University of Amsterdam
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AMLAB Amsterdam Machine Learning Lab

Machine Learning 1

Lecture 11.2 - Kernel Methods
Kernel Trick - Valid Kernels

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(Bishop 6.2)


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Kernel Trick/Kernel substitution

- Formulate your optimization problem in such a way that the input vectors $\mathbf{x}_n$ enter only in the form of scalar products:

$$\mathbf{x}_n^T \mathbf{x}_n \qquad \text{(or when using basis functions } \boldsymbol{\phi}(\mathbf{x}_n)^T \boldsymbol{\phi}(\mathbf{x}_n))$$

- Replace all instances of $\mathbf{x}_n^T \mathbf{x}_m$ with a kernel function

$$k(\mathbf{x}_n, \mathbf{x}_m) = K_{nm}$$

store in Gram matrix $N \times N$

- Kernel $k(\mathbf{x}_n, \mathbf{x}_m)$ corresponds to a scalar product in some (possibly infinite dimensional) feature space.

- Valid kernel: $\boxed{\text{Gram Matrix } \mathbf{K}}$ must be symmetric positive semi definite for all possible choices of $\{\mathbf{x}_n\}_{n=1}^N$

$\underline{z}^T K \underline{z} \geq 0, \; \underline{z} \in \mathbb{R}^N, \; K \in \mathbb{R}^{N \times N}$

$k(\underline{x}, \underline{x}') = \phi(x)^T \phi(x')$:

$\underline{z}^T K \underline{z} = \underline{z}^T \Phi \Phi^T \underline{z} = (\Phi^T \underline{z})^T (\Phi^T \underline{z}) = \|\Phi^T \underline{z}\|^2 \geq 0$

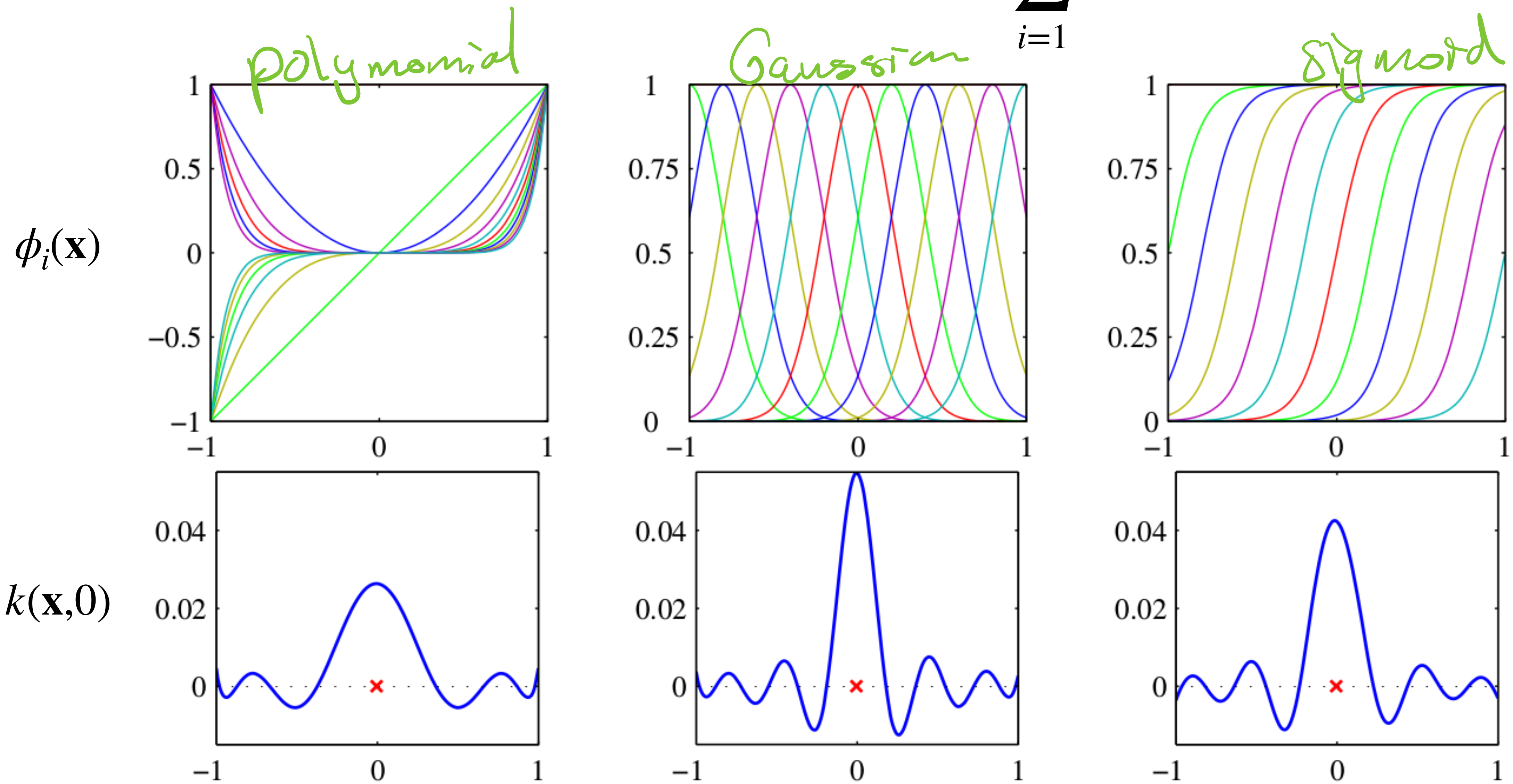
Constructing valid kernels

- Construct kernel from explicit set of basis functions:

$$k(\mathbf{x},\mathbf{x}') = \boldsymbol{\phi}(\mathbf{x})^T\boldsymbol{\phi}(\mathbf{x}') = \sum_{i=1}^{M} \phi_i(\mathbf{x})\phi_i(\mathbf{x}')$$

$$\begin{pmatrix} \boldsymbol{\Sigma} = \mathbf{U}^T\boldsymbol{\Lambda}\mathbf{U} \\ \boldsymbol{\Sigma}^{1/2} = \mathbf{U}^T\boldsymbol{\Lambda}^{1/2}\mathbf{U} \\ \boldsymbol{\psi}(\mathbf{x}) = \boldsymbol{\Sigma}^{1/2}\boldsymbol{\phi}(\mathbf{x}) \end{pmatrix}$$

$$k(\mathbf{x},\mathbf{x}') = \boldsymbol{\phi}(\mathbf{x})^T\boldsymbol{\Sigma}\boldsymbol{\phi}(\mathbf{x}') = \boldsymbol{\psi}(\mathbf{x})^T\boldsymbol{\psi}(\mathbf{x}') = \sum_{i=1}^{M} \psi_i(\mathbf{x})\psi_i(\mathbf{x}')$$



Deriving the corresponding feature vector

- For every positive definite kernel there exists $\boldsymbol{\phi} : \mathbb{R}^d \rightarrow \mathbb{R}^M$ such that

$$k(\mathbf{x}, \mathbf{x}') = \boldsymbol{\phi}(\mathbf{x})^T \boldsymbol{\phi}(\mathbf{x})$$

- Depending on the kernel, M can be infinite!

- In general difficult to retrieve the corresponding $\boldsymbol{\phi}(\mathbf{x})$ for a given kernel

Example: polynomial kernel

- Polynomial kernel of order $M = 2$ for $\mathbf{x}, \mathbf{z} \in \mathbb{R}^2$

$$k(\mathbf{x}, \mathbf{z}) = (1 + \mathbf{x}^T\mathbf{z})^2 = (1 + x_1 z_1 + x_2 z_2)^2 = (1 + x_1 z_1 + x_2 z_2)(1 + x_1 z_1 + x_2 z_2)$$

$$= 1 + 2x_1z_1 + 2x_2z_2 + (x_1z_1)^2 + (x_2z_2)^2 + 2x_1z_1x_2z_2$$

rewrite in the form $\phi(x)^T \phi(z)$

$\phi_0(z) = 1$, $\phi_1(z) = \sqrt{2}z_1$, - - - -, $\phi_5(z) = \sqrt{2}z_1z_2$

$$= \underbrace{(1, \sqrt{2}x_1, \sqrt{2}x_2, x_1^2, x_2^2, \sqrt{2}x_1x_2)}_{\phi(x)}{}^T \underbrace{(1, \sqrt{2}z_1, \sqrt{2}z_2, z_1^2, z_2^2, \sqrt{2}z_1z_2)}_{\phi(z)}$$

$$= \boldsymbol{\phi}(\mathbf{x})^T \boldsymbol{\phi}(\mathbf{z})$$

- And thus the corresponding kernel $\boldsymbol{\phi}(\mathbf{x}) \in \mathbb{R}^6$

Examples

- Generalized polynomial kernel

$$k(\mathbf{x}, \mathbf{x}') = (c + \mathbf{x}^T\mathbf{x}')^M$$

- Gaussian kernel/squared exponential kernel: infinite dimensional space!

$$\underline{\phi}(\underline{x}) \in \mathbb{R}^{M = \infty}$$

$$k(\mathbf{x}, \mathbf{x}') = \exp(-\frac{1}{2\sigma^2}||\mathbf{x} - \mathbf{x}'||^2)$$

- Radial basis functions:

$$k(\mathbf{x}, \mathbf{x}') = k(||\mathbf{x} - \mathbf{x}'||^2)$$

Construct new kernels from other kernels

Example Bishop 6.2

$k(\underline{x}, \underline{x}') = \exp(-\|\underline{x}-\underline{x}'\|^2/2)$

derived from

$k_0(\underline{x}, \underline{x}') = \underline{x}^T \underline{x}'$

Each of these kernels correspond to some

$k(\underline{x}, \underline{x}') = \underline{\phi}(\underline{x})^T \underline{\phi}(\underline{x}')$

$$
\begin{aligned}
k(\mathbf{x}, \mathbf{x}') &= c k_1(\mathbf{x}, \mathbf{x}') \\
k(\mathbf{x}, \mathbf{x}') &= f(\mathbf{x}) k_1(\mathbf{x}, \mathbf{x}') f(\mathbf{x}') \\
k(\mathbf{x}, \mathbf{x}') &= q\left(k_1(\mathbf{x}, \mathbf{x}')\right) \\
k(\mathbf{x}, \mathbf{x}') &= \exp\left(k_1(\mathbf{x}, \mathbf{x}')\right) \\
k(\mathbf{x}, \mathbf{x}') &= k_1(\mathbf{x}, \mathbf{x}') + k_2(\mathbf{x}, \mathbf{x}') \\
k(\mathbf{x}, \mathbf{x}') &= k_1(\mathbf{x}, \mathbf{x}') k_2(\mathbf{x}, \mathbf{x}') \\
k(\mathbf{x}, \mathbf{x}') &= k_3\left(\boldsymbol{\phi}(\mathbf{x}), \boldsymbol{\phi}(\mathbf{x}')\right) \\
k(\mathbf{x}, \mathbf{x}') &= \mathbf{x}^{\mathrm{T}} \mathbf{A} \mathbf{x}' \\
k(\mathbf{x}, \mathbf{x}') &= k_a(\mathbf{x}_a, \mathbf{x}'_a) + k_b(\mathbf{x}_b, \mathbf{x}'_b) \\
k(\mathbf{x}, \mathbf{x}') &= k_a(\mathbf{x}_a, \mathbf{x}'_a) k_b(\mathbf{x}_b, \mathbf{x}'_b)
\end{aligned}
$$