GENERAL ASSEMBLY

INTRO TO DATA SCIENCE

SUPPORT VECTOR MACHINES

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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recall:

binary classifier – solves two-class problem

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

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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.

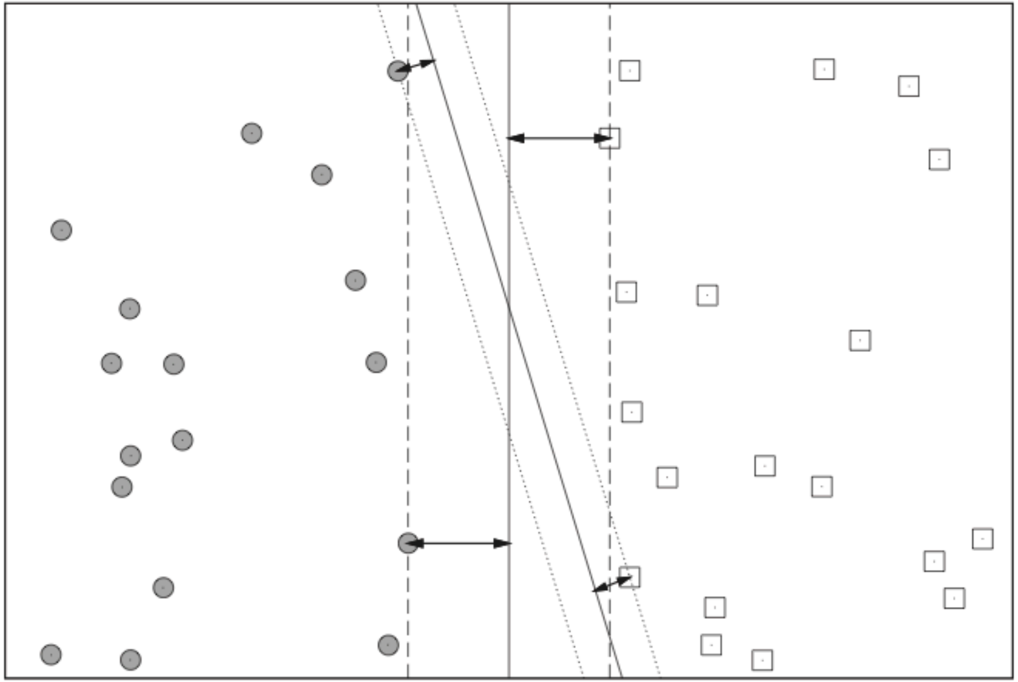

FIGURE 18-4. Two decision boundaries and their margins. Note that the vertical decision boundary has a wider margin than the other one. The arrows indicate the distance between the respective support vectors and the decision boundary.

source: Data Analysis with Open Source Tools, by Philipp K. Janert. O'Reilly Media, 2011.

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The goal of an SVM is to create the linear decision boundary with the largest margin. This is commonly called the **maximum margin hyperplane**.

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A: Using *geometric reasoning* (as opposed to the algebraic we've used to derive other classifiers).

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**,

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

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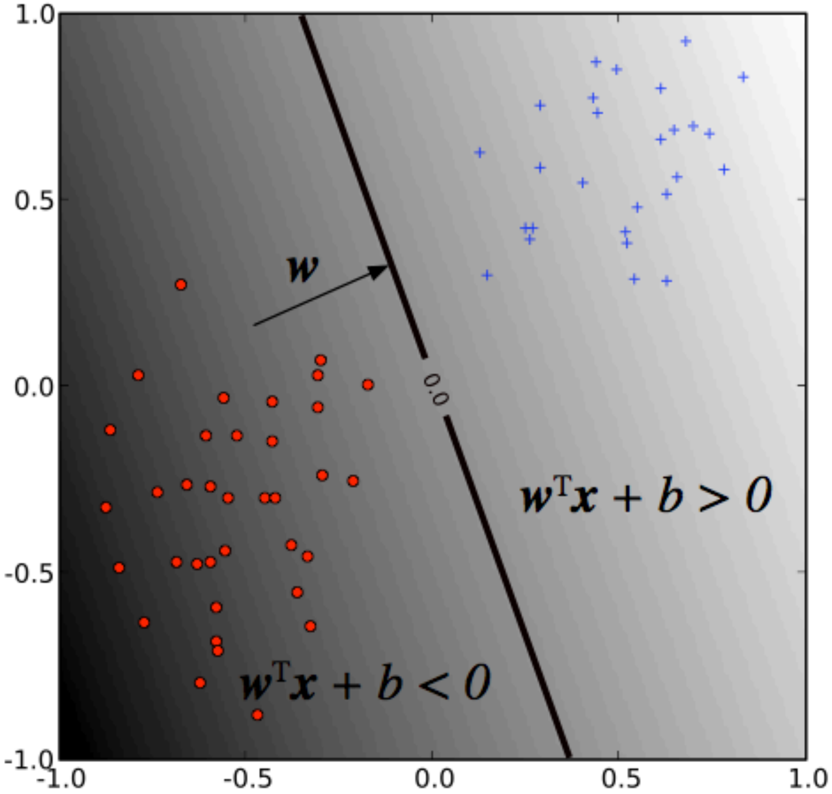
The sign of *f(x)* determines the (binary) class label of a record *x*.

MAXIMUM MARGIN HYPERPLANES



source: *http://pyml.sourceforge.net/doc/howto.pdf*

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.

Q: Why are these the same thing?

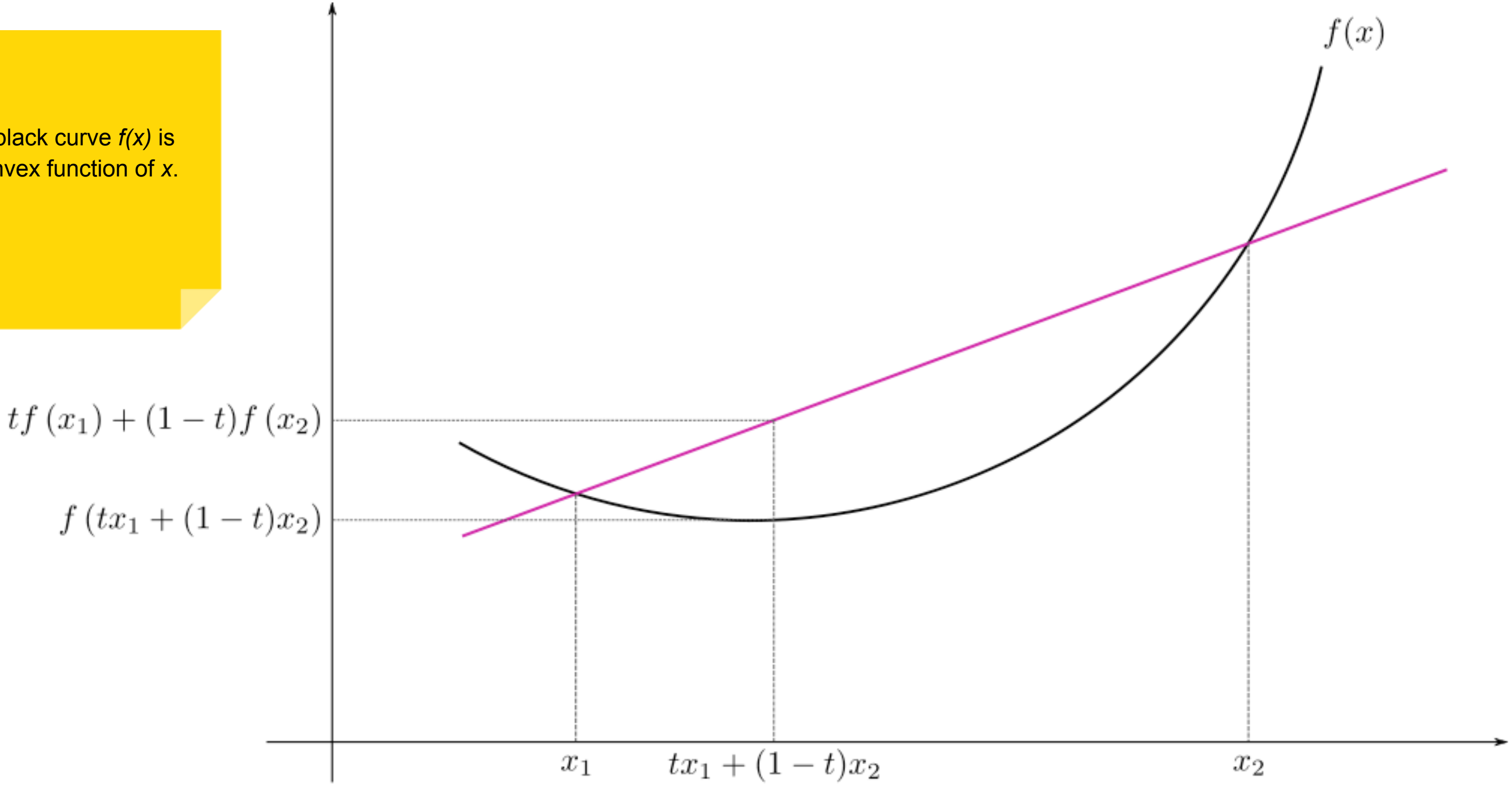
A: Because using the mmh as the decision boundary minimizes the probability that a small perturbation in the position of a point produces a classification error.

Selecting the mmh is an exercise in analytic geometry.

In particular, this task reduces to the optimization of a **convex** objective function.

NOTE

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



source: http://en.wikipedia.org/wiki/File:ConvexFunction.svg

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This is nice because convex optimization problems are guaranteed to give **global optima** (and they're easy to solve numerically too).

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

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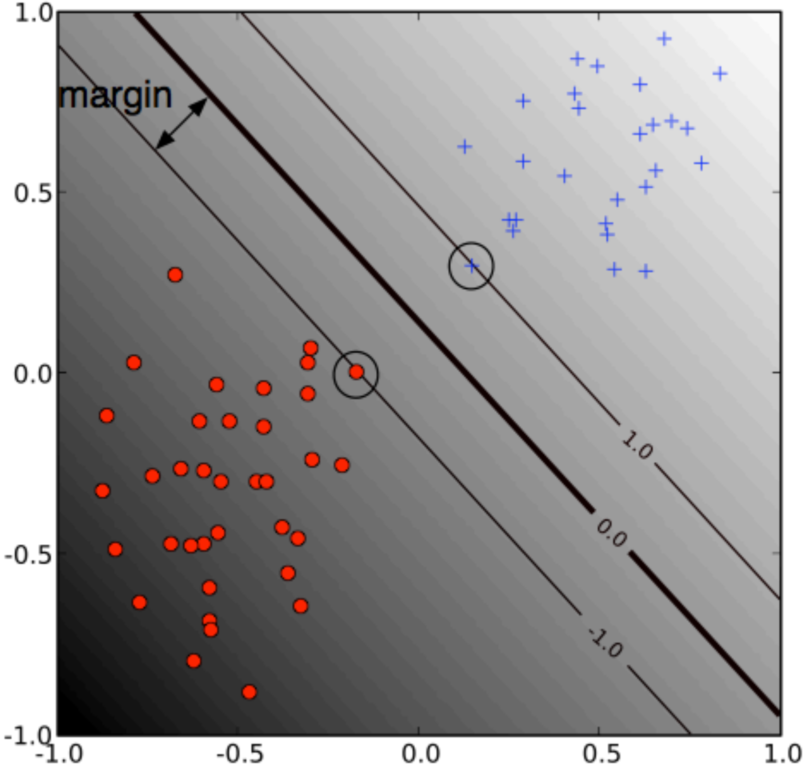
MAXIMUM MARGIN HYPERPLANES



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The other points (far from the decision boundary) don't affect the construction of the mmh at all!

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The optimization problem that this SVM solves is:

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

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NOTE

This type of optimization problem can be solved with *quadratic programming*.

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

III. SLACK VARABLES

Recall that in building the hard margin classifier, we assumed that our data was **linearly separable** (eg, that we could perfectly classify each record with a linear decision boundary).

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

Slack variables ξ_i generalize the optimization problem to permit some misclassified training records (which come at a cost C).

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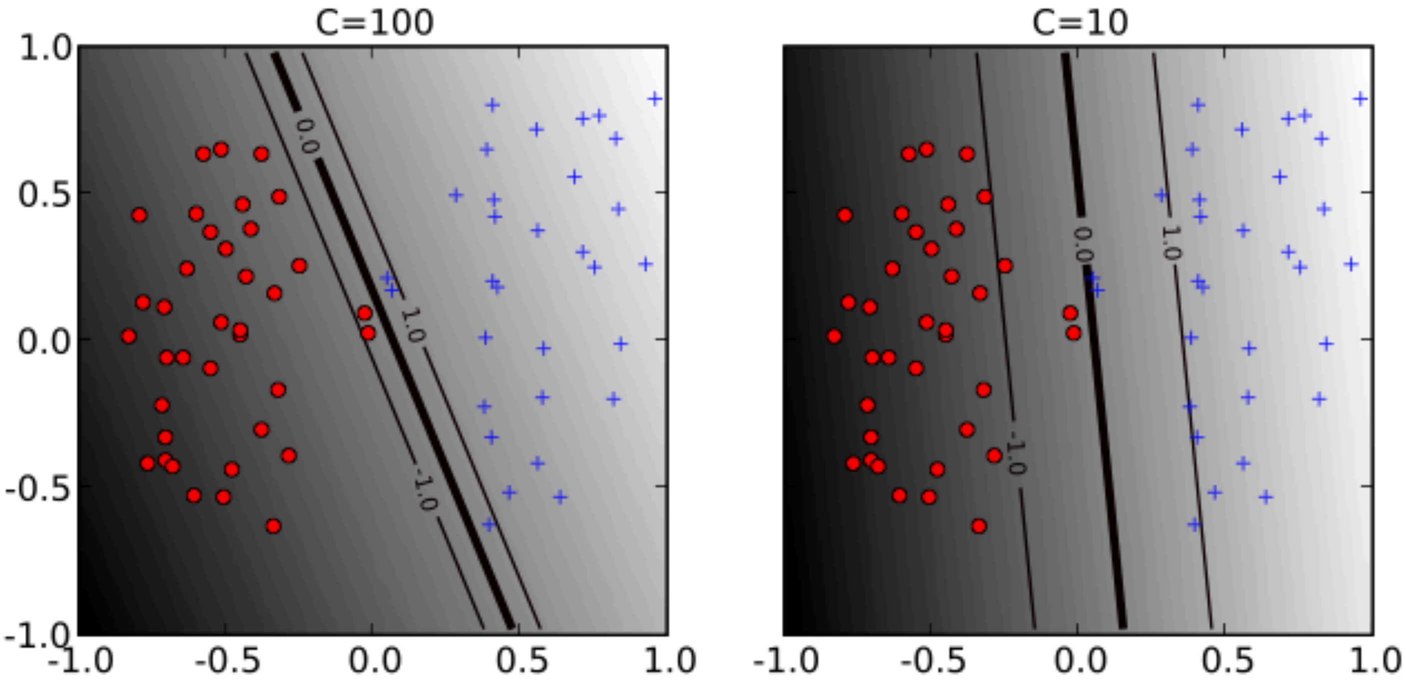
This an example of *bias-variance tradeoff*.

SLACK VARIABLES – SOFT MARGIN CONSTANT



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The soft-margin optimization problem can be rewritten as:

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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 x_i only via the **inner product**

$$\langle x_i, x_j \rangle = x_i^T x_j$$

The inner product is an operation that takes two vectors and returns a real number.

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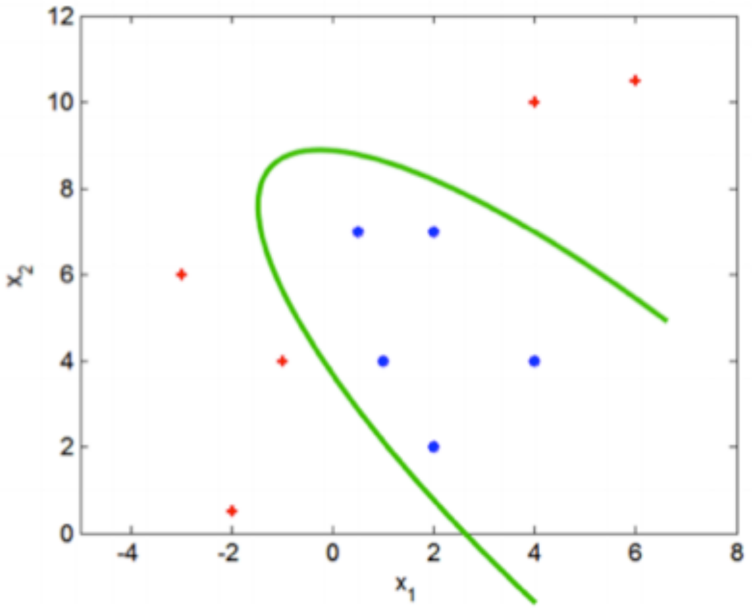
In particular, we can easily change K to be some other space K'.

IV. NONLINEAR CLASSIFICATION

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



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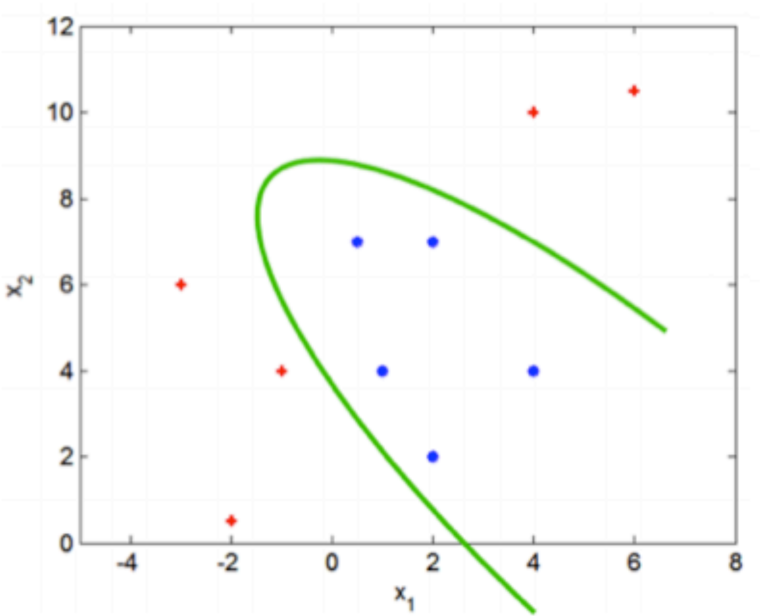
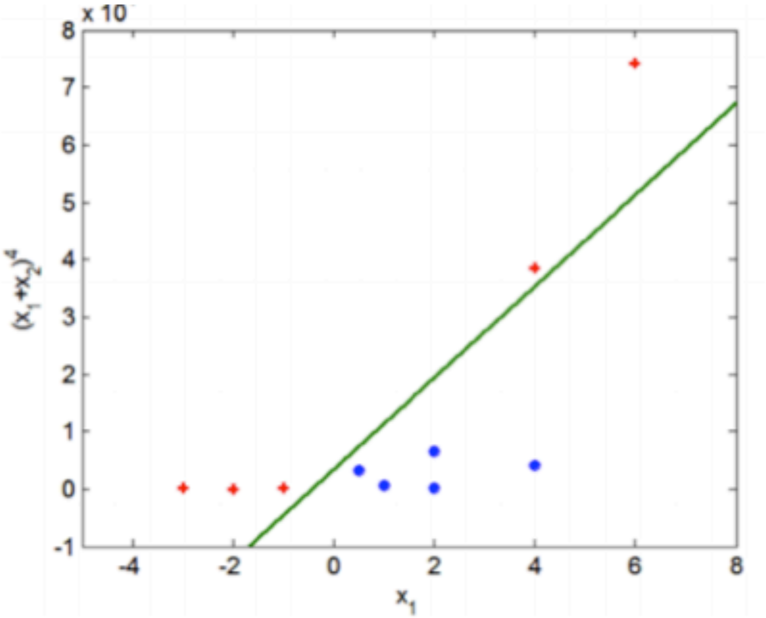
This *linear* decision boundary will be mapped to a *nonlinear* decision boundary in the original feature space.



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 $x^T x$:

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

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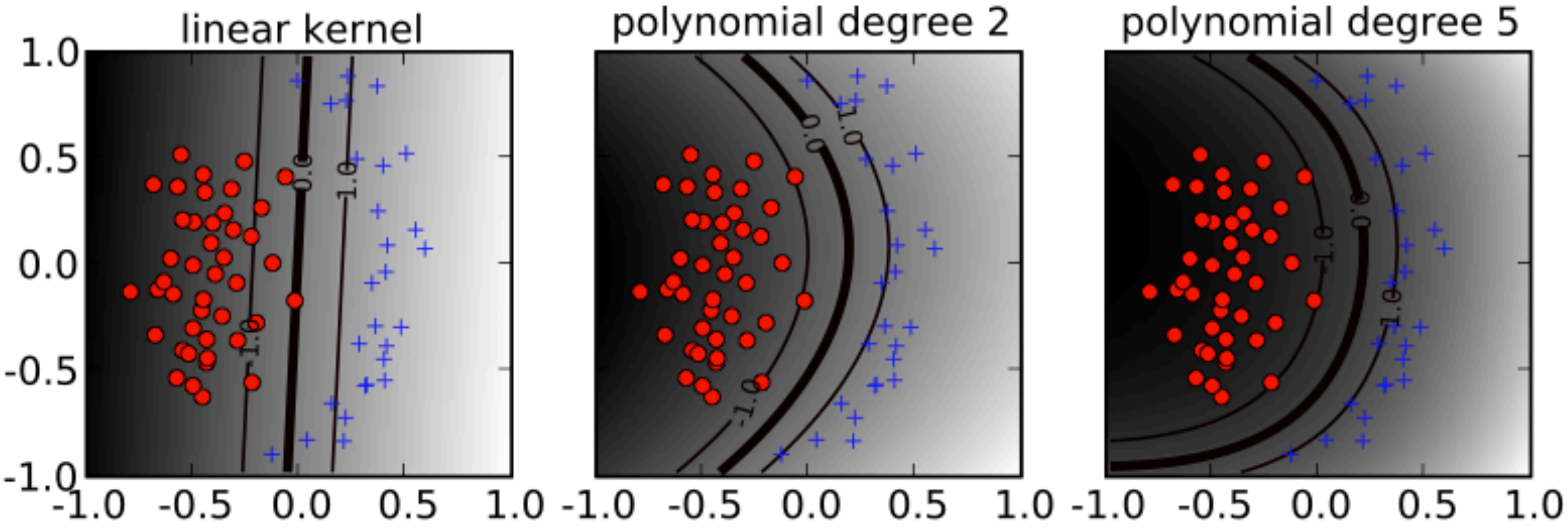
The **hyperparameters** d, γ affect the flexibility of the decision bdy.



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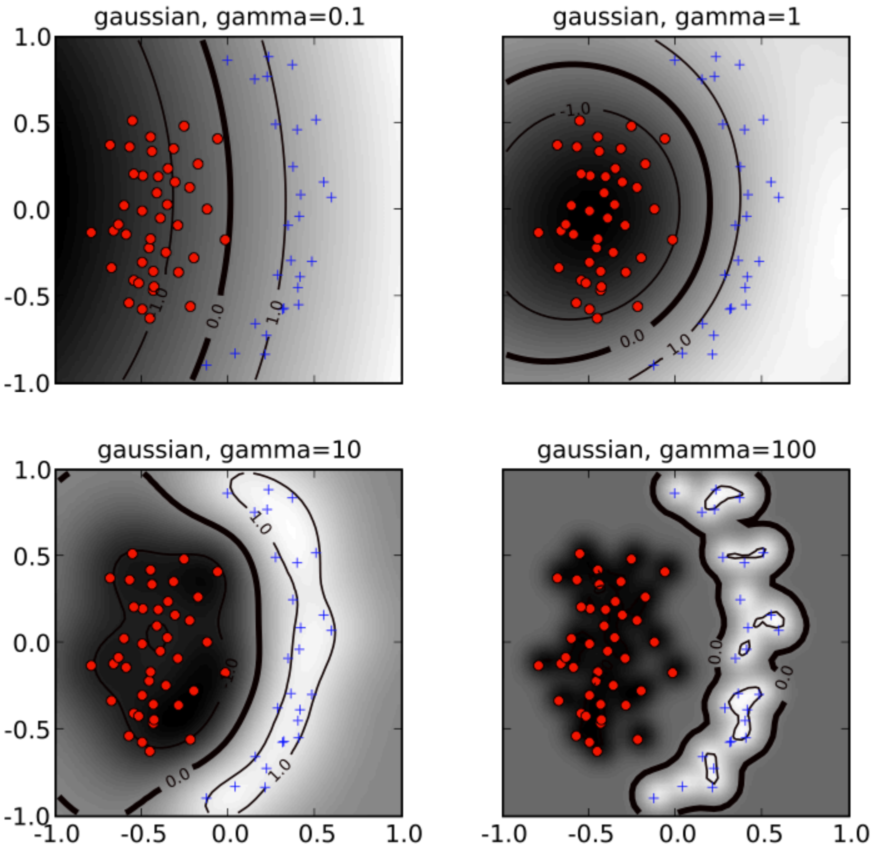
NONLINEAR CLASSIFICATION – GAUSSIAN KERNEL



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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!

EX: SVM IN SCIKIT-LEARN