# Kernels and the Kernel Trick

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Reading Club "Support Vector Machines"

# Optimization Problem

- maximize:

$$W(\alpha) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} \alpha_j \alpha_j y_i y_j \langle x_i \cdot x_j \rangle$$

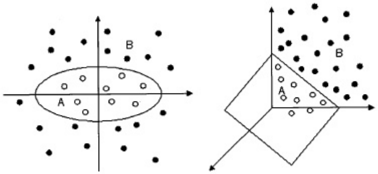
subject to $\alpha_i \geq 0, i = 1, \ldots, m$ and $\sum_{i=1}^{m} \alpha_i y_i = 0$

- data not linear separable in input space

$\longrightarrow$ map into some feature space where data is linear separable

# Mapping Example

- map data points into feature space with some function $\phi$
- e.g.:
  - $\phi : \mathbb{R}^2 \rightarrow \mathbb{R}^2$
  - $(x_2, x_2) \rightarrow (z_1, z_2, z_3) := (x_1^2, \sqrt{2}x_1x_2, x_2^2)$




- hyperplane $\langle w \cdot z \rangle = 0$, as a function of x:

$$w_1x_1^2 + w_2\sqrt{2}x_1x_2 + w_3x_2^2 = 0$$

# Kernel Trick

- solve maximisation problem using mapped data points

$$W(\alpha) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} \alpha_j \alpha_j y_i y_j \langle \phi(x_i) \cdot \phi(x_j) \rangle$$

- Dual Representation of Hyperplane (↺ primal Lagrangian):

$$f(x) = \langle w \cdot x \rangle + b = \sum \alpha_i y_i \langle x_i \cdot x \rangle \quad \text{with} \quad w = \sum \alpha_i y_i x_i$$

- weight vector represented only by data points
- only inner product of data points necessary, no coordinates
- kernel function $K(x_1, x_2) = \langle \phi(x_i) \cdot \phi(x_j) \rangle$

  $\longrightarrow$ $\phi$ not necessary any more

  $\longrightarrow$ possible to operate in any n-dimensional $FS$

  $\longrightarrow$ complexity independent of $FS$

# Example Kernel Trick

$$\vec{x} = (x_1, x_2)$$
$$\vec{z} = (z_1, z_2)$$
$$K(x, z) = \langle \vec{x} \cdot \vec{z} \rangle^2$$

$$\begin{aligned}
K(x, z) &= \langle \vec{x} \cdot \vec{z} \rangle^2 \\
&= (x_1 z_1 + x_2 z_2)^2 \\
&= (x_1^2 z_1^2 + 2 x_1 z_1 x_2 z_2 + x_2^2 z_2^2) \\
&= \left\langle (x_1^2, \sqrt{2} x_1 x_2, x_2^2) \cdot (z_1^2, \sqrt{2} z_1 z_2, z_2^2) \right\rangle \\
&= \langle \phi(\vec{x}) \cdot \phi(\vec{z}) \rangle
\end{aligned}$$

mapping function $\phi$ fused in $K$

$\rightarrow$ implicit $\phi(\vec{x}) = (x_1^2, \sqrt{2} x_1 x_2, x_2^2)$

# Typical Kernels

- **Polynomial Kernel**

$$K(x,z) = \left(\langle x \cdot z \rangle + \theta\right)^d, \qquad for \;\; d \geq 0$$

- **Radial Basis Function** (Gaussian Kernel)

$$K(x,z) = e^{-\frac{\|x-z\|^2}{2\sigma^2}} \qquad \|x\| := \sqrt{\langle x \cdot x \rangle}$$

- (**Sigmoid Kernel**)

$$K(x,z) = tanh(\eta \langle x \cdot z \rangle + \theta$$

- **Inverse multi-quadric**

$$K(x,z) = \frac{1}{\sqrt{\|x-z\|^2 2\sigma^2 + c^2}}$$

# Typical Kernels Cont.

- **Kernels for Sets** - $\chi, \chi'$

$$K - s(\chi, \chi') = \sum_{i=1}^{N_\chi} \sum_{j=1}^{N_{\chi'}} k(x_i, x_j')$$

where $k(x_i, x_j')$ is a kernel on elements in $\chi, \chi'$

- Kernels for strings (Spectral Kernels) and trees

$\longrightarrow$ no one-fits-all kernel

$\longrightarrow$ model search and cross-validation in practice

$\longrightarrow$ low polynomial or RBF a good initial try

# Kernel Properties

- Symmetry

$$K(x,z) = \langle \phi(x) \cdot \phi(z) \rangle = \langle \phi(z) \cdot \phi(x) \rangle = K(z,x)$$

- Cauchy-Schwarz Inequality

$$\begin{aligned} K(x,z)^2 &= \langle \phi(x) \cdot \phi(z) \rangle^2 \leq \|\phi(x)\|^2 \|\phi(z)\|^2 \\ &= \langle \phi(x) \cdot \phi(x) \rangle \langle \phi(z) \cdot \phi(z) \rangle \\ &= K(x,x) K(z,z) \end{aligned}$$

# Making Kernels from Kernels

- create complex Kernels by combining simpler ones
- Closure Properties:

$$
\begin{aligned}
K(x,z) &= c \cdot K_1(x,z) \\
K(x,z) &= c + K_1(x,z) \\
K(x,z) &= K_1(x,z) + K_2(x,z) \\
K(x,z) &= K_1(x,z) \cdot K_2(x,z) \\
K(x,z) &= f(x) \cdot f(z)
\end{aligned}
$$

if $K_1$ and $K_2$ are kernels, $\forall f : X \to \mathbb{R}$, and $c > 0$

# Gram Matrix

- Kernel function as similarity measure between input objects
- Gram Matrix (Similarity/Kernel Matrix) represents similarities between input vectors
- let $V = \vec{v}_1, \ldots, \vec{v}_n$ a set of input vectors, then the Gram Matrix $\mathbf{K}$ is defined as:

$$\mathbf{K} = \begin{pmatrix} \langle \phi(\vec{v}_1) \cdot \phi(\vec{v}_1) \rangle & \ldots & \langle \phi(\vec{v}_1) \cdot \phi(\vec{v}_n) \rangle \\ \langle \phi(\vec{v}_2) \cdot \phi(\vec{v}_1) \rangle & \ddots & \vdots \\ \vdots & & \\ \langle \phi(\vec{v}_n) \cdot \phi(\vec{v}_1) \rangle & \ldots & \langle \phi(\vec{v}_n) \cdot \phi(\vec{v}_n) \rangle \end{pmatrix}$$

- $\mathbf{K}$ is symmetric and positive semis-definite (positive eigenvalues)

# Mercer's Theorem

- assume:
  - finite input space $X = \{\mathbf{x_1}, \dots, \mathbf{x_n}\}$
  - symmetric function $K(\mathbf{x}, \mathbf{z})$ on X
  - Gram Matrix $\mathbf{K} = (K(x_i, x_j))_{i,j=1}^n$
  - since $\mathbf{K}$ is symmetric there exists an orthogonal matrix $\mathbf{V}$ s.t. $\mathbf{K} = \mathbf{V\Lambda V'}$
  - diagonal $\Lambda$ containing eigenvalues $\lambda_t$ of $\mathbf{K}$
  - and eigenvectors $\mathbf{v_t} = (v_{ti})_{i=1}^n$ as columns of $\mathbf{V}$
  - all eigenvalues are non-negative and let feature mapping be

$$\phi : \mathbf{x_i} \mapsto \left(\sqrt{\lambda_i} v_{ti}\right)_{t=1}^n \in \mathbb{R}^n, i = 1, \dots, n.$$

- then

$$\langle \phi(x_i) \cdot \phi(x_j) \rangle = \sum_{t=1}^n \lambda_t v_{ti} v_{tj} = (\mathbf{V\Lambda V'})_{ij} = \mathbf{K}_{ij} = K(x_i, x_j)$$

# Mercer's Theorem Cont.

- every Gram Matrix is symmetric and positive semi-definite
- every spsd matrix can be regarded as a Kernel Matrix, i.e. as an inner product matrix in some space
- diagonal matrix satisfies Mercer's criteria, but not good as Gram Matrix
  - self-similarity dominates between-sample similarity
  - represents orthogonal samples
- generalization for infinite input space
  - ⇝ eigenvectors of the data in can be used to detect directions of maximum variance
  - ⇝ kernel principal components analysis

# Summary

- Kernel calculates dot product of mapped data points without mapping function $\phi$
- represented by symmetric, positive semi-definite Gram Matrix
  - fuses information about data *and* kernel
- standard kernels (cross validation)
- every similarity matrix can be used as kernel (satisfying Mercer's criteria)
- ongoing research to estimate Kernel Matrix from available data