DSC 140A

Probabilistic Modeling & Machine Learning

Lecture 10 | Part 1

High-Dimensional Feature Maps

Linear Prediction Rules

- We have seen how to fit linear functions:

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

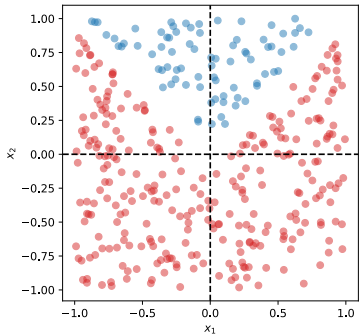
- Used for both **regression** and **classification**

- **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 $H(x_1, x_2) = w_0 + w_1 x_1 + w_2 x_2$ will work well

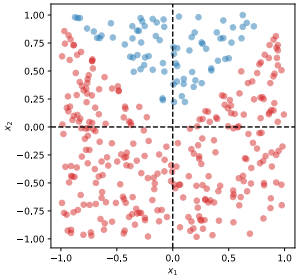


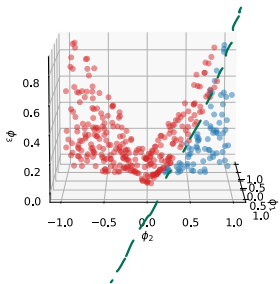
However...

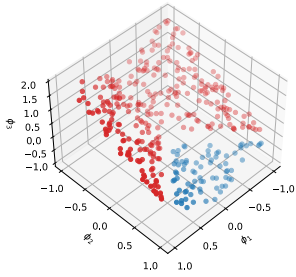
- We have seen a way around this limitation: **basis functions**.
- **Idea:** design a function $\vec{\phi}(\vec{x})$ that maps data to a new space in which it is **linearly separable**.

Example

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







Procedure

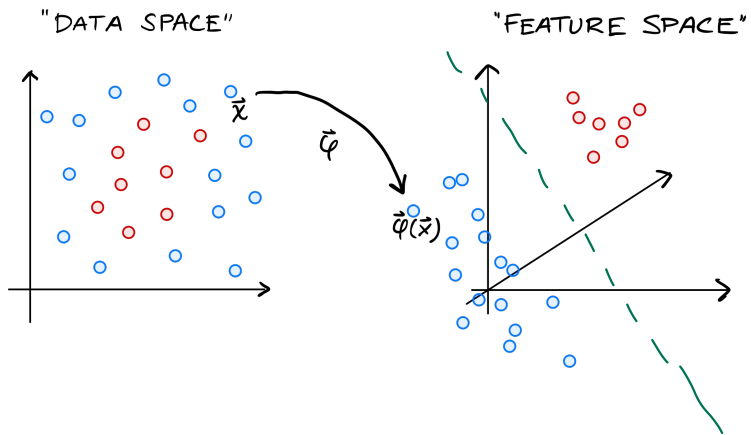
1. Define feature map $\vec{\phi}(\vec{x}) : \mathbb{R}^d \to \mathbb{R}^k$
   - $\vec{\phi}(\vec{x}) = (\phi_1(\vec{x}), \ldots, \phi_k(\vec{x}))^T$
   - Number of basis functions k can be $>$ or $\leq$ than d

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

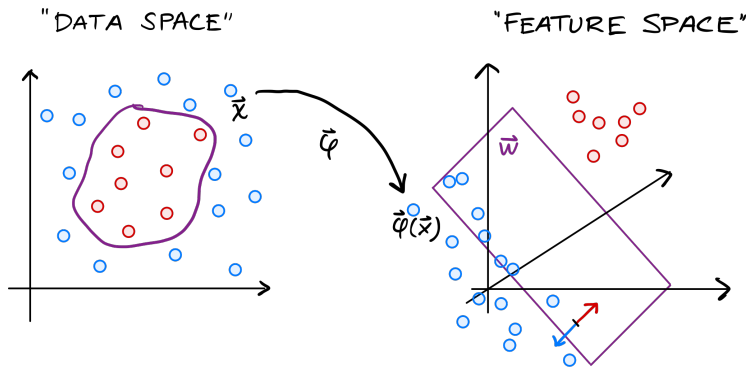
3. Learn a linear predictor in feature space:

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

Procedure

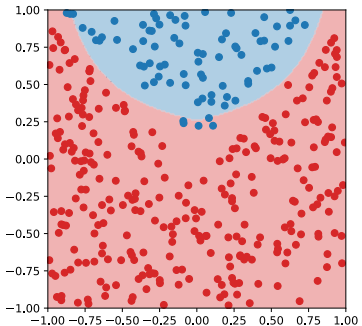


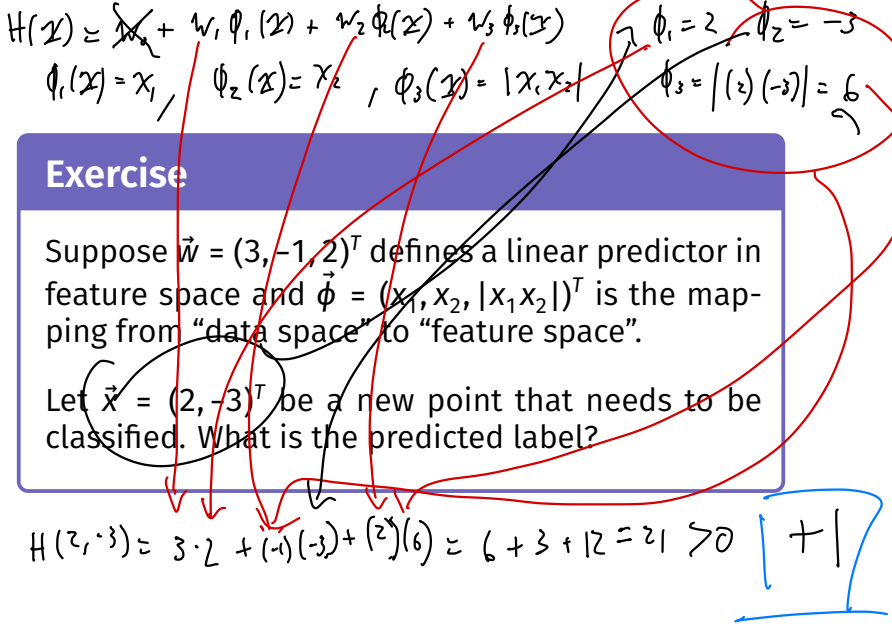
Procedure



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

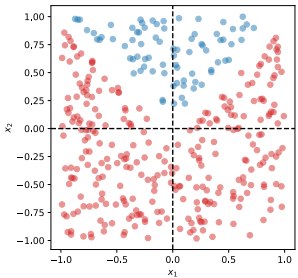
- How do we choose $\vec{\phi}$?
- **Hope:** data is linearly separable in feature space
- Appears difficult to engineer $\vec{\phi}$ to satisfy this.
  - Need to design ~~$\vec{\phi}$ for each new~~ data set?

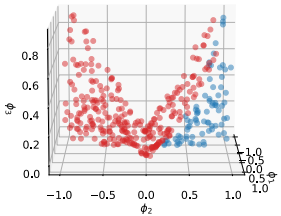
"feature engineering"

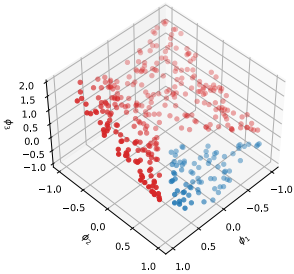
- **Goal:** design a general feature map that is likely to make any data set linearly separable

High-Dimensional Feature Maps

- **Observe:** in our example, $\vec{\phi}$ mapped to space of larger dimension "lifting" into a higher-dimensional feature space







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

order - 2

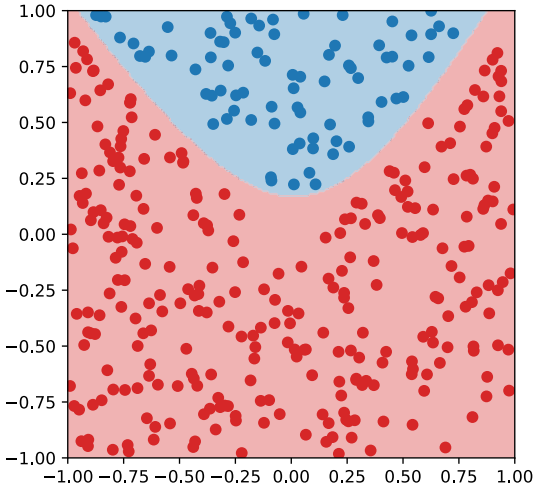
- Define a feature map $\vec{\phi} : \mathbb{R}^2 \to \mathbb{R}^6$ as follows:

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

- 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...

Example: Monomials

- 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**.

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Lecture 10 | Part 2

The Kernel Trick

Recap

- We can learn non-linear patterns by:

1. Defining a high-dimensional feature map, $\vec{\phi} : \mathbb{R}^d \to \mathbb{R}^k$ $k > d$
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

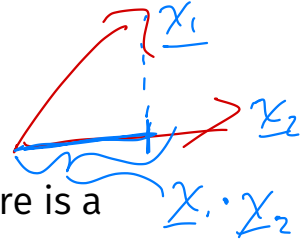
- In many algorithms, when $\vec{\phi}(\vec{x})$ appears, it always appears as part of a dot product:

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

- 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:

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

- $\kappa(\vec{x}, \vec{x}') = (1 + \vec{x} \cdot \vec{x}')^2$ 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

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**. of order 2

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:

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

- 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 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.

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Probabilistic Modeling & Machine Learning

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:

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

Problem

There are $\phi(x) \cdot \phi(x')$ in here when expanded

- To perform ridge regression, solve:

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

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

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

$$\Phi^T = \left(\phi(x^{(1)}), \phi(x^{(2)}), \ldots, \phi(x^{(n)}) \right)$$

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**:

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

product of matrices

Main Idea

To do ridge regression, you can either solve:

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

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

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

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

Kernelizing

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

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

- Inside Φ:

feature vector for 1 sample

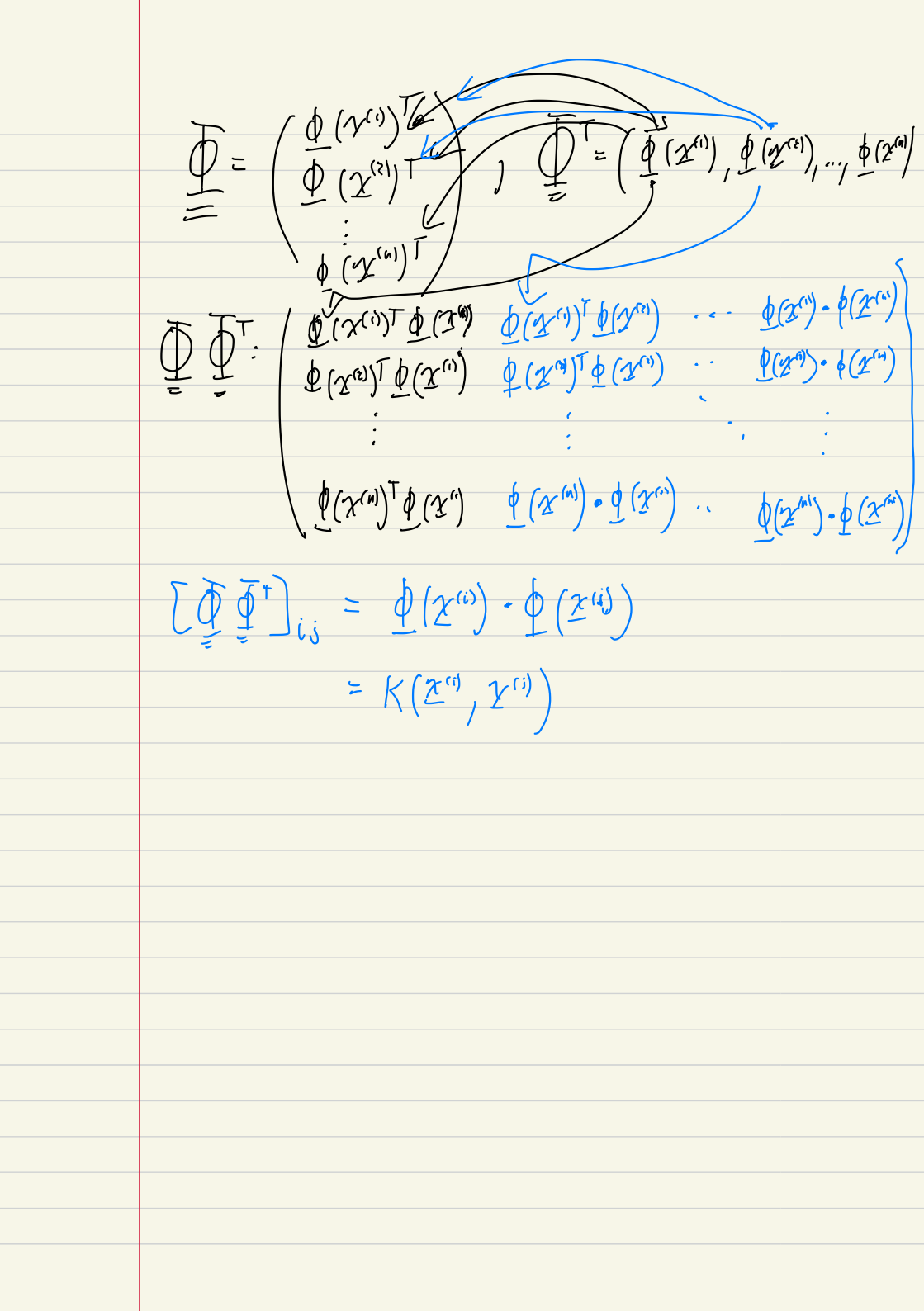
$$\Phi = \begin{pmatrix} \vec{\phi}(\vec{x}^{(1)}) \\ \vec{\phi}(\vec{x}^{(2)}) \\ \vdots \\ \vec{\phi}(\vec{x}^{(n)}) \end{pmatrix}$$

$n \times k$

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 $\vec{\phi}(\vec{x}^{(i)}) \cdot \vec{\phi}(\vec{x}^{(j)}) = \kappa(\vec{x}^{(i)}, \vec{x}^{(j)})$

a matrix of kernel evaluations

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

- 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**.

$$(\underline{\underline{K}})^T = (\underline{\underline{\Phi}}\,\underline{\underline{\Phi}}^T)^T = (\underline{\underline{\Phi}}^T)^T \underline{\underline{\Phi}}^T = \underline{\underline{\Phi}}\,\underline{\underline{\Phi}}^T \Rightarrow \underline{\underline{K}}^T = \underline{\underline{K}}$$

$$\underline{\alpha}^* = \underset{\underline{\alpha}}{\operatorname{argmin}} \underbrace{\frac{1}{n}\|\underline{\underline{K}}\underline{\alpha} - \underline{y}\|_2^2}\, + \lambda \underline{\alpha}^T \underline{\underline{K}}\,\underline{\alpha}$$

$$= \underbrace{\frac{1}{n}(\underline{\underline{K}}\underline{\alpha} - \underline{y})^T(\underline{\underline{K}}\underline{\alpha} - \underline{y}) + \lambda \underline{\alpha}^T \underline{\underline{K}}\,\underline{\alpha}}_{J}$$

$$\Rightarrow \nabla_{\underline{\alpha}} J = 2\frac{1}{n}\underline{\underline{K}}^T(\underline{\underline{K}}\underline{\alpha} - \underline{y}) + 2\lambda \underline{\underline{K}}\,\underline{\alpha} = 0$$

$$= \underbrace{2\underline{\underline{K}}}_{\neq 0}\underbrace{\left(\frac{1}{n}(\underline{\underline{K}}\underline{\alpha} - \underline{y}) + \lambda \underline{\alpha}\right)}_{0} = 0$$

$$\frac{1}{n}\underline{\underline{K}}\underline{\alpha} - \frac{1}{n}\underline{y} + \lambda \underline{\alpha} = 0$$

$$\Rightarrow \left(\frac{1}{n}\underline{\underline{K}} + \lambda \underline{\underline{I}}\right)\underline{\alpha} - \frac{1}{n}\underline{y} = 0$$

$$\Rightarrow (\underline{\underline{K}} + n\lambda \underline{\underline{I}})\underline{\alpha} - \underline{y} = 0$$

$$(\underline{\underline{K}} + n\lambda \underline{\underline{I}})\underline{\alpha} = \underline{y}$$

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

Kernelization

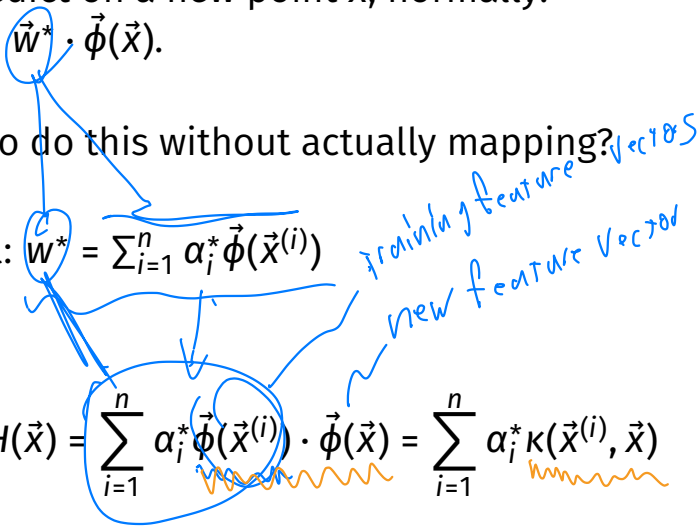
- **Observe:** we train linear predictor in feature space without actually mapping to feature space:

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

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

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

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!

memory - $\mathcal{O}(n^2)$
time - $\Theta(n^3)$

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

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Probabilistic Modeling & Machine Learning

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 $\kappa_1, \kappa_2, \kappa_3$ 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**):

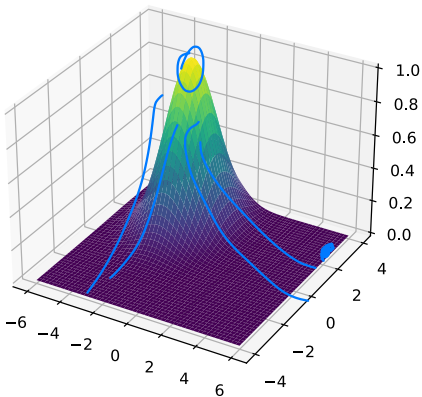
$$\kappa(\vec{x}, \vec{x}') = e^{\frac{-\|\vec{x}-\vec{x}'\|^2}{2\sigma^2}} = e^{-\gamma\|\vec{x}-\vec{x}'\|^2} \qquad \text{where } \gamma = 1/(2\sigma^2)$$

"gamma"

"bandwidth"

makes more precision
edgy

RBF Kernel



RBF Kernel Interpretation

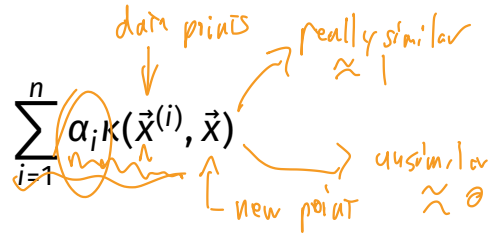
$$\kappa(\vec{x}, \vec{x}') = e^{\frac{-\|\vec{x}-\vec{x}'\|^2}{2\sigma^2}} = e^{-\gamma\|\vec{x}-\vec{x}'\|^2}$$

- **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:

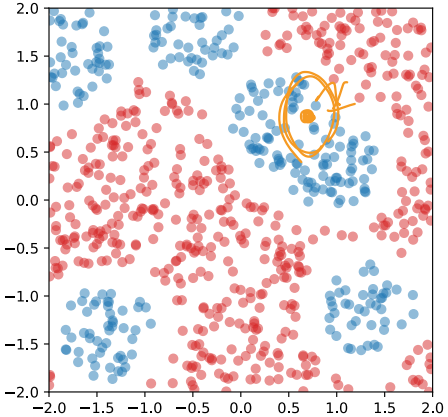
$$H(\vec{x}) = \sum_{i=1}^{n} \alpha_i \kappa(\vec{x}^{(i)}, \vec{x})$$



- **Observations:**
  - One parameter α_i learned for **each** training point $\vec{x}^{(i)}$
  - $\kappa(\vec{x}^{(i)}, \vec{x})$ 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

like a weighted nearest neighbor

k-NN:

$$\text{sign}\left(\sum_{i=1}^{n} y_i \mathbb{1}(\vec{x}^{(i)} \text{ is a } k\text{-nn of } \vec{x})\right)$$

indicator function $\mathbb{1}(\vec{x}^{(i)} \text{ closest to } \vec{x}) = \begin{cases} 1 & \text{if true} \\ 0 & \text{o/w} \end{cases}$

RBF kernel predictor:

$$\text{sign}\left(\sum_{i=1}^{n} \alpha_i \kappa(\vec{x}^{(i)}, \vec{x})\right)$$

RBF Kernel Map

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

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

- This is a mapping to an **infinite dimensional Hilbert space**!

Other Kernels

"modelling"

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

DSC 140A

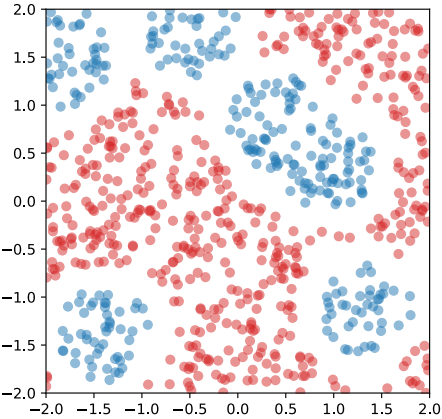
Probabilistic Modeling & Machine Learning

Lecture 10 | Part 5

Demo: Kernel SVM

Demo

- Train an RBF kernel SVM on the data below.

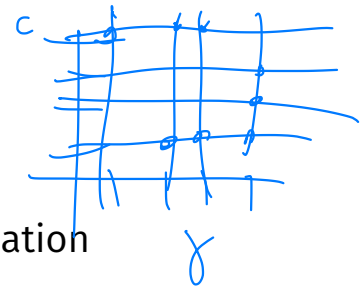


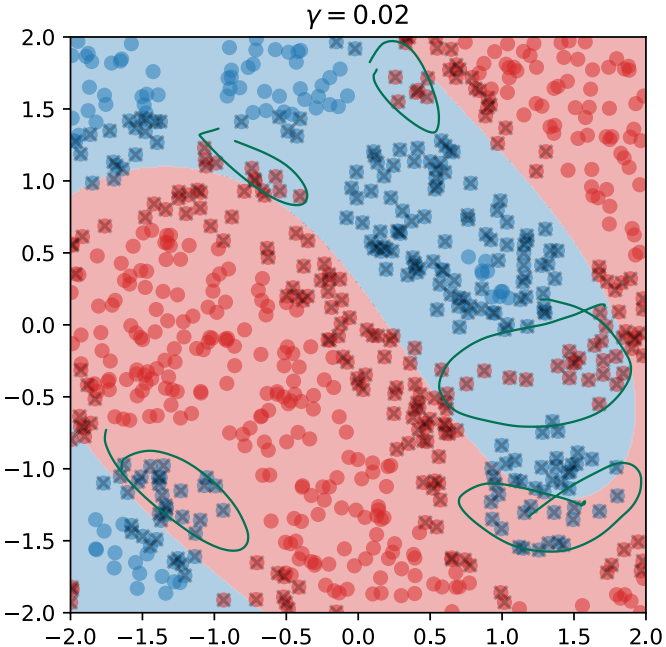
Aside: Hyperparameter Selection

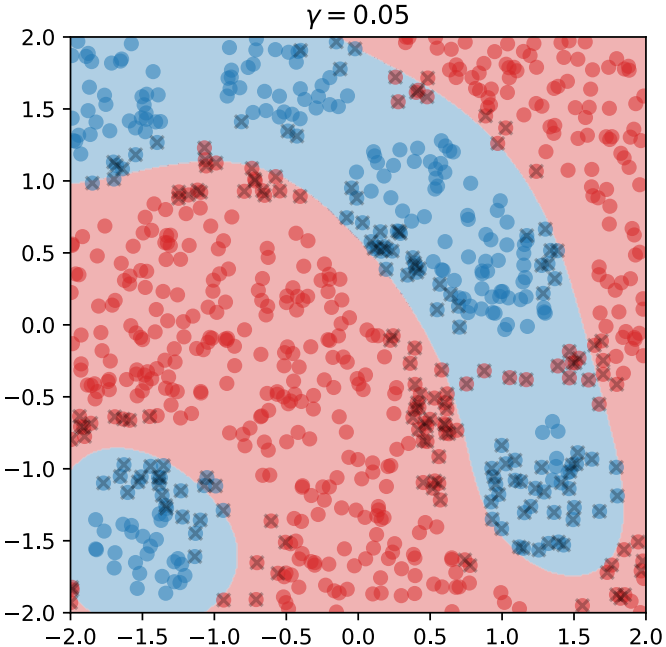
- Two hyperparameters to specify:
  - Slack: C
  - Kernel width: γ

precision

- 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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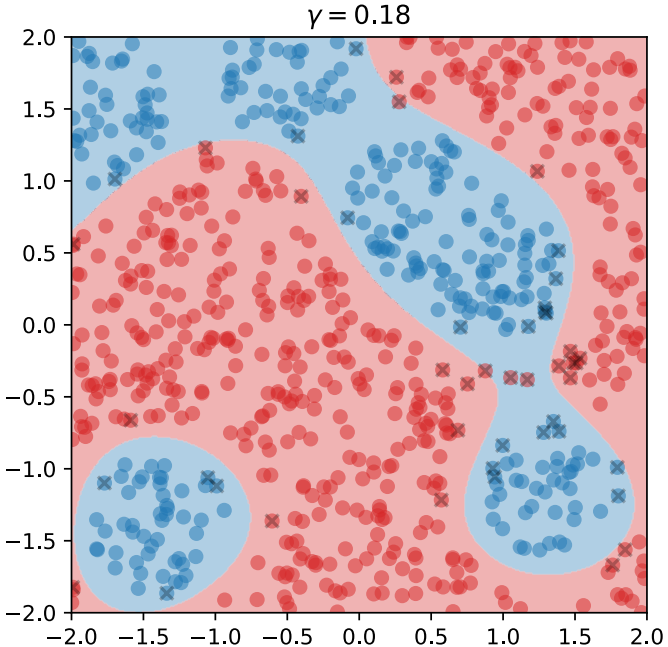
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0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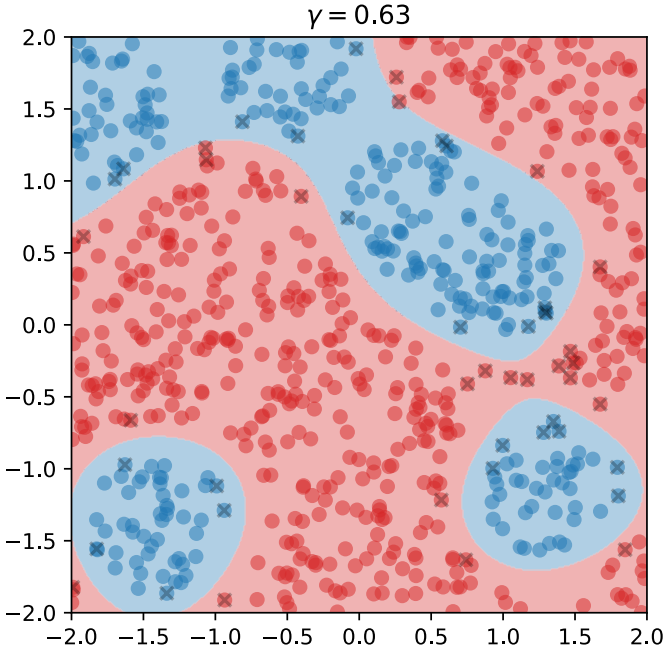
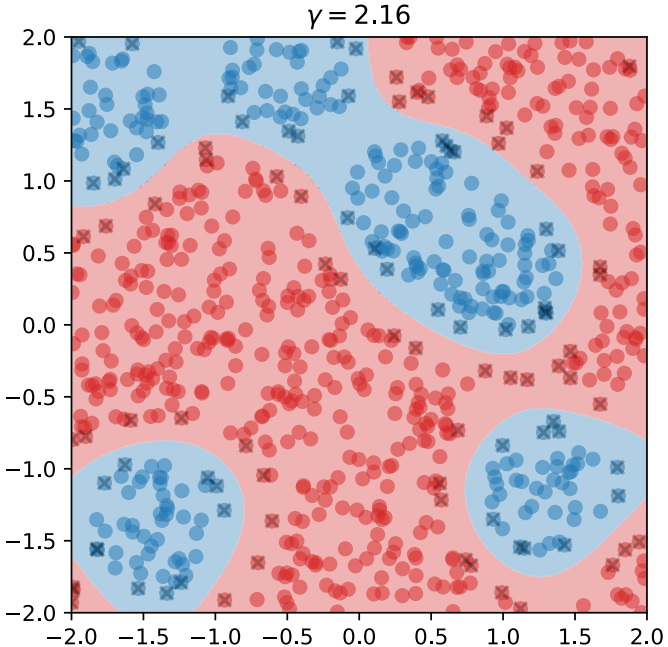
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0


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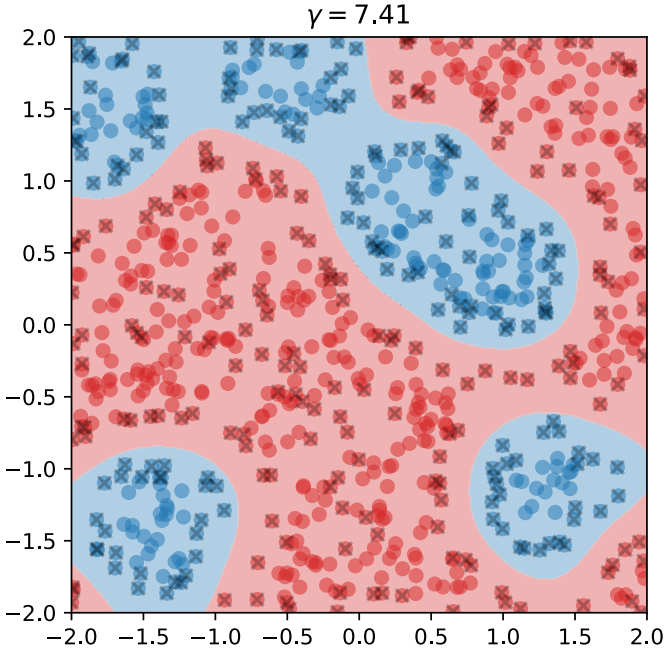
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0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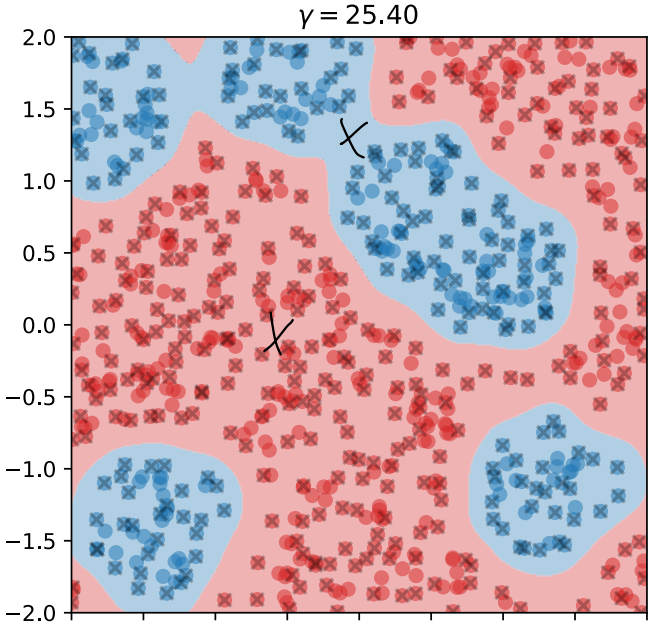
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0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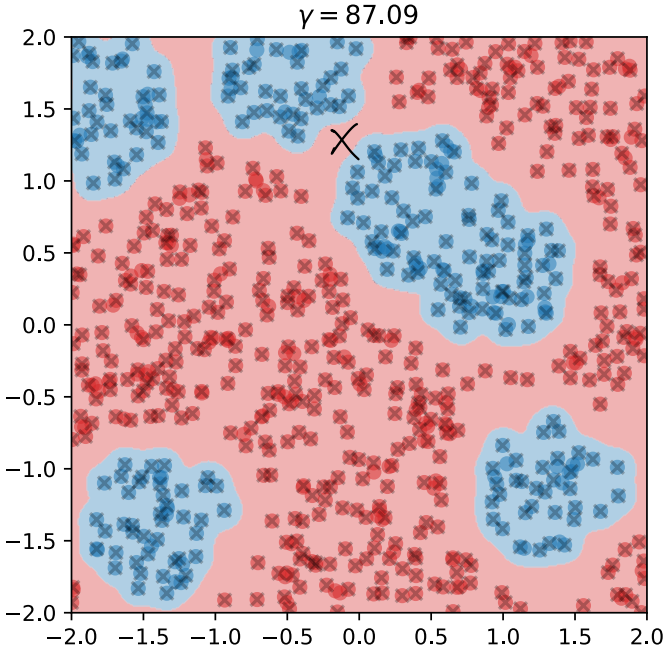
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0


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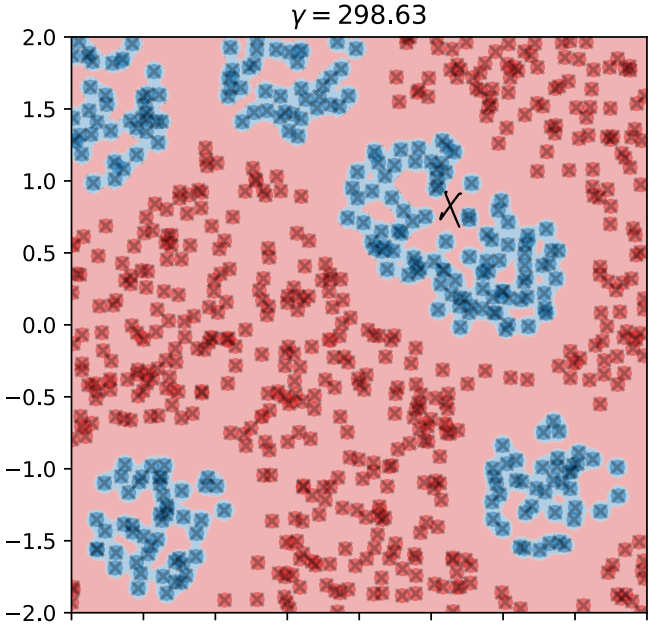
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0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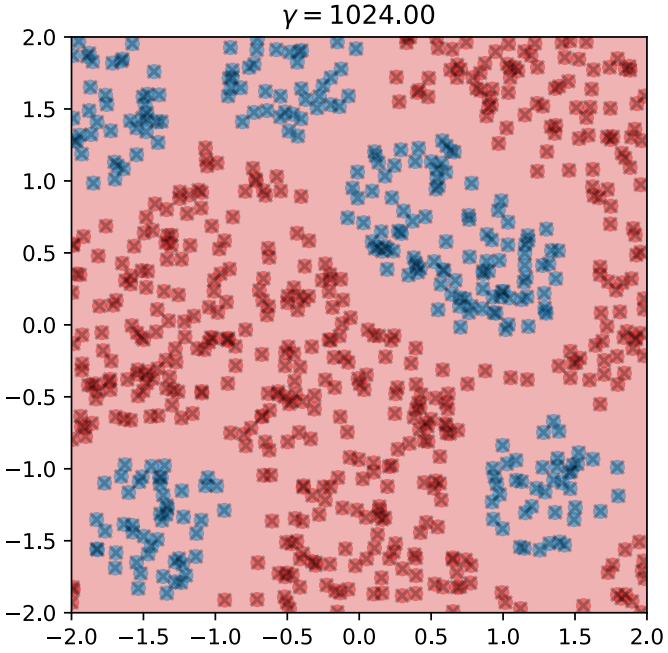
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0
X


$\gamma = 1024.00$
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