CS-E4710 Machine Learning: Supervised Methods

Lecture 7: Kernel methods

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Kernel methods

Key characteristics of kernel methods:

- **Embedding:** Inputs $\mathbf{x} \in X$ from some input space X are embedded into a *feature space* F via a feature map $\phi : X \mapsto F$. ϕ may be highly **non-linear** and F potentially very high-dimensional vector space
- **Linear models:** are built for the the patterns in the feature space (typically $\mathbf{w}^T \phi(\mathbf{x})$); efficient to find the optimal model, convex optimization
- **Kernel trick:** Algorithms work with kernels, inner products of feature vectors $\kappa(\mathbf{x}, \mathbf{z}) = \sum_j \phi_j(\mathbf{x})\phi_j(\mathbf{z})$ rather than the explicit features $\phi(\mathbf{x})$; side-step the efficiency problems of high-dimensionality
- **Regularized learning:** To avoid overfitting, large feature weights are penalized, separation by large margin is favoured

Data analysis tasks via kernels

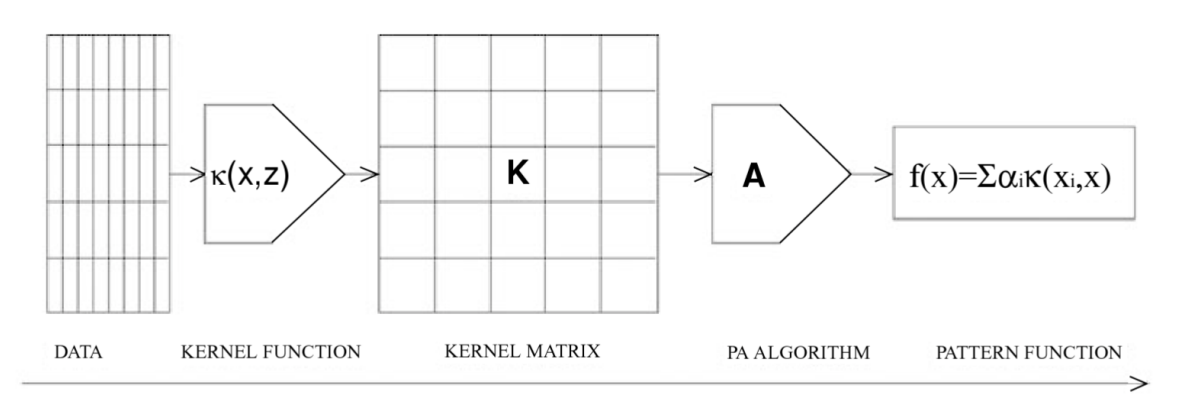
Many data analysis algorithms can be 'kernelized', i.e. transformed to an **equivalent** form by replacing object descriptions (feature vectors) by pairwise similarities (kernels):

- Classification (SVM)
- Regression
- Ranking
- Novelty detection
- Clustering
- Principal component analysis, canonical correlation analysis
- Multi-label/Multi-task/Structured output
- ...

More of the tasks beyond classification will be discussed at the course Kernel Methods in Machine Learning (Spring 2022 by Rohit Babbar)

Modularity of kernel methods

- Algorithms are designed that work with arbitrary inner products (or kernels) between inputs
- The same algorithm will work with any inner product (or kernel)
- This allows theoretical properties of the learning algorithm to be investigated and the results will carry to all application domains
- Kernel will depend on the application domain; prior information is encoded into the kernel



What is a kernel?

- Informally, a **kernel** is a function that calculates the similarity between two objects, e.g.
  - two proteins
  - two images
  - two documents
  - ...
- $x_i \in X$ and $x_j \in X$
  - $X =$ set of all proteins in the nature (finite set)
  - $X =$ all possible images (infinite set)
  - $X =$ all possible documents (infinite set)
- $\kappa \colon X \times X \to \mathbb{R}$

Data and Feature maps

- We assume inputs $\mathbf{x}$ to come from an arbitrary set X:
  - Vectors, matrices, tensors
  - Structured objects: Sequences, hierarchies, graphs
- We further assume the data items can be expressed as objects in some feature space F
- Typically F is a space of feature vectors, $F \subseteq \mathbb{R}^N$, where N is the dimension of the feature space, or more generally matrices or tensors.
- Inputs $\mathbf{x}$ are mapped to this space by a feature map $\phi : X \mapsto F$
- $\phi(\mathbf{x})$ is the image of the data item in the feature space

What is a kernel?

- Formally: a kernel function is an inner product (scalar product, dot product) in a feature space F,denoted by $\langle \cdot, \cdot \rangle_F$
  - Often the subscript F is dropped when it is clear from context
- Linear kernel: If $\mathbf{x} \in \mathbb{R}^n$ and the feature map $\phi(\mathbf{x}) = \mathbf{x}$ is the identity, then $F = \mathbb{R}^n$ and the resulting kernel

$$\kappa_{lin}(\mathbf{x}, \mathbf{z}) = \langle \phi(\mathbf{x}), \phi(\mathbf{z}) \rangle_F = \langle \mathbf{x}, \mathbf{z} \rangle_{\mathbb{R}^n}$$

  is called the linear kernel
- Linear kernel therefore corresponds to the dot product in $\mathbb{R}^n$

$$\kappa_{lin}(\mathbf{x}, \mathbf{z}) = \sum_{j=1}^{n} x_j z_j = \mathbf{x}^T \mathbf{z}$$

Geometric interpretation

- Geometric interpretation of the linear kernel: cosine angle between two feature vectors

$$\cos\beta = \frac{\mathbf{x}^T\mathbf{z}}{\|\mathbf{x}\|_2 \|\mathbf{z}\|_2} = \frac{\kappa_{lin}(\mathbf{x},\mathbf{z})}{\sqrt{\kappa_{lin}(\mathbf{x},\mathbf{x})}\sqrt{\kappa_{lin}(\mathbf{z},\mathbf{z})}},$$

  where

$$\|\mathbf{x}\|_2 = \sqrt{\kappa_{lin}(\mathbf{x},\mathbf{x})} = \sqrt{\langle \mathbf{x},\mathbf{x}\rangle} = \sqrt{\sum_{j=1}^{n} x_j^2}$$

  is the Euclidean norm.

Kernel vs. Euclidean distance

- Assume two vectors $\mathbf{x}, \mathbf{z} \in \mathbb{R}^n$ with unit length $\|\mathbf{x}\|_2 = \|\mathbf{z}\|_2 = 1$
- Kernel: $\kappa(\mathbf{x}, \mathbf{z}) = \mathbf{x}^T\mathbf{z}$
- Euclidean Distance: $d(\mathbf{x}, \mathbf{z}) = \|\mathbf{x} - \mathbf{z}\|_2 = \sqrt{\sum_{k=1}^{n}(x_k - z_k)^2}$
- Expanding the squares and using unit length of the vectors we get:

$$\frac{1}{2}d(\mathbf{x}, \mathbf{z})^2 = \frac{1}{2}\|\mathbf{x} - \mathbf{z}\|_2^2 = \frac{1}{2}(\mathbf{x} - \mathbf{z})^T(\mathbf{x} - \mathbf{z}) =$$

$$= \frac{1}{2}\left(\|\mathbf{x}\|_2^2 - 2\mathbf{x}^T\mathbf{z} + \|\mathbf{z}\|_2^2\right)$$

$$= 1 - \mathbf{x}^T\mathbf{z} = 1 - \kappa(\mathbf{x}, \mathbf{z})$$

Hilbert space*

Formally the underlying space of a kernel is required to be a Hilbert space

A Hilbert space is a real vector space $\mathcal{H}$, with the following additional properties

- Equipped with a **inner product**, a map $\langle ., . \rangle$, which satisfies for all objects $x, x', z \in \mathcal{H}$
  - linear: $\langle ax + bx', z \rangle = a\langle x, z \rangle + b\langle x', z \rangle$
  - symmetric: $\langle x, x' \rangle = \langle x', x \rangle$
  - positive semi-definite: $\langle x, x \rangle \geq 0$, $\langle x, x \rangle = 0$ if and only if $x = 0$
- Complete: every Cauchy sequence $\{h_n\}_{n \geq 1}$ of elements in $\mathcal{H}$ converges to an element of $\mathcal{H}$
- Separable: there is a countable set of elements $\{h_1, h_2, \ldots, \}$ in $\mathcal{H}$ such that for any $h \in \mathcal{H}$ and every $\epsilon > 0$ $\|h_i - h\| < \epsilon$.

On this lecture $\mathcal{H} = \mathbb{R}^N$, where the dimension N is finite or infinite. Both cases are Hilbert spaces.

* Advanced material; will not be examined

The kernel matrix

- In kernel methods, a **kernel matrix**, also called the **Gram matrix**, an $m \times m$ matrix of pairwise similarity values is used:

$$\mathbf{K} = \begin{bmatrix} \kappa(\mathbf{x}_1, \mathbf{x}_1) & \kappa(\mathbf{x}_1, \mathbf{x}_2) & \dots & \kappa(\mathbf{x}_1, \mathbf{x}_m) \\ \kappa(\mathbf{x}_2, \mathbf{x}_1) & \kappa(\mathbf{x}_2, \mathbf{x}_2) & \dots & \kappa(\mathbf{x}_2, \mathbf{x}_m) \\ \vdots & \vdots & \ddots & \vdots \\ \kappa(\mathbf{x}_m, \mathbf{x}_1) & \kappa(\mathbf{x}_m, \mathbf{x}_2) & \dots & \kappa(\mathbf{x}_m, \mathbf{x}_m) \end{bmatrix}$$

- Each entry is an inner product between two data points $\kappa(\mathbf{x}_i, \mathbf{x}_j) = \langle \phi(\mathbf{x}_i), \phi(\mathbf{x}_j) \rangle$, where $\phi : X \mapsto \mathcal{F}$ is a feature map
- Since an inner product is symmetric, $\mathbf{K}$ is a symmetric matrix

The kernel matrix

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- Processing the kernel matrix during preprocessing, training and prediction time is the major factor of the time-complexity of kernel methods
- Compare the two matrices assuming m examples of dimension $\mathbb{R}^N$
  - The kernel matrix has m^2 items, independently from N
  - The data matrix, matrix of feature vectors of the training data has size mN
- Consequently, the kernel matrix scales better than the data matrix when $N > m$

The kernel matrix

- A symmetric matrix $\mathbf{A} \in \mathbb{R}^{m \times m}$ is positive semi-definite (PSD) if for any vector $\mathbf{v} \in \mathbb{R}^m$, we have $\mathbf{v}^T \mathbf{A} \mathbf{v} \geq 0$
- The **kernel matrix** corresponding to the kernel function $\kappa(\mathbf{x}, \mathbf{z}) = \langle \phi(\mathbf{x}), \phi(\mathbf{z}) \rangle$ on a set of data points $\{\mathbf{x}_i\}_{i=1}^m$ is positive semidefinite:

$$\mathbf{v}^T \mathbf{K} \mathbf{v} = \sum_{i,j=1}^{n} v_i \mathbf{K}_{ij} v_j = \sum_{i,j=1}^{m} v_i \langle \phi(x_i), \phi(x_j) \rangle v_j =$$

$$= \langle \sum_{i=1}^{m} v_i \phi(x_i), \sum_{j=1}^{m} v_j \phi(x_j) \rangle = \| \sum_{i=1}^{m} v_i \phi(x_i) \|^2 \geq 0$$

- Consequence: as a symmetric PSD matrix, kernel matrix $\mathbf{K}$ has non-negative eigenvalues $\lambda_1 \geq \cdots \geq \lambda_m \geq 0$

PSD property and optimization

- Consider objective of the dual SVM optimization problem

$$OBJ(\boldsymbol{\alpha}) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{m} \alpha_i \alpha_j y_i y_j \kappa(\mathbf{x}_i, \mathbf{x}_j) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \boldsymbol{\alpha}^T \mathbf{H} \boldsymbol{\alpha}$$

  where

$$\mathbf{H} = \left(\frac{\partial^2 OBJ(\boldsymbol{\alpha})}{\partial \alpha_i \partial \alpha_j} \right)_{i,j=1}^{m} = (y_i y_j \kappa(\mathbf{x}_i, \mathbf{x}_j))_{i,j=1}^{m}$$

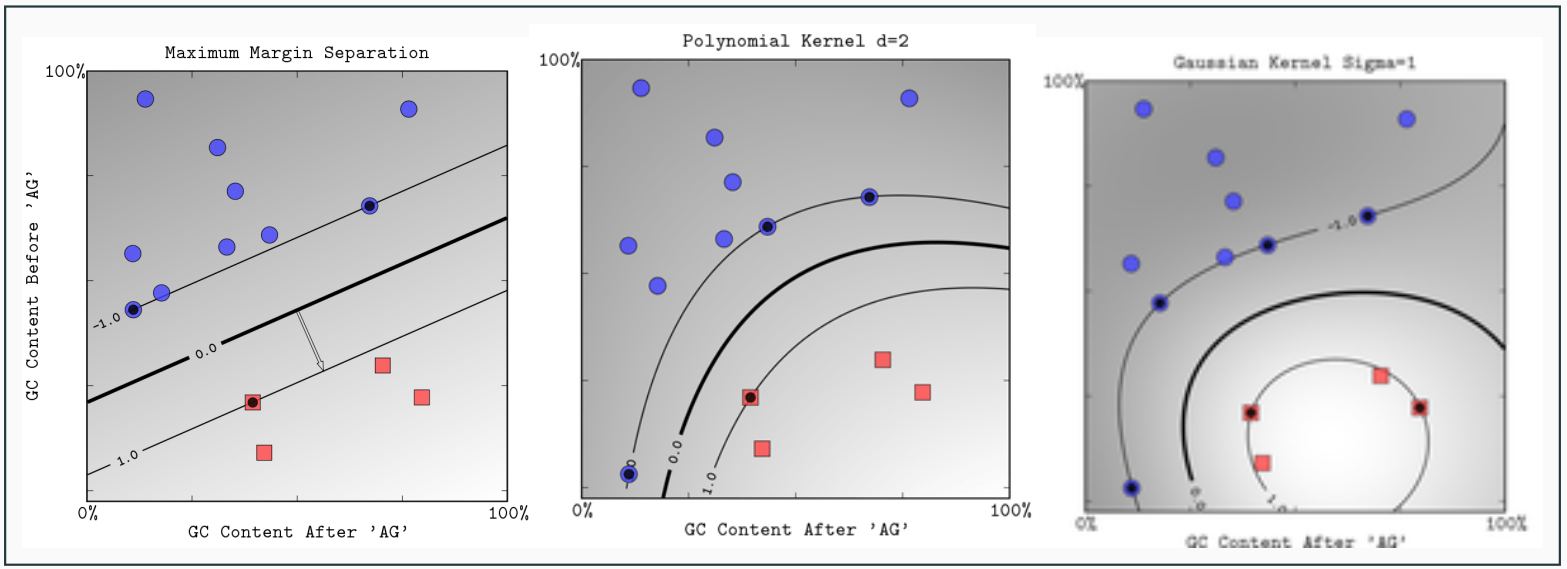
  is the Hessian matrix of second derivatives of the objective

- If $\mathbf{H}$ is PSD $OBJ(\boldsymbol{\alpha})$ is concave ($-OBJ(\boldsymbol{\alpha})$ is convex), and has no non-optimal local maxima
- However, $\mathbf{H}$ is PSD if and only if $\mathbf{K}$ is PSD
- Thus, a PSD kernel matrix $\mathbf{K}$ ensures that we can find a global optimum by gradient descent approaches

Non-linear kernels

Non-linear kernels

- By defining kernels that are non-linear functions of the original feature vectors, a linear models (e.g. SVM classifier) can be turned into a non-linear model
- However, the learning algorithm does not need to be changes, apart from plugging in the new kernel matrix
- The most commonly used non-linear kernels:
  - Polynomial kernel: $\kappa_{pol}(\mathbf{x}, \mathbf{z}) = (\mathbf{x}^T \mathbf{z} + c)^q$
  - Gaussian (or radial basis function, RBF) kernel: $\kappa_{RBF}(\mathbf{x}, \mathbf{z}) = \exp\left(-\|\mathbf{x} - \mathbf{z}\|^2/(2\,\sigma^2)\right)$



Non-linear kernels: Polynomial kernel

- Given inputs $\mathbf{x} \in \mathbb{R}^d$, the **polynomial kernel** is given by

$$\kappa_{pol}(\mathbf{x}, \mathbf{z}) = (\mathbf{x}^T \mathbf{z} + c)^q$$

- Integer $q > 0$ gives the **degree** of the polynomial kernel
- Real value $c \geq 0$ is a weighting factor for lower order polynomial terms
- The underlying features are **non-linear**: monomial combinations $x_1 \cdot x_2 \cdots x_k$ of degree $k \leq q$ of the original features x_j

Example: Polynomial kernel on 2D inputs

- Consider two-dimensional inputs $\mathbf{x} = [x_1, x_2]^T \in \mathbb{R}^2$
- The second degree polynomial kernel is given by $\kappa(\mathbf{x}, \mathbf{x}') = (\mathbf{x}^T\mathbf{x}' + c)^2$
- We can write it as a inner product in $\mathbb{R}^6$:

$$\begin{aligned}
\kappa(\mathbf{x}, \mathbf{x}') &= (\mathbf{x}^T\mathbf{x}' + c)^2 = (x_1x_1' + x_2x_2' + c)^2 = \\
&= x_1x_1'x_1x_1' + x_2x_2'x_2x_2' + c^2 + \\
&+ 2x_1x_1'x_2x_2' + 2cx_1x_1' + 2cx_2x_2' \\
&= \begin{bmatrix} x_1^2 \\ x_2^2 \\ \sqrt{2}x_1x_2 \\ \sqrt{2c}x_1 \\ \sqrt{2c}x_2 \\ c \end{bmatrix}^T \begin{bmatrix} x_1'^2 \\ x_2'^2 \\ \sqrt{2}x_1'x_2' \\ \sqrt{2c}x_1' \\ \sqrt{2c}x_2' \\ c \end{bmatrix} \\
&= \phi(\mathbf{x})^T\phi(\mathbf{x}'),
\end{aligned}$$

where $\phi(\mathbf{x}) = [x_1^2, x_2^2, \sqrt{2}x_1x_2, \sqrt{2c}x_1, \sqrt{2c}x_2, c]^T$

Non-linear kernels: Polynomial kernel

$$\kappa_{pol}(\mathbf{x}, \mathbf{z}) = (\langle \mathbf{x}, \mathbf{z} \rangle + c)^q$$

A linear model in the polynomial feature space corresponds to a **non-linear model** in the original feature space

- In the previous example, the model

  $$\mathbf{w}^T \phi(\mathbf{x}) = w_1 x_1^2 + w_2 x_2^2 + w_3 \sqrt{2} x_1 x_2 + w_4 \sqrt{2c} x_1 + w_5 \sqrt{2c} x_2 + w_6 c = 0$$

  is a second degree polynomial in the original inputs space, but a hyperplane in the new 6-dimensional feature space
- Using the dual representation $\mathbf{w} = \sum_{i=1}^{m} \alpha_i y_i \phi(\mathbf{x}_i)$, the polynomial kernel allows non-linear classification in the input space by

  $$\mathbf{w}^T \phi(\mathbf{x}) = \sum_i \alpha_i y_i \langle \phi(\mathbf{x}_i), \phi(\mathbf{x}) \rangle = \sum_i \alpha_i y_i \kappa(\mathbf{x}_i, \mathbf{x})$$

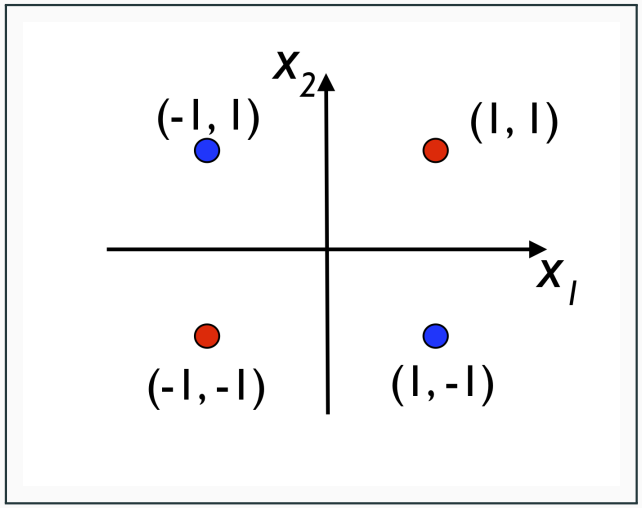
Example: XOR with polynomial kernel

Consider the following simple example:

- Input data points $\{(-1,-1),(-1,1),(1,-1),(1,1)\}$ and the label (red $= 1$, blue $=$-1) given by a XOR type function

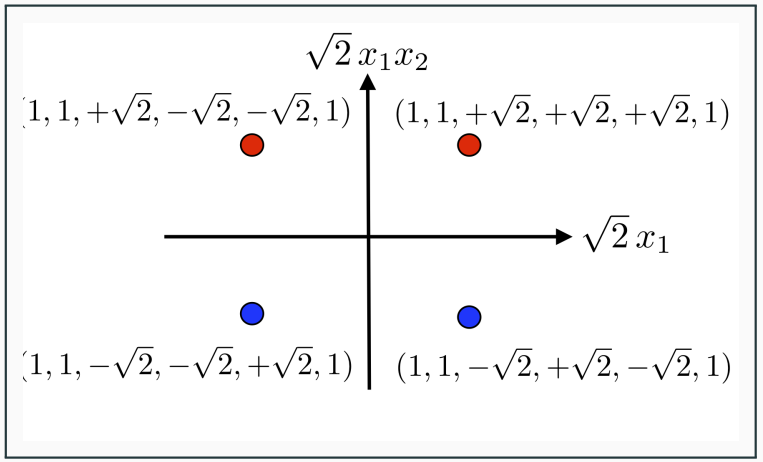
$$y = x_1 x_2 = \begin{cases} +1 & \text{if } x_1 = x_2 \\ -1 & \text{if } x_1 \neq x_2 \end{cases}$$

- The classes are not linearly separable: there is no consistent line that separates the two classes



Example: XOR with polynomial kernel

- However, map the data using the feature map $\phi(\mathbf{x}) = [x_1^2, x_2^2, \sqrt{2}x_1x_2, \sqrt{2c}x_1, \sqrt{2c}x_2, c]^T$ underlying the polynomial kernel function



- Now, the example data is linearly separable in the feature space, for example, choose $\alpha_i = 1/(4\sqrt{2})$, for all i:

$$\begin{aligned}\mathbf{w} &= \sum_i \alpha_i y_i \phi(\mathbf{x}_i) = \\ &= (\phi([-1,-1]^T) - \phi([-1,1]^T) - \phi([1,-1]^T) + \phi([1,1]^T))/(4\sqrt{2}) \\ &= [0,0,1,0,0,0]^T\end{aligned}$$

- We can consistently classify the example data by using the kernel function $\kappa(\mathbf{x}, \mathbf{x}') = \langle \phi(\mathbf{x}), \phi(\mathbf{x}') \rangle$: $h(\mathbf{x}) = \text{sgn}\left(\sum_{i=1}^m \alpha_i y_i \kappa(\mathbf{x}_i, \mathbf{x})\right)$

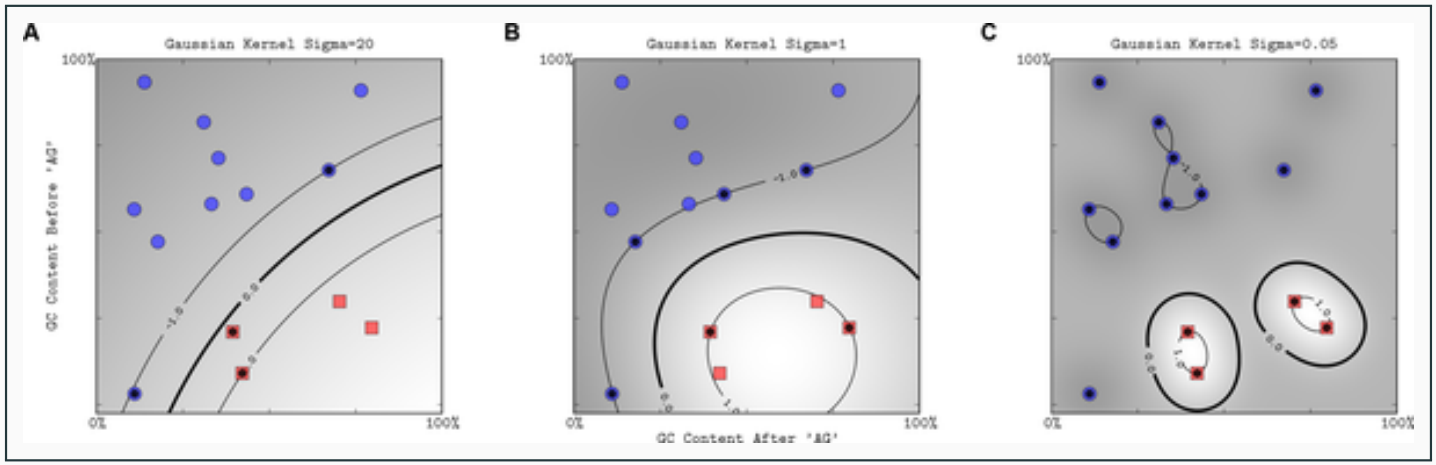
Non-linear kernels: Polynomial kernel

- The dimension of the polynomial feature space is $\binom{d+q}{q} = O((d+q)^q)$ where d is the dimension of the input space X and q is the degree of the polynomial.
- Explicitly maintaining the feature map $\phi(\mathbf{x})$ and the weight vector $\mathbf{w}$, and evaluating the model $\mathbf{w}^T\phi(\mathbf{x})$ takes $O(d^q)$ time and space
- However, the polynomial kernel $\kappa(\mathbf{x}, \mathbf{x}') = (\langle \mathbf{x}, \mathbf{x}' \rangle + c)^q$ can be computed in time $O(d)$ in preprocessing, and evaluated in constant time
- Evaluating the model using the dual representation $\sum_{i=1}^{m} \alpha_i y_i \kappa(\mathbf{x}_i, \mathbf{x})$ takes $O(m)$ time
- Trade-off: No computational overhead from working in the high-dimensional feature space, but linear dependency in the size of training data

Non-linear kernels: Gaussian kernel (Radial basis function kernel, RBF)

$$\kappa_{RBF}(\mathbf{x}, \mathbf{z}) = \exp\left(-\|\mathbf{x} - \mathbf{z}\|^2/(2\,\sigma^2)\right)$$

- Gaussian kernel can be seen as a limit of polynomial kernels $\Longrightarrow$ corresponds to an **infinite dimensional** polynomial kernel
- Smoothness of Gaussian kernel is controlled by the parameter σ
- Higher-order features are exponentially downweighted.
- Proof: through power series expansion of $e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!}$ and using elementary properties of kernels (see Mohri book ch. 6 for details)



Kernels and generalization

Rademacher complexity

- Assume a symmetric positive definite kernel $\kappa : X \times X \mapsto \mathbb{R}$ with associated feature map ϕ, and a sample S of size m, with the kernel matrix $\mathbf{K} = (\kappa(x_i, x_j))_{i,j=1}^m$, and $\kappa(\mathbf{x}_i, \mathbf{x}_i) \leq r^2$ for all $i = 1, \ldots, m$
- Empirical Rademacher complexity of the hypothesis class

$$\mathcal{H} = \{\mathbf{x} \mapsto \langle \mathbf{w}, \phi(\mathbf{x}) \rangle : \|\mathbf{w}\| \leq B\}$$

  for some $B \geq 0$ satisfies (c.f. Mohri book for the proof)

$$\hat{\mathcal{R}}_S(\mathcal{H}) \leq \frac{B\sqrt{trace(\mathbf{K})}}{m}$$

- The key quantities are
  - the upper bound B of the norm of weight vector – relates to the margin
  - the trace of the kernel matrix $trace(\mathbf{K}) = \sum_{i=1}^m \kappa(\mathbf{x}_i, \mathbf{x}_i) = \sum_{i=1}^m \|\phi(\mathbf{x}_i)\|^2 \leq mr^2$ – relates to the norm of the data points

Generalization error bound

- We can plug the above to a Rademacher complexity based generalization bound (c.f. Lecture 3)

$$R(h) \leq \hat{R}(h) + \hat{\mathcal{R}}(\mathcal{H}) + 3\sqrt{\frac{\log \frac{2}{\delta}}{2m}}$$

$$\leq \hat{R}(h) + \frac{B\sqrt{trace(\mathbf{K})}}{m} + 3\sqrt{\frac{\log \frac{2}{\delta}}{2m}}$$

- Evaluating this bound required observing the empirical risk of the hypothesis $\hat{R}(h)$, the norm of the weight vector $B = \sqrt{\sum_{i,j=1}^{m} \alpha_i \alpha_j y_i y_j \kappa(\mathbf{x}_i, \mathbf{x}_j)}$, and the trace of the kernel matrix
- Note that we do not need to run simulations with random labelings the above only requires computing the kernel matrix and the hypothesis with the real training data

Designing kernels

Several ways to get to a kernel

Approach I. Construct a feature map ϕ and think about efficient ways to compute the inner product $\langle \phi(x), \phi(x) \rangle$

- If $\phi(x)$ is very high-dimensional, computing the inner product element by element is slow, we don't want to do that
- For several cases, there are efficient algorithms to compute the kernel in low polynomial time, even with exponential or infinite dimension of ϕ

Several ways to get to a kernel

Approach II. Construct similarity measure and show that it qualifies as a kernel:

- Show that for any set of examples the matrix $K = (\kappa(\mathbf{x}_i, \mathbf{x}_j))_{i,j=1}^{m}$ is positive semi-definite (PSD).
- In that case, there always is an underlying feature representation, for which the kernel represents the inner product
- Example: if you can show the matrix is a covariance matrix for some variates, you will know the matrix will be PSD.

Several ways to get to a kernel

Approach III. Convert a distance or a similarity into a kernel

- Take any distance $d(\mathbf{x}, \mathbf{z})$ or a similarity measure $s(\mathbf{x}, \mathbf{z})$ (that do not need to be a kernel)
- In addition a set of data points $Z = \{\mathbf{z}_j\}_{j=1}^m$ from the same domain is required (e.g. training data)
- Construct feature vector from distances (similarly for s): $\phi(x) = (d(\mathbf{x}, \mathbf{z}_1), d(\mathbf{x}, \mathbf{z}_2), \ldots, d(\mathbf{x}, \mathbf{z}_m))$
- Compute linear kernel, also know as the **empirical kernel map**: $\kappa(\mathbf{x}, \mathbf{x}') = \langle \phi(\mathbf{x}), \phi(\mathbf{x}') \rangle$
- This will always work technically, but requires that the data Z captures the essential patterns in the input space $\implies$ need enough data

Several ways to get to a kernel

Approach IV. Making kernels from kernels

- Examples of elementary operations that give valid kernels when applied to kernels $\kappa_n, n = 1, 2, \ldots$
  1. Sum: $\kappa(\mathbf{x}, \mathbf{z}) = \kappa_1(\mathbf{x}, \mathbf{z}) + \kappa_2(\mathbf{x}, \mathbf{z})$
  2. Scaling with a positive scalar: $\kappa(\mathbf{x}, \mathbf{z}) = a\kappa_1(\mathbf{x}, \mathbf{z}), a > 0$
  3. Itemwise product: $\kappa(\mathbf{x}, \mathbf{z}) = \kappa_1(\mathbf{x}, \mathbf{z})\kappa_2(\mathbf{x}, \mathbf{z})$
  4. Normalization: $\kappa(\mathbf{x}, \mathbf{z}) = \frac{\kappa_1(\mathbf{x},\mathbf{z})}{\sqrt{\kappa_1(\mathbf{x},\mathbf{x})\kappa_1(\mathbf{z},\mathbf{z})}} = \left\langle \frac{\phi(\mathbf{x})}{\|\phi(\mathbf{x})\|}, \frac{\phi(\mathbf{z})}{\|\phi(\mathbf{z})\|} \right\rangle$
  5. Pointwise limit: $\kappa(\mathbf{x}, \mathbf{z}) = \lim_{n\to\infty} \kappa_n(\mathbf{x}, \mathbf{z})$
  6. Composition with a power series of radius of convergence ρ: $\kappa(\mathbf{x}, \mathbf{z}) = \sum_{n=0}^{\infty} a_n \kappa(\mathbf{x}, \mathbf{z})^n$, with $a_n \geq 0$ for all n, and $|\kappa(\mathbf{x}, \mathbf{z})| < \rho$
- The operations can be combined to construct arbitrarily complex kernels, e.g. polynomial kernels and Gaussian kernels can be derived this way (see details in the Mohri book ch. 6)

Kernels for structured data

Kernels for structured data

- In many applications the data does not come in the form of numerical vectors or data matrices, but from a general set of objects X, for example:
  - Sequential data - text analysis kernels, string kernels
  - Molecular data - graph kernels
  - Structured documents, context-free grammars, classification taxonomies, ... - tree kernels
- To compute kernels we could define a feature map $\phi : X \mapsto F$ and compute feature vectors $\phi(x)$ for our data, and the kernel as the inner product: $\kappa(x_i, x_j) = \langle \phi(x_i), \phi(x_j) \rangle_F$
- Alternatively, we can use an algorithm that directly computes the kernel values $\kappa(x_i, x_j)$for any pair or objects x_i, x_j
- The latter approach can be very effective if the feature space F has a high dimension

Kernels for structured data

- The commonly seen form for kernels for two structured objects x_i and x_j

$$\kappa(x_i, x_j) = \sum_{s \in S} \phi_s(x_i)\phi_s(x_j),$$

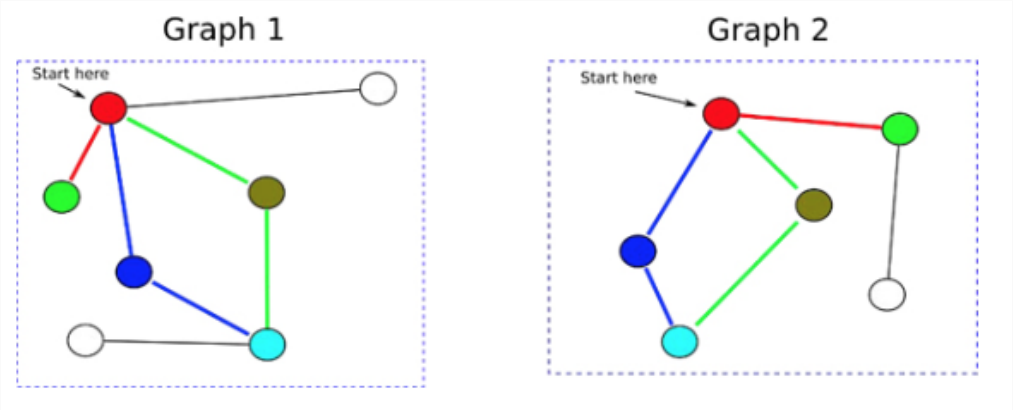
  where S is the set of substructures of interest and $\phi_s(x)$ is either
  - An indicator function: $\phi_s(x) = 1$ if and only if x contains s
  - A count: x contains $\phi_s(x)$ instances of s
- In many cases, the set S has exponential size in the size of the objects and the feature vectors $\phi(x)$ are high dimensional and sparse
- Efficient algorithms exist for computing the kernels $\kappa(x_i, x_j)$ directly from the structured data, skipping writing down the feature vectors $\phi(x)$

Example: String kernels

- String kernels is a family of kernels between sequences based on "counting" common subsequences two sequences have
- Underlying feature map, also called subsequence spectrum, contains a feature for each possible substring
- The feature spaces induced by subsequences are generally exponential in the length of the subsequences
- However, low polynomial time algorithms (linear to quadratic time) exist to compute string kernels
- For more information see Lodhi et al. "Text classification using string kernels." Journal of Machine Learning Research 2.Feb (2002): 419-444.

Example: Graph kernels

- Basic idea: count common substructures in two graphs
- Challenging problem in general due to the underlying NP-hard subgraph isomorphism problem: given two graphs G and S, does a graph S appear in G as a subgraph
- Polynomial-time kernel computation possible for restricted substructures:
  - Random walks
  - Tree-shaped subgraphs
  - Small general subgraphs
- For more information see Vishwanathan et al. "Graph kernels." Journal of Machine Learning Research 11 (2010): 1201-1242.



Summary

- Kernel methods are a broad class of data analysis methods
- Kernels allow efficient non-linear learning in high-dimensional feature spaces
- Special kernels can be designed for different data types such as sequential or graph data
- Time-complexity of kernel methods generally scale quadratically in the number of training points (due to the kernel matrix), which can be a limitation when huge datasets are processed
- More on kernel methods on the course CS-E4830 Kernel methods in machine learning (Spring 2022)