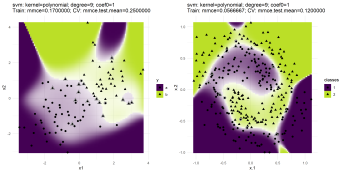
Introduction to Machine Learning

The Polynomial Kernel



Learning goals

- Know the homogeneous and non-homogeneous polynomial kernel
- Understand the influence of the choice of the degree on the decision boundary

HOMOGENEOUS POLYNOMIAL KERNEL

$$k(\mathbf{x}, \tilde{\mathbf{x}}) = (\mathbf{x}^T \tilde{\mathbf{x}})^d, \text{ for } d \in \mathbb{N}$$

The feature map contains all monomials of exactly order d.

$$\phi(\mathbf{x}) = \left(\sqrt{\binom{d}{k_1, \ldots, k_p}} x_1^{k_1} \ldots x_p^{k_p} \right)_{k_i \geq 0, \sum_i k_i = d}$$

That $\langle \phi(\mathbf{x}), \phi(\tilde{\mathbf{x}}) \rangle = k(\mathbf{x}, \tilde{\mathbf{x}})$ holds can easily be checked by simple calculation and using the multinomial formula

$$(x_1 + \ldots + x_p)^d = \sum_{k_i \geq 0, \sum_i k_i = d} \binom{d}{k_1, \ldots, k_p} x_1^{k_1} \ldots x_p^{k_p}$$

The map $\phi(\mathbf{x})$ has $\binom{p+d-1}{d}$ dimensions. We see that $\phi(\mathbf{x})$ contains no terms of "lesser" order, so, e.g., linear effects. As an example for $p = d = 2$: $\phi(\mathbf{x}) = (x_1^2, x_2^2, \sqrt{2} x_1 x_2)$.

NONHOMOGENEOUS POLYNOMIAL KERNEL

$$k(\mathbf{x}, \tilde{\mathbf{x}}) = (\mathbf{x}^T \tilde{\mathbf{x}} + b)^d, \text{ for } b \geq 0, d \in \mathbb{N}$$

The maths is very similar as before, we kind of add a further constant term in the original space, with

$$(\mathbf{x}^T \tilde{\mathbf{x}} + b)^d = (x_1 \tilde{x}_1 + \ldots + x_p \tilde{x_p} + \sqrt{b}\sqrt{b})^d$$

The feature map contains all monomials up to order d.

$$\phi(\mathbf{x}) = \left(\sqrt{\binom{d}{k_1, \ldots, k_{p+1}}} x_1^{k_1} \ldots x_p^{k_p} b^{k_{p+1}/2} \right)_{k_i \geq 0, \sum_i k_i = d}$$

The map $\phi(\mathbf{x})$ has $\binom{p+d}{d}$ dimensions. For $p = d = 2$:

$$\phi(\mathbf{x}) = (x_1^2, x_2^2, \sqrt{2} x_1 x_2, \sqrt{2b} x_1, \sqrt{2b} x_2, b)$$

NONHOMOGENEOUS POLYNOMIAL KERNEL

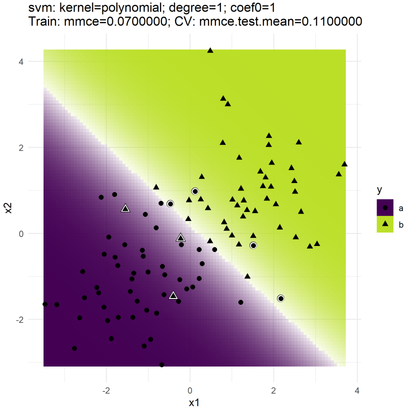
The relationship between the kernel and the feature map can be shown by unraveling the polynomial formula. For p=d=2:

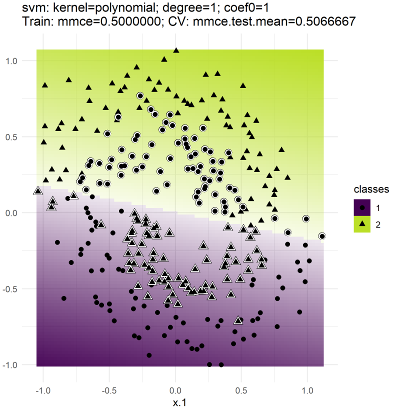
$$\left(\mathbf{x}^T\tilde{\mathbf{x}} + b\right)^2 = \left(\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \cdot (\tilde{x}_1 \ \tilde{x}_2) + b\right) \cdot \left(\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \cdot (\tilde{x}_1 \ \tilde{x}_2) + b\right)$$

$$\begin{aligned}
&= (x_1\tilde{x}_1 + x_1\tilde{x}_2 + x_2\tilde{x}_1 + x_2\tilde{x}_2 + b) \cdot \\
&\quad (x_1\tilde{x}_1 + x_1\tilde{x}_2 + x_2\tilde{x}_1 + x_2\tilde{x}_2 + b) \\
&= x_1^2\tilde{x}_1^2 + x_2^2\tilde{x}_2^2 + 2x_1\tilde{x}_1x_2\tilde{x}_2 + 2bx_1\tilde{x}_1 + 2bx_2\tilde{x}_2 + b^2 \\
&= (x_1^2, x_2^2, \sqrt{2}x_1x_2, \sqrt{2b}x_1, \sqrt{2b}x_2, b)^T \cdot \\
&\quad (\tilde{x}_1^2, \tilde{x}_2^2, \sqrt{2}\tilde{x}_1\tilde{x}_2, \sqrt{2b}\tilde{x}_1, \sqrt{2b}\tilde{x}_2, b) \\
&= \phi(\mathbf{x})^T \cdot \phi(\tilde{\mathbf{x}})
\end{aligned}$$

POLYNOMIAL KERNEL

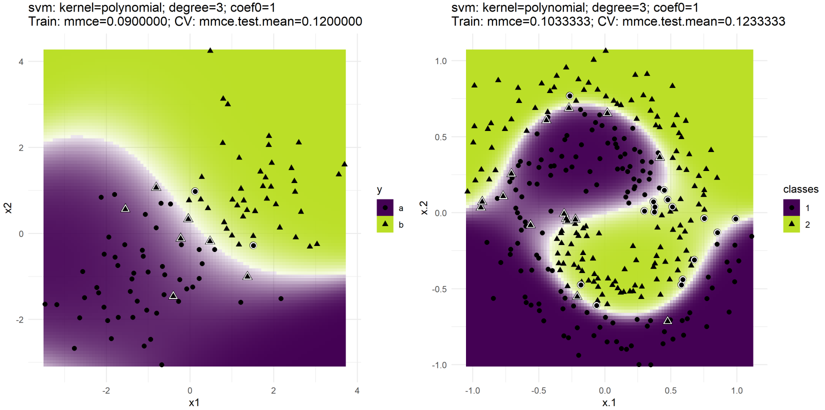
Degree $d = 1$ yields a linear decision boundary.





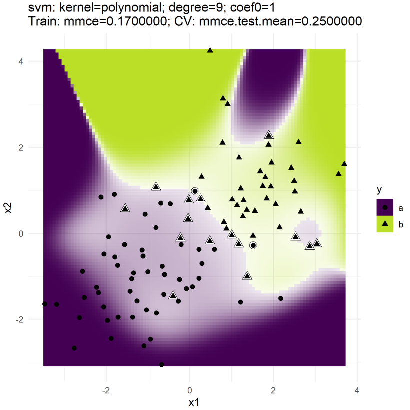
POLYNOMIAL KERNEL

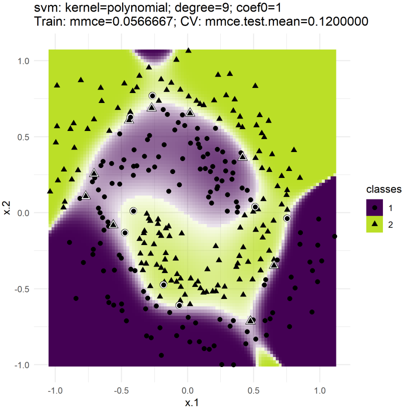
The higher the degree, the more nonlinearity in the decision boundary.



POLYNOMIAL KERNEL

The higher the degree, the more nonlinearity in the decision boundary.





POLYNOMIAL KERNEL

For $k(\mathbf{x}, \tilde{\mathbf{x}}) = (\mathbf{x}^\top \tilde{\mathbf{x}} + 0)^d$ we get no lower order effects.