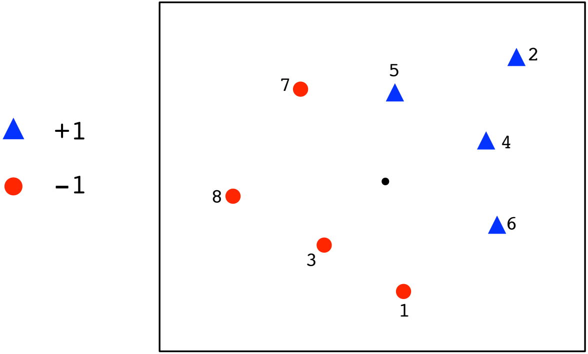
Kernels

DSE 220

Recall: Perceptron

Input space $\mathcal{X} = \mathbb{R}^p$, label space $\mathcal{Y} = \{-1, 1\}$

- $w = 0$
- while some (x, y) is misclassified:
  - $w = w + yx$



Separator: $w = 0$

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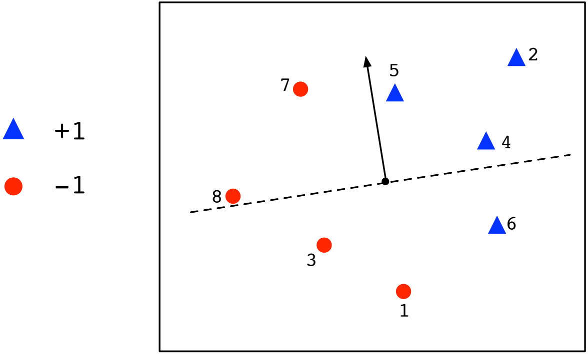

Separator: $w = -x^{(1)}$

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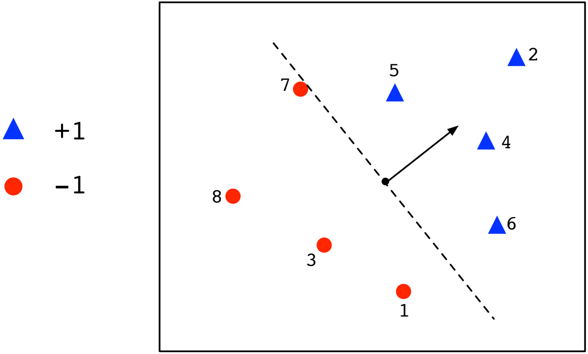
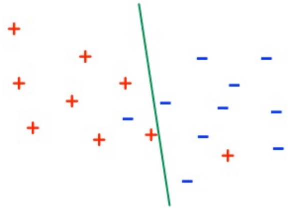


Separator: $w = -x^{(1)} + x^{(6)}$

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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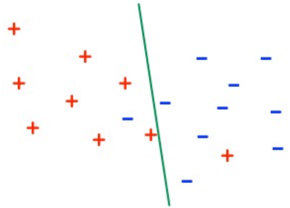

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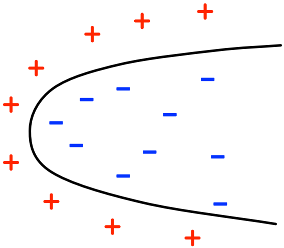
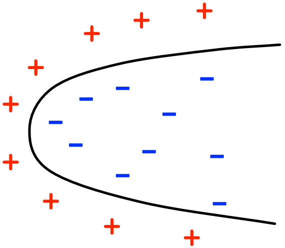
Systematic deviation



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:

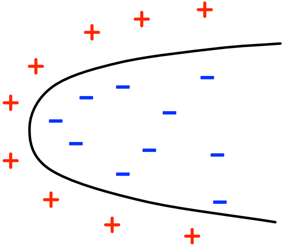
$$x_1^2,\ x_2^2,\ \ldots,\ x_p^2$$

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

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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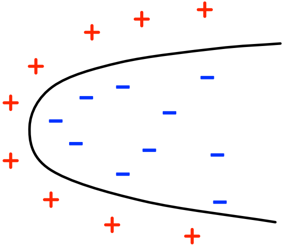

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- This is quadratic in $x = (1, x_1, x_2)$
- But it is linear in $\Phi(x) = (1, x_1, x_2, x_1^2, x_2^2, x_1 x_2)$

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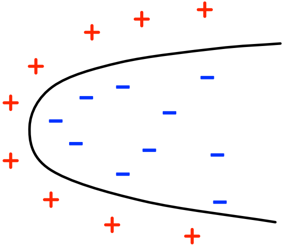

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By embedding the data in a higher-dimensional feature space, we can keep using a linear classifier!

Quick quiz

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2. What if $x = (1, x_1, \ldots, x_p)$?

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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For MNIST, from 784 to 307720!

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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,

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

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

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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:

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\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) \\
&= 1 + 2x_1z_1 + 2x_2z_2 + x_1^2z_1^2 + x_2^2z_2^2 + 2x_1x_2z_1z_2 \\
&= (1 + x_1z_1 + x_2z_2)^2 \quad = \quad (1 + x \cdot z)^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!

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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 $[(1, \alpha_1), (22, \alpha_{22}), (37, \alpha_{37})]$.

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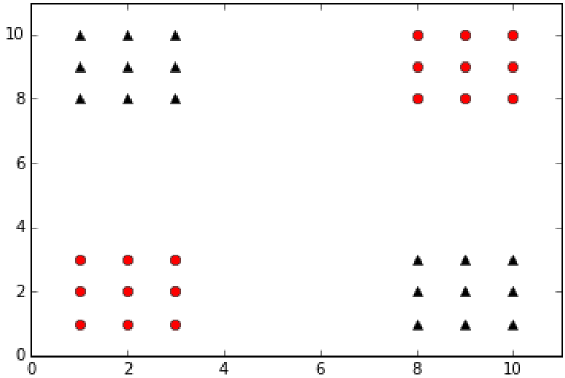
To classify a new point x: Return sign $\left(\sum_j \alpha_j y^{(j)} \Phi(x^{(j)}) \cdot \Phi(x)\right)$.

Kernel Perceptron: Examples



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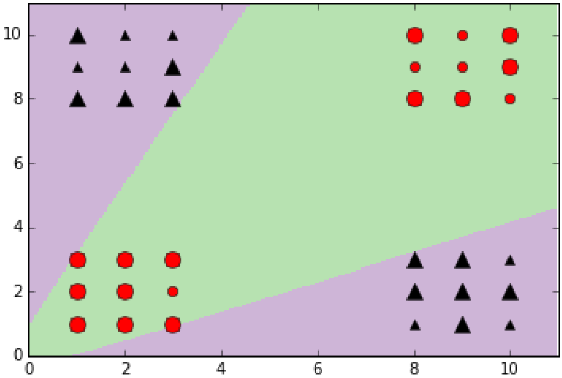

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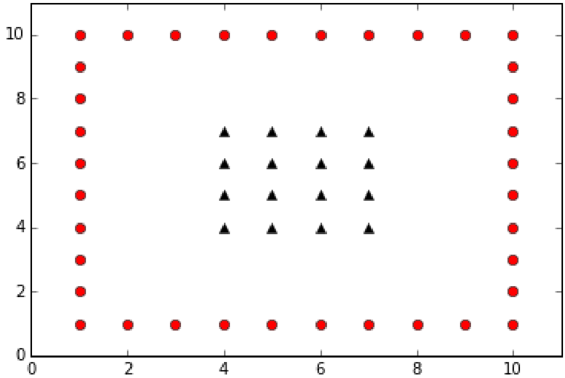

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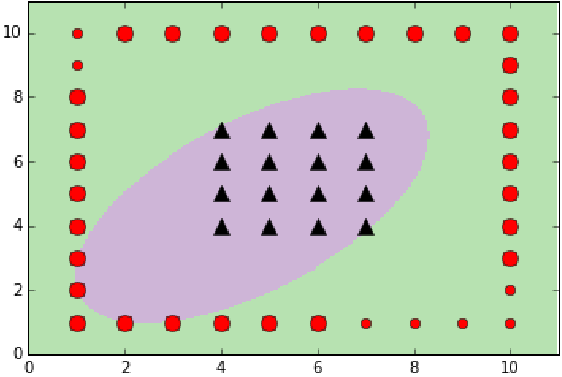

Quick quiz

Recall the kernel perceptron algorithm:

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Suppose we run it on a data set and find that it converges after k updates.

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Suppose we run it on a data set and find that it converges after k updates.

1. How many dot product computations are needed to classify a new point?
2. What is the total number of dot product computations during learning?

Does this work with SVMs?

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

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

$$\xi \geq 0$$

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

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

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

At optimality, $w = \sum_i \alpha_i y^{(i)} x^{(i)}$, with

$$0 < \alpha_i < C \quad \Rightarrow \quad y^{(i)}(w \cdot x^{(i)} + b) = 1$$

$$\alpha_i = C \quad \Rightarrow \quad y^{(i)}(w \cdot x^{(i)} + b) = 1 - \xi_i$$

Kernel SVM

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   This yields $w = \sum_i \alpha_i y^{(i)} \Phi(x^{(i)})$.
   Offset b is obtained from the complementary slackness conditions.
3. **Classification.** Given a new point x, classify as

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

Kernel Perceptron vs. Kernel SVM: examples

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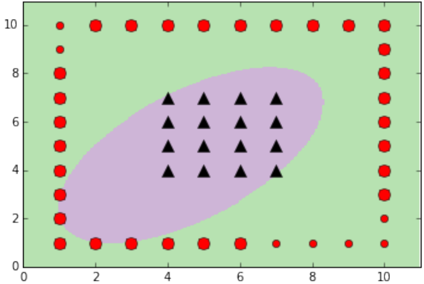

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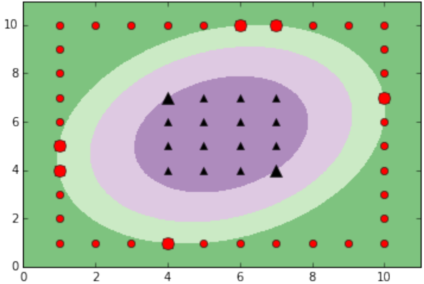

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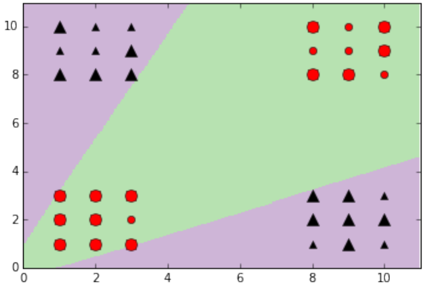

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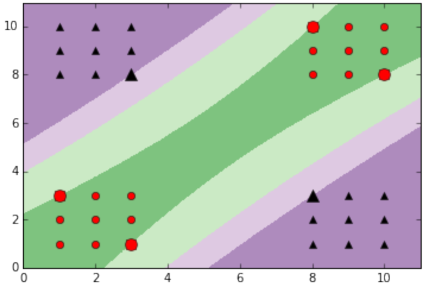
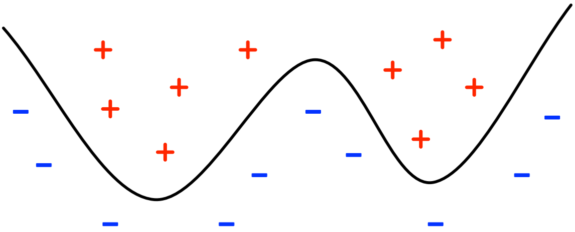


Polynomial decision boundaries

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



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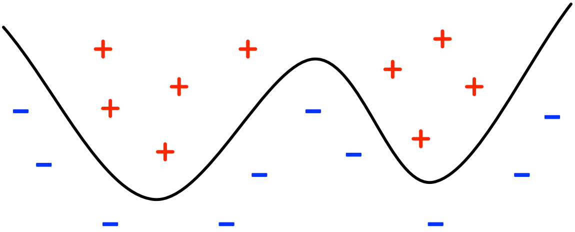

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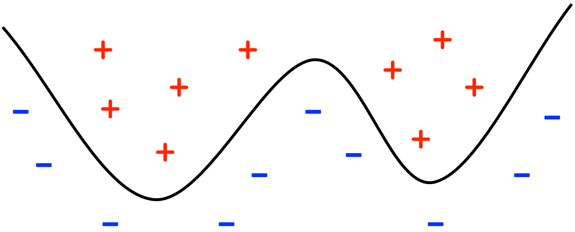

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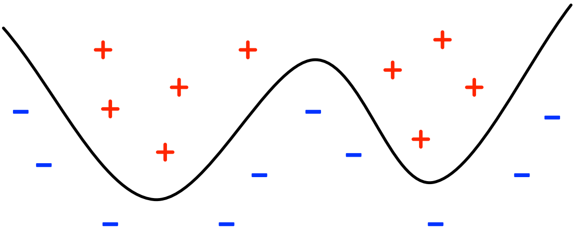

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The **kernel function**, a measure of similarity:

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

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Sequence data:

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We will use an infinite-dimensional embedding!

String kernels, cont'd

For each substring s, define *feature*:

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

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Example: the embedding of "aardvark" includes features

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

A linear classifier based on such features is potentially very powerful.

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 possible string:

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

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

Quick quiz

For each of the following kernel functions, find a corresponding embedding $x \to \Phi(x)$.

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2. $k(x, z) = x^T Az$, where A is a symmetric positive semidefinite matrix.

Mercer's condition

A function $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is a valid kernel function if it corresponds to some embedding: that is, if there exists Φ defined on $\mathcal{X}$ such that

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Mercer (1909): This is equivalent to requiring that for any finite subset $\{x^{(1)}, \ldots, x^{(m)}\} \subset \mathcal{X}$, the $m \times m$ similarity matrix

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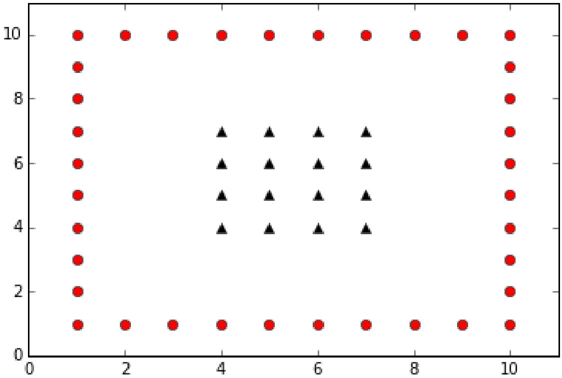
A popular similarity function: the **Gaussian kernel** or **RBF kernel**

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

where σ is an adjustable scale parameter.

RBF kernel: examples



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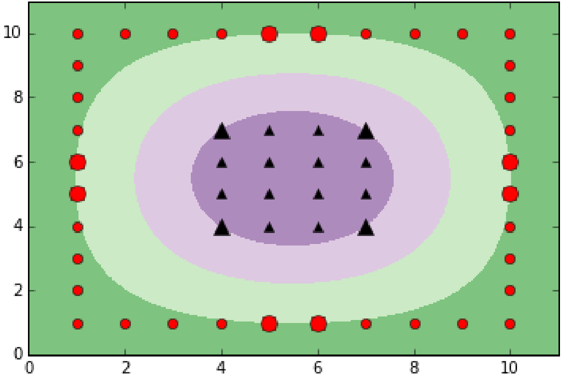

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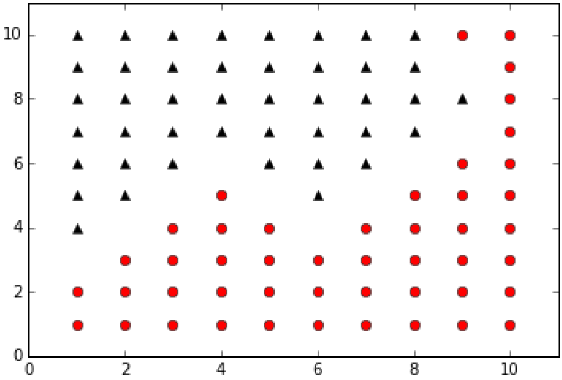

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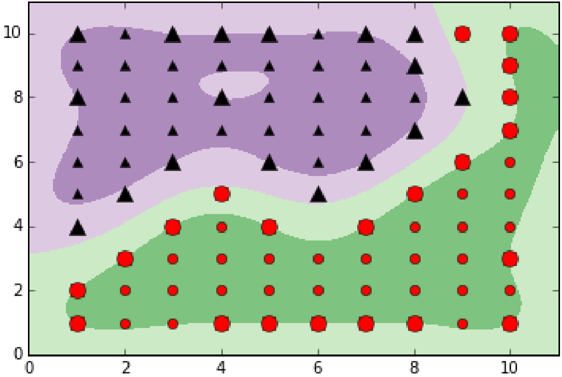

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Quick quiz

Recall that the RBF kernel is given by $k(x,z) = e^{-\|x-z\|^2/2\sigma^2}$.

1. How does this function behave as $\sigma \uparrow \infty$?
2. How does this function behave as $\sigma \downarrow 0$?
3. As the amount of data increases, would it make sense to increase σ or to decrease it?

Kernels: postscript

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

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2. Learning the kernel function
   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.