Kernel Models

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[Adriano Koshiyama]

Overview

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Back to Feature Maps

- Overview
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Overview

- We show how a linear method such as least squares may be lifted to a (potentially) higher dimensional space to provide a nonlinear regression.

Map // Selection	Explicit	Implicit
Explicit	Basis Functions with Stepwise	Regularization
Implicit	Kernelization with Stepwise	**Kernel Methods with Regularization**

- **Implicit** Selection are widely adopted in Machine Learning
- **Explicit** Mapping is not very systematic, being more problem-dependent, but some recipes are universal (interactions, z-scores, etc.)
- **Implicit** Mapping with **Implicit** Feature selection is **Our Focus Today!**
- **Implicit** mapping with **Explicit** feature selection is not generally used

Back to Ridge Regression

- If we consider the Ridge Regression case, we have

$$\min_{\boldsymbol{\beta}(\lambda)} \boldsymbol{MSE}[\boldsymbol{\beta}(\lambda)] = \left|\left|\boldsymbol{y} - \boldsymbol{X\beta}\right|\right|_2^2 + \lambda\left|\left|\boldsymbol{\beta}\right|\right|_2^2, \text{ for a given } \lambda \geq 0$$

- we can rewrite this expression as

$$\min_{\boldsymbol{\beta}(\lambda)} \boldsymbol{MSE}[\boldsymbol{\beta}(\lambda)] = \boldsymbol{y}^T\boldsymbol{y} - 2\boldsymbol{\beta}^T\boldsymbol{X}^T\boldsymbol{y} + \boldsymbol{\beta}^T\boldsymbol{X}^T\boldsymbol{X\beta} + \lambda\boldsymbol{\beta}^T\boldsymbol{I}_{JxJ}\boldsymbol{\beta}$$

- First order condition: $\nabla_{\boldsymbol{\beta}(\lambda)} \boldsymbol{MSE}[\boldsymbol{\beta}(\lambda)] = 0$, then

$$-2\boldsymbol{X}^T\boldsymbol{y}^T + \boldsymbol{X}^T\boldsymbol{X\beta} + \lambda\boldsymbol{I}_{JxJ}\boldsymbol{\beta} = \boldsymbol{0} \rightarrow -2\boldsymbol{X}^T\boldsymbol{y} + (\boldsymbol{X}^T\boldsymbol{X} + \lambda\boldsymbol{I}_{JxJ})\boldsymbol{\beta} = \boldsymbol{0}$$

- Yielding the solution, akin to Linear Regression, but with a new param

$$\boldsymbol{\beta} = \left(\boldsymbol{X}^T\boldsymbol{X} + \lambda\boldsymbol{I}_{JxJ}\right)^{-1}\boldsymbol{X}^T\boldsymbol{y}$$

- Second order condition: $\boldsymbol{H}[\boldsymbol{MSE}[\boldsymbol{\beta}(\lambda)]]$ is positive semi-definite

$$\boldsymbol{H}\left[\boldsymbol{MSE}[\boldsymbol{\beta}(\lambda)]\right] = \left(\boldsymbol{X}^T\boldsymbol{X} + \lambda\boldsymbol{I}_{JxJ}\right)^{\boldsymbol{T}} = \left(\boldsymbol{X}^T\boldsymbol{X} + \lambda\boldsymbol{I}_{JxJ}\right)$$

since $\boldsymbol{X}^T\boldsymbol{X}$ is positive semi-definite, $\boldsymbol{I}_{JxJ}$ is positive definite, the hessian matrix will be positive semi-definite for a suitable choice of λ (usually $\lambda \geq 0$)

PS: remember to scale $\boldsymbol{X}$ columns (like having zero mean and unit std)

Explicit Feature Maps

- Overall, the main idea is to extend the model, including new features engineered using some **nonlinear mapping** (a.k.a. basis function)

$$y_i = \boldsymbol{\alpha}^T \phi(\boldsymbol{x}_i) + \varepsilon_i$$

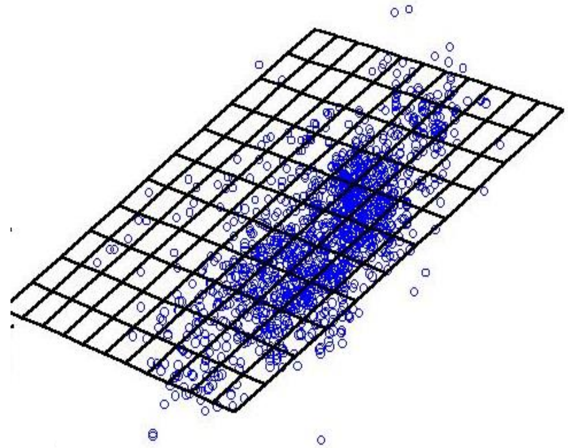
with $\phi: S^J \to \mathcal{R}^M$, usually $M > J$; hence more coefficients have to be fitted

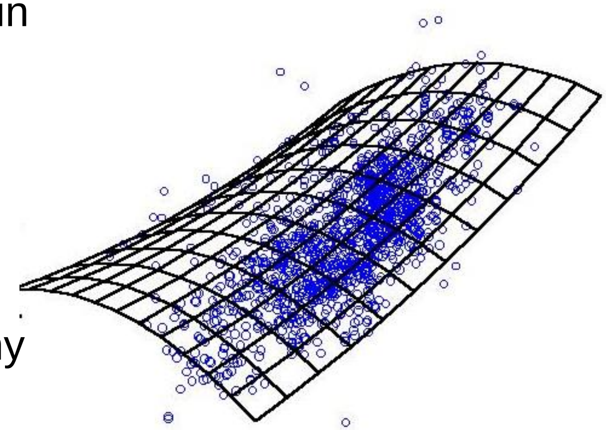
- Since the model is linear in the parameters $\boldsymbol{\alpha}^T$, we can call $\phi(\boldsymbol{x}_i) = \boldsymbol{z_i}$ and use the usual solution $\boldsymbol{w} = \left(\boldsymbol{Z^T Z}\right)^{-1} \boldsymbol{Z^T y}$, with $\boldsymbol{Z} = [\boldsymbol{z_1}, \dots, \boldsymbol{z_n}]^{\boldsymbol{T}}$

- Some commonly used feature maps, adopted in many situations
  - Polynomial: ϕ: $x_i \to (1, x_i, x_i^2, x_i^3, \dots)$
  - Veronese/ANOVA/Interaction mapping

ϕ: $x_{i1}, x_{i2} \to (1, x_{i1}, x_{i2}\ x_{i1}^2, x_{i2}^2, x_{i1} x_{i2}, \dots)$

- In fact, log, sqrt, one-hot encoding, etc. and any other transformation





Kernel Ridge Regression

- Is it possible to create polynomial features, without incurring in all the additional calculations, memory storage, etc.? **A: Yes**
- **First step**: rewrite Ridge Regression solution by

$$\boldsymbol{X^T X \beta} + \lambda \boldsymbol{I}_{JxJ}\boldsymbol{\beta} = \boldsymbol{X^T y} \Rightarrow \lambda \boldsymbol{I}_{JxJ}\boldsymbol{\beta} = \boldsymbol{X^T y} - \boldsymbol{X^T X \beta} \Rightarrow \boldsymbol{\beta} = \left(\frac{1}{\lambda}\right)\boldsymbol{X^T}[\boldsymbol{y} - \boldsymbol{X\beta}]$$

hence, $\boldsymbol{\beta}$ can be expressed as a linear combination of the columns of $\boldsymbol{X^T}$

$$\boldsymbol{\beta} = \boldsymbol{X^T \alpha}$$

with $\boldsymbol{\alpha} \in \mathbb{R}^n$ being the dual coefficient vector; further manipulation show

$$\boldsymbol{\alpha} = \left(\frac{1}{\lambda}\right)[\boldsymbol{y} - \boldsymbol{X\beta}] \Rightarrow \boldsymbol{\alpha}\lambda = [\boldsymbol{y} - \boldsymbol{XX^T \alpha}] \Rightarrow (\boldsymbol{XX^T} + \lambda \boldsymbol{I}_{nxn})\boldsymbol{\alpha} = \boldsymbol{y}$$

- therefore, $\boldsymbol{\alpha} = \left(\boldsymbol{XX^T} + \lambda \boldsymbol{I}_{nxn}\right)^{-\mathbf{1}}\boldsymbol{y}$, implying that $\boldsymbol{\alpha}$
  - minimizes $\boldsymbol{MSE}[\boldsymbol{\alpha}(\lambda)] = \left|\left|\boldsymbol{y} - \boldsymbol{XX^T\alpha}\right|\right|_{\mathbf{2}}^{\mathbf{2}} + \lambda\, \boldsymbol{\alpha^T XX^T \alpha}$
  - written in terms of inner products of rows ($\boldsymbol{XX^T}$) not columns ($\boldsymbol{X^T X}$)

Kernel Trick

- **Second step**: since $\boldsymbol{\alpha}$ is written in terms of inner products of rows

$$\boldsymbol{X}\boldsymbol{X}^T = \begin{bmatrix} \langle \boldsymbol{x_1}, \boldsymbol{x_1} \rangle & \cdots & \langle \boldsymbol{x_1}, \boldsymbol{x_n} \rangle \\ \vdots & \ddots & \vdots \\ \langle \boldsymbol{x_n}, \boldsymbol{x_1} \rangle & \cdots & \langle \boldsymbol{x_n}, \boldsymbol{x_n} \rangle \end{bmatrix}$$

- if, we consider a feature map of $\boldsymbol{x_i}$, $\boldsymbol{\phi}: S^J \rightarrow \mathcal{R}^M$, we can rewrite the Gram-Matrix $\boldsymbol{X}\boldsymbol{X}^T$ after feature mapping by

$$. = \begin{bmatrix} \langle \boldsymbol{\phi}(\boldsymbol{x_1}), \phi(\boldsymbol{x_1}) \rangle & \cdots & \langle \boldsymbol{\phi}(\boldsymbol{x_1}), \boldsymbol{\phi}(\boldsymbol{x_n}) \rangle \\ \vdots & \ddots & \vdots \\ \langle \boldsymbol{\phi}(\boldsymbol{x_n}), \boldsymbol{\phi}(\boldsymbol{x_1}) \rangle & \cdots & \langle \boldsymbol{\phi}(\boldsymbol{x_n}), \boldsymbol{\phi}(\boldsymbol{x_n}) \rangle \end{bmatrix} = \begin{bmatrix} k(\boldsymbol{x_1}, \boldsymbol{x_1}) & \cdots & k(\boldsymbol{x_1}, \boldsymbol{x_n}) \\ \vdots & \ddots & \vdots \\ k(\boldsymbol{x_n}, \boldsymbol{x_1}) & \cdots & k(\boldsymbol{x_n}, \boldsymbol{x_n}) \end{bmatrix} = \boldsymbol{K}$$

- where $k(\boldsymbol{x_k}, \boldsymbol{x_i}) \coloneqq \langle \boldsymbol{\phi}(\boldsymbol{x_k}), \boldsymbol{\phi}(\boldsymbol{x_i}) \rangle$ is a (**kernel**) function that **replicates** a certain **feature mapping plus an inner product**!
- Example: consider that $\boldsymbol{x}, \boldsymbol{z} \in \mathbb{R}^{\mathbf{2}}$ (think as two rows of a 2-d dataset) and $k(\boldsymbol{x}, \boldsymbol{z}) = \langle \boldsymbol{x}, \boldsymbol{z} \rangle^2$, then $k(\boldsymbol{x}, \boldsymbol{z}) = x_1^2 z_1^2 + x_2^2 z_2^2 + 2 x_1 x_2 z_1 z_2 = \cdots$

$$\ldots = \left[x_1^2\,, x_2^2, \sqrt{2} x_1 x_2\right]^T \left[z_1^2\,, z_2^2, \sqrt{2} z_1 z_2\right] = \langle \boldsymbol{\phi}(\boldsymbol{x}), \boldsymbol{\phi}(\boldsymbol{z}) \rangle$$

for a map $\boldsymbol{\phi}(\boldsymbol{x}) = [x_1^2, x_2^2, \sqrt{2} x_1 x_2]$, close to a second degree polynomial

- hence,$\langle \boldsymbol{\phi}(\boldsymbol{x}), \boldsymbol{\phi}(\boldsymbol{z}) \rangle$ takes roughly $O(n^2)$ whilst $k(\boldsymbol{x}, \boldsymbol{z})$ takes $O(n)$

Dual Representation – Pros and Cons

- **Primal Form: Computation with Basis Functions**
  - **Training**: $O(J^p)$ for feature mapping and $O(nJ^2 + J^3)$ for estimation
    - Dataset $D = \{(\boldsymbol{x_i}, y_i)\}_{i=1}^n$
    - Basis functions: ϕ_1, ..., ϕ_k where ϕ: $\mathbb{R}^J \rightarrow \mathbb{R}$
    - Feature map: $\boldsymbol{\phi}(\boldsymbol{x}) = [\phi_1(\boldsymbol{x}), \dots, \phi_k(\boldsymbol{x})]$
    - Solution: $\boldsymbol{\beta} = \left(\boldsymbol{Z^T Z}\right)^{-1} \boldsymbol{Z^T y}$, with $\boldsymbol{Z} = [\boldsymbol{\phi}(\boldsymbol{x_1}), \dots, \boldsymbol{\phi}(\boldsymbol{x_n})]^{\boldsymbol{T}}$
  - **Prediction**: $\hat{y}(\boldsymbol{x_i}) = \boldsymbol{\beta^T \phi}(\boldsymbol{x_i})$, taking $O(k)$ operations
- **Dual Form: Implicit Feature Map**
  - **Training**: $O(Jn)$ to create $\boldsymbol{K}$ and $O(Jn^2 + n^3)$ for estimation
    - Dataset $D = \{(\boldsymbol{x_i}, y_i)\}_{i=1}^n$
    - Kernel Function: k: $\mathbb{R}^J \times \mathbb{R}^J \rightarrow \mathbb{R}$
    - Kernel Matrix: $\boldsymbol{K} = \begin{bmatrix} k(\boldsymbol{x_1}, \boldsymbol{x_1}) & \cdots & k(\boldsymbol{x_1}, \boldsymbol{x_n}) \\ \vdots & \ddots & \vdots \\ k(\boldsymbol{x_n}, \boldsymbol{x_1}) & \cdots & k(\boldsymbol{x}_n, \boldsymbol{x}_n) \end{bmatrix}$
    - Solution: $\boldsymbol{\alpha} = (\boldsymbol{K} + \lambda \boldsymbol{I}_{nxn})^{-\boldsymbol{1}} \boldsymbol{y}$
  - **Prediction**: $\hat{y}(\boldsymbol{v}) = \sum_{\boldsymbol{i}} \alpha_i \, k(\boldsymbol{x_i}, \boldsymbol{v})$, taking $O(nJ)$ operations

Kernels

- Definition
- Kernelization
- Some key facts and results
- A bestiary of kernels

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Definition

- **Kernel**
  - A function k: $\mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ is called a kernel on $\mathcal{X}$ if there exists a Hilbert space $\mathcal{F}$ and a map $\boldsymbol{\phi}$: $\mathcal{X} \rightarrow \mathcal{F}$, such that $k(x, z) = \langle \boldsymbol{\phi}(\boldsymbol{x}), \boldsymbol{\phi}(\boldsymbol{z}) \rangle_{\mathcal{F}}$

- In our more usual terminology
  - $\boldsymbol{\phi}$: $\mathcal{X} \rightarrow \mathcal{F}$ is called a **feature map**
  - $\mathcal{F}$ is called a **feature space**

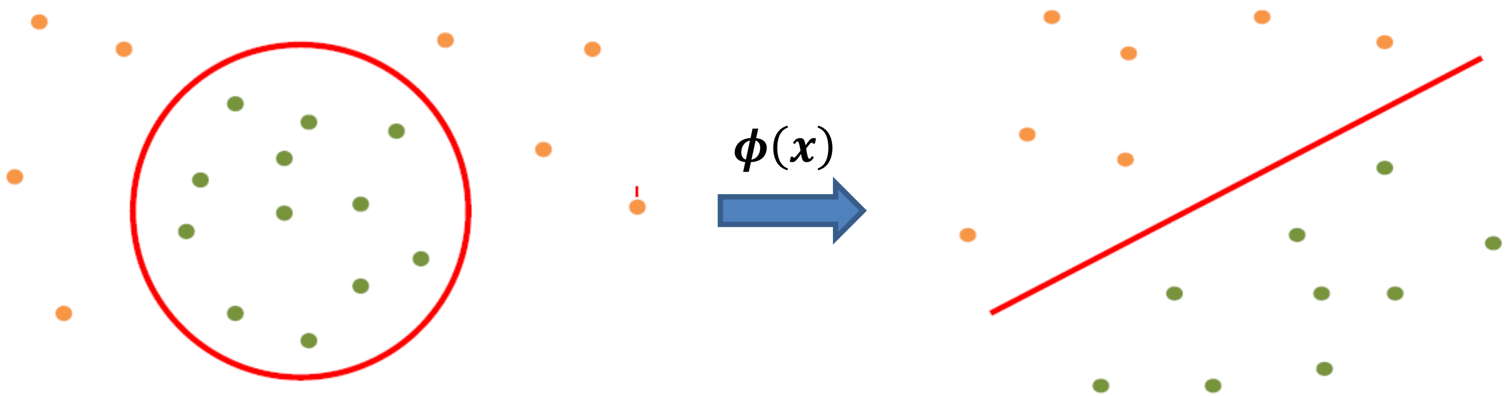
- Hence, a kernel function is a composition of "feature map" with scalar product. Our previous example, $\boldsymbol{x}, \boldsymbol{z} \in \mathbb{R}^2$, we have:
  - $k(\boldsymbol{x}, \boldsymbol{z}) = \langle \boldsymbol{x}, \boldsymbol{z} \rangle^{\mathbf{2}}$ (homogenous 2-degree polynomial kernel)
  - $\boldsymbol{\phi}(\boldsymbol{x}) = [x_1^2, x_2^2, \sqrt{2} x_1 x_2]$ or $\boldsymbol{\phi}(\boldsymbol{x}) = [x_1^2, x_2^2, x_1 x_2, x_1 x_2]$

is one of the most common instantiations of a kernel function

- **Note that a kernel function is not always is associated with an unique feature map!**

Kernelization

- Kernels allow to make linear algorithms work on non-linear features, by replicating a very complicated feature mapping by a kernel function over the raw features
- Example: Support Vector Machine: $D = \{(\boldsymbol{x_i}, y_i)\}_{i=1}^{n}, y_i \in \{-1,1\}$



$$f(\boldsymbol{x}) = \operatorname{sgn}(\beta_0 + \boldsymbol{\beta}^T \boldsymbol{x})$$

$\boldsymbol{\beta} = \sum_i \alpha_i \boldsymbol{x}_i y_i$ solves a QP involving $\boldsymbol{X^T X}$, with α_i representing “dual variables

$$f(\boldsymbol{z}) = \operatorname{sgn}\left(\beta_0 + \sum_i \alpha_i\, k(\boldsymbol{x}_i, \boldsymbol{z})\right)$$

$$= \boldsymbol{\alpha^T k(X, z)}$$

$\boldsymbol{\alpha}$ solves a QP involving kernel matrix $\boldsymbol{K}$

Key facts and results

- **What functions are kernels?**

- Given a function k: $\mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$, which properties of k guarantee that there exists a Hilbert space $\mathcal{F}$ and a map $\boldsymbol{\phi}$: $\mathcal{X} \rightarrow \mathcal{F}$, such that $k(\boldsymbol{x}, \boldsymbol{z}) = \langle \boldsymbol{\phi}(\boldsymbol{x}), \boldsymbol{\phi}(\boldsymbol{z}) \rangle_{\mathcal{F}}$?
- **Subtle note**: we have generalized the definition of **finite-dimensional** feature maps $\boldsymbol{\phi}$: $\mathbb{R}^J \rightarrow \mathbb{R}^m$ to **infinite-dimensional** feature maps $\boldsymbol{\phi}$: $\mathbb{R}^J \rightarrow \mathcal{F}$ (Hilbert space)

- **First**: a function h: $\mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ **is positive semidefinite** if is symmetric and the matrix $\boldsymbol{H}$ made of $\boldsymbol{H}_{ixj} = h(\boldsymbol{x}_i, \boldsymbol{x}_j)$ for every *i* and *j* is positive semidefinite ($\boldsymbol{v}^T \boldsymbol{H} \boldsymbol{v} \geq 0$)
- **Theorem (Positive Semidefinite Kernels)**
  - A function k is positive semidefinite if and only if

$$k(\boldsymbol{x}, \boldsymbol{z}) = \langle \boldsymbol{\phi}(\boldsymbol{x}), \boldsymbol{\phi}(\boldsymbol{z}) \rangle,\ \boldsymbol{x}, \boldsymbol{z} \in \mathbb{R}^J$$

for some feature map $\boldsymbol{\phi}$: $\mathbb{R}^J \rightarrow \mathcal{F}$ and Hilbert space $\mathcal{F}$

Key facts and results

- **Theorem (Moore-Aronszajn, 1950)**
- For every positive semidefinite kernel $k\colon \mathcal{X} \times \mathcal{X} \to \mathbb{R}$, there is an unique feature map $\boldsymbol{\phi}\colon \mathcal{X} \to \mathcal{F}$ (up to a isomorphism) into an unique Hilbert space $\mathcal{F}$ (the so-called Reproducing Kernel Hilbert Space – RKHS)
  - **RKHS**: $\boldsymbol{\phi}\colon \boldsymbol{x} \to \boldsymbol{k}(\boldsymbol{x},.)$ and $\langle \boldsymbol{k}(\boldsymbol{x},.), \boldsymbol{f}(.)\rangle_{\mathcal{F}} = f(\boldsymbol{x})$, $\forall f \in \mathcal{F}$
- **Theorem (Kimeldorf-Wahba, 1971) "Representer Theorem"**
  - Let $D = \{(\boldsymbol{x_i}, y_i)\}_{i=1}^{n}$ be data points
  - Let k be a positive semidefinite kernel with RHKS $\mathcal{F}$
  - Let $\mathcal{L}\colon \mathbb{R}^J \times \mathbb{R} \times \mathbb{R} \to \mathbb{R}$ be any loss function
  - Let $\Omega\colon [0, \infty) \to \mathbb{R}$ strictly increasing penalty function
- Then, there is a minimizer of the type $f(x) = \alpha^T \boldsymbol{k}(x,.)$ to $R(f) = \sum_i \mathcal{L}\left(\boldsymbol{x}_i, y_i, f(\boldsymbol{x}_i)\right) + \Omega\left(||f||_{\mathcal{F}}\right)$

A bestiary of kernels

- **Linear**: $k(\boldsymbol{x},\boldsymbol{z}) = \boldsymbol{x}^T \boldsymbol{A}\boldsymbol{z}$ (usually $\boldsymbol{A}$ is a positive definite matrix)
- **Dot-product**: $k(\boldsymbol{x},\boldsymbol{z}) = f(\langle \boldsymbol{x},\boldsymbol{z}\rangle)$ (usually f is a positive definite)
- **Polynomial**: $k(\boldsymbol{x},\boldsymbol{z}) = (\theta\langle \boldsymbol{x},\boldsymbol{z}\rangle + c)^d$ (general formulation)
- **Sigmoid**: $k(\boldsymbol{x},\boldsymbol{z}) = tanh(\sigma\langle \boldsymbol{x},\boldsymbol{z}\rangle + c))$ (not positive definite…)
- **Radial basis function kernels**

Gaussian/RBF Kernel

$$k(\boldsymbol{x},\boldsymbol{z}) = \exp\left(-\frac{\|\boldsymbol{x}-\boldsymbol{z}\|_2^2}{2\sigma^2}\right)$$

Laplacian Kernel

$$k(\boldsymbol{x},\boldsymbol{z}) = \exp\left(-\frac{\|\boldsymbol{x}-\boldsymbol{z}\|}{\sigma}\right)$$

- **Proposition**
- For positive definite kernels $k_1, k_2, \ldots$ and $c_i > 0$, any of the composition below is also a positive definite kernel

$$k_1(\boldsymbol{x},\boldsymbol{z}) + c_1 \qquad c_1 k_1(\boldsymbol{x},\boldsymbol{z}) + c_2 k_2(\boldsymbol{x},\boldsymbol{z}) \qquad k_1(\boldsymbol{x},\boldsymbol{z}) k_2(\boldsymbol{x},\boldsymbol{z})$$

$$\frac{k_1(\boldsymbol{x},\boldsymbol{z})}{\sqrt{k_1(\boldsymbol{x},\boldsymbol{x}) k_1(\boldsymbol{z},\boldsymbol{z})}}$$

$\sum_{i=1}^{\infty} c_i \langle \boldsymbol{x},\boldsymbol{z}\rangle^i$
(in case of convergence)

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Support Vector Machines

- Main Idea and Details
- Linear Support Vector Machines
- Kernel/Nonlinear Support Vector Machines
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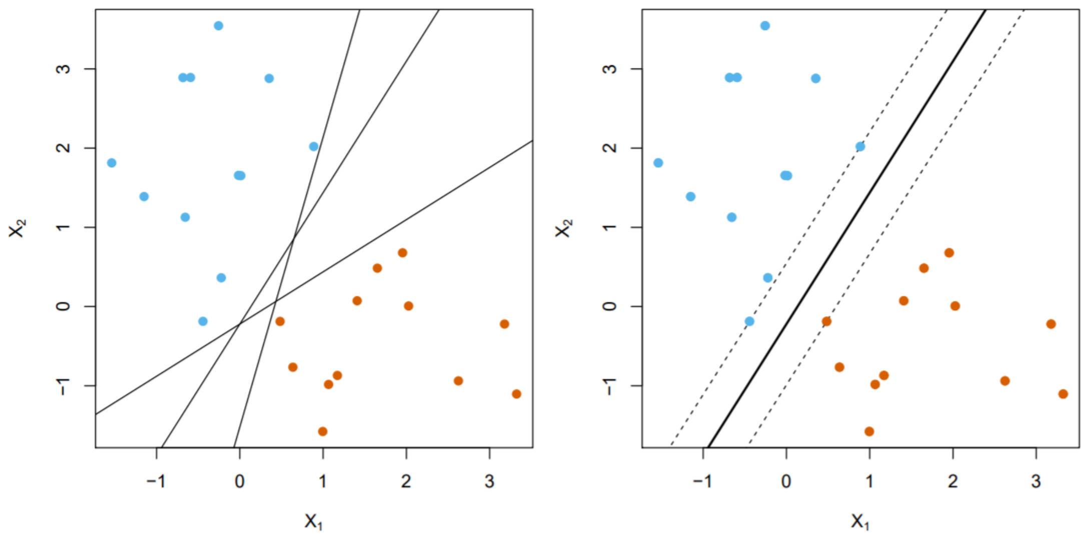
Main Idea and Details

- **Main idea**: given a $D = \{(\boldsymbol{x_i}, y_i)\}_{i=1}^{n}$, $y_i \in \{-1, 1\}$, $H = \{\boldsymbol{x} \in \mathbb{R}^J : < \boldsymbol{w}, \boldsymbol{x} > = c\}$, with normal vector $\boldsymbol{w}$ and offset *c*, separating points from class -1 and class 1 with the largest symmetric **margin of $\pm\boldsymbol{\eta}$**



- **A contrast**: whilst Logistic Regression first build a conditional probability model, and then classify based in a threshold, SVMs bypass the first step, and build a classifier directly!

Linear Support Vector Machines

- **Hard margin Linear SVM**: Find a hyperplane $H = \{\boldsymbol{x} \in \mathbb{R}^J : < \boldsymbol{w}, \boldsymbol{x} > = c\}$, with normal vector $\boldsymbol{w}$ and offset c, separating points from class -1 and class 1 with the largest symmetric **margin of** $\pm\boldsymbol{\eta} = \frac{\mathbf{1}}{||\boldsymbol{w}||}$

$$\max_{\boldsymbol{w},c} \eta\,, \qquad s.t. \, y_i \cdot (< \boldsymbol{w}, \boldsymbol{x_i} > -c) \geq 1, \qquad y_i \in \{-1, 1\}$$

Too strict in practice!

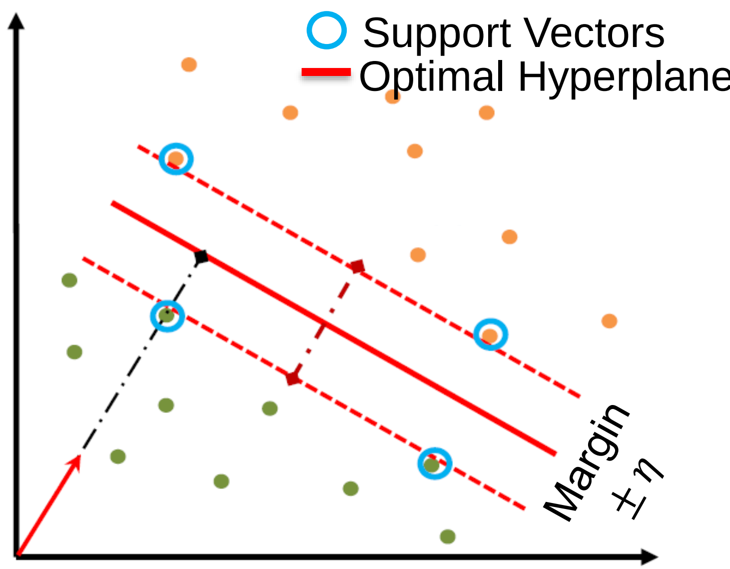
- **Soft margin Linear SVM**

$$\min_{\boldsymbol{w},c} \frac{1}{2} ||\boldsymbol{w}||^2 + C \sum_i \xi_i\,,$$

$$s.t.: \; y_i \cdot (< \boldsymbol{w}, \boldsymbol{x_i} > -c) \geq 1 - \xi_i \text{ and } \xi_i \geq 0$$

where ξ_i is a slack variable for each data point; it measures how much the i-th sample is allowed to violate the margin. Two conflicting objectives, maximize $\boldsymbol{\eta}$ but minimizing ξ_i as possible; C **is the hyperparameter that control this trade-off**

Both problems can be solved via Quadratic Programming solvers



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Kernel Support Vector Machines

Primal form

$$\min_{\boldsymbol{w},c} \frac{1}{2}\left|\left|\boldsymbol{w}\right|\right|^2 + C\sum_i \xi_i\,,$$

$$s.t.\, y_i \cdot (<\boldsymbol{w}, \boldsymbol{x_i}> - c) \geq 1 - \xi_i \text{ and } \xi_i \geq 0$$

Dual form

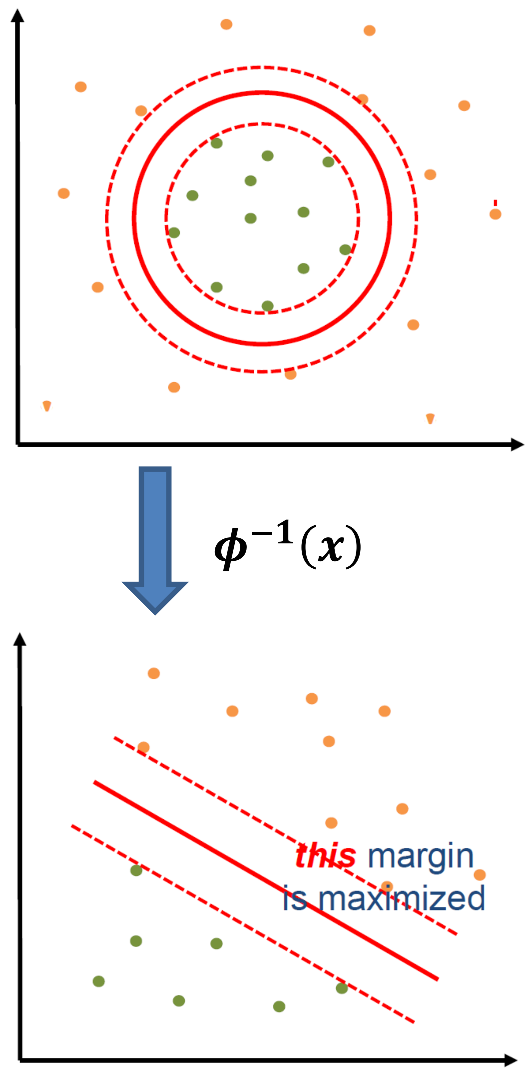
$$\min_{\boldsymbol{\alpha}} \frac{1}{2}\boldsymbol{\alpha}^T\boldsymbol{Q}\boldsymbol{\alpha} - \sum_i \alpha_i$$

$s.t.\, \boldsymbol{y}^T\boldsymbol{\alpha} = 0$, with $0 \leq \alpha_i \leq C$, *i=1,…,n*

with $\boldsymbol{Q}_{ik} \coloneqq y_i y_k k(\boldsymbol{x}_i, \boldsymbol{x}_k)$ is an *n x n positive definite matrix* and C an upper bound for the dual weights

Decision function

$$f(\boldsymbol{z}) = \operatorname{sgn}\left(\sum_i y_i \alpha_i\, K(\boldsymbol{x}_i, \boldsymbol{z}) \; + c\right)$$



Also solvable via QP, via Slater Theorem

Kernel selection and fine-tuning

- **Kernel Ridge Regression** (remember to scale input variables)
  - Start with a **Grid-search strategy, making it fine-grained** after a certain range looks promising
  - Try a range of regularization values: $\lambda = [0.0001, 1.0]$
  - RBF Kernel is preferred; values ranging: $\sigma = [0.01, 10.0]$
  - Use RMSE, **but also MAD and Pseudo-R2** (Square of the Correlation) for hyperparameter selection
- **Support Vector Machines** (remember to scale input variables)
  - **Grid-search strategy**: similar to KRR
  - Try a range of penalty values: $C = [0.001, 10.0]$
  - RBF Kernel is preferred; values ranging: $\sigma = [0.01, 10.0]$
  - **F1-Score tends to be a good generic metric**, but also Area Under the ROC curve (AUC), and precision/recall are important metrics. Accuracy is fine when the classes are well-balanced

Main Reading

- Chapters 5.8 and 12, of Elements of Statistical Learning, Hastie T., Tibshirani R. and Friedman J.
- Chapelle, O. (2007). Training a support vector machine in the primal. Neural computation, 19(5), 1155-1178.

email: faculty@mlinstitute.com

Further Reading

- Chapters 2 and 3 of Kernel Methods for Pattern Analysis,Shawe-Taylor J., and Cristianini N., Cambridge University Press
- Chapter 19, Support Vector Machines and Kernel Methods, Computer Age Statistical Inference, Efron B., Hastie T.
- Hofmann, T., Schölkopf, B., & Smola, A. J. (2008). Kernel methods in machine learning. The annals of statistics, 1171-1220.
- General Reference: Scholkopf, B., & Smola, A. J. (2001). Learning with kernels: support vector machines, regularization, optimization, and beyond. MIT press.

email: faculty@mlinstitute.com

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