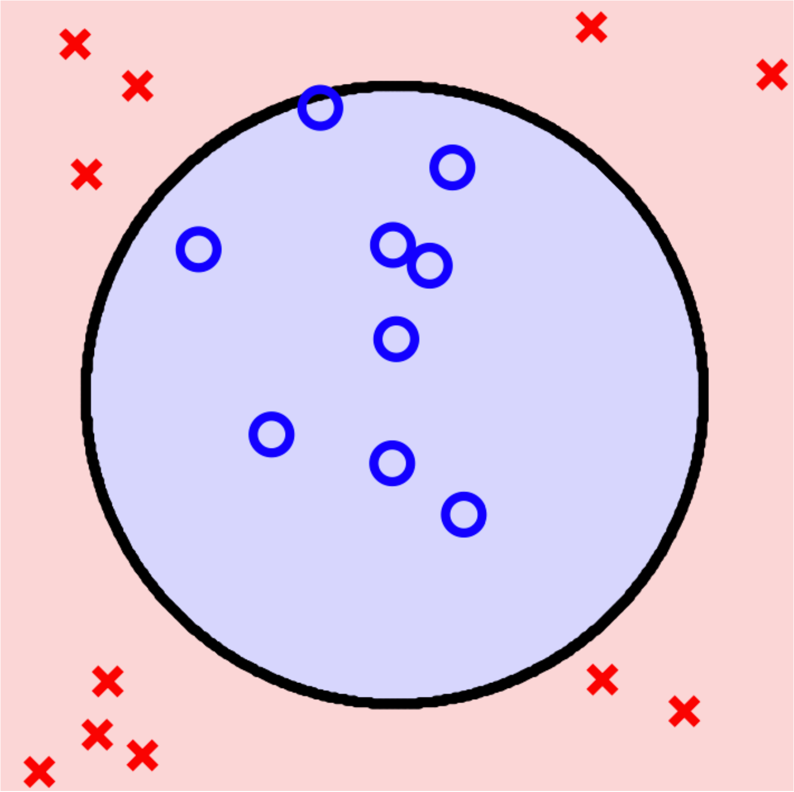
Lecture 7
Kernel Method
(Going Beyond Linear Hypothesis Efficiently)

A simple way to go beyond linear hypothesis space: feature mapping



Not linearly separable in 2 dimensions.
Using logistic regression will also give large error.

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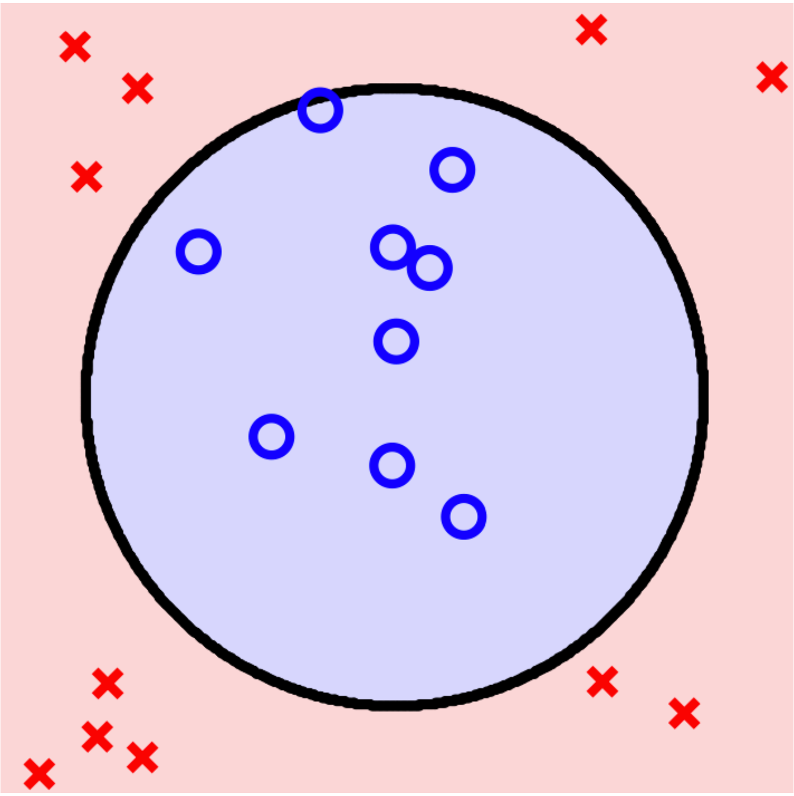

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Using logistic regression will also give large error.

Solution: go to higher dimension via *a feature map!*

$$\Phi(x_1, x_2) = \left(x_1, x_2, x_1^2 + x_2^2\right)$$

This clearly will be linearly separable in 3 dimensions!

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$$\Phi : X \to F$$

where typically $|X| = d \ll |F| = p$.

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An illustrative simple example could be $\mathbf{x} = \left(x_1, x_2\right) \mapsto \Phi(\mathbf{x}) = \left(x_1^2, \sqrt{2}x_1x_2, x_2^2\right)$,

so the hypothesis space is no longer linear, but a polynomial of degree 2.
This is particularly useful, because points that are not classified by a linear model might be easily classified by a linear model in a *feature space*.

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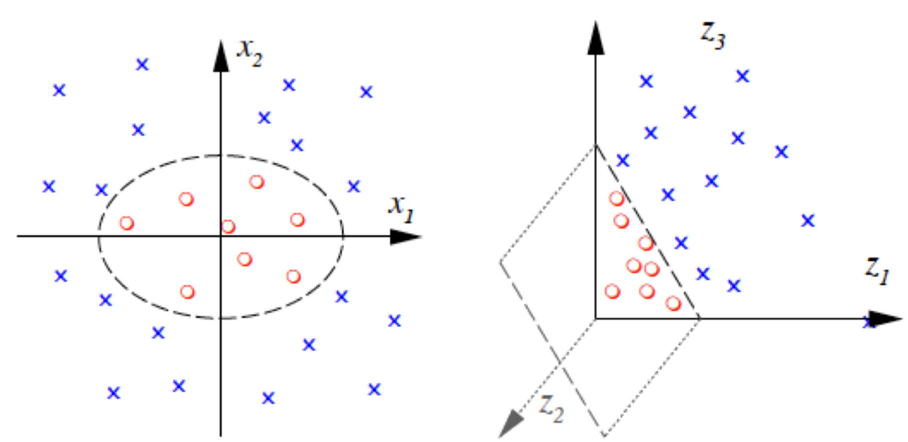
$$\Phi : R^2 \to R^3$$
$$(x_1, x_2) \mapsto (z_1, z_2, z_3) := (x_1^2, \sqrt{2}x_1x_2, x_2^2)$$



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Importantly, it's not difficult to see that solving Tikhonov regularization problem

$$\min_{\mathbf{w} \in \mathbb{R}^p} \frac{1}{n} \sum_{i=1}^{n} \ell \left(y_i, f_{\mathbf{w}}\left(\mathbf{x}_i\right)\right) + \lambda \|\mathbf{w}\|^2$$

is essentially the same, up to replacing $\mathbf{x} \in \mathbb{R}^D$ by the *feature vector* $\Phi(\mathbf{x}) \in \mathbb{R}^p$, as what we have done earlier in this class!

A simple way to go beyond linear hypothesis space: feature mapping

Consider

$$\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_d \end{pmatrix} \qquad \text{and} \qquad \phi(\mathbf{x}) = \begin{pmatrix} 1 \\ x_1 \\ \vdots \\ x_d \\ x_1 x_2 \\ \vdots \\ x_{d-1} x_d \\ \vdots \\ x_1 x_2 \dots x_d \end{pmatrix}$$

This feature map is *very expressive*, and allows complicated *non-linear decision boundaries*; however, its dimension is $p = 2^d$ and hence is *prohibitively unbearable* (computationally)!

The Kernel Trick

The kernel trick is a way to get around this dilemma by learning a function in a much higher dimensional space, without ever computing a single vector $\Phi(\mathbf{x})$ or $\mathbf{w}$. The magic sauce behind this is the *representer theorem*, which we will not prove here but provides a note for you to read.

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The representer theorem states that the solution to the Tikhonov regularization problem

$$\min_{\mathbf{w}\in\mathbb{R}^D} \frac{1}{n}\sum_{i=1}^{n} \ell\left(y_i, f_{\mathbf{w}}\left(\mathbf{x}_i\right)\right) + \lambda\|\mathbf{w}\|^2$$

can always be written as a linear combination of input features as

$$\boxed{\hat{\mathbf{w}}^T = \sum_{i=1}^{n} \Phi(\mathbf{x}_i)^T w_i}$$

where w_i is a scalar coefficient.

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This implies that the empirically optimal hypothesis function can be written as an inner-product

$$\underbrace{\hat{f}_{\hat{\mathbf{w}}}(\mathbf{x})}_{}\overset{O(p^2)!!}{} = \hat{\mathbf{w}}^T\Phi(\mathbf{x}) = \sum_{i=1}^{n} w_i \Phi(\mathbf{x}_i)^T\Phi(\mathbf{x})$$

The solution depends on the input feature only via the inner product!

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The solution depends on the input feature only via the inner product!

$$= \sum_{i=1}^{n} w_i \underbrace{\langle \Phi(\mathbf{x}_i), \Phi(\mathbf{x})\rangle}_{\equiv K(\mathbf{x}_i,\mathbf{x})}$$

$O(n^2)$

Kernel Trick

Replace an inner product with a more general function, with inner product-like property (hence the name *kernel*)

save computational resource!

General Kernels

So Kernel method converts risk minimisation problem in high-dimensional feature space to learning the linear combination

$$\hat{f}(\mathbf{x}) = \sum_{i=1}^{n} w_i K(\mathbf{x}_i, \mathbf{x})$$

where a kernel function $K(\mathbf{x}, \mathbf{x}')$ must behave like an inner-product, that is $K(\mathbf{x}, \mathbf{x}')$ must be symmetric, and positive semi-definite.

Examples

Linear Kernel

$$K(\mathbf{x}, \mathbf{x}') = \mathbf{x}^T \mathbf{x}'$$

Similar to a good old linear classifier,
but can be faster if the dimension of data
is large compared to the number of data.

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Gaussian Kernel
Radial Basis Function (RBF)

$$K(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{\| \mathbf{x} - \mathbf{x}' \|^2}{2\sigma^2}\right)$$

The most popular kernel

- It is a universal approximator. (hence the name basis function)

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Note that for RBF the feature space of the kernel has an infinite number of dimensions; for $\sigma = 1$, for example, it can be expanded as

$$\exp\left(-\frac{1}{2} \| \mathbf{x} - \mathbf{x}' \|^2\right) = \sum_{j=0}^{\infty} \frac{(\mathbf{x}^\top \mathbf{x}')^j}{j!} \exp\left(-\frac{1}{2}\|\mathbf{x}\|^2\right) \exp\left(-\frac{1}{2} \| \mathbf{x}' \|^2\right)$$

$$= \sum_{j=0}^{\infty} \sum_{\sum n_i = j} \exp\left(-\frac{1}{2}\|\mathbf{x}\|^2\right) \frac{x_1^{n_1} \cdots x_k^{n_k}}{\sqrt{n_1! \cdots n_k!}} \exp\left(-\frac{1}{2} \| \mathbf{x}' \|^2\right) \frac{x_1'^{n_1} \cdots x'^{n_k}_k}{\sqrt{n_1! \cdots n_k!}}$$

Kernel Machines and How to Train Them

$$\hat{\mathbf{w}} = \min_{\mathbf{w} \in \mathbb{R}^D} \sum_{i=1}^{n} \left(y_i - f_{\mathbf{w}}\left(\mathbf{x}_i\right) \right)^2 + \lambda \|\mathbf{w}\|^2$$

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$$= \min_{\mathbf{w}\in\mathbb{R}^D} \sum_{i,j=1}^{n} \left(y_j - w_i K(\mathbf{x}_i, \mathbf{x}_j)\right)^2 + \lambda\|\mathbf{w}\|^2$$

$\mathbf{K}$ matrix of size n^2

ridge regression

$$\hat{\mathbf{w}} = \left(X^T X + \lambda I\right)^{-1} X^T \mathbf{y}$$

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$$\hat{\mathbf{w}} = \left(X^T X + \lambda I\right)^{-1} X^T \mathbf{y}$$

kernel ridge regression

$$\hat{\mathbf{w}} = (\mathbf{K} + \lambda I)^{-1} \mathbf{y}$$

Example usage of Kernel method: RBFs for Regression (Curve-fitting)

$$h(\mathbf{x}) = \sum_{i=1}^{n} w_i \exp\left(- \parallel \mathbf{x} - \mathbf{x}_i \parallel ^2 / 2\sigma^2\right)$$

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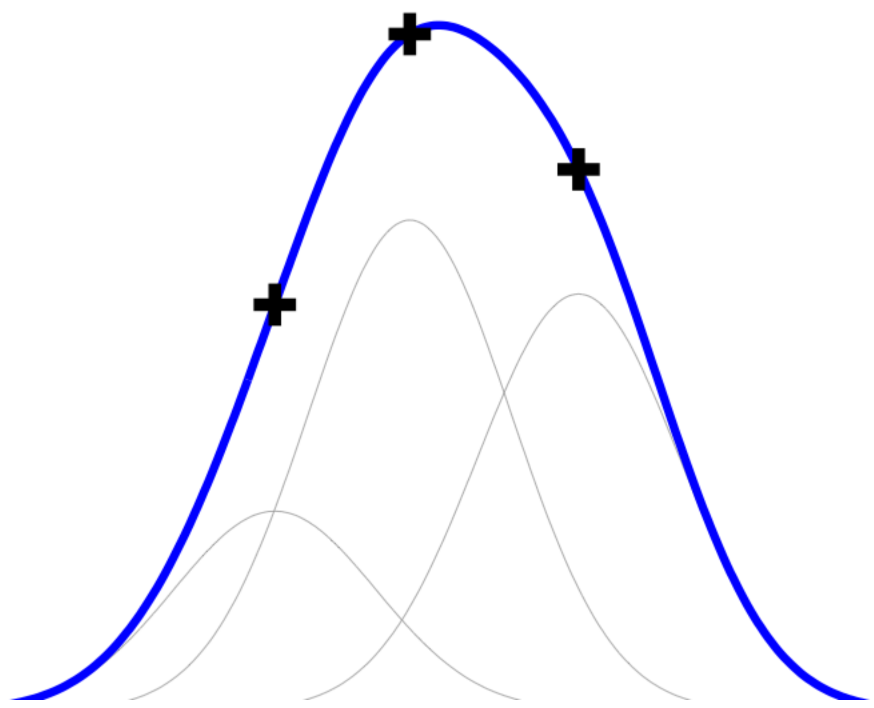
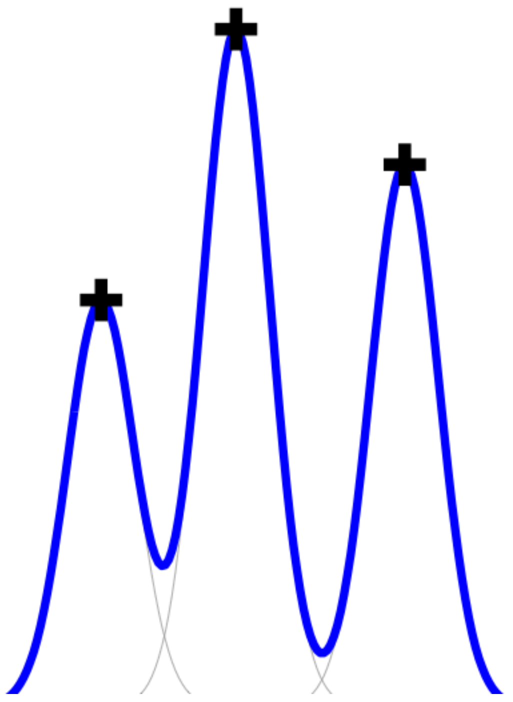
$n = 3$



large σ



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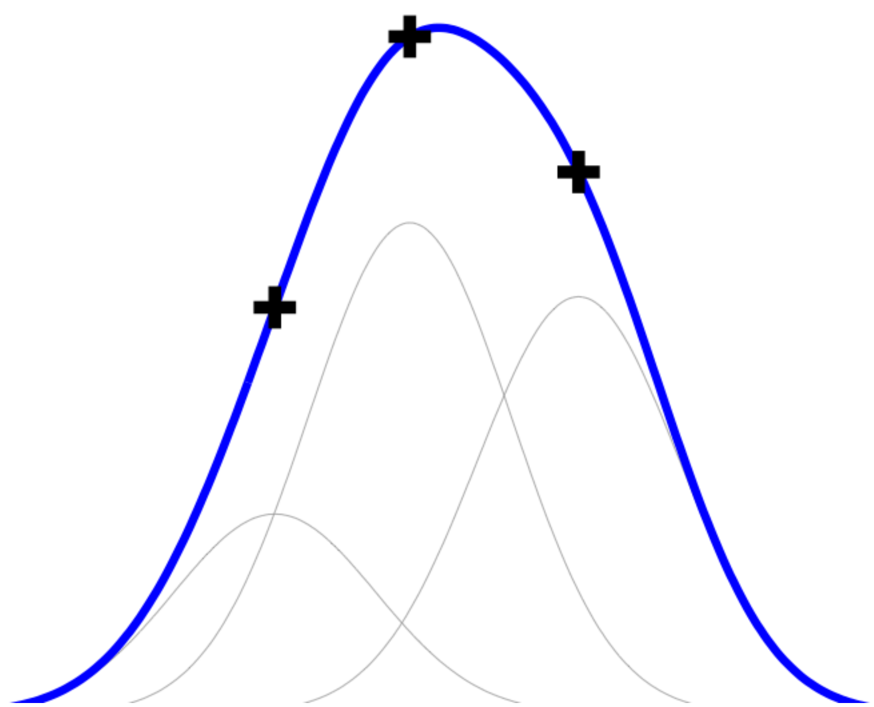

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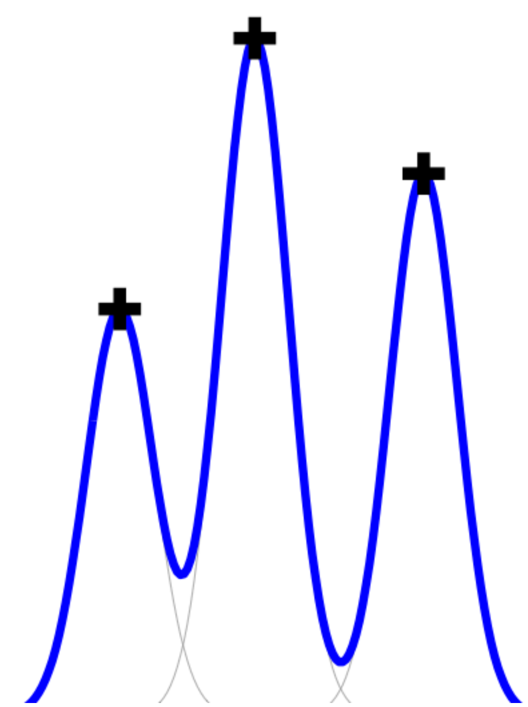
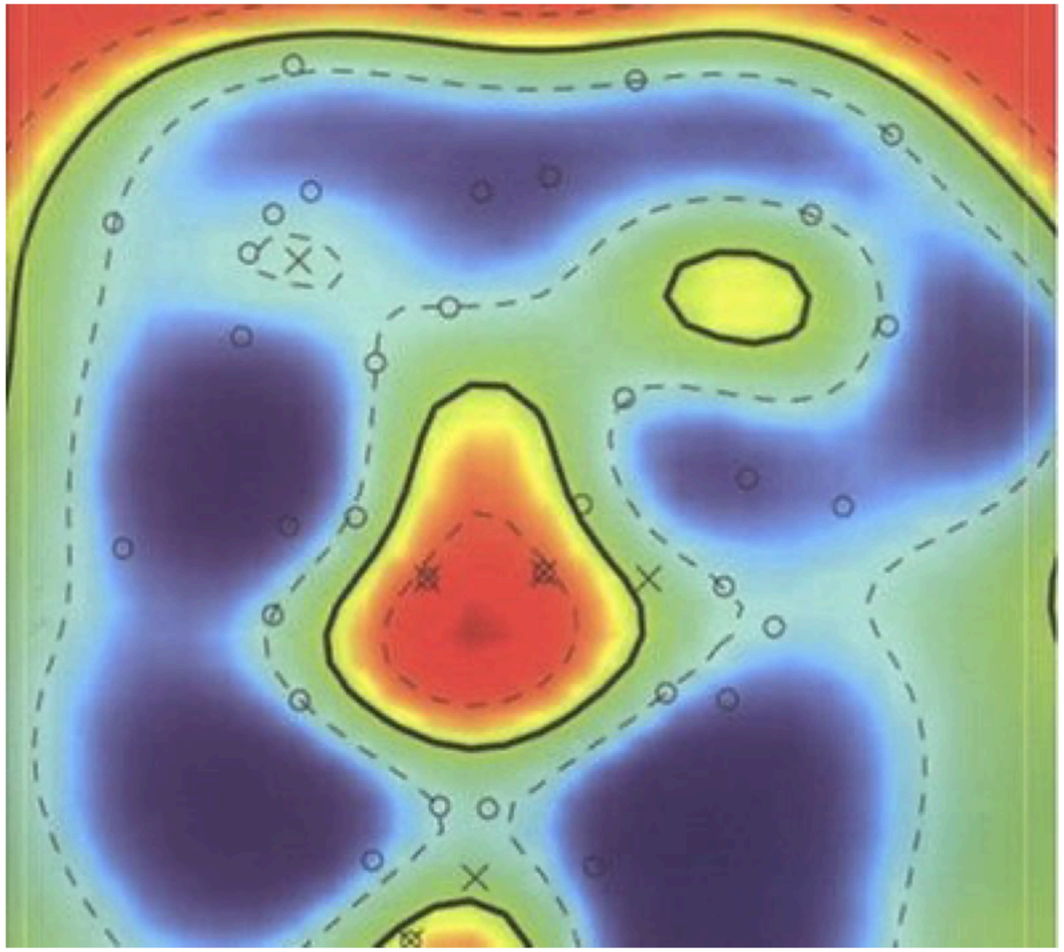


small σ

more expressive, but can overfit

Example usage of Kernel method: RBFs for Classification

$$h(\mathbf{x}) = \text{sign}\left[\sum_{i=1}^{n} w_i \exp\left(- \| \mathbf{x} - \mathbf{x}_i \|^2 / 2\sigma^2\right)\right]$$



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