DSC 140A

Probabilistic Modeling & Machine Learning

Lecture 8 | Part 1

High-Dimensional Feature Maps

Linear Prediction Rules

- We have seen how to fit linear functions:

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

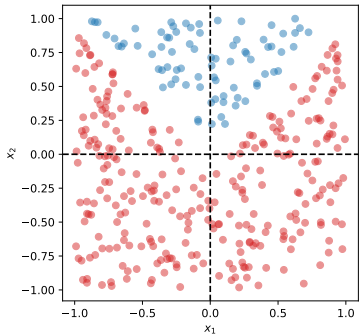
- Used for both **regression** and **classification**

- **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 $H(x_1, x_2) = w_0 + w_1 x_1 + x_2 x_2$ will work well

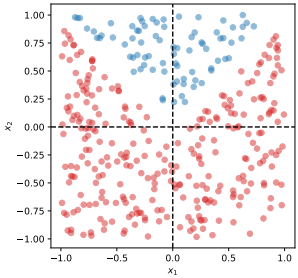


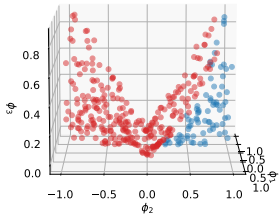
However...

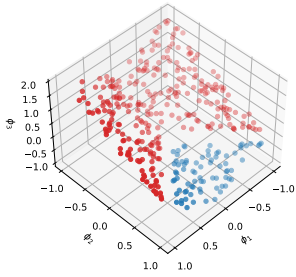
- We have seen a way around this limitation: **basis functions**.
- **Idea:** design a function $\vec{\phi}(\vec{x})$ that maps data to a new space in which it is **linearly separable**.

Example

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







Procedure

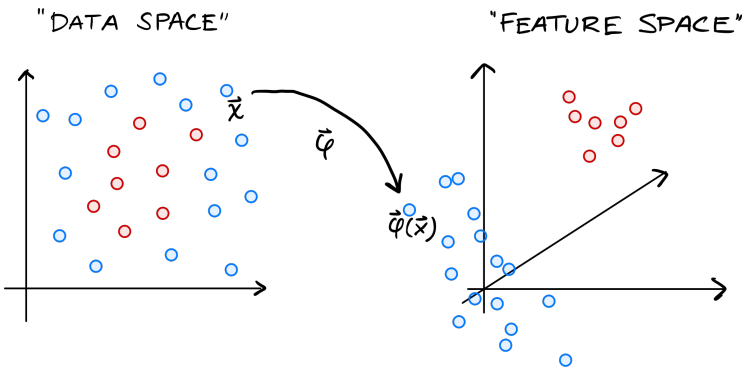
1. Define feature map $\vec{\phi}(\vec{x}) : \mathbb{R}^d \to \mathbb{R}^k$
   - $\vec{\phi}(\vec{x}) = (\phi_1(\vec{x}), \ldots, \phi_k(\vec{x}))^T$
   - Number of basis functions k can be $>$ or $\leq$ than d

2. Map each training point to k-dimensional **feature space**: $\vec{x}^{(i)} \mapsto \vec{\phi}(\vec{x}^{(i)})$

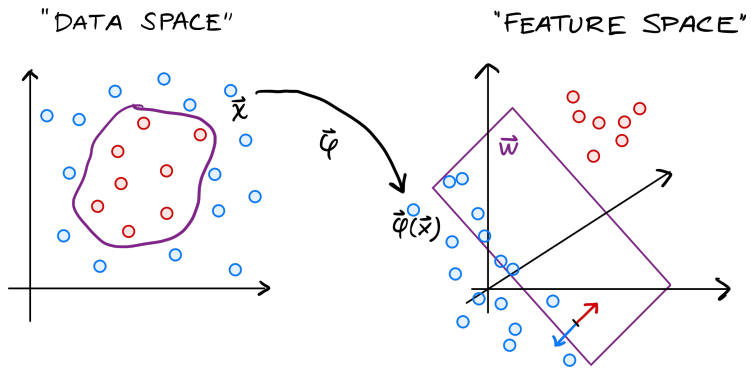
3. Learn a linear predictor in feature space:

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

Procedure

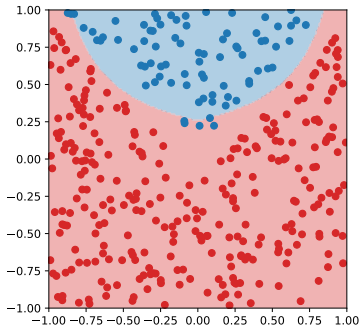


Procedure


"DATA SPACE"
"FEATURE SPACE"
$\vec{x}$
$\vec{\varphi}$
$\vec{\varphi}(\vec{x})$
$\vec{w}$

Example

- Use mapping $\vec{\phi}(\vec{x}) = (x_1, x_2, |x_1 x_2|)^T$
- 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 $\vec{\phi} = (x_1, x_2, |x_1 x_2|)^T$ is the mapping from "data space" to "feature space".

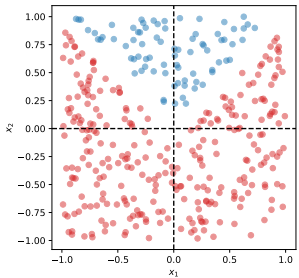
Let $\vec{x} = (2, -3)^T$ be a new point that needs to be classified. What is the predicted label?

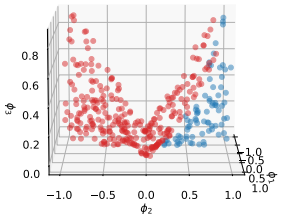
Feature Maps

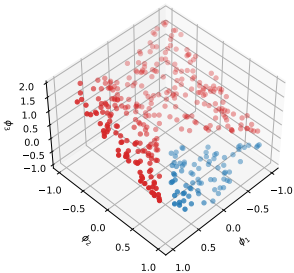
- How do we choose $\vec{\phi}$?
- **Hope:** data is linearly separable in feature space
- Appears difficult to engineer $\vec{\phi}$ to satisfy this.
  - Need to design $\vec{\phi}$ for each new data set?
- **Goal:** design a general feature map that is likely to make any data set linearly separable

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.

Example: Monomials

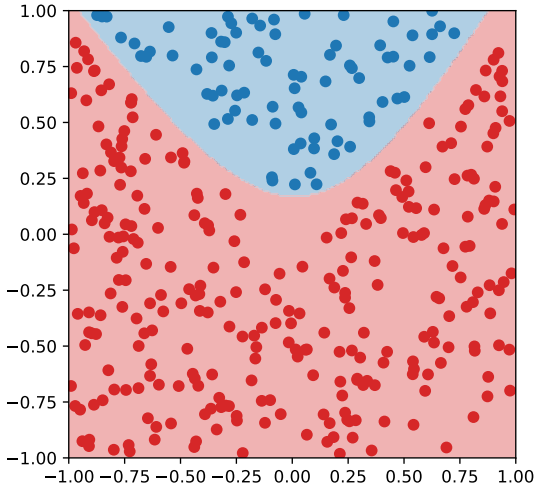
- Define a feature map $\vec{\phi} : \mathbb{R}^2 \to \mathbb{R}^6$ as follows:

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

- We fit a prediction function of the form:

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

Example: Monomials



Example: Monomials

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

$$1, \qquad x_i, \qquad x_i x_j, \qquad x_i^2$$

- 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 $\vec{\phi}(\vec{x}) \in \mathbb{R}^{1{,}326}$.

Example: Monomials

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

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

- 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...

Problem

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

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Lecture 8 | 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.

The Kernel Trick

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

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

- 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 mapping to feature space.

- This is called the **kernel trick**.

Example: Polynomial Kernel

- Define the feature map:

$$\vec{\phi}(\vec{x}) = (1, x_1^2, x_2^2, x_3^2, \sqrt{2}\,x_1, \sqrt{2}\,x_2, \sqrt{2}\,x_3, \sqrt{2}\,x_1x_2, \sqrt{2}\,x_1x_3, \sqrt{2}\,x_2x_3)^T$$

- $\kappa(\vec{x}, \vec{x}') = (1 + \vec{x} \cdot \vec{x}')^2$ is a kernel for this $\vec{\phi}$.
  - That is, $\kappa(\vec{x}, \vec{x}') = \vec{\phi}(\vec{x}) \cdot \vec{\phi}(\vec{x}')$

- Called the **polynomial kernel**[1]

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

Kernelized Algorithms

- Only certain mappings 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.

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

Kernel Ridge Regression

- Suppose $\vec{\phi}(\vec{x})$ is a feature map with kernel k.
- 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:

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

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 $\vec{\alpha} = (\alpha_1, \ldots, \alpha_n)^T$:

$$\vec{w}^* = \Phi^T \vec{\alpha}$$

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:

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

  is equivalent to the **dual** problem:

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

Kernelizing

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

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

- 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:

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

- This is **kernel ridge regression**.

Kernelization

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

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

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.
2. Solve linear system: $\vec{\alpha}^* = (K - \lambda I)^{-1}\vec{y}$
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):

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

3. To make new prediction, $H(\vec{x}) = \sum_{i \in S} \alpha_i^* \kappa(\vec{x}^{(i)}, \vec{x})$
   - Where S is the set of indices of support vectors.

Kernelization Downsides

- Often, training involves the $n \times n$ kernel matrix.
  - Can be very large!

- There are ways to mitigate this:
  - Small-batch stochastic gradient descent.
  - Nyström method.

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Lecture 8 | Part 3

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 $\kappa_1, \kappa_2, \kappa_3$ are kernels and f is any function. Then the below are kernels:
  - $\kappa(\vec{x}, \vec{x}') = \kappa_1(\vec{x}, \vec{x}') + \kappa_2(\vec{x}, \vec{x}')$
  - $\kappa(\vec{x}, \vec{x}') = \kappa_1(\vec{x}, \vec{x}') \times \kappa_2(\vec{x}, \vec{x}')$
  - $\kappa(\vec{x}, \vec{x}') = \kappa_3(\vec{\phi}(\vec{x}), \vec{\phi}(\vec{x}'))$
  - $\kappa(\vec{x}, \vec{x}') = f(\vec{x})\kappa_1(\vec{x}, \vec{x}')f(\vec{x}')$

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, $\vec{x}^{(1)}, \ldots, \vec{x}^{(n)}$.

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**):

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

RBF Kernel Interpretation

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

- **Interpretation:** RBF kernel measures similarity of $\vec{x}$ and $\vec{x}'$
  - 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

RBF Kernel Interpretation

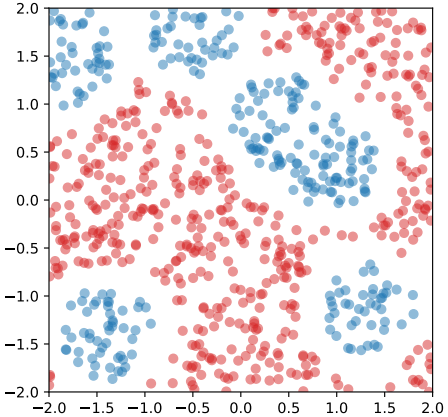
- Recall that in kernel ridge regression / SVM, the prediction is:

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

- **Observations:**
  - One parameter α_i learned for **each** training point $\vec{x}^{(i)}$
  - $K(\vec{x}^{(i)}, \vec{x})$ will be ≈ 0 for any $\vec{x}^{(i)}$ far from $\vec{x}$
  - $H(\vec{x})$ is largely determined by the training points closest to $\vec{x}$

RBF Kernel Interpretation

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



RBF Kernel Interpretation

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

RBF Kernel Map

- What ϕ is the RBF kernel a kernel for?
- The mapping $\vec{\phi}(\vec{x})$ with entries of the form:

$$e^{-\|\vec{x}\|^2/2}x_i, \quad \frac{1}{\sqrt{2!}}e^{-\|\vec{x}\|^2/2}x_i x_j, \quad \frac{1}{\sqrt{3!}}e^{-\|\vec{x}\|^2/2}x_i x_j x_k, \quad \ldots$$

- 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.

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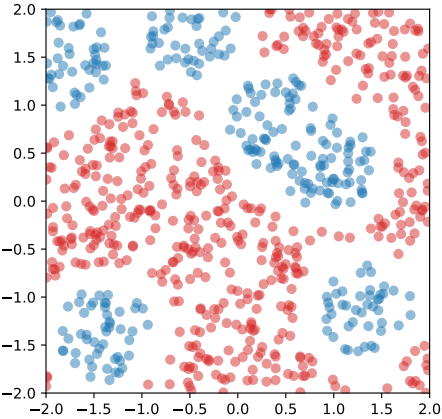
Lecture 8 | Part 4

Demo: Kernel SVM

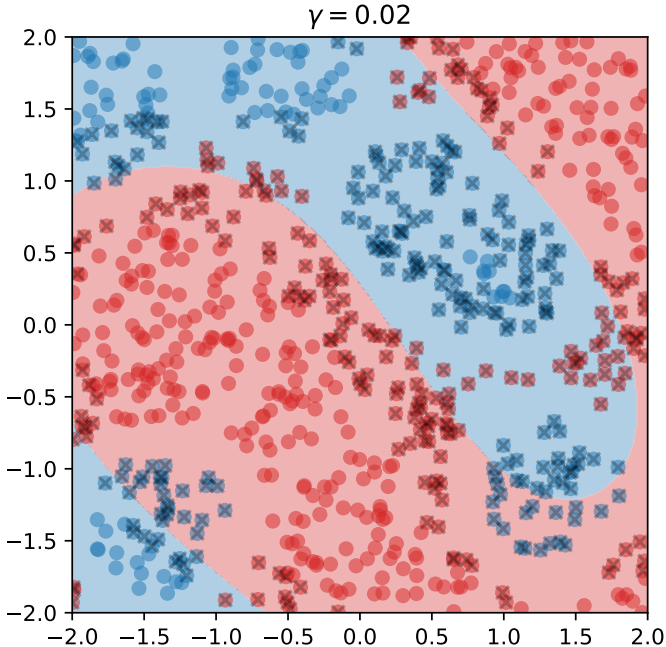
Demo

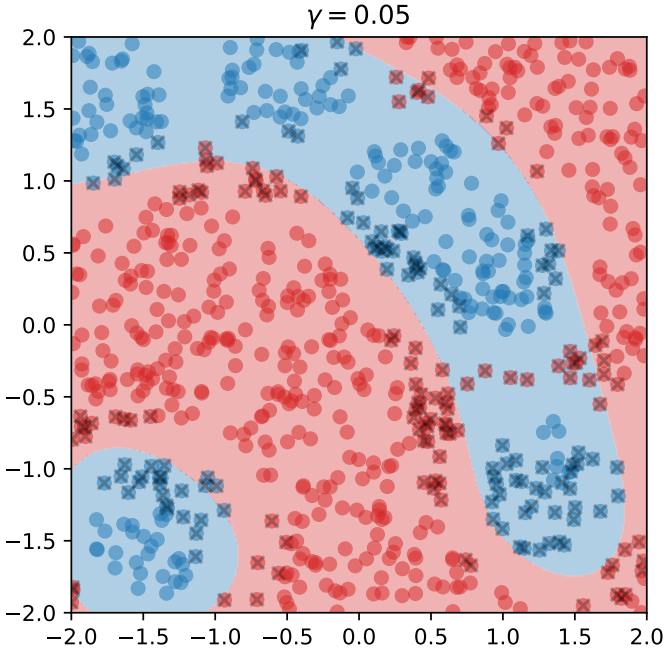
- Train an RBF kernel SVM on the data below.

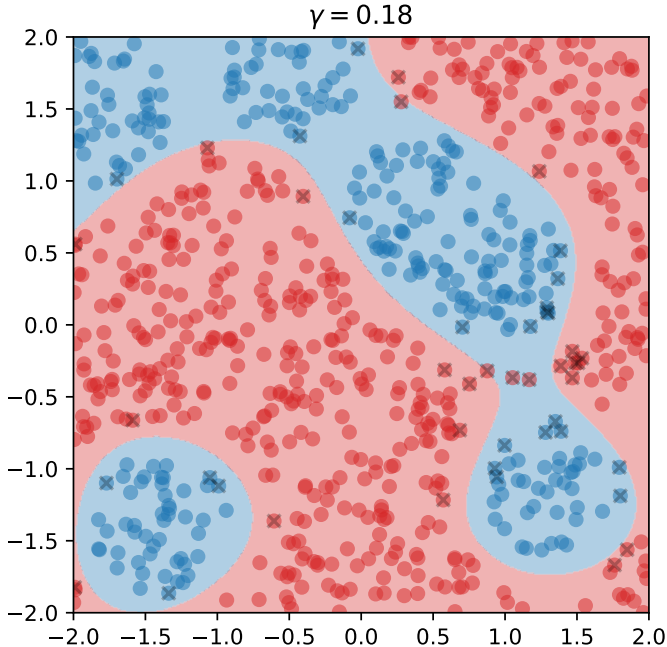


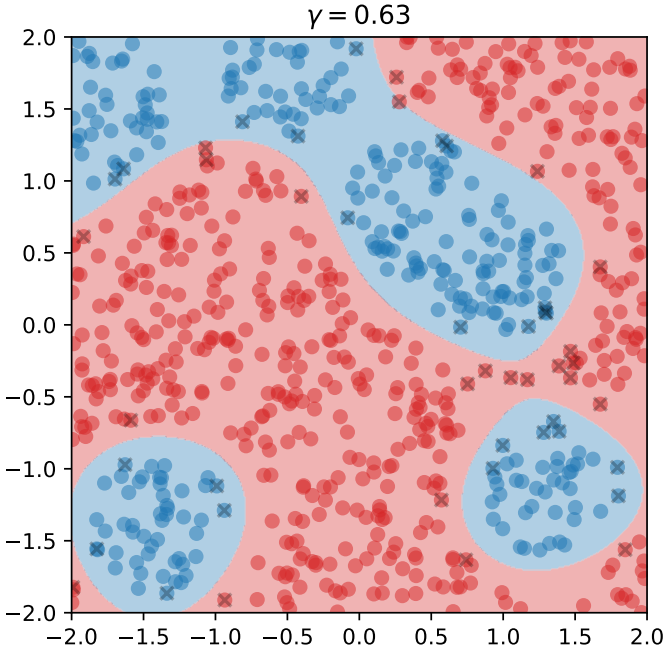
Aside: Hyperparameter Selection

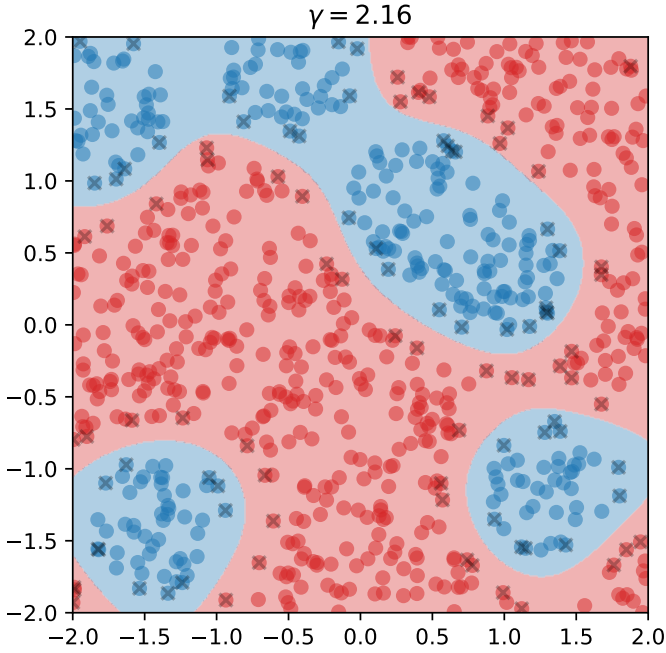
- Two hyperparameters to specify:
  - Slack: C
  - Kernel width: γ
- Choose with grid search cross-validation

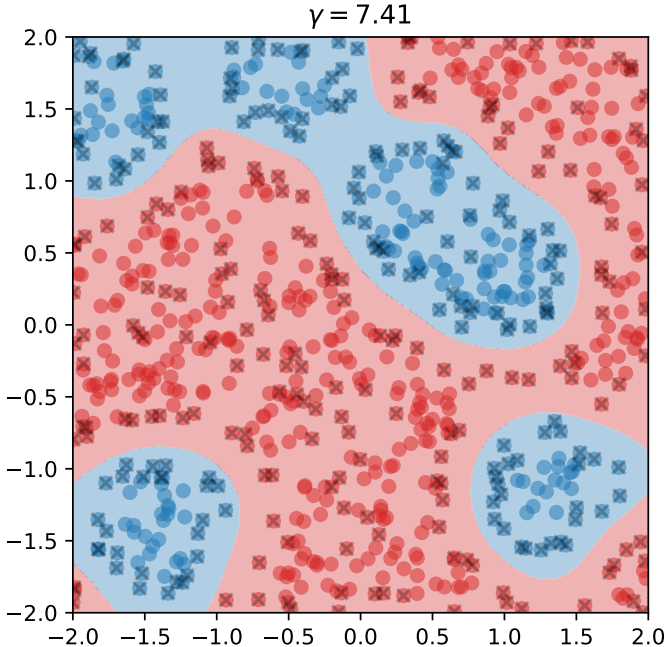

$\gamma = 0.02$
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0

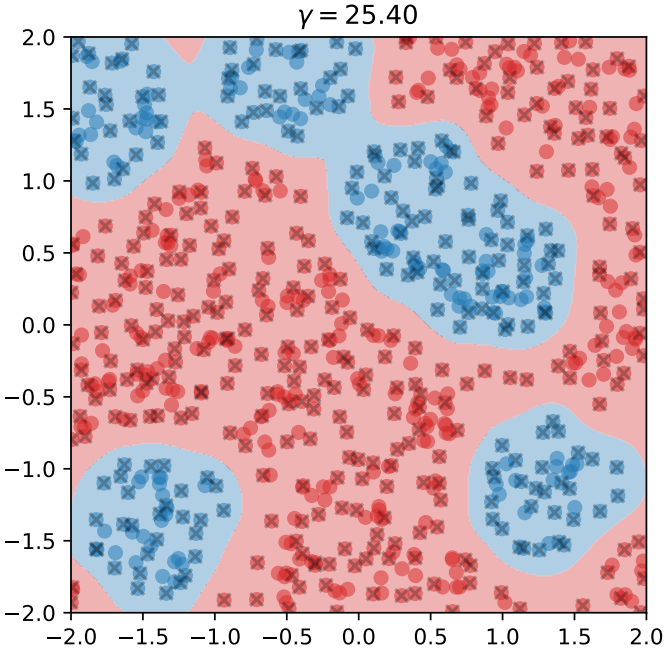

$\gamma = 0.05$
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0

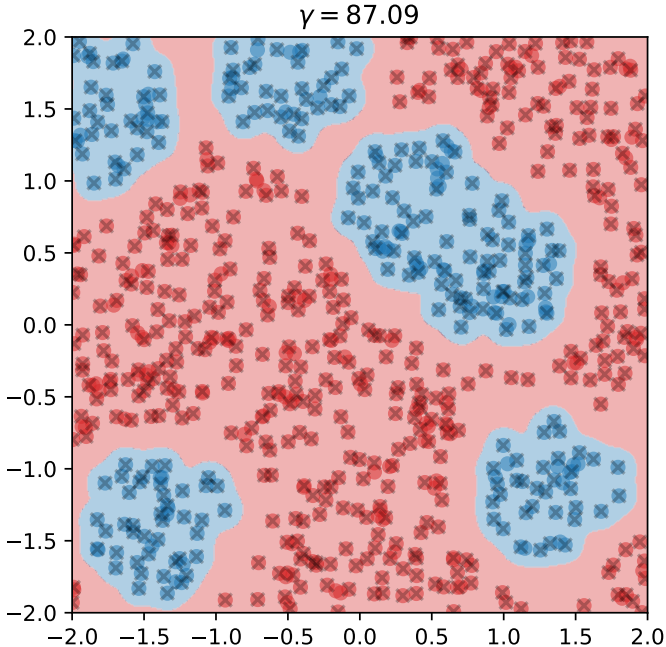

$\gamma = 0.18$
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0

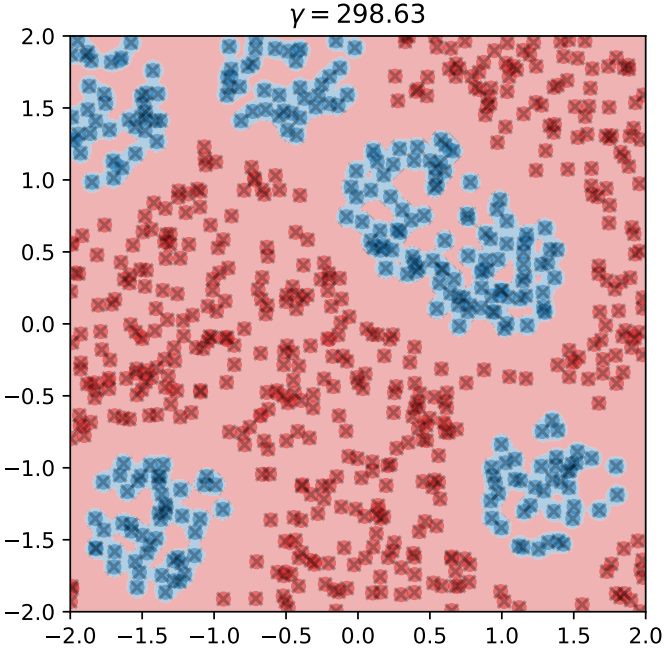

$\gamma = 0.63$
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0

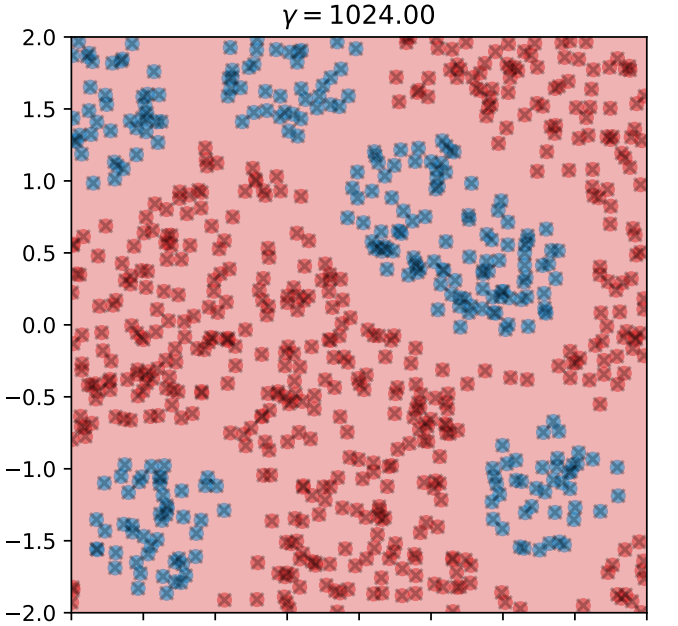

$\gamma = 2.16$
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0


$\gamma = 7.41$
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0


$\gamma = 25.40$
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0


$\gamma = 87.09$
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0


$\gamma = 298.63$
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0


$\gamma = 1024.00$
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0