# Lecture 11. Kernel Methods

COMP90051 Statistical Machine Learning

Semester 2, 2018
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# This lecture

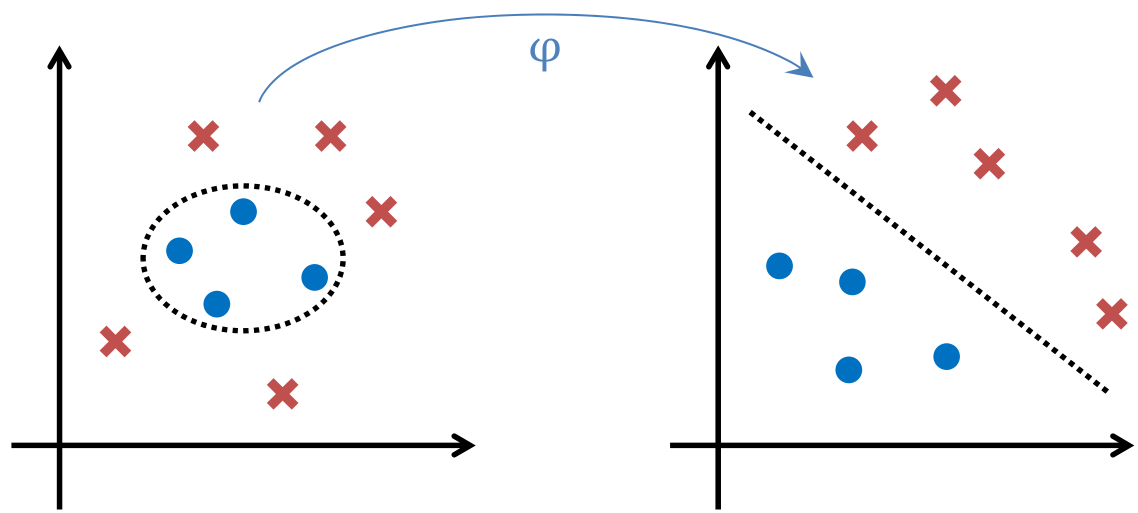
- Kernelisation
  - Basis expansion on dual formulation of SVMs
  - "Kernel trick"; Fast computation of feature space dot product
- Modular learning
  - Separating "learning module" from feature transformation
  - Representer theorem
- Constructing kernels
  - Overview of popular kernels and their properties
  - Mercer's theorem
  - Learning on unconventional data types

# Kernelising the SVM

Feature transformation by basis expansion; sped up by direct evaluation of kernels – the ‘kernel trick’

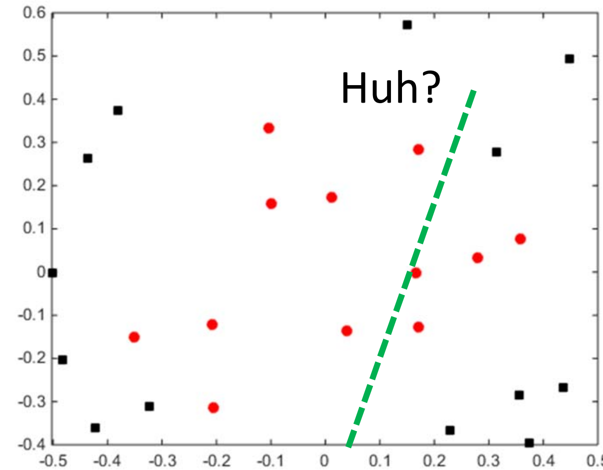
# Handling non-linear data with the SVM

- Method 1: Soft-margin SVM (deck #10)
- Method 2: Feature space transformation (deck #4)
  - Map data into a new feature space
  - Run hard-margin or soft-margin SVM in new space
  - Decision boundary is non-linear in original space

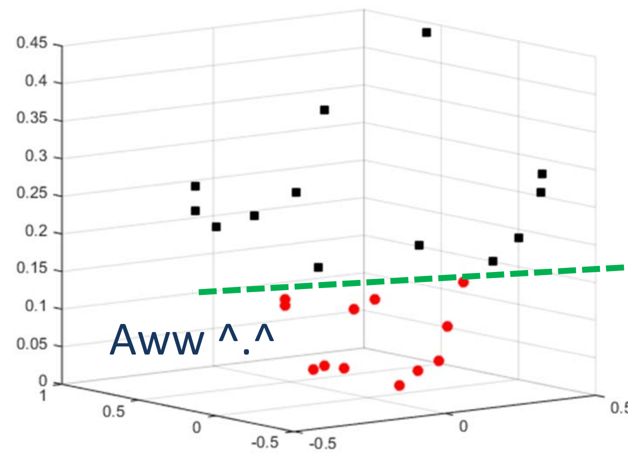


# Feature transformation (Basis expansion)

- Consider a binary classification problem
- Each example has features $[x_1, x_2]$
- Not linearly separable




- Now ‘add’ a feature $x_3 = x^2 + x_2^2$
- Each point is now $[x_1, x_2, x_1^2 + x_2^2]$
- Linearly separable!



# Naïve workflow

- Choose/design a linear model
- Choose/design a high-dimensional transformation $\varphi(\boldsymbol{x})$
  - Hoping that after adding a lot of various features some of them will make the data linearly separable
- For each training example, and for each new instance compute $\varphi(\boldsymbol{x})$
- Train classifier/Do predictions

- Problem: impractical/impossible to compute $\varphi(\boldsymbol{x})$ for high/infinite-dimensional $\varphi(\boldsymbol{x})$

# Hard-margin SVM's dual formulation

- Training: finding $\boldsymbol{\lambda}$ that solve

dot-product

$$\underset{\boldsymbol{\lambda}}{\operatorname{argmax}} \sum_{i=1}^{n} \lambda_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \lambda_i \lambda_j y_i y_j \boxed{\boldsymbol{x}_i' \boldsymbol{x}_j}$$

$$\text{s.t. } \lambda_i \geq 0 \text{ and } \sum_{i=1}^{n} \lambda_i y_i = 0$$

- Making predictions: classify instance $\boldsymbol{x}$ as sign of

dot-product

$$s = b^* + \sum_{i=1}^{n} \lambda_i^* y_i \boxed{\boldsymbol{x}_i' \boldsymbol{x}}$$

Note: $b^*$ found by solving for it in $y_j\left(b^* + \sum_{i=1}^{n} \lambda_i^* y_i \boxed{\boldsymbol{x}_i' \boldsymbol{x}_j}\right) = 1$ for any support vector $j$

# Hard-margin SVM in *feature space*

- Training: finding $\boldsymbol{\lambda}$ that solve

$$\underset{\boldsymbol{\lambda}}{\operatorname{argmax}} \sum_{i=1}^{n} \lambda_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \lambda_i \lambda_j y_i y_j \boxed{\varphi(\boldsymbol{x}_i)' \varphi(\boldsymbol{x}_j)}$$

$$\text{s.t. } \lambda_i \geq 0 \text{ and } \sum_{i=1}^{n} \lambda_i y_i = 0$$

- Making predictions: classify new instance $\boldsymbol{x}$ as sign of

$$s = b^* + \sum_{i=1}^{n} \lambda_i^* y_i \boxed{\varphi(\boldsymbol{x}_i)' \varphi(\boldsymbol{x})}$$

Note: $b^*$ found by solving for it in $y_j\left(b^* + \sum_{i=1}^{n} \lambda_i^* y_i \boxed{\varphi(\boldsymbol{x}_i)' \varphi(\boldsymbol{x}_j)}\right) = 1$ for support vector $j$

# Observation: Kernel representation

- Both parameter estimation and computing predictions depend on data only in a form of a dot product
  - In original space $\boldsymbol{u}'\boldsymbol{v} = \sum_{i=1}^{m} u_i v_i$
  - In transformed space $\varphi(\boldsymbol{u})'\varphi(\boldsymbol{v}) = \sum_{i=1}^{l} \varphi(\boldsymbol{u})_i \varphi(\boldsymbol{v})_i$

- Kernel is a function that can be expressed as a dot product in some feature space $K(\boldsymbol{u}, \boldsymbol{v}) = \varphi(\boldsymbol{u})'\varphi(\boldsymbol{v})$

# Kernel as shortcut: Example

- For *some* $\varphi(\boldsymbol{x})$'s, kernel is faster to compute directly than first mapping to feature space then taking dot product.
- For example, consider two vectors $\boldsymbol{u} = [u_1]$ and $\boldsymbol{v} = [v_1]$ and transformation $\varphi(\boldsymbol{x}) = [x_1^2, \sqrt{2c}x_1, c]$, some $c$
  - So $\varphi(\boldsymbol{u}) = \underbrace{\left[u_1^2, \sqrt{2c}u_1, c\right]'}_{\text{2 operations}}$ and $\varphi(\boldsymbol{v}) = \underbrace{\left[v_1^2, \sqrt{2c}v_1, c\right]'}_{\text{+2 operations}}$
  - Then $\varphi(\boldsymbol{u})'\varphi(\boldsymbol{v}) = \left(u_1^2 v_1^2 + 2cu_1v_1 + c^2\right)$ +5 operations = 9 ops.
- This can be alternatively computed directly as

$$\varphi(\boldsymbol{u})'\varphi(\boldsymbol{v}) = (u_1v_1 + c)^2 \quad \text{3 operations}$$

  - Here $K(\boldsymbol{u}, \boldsymbol{v}) = (u_1v_1 + c)^2$ is the corresponding kernel

# More generally: The "kernel trick"

- Consider two training points $\boldsymbol{x}_i$ and $\boldsymbol{x}_j$ and their dot product in the transformed space.
- $k_{ij} \equiv \varphi(\boldsymbol{x}_i)'\varphi(\boldsymbol{x}_j)$ can be computed as:
  1. Compute $\varphi(\boldsymbol{x}_i)'$
  2. Compute $\varphi(\boldsymbol{x}_j)$
  3. Compute $k_{ij} = \varphi(\boldsymbol{x}_i)'\varphi(\boldsymbol{x}_j)$
- However, for some transformations $\varphi$, there's a "shortcut" function that gives exactly the same answer $K(\boldsymbol{x}_i, \boldsymbol{x}_j) = k_{ij}$
  * Doesn't involve steps 1 – 3 and no computation of $\varphi(\boldsymbol{x}_i)$ and $\varphi(\boldsymbol{x}_j)$
  * Usually $k_{ij}$ computable in $O(m)$, but computing $\varphi(\boldsymbol{x})$ requires $O(l)$, where $l \gg m$ (impractical) and even $l = \infty$ (infeasible)

# Kernel hard-margin SVM

- Training: finding $\boldsymbol{\lambda}$ that solve

feature mapping is implied by kernel

$$\underset{\boldsymbol{\lambda}}{\operatorname{argmax}} \sum_{i=1}^{n} \lambda_i - \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} \lambda_i \lambda_j y_i y_j \boxed{K\left(\boldsymbol{x}_i, \boldsymbol{x}_j\right)}$$

$$\text{s.t. } \lambda_i \geq 0 \text{ and } \sum_{i=1}^{n} \lambda_i y_i = 0$$

- Making predictions: classify new instance $\boldsymbol{x}$ based on the sign of

$$s = b^* + \sum_{i=1}^{n} \lambda_i^* y_i \boxed{K\left(\boldsymbol{x}_i, \boldsymbol{x}_j\right)}$$

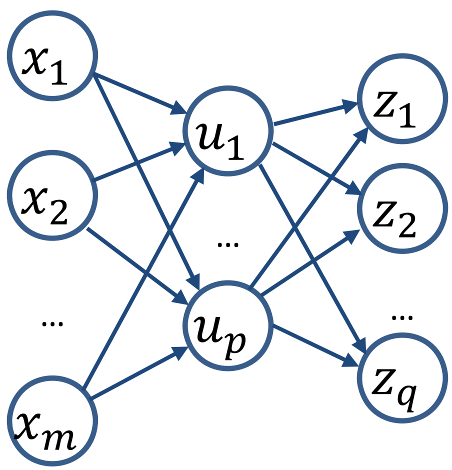
feature mapping is implied by kernel

- Here $b^*$ can be found by noting that for support vector $j$ we have $y_j\left(b^* + \sum_{i=1}^{n} \lambda_i^* y_i \boxed{K\left(\boldsymbol{x}_i, \boldsymbol{x}_j\right)}\right) = 1$

# Approaches to non-linearity

## ANNs

- Elements of $\boldsymbol{u} = \varphi(\boldsymbol{x})$ are transformed input $\boldsymbol{x}$
- This $\varphi$ has weights learned from data




## SVMs

- Choice of kernel $K$ determines features $\varphi$
- Don't learn $\varphi$ weights
- But, don't even need to compute $\varphi$ so can support v high dim. $\varphi$
- Also support arbitrary data types

# Any method that uses a feature space transformation $\varphi(x)$ uses kernels

When poll is active, respond at **PollEv.com/bipr**

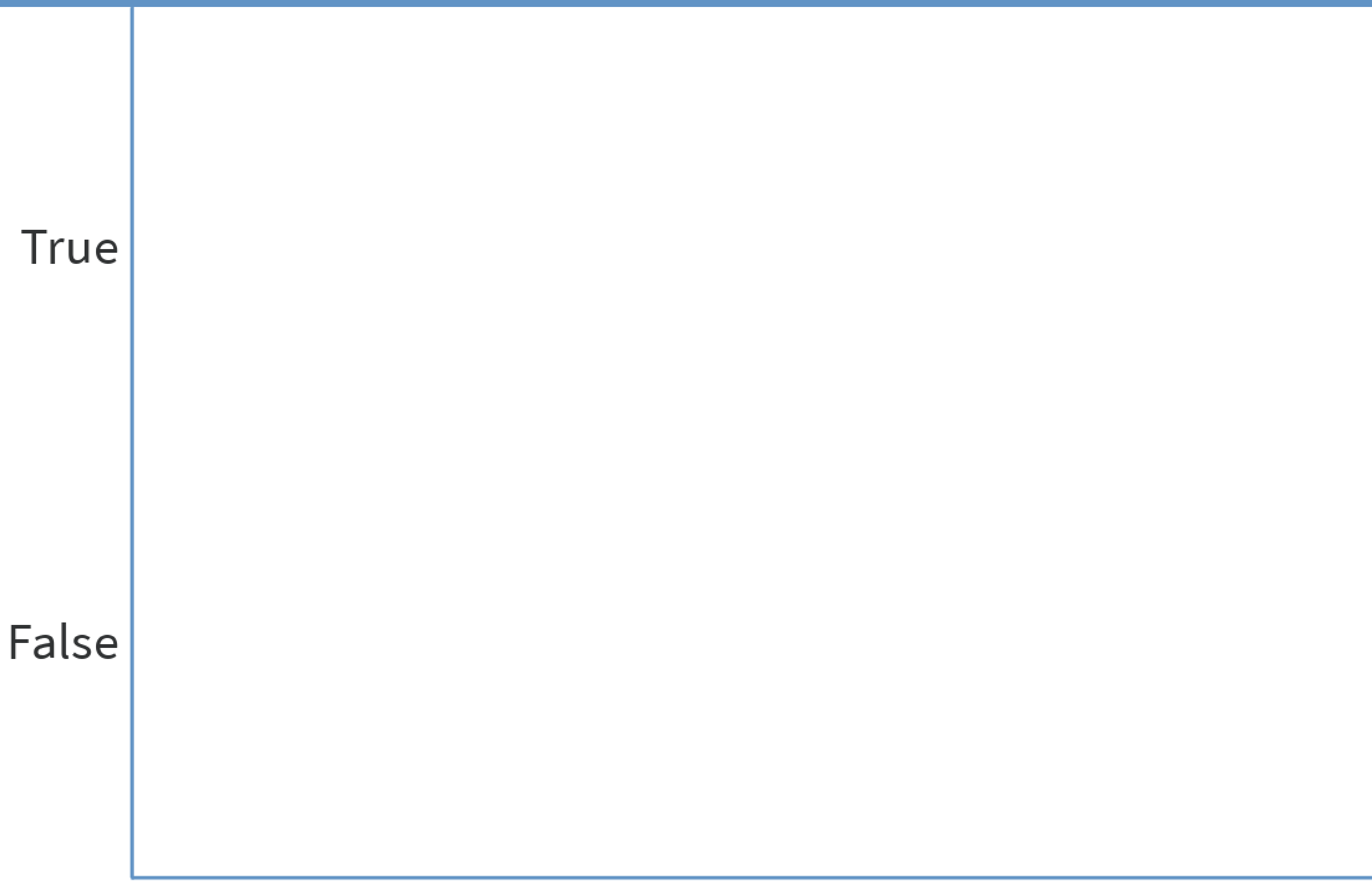
Text **BIPR** to **+61 427 541 357** once to join

Answers to this poll are anonymous

True

False

# Support vectors are points from the training set



# Feature mapping $\varphi(x)$ makes data linearly separable

True

False

# Modular Learning

Kernelisation beyond SVMs;
Separating the “learning module”
from feature space transformation

# Modular learning

- All information about feature mapping is concentrated within the kernel
- In order to use a different feature mapping, simply change the kernel function
- Algorithm design decouples into choosing a “learning method” (e.g., SVM vs logistic regression) and choosing feature space mapping, i.e., kernel

# Kernelised perceptron (1/3)

When classified correctly, weights are unchanged

When misclassified: $\boldsymbol{w}^{(k+1)} = -\eta(\pm\boldsymbol{x})$
($\eta > 0$ is called *learning rate)*

<u>If $y = 1$, but $s < 0$</u>
$w_i \leftarrow w_i + \eta x_i$
$w_0 \leftarrow w_0 + \eta$

<u>If $y = -1$, but $s \geq 0$</u>
$w_i \leftarrow w_i - \eta x_i$
$w_0 \leftarrow w_0 - \eta$

Suppose weights are initially set to 0

First update: $\boldsymbol{w} = \eta y_{i_1} \boldsymbol{x}_{i_1}$
Second update: $\boldsymbol{w} = \eta y_{i_1} \boldsymbol{x}_{i_1} + \eta y_{i_2} \boldsymbol{x}_{i_2}$
Third update $\boldsymbol{w} = \eta y_{i_1} \boldsymbol{x}_{i_1} + \eta y_{i_2} \boldsymbol{x}_{i_2} + \eta y_{i_3} \boldsymbol{x}_{i_3}$
etc.

# Kernelised perceptron (2/3)

- Weights always take the form $\boldsymbol{w} = \sum_{i=1}^{n} \alpha_i y_i \boldsymbol{x}_i$, where $\boldsymbol{\alpha}$ some coefficients
- Perceptron weights are always a linear combination of data!
- Recall that prediction for a new point $\boldsymbol{x}$ is based on sign of $w_0 + \boldsymbol{w}'\boldsymbol{x}$
- Substituting $\boldsymbol{w}$ we get $w_0 + \sum_{i=1}^{n} \alpha_i y_i \boldsymbol{x}_i'\boldsymbol{x}$
- The dot product $\boldsymbol{x}_i'\boldsymbol{x}$ can be replaced with a kernel

# Kernelised perceptron (3/3)

Choose initial guess $\boldsymbol{w}^{(0)}$, $k = 0$

Set $\boldsymbol{\alpha} = \mathbf{0}$

For $t$ from 1 to $T$ (epochs)

For each training example $\{\boldsymbol{x}_i, y_i\}$

Predict based on $w_0 + \sum_{j=1}^{n} \alpha_j y_j \boldsymbol{x}_i' \boldsymbol{x}_j$

If misclassified, update $\alpha_i \leftarrow \alpha_i + 1$

# Representer theorem

- Theorem: For any training set $\{\boldsymbol{x}_i, y_i\}_{i=1}^{n}$, any empirical risk function $E$, monotonic increasing function $g$, then any solution

$$f^* \in \arg\min_f E(\boldsymbol{x}_1, y_1, f(\boldsymbol{x}_1), \dots, \boldsymbol{x}_n, y_n, f(\boldsymbol{x}_n)) + g(\|f\|)$$

has representation for some coefficients

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

Aside: f sits in a reproducing kernel Hilbert space (RKHS)

- Tells us when a (decision-theoretic) learner is kernelizable
- The dual tells us the form this linear kernel representation takes
- SVM is but one example!
  * Ridge regression
  * Logistic regression
  * Principal component analysis (PCA)
  * Canonical correlation analysis (CCA)
  * Linear discriminant analysis (LDA)
  * and many more …

# Constructing Kernels

An overview of popular kernels
and kernel properties

# Polynomial kernel

- Function $K(\boldsymbol{u}, \boldsymbol{v}) = (\boldsymbol{u}'\boldsymbol{v} + c)^d$ is called *polynomial kernel*
  - Here $\boldsymbol{u}$ and $\boldsymbol{v}$ are vectors with $m$ components
  - $d \geq 0$ is an integer and $c \geq 0$ is a constant
- Without the loss of generality, assume $c = 0$
  - If it's not, add $\sqrt{c}$ as a dummy feature to $\boldsymbol{u}$ and $\boldsymbol{v}$
- $(\boldsymbol{u}'\boldsymbol{v})^d = (u_1 v_1 + \cdots + u_m v_m)(u_1 v_1 + \cdots + u_m v_m) \ldots (u_1 v_1 + \cdots + u_m v_m)$
- $= \sum_{i=1}^{l} (u_1 v_1)^{a_{i1}} \ldots (u_m v_m)^{a_{im}}$
  - Here $0 \leq a_{ij} \leq d$ and $l$ are integers
- $= \sum_{i=1}^{l} \left(u_1^{a_{i1}} \ldots u_m^{a_{im}}\right)\left(v_1^{a_{i1}} \ldots v_m^{a_{im}}\right)$
- $= \sum_{i=1}^{l} \varphi(\boldsymbol{u})_i \varphi(\boldsymbol{v})_i$
- Feature map $\varphi: \mathbb{R}^m \rightarrow \mathbb{R}^l$, where $\varphi_i(\boldsymbol{x}) = \left(x_1^{a_{i1}} \ldots x_m^{a_{im}}\right)$

# Identifying new kernels

- Method 1: Let $K_1(\boldsymbol{u}, \boldsymbol{v})$, $K_2(\boldsymbol{u}, \boldsymbol{v})$ be kernels, $c > 0$ be a constant, and $f(\boldsymbol{x})$ be a real-valued function. Then each of the following is also a kernel:
  * $K(\boldsymbol{u}, \boldsymbol{v}) = K_1(\boldsymbol{u}, \boldsymbol{v}) + K_2(\boldsymbol{u}, \boldsymbol{v})$
  * $K(\boldsymbol{u}, \boldsymbol{v}) = cK_1(\boldsymbol{u}, \boldsymbol{v})$
  * $K(\boldsymbol{u}, \boldsymbol{v}) = f(\boldsymbol{u})K_1(\boldsymbol{u}, \boldsymbol{v})f(\boldsymbol{v})$
  * *See Bishop for more identities*

Prove these!

- Method 2: Using Mercer's theorem (coming up!)

# Radial basis function kernel

- Function $K(\boldsymbol{u},\boldsymbol{v}) = \exp\left(-\gamma\|\boldsymbol{u}-\boldsymbol{v}\|^2\right)$ is the *radial basis function kernel* (aka Gaussian kernel)
  - Here $\gamma > 0$ is the spread parameter
- $\exp\left(-\gamma\|\boldsymbol{u}-\boldsymbol{v}\|^2\right) = \exp\left(-\gamma(\boldsymbol{u}-\boldsymbol{v})'(\boldsymbol{u}-\boldsymbol{v})\right)$
- $= \exp\left(-\gamma(\boldsymbol{u}'\boldsymbol{u} - 2\boldsymbol{u}'\boldsymbol{v} + \boldsymbol{v}'\boldsymbol{v})\right)$
- $= \exp(-\gamma\boldsymbol{u}'\boldsymbol{u})\exp(2\gamma\boldsymbol{u}'\boldsymbol{v})\exp(-\gamma\boldsymbol{v}'\boldsymbol{v})$
- $= f(\boldsymbol{u})\exp(2\gamma\boldsymbol{u}'\boldsymbol{v})f(\boldsymbol{v})$
- $= f(\boldsymbol{u})\left(\sum_{d=0}^{\infty} r_d(\boldsymbol{u}'\boldsymbol{v})^d\right)f(\boldsymbol{v})$

Power series expansion

- Here, each $(\boldsymbol{u}'\boldsymbol{v})^d$ is a polynomial kernel. Using kernel identities, we conclude that the middle term is a kernel, and hence the whole expression is a kernel

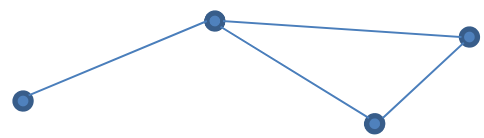
# Mercer's Theorem

- Question: given $\varphi(\boldsymbol{u})$, is there a good kernel to use?
- Inverse question: given some function $K(\boldsymbol{u}, \boldsymbol{v})$, is this a valid kernel? In other words, is there a mapping $\varphi(\boldsymbol{u})$ implied by the kernel?

- Mercer's theorem:
  * Consider a finite sequences of objects $\boldsymbol{x}_1, \dots, \boldsymbol{x}_n$
  * Construct $n \times n$ matrix of pairwise values $K(\boldsymbol{x}_i, \boldsymbol{x}_j)$
  * $K(\boldsymbol{x}_i, \boldsymbol{x}_j)$ is a valid kernel if this matrix is positive-semidefinite, and this holds for all possible sequences $\boldsymbol{x}_1, \dots, \boldsymbol{x}_n$

# Data comes in a variety of shapes

- So far in COMP90051 data has been vectors of numbers
- But what if we wanted to do machine learning on …
- Graphs
  - Facebook, Twitter, …



- Sequences of variable lengths
  - “science is organized knowledge”, “wisdom is organized life”*, …
  - “CATTC”, “AAAGAGA”
- Songs, movies, etc.

* Immanuel Kant

# Handling arbitrary data structures

- Kernels are powerful approach to deal with many data types
- Could define similarity function on variable length strings

*K("science is organized knowledge", "wisdom is organized life")*

- However, not every function on two objects is a valid kernel
- Remember that we need that function $K(\boldsymbol{u}, \boldsymbol{v})$ to imply a dot product in some feature space

# A large variety of kernels

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# This lecture

- Kernels
  - Nonlinearity by basis expansion
  - Kernel trick to speed up computation
- Modular learning
  - Separating "learning module" from feature transformation
  - Representer theorem
- Constructing kernels
  - An overview of popular kernels and their properties
  - Mercer's theorem
  - Extending machine learning beyond conventional data structure

Next lecture: Ensemble methods