GENERAL ASSEMBLY

INTRO TO DATA SCIENCE

LECTURE 11: SUPPORT VECTOR MACHINES

LAST TIME:

- ENSEMBLE TECHNIQUES
- PROBLEMS IN CLASSIFICATION
- BAGGING, BOOSTING, RANDOM FORESTS

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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recall:

binary classifier – *solves two-class problem*

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

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

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

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.*

SUPPORT VECTOR MACHINES

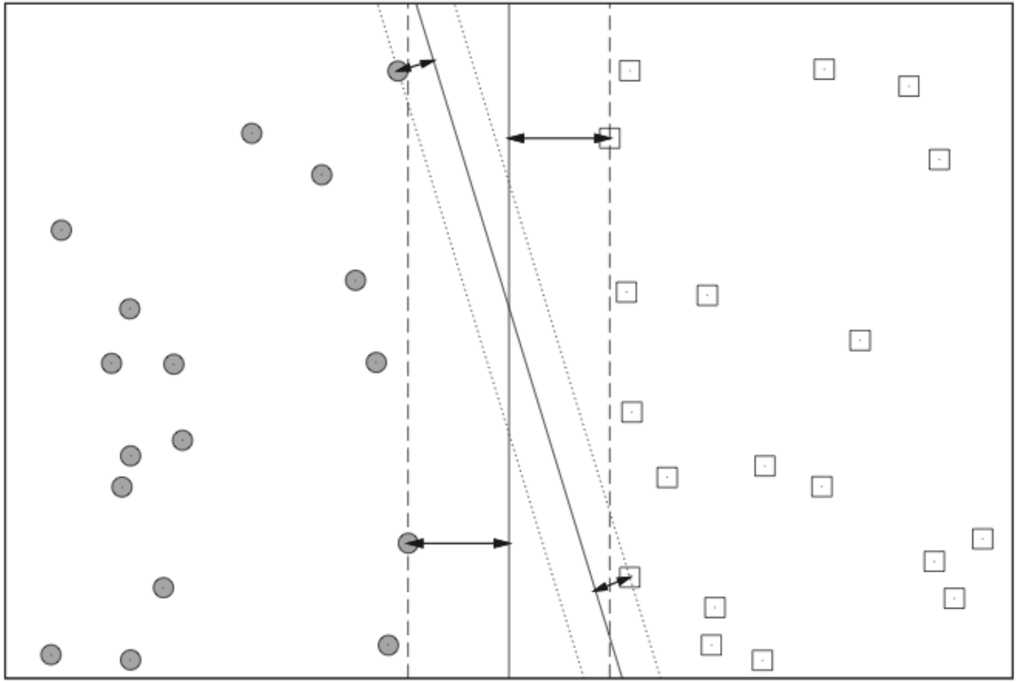

FIGURE 18-4. Two decision boundaries and their margins. Note that the vertical decision boundary has a wider margin than the other one. The arrows indicate the distance between the respective support vectors and the decision boundary.

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

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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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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,**

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

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

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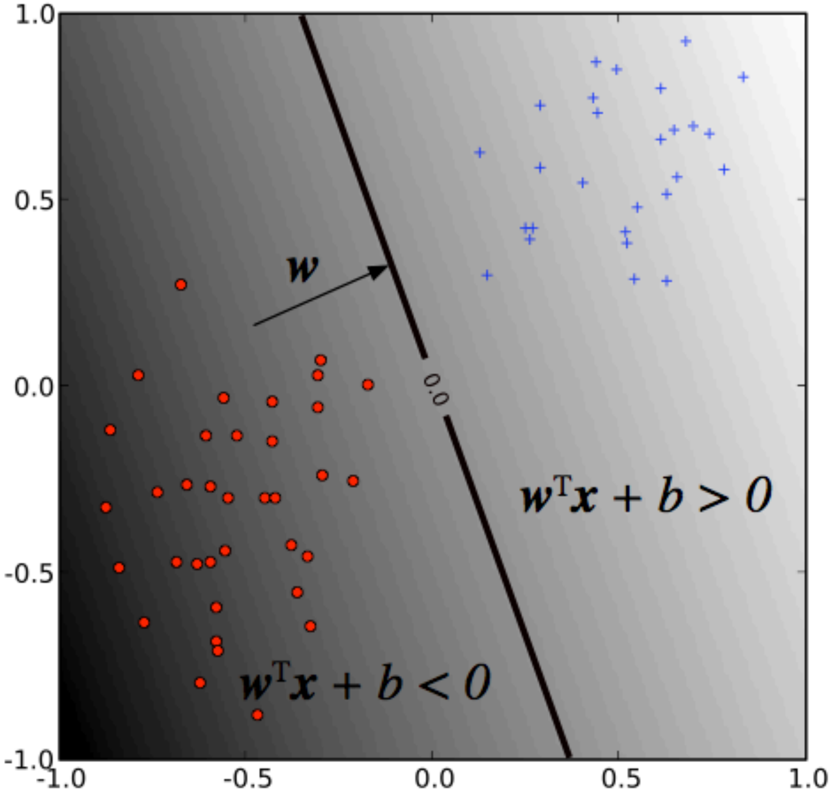
The sign of $f(x)$ determines the (binary) class label of a record x.

MAXIMUM MARGIN HYPERPLANES



NOTE

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

The bias determines its *translation* from the origin.

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

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.

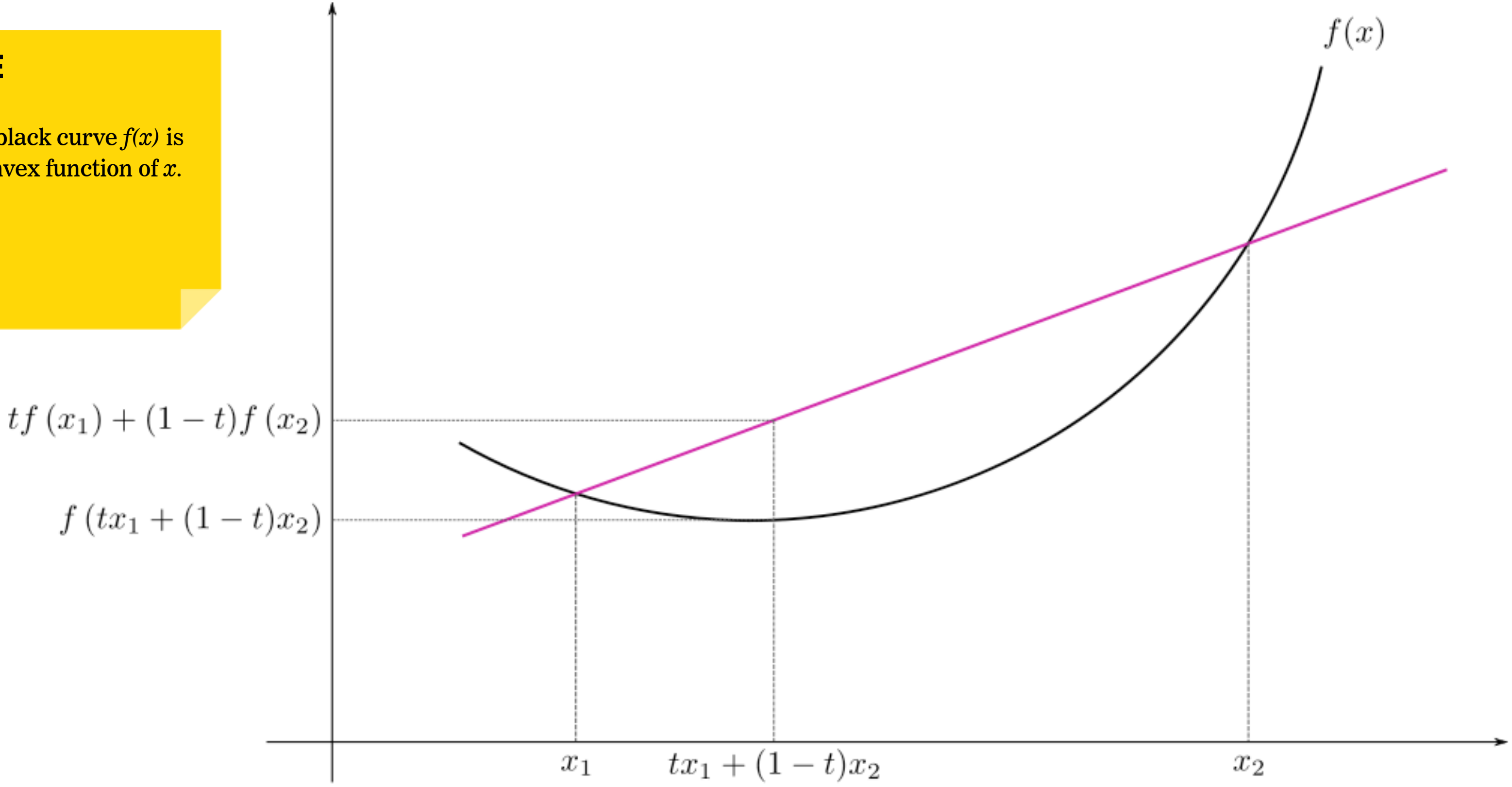
Selecting the mmh is a straightforward exercise in analytic geometry (we won't go through the details here).

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

CONVEX FUNCTIONS

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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NOTE

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

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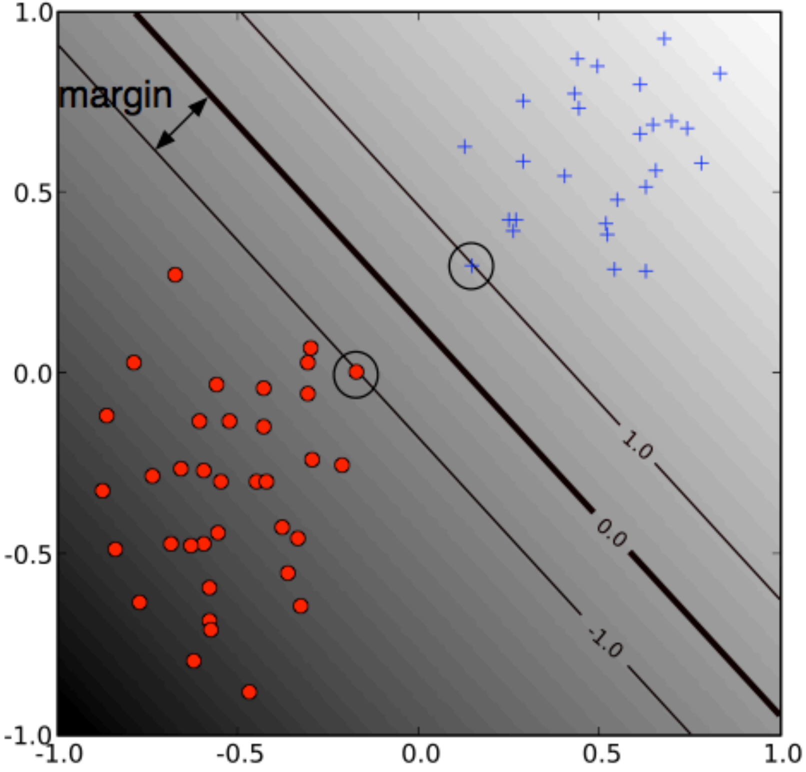
MAXIMUM MARGIN HYPERPLANES



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These points are called the **support vectors**.

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:

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

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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 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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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.**

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

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

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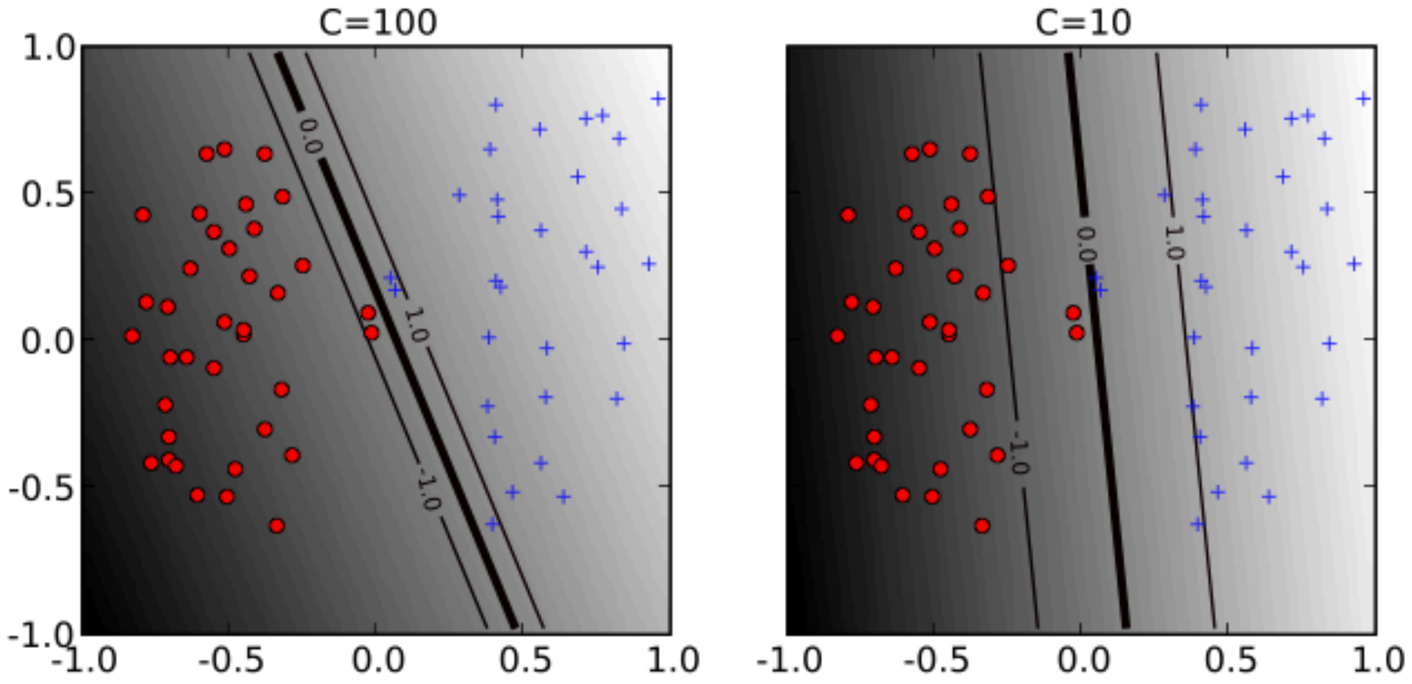
This an example of bias-variance tradeoff.



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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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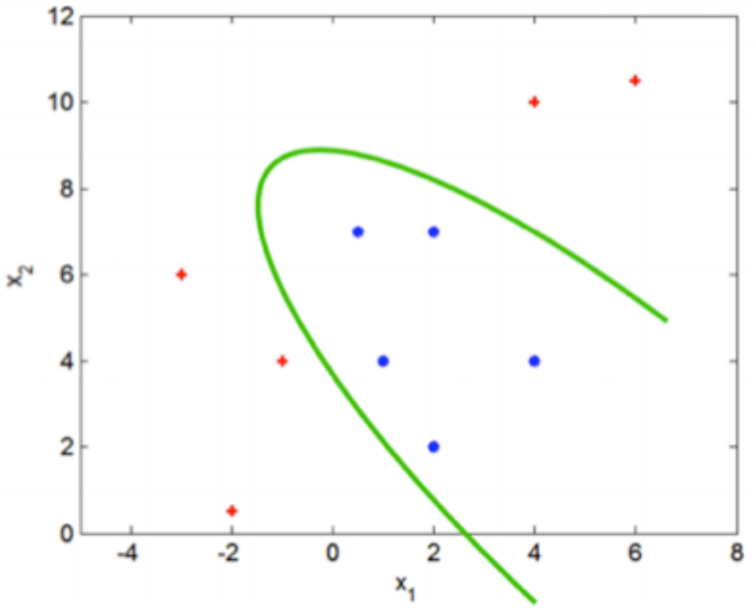
The fact that we we can rewrite the optimization problem in terms of the inner product means that we don't actually have to do any calculations in the feature space $\mathbb{K}$.

In particular, we can easily change $\mathbb{K}$ to be some other space $\mathbb{K}$'.

IV. NONLINEAR CLASSIFICATION

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



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One possibility is to add nonlinear combinations of features to the data, and then to create a linear decision boundary in the enhanced (higher-dimensional) feature space.

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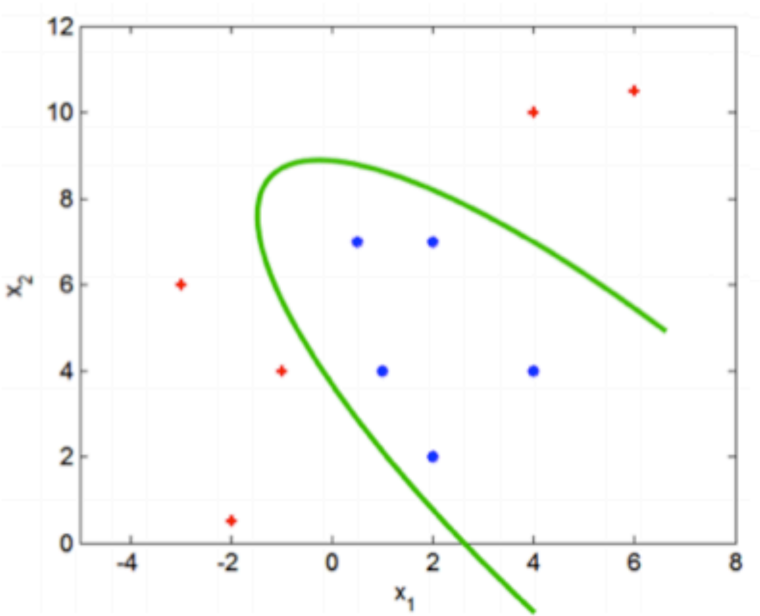
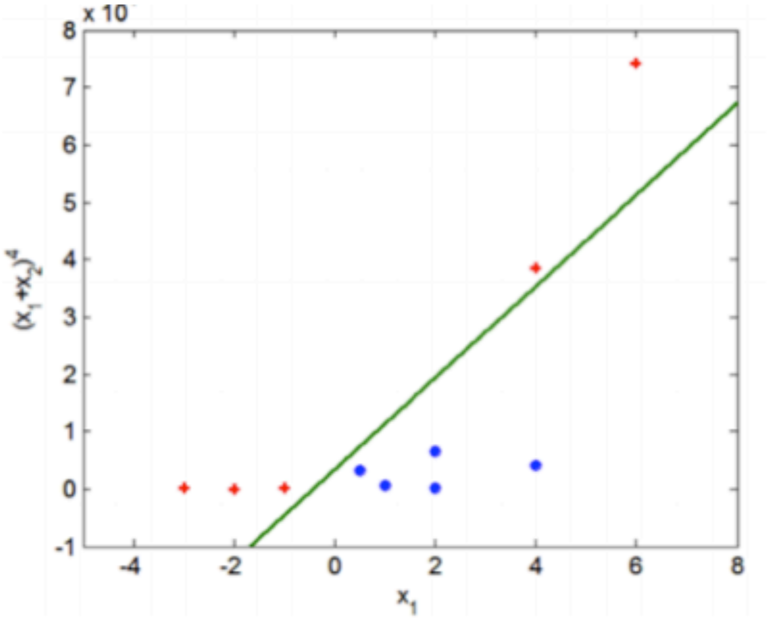
This linear *decision boundary will be mapped to a* nonlinear *decision boundary in the original feature space.*



original feature space *K*



higher-dim feature space *K'*

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In particular, this will not scale well, since it requires many high-dimensional calculations.

Warning:

In particular, this will be expensive, since it requires many high-dimensional calculations.

It can sometimes lead to more complexity (both modeling complexity and computational complexity) than we want.

To recap:

- *remap the feature vectors* x_i *into a higher-dimensional space* K'
- *create a linear decision boundary in* K'
- *back out the nonlinear decision boundary in* K *from the result*

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

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

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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* $\mathbb{R}$ *.*

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!*

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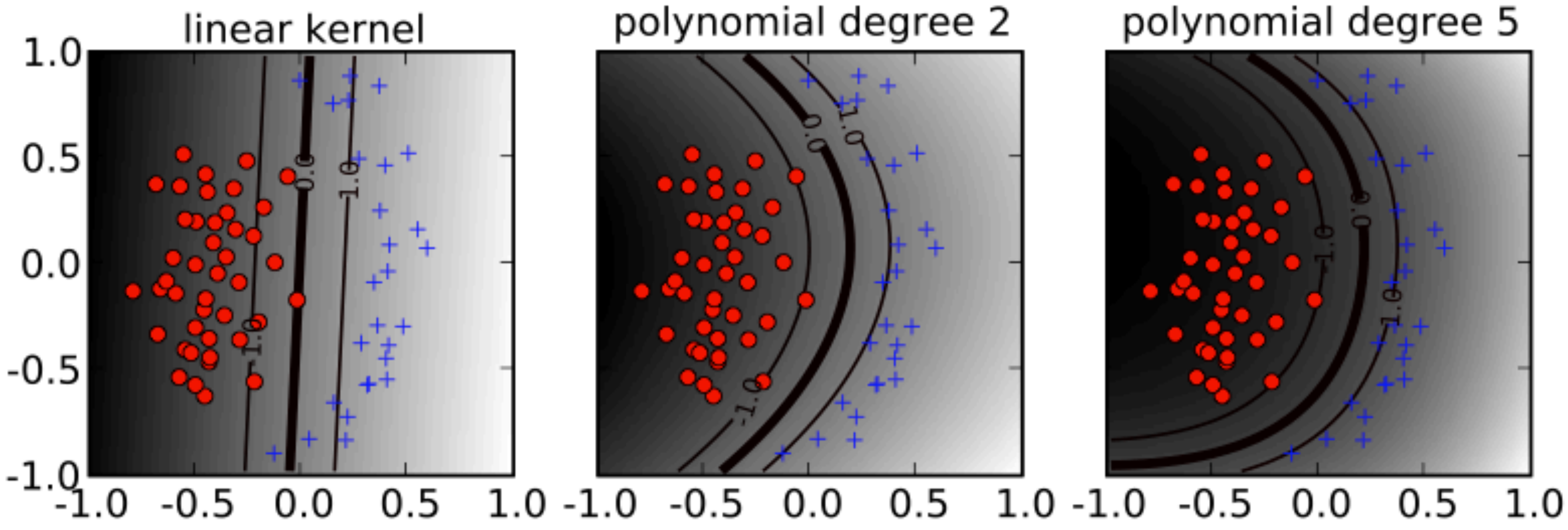
The **hyperparameters** d, γ *affect the flexibility of the decision bdy.*

NONLINEAR CLASSIFICATION – POLYNOMIAL KERNEL



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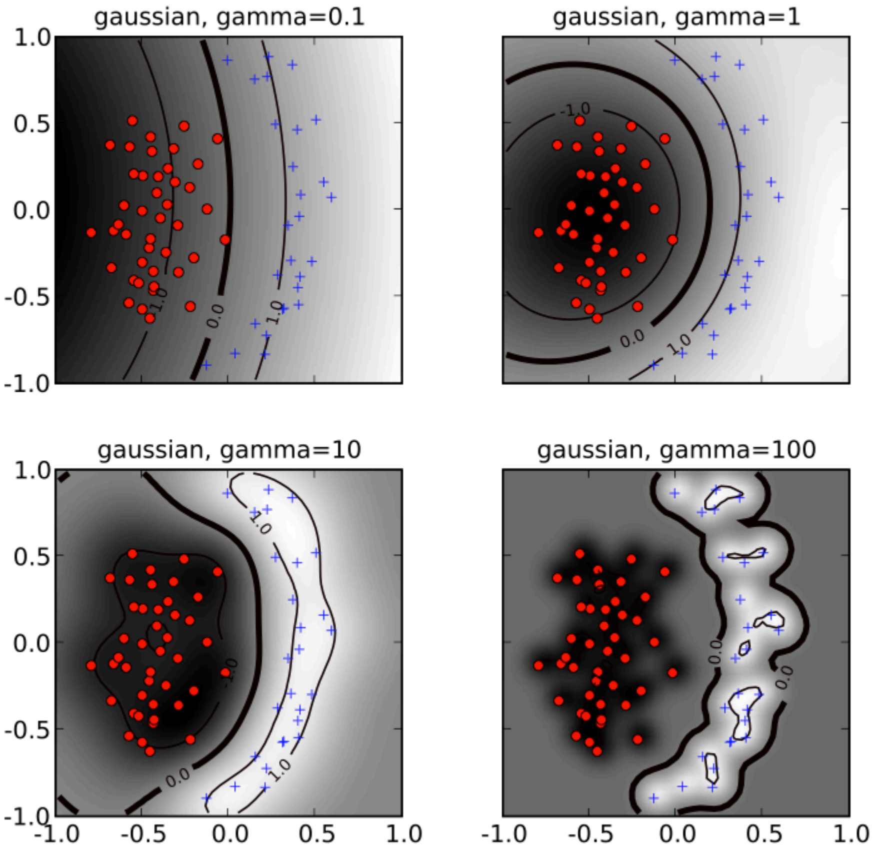

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SVMs (and **kernel methods** *in general) are versatile, powerful, and popular techniques that can produce accurate results for a wide array of classification problems.*

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

EX: SVM IN SCIKIT-LEARN