

INTRO to DATA SCIENCE:

NON-LINEAR CLASSIFICATION AND SUPPORT VECTOR MACHINES

AGENDA

I. SUPPORT VECTOR MACHINES

II. MAXIMUM MARGIN HYPERPLANES

III. SLACK VARIABLES

IV. NONLINEAR CLASSIFICATION

EXERCISE:

V. SVM IN SCIKIT-LEARN

I. SUPPORT VECTOR MACHINES

Q: What is a support vector machine?

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A: A binary linear classifier whose decision boundary is explicitly constructed to minimize generalization error.

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Quick review – who can define one of the underlined terms for us...?

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recall:

binary classifier – *solves two-class problem*

linear classifier – *creates linear decision boundary (in 2d)*

	<i>continuous</i>	<i>categorical</i>
<i>supervised</i>	???	???
<i>unsupervised</i>	???	???

	<i>continuous</i>	<i>categorical</i>
<i>supervised</i>	<i>regression</i>	<i>classification</i>
<i>unsupervised</i>	<i>dimension reduction</i>	<i>clustering</i>

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NOTE

These are two different ways of looking at the same problem.

Familiarity with both leads to deeper understanding!

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*The generalization error is equated with the geometric concept of **margin**, which is the region along the decision boundary that is free of data points.*

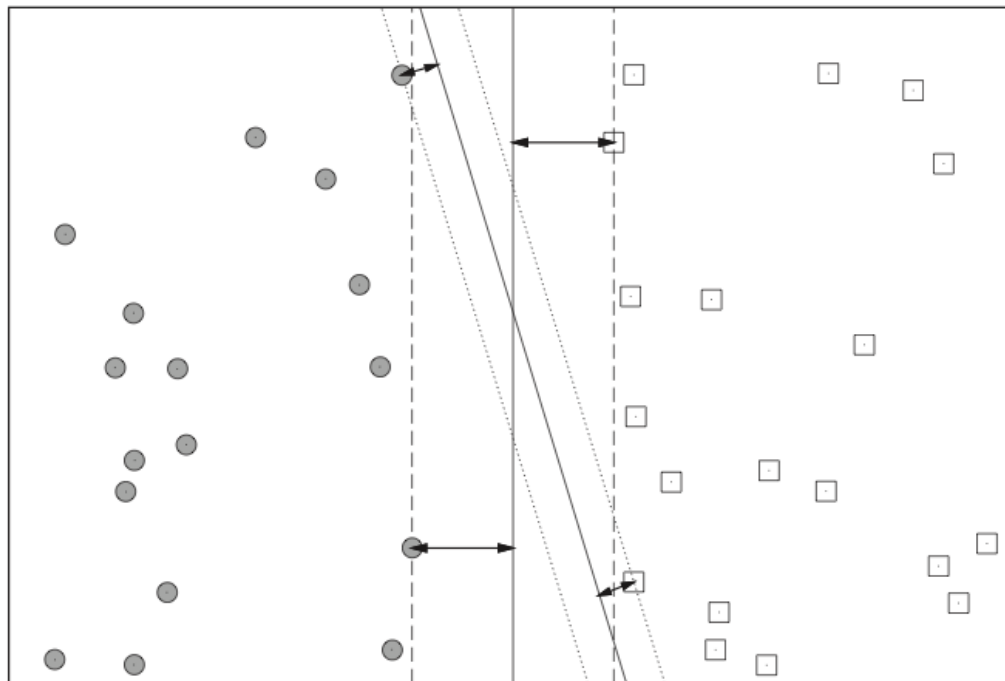


FIGURE 18-4. Two decision boundaries and their margins. Note that the vertical decision boundary has a wider margin than the other one. The arrows indicate the distance between the respective support vectors and the decision boundary.

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NOTE

A *hyperplane* is just a high-dimensional generalization of a line.

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*A: Using a clever maneuver called the **kernel trick**.*

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Nonlinear classification in K is then obtained by creating a linear decision boundary in K' .

In practice, this involves no computations in the higher dimensional space!

II. MAXIMUM MARGIN HYPERPLANES

Q: How is the decision boundary (MMH) derived?

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A: By the discriminant function,

$$f(\mathbf{x}) = \mathbf{w}^T \mathbf{x} + b.$$

such that w is the weight vector and b is the bias.

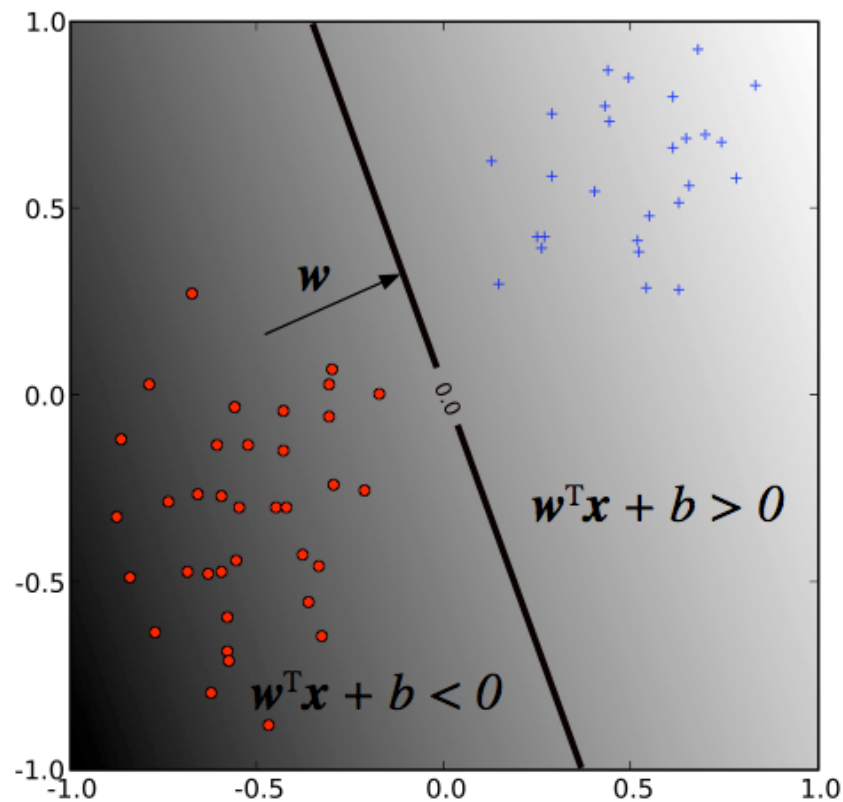
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*A: By the **discriminant function**,*

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such that w is the weight vector and b is the bias.

The sign of $f(x)$ determines the (binary) class label of a record x .



NOTE

The weight vector determines the *orientation* of the decision boundary.

The bias determines its *translation* from the origin.

As we said before, SVM solves for the decision boundary that minimizes generalization error, or equivalently, that has the maximum margin.

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NOTE

Intuitively, the wider the margin, the clearer the distinction between classes.

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A: Because using the MMH as the decision boundary minimizes the probability that a small perturbation in the position of a point produces a classification error.

Selecting the MMH is a straightforward exercise in analytic geometry (we won't go through the details here).

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Remember what convex means in this context...?

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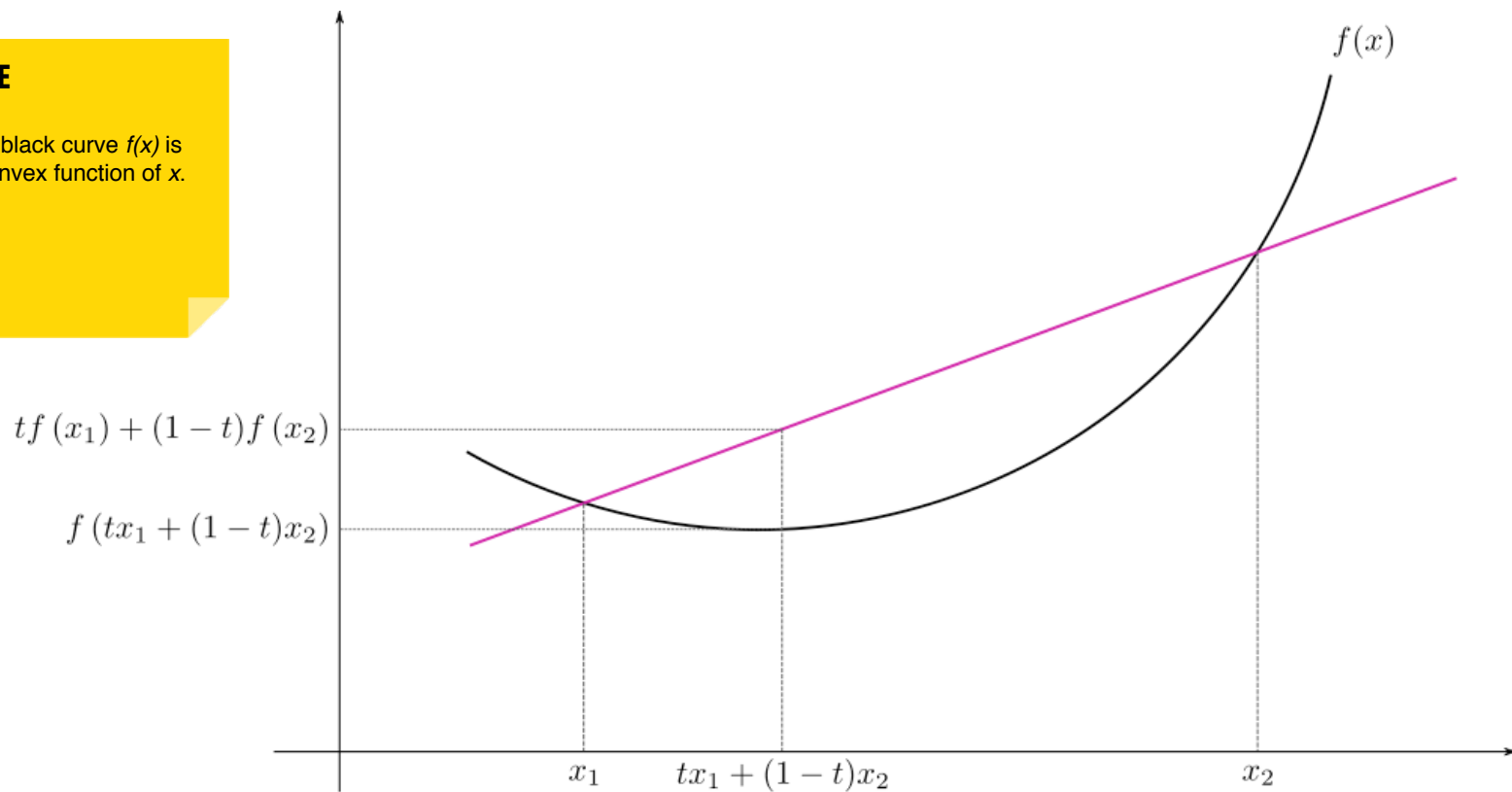
NOTE

The heuristic techniques we've discussed (eg greedy algorithms) are not necessary with convex optimization!

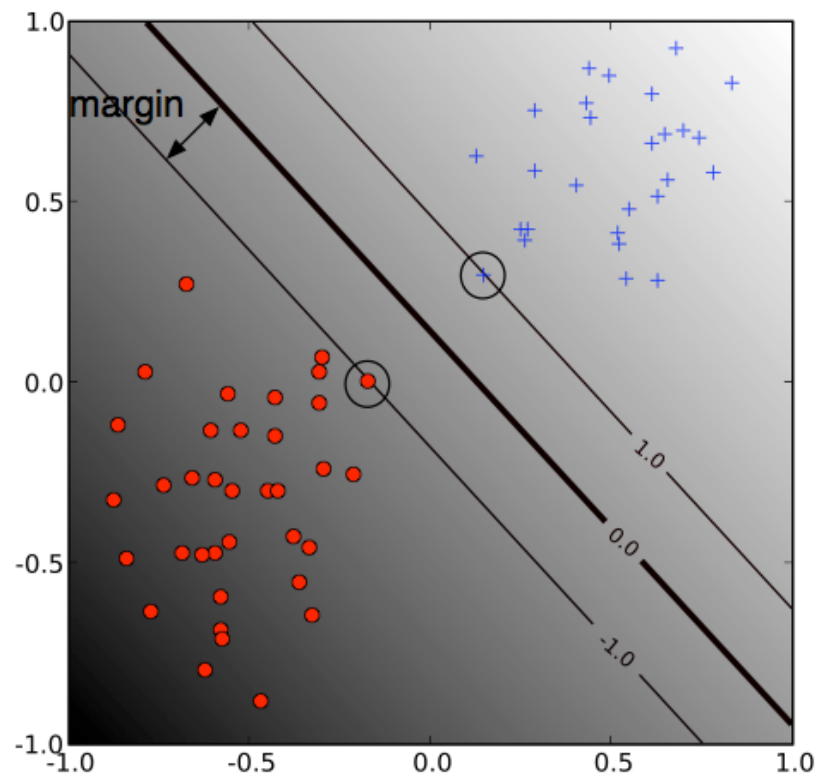
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NOTE

The black curve $f(x)$ is a convex function of x .



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The other points (far from the decision boundary) don't affect the construction of the MMH at all! However, the global (convex) nature of the algorithm means that for those support vectors, the optimal MMH will be found!

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The optimization problem that this SVM solves is:

$$\begin{array}{ll} \underset{\mathbf{w}, b}{\text{minimize}} & \frac{1}{2} \|\mathbf{w}\|^2 \\ \text{subject to:} & y_i(\mathbf{w}^\top \mathbf{x}_i + b) \geq 1 \quad i = 1, \dots, n. \end{array}$$

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NOTE

This type of optimization problem is called a *quadratic program*.

The result of this qp is the *hard margin classifier* we've been discussing.

III. SLACK VARIABLES

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Suppose that this was not true, or suppose that we wanted to use a larger margin at the expense of incurring some training error.

*This can be done using by introducing **slack variables**.*

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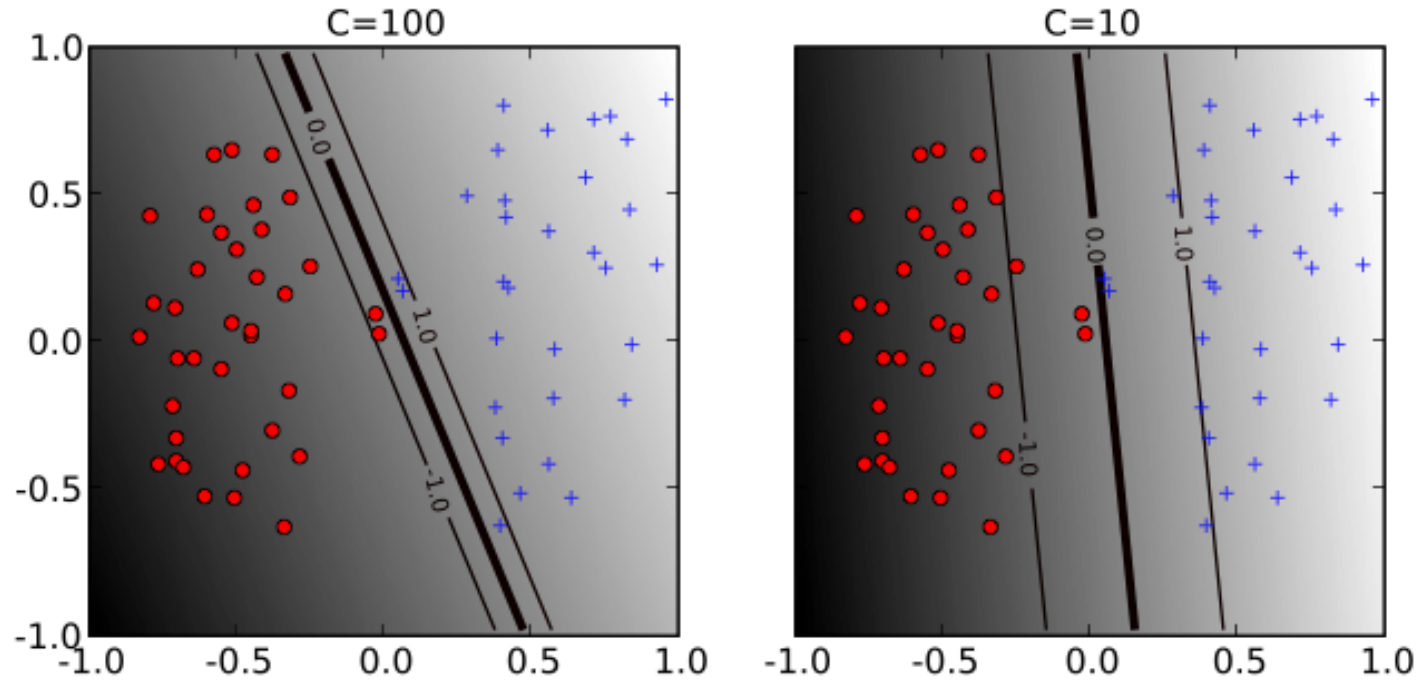
$$\begin{aligned} & \underset{\mathbf{w}, b}{\text{minimize}} && \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{i=1}^n \xi_i \\ & \text{subject to:} && y_i(\mathbf{w}^\top \mathbf{x}_i + b) \geq 1 - \xi_i, \quad \xi_i \geq 0. \end{aligned}$$

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This an example of bias-variance tradeoff.



The soft-margin optimization problem can be rewritten as:

$$\begin{aligned} & \underset{\alpha}{\text{maximize}} && \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n y_i y_j \alpha_i \alpha_j \mathbf{x}_i^T \mathbf{x}_j \\ & \text{subject to:} && \sum_{i=1}^n y_i \alpha_i = 0, \quad 0 \leq \alpha_i \leq C. \end{aligned}$$

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NOTE

This is called the *dual formulation* of the optimization problem.

(reached via Lagrange multipliers)

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Notice that this expression depends on the features \mathbf{x}_i only via the inner product

$$\langle \mathbf{x}_i, \mathbf{x}_j \rangle = \mathbf{x}_i^T \mathbf{x}_j$$

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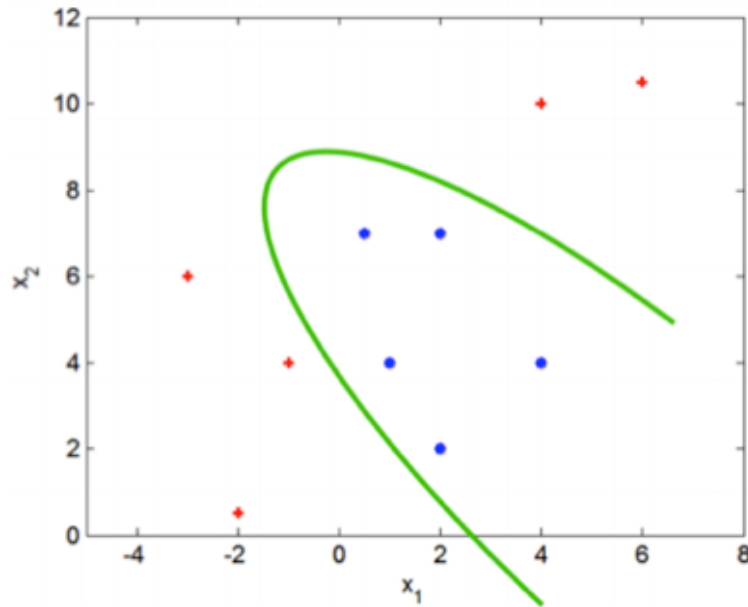
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In particular, we can easily change K to be some other space K' .

IV. NONLINEAR CLASSIFICATION

Suppose we need a more complex classifier than a linear decision boundary allows.



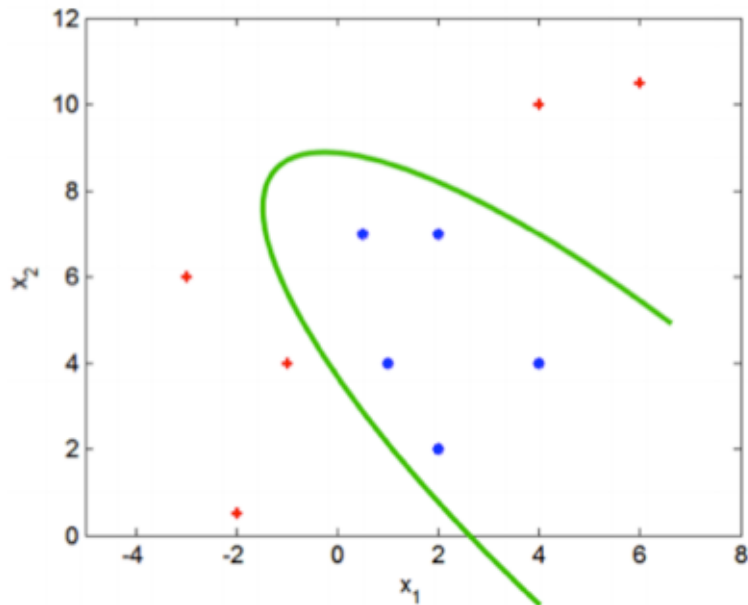
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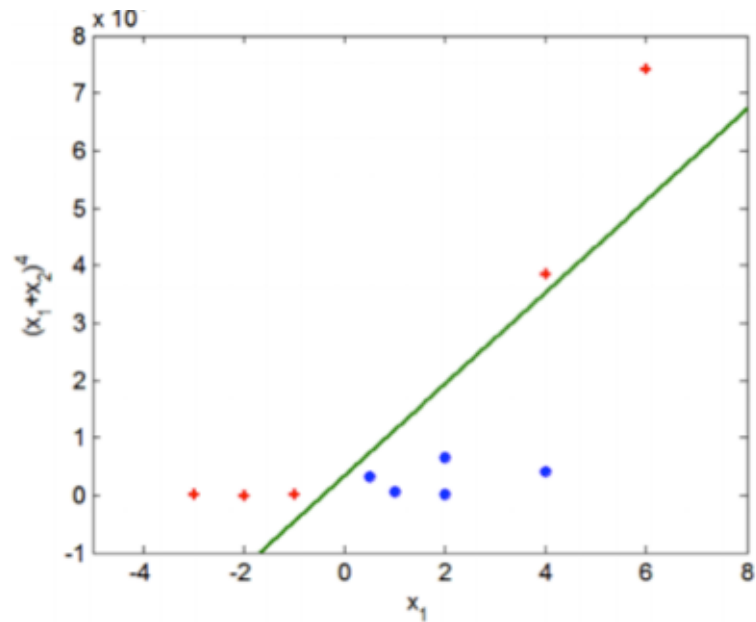
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This linear decision boundary will be mapped to a nonlinear decision boundary in the original feature space.



original feature space K



higher-dim feature space K'

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It will likely lead to more complexity (both modeling complexity and computational complexity) than we want.

Let's hang on to the logic of the previous example, namely:

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- remap the feature vectors x_i into a higher-dimensional space K'*
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But we want to save ourselves the trouble of doing a lot of additional high-dimensional calculations. How can we do this?

Recall that our optimization problem depends on the features only through the inner product $\mathbf{x}^T \mathbf{x}$:

$$\begin{aligned} & \underset{\alpha}{\text{maximize}} && \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n y_i y_j \alpha_i \alpha_j \mathbf{x}_i^T \mathbf{x}_j \\ & \text{subject to:} && \sum_{i=1}^n y_i \alpha_i = 0, \quad 0 \leq \alpha_i \leq C. \end{aligned}$$

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We can replace this inner product with a more general function that has the same type of output as the inner product.

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*We can replace this with a generalization of the inner product called a **kernel function** that maps two vectors in a higher-dimensional feature space K' into \mathbb{R} .*

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NOTE

These conditions are contained in a result called *Mercer's theorem*.

The upshot is that we can use a kernel function to implicitly train our model in a higher-dimensional feature space, without incurring additional computational complexity!

As long as the kernel function satisfies certain conditions, our conclusions above regarding the mmh continue to hold.

In other words, no algorithmic changes are necessary, and all the benefits of a linear SVM are maintained.

some popular kernels:

linear kernel

$$k(\mathbf{x}, \mathbf{x}') = \langle \mathbf{x}, \mathbf{x}' \rangle$$

polynomial kernel

$$k(\mathbf{x}, \mathbf{x}') = (\mathbf{x}^\top \mathbf{x}' + 1)^d$$

Gaussian kernel

$$k(\mathbf{x}, \mathbf{x}') = \exp(-\gamma \|\mathbf{x} - \mathbf{x}'\|^2)$$

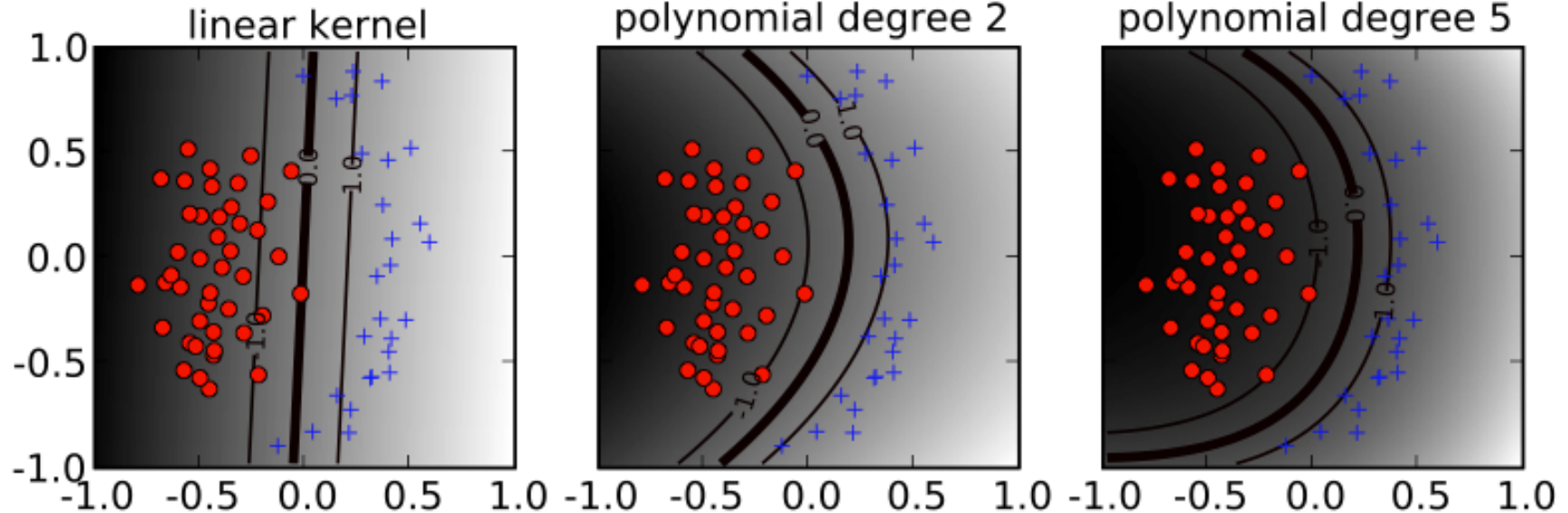
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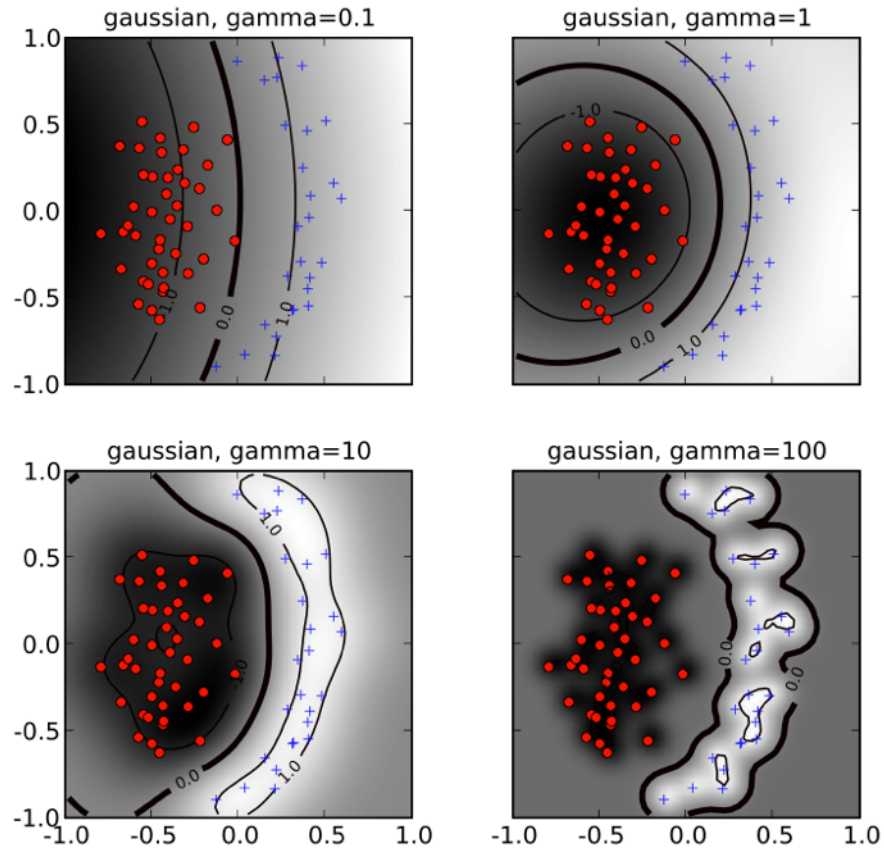
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The hyperparameters d, γ affect the flexibility of the decision bdy.





*SVMs (and **kernel methods** in general) are versatile, powerful, and popular techniques that can produce accurate results for a wide array of classification problems.*

The main disadvantage of SVMs is the lack of intuition they produce. These models are truly black boxes!

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