Lecture 14. Kernel Methods

COMP90051 Statistical Machine Learning

Semester 2, 2015
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Based on slides provided by
Ben Rubinstein and
http://kernel-methods.net

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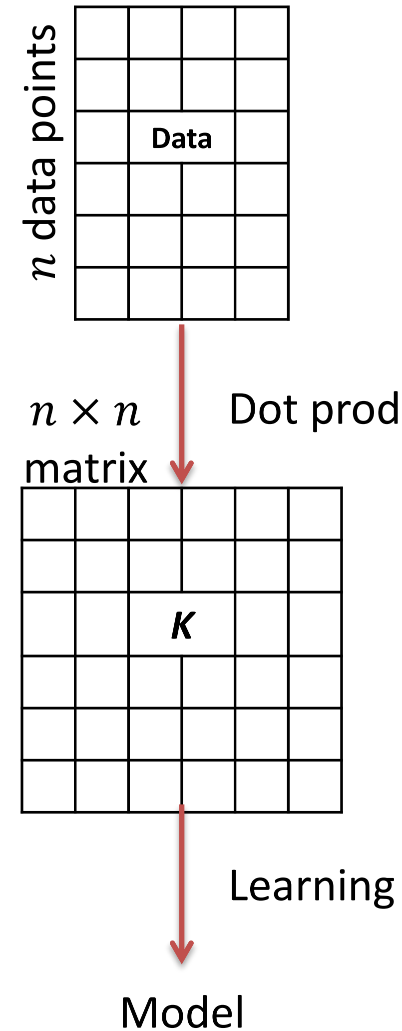
Kernel Methods

Very general family of linear techniques that can be made non-linear in a multitude of ways

Overview

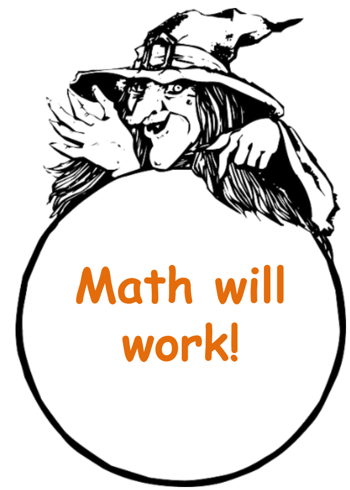
- Kernel matrix $\boldsymbol{K}$
  - Square *n* x *n* matrix measuring pairwise similarity
  - Entries $K_{ij} = \boldsymbol{x}_i \cdot \boldsymbol{x}_j$
- Kernel methods
  - Linear methods relying on training data only through $\boldsymbol{K}$
  - **Make non-linear** by running linear approach in new feature space; but don't need to map the data, just need $\boldsymbol{K}$
- **Modular**: learning algorithm, feature space, decouple
  - Can design general learning algorithms
  - Can design general feature mappings/kernels



Dot products, dot products, …

- How does the SVM depend on the data?

$$\min_{\boldsymbol{w}} \left(\frac{1}{2} \|\boldsymbol{w}\|^2 + \frac{C}{n} \sum_{i=1}^{n} l(1 - y_i \boldsymbol{w} \cdot \boldsymbol{x}_i - b) \right)$$



- Famous result: "Representer Theorem"
  * Solution in span of data!! $\boldsymbol{w}^* = \sum_{i=1}^{n} \alpha_i y_i \boldsymbol{x}_i$
  * Predictions become $f(\boldsymbol{x}) = \boldsymbol{w} \cdot \boldsymbol{x} = \sum_{i=1}^{n} \alpha_i y_i \boldsymbol{x}_i \cdot \boldsymbol{x}$
  * Support vectors are those $\boldsymbol{x}_i$ with $\alpha_i \neq 0$
    → why the SVM is non-parametric!
  * Finding the α_i involves only dot products between data

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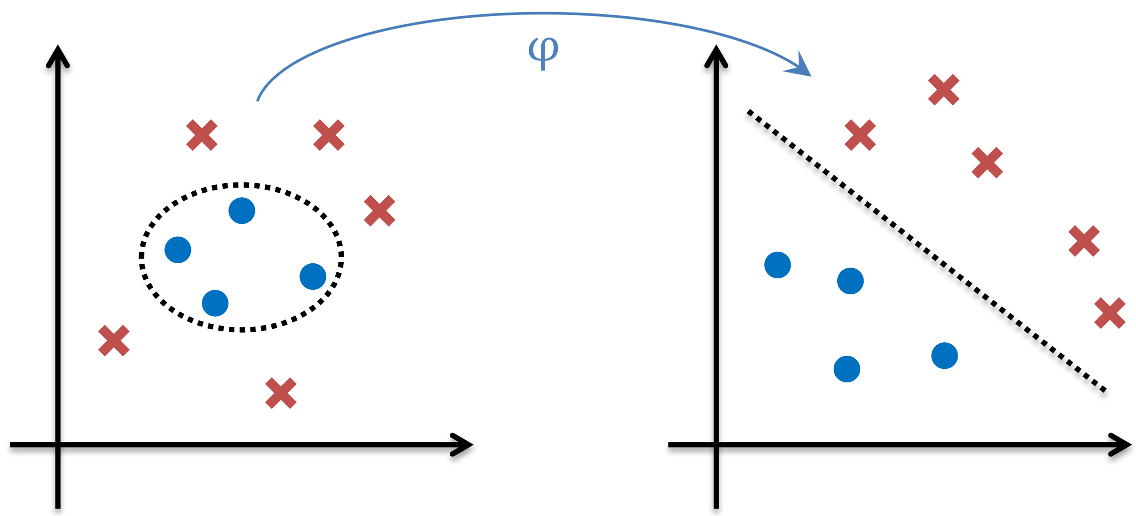
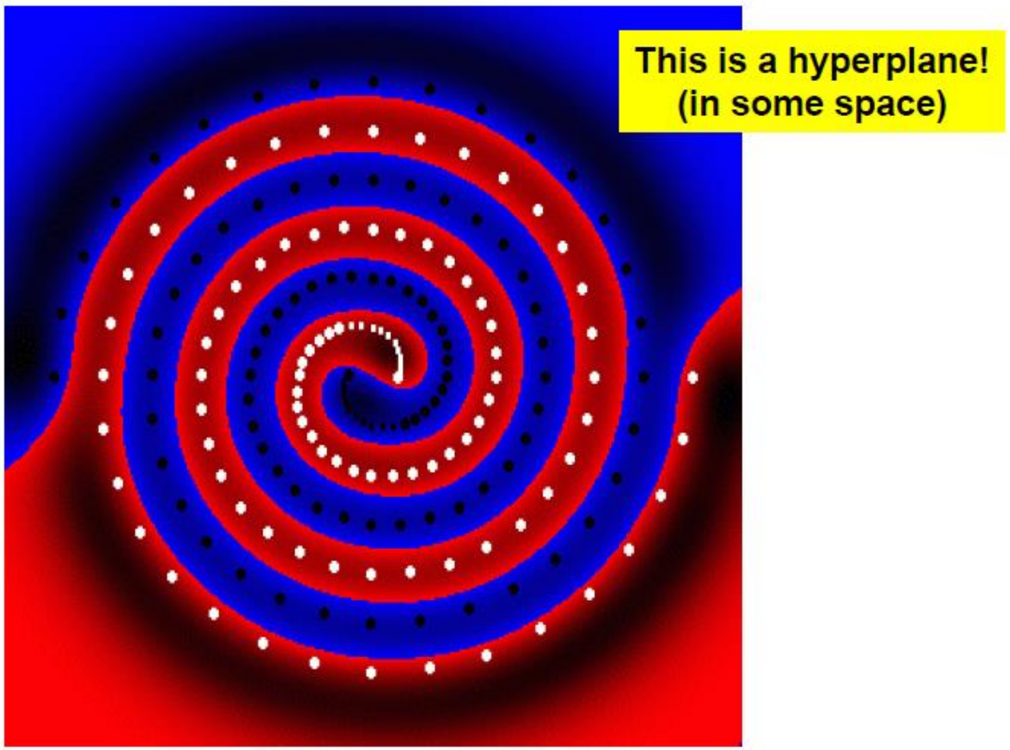
Non-linear SVM

- Map data into a new feature space
  - Example: original features and products of pairs
    $\varphi(x_1, \ldots, x_d) = (x_1, \ldots, x_d, x_1 x_1, x_1 x_2, \ldots, x_d x_d)$
- Run linear SVM in new space (use kernel matrix)
- Decision boundary is non-linear in original space



Flexibility of non-linear SVM



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Blessing of dimensionality

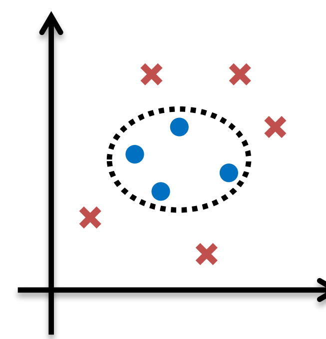
- Kernels implicitly map data to a very high dimensional features space
- Potentially dangerous because it looks like we now have many more parameters than data points
  - That is, $\boldsymbol{w}$ for the transformed features space is high dimensional
  - Curse of dimensionality
  - Danger of overfitting
- Representer theorem: $f(\boldsymbol{x}) = \sum_{i=1}^{n} \alpha_i y_i \boldsymbol{x}_i \cdot \boldsymbol{x}$
  - The number of parameters is at most n, independent of dimensionality
  - Support vectors are those data points with non-zero α_i
- Usually the number of non-zero α_i is smaller than n
  - Sparse kernel machines

Danger!! Potential problem

- Training linear SVM cubic in dimension *d*
- Non-linear → more dimensions → intractable?
- Representer Theorem to the rescue
  - Need only find α_i's which determine weight vector
  - "Only" *n* of them, independent of *d*
    … problematic if "big data"

But wait… what about the kernel matrix?

- *Computing* kernel matrix naïvely expensive
  - Map data to d'-dim feature space, then dot product; takes $O(d'n^2)$
- Computing kernels *directly* can be **cheap as**
- Example: p-degree polynomial kernel
  - $\varphi(x_1, \ldots, x_d) = (x_1, \ldots, x_d, x_1x_1, x_1x_2, \ldots, x_dx_d, \ldots)$
  - $d' = O(d^p)$ is pretty yuck → $O(d^p)$ per matrix entry
  - Trick to cut down to $O(d)$: $\varphi(\boldsymbol{u}) \cdot \varphi(\boldsymbol{v}) = (1 + \boldsymbol{u} \cdot \boldsymbol{v})^p$



- In fact, don't bother with feature spaces just make up matrix
  - Mercer's Theorem: provides a tool for identifying valid kernels

Some popular kernels

Kernel	$k(\boldsymbol{u}, \boldsymbol{v})$	Parameters	Mapping *x* to features
Linear	$\boldsymbol{u} \cdot \boldsymbol{v}$	-	Identity
Polynomial	$(1 + \boldsymbol{u} \cdot \boldsymbol{v})^p$	Integer degree p>1	Degree *p* polynomial in the x_i's
Gaussian aka Radial Basis Function (RBF)	$\exp\left(\frac{-\lVert\boldsymbol{u} - \boldsymbol{v}\rVert^2}{2\sigma^2}\right)$	Width σ	Infinite dimensional, nothing explicit!

Many more…

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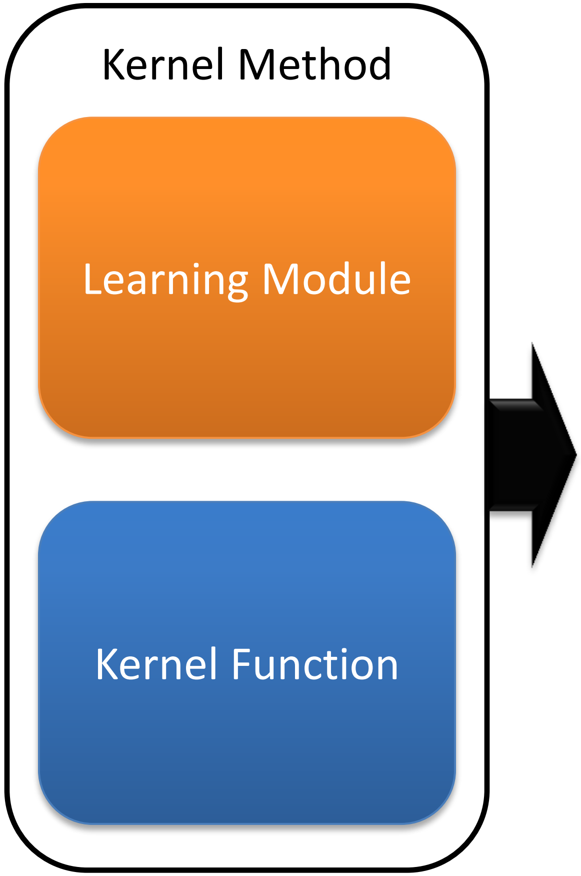
Modular learning

- More sophisticated learning algorithms, and kernels, exist
- Representer + Mercer Theorems imply their design decouples



$$f(x) = \sum_{i=1}^{n} \alpha_i K(\boldsymbol{x}_i, \boldsymbol{x})$$

…and the algorithms

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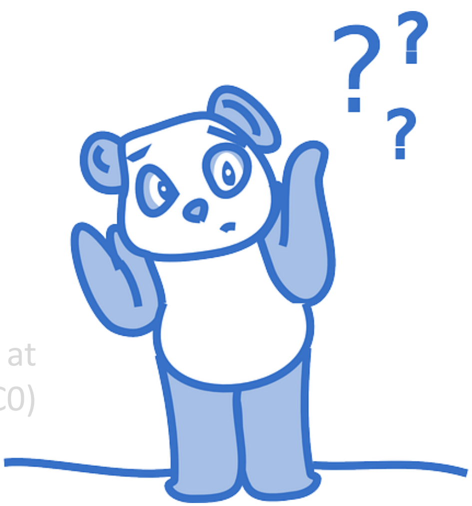
Checkpoint

- Which of the following statements is true?

 Any method that uses a feature space transformation $\varphi(\boldsymbol{x})$ is a kernel method

 Support vectors are points from the training set

 Feature mapping $\varphi(\boldsymbol{x})$ makes data linearly separable



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Kernelised SVM

Historically first kernel method

Feature transformations and kernels

- A feature transformation $\varphi(\boldsymbol{x})$ can help transforming data into a linearly separable form
- The kernel trick can be used to perform the transformation implicitly, without actually computing the transformation for each point
- One <u>does not have to use kernels</u>: feature transformation $\varphi(\boldsymbol{x})$ can be also use explicitly
  - If the number of resulting features is reasonable

Solutions to the SVM problem

- Recall the soft-margin SVM problem statement:

$$\min_{\boldsymbol{w}} \left(\frac{1}{2} \|\boldsymbol{w}\|^2 + \frac{C}{2} \sum_{i=1}^{n} \xi_i \right)$$

Subject to $\xi_i \geq 0$, $y_i(\boldsymbol{w}\boldsymbol{x}_i + b) \geq 1 - \xi_i$ for $i = 1, \ldots, n$

- This optimization problem (and many others) can be solved in two ways, called the primal formulation and dual formulation

- The primal approach is to solve the problem as it is stated here
  * If you wish, you can first apply $\varphi(\boldsymbol{x})$ here directly

- The complexity of training is $O(d^3)$, where d is the dimensionality of data
  * Recall that [solving optimization = training]
  * If you have applied $\varphi(\boldsymbol{x})$ then d is the dimensionality of resulting space

The dual formulation

- The idea of the dual formulation is to combine equations for the objective function and constraints into a single new objective function without constraints
  - This can be analytically convenient
  - Also this can lead to a different perspective on the problem
- This method is called *Lagrange multipliers*, and the corresponding new objective function is called *Lagrangian*

Formulating the dual SVM problem

- Soft-margin SVM original problem:

$$\min_{\boldsymbol{w},b} \boxed{\left(\frac{1}{2}\|\boldsymbol{w}\|^2 + \frac{C}{n}\sum_{i=1}^{n} \xi_i\right)}$$

  - Subject to $\boxed{\xi_i \geq 0}$, $\boxed{y_i(\boldsymbol{w}\boldsymbol{x}_i + b) \geq 1 - \xi_i}$ for $i = 1, \dots, n$

- Lagrangian

$$L_P \stackrel{\text{def}}{=} \boxed{\frac{1}{2}\|\boldsymbol{w}\|^2 + C\sum_{i=1}^{n} \xi_i} - \sum_{i=1}^{n} \alpha_i \boxed{\left[y_i(\boldsymbol{w}\boldsymbol{x}_i + b) \geq 1 - \xi_i\right]} - \sum_{i=1}^{n} \mu_i \boxed{\xi_i}$$

- Fix α_i, μ_i and minimise Lagrangian with respect to $\boldsymbol{w}, b, \xi$:
  - Set partial derivatives $\frac{\partial L_P}{\partial w_i}, \frac{\partial L_P}{\partial b}, \frac{\partial L_P}{\partial \xi_i}$ to zero

Solving the SVM problem

- Setting the partial derivatives to zero gives
  - $w^* = \sum_{i=1}^{n} \alpha_i y_i \boldsymbol{x}_i$
  - $0 = \sum_{i=1}^{n} \alpha_i y_i$
  - $\alpha_i = C/n - \mu_i$
  - $\alpha_i, \mu_i, \xi_i \geq 0$
- Substituting these back into L_P gives
  - $L_D = \sum_{i=1}^{n} \alpha_i - \frac{1}{2}\sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j \boldsymbol{x}_i \boldsymbol{x}_j$

Proofs are outside the scope

- L_D gives a lower bound on the original solution
- Therefore we maximize L_D w.r.t. α_i, s.t. $0 = \sum_{i=1}^{n} \alpha_i y_i$ and $0 \leq \alpha_i \leq \frac{C}{n}$
- In addition, Karush-Kuhn-Tucker conditions complete unique characterization of solution

About those alpha's

- Transform

$$\min_{\boldsymbol{w}} \frac{1}{2}\|\boldsymbol{w}\|^2 + \frac{C}{2}\sum_{i=1}^{n} \xi_i$$

into "dual problem"

$$\max_{\boldsymbol{\alpha}} \ \boldsymbol{\alpha} \cdot \mathbf{1} - \frac{1}{2}\boldsymbol{\alpha}^T G \boldsymbol{\alpha}$$

subject to $0 \leq \alpha_i \leq \frac{C}{n}$

where $\underbrace{G_{ij}}_{\text{Gram matrix}} = y_i y_j \boldsymbol{x}_i \cdot \boldsymbol{x}_j = y_i y_j \underbrace{K_{ij}}_{\text{Kernel matrix}}$

Want different non-linear mapping? Swap out *K*

- Quadratic program but in *n*, not *d* variables
- See how regularisation restricts data influence?

Solutions to the SVM problem

- The complexity of the primal solution is $O(d^3)$, where d is the dimensionality of data (after applying φ)
- The complexity of the dual solution is $O(n^3)$
- For “big data”, and finite-dimensional explicit transformation $\varphi(\boldsymbol{x})$ the primal form can be preferable

SVM: decisions to make

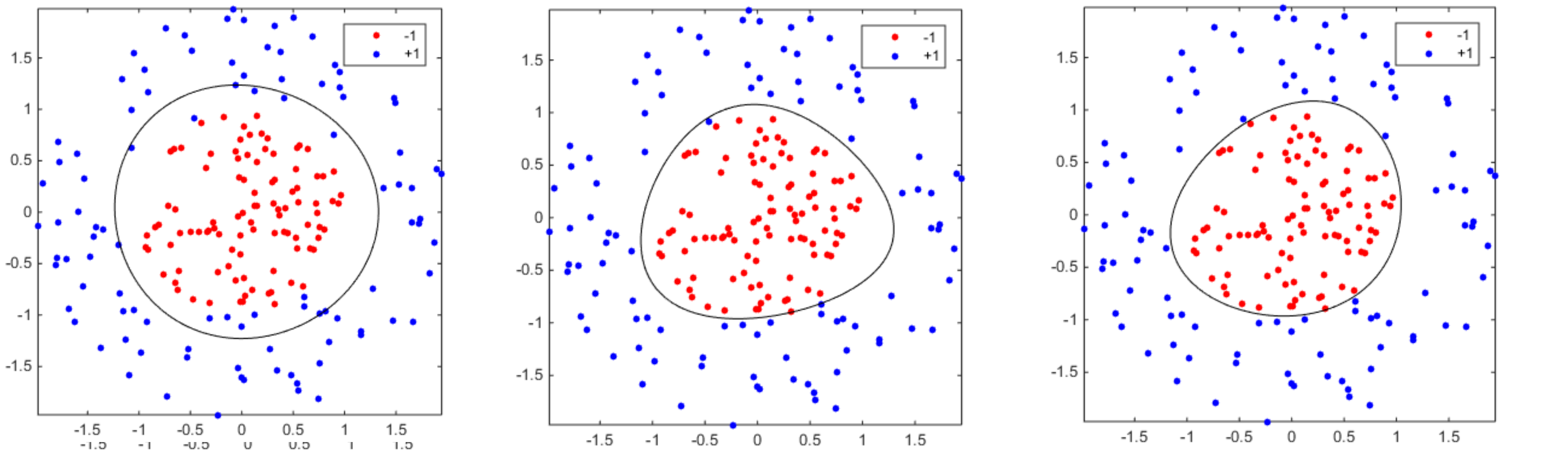
- Regularisation parameter C
- Choice of a kernel
- Note that some kernels introduce additional parameters, e.g., p in polynomial kernel $(1 + \boldsymbol{u} \cdot \boldsymbol{v})^p$

- SVM is a sparse kernel machine
- Regularisation also helps avoid the curse of dimensionality
- In practice: everything is set using cross-validation

Varying regularization parameter

Low C, tendency to underfit

High C, tendency to overfit



Polynomial kernel is used in all cases

SVMs for multiclass classification

- Multiclass classification has to be reduced to binary classification
- ***One-versus-all***: K binary classifications are made for each of the K classes. Each time, classification is "class k" vs "the rest". A new instance is assigned to class for which it has the strongest confidence (furthest away from the boundary).
- ***One-versus-one***: $K(K-1)/2$ classifications are made, covering all possible pairs of classes. A new instance is assigned the most voted class (class that gets most number of "wins").

SVM vs Neural Networks

Kernelised SVM	Feed-forward ANN
Linear SVM applied to non-linear data using kernelisation	Non-linear model by design (non-linear transfer functions)
Variable number of parameters, up to N (data points): predictions are made using support vectors	Parametric model: fixed number of parameters
Inherently batch training (see dual formulation, Kernel matrix)	Naturally amenable to online training (e.g., stochastic gradient descent)
SVM training always finds a global minimum (convex problem)	Global minimum is not guaranteed
Single dimensional output	Naturally adaptable for multiclass classification and multidimensional output

Summary

- Kernel methods
  - Modular decoupling of linear learner and feature mapping
  - Built on Representer Theorem, Mercer’s Theorem
  - Tonnes of kernel functions
  - Tonnes of kernel methods (SVM, PCA)