GENERAL ASSEMBLY

INTRO TO DATA SCIENCE
LECTURE 10: SUPPORT VECTOR MACHINES

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LAST TIME:

- DECISION TREES
- BUILDING DECISION TREES
- OBJECTIVE SPLITTING FUNCTIONS
- PREVENTING OVERFITTING IN DECISION TREES

QUESTIONS?

I. SUPPORT VECTOR MACHINES
II. SOFT-MARGIN SVM
III. NONLINEAR SVM
HANDS-ON: SVM

I. SUPPORT VECTOR MACHINES

Q: *What is a support vector machine?*

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

recall:

binary classifier – solves two-class problem

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

Q: *How is the decision boundary derived?*

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.*

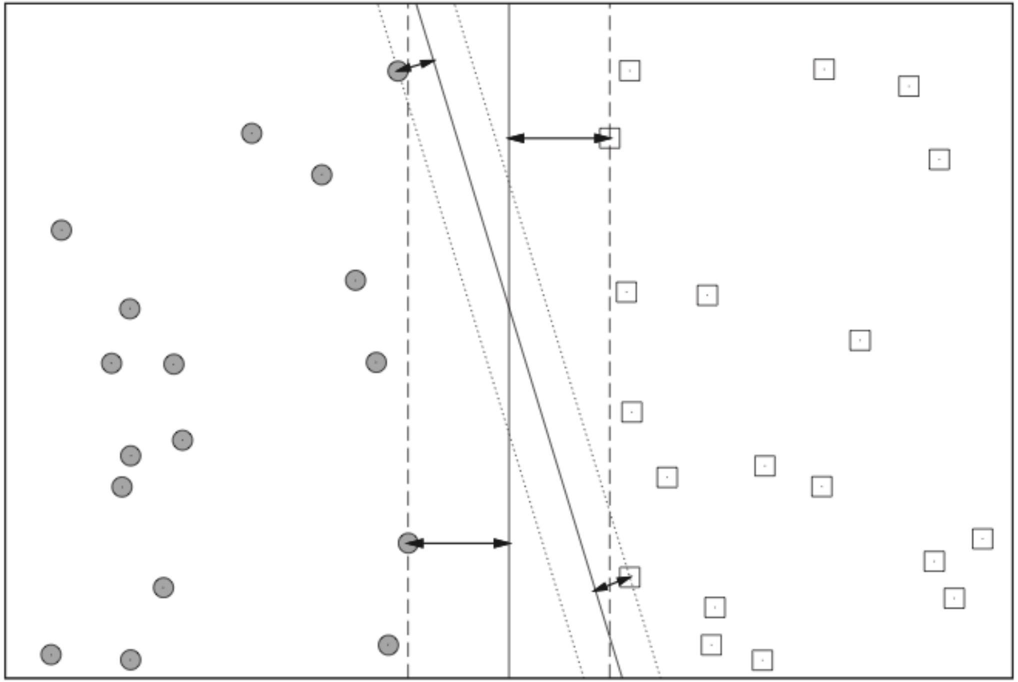


FIGURE 18-4. Two decision boundaries and their margins. Note that the vertical decision boundary has a wider margin than the other one. The arrows indicate the distance between the respective support vectors and the decision boundary.

Q: *How is the decision boundary derived?*
A: *Using **geometric reasoning** (as opposed to the algebraic reasoning we've used to derive other classifiers).*

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

Q: *How is the decision boundary (**mmh**) derived?*

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

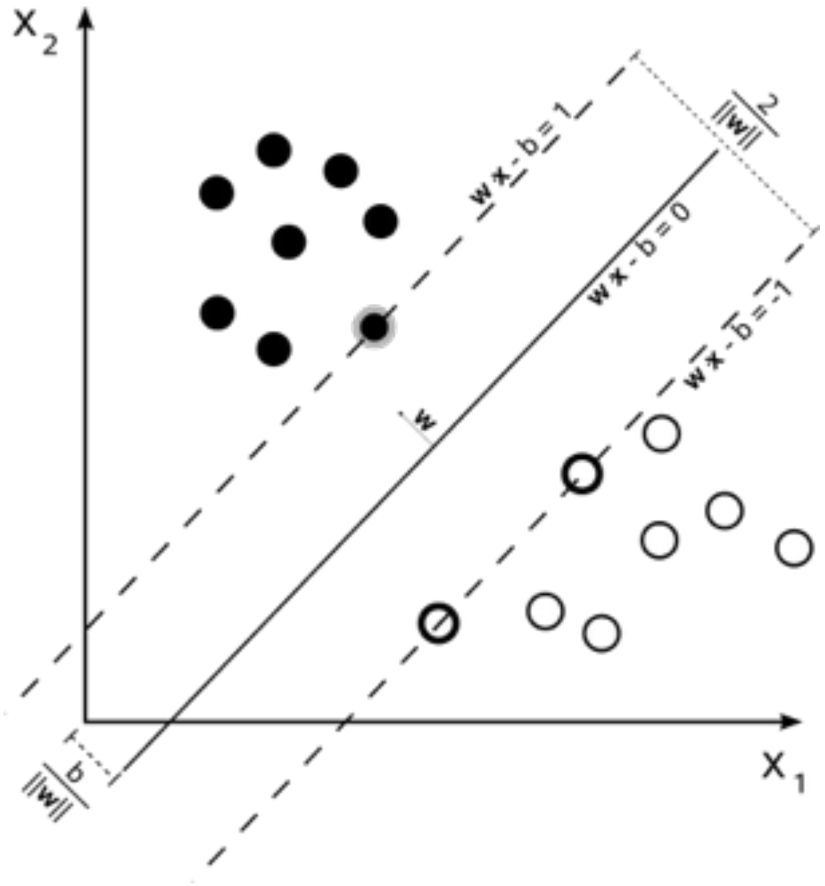
$$f(\mathbf{x}) = \mathbf{w}^\mathsf{T}\mathbf{x} + b.$$

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.

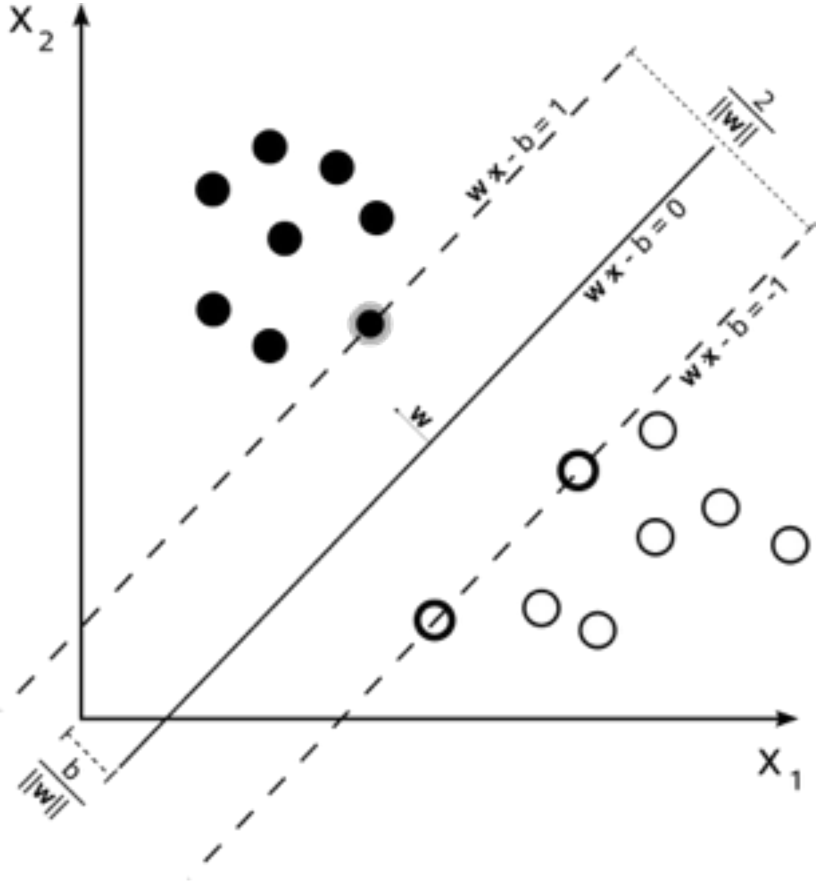
*How is the decision boundary (**mmh**) derived?*

- Any hyperplane can be written as the set of points where $\boldsymbol{w^T x - b = 0}$
  - $\boldsymbol{w}$ sets the plane's orientation (it's perpendicular to the plane)
  - $\boldsymbol{b}$ sets the offset from the origin
- Set the margin planes for each class such that $\boldsymbol{w^T - b = +/-1}$
  - +1 for positive class, -1 for negative class



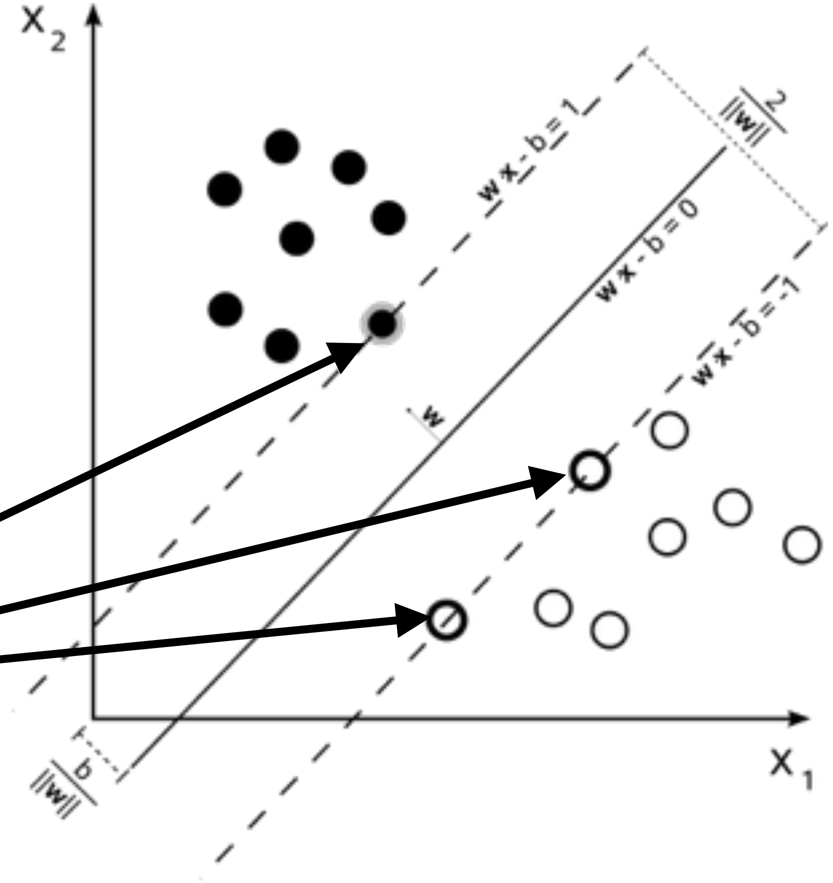
*How is the decision boundary (**mmh**) derived?*

- Thus, our goal of maximizing the margin width amounts to maximizing ***2/||w||***
  - To do this, we must minimize **||*w*||**
  - Easier to minimize ***||w||²/2***
- We do this subject to the constraint: $y_i * (w^T x_i - b) \geq 1$
- This is a **Quadratic Programming (QP)** optimization problem, yielding ***w*** and ***b***



*How is the decision boundary (**mmh**) derived?*

- This is a **Quadratic Programming (QP)** optimization problem, yielding ***w*** and ***b***
- Solving this QP problem yields a solution of the form: $w = \sum_i \alpha_i y_i x_i$
- Most of these alpha are 0
- Only the "***support vectors***" will be nonzero
- Thus only they contribute!



II. SOFT-MARGIN SVM

- *So far we've been dealing with what's called a **hard margin SVM** - what does this mean?*
  - *We assume the data is perfectly separable by our hyperplane*
  - *No classification instances will fall within the margin*
- *As we've seen, probably not realistic (especially in linear case)*
- *So how do we allow for some error/noise in our model?*

Q: *How do we handle potentially inseparable data?*

A: *By training a **soft margin SVM** rather than a hard margin*

soft margin – basically allows for a fuzzy boundary, where some proportion of elements may be misclassified in order to maintain a simpler boundary

Remember, simpler boundaries are probably more likely to generalize.

Q: *How do we train a **soft margin SVM**?*

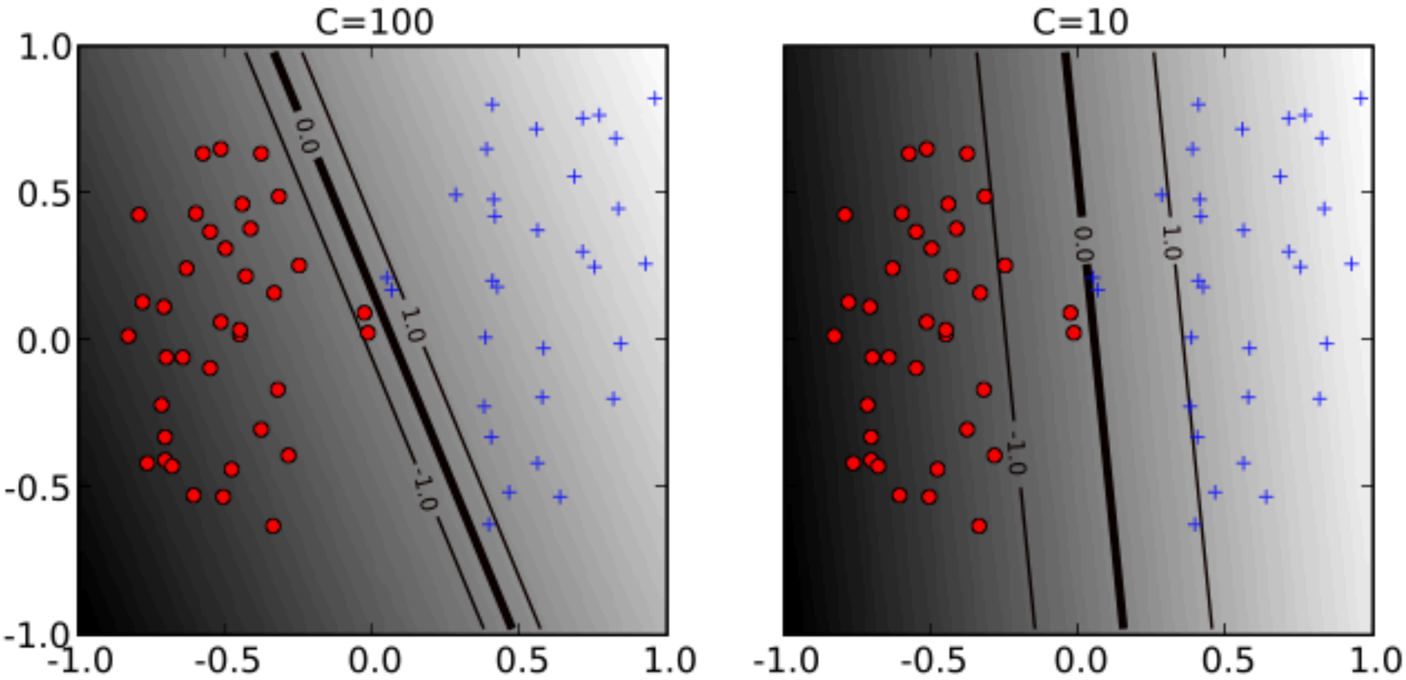
A: *By making use of **slack variables** that allow a proportion of instances to be misclassified*

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

The resulting soft margin QP problem is given by:

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

SOFT-MARGIN SVM



III. NONLINEAR SVM

Recall that our soft-margin SVM optimization function can be written as follows:

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

This can be rewritten in the following form:

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

NOTE

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

(reached via Lagrange multipliers)

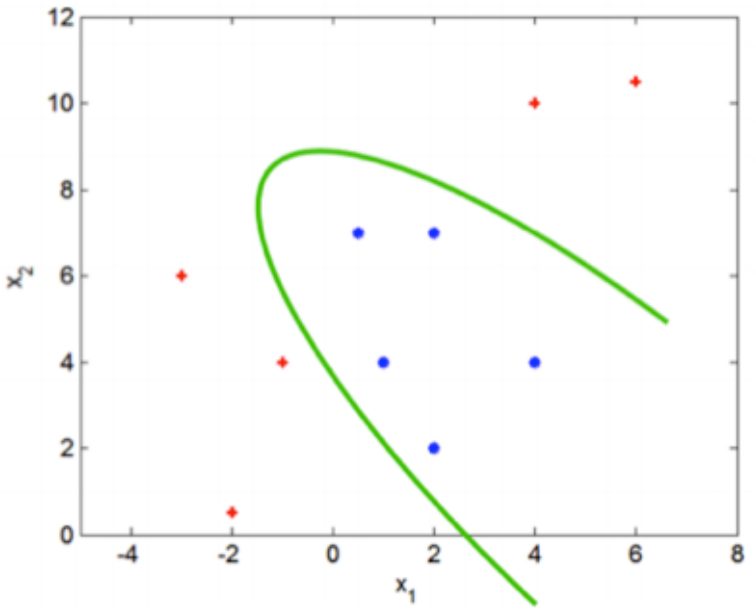
Notice that this expression depends only on ***inner products*** $\mathbf{x}_i^T\mathbf{x}_j$

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

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 K, ***just dot products***.

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

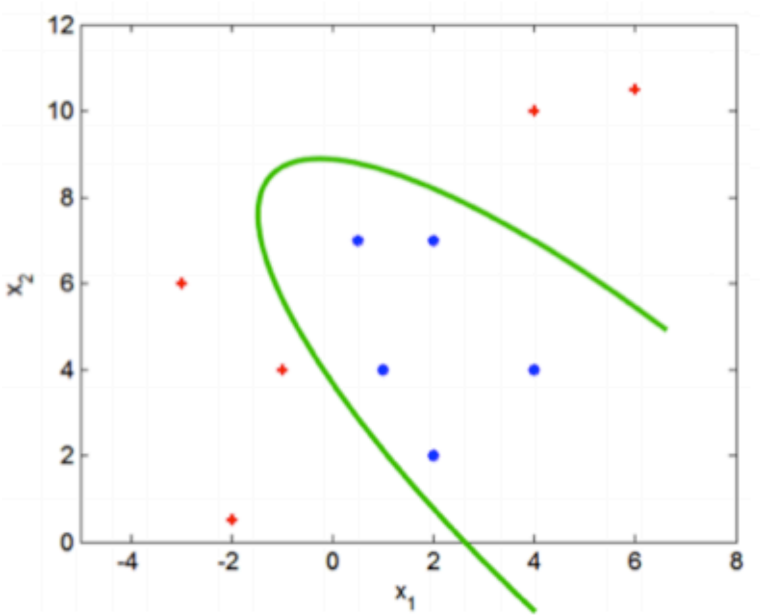
Suppose we need a more complex classifier than a linear decision boundary allows.



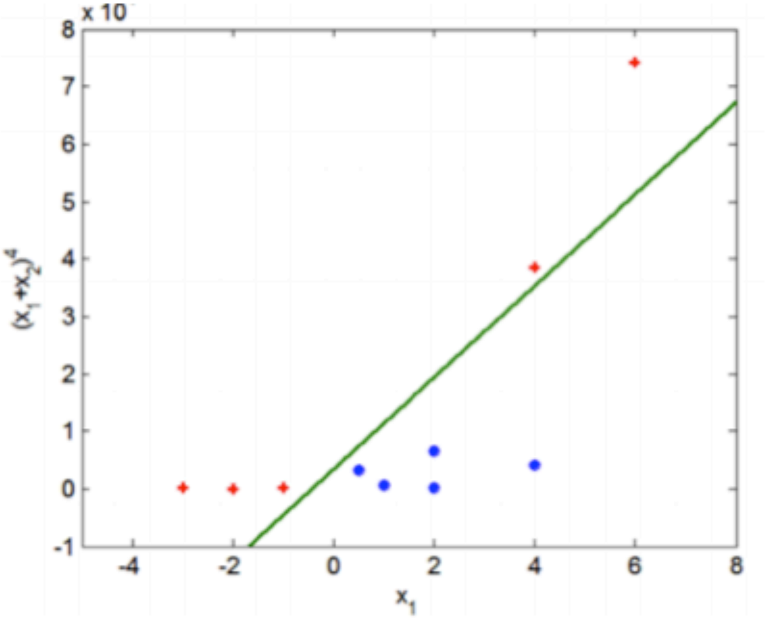
Suppose we need a more complex classifier than a linear decision boundary allows.

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.

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'*

The logic of this approach is sound, but there are a few problems with this version.

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

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:

- 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

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 $x^T x$:

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

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

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.

NOTE

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

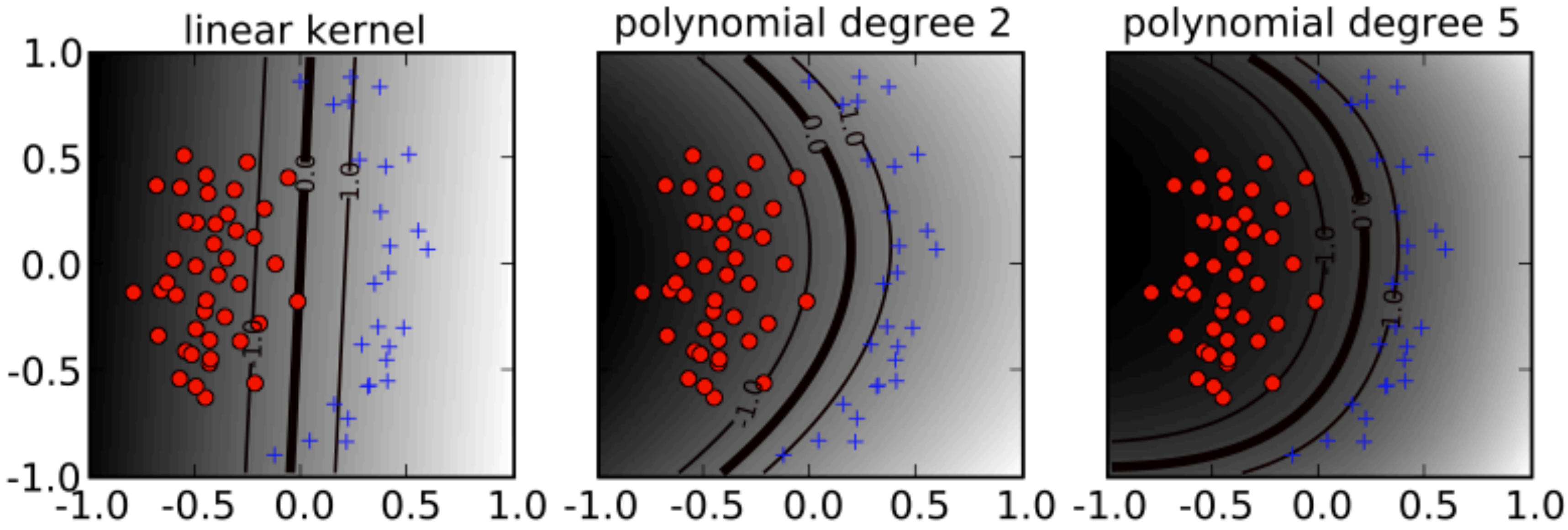
some popular kernels:

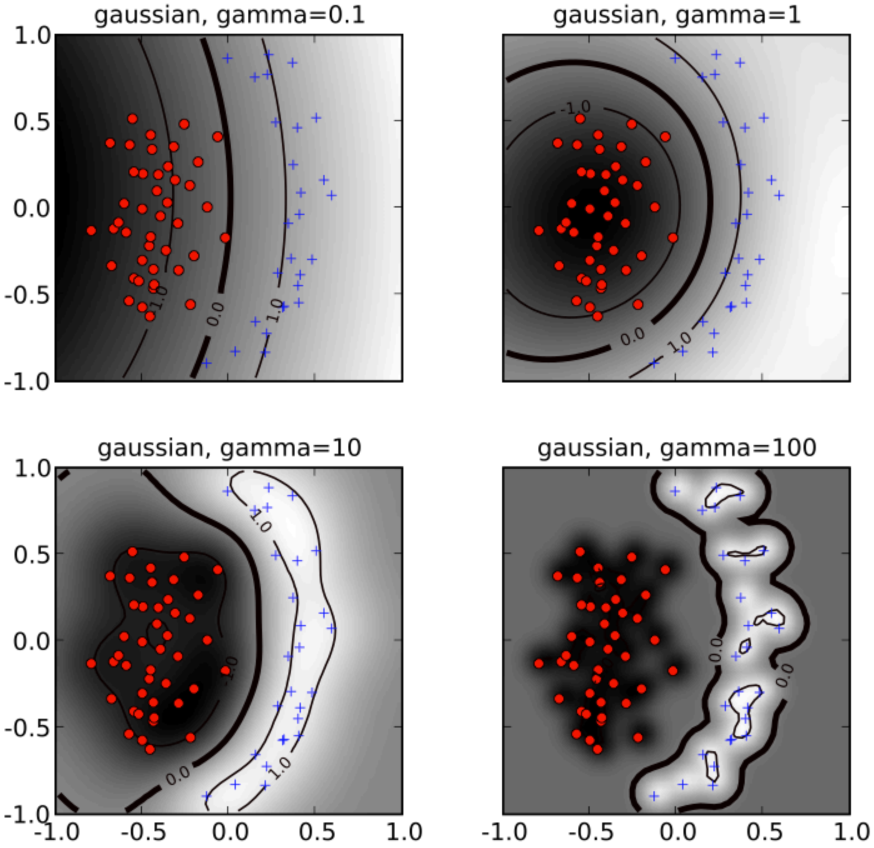
linear kernel $$k(\mathbf{x}, \mathbf{x}') = \langle \mathbf{x}, \mathbf{x}' \rangle$$

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

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

The **hyperparameters** ***d***, **γ** affect the flexibility


linear kernel
polynomial degree 2
polynomial degree 5
1.0
0.5
0.0
-0.5
-1.0
-1.0 -0.5 0.0 0.5 1.0
0.0
1.0
-1.0


gaussian, gamma=0.1
gaussian, gamma=1
gaussian, gamma=10
gaussian, gamma=100
1.0
0.5
0.0
-0.5
-1.0
-1.0
-0.5
0.0
0.5
1.0
-1.0
0.0
1.0

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!

HANDS-ON: SVM