Kernel Methods

AI534

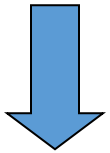
Key concepts:

Feature mapping to address non-linear separability
The kernel trick to avoid explicit feature mapping
Definition of Kernel functions
Kernelized perceptron
Kernelized linear regression with L2 regularization

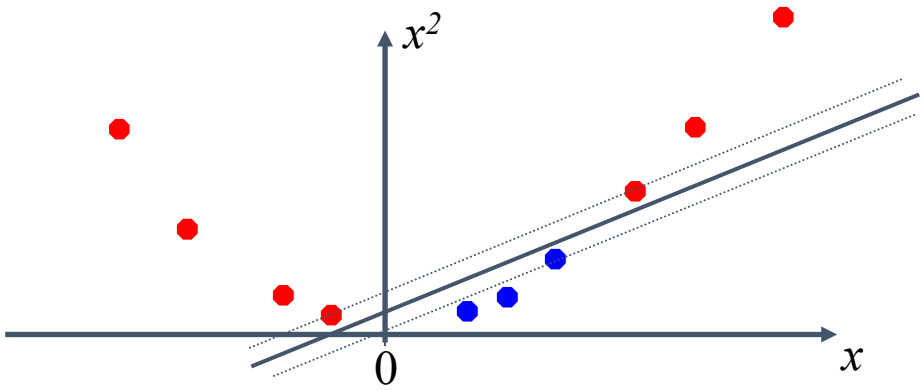
Nonlinearly Separable Data

Original
1-d space

x



Mapped
2-d space

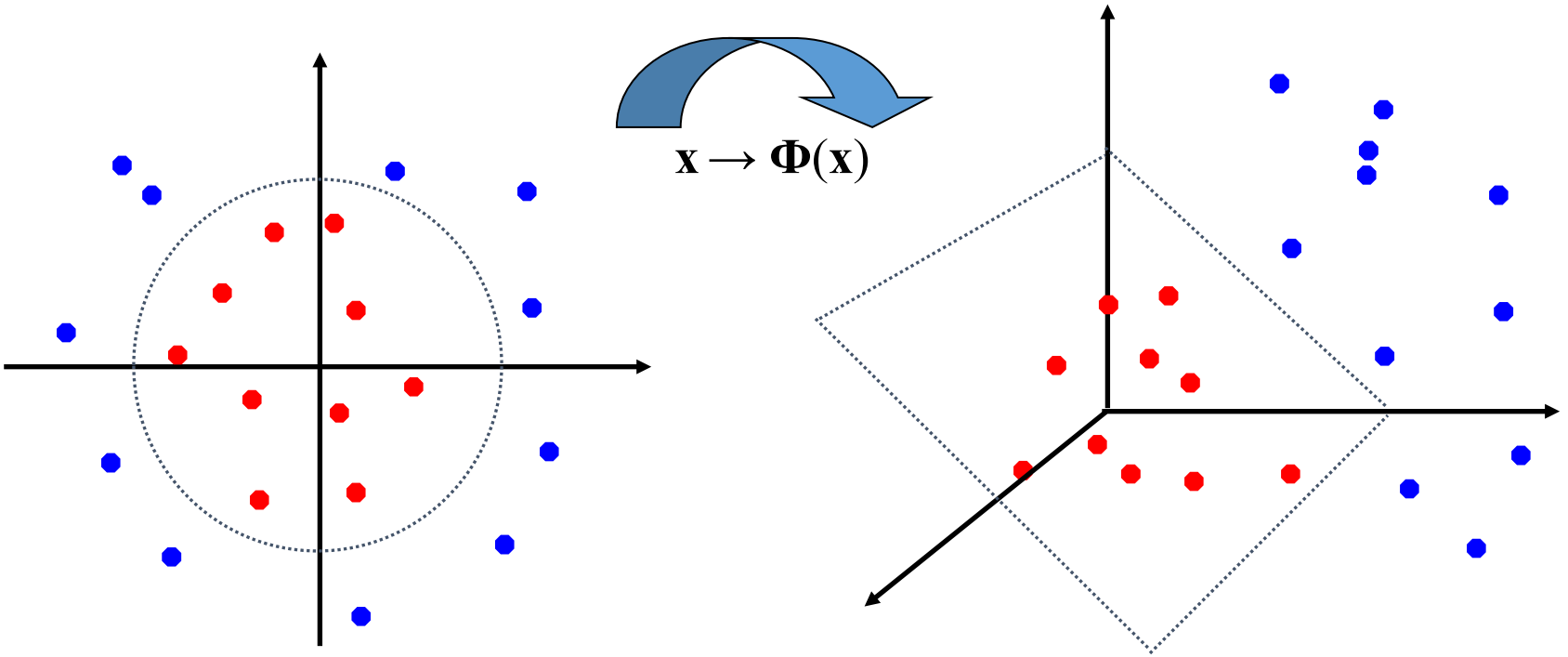


(x, x^2)

Mapping the data to a higher dimensional space can introduce linear separability for data that is not linearly separable in the original input space

Non-linear Classifier via Feature Mapping

- General idea: For <u>any</u> data set, the ***original input space*** can always be mapped to some higher-dimensional **feature spaces** such that the data is linearly separable:



Original input space

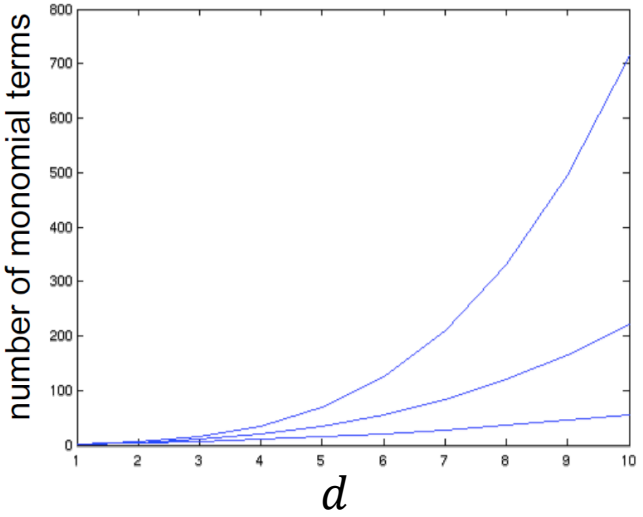
Mapped feature space

Example: Quadratic Feature Space

- Assume d input dimensions $\boldsymbol{x} = (x_1, \cdots, x_d)$
- Number of quadratic terms:

$$1 + d + d + d(d-1)/2 \approx O(d^2)$$

- What if we want to consider even higher order features?
  - For cubic feature space: $O(d^3)$
  - The number of dimensions after mapping increase rapidly with increasing **order $\boldsymbol{m}$**



$$\Phi(x) = \begin{pmatrix} 1 \\ \sqrt{2}x_1 \\ \sqrt{2}x_2 \\ \vdots \\ \sqrt{2}x_d \\ x_1^2 \\ x_2^2 \\ \vdots \\ x_d^2 \\ \sqrt{2}x_1x_2 \\ \sqrt{2}x_1x_3 \\ \vdots \\ \sqrt{2}x_1x_d \\ \vdots \\ \sqrt{2}x_{d-1}x_d \end{pmatrix}$$

Constant term

Linear terms

Pure quadratic terms

Quadratic Cross-terms

Quadratic Features

Revisiting Perceptron (using nonlinear feature mapping)

Given current weight $\mathbf{w}_t$, predict for $\mathbf{x}$ by: $\hat{y}(\mathbf{x}) = sign(\mathbf{w}_t^T \mathbf{x})$

$\mathbf{w}_t$ was created when $\mathbf{w}_{t-1}$ makes a mistake on a training example $(\mathbf{x}, y)$ via:

$$\mathbf{w}_t = \mathbf{w}_{t-1} + y\mathbf{x}$$

Let S_t stores (the indices of) all the previous mistakes leading up to $\mathbf{w}_t$, we have:

$$\mathbf{w}_t = \sum_{i \in S_t} y_i \mathbf{x}_i$$

Note S_t may contain repetitions: if an example was misclassified multiple times, it will appear multiple times.

We can then rewrite the prediction rule as:

$$\hat{y}(\mathbf{x}) = sign(\sum_{i \in S_t} y_i \mathbf{x}_i^T \mathbf{x})$$

Now if data is mapped to a higher dimension by Φ, we simply replace $\mathbf{x}$ with $\Phi(\mathbf{x})$:

$$\hat{y}(\mathbf{x}) = sign\left(\sum_{i \in S_t} y_i \Phi(\mathbf{x}_i)^T \Phi(\mathbf{x})\right)$$

Restructuring the Perceptron algorithm

Let $\mathbf{w} \leftarrow (0,0,\dots,0)$
Repeat if $iter \leq iters$
  for every training example $i = 1,\dots,n$
    $u_i = \mathbf{w}^T \mathbf{x}_i$
    if $y_i u_i \leq 0$ $\mathbf{w} \leftarrow \mathbf{w} + y_i \mathbf{x}_i$
  $iter = iter + 1$

Original Perceptron

New version by Remembering all mistakes in S

$S = [\,]$ //list of mistaken examples
Repeat if $iter \leq iters$
  for every training example $i = 1,\dots,n$
    $u_i = \sum_{j \in S} y_j \mathbf{x}_j^T \mathbf{x}_i$
    if $y_i u_i \leq 0$ add i to S
  $iter = iter + 1$

If we wish to use mapped feature space, simply replace $\mathbf{x}_j^T \mathbf{x}_i$ with $\Phi(\mathbf{x}_j)^T \Phi(\mathbf{x}_i)$

Dot product in the Quadratic Feature Space

Explicit mapping takes $O(d^2)$ time. Consider two d-dimensional vectors $\mathbf{a}$ and $\mathbf{b}$:

$$\Phi(\boldsymbol{a})^T\Phi(\boldsymbol{b}) = \begin{pmatrix} 1 \\ \sqrt{2}a_1 \\ \sqrt{2}a_2 \\ \vdots \\ \sqrt{2}a_d \\ a_1^2 \\ a_2^2 \\ \vdots \\ a_d^2 \\ \sqrt{2}a_1a_2 \\ \sqrt{2}a_1a_3 \\ \vdots \\ \sqrt{2}a_1a_d \\ \vdots \\ \sqrt{2}a_{d-1}a_d \end{pmatrix} \cdot \begin{pmatrix} 1 \\ \sqrt{2}b_1 \\ \sqrt{2}b_2 \\ \vdots \\ \sqrt{2}b_d \\ b_1^2 \\ b_2^2 \\ \vdots \\ b_d^2 \\ \sqrt{2}b_1b_2 \\ \sqrt{2}b_1b_3 \\ \vdots \\ \sqrt{2}b_1b_d \\ \vdots \\ \sqrt{2}b_{d-1}b_d \end{pmatrix}$$

$$\Phi(\boldsymbol{a})^T\Phi(\boldsymbol{b}) = 1 + 2\sum_{i=1}^{d} a_ib_i + \sum_{i=1}^{d} a_i^2b_i^2 + \sum_{i=1}^{d}\sum_{j=i+1}^{d} 2a_ia_jb_ib_j$$

Consider the following function:

$$(\mathbf{a}^T\mathbf{b}+1)^2 = (\mathbf{a}^T\mathbf{b})^2 + 2(\mathbf{a}^T\mathbf{b}) + 1$$

$$= \left(\sum_{i=1}^{d} a_ib_i\right)^2 + 2\sum_{i=1}^{d} a_ib_i + 1$$

$$= \sum_{i=1}^{d}\sum_{j=1}^{d} a_ia_jb_ib_j + 2\sum_{i=1}^{d} a_ib_i + 1$$

$$= \sum_{i=1}^{d} a_i^2b_i^2 + 2\sum_{i=1}^{d}\sum_{j=i+1}^{d} a_ia_jb_ib_j + 2\sum_{i=1}^{d} a_ib_i + 1$$

$\kappa(\mathbf{a},\mathbf{b}) = (\mathbf{a}^T\mathbf{b}+1)^2$ computes the dot product in quadratic space in $O(d)$ time

The kernel trick

- **Definition:** A function $\kappa(\mathbf{x}, \mathbf{x}')$ is called a ***kernel function*** if $\kappa(\mathbf{x}, \mathbf{x}') =< \phi(\mathbf{x}), \phi(\mathbf{x}') >$ for some mapping function ϕ
- **Implication**: we can simply replace any occurrences of dot product $< \mathbf{x} \cdot \mathbf{x}' >$ with a kernel function κ that computes $\kappa(\mathbf{x}, \mathbf{x}') =< \phi(\mathbf{x}), \phi(\mathbf{x}') >$
- **Implication**: we do not need to explicitly compute the mapping of the features --- significant computational savings

- For example, to compute the dot product in the quadratic space:
  - With the quadratic kernel function $\kappa(\mathbf{x}, \mathbf{x}') = (\mathbf{x}^T\mathbf{x}' + 1)^2 : O(d)$
  - With explicit mapping $< \phi(\mathbf{x}), \phi(\mathbf{x}') > : O(d^2)$

Kernelizing Perceptron

$S = [\,]$ //list of mistaken examples
Repeat if $iter \leq iters$
  for every training example $i = 1, \ldots, n$
    $u_i = \sum_{j \in S} y_j \mathbf{x}_j^T \mathbf{x}_i$
    if $y_i u_i \leq 0$ add i to S
  $iter = iter + 1$

Original Perceptron (restructured)

Replacing $\mathbf{x}_j^T \mathbf{x}_i$ with $\kappa(\mathbf{x}_j, \mathbf{x}_i)$

$S = [\,]$ //list of mistaken examples
Repeat if $iter \leq iters$
  for every training example $i = 1, \ldots, n$
    $u_i = \sum_{j \in S} y_j \kappa(\mathbf{x}_j, \mathbf{x}_i)$
    if $y_i u_i \leq 0$ add i to S
  $iter = iter + 1$

Making it better

$S = [\,]$ //list of mistaken examples

Repeat if $iter \leq iters$

for every training example $i = 1, \ldots, n$

$$u_i = \sum_{j \in S} y_j \kappa(\mathbf{x}_j, \mathbf{x}_i)$$

if $y_i u_i \leq 0$ add i to S

$iter = iter + 1$

Remember all mistakes in S

Keep a counter for each example

Let $\alpha_i = 0 \;\; \forall i = 1, \ldots, n$

Repeat if $iter \leq iters$

for every training example $i = 1, \ldots, n$

$$u_i = \sum_{j=1 \text{ to } n} \alpha_j y_j \kappa(\mathbf{x}_j, \mathbf{x}_i)$$

if $y_i u_i \leq 0$ $\alpha_i \leftarrow \alpha_i + 1$

$iter = iter + 1$

Kernel perceptron

Kernel functions

- A kernel function can be intuitively viewed as computing some similarity measure between examples
- In practice, we directly use the kernel functions without explicitly stating the transformation Φ
- Given a kernel function, finding its corresponding transformation can be very cumbersome or impossible
  - RBF kernel's mapped space has infinite dimensions
- Not all functions are kernels
  - For some functions there does not exist a corresponding mapping $\Phi(\mathbf{x})$
- If you have a good similarity measure, can we use it as a kernel?

Kernel Function or Not

- Consider a finite set of m points, we define the kernel (Gram) marix as

$$K = \begin{bmatrix} \kappa(\mathbf{x}_1, \mathbf{x}_1) & \kappa(\mathbf{x}_1, \mathbf{x}_2) & \dots & \kappa(\mathbf{x}_1, \mathbf{x}_n) \\ \kappa(\mathbf{x}_2, \mathbf{x}_1) & \kappa(\mathbf{x}_2, \mathbf{x}_2) & \dots & \kappa(\mathbf{x}_2, \mathbf{x}_n) \\ \dots & \dots & \dots & \dots \\ \kappa(\mathbf{x}_n, \mathbf{x}_1) & \kappa(\mathbf{x}_n, \mathbf{x}_2) & \dots & \kappa(\mathbf{x}_n, \mathbf{x}_n) \end{bmatrix}_{n \times n}$$

- Kernel matrices by definition are square and symmetric

Mercer theorem:

A function κ is a kernel function if and only if for any finite sample $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n$, its corresponding kernel matrix is positive semi-definite ($c^T K c \geq 0$ for all $c \in R^n$, or alternatively, only has non-negative eigenvalues)

Understanding mercer theorem

- If $\kappa(\cdot)$ is a kernel and K is the kernel matrix with $K_{ij} = \kappa(x_i, x_j)$, then

$$c^T K c = \sum_{ij} c_i c_j K_{ij} = \sum_{ij} c_i c_j \phi(x_i)\phi(x_j)$$

$$= \left(\sum_i c_i \phi(x_i)\right)\left(\sum_j c_j \phi(x_j)\right)$$

$$= \left\|\sum_i c_i \phi(x_i)\right\|^2 \geq 0$$

You can use mercer theorem or the original definition to show that a function is a kernel function. Alternatively, you can also show a function is kernel by linking it to some well known kernel functions using closure property.

Some common kernel functions

- Linear kernel: $\kappa(a, b) = (a \cdot b)$ (ϕ is identity mapping)
- $\kappa(a, b) = (a \cdot b)^d$
  - ϕ maps to d-th order (**only**) polynomial features
- $\kappa(a, b) = (a \cdot b + 1)^d$
  - ϕ maps to **up to** d-th order polynomial features
- Radial-Basis-Function (RBF) or Gaussian kernel:

$$\kappa(a, b) = \exp\left(-\frac{(a-b)^2}{2\sigma^2}\right)$$

  - ϕ maps to infinite dimensional feature space
  - Proof is based on the identity of

$$e^x = \frac{\sum_{k=0}^{\infty} x^k}{k!}$$

Closure Property of Kernels

If κ_1 and κ_2 are kernel functions, then the following are all kernel functions:

- $\kappa(x, y) = \kappa_1(x, y) + \kappa_2(x, y)$
  - $\Phi = \text{concatenation of } \Phi_1 \text{and } \Phi_2$
- $\kappa(x, y) = a\kappa_1(x, y)$, where $a > 0$
  - $\Phi = \sqrt{a}\Phi_1$
- $\kappa(x, y) = \kappa_1(x, y)\kappa_2(x, y)$
  - If Φ_1 has N_1 features and Φ_2 has N_2 features
  - Φ will have $N_1 \times N_2$ features: $\Phi_{ij} = \Phi_{1i} \cdot \Phi_{2j}$

One can repeatedly apply the closure property to compose kernel functions, e.g., $a\kappa_1 + b\kappa_2 + \kappa_1\kappa_2$ is a kernel function for $a, b > 0$

Key Choices in Applying Kernel

- Selecting the kernel function
  - (cross-) validation to rescue
  - Popular choices: Linear kernel, polynomial kernels (with low degrees)
  - Start simple, go more complex only if needed.
  - Can learn to combine different kernels (kernel learning)
    - $K = \alpha_1 K_1 + \alpha_2 K_2 + \cdots + \alpha_k K_k,$ s.t. $\alpha_i \geq 0$ for $i = 1, \ldots, k$
  - Kernel functions are defined for many non-traditional non-Euclidean data, e.g., graph kernel, set kernel, string kernel etc.
- Selecting the kernel parameter
  - can have strong impact on performance
  - the optimal range can be reasonably large
  - grid search with (cross-)validation is commonly used

Question break

It can be shown that for any dataset, we can map the original input features to a higher dimensional feature space such that the positive and negative examples are linearly separable in the mapped space. What are the implications of such feature mapping?

A. Feature engineering is no longer important because feature mapping can create the separation that we need.
B. Feature engineering is still important because without the right features, the separation in the mapped space will not be generalizable.

The kernel trick uses a kernel function instead of explicitly mapping the features then taking the dot product. Among the following statements, which ones are true?

A. Using kernel functions (as opposed to mapping then dot product) is a faster way to compute the dot product in the mapped space.
B. Using kernel functions (as opposed to mapping then dot product) is more sample efficient, i.e., it needs fewer training examples to learn effectively.
C. Using kernel functions (as opposed to mapping then dot product) allows us to consider mappings that are not explicitly possible, e.g., due to infinite dimensions.

Revisiting Linear Regression

- Consider the L2 regularized linear regression

$$\max_{\mathbf{w}} \frac{1}{2}\|\mathbf{y} - \boldsymbol{X}\mathbf{w}\|^2 + \frac{\lambda}{2}\mathbf{w}^T\mathbf{w}$$

where $\mathbf{X}$ is the data matrix, each row contains the features of one training example, $\mathbf{y}$ is the vector of ground truth predictions for all training examples

- Closed form solution:

$$\mathbf{w} = (\lambda \boldsymbol{I} + \mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

where $\boldsymbol{I}$ is the identity matrix

- $\mathbf{w}$ lies in the space spanned by the training examples, i.e., $\mathbf{w} = \sum_i \alpha_i \mathbf{x}_i$
- Instead of solving the optimization problem in the space of $\mathbf{w}$, instead, we can directly solve for $\alpha_i' s$

Kernelizing Linear Regression

- Learned Function:
  - Original: $\hat{f}(\mathbf{x}) = \mathbf{w}^T\mathbf{x}$
  - Kernelized: $\hat{f}(\mathbf{x}) = \sum_i \alpha_i \kappa(\mathbf{x}_i, \mathbf{x})$ (plug in $\mathbf{w} = \sum_i \alpha_i \Phi(\mathbf{x}_i)$ and replace dot product with κ)
- Objective:
  - Original: $\frac{1}{2}\|\mathbf{y} - \boldsymbol{X}\mathbf{w}\|^2 + \frac{\lambda}{2}\mathbf{w}^T\mathbf{w}$ ← solving for **w,** primal problem
  - Kernelized: $\frac{1}{2}\|\mathbf{y} - K\boldsymbol{\alpha}\|^2 + \frac{\lambda}{2}\boldsymbol{\alpha}^T K\boldsymbol{\alpha}$ ← solving for $\boldsymbol{\alpha}$**,** dual problem

K is the kernel (gram) matrix of the training data: $K_{ij} = \kappa(\mathbf{x}_i, \mathbf{x}_j)$

- Closed form solution:

$$\alpha = (K + \lambda I)^{-1}\mathbf{y}$$

General Applications of Kernel Methods

- Many learning algorithms formulate optimization problems and the solutions are some weighted sum of the input training examples
- Explicitly express the weights as sum of weighted sum of training examples allows us to perform learning using dot products between examples, in the dual space
- Apply the kernel trick by replacing dot product with kernel functions.
- This enables the use of high dimensional nonlinear feature spaces without having to pay the price of computing and working with high dimensional mapped features
- Many types of kernels, wide applicability including some for data that are not naturally in vector form, like graphs, strings, sets etc.