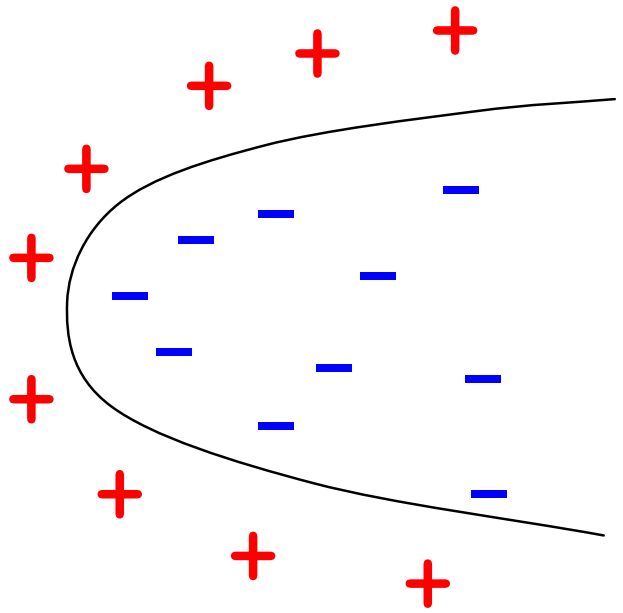

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- This is quadratic in $x = (1, x_1, x_2)$
- But it is linear in $\Phi(x) = (1, x_1, x_2, x_1^2, x_2^2, x_1 x_2)$

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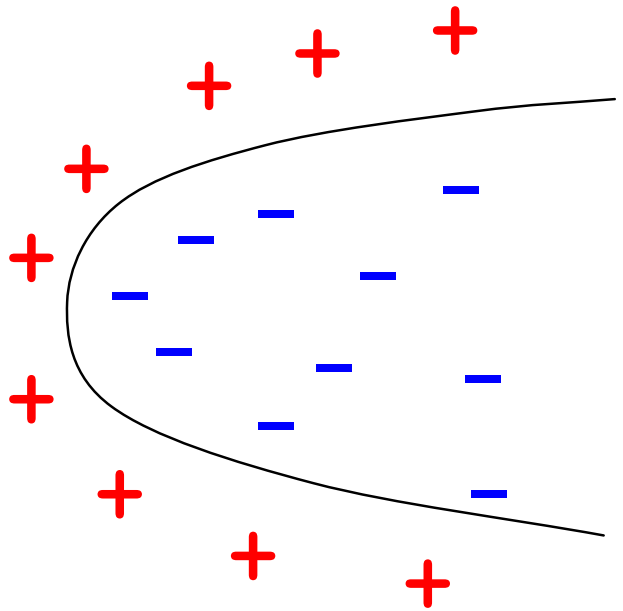

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By embedding the data in a higher-dimensional feature space, we can keep using a linear classifier!

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Use the formula – $(1 + 2p + \binom{p}{2})$

Perceptron revisited

Learning in the higher-dimensional feature space:

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

Final w is a weighted linear sum of various $\Phi(x)$.

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The **kernel trick** (Aizenman, Braverman, Rozonoer (1964)):

- The only time we ever access $\Phi(x)$ is to compute $w \cdot \Phi(x)$. If, say,

$$w = a_1\Phi(x^{(1)}) + a_2\Phi(x^{(2)}) + a_3\Phi(x^{(3)}),$$

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  then $w \cdot \Phi(x)$ is a weighted sum of dot products $\Phi(x) \cdot \Phi(x^{(i)})$.

- Can we compute such dot products without writing out the $\Phi(x)$'s?

Computing dot products

In 2-d:

$$
\begin{aligned}
&\Phi(x) \cdot \Phi(z) \\
&= (1, \sqrt{2}x_1, \sqrt{2}x_2, x_1^2, x_2^2, \sqrt{2}x_1x_2) \cdot (1, \sqrt{2}z_1, \sqrt{2}z_2, z_1^2, z_2^2, \sqrt{2}z_1z_2) \\
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For MNIST: computing dot products in the 307720-dimensional quadratic feature space takes time proportional to just 784, the original dimension!

The kernel trick

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1. The only time we ever look at data – during training or subsequent classification – is to compute dot products $w \cdot \Phi(x)$.

2. And w itself is a linear combination of $\Phi(x)$'s. If, say,

$$w = \alpha_1 \Phi(x^{(1)}) + \alpha_{22} \Phi(x^{(22)}) + \alpha_{37} \Phi(x^{(37)}),$$

we can store w as $[(1, \alpha_1), (22, \alpha_{22}), (37, \alpha_{37})]$.

3. Dot products $\Phi(x) \cdot \Phi(x')$ can be computed efficiently, without ever writing out the high-dimensional embedding $\Phi(\cdot)$.

Kernel Perceptron

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

Primal form:

- $w = 0$
- while there is some i with $y^{(i)}(w \cdot \Phi(x^{(i)})) < 0$:
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- $\alpha = 0$
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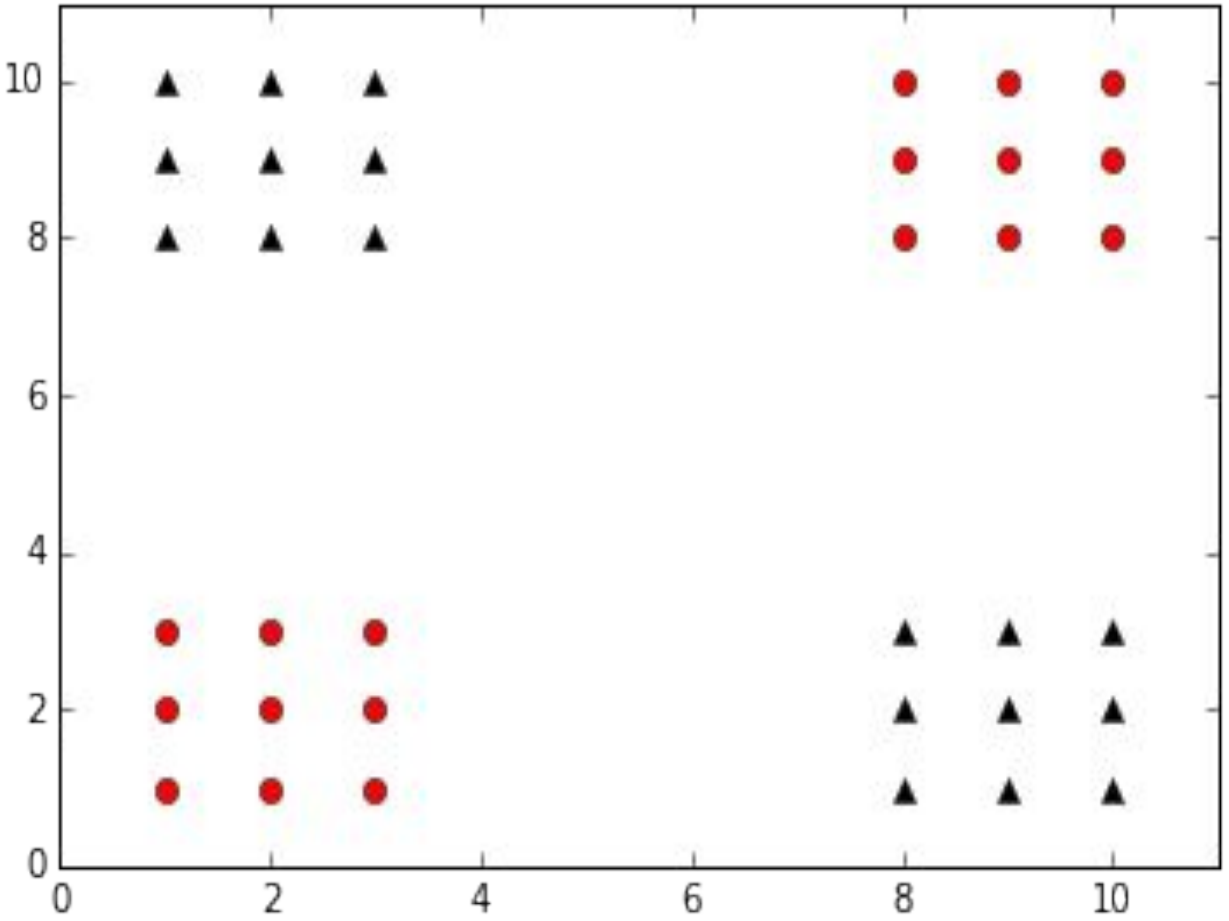
To classify a new point x: Return sign $\left(\sum_j \alpha_j y^{(j)} \Phi(x^{(j)}) \cdot \Phi(x) \right)$.

Kernel Perceptron: Examples



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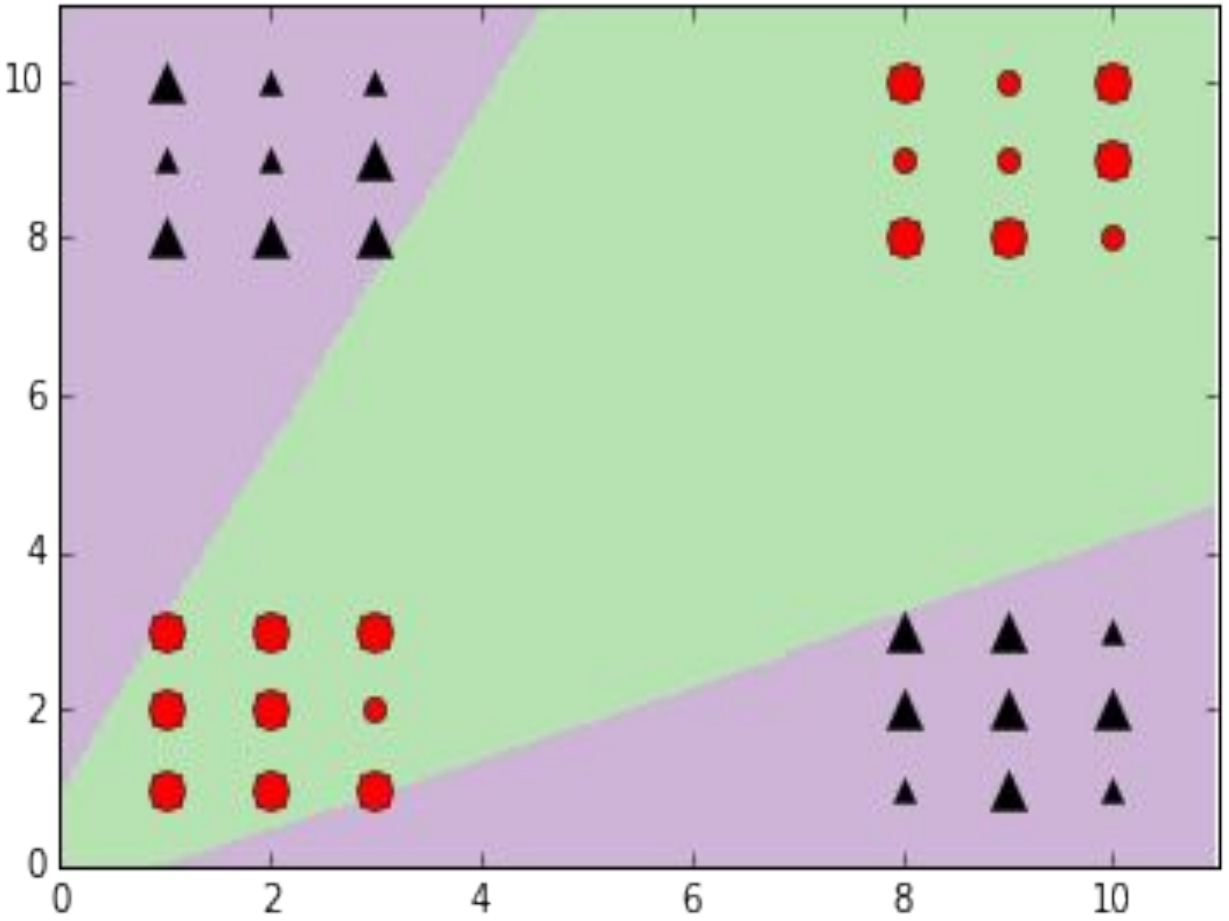

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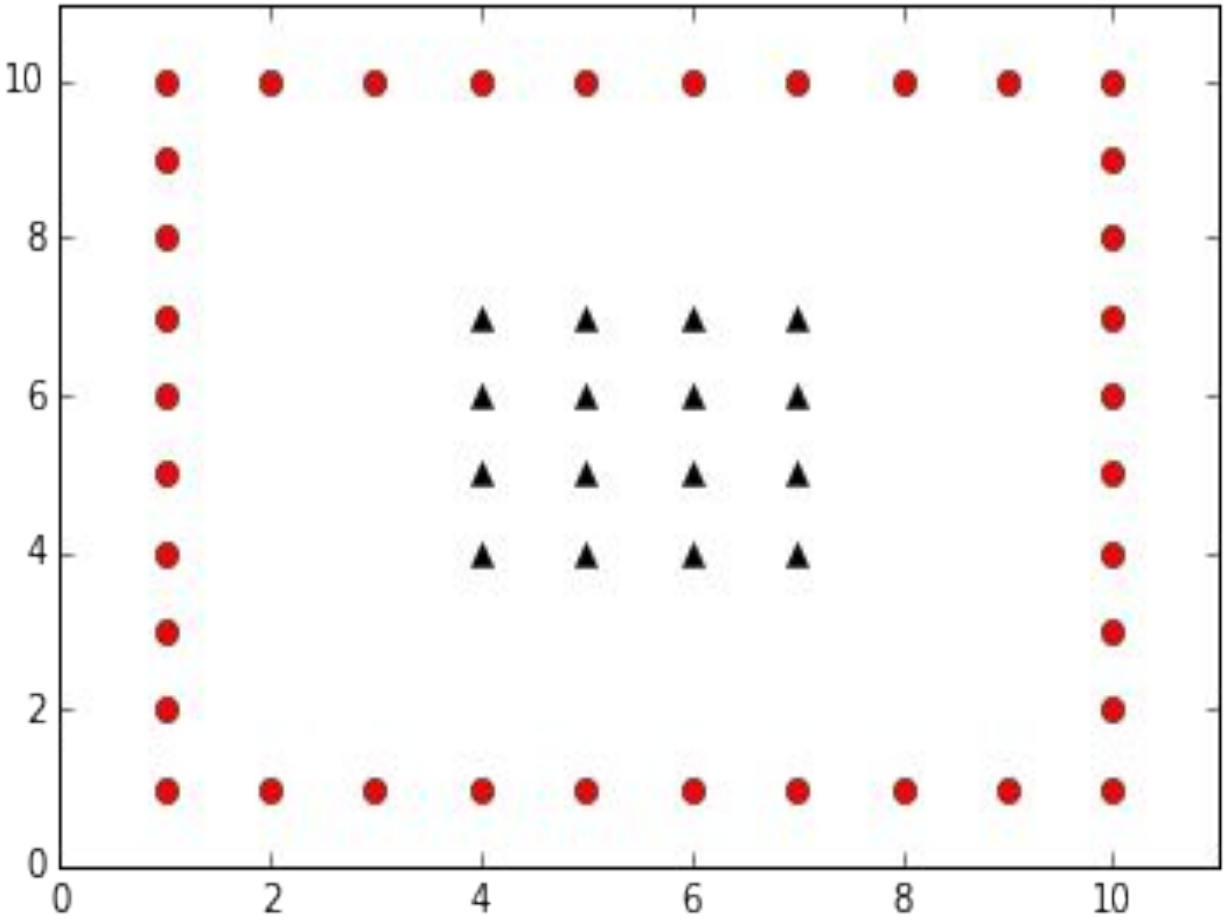

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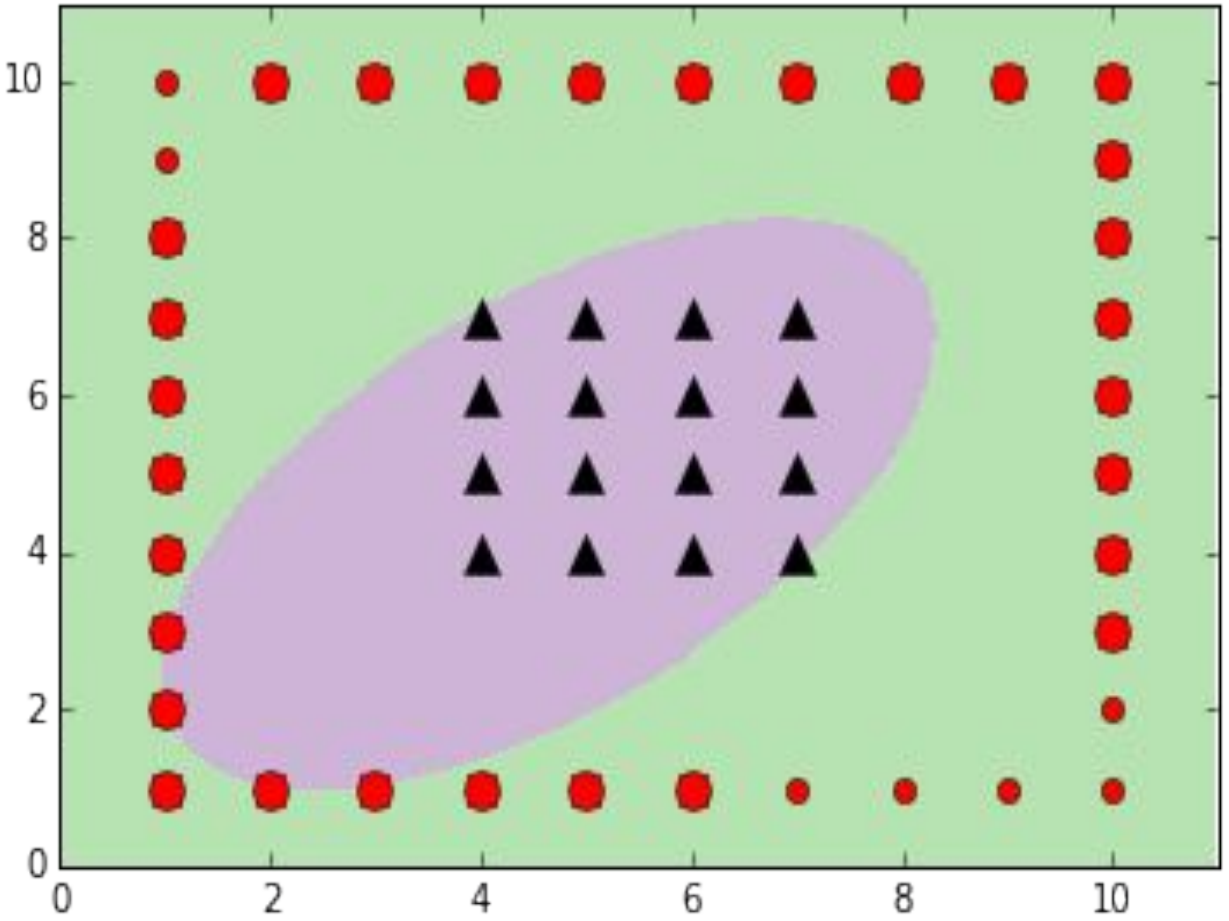

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Recall the kernel perceptron algorithm:

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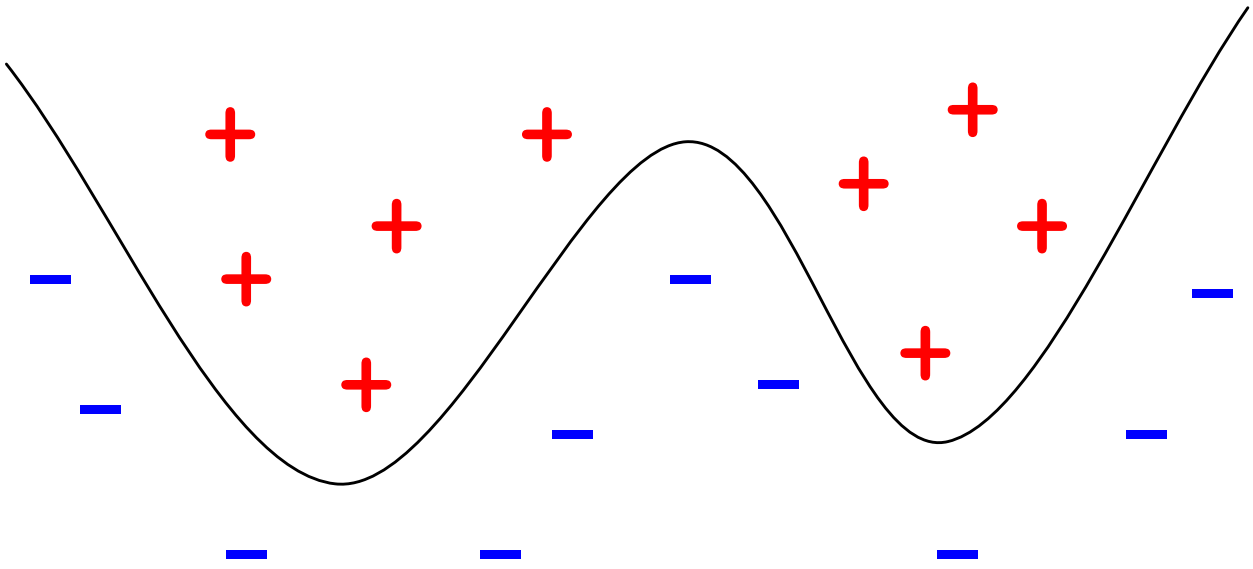
Solution: 1 term after first update, 2 terms after second update and so on till k updates. Therefore, in order of (1 + 2 + … + k) = **at least $\binom{k}{2}$** updates.

Polynomial decision boundaries

To get a decision surface which is an arbitrary polynomial of order *d* :



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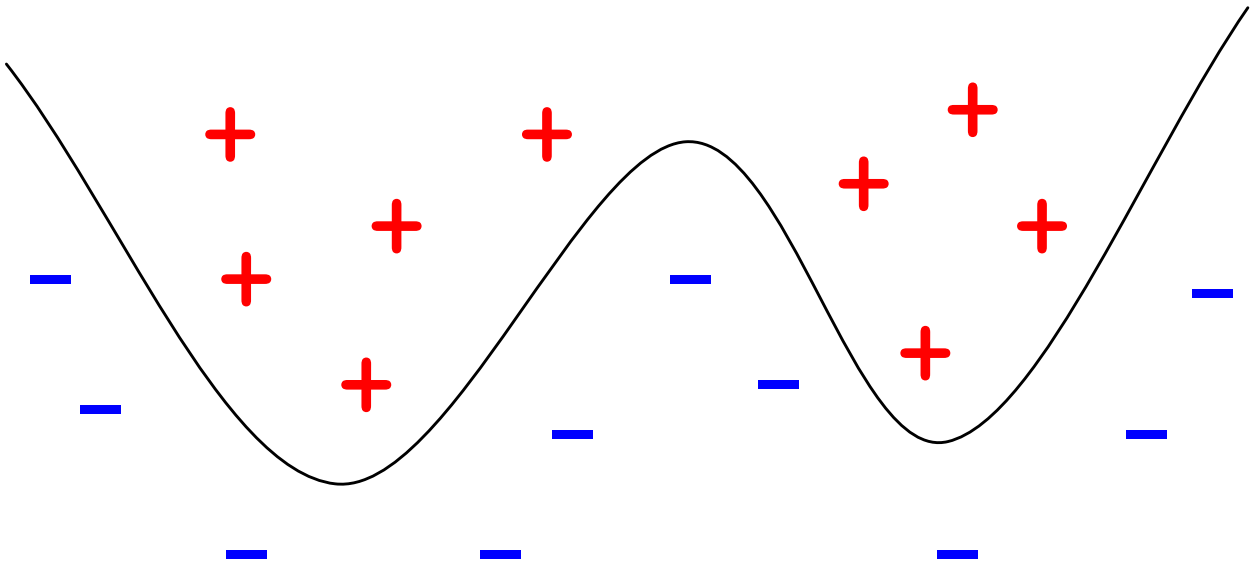

- Let $\Phi(x)$ consist of all terms of order $\leq d$, such as $x_1 x_2^2 x_3^{d-3}$. (How many such terms are there, roughly?)

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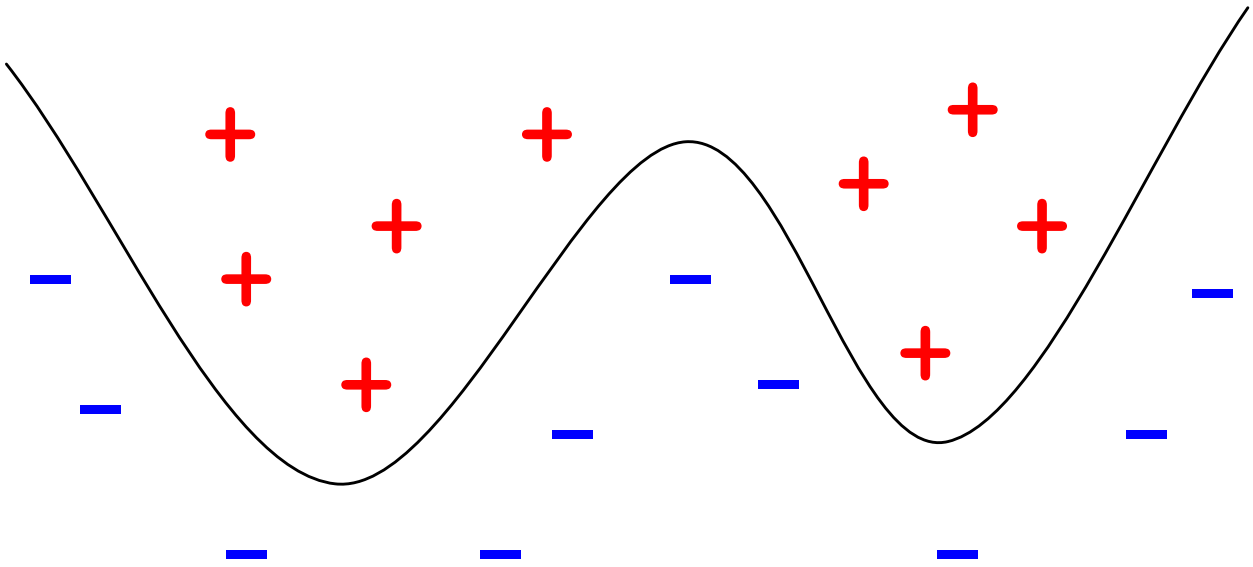

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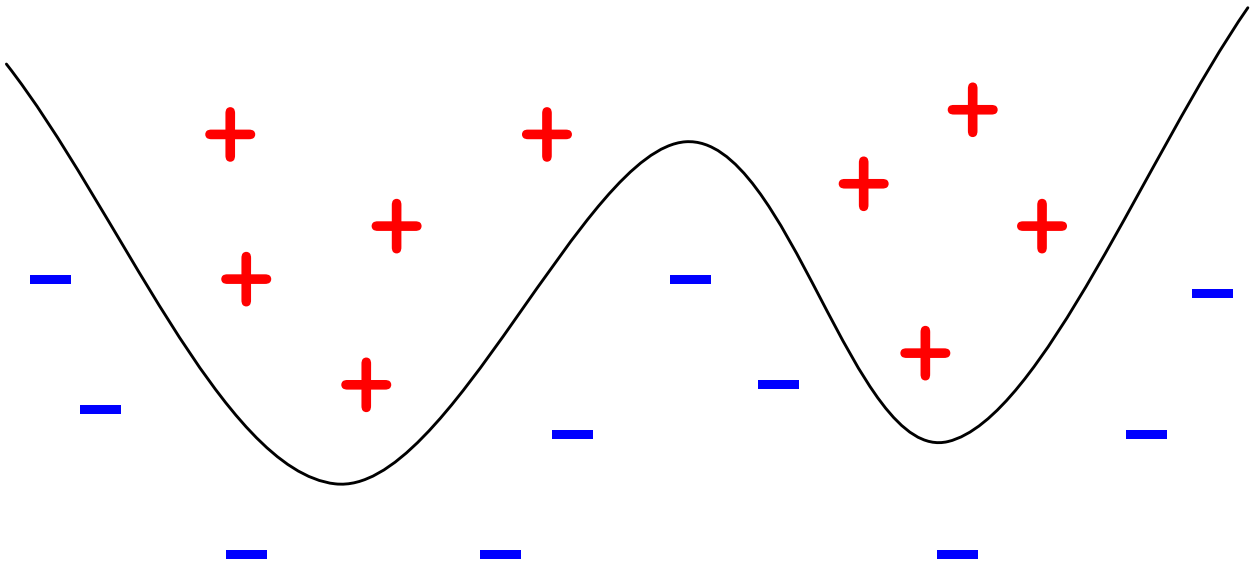

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The **kernel function**, a measure of similarity:

$$k(x, z) = \Phi(x) \cdot \Phi(z).$$

The kernel function

Now shift attention: away from the embedding $\Phi(x)$, which we never explicitly construct, towards the thing we actually use:

- the **similarity measure** $k(x, z)$

Rewrite learning algorithm and final classifier in terms of k .

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The classifier $w \cdot \Phi(x)$, for

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

becomes a **similarity-weighted vote**,

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

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Can we choose k to be any similarity function suitable for the application domain?

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2. Since A is PSD, we can re-write it as UU^T

$$x^T Az = x^T UU^T z = (U^T x)^T (zU)^T$$
$$\Rightarrow \phi(x) = U^T x$$

Kernels: postscript

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   - Over many different structures (sequences, sets, trees, graphs, ...)

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   - Over many different structures (sequences, sets, trees, graphs, ...)
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Kernels: postscript

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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

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