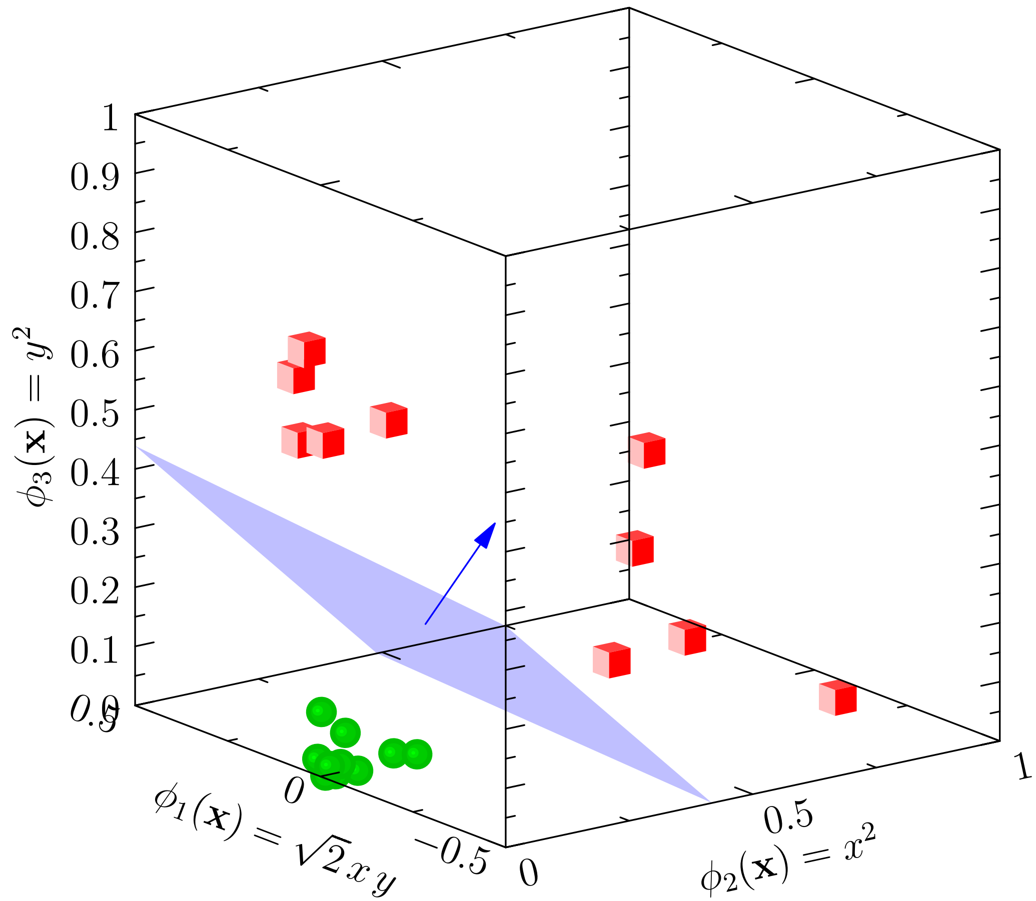
Advanced Machine Learning

Kernel Trick



The Kernel Trick, SVMs, Regression

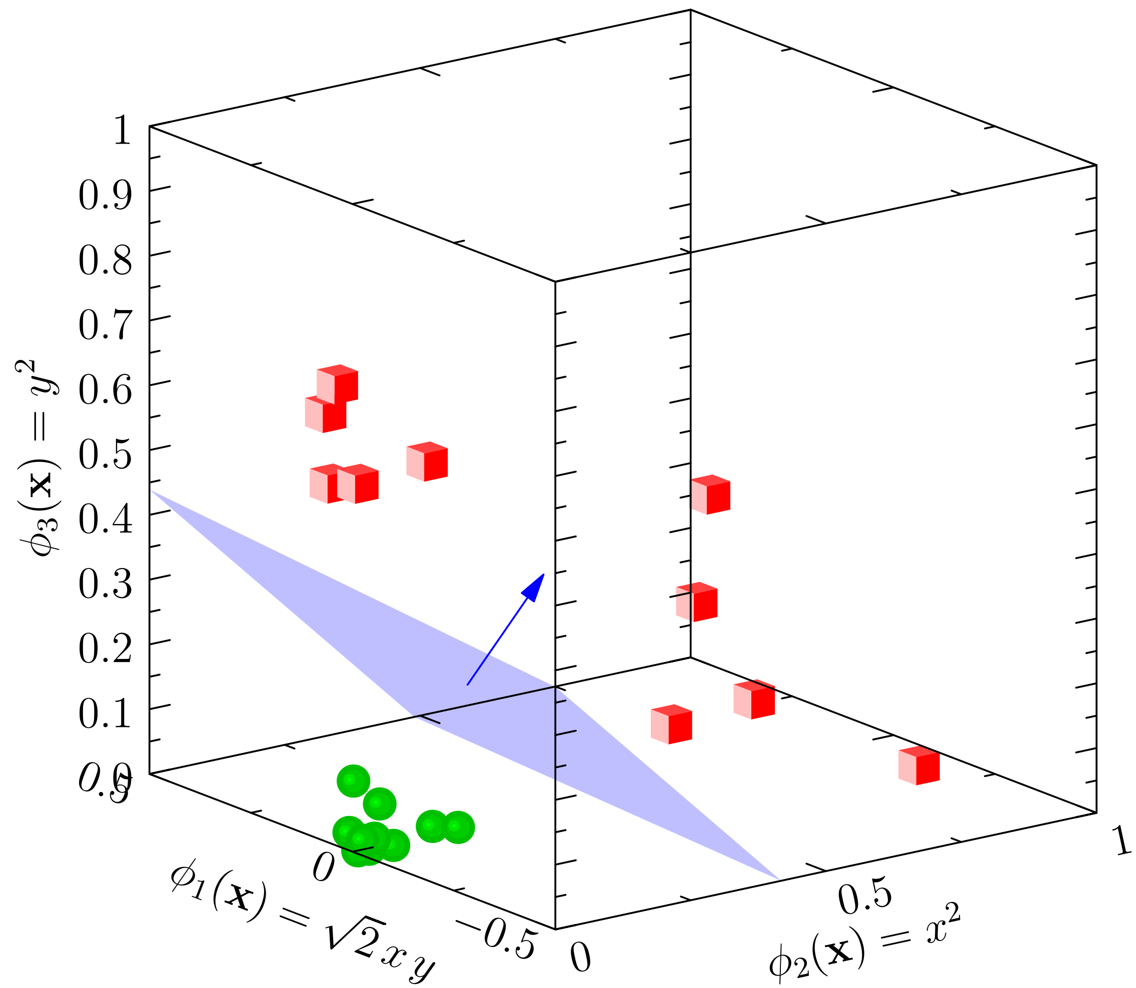
Outline

1. **The Kernel Trick**

2. Positive Semi-Definite Kernels

3. Kernel Properties

4. Beyond Classification



SVM Kernels

- SVM Kernels are functions of two variables that can be factorised

$$K(\boldsymbol{x},\boldsymbol{y}) = \langle \boldsymbol{\phi}(\boldsymbol{x}),\boldsymbol{\phi}(\boldsymbol{y})\rangle = \sum_i \phi_i(\boldsymbol{x})\,\phi_i(\boldsymbol{y})$$

- where $\boldsymbol{\phi}(\boldsymbol{x}) = (\phi_1(\boldsymbol{x}), \phi_2(\boldsymbol{x}), \ldots)^{\mathsf{T}}$ and $\phi_i(\boldsymbol{x})$ are real valued functions of $\boldsymbol{x}$

- $K(\boldsymbol{x},\boldsymbol{y})$ will be positive semi-definite (because it is an inner-product)

- Furthermore, any positive semi-definite function will factorise

- This factorisation is not always obvious (we return to this later)

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Dual Form

- Recall that the dual problem for an SVM is

$$\max_{\boldsymbol{\alpha}} \sum_{k=1}^{m} \alpha_k - \frac{1}{2} \sum_{k,l=1}^{m} \alpha_k \alpha_l y_k y_l \langle \boldsymbol{\phi}(\boldsymbol{x}_k), \boldsymbol{\phi}(\boldsymbol{x}_l) \rangle$$

- subject to $\sum_{k=1}^{m} y_k \alpha_k = 0$ and $0 \leq \alpha_k (\leq C)$
- But since $K(\boldsymbol{x}_k, \boldsymbol{x}_l) = \langle \boldsymbol{\phi}(\boldsymbol{x}_k), \boldsymbol{\phi}(\boldsymbol{x}_l) \rangle$ the dual problem becomes

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- This is the **kernel trick**—we never have to compute $\boldsymbol{\phi}(\boldsymbol{x})$!

Classifying New Data

- Having trained the SVM we now have to use it
- Given a new input $\boldsymbol{x}$ we decide on the class

$$y = \operatorname{sgn}(\langle \boldsymbol{w}, \boldsymbol{\phi}(\boldsymbol{x}) \rangle - b) \qquad \text{but} \qquad \boldsymbol{w} = \sum_{k=1}^{m} \alpha_k y_k \boldsymbol{\phi}(\boldsymbol{x}_k)$$

- In the dual representation this becomes

$$\operatorname{sgn}\left(\sum_{k=1}^{m} \alpha_k y_k K(\boldsymbol{x}_k, \boldsymbol{x}) - b \right)$$

where we only need to sum over the non-zero α_k (i.e. the support vectors SVs)

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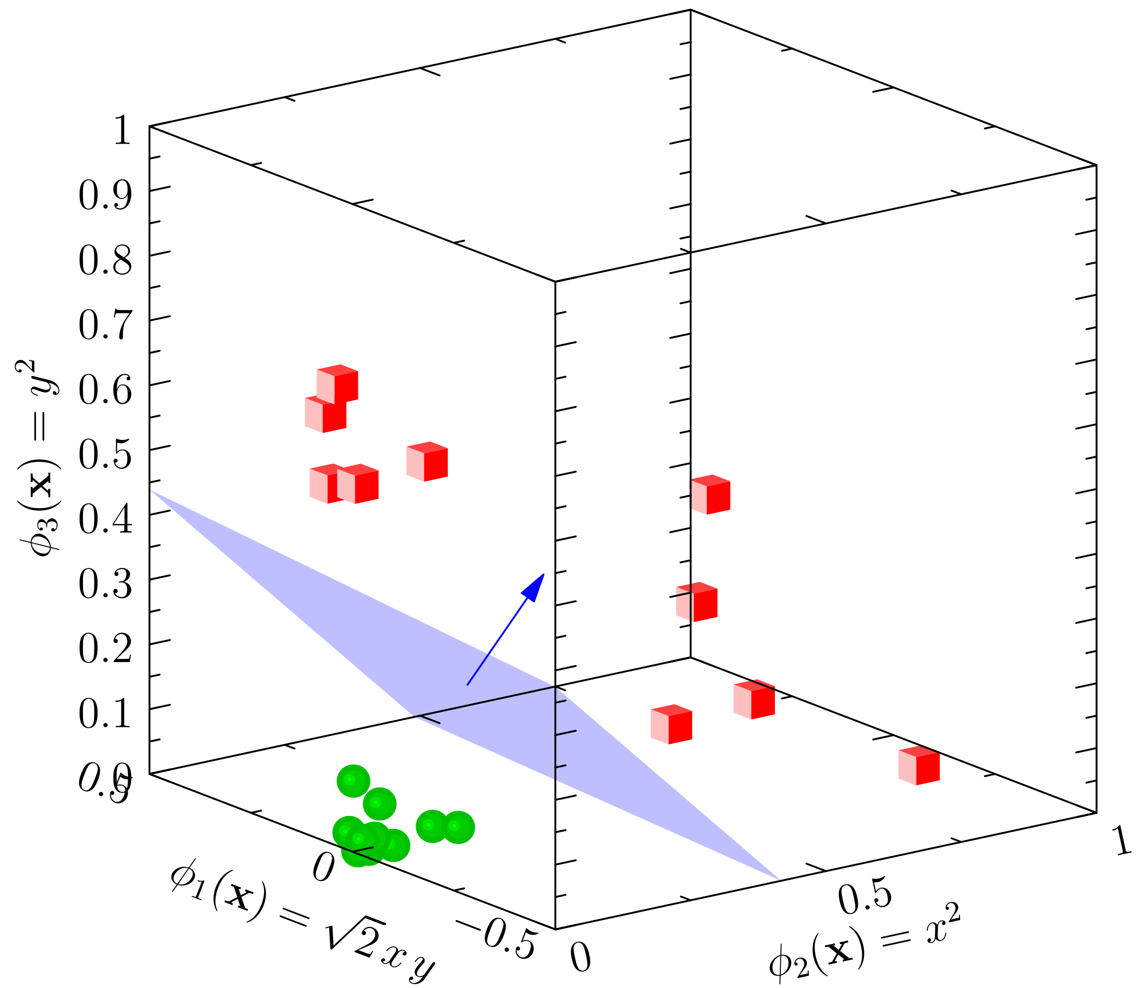

Recap on Eigen Systems

- Recall for a symmetric $(n \times n)$ matrix $\boldsymbol{M}$ an eigenvector, $\boldsymbol{v}$

$$\boldsymbol{M}\boldsymbol{v} = \lambda \boldsymbol{v}$$

- There are n independent eigenvectors $\boldsymbol{v}^{(i)}$ with real eigenvalues $\lambda^{(i)}$

- The eigenvectors are orthogonal so that $\boldsymbol{v}^{(i)\mathsf{T}}\boldsymbol{v}^{(j)} = 0$ if $i \neq j$

- Forming a matrix of eigenvectors $\mathbf{V} = (\boldsymbol{v}^{(1)}, \boldsymbol{v}^{(2)}, \ldots \boldsymbol{v}^{(n)})$ the matrix satisfies

$$\mathbf{V}^{\mathsf{T}}\mathbf{V} = \mathbf{V}\mathbf{V}^{\mathsf{T}} = \mathbf{I}$$

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Eigen Decomposition

- From the eigenvalue equation $\mathbf{M}\boldsymbol{v}^{(k)} = \lambda^{(k)}\boldsymbol{v}^{(k)}$

$$\mathbf{M}\mathbf{V} = \mathbf{V}\boldsymbol{\Lambda} \qquad \text{where} \quad \boldsymbol{\Lambda} = \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{pmatrix}$$

- Multiplying on the right by $\mathbf{V}^{\mathsf{T}}$ we get

$$\mathbf{M} = \mathbf{V}\boldsymbol{\Lambda}\mathbf{V}^{\mathsf{T}} = \sum_{k=1}^{n} \lambda^{(k)} \boldsymbol{v}^{(k)} \boldsymbol{v}^{(k)\mathsf{T}}$$

Or

$$M_{ij} = \sum_{k=1}^{n} \lambda^{(k)} v_i^{(k)} v_j^{(k)}$$

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$$M_{ij} = \sum_{k=1}^{n} \lambda^{(k)} v_i^{(k)} v_j^{(k)} = \sum_{k=1}^{n} u_i^{(k)} u_j^{(k)} = \langle \boldsymbol{u}_i, \boldsymbol{u}_j \rangle$$

$$u_i^{(k)} = \sqrt{\lambda^{(k)}}\, v_i^{(k)}$$

Eigenfunctions

- By analogy for a symmetric function of two variables we can define an *eigenfunction*

$$\int K(\boldsymbol{x},\boldsymbol{y})\psi(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y} = \lambda\psi(\boldsymbol{x})$$

- In general there will be a denumerable set of eigenfunctions $\psi^{(k)}(\boldsymbol{x})$ where

$$K(\boldsymbol{x},\boldsymbol{y}) = \sum_k \lambda^{(k)}\psi^{(k)}(\boldsymbol{x})\psi^{(k)}(\boldsymbol{y})$$

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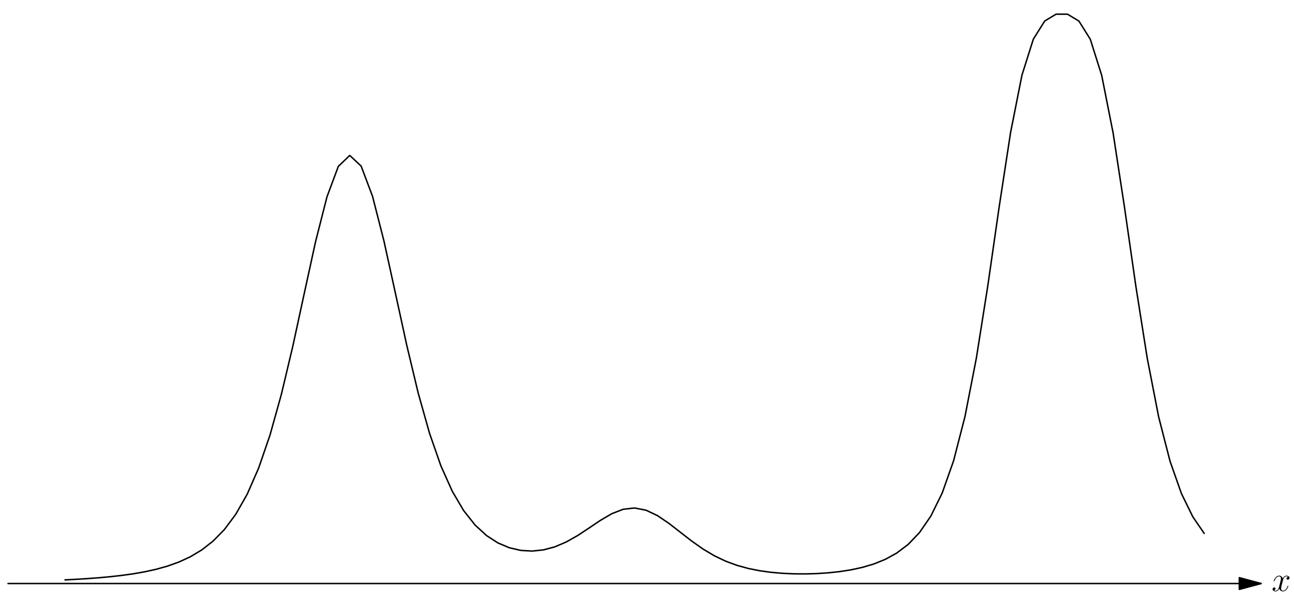
Limit Process

- Consider sampling a function at a set of points



- In the limit where the number of sample points goes to infinity the vector more closely approximates a function

- Instead of the indices being numbers we use $k \leftarrow x_k$

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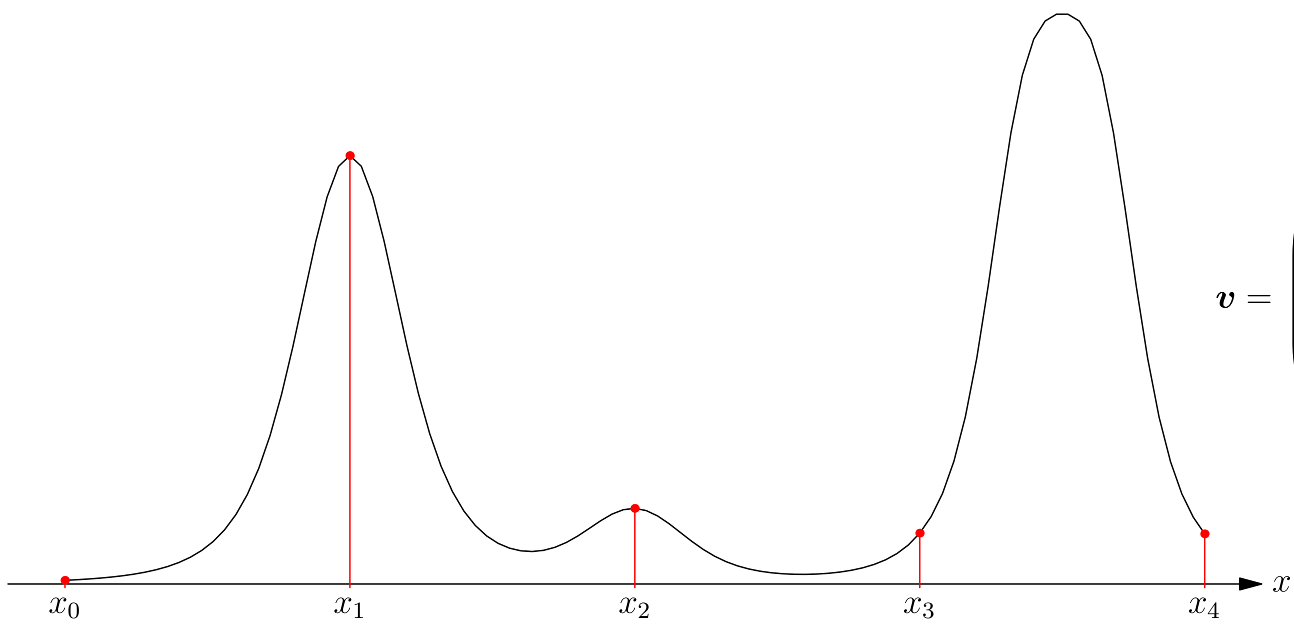

$$\boldsymbol{v} = \begin{pmatrix} 0.0512 \\ 6.01 \\ 1.06 \\ 0.714 \\ 0.703 \end{pmatrix}$$

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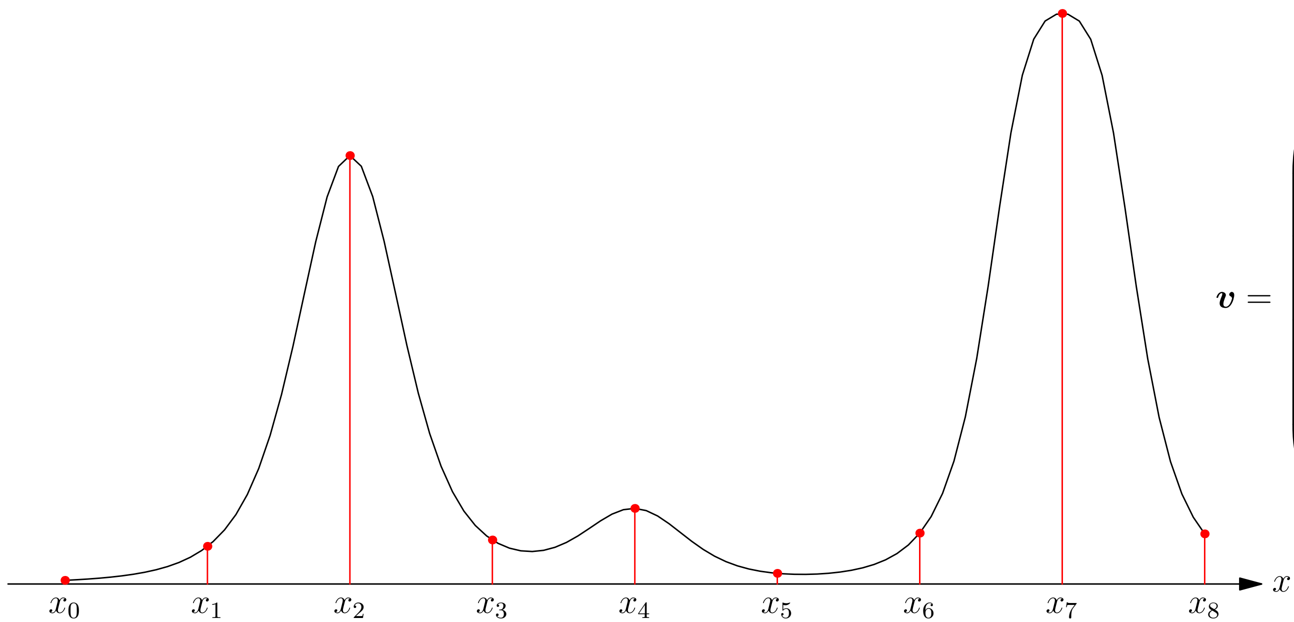

$$\boldsymbol{v} = \begin{pmatrix} 0.0512 \\ 0.529 \\ 6.01 \\ 0.617 \\ 1.06 \\ 0.149 \\ 0.714 \\ 8 \\ 0.703 \end{pmatrix}$$

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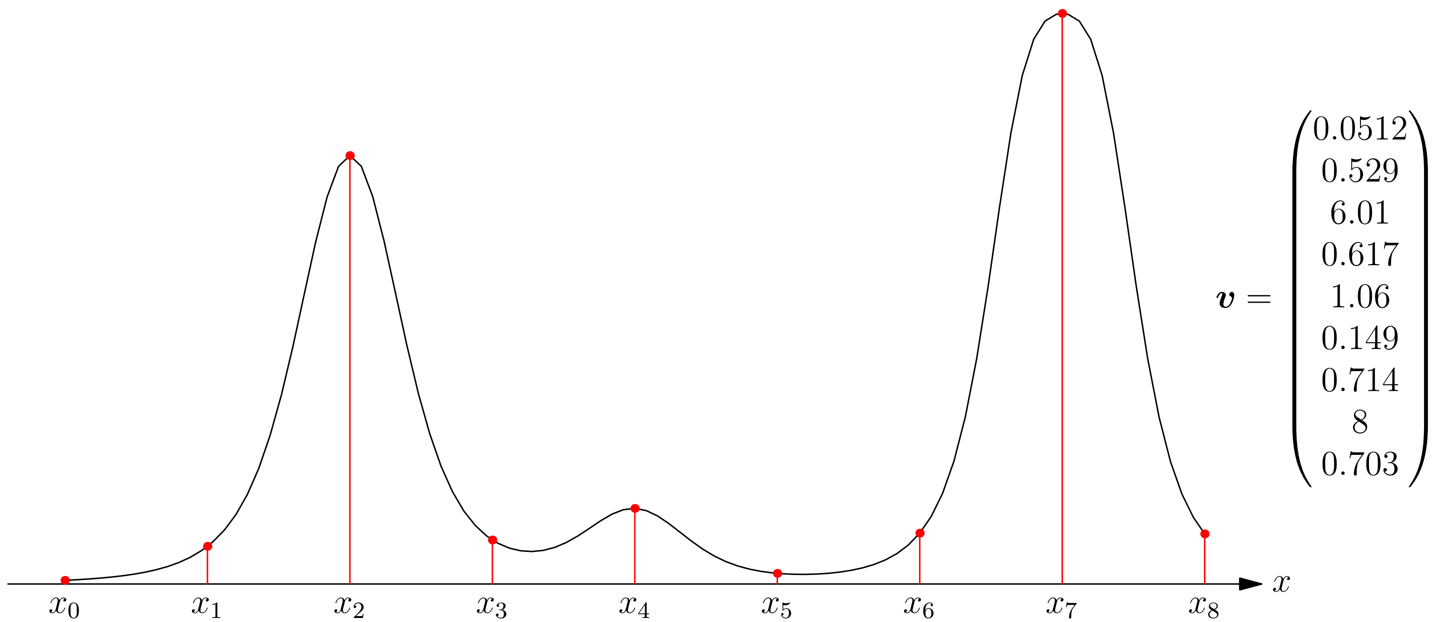

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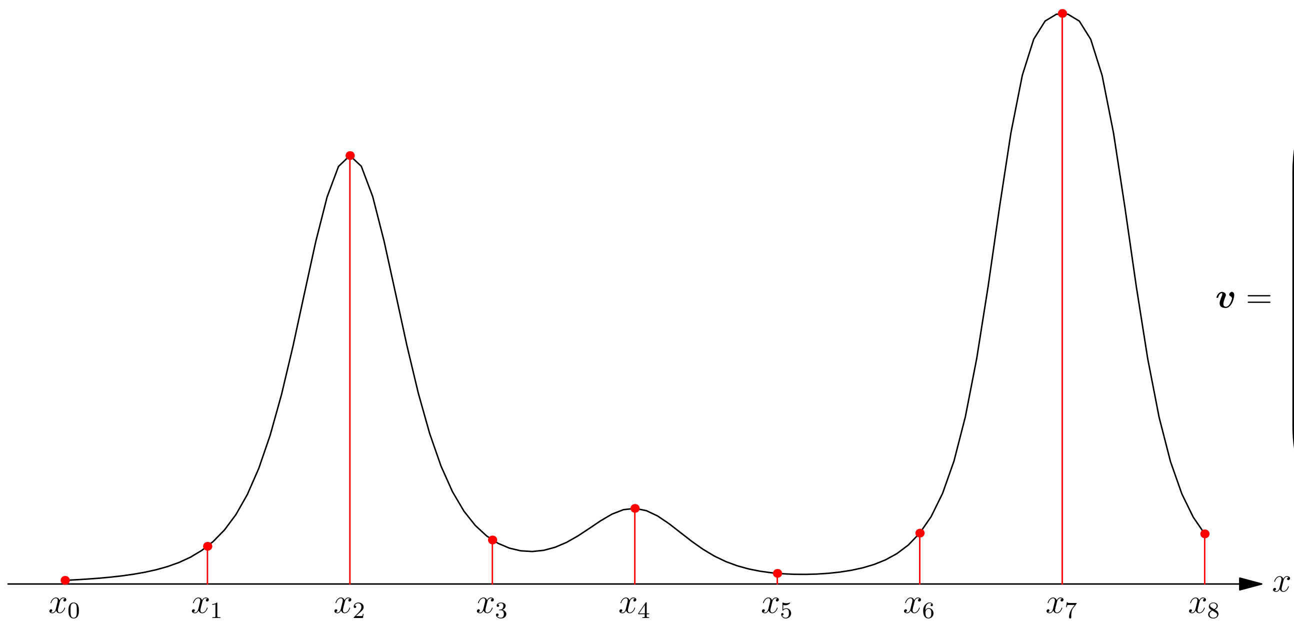

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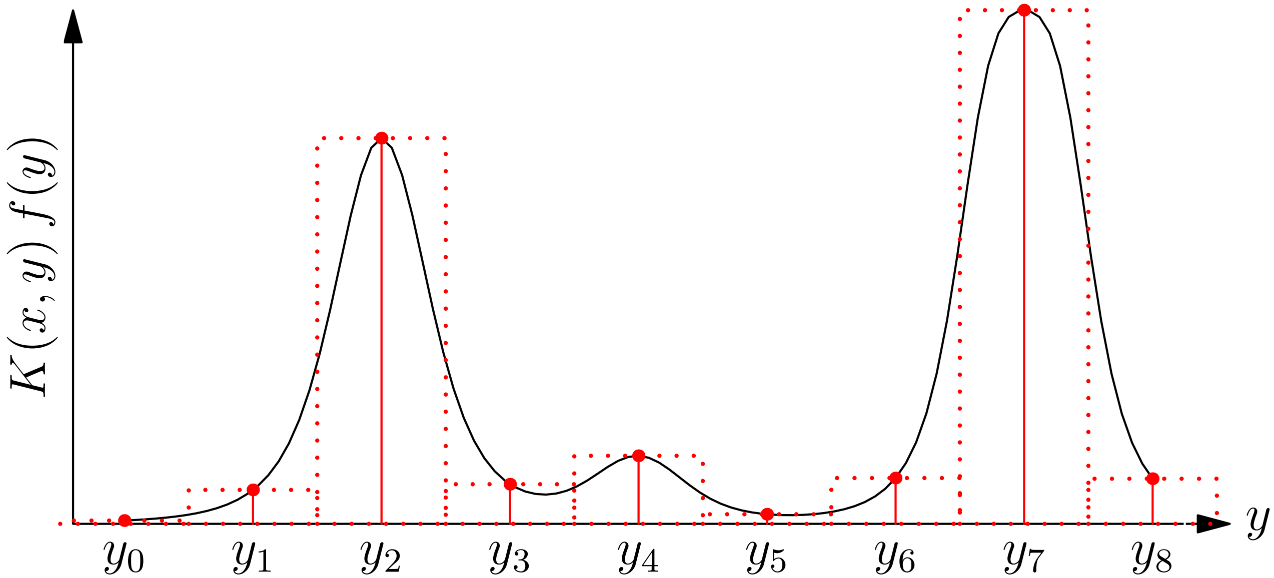
Linear Operators

- Recall a linear function $\mathcal{T}[f(x)]$ can be represented by a kernel

$$\mathcal{T}[f(x)] = \int_{y\in\mathcal{I}} K(x,y)\, f(y)\,\mathrm{d}y$$



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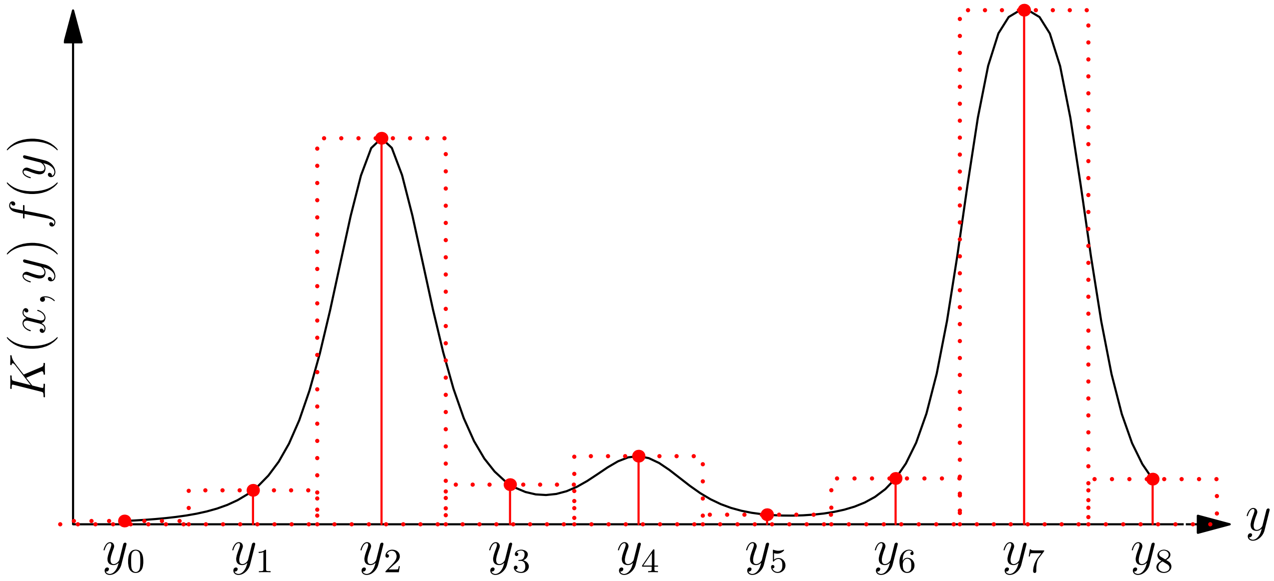

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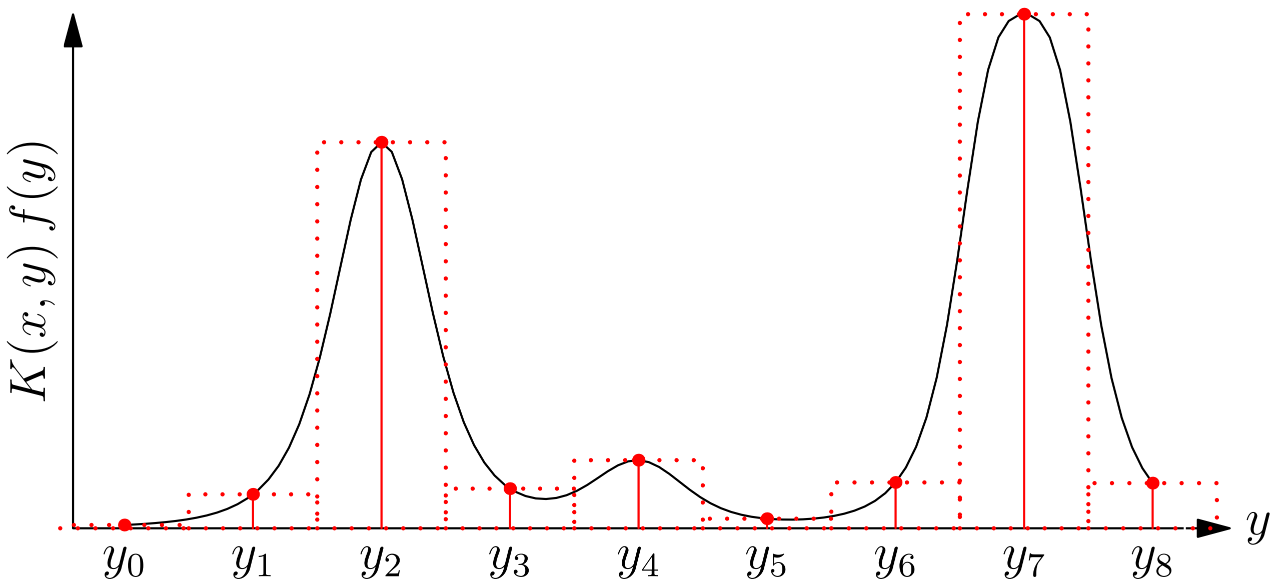

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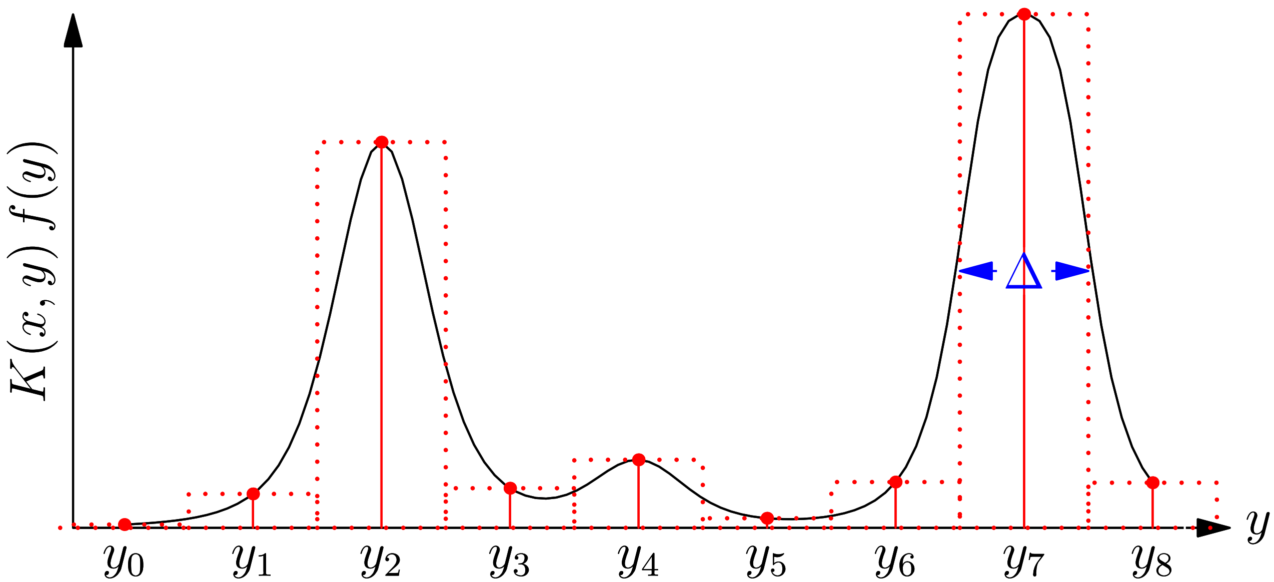

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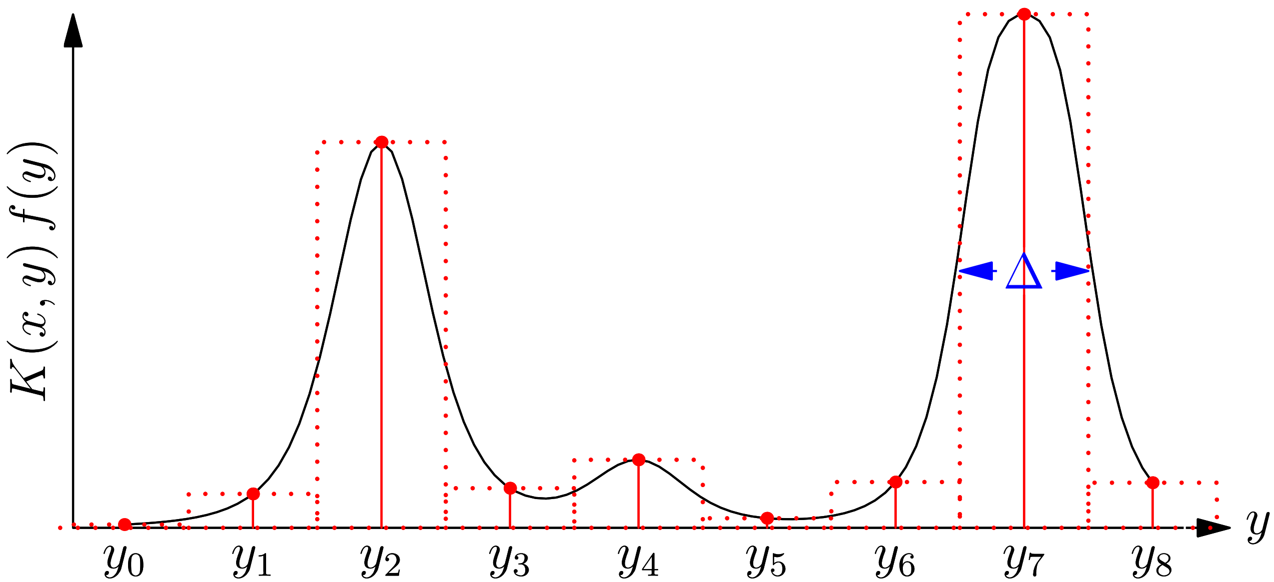

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SVM Kernels

- If we define $\phi^{(k)}(\boldsymbol{x}) = \sqrt{\lambda^{(k)}}\psi^{(k)}(\boldsymbol{x})$ then

$$K(\boldsymbol{x},\boldsymbol{y}) = \sum_k \lambda^{(k)}\psi^{(k)}(\boldsymbol{x})\psi^{(k)}(\boldsymbol{y}) = \sum_k \phi^{(k)}(\boldsymbol{x})\phi^{(k)}(\boldsymbol{y})$$

- This is the definition of a SVM kernel we started with
- Note that for $\phi^{(k)}(\boldsymbol{x})$ to be real $\lambda^{(k)} \geq 0$ for all k
- If $\lambda^{(k)} < 0$ then $\langle \boldsymbol{\phi}(\boldsymbol{x}), \boldsymbol{\phi}(\boldsymbol{x}) \rangle = \|\phi(\boldsymbol{x})\|^2$ might be negative and "distance" between points in the extended feature space can be negative!
- If we use a kernel that isn't positive semi-definite then the Hessian of the dual objective function will not be negative semi-definite and there will be a maximum where $\boldsymbol{\alpha}$ diverges

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$$K(\boldsymbol{x},\boldsymbol{y}) = \sum_k \lambda^{(k)}\psi^{(k)}(\boldsymbol{x})\psi^{(k)}(\boldsymbol{y}) = \sum_k \phi^{(k)}(\boldsymbol{x})\phi^{(k)}(\boldsymbol{y})$$

- This is the definition of a SVM kernel we started with
- Note that for $\phi^{(k)}(\boldsymbol{x})$ to be real $\lambda^{(k)} \geq 0$ for all k
- If $\lambda^{(k)} < 0$ then $\langle \boldsymbol{\phi}(\boldsymbol{x}), \boldsymbol{\phi}(\boldsymbol{x})\rangle = \|\phi(\boldsymbol{x})\|^2$ might be negative and "distance" between points in the extended feature space can be negative!
- If we use a kernel that isn't positive semi-definite then the Hessian of the dual objective function will not be negative semi-definite and there will be a maximum where $\boldsymbol{\alpha}$ diverges

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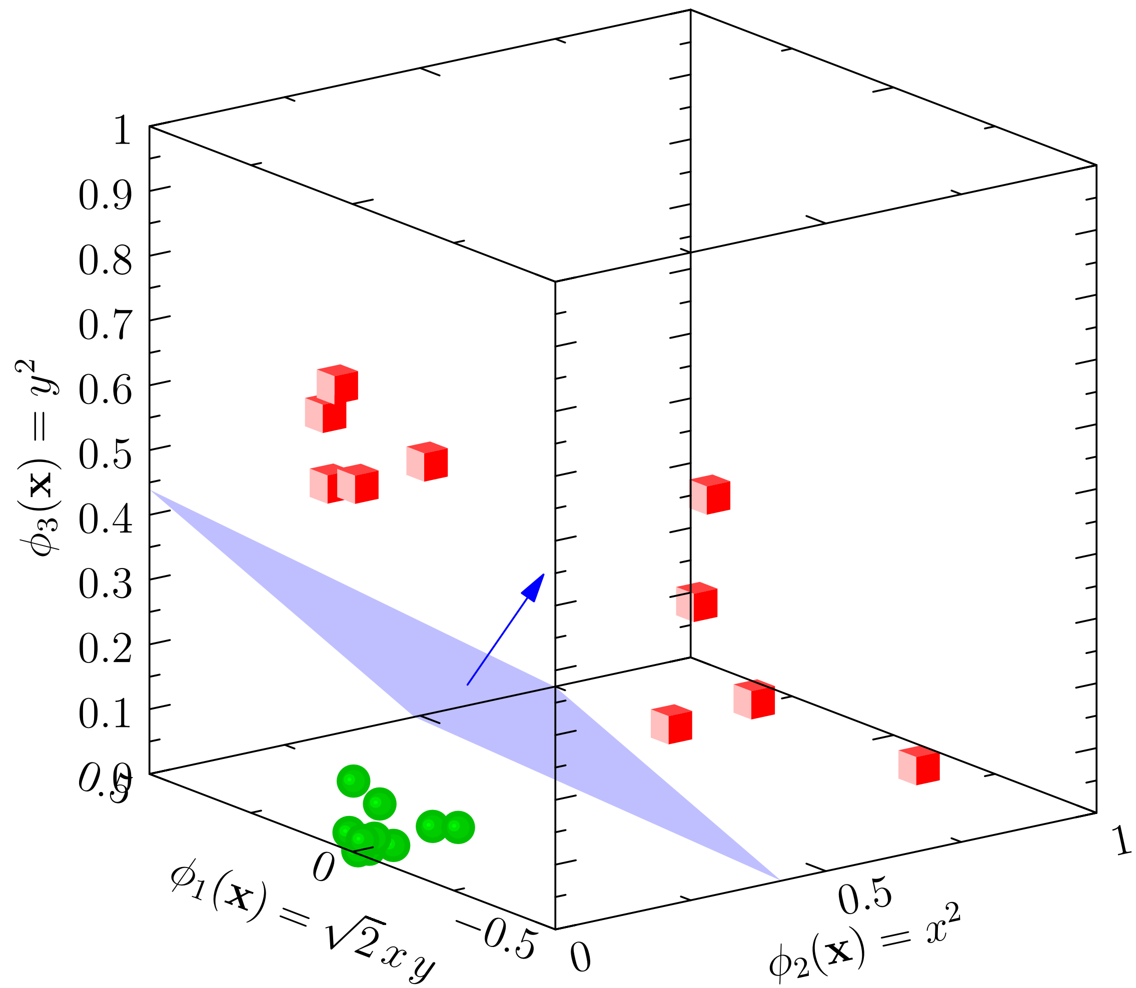
Outline

1. The Kernel Trick
2. Positive Semi-Definite Kernels
3. **Kernel Properties**
4. Beyond Classification



Positive Semi-Definite Kernels

- Kernels (or matrices) that have eigenvalues $\lambda^{(k)} \geq 0$ are called positive semi-definite

- (If the eigenvalues are strictly positive $\lambda^{(k)} > 0$ the kernels or matrices are called positive definite)

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Properties of Positive Semi-Definiteness

- Since

$$K(\boldsymbol{x},\boldsymbol{y}) = \langle \boldsymbol{\phi}(\boldsymbol{x}),\boldsymbol{\phi}(\boldsymbol{y}) \rangle$$

- An immediate consequence is that for any function $f(\boldsymbol{x})$

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&= \left\| \int f(\boldsymbol{x}) \boldsymbol{\phi}(\boldsymbol{x}) \mathrm{d}\boldsymbol{x} \right\|^2 \geq 0
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- The following statements are equivalent
  - ⋆ $K(\boldsymbol{x},\boldsymbol{y})$ is positive semi-definite (written $K(\boldsymbol{x},\boldsymbol{y}) \succeq 0$)
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  - ⋆ The kernel can be written

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Adding Kernels

- We can construct SVM kernels from other kernels
- If $K_1(\boldsymbol{x},\boldsymbol{y})$ and $K_2(\boldsymbol{x},\boldsymbol{y})$ are valid kernels then so is $K_3(\boldsymbol{x},\boldsymbol{y}) = K_1(\boldsymbol{x},\boldsymbol{y}) + K_2(\boldsymbol{x},\boldsymbol{y})$

$$
\begin{aligned}
Q &= \int f(\boldsymbol{x})\, K_3(\boldsymbol{x},\boldsymbol{y})\, f(\boldsymbol{y})\, \mathrm{d}\boldsymbol{x}\, \mathrm{d}\boldsymbol{y} \\
&= \int f(\boldsymbol{x}) \left(K_1(\boldsymbol{x},\boldsymbol{y}) + K_2(\boldsymbol{x},\boldsymbol{y})\right) f(\boldsymbol{y})\, \mathrm{d}\boldsymbol{x}\, \mathrm{d}\boldsymbol{y} \\
&= \int f(\boldsymbol{x})\, K_1(\boldsymbol{x},\boldsymbol{y})\, f(\boldsymbol{y})\, \mathrm{d}\boldsymbol{x}\, \mathrm{d}\boldsymbol{y} + \int f(\boldsymbol{x})\, K_2(\boldsymbol{x},\boldsymbol{y})\, f(\boldsymbol{y})\, \mathrm{d}\boldsymbol{x}\, \mathrm{d}\boldsymbol{y} \geq 0
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- If $K(\boldsymbol{x},\boldsymbol{y})$ is a valid kernel so is $cK(\boldsymbol{x},\boldsymbol{y})$ for $c > 0$

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Product of Kernels

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Exponentiating Kernels

- If $K(\boldsymbol{x},\boldsymbol{y})$ is a valid kernel so is $K^n(\boldsymbol{x},\boldsymbol{y})$ (by induction)
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  - ⋆ If $K^{n-1}(\boldsymbol{x},\boldsymbol{y}) \succeq 0$ then

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- and $\exp(K(\boldsymbol{x},\boldsymbol{y}))$ is also a valid kernel since

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RBF Kernel

- Now $\boldsymbol{x}^{\mathsf{T}}\boldsymbol{y} = \langle \boldsymbol{x}, \boldsymbol{y} \rangle$ is a valid kernel because it is an inner product of functions $\boldsymbol{\phi}(\boldsymbol{x}) = \boldsymbol{x}$

- For $\gamma > 0$ we have $2\gamma \boldsymbol{x}^{\mathsf{T}}\boldsymbol{y} \succeq 0$

- Thus $\exp(2\gamma \boldsymbol{x}^{\mathsf{T}}\boldsymbol{y}) \succeq 0$

- If $K(\boldsymbol{x}, \boldsymbol{y}) \succeq 0$ then $g(\boldsymbol{x}) K(\boldsymbol{x}, \boldsymbol{y}) g(\boldsymbol{y}) \succeq 0$

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where $f(\boldsymbol{x})g(\boldsymbol{x}) = h(\boldsymbol{x})$

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Other Kernels

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- The condition that a SVM kernel must be positive semi-definite is quite restrictive
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Spectrum Kernel

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- This is known as a p-spectrum

- A p-spectrum kernel counts the number of common substrings

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- A more sophisticated kernel is to count all of the common subsequences that occur in two documents
- Naively this would take an exponential amount of time to compute
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- Kernels have been developed for comparing trees (e.g. for computer program evaluation, XML, etc.)
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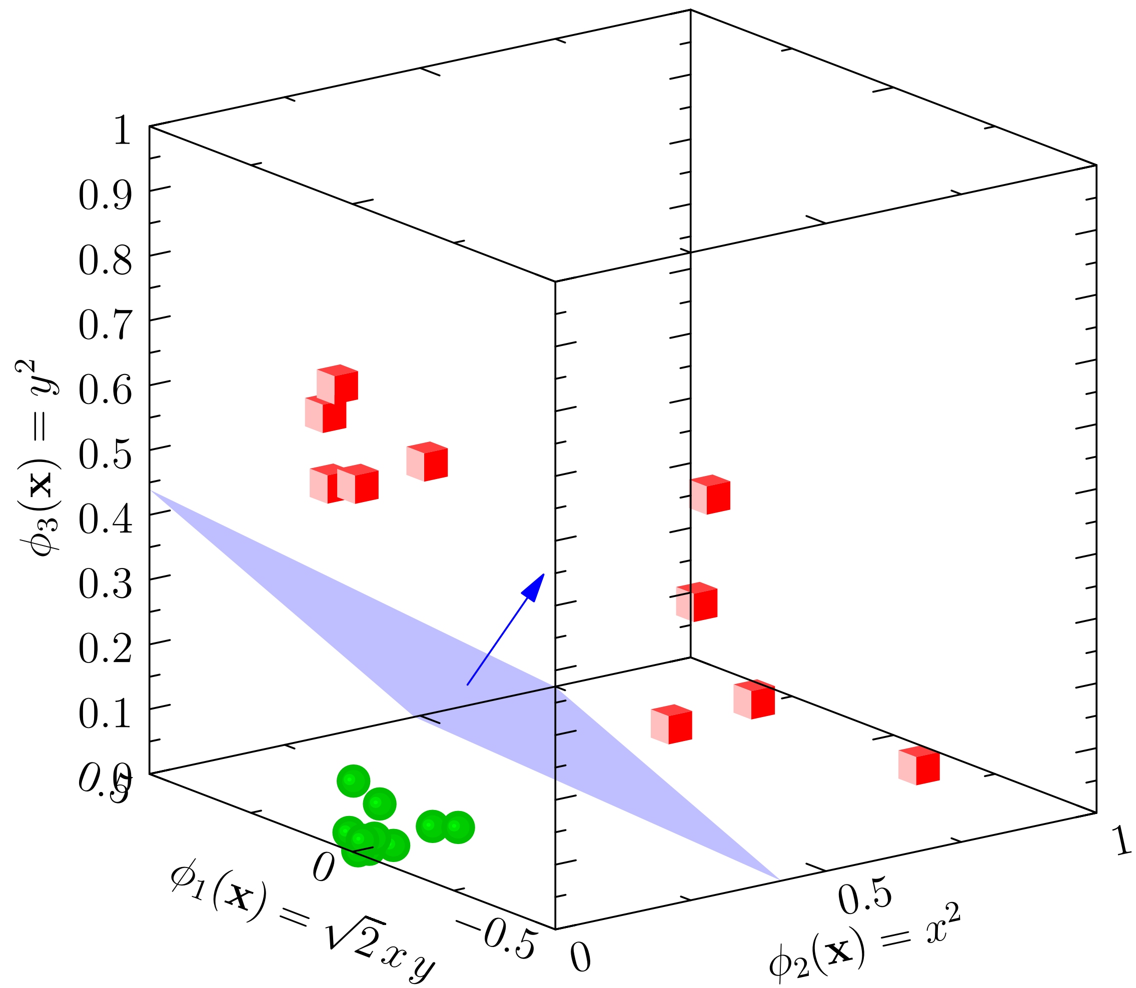
Outline

1. The Kernel Trick

2. Positive Semi-Definite Kernels

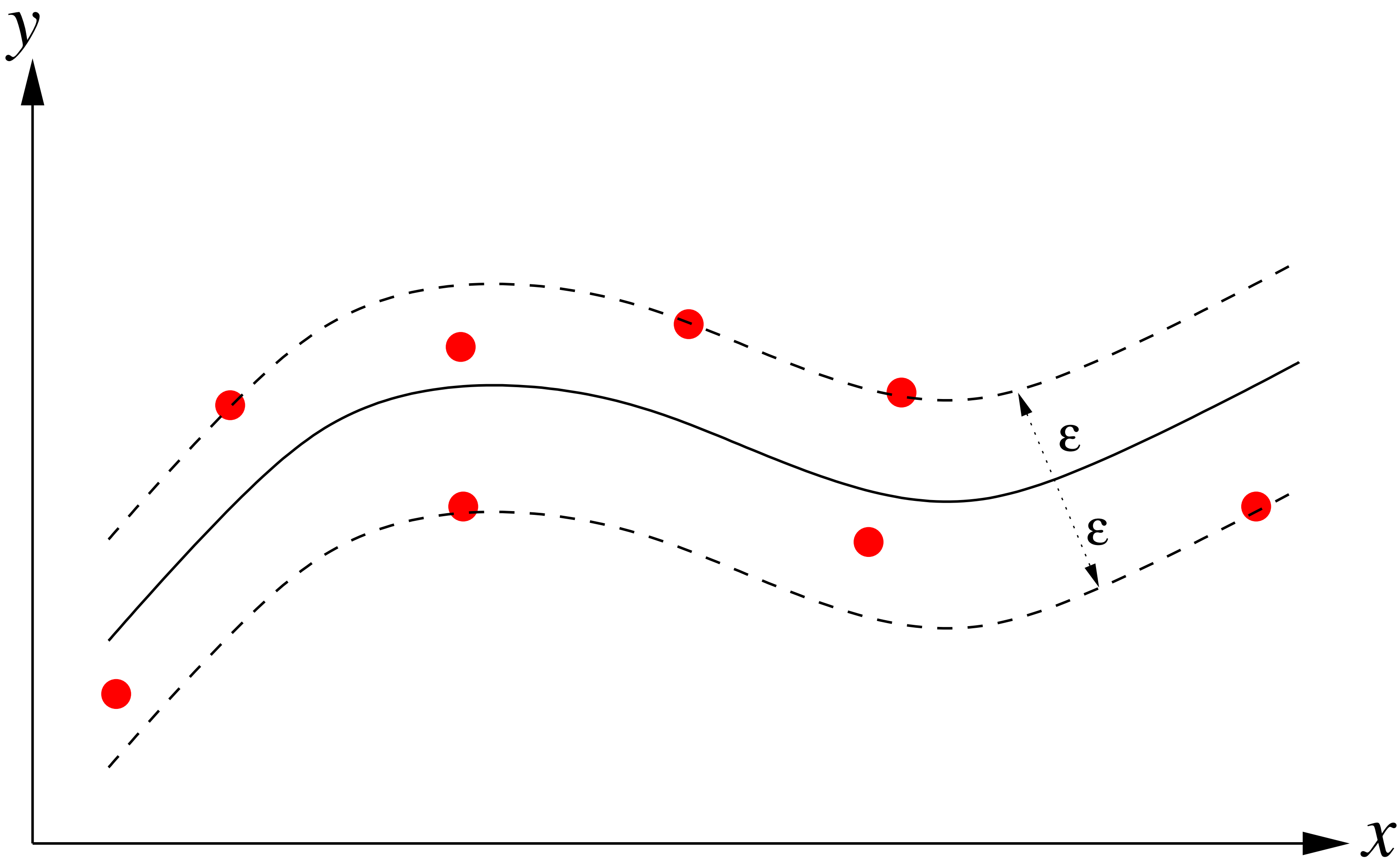
3. Kernel Properties

4. **Beyond Classification**



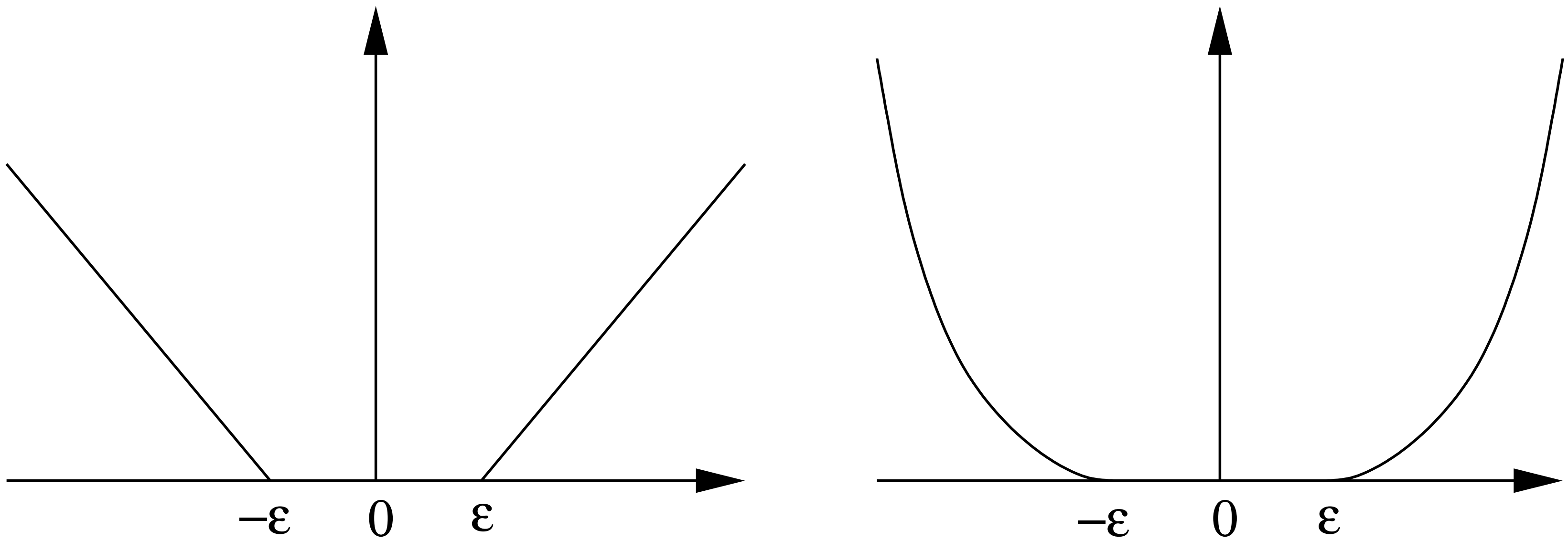
Regression with Margins

- SVMs can be modified to perform regression



Error Functions

- Can introduce slack variables with different errors



- This can be transformed to a quadratic programming problem

Ridge Regression Using Kernels

- We can also solve regression problems without using margins
- To solve a regression problem once again the problem is set up as a quadratic programming problem

$$\min_{\boldsymbol{w}} \lambda \|\boldsymbol{w}\|^2 + \sum_{i=1}^{m} \big(y_i - \boldsymbol{w}^{\mathsf{T}} \boldsymbol{\phi}(\boldsymbol{x}_i)\big)^2$$

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