

Lecture 10 | Part 1

High-Dimensional Feature Maps

Linear Prediction Rules

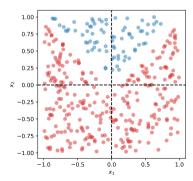
We have seen how to fit linear functions:

$$H(\vec{x}) = w_0 + w_1 x_1 + \dots + w_d x_d$$

- Used for both regression and classification
- Limitation: regression function / decision boundary is a straight line / plane / hyperplane

Example

- The data below is not linearly separable
- No prediction function of the form $H(x_1, x_2) = w_0 + w_1 x_1 + w_2 x_2$ will work well

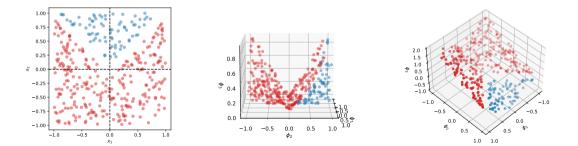


However...

- We have seen a way around this limitation: basis functions.
- Idea: design a function $\vec{\phi}(\vec{x})$ that maps data to a new space in which it is **linearly separable**.

Example

• Consider the mapping $\vec{\phi}(x_1, x_2) = (x_1, x_2, |x_1x_2|)^T$

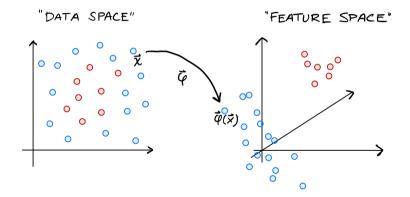


Procedure

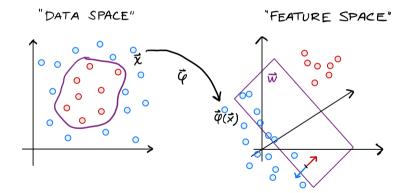
- 1. Define feature map $\vec{\phi}(\vec{x}) : \mathbb{R}^d \to \mathbb{R}^k$
 - $\blacktriangleright \vec{\phi}(\vec{x}) = (\phi_1(\vec{x}), \dots, \phi_k(\vec{x}))^T$
 - Number of basis functions k can be > or ≤ than d
- 2. Map each training point to *k*-dimensional feature space: $\vec{x}^{(i)} \mapsto \vec{\phi}(\vec{x}^{(i)})$
- 3. Learn a linear predictor in feature space:

$$H(\vec{x}) = w_0 + w_1 \phi_1(\vec{x}) + \dots + \phi_k(\vec{x})$$

Procedure



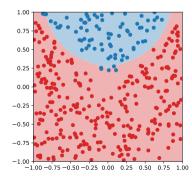
Procedure



Example

• Use mapping $\vec{\phi}(\vec{x}) = (x_1, x_2, |x_1x_2|)^T$

Decision boundary in "data space" no longer a straight line.



Exercise

Suppose $\vec{w} = (3, -1, 2)^T$ defines a linear predictor in feature space and $\vec{\phi} = (x_1, x_2, |x_1x_2|)^T$ is the mapping from "data space" to "feature space".

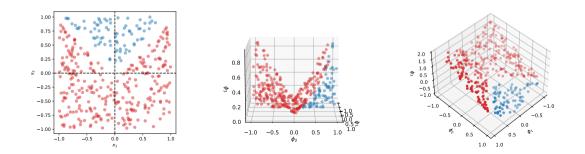
Let $\vec{x} = (2, -3)^T$ be a new point that needs to be classified. What is the predicted label?

Feature Maps

- How do we choose $\vec{\phi}$?
- **Hope:** data is linearly separable in feature space
- Appears difficult to engineer φ to satisfy this.
 Need to design φ for each new data set?
- Goal: design a general feature map that is likely to make any data set linearly separable

High-Dimensional Feature Maps

• **Observe:** in our example, $\vec{\phi}$ mapped to space of larger dimension



High-Dimensional Feature Maps

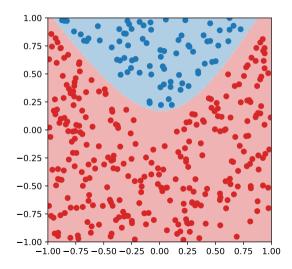
- Intuition: each additional feature makes the data easier to classify.
- Intuition: a high-dimensional feature map is likely to make the data linearly separable.
- Idea: design very high-dimensional generic feature maps.

▶ Define a feature map $\vec{\phi}$: $\mathbb{R}^2 \rightarrow \mathbb{R}^6$ as follows:

$$\vec{\phi}(\vec{x}) = (1, x_1, x_2, x_1 x_2, x_1^2, x_2^2)^T$$

We fit a prediction function of the form:

$$H(\vec{x}) = w_0 + w_1 x_1 + w_2 x_2 + w_3 x_1 x_2 + w_4 x_1^2 + w_5 x_2^2$$



In general, define a feature map $\vec{\phi}$ to contain all **monomials** of the form:

1,
$$x_i$$
, $x_i x_j$, x_i^2

▶ If $\vec{x} \in \mathbb{R}^d$, then $\vec{\phi}(\vec{x}) \in \mathbb{R}^{1+2d+\binom{d}{2}}$.

• **Example:** if $\vec{x} \in \mathbb{R}^{50}$, then $\vec{\phi}(\vec{x}) \in \mathbb{R}^{1,326}$.

• Why stop there? Design $\vec{\phi}$ to contain all terms of form:

1,
$$x_i$$
, $x_i x_j$, x_i^2 , $x_i x_j x_k$, x_i^3

► If $\vec{x} \in \mathbb{R}^d$, then $\vec{\phi}(\vec{x}) \in \mathbb{R}^{1+3d+\binom{d}{2}+\binom{d}{3}}$.

• **Example:** if $\vec{x} \in \mathbb{R}^{50}$, then $\vec{\phi}(\vec{x}) \in \mathbb{R}^{20,976}$!

And so on...

- Monomial feature maps take low-dimensional data and map it to very high-dimensional space.
- It is very general: the data is likely to be linearly separable in this space.
- It solves the problem of needing to manually craft basis functions for each new data set.

Problem

- Mapping to very high dimensions is likely to make the data linearly separable.
- But fitting a linear prediction rule in very high dimensions is computationally costly.



Lecture 10 | Part 2 The Kernel Trick

Recap

- We can learn non-linear patterns by:
 - 1. Defining a high-dimensional feature map, $\vec{\phi}: \mathbb{R}^d \to \mathbb{R}^k$
 - 2. Mapping each training point to *k*-dimensional feature space: $\vec{x}^{(i)} \mapsto \vec{\phi}(\vec{x}^{(i)})$
 - 3. Training a linear predictor in feature space.

Problem

Learning in a very high-dimensional space can be costly, or even infeasible.

The Trick

We can train many linear predictors as if we have mapped data to feature space, without actually doing so.

Idea

▶ In many algorithms, when $\vec{\phi}(\vec{x})$ appears, it always appears as part of a dot product:

$$\vec{\phi}(\vec{x})\cdot\vec{\phi}(\vec{x}')$$

- To compute, we could map and do dot product in feature space.
- But this is costly!

Kernels

But some $\vec{\phi}$ are special; for them, there is a function κ satisfying:

$$\kappa(\vec{x},\vec{x}')=\vec{\phi}(\vec{x})\cdot\vec{\phi}(\vec{x}')$$

Crucially, computing κ does not require mapping to feature space!

κ is called a kernel function.

Example: Polynomial Kernel

• Define the feature map $\vec{\phi}: \mathbb{R}^2 \to \mathbb{R}^6$ as follows:

$$\vec{\phi}(\vec{x}) = (1, x_1^2, x_2^2, \sqrt{2} x_1, \sqrt{2} x_2, \sqrt{2} x_1 x_2,)^T$$

Called the polynomial kernel¹

¹In general, $\kappa(\vec{x}, \vec{x}') = (1 + \vec{x} \cdot \vec{x}')^k$ is kernel for *k*-order monomial mappings

Exercise

As before, define

$$\vec{\phi}(\vec{x}) = (1, x_1^2, x_2^2, \sqrt{2} x_1, \sqrt{2} x_2, \sqrt{2} x_1 x_2)^T,$$

and let $\kappa(\vec{x}, \vec{x}') = (1 + \vec{x} \cdot \vec{x}')^2$ be the **polynomial** kernel.

Let $\vec{x} = (2, -3)^T$ and $\vec{x}' = (1, 4)^T$.

1. Compute $\vec{\phi}(\vec{x})$ and $\vec{\phi}(\vec{x}')$. 2. Use that to compute $\vec{\phi}(\vec{x}) \cdot \vec{\phi}(\vec{x}')$. 3. Now compute $\kappa(\vec{x}, \vec{x}')$ by evaluating $(1 + \vec{x} \cdot \vec{x}')^2$. 4. Are they the same?

Main Idea

For certain feature maps $\vec{\phi}$, there is an **easy** way to compute $\vec{\phi}(\vec{x}) \cdot \vec{\phi}(\vec{x}')$ without actually computing $\vec{\phi}(\vec{x})$ and $\vec{\phi}(\vec{x}')$: use the **kernel** function $\kappa(\vec{x}, \vec{x}')$.

The Kernel Trick

In many algorithms, when $\vec{\phi}(\vec{x})$ appears, it always appears as part of a dot product of the form:

$$ec{\phi}(ec{x})\cdotec{\phi}(ec{x}')$$

- By replacing all instances of $\vec{\phi}(\vec{x}) \cdot \vec{\phi}(\vec{x}')$ with $\kappa(\vec{x}, \vec{x}')$, we kernelize the algorithm; avoid explicitly mapping to feature space.
- This is called the kernel trick.

Kernelized Algorithms

- Only certain feature maps have efficiently-computed kernels.
- Only certain learning algorithms can be kernelized.
- All of the linear algorithms we've learned can.
 Least squares, perceptron, SVMs, etc.



Lecture 10 | Part 3

Kernel Ridge Regression (and Kernel SVM)

Kernel Ridge Regression

Let's kernelize **ridge regression**.

First: verify that all instances of $\vec{\phi}(\vec{x})$ appear as part of a dot product: $\vec{\phi}(\vec{x}) \cdot \vec{\phi}(\vec{x}')$

Review: Ridge Regression

Suppose $\vec{\phi}(\vec{x})$ is a feature map. To train a ridge regressor in feature space, we'd solve

$$\arg\min_{\vec{w}} \frac{1}{n} \sum_{i=1}^{n} \left(\vec{\phi}(\vec{x}^{(i)}) \cdot \vec{w} - y_i \right)^2 + \lambda \|\vec{w}\|^2$$

In matrix-vector form, where Φ is the design matrix, solve:

$$\underset{\vec{w}}{\arg\min} \frac{1}{n} \| \Phi \vec{w} - \vec{y} \|^2 + \lambda \vec{w}^T \vec{w}$$

Problem

► To perform ridge regression, solve:

$$\underset{\vec{w}}{\arg\min} \frac{1}{n} \| \Phi \vec{w} - \vec{y} \|^2 + \lambda \vec{w}^T \vec{w}$$

To **kernelize** this, we need to replace all instances of $\vec{\phi}(\vec{x}) \cdot \vec{\phi}(\vec{x}')$ with $\kappa(\vec{x}, \vec{x}')$.

But $\vec{\phi}(\vec{x}) \cdot \vec{\phi}(\vec{x}')$ doesn't appear here!

Fix: rewrite this problem in a **dual** form.

Fact

The solution w^* is a linear combination of $\vec{\phi}(\vec{x}^{(i)})$: $\vec{w}^* = \sum_{i=1}^n \alpha_i \vec{\phi}(\vec{x}^{(i)})$

Why? The gradient of the regularized risk is: $\frac{2}{n} \sum_{i=1}^{n} \left(\vec{\phi}(\vec{x}^{(i)}) \cdot \vec{w} - y_i \right) \vec{\phi}(\vec{x}^{(i)}) + 2\lambda \vec{w}$

Setting to zero, solving for \vec{w} gives:

$$\vec{w}^* = \sum_{i=1}^n \underbrace{\left(-\frac{1}{n\lambda}\vec{\phi}(\vec{x}^{(i)}) \cdot \vec{w}^* - y_i\right)}_{\alpha_i} \vec{\phi}(\vec{x}^{(i)})$$

Fact

• The solution w^* is a linear combination of $\vec{\phi}(\vec{x}^{(i)})$:

$$\vec{w}^* = \sum_{i=1}^n \alpha_i \vec{\phi}(\vec{x}^{(i)})$$

In matrix-vector form, where $\vec{\alpha} = (\alpha_1, ..., \alpha_n)^T$: $\vec{w}^* = \Phi^T \vec{\alpha}$

Dual Problem

• Using the fact that $\vec{w}^* = \sum_{i=1}^n \alpha_i \vec{\phi}(\vec{x}^{(i)}) = \Phi^T \vec{\alpha}$ for some $\vec{\alpha}$, the problem:

$$\underset{\vec{w}}{\arg\min} \frac{1}{n} \| \Phi \vec{w} - \vec{y} \|^2 + \lambda \vec{w}^T \vec{w}$$

is equivalent to the **dual problem**:

$$\arg\min_{\vec{\alpha}} \frac{1}{n} \| \Phi \Phi^{\mathsf{T}} \vec{\alpha} - \vec{y} \|^2 + \lambda \vec{\alpha}^{\mathsf{T}} \Phi \Phi^{\mathsf{T}} \vec{\alpha}$$

Main Idea

To do ridge regression, you can either solve:

$$\underset{\vec{w}}{\arg\min} \frac{1}{n} \| \Phi \vec{w} - \vec{y} \|^2 + \lambda \vec{w}^T \vec{w}$$

or you can solve the **dual problem**:

$$\arg\min_{\vec{\alpha}} \frac{1}{n} \| \Phi \Phi^{\mathsf{T}} \vec{\alpha} - \vec{y} \|^2 + \lambda \vec{\alpha}^{\mathsf{T}} \Phi \Phi^{\mathsf{T}} \vec{\alpha}$$

They give the same answer! But the dual problem can be kernelized.

Kernelizing

• Where does $\vec{\phi}(\vec{x})$ appear in this problem?

$$\arg\min_{\vec{\alpha}} \frac{1}{n} \| \Phi \Phi^{\mathsf{T}} \vec{\alpha} - \vec{y} \|^2 + \lambda \vec{\alpha}^{\mathsf{T}} \Phi \Phi^{\mathsf{T}} \vec{\alpha}$$

Inside Φ:

$$\Phi = \begin{pmatrix} \vec{\phi}(\vec{x}^{(1)}) & \longrightarrow \\ \vec{\phi}(\vec{x}^{(2)}) & \longrightarrow \\ \vdots & \\ \vec{\phi}(\vec{x}^{(n)}) & \longrightarrow \end{pmatrix}$$

Exercise

Argue that the (i, j) entry of $\Phi \Phi^T$ is equal to $\kappa(\vec{x}^{(i)}, \vec{x}^{(j)})$.

$$\Phi = \begin{pmatrix} \vec{\phi}(\vec{x}^{(1)}) & \longrightarrow \\ \vec{\phi}(\vec{x}^{(2)}) & \longrightarrow \\ \vdots \\ \vec{\phi}(\vec{x}^{(n)}) & \longrightarrow \end{pmatrix}$$

Kernelizing

The (i, j) entry of $\Phi \Phi^T$ is $\vec{\phi}(\vec{x}^{(i)}) \cdot \vec{\phi}(\vec{x}^{(j)}) = \kappa(\vec{x}^{(i)}, \vec{x}^{(j)})$

$$\Phi\Phi^{T} = \underbrace{\begin{pmatrix} \kappa(\vec{x}^{(1)}, \vec{x}^{(1)}) & \kappa(\vec{x}^{(1)}, \vec{x}^{(2)}) & \cdots & \kappa(\vec{x}^{(1)}, \vec{x}^{(n)}) \\ \kappa(\vec{x}^{(2)}, \vec{x}^{(1)}) & \kappa(\vec{x}^{(2)}, \vec{x}^{(2)}) & \cdots & \kappa(\vec{x}^{(2)}, \vec{x}^{(n)}) \\ \vdots & \vdots & \ddots & \vdots \\ \kappa(\vec{x}^{(n)}, \vec{x}^{(1)}) & \kappa(\vec{x}^{(n)}, \vec{x}^{(2)}) & \cdots & \kappa(\vec{x}^{(n)}, \vec{x}^{(n)}) \end{pmatrix}}_{K}$$

K is called the Kernel matrix (or Gram matrix).

Kernel Ridge Regression

The dual problem becomes:

$$\arg\min_{\vec{\alpha}} \frac{1}{n} \| K\vec{\alpha} - \vec{y} \|^2 + \lambda \vec{\alpha}^T K\vec{\alpha}$$

Exact solution to the dual problem:

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

► This is kernel ridge regression.

Kernelization

Observe: we train linear predictor in feature space without actually mapping to feature space:

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

Making Predictions

To predict on a new point \vec{x} , normally: $H(\vec{x}) = \vec{w}^* \cdot \vec{\phi}(\vec{x}).$

How to do this without actually mapping?

• Recall:
$$w^* = \sum_{i=1}^n \alpha_i^* \vec{\phi}(\vec{x}^{(i)})$$

• So:

$$H(\vec{x}) = \sum_{i=1}^{n} \alpha_i^* \vec{\phi}(\vec{x}^{(i)}) \cdot \vec{\phi}(\vec{x}) = \sum_{i=1}^{n} \alpha_i^* \kappa(\vec{x}^{(i)}, \vec{x})$$

Making Predictions

To make a prediction on a new point:

$$H(\vec{x}) = \sum_{i=1}^{n} \alpha_i^* \kappa(\vec{x}^{(i)}, \vec{x})$$

- No need to map to feature space.
- Interpretation: A weighted sum of kernel evaluations.

Procedure: Kernel Ridge Regression

- 1. Pick a kernel function, *κ*, and compute the kernel matrix, *K*.
- 2. Solve linear system: $\vec{\alpha}^* = (K + n\lambda I)^{-1}\vec{y}$
- 3. To make new prediction, $H(\vec{x}) = \sum_{i=1}^{n} \alpha_i^* \kappa(\vec{x}^{(i)}, \vec{x})$

Kernel Soft-SVM

- Soft-SVM can also be **kernelized**.
- 1. Pick a kernel function, κ.
- 2. Solve dual problem (e.g., with SGD):

$$\arg\min_{\vec{\alpha}} \left(\lambda \vec{\alpha}^{\mathsf{T}} K \vec{\alpha} + \frac{1}{n} \sum_{i=1}^{n} \max\{0, 1 - y_i (K \vec{\alpha})_i\} \right)$$

3. To make new prediction, H(x) = Σ_{i∈S} α_i^{*}κ(x⁽ⁱ⁾, x)
 ▶ Where S is the set of indices of support vectors.

Kernelization Downsides

- Often, training involves the n × n kernel matrix.
 Can be very large!
- There are ways to mitigate this:
 - Small-batch stochastic gradient descent.
 - Nyström method.



Lecture 10 | Part 4

Kernel Functions

Valid Kernels

- The first step in kernel learning is to pick a kernel function, κ.
- To be a valid kernel, must compute the dot product w.r.t., some mapping, $\vec{\phi}(\vec{x})$.
- That is, it must be that

$$\kappa(\vec{x},\vec{x}')=\vec{\phi}(\vec{x})\cdot\vec{\phi}(\vec{x}')$$

for some $\vec{\phi}$.

Constructing Kernels: Approach #1

- How do we come up with valid kernel functions?
- Approach #1:
 - 1. Start by picking $\vec{\phi}$
 - 2. Find a function κ that efficiently computes $\vec{\phi}(\vec{x}) \cdot \vec{\phi}(\vec{x}')$, if one exists.

Constructing Kernels: Approach #2

- New kernels can be constructed from other kernels.
- Suppose κ₁, κ₂, κ₃ are kernels and f is any function. Then the below are kernels:

$$\kappa(\vec{x},\vec{x}') = \kappa_1(\vec{x},\vec{x}') + \kappa_2(\vec{x},\vec{x}')$$

 $\blacktriangleright \kappa(\vec{x},\vec{x}') = \kappa_1(\vec{x},\vec{x}') \times \kappa_2(\vec{x},\vec{x}')$

$$\blacktriangleright \ \kappa(\vec{x},\vec{x}') = \kappa_3(\vec{\phi}(\vec{x}),\vec{\phi}(\vec{x}'))$$

$$\blacktriangleright \kappa(\vec{x},\vec{x}') = f(\vec{x})\kappa_1(\vec{x},\vec{x}')f(\vec{x}')$$

Verifying Kernels

Theorem

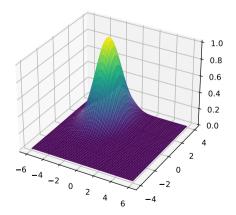
A symmetric function κ is a valid kernel if and only if the kernel matrix, K, is positive semi-definite for any choice of data, $\vec{x}^{(1)}, \dots, \vec{x}^{(n)}$.

Radial Basis Function Kernel

- Often, though, we don't design our own kernel.
- A very popular choice: the radial basis function (RBF) kernel (or Gaussian kernel):

$$\kappa(\vec{x}, \vec{x}') = e^{\frac{-\|\vec{x}-\vec{x}'\|^2}{2\sigma^2}} = e^{-\gamma \|\vec{x}-\vec{x}'\|^2}$$
 where $\gamma = 1/(2\sigma^2)$

RBF Kernel



$$\kappa(\vec{x}, \vec{x}') = e^{\frac{-\|\vec{x}-\vec{x}'\|^2}{2\sigma^2}} = e^{-\gamma \|\vec{x}-\vec{x}'\|^2}$$

- Interpretation: RBF kernel measures similarity of x and x'
 - Very similar: $\kappa(\vec{x}, \vec{x}') \approx 1$.
 - Very different: $\kappa(\vec{x}, \vec{x}') \approx 0$.
- Parameter σ (or γ) controls the scale
 The larger σ (smaller γ), the wider the Guassian

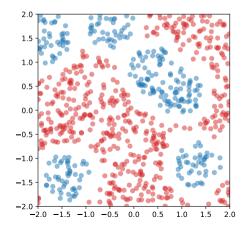
Recall that in kernel ridge regression / SVM, the prediction is:

$$H(\vec{x}) = \sum_{i=1}^{n} \alpha_i \kappa(\vec{x}^{(i)}, \vec{x})$$

Observations:

- One parameter α_i learned for **each** training point $\vec{x}^{(i)}$
- H(x) is largely determined by the training points closest to x

- RBF function placed at each training point.
- $H(\vec{x})$ is largely determined by training points closest to \vec{x}



An RBF Kernel predictor can be seen as a generalization of the k-nearest neighbor rule

k-NN: RBF kernel predictor: sign $\left(\sum_{i=1}^{n} y_i \mathbf{1}(\vec{x}^{(i)} \text{ is a } k \text{-nn of } \vec{x})\right)$ sign $\left(\sum_{i=1}^{n} \alpha_i \kappa(\vec{x}^{(i)}, \vec{x})\right)$

RBF Kernel Map

- What ϕ is the RBF kernel a kernel for?
- The mapping $\vec{\phi}(\vec{x})$ with entries of the form: $e^{-\|\vec{x}\|^2/2}x_i, \quad \frac{1}{\sqrt{2!}}e^{-\|\vec{x}\|^2/2}x_ix_j, \quad \frac{1}{\sqrt{3!}}e^{-\|\vec{x}\|^2/2}x_ix_jx_k, \quad \dots$
- This is a mapping to an infinite dimensional Hilbert space!

Other Kernels

- There are other interesting kernels useful for specific domains.
- Example: string kernels for text classification.
 Dot product in space generated by all substrings.

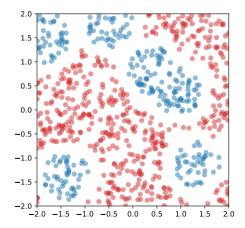


Lecture 10 | Part 5

Demo: Kernel SVM

Demo

▶ Train an RBF kernel SVM on the data below.



Aside: Hyperparameter Selection

- Two hyperparameters to specify:
 - Slack: C
 - Kernel width: γ
- Choose with grid search cross-validation

