DSC 140B
Representation Learning

Lecture 20 | Part 1

Feature Maps

Recap

- Linear prediction functions are limited.
- Idea: transform the data to a new space where prediction is “easier”.
- To do so, we used **basis functions**.

Overview: Feature Mapping

1. Start with data in original space, $\mathbb{R}^d$.

2. Choose some basis functions, $\varphi_1, \varphi_2, \ldots, \varphi_{d'}$

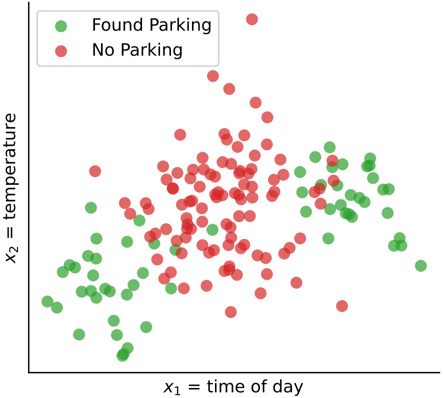
3. Map each data point to **feature space** $\mathbb{R}^{d'}$:

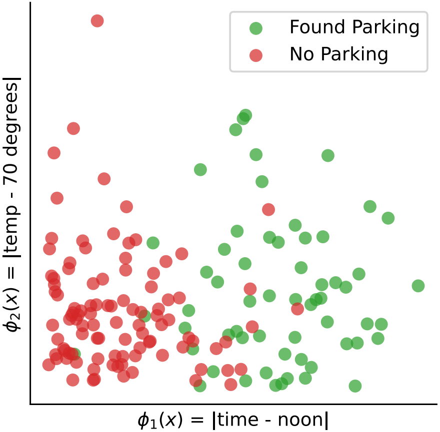
$$\vec{x} \mapsto (\varphi_1(\vec{x}), \varphi_2(\vec{x}), \ldots, \varphi_{d'}(\vec{x}))^t$$

4. Fit linear prediction function in new space:

$$H(\vec{x}) = w_0 + w_1 \varphi_1(\vec{x}) + w_2 \varphi_2(\vec{x})$$

Feature Space, Visualized





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Representation Learning

Lecture 20 | Part 2

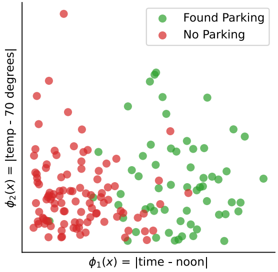
A Tale of Two Spaces

A Tale of Two Spaces

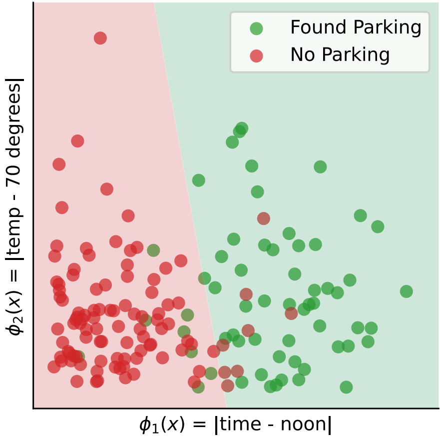
- The **original space**: where the raw data lies.
- The **feature space**: where the data lies after feature mapping $\vec{\varphi}$
- Remember: we fit a linear prediction function in the **feature space**.

Exercise

- In **feature space**, what does the decision boundary look like?
- What does the prediction function surface look like?

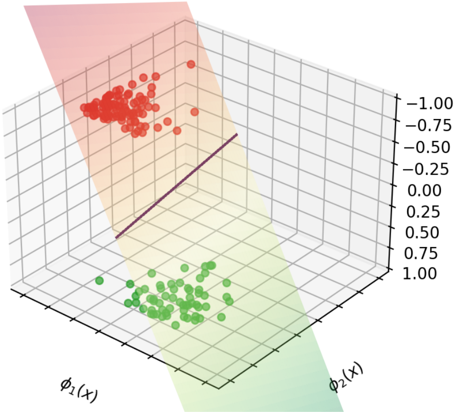


Decision Boundary in Feature Space[2]



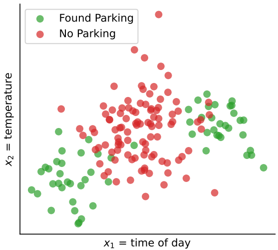
[2]Fit by minimizing square loss

Prediction Surface in Feature Space

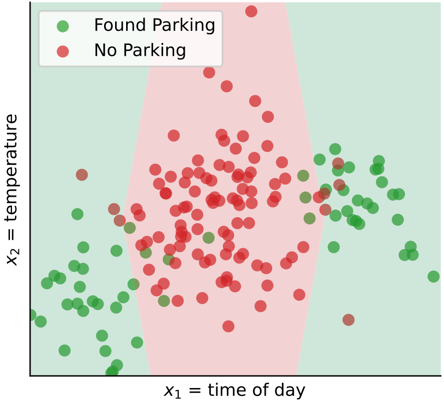


Exercise

- In the **original space**, what does the decision boundary look like?
- What does the prediction function surface look like?

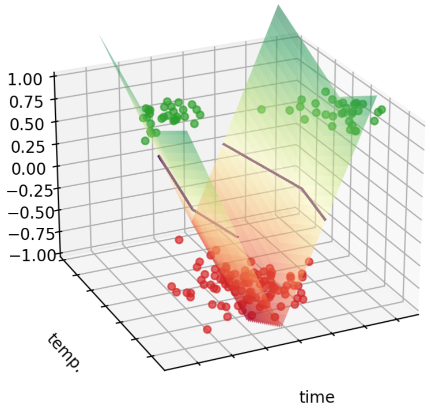


Decision Boundary in Original Space[3]



[3]Fit by minimizing square loss

Prediction Surface in Original Space



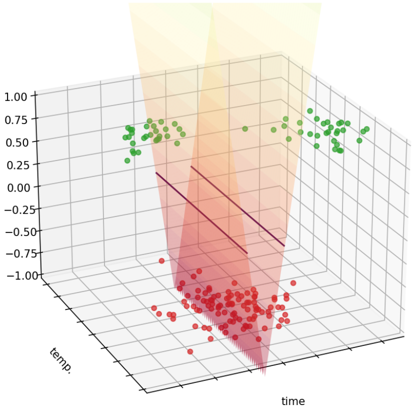
Insight

- H is a sum of basis functions, φ_1 and φ_2.
  - $H(\vec{x}) = w_0 + w_1\varphi_1(\vec{x}) + w_2\varphi_2(\vec{x})$

- The prediction surface is a sum of other surfaces.

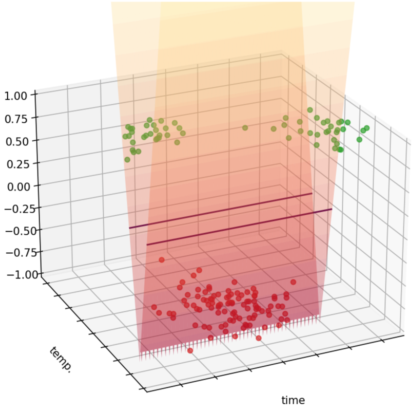
- Each basis function is a “building block”.

Visualizing the Basis Function φ_1



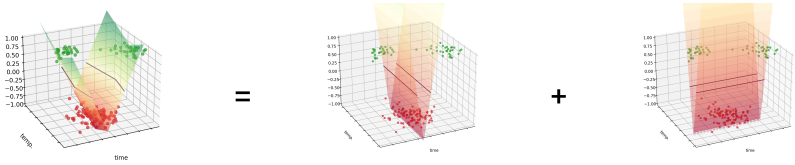
- $w_0 + w_1 |x_1 - \text{noon}|$

Visualizing the Basis Function φ_2

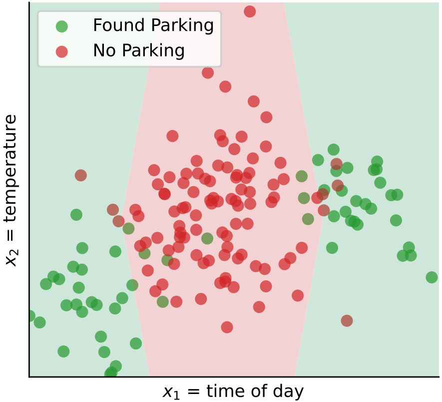


- $w_0 + w_2 |x_2 - 72^{\circ}|$

Visualizing the Prediction Surface



View: Function Approximation



- Find a function that is ≈ 1 near green points and ≈ −1 near red points.

What’s Wrong?

- We’ve discovered how to learn non-linear patterns using linear prediction functions.
  - Use non-linear basis functions to map to a feature space.

- Something should bug you, though...

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Representation Learning

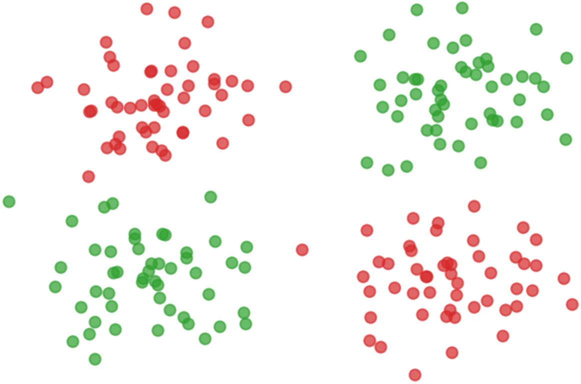
Lecture 20 | Part 3

Radial Basis Functions

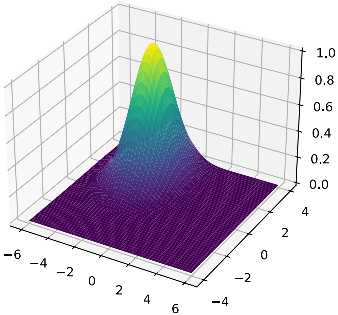
Generic Basis Functions

- The basis functions we used before were engineered using domain knowledge.
- They were specific to the problem at hand.
- **Very manual process!**
- **Now:** features that work for many problems.

Example



Gaussian Basis Functions



- A common choice: **Gaussian** basis functions:

$$\varphi(\vec{x}; \vec{\mu}, \sigma) = e^{-\|\vec{x}-\vec{\mu}\|^2/\sigma^2}$$

- $\vec{\mu}$ is the center.
- σ controls the "width"

Gaussian Basis Function

- If $\vec{x}$ is close to $\vec{\mu}$, $\varphi(\vec{x}; \vec{\mu}, \sigma)$ is large.
- If $\vec{x}$ is far from $\vec{\mu}$, $\varphi(\vec{x}; \vec{\mu}, \sigma)$ is small.
- Intuition: φ measures how "similar" $\vec{x}$ is to $\vec{\mu}$.
  - Assumes that "similar" objects have close feature vectors.

New Representation

- Pick number of new features, d'.
- Pick centers for Gaussians $\vec{\mu}^{(1)}, \ldots, \vec{\mu}^{(2)}, ..., \vec{\mu}^{(d')}$
- Pick widths: $\sigma_1, \sigma_2, \ldots, \sigma_{d'}$ (usually all the same)
- Define ith basis function:

$$\varphi_i(\vec{x}) = e^{-\|\vec{x}-\vec{\mu}^{(i)}\|^2/\sigma_i^2}$$

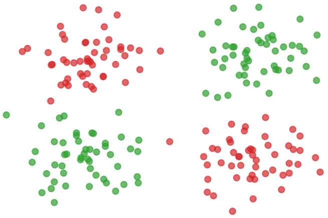
New Representation

- For any feature vector $\vec{x} \in \mathbb{R}^d$, map to vector $\vec{\varphi}(\vec{x}) \in \mathbb{R}^{d'}$.
  - φ_1: "similarity" of $\vec{x}$ to $\vec{\mu}^{(1)}$
  - φ_2: "similarity" of $\vec{x}$ to $\vec{\mu}^{(2)}$
  - ...
  - $\varphi_{d'}$: "similarity" of $\vec{x}$ to $\vec{\mu}^{(d')}$

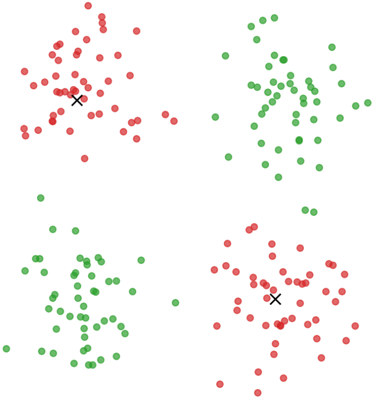
- Train linear classifier in this new representation.
  - E.g., by minimizing expected square loss.

Exercise

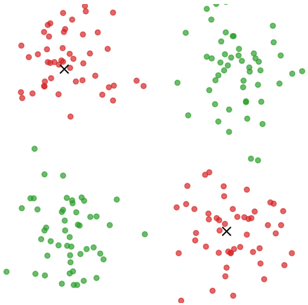
How many Gaussian basis functions would you use, and where would you place them to create a new representation for this data?

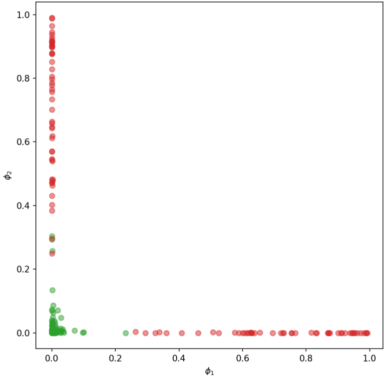


Placement



Feature Space





Prediction Function

- $H(\vec{x})$ is a sum of Gaussians:

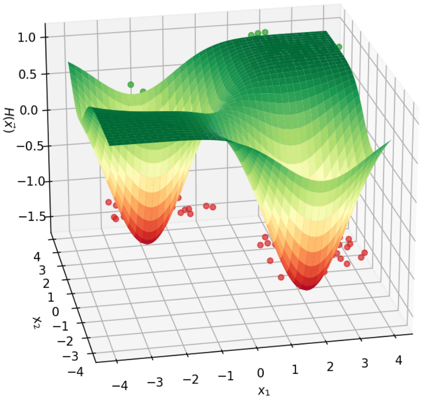
$$\begin{aligned} H(\vec{x}) &= w_0 + w_1 \varphi_1(\vec{x}) + w_2 \varphi_2(\vec{x}) + \ldots \\ &= w_0 + w_1 e^{-\|\vec{x}-\vec{\mu}_1\|^2/\sigma^2} + w_2 e^{-\|\vec{x}-\vec{\mu}_2\|^2/\sigma^2} + \ldots \end{aligned}$$

Exercise

What does the surface of the prediction function look like?

Hint: what does the sum of 1-d Gaussians look like?

Prediction Function Surface

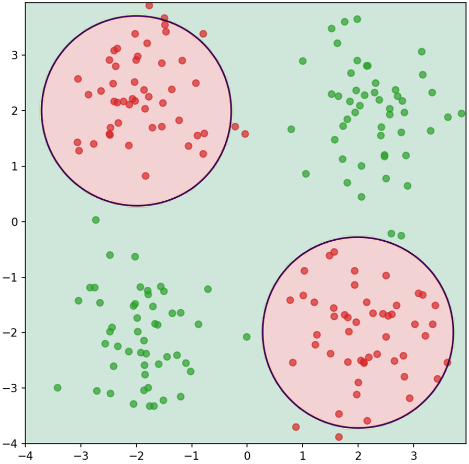


$$H(\vec{x}) = w_0 + w_1 e^{-\|\vec{x}-\vec{\mu}_1\|^2/\sigma^2} + w_2 e^{-\|\vec{x}-\vec{\mu}_2\|^2/\sigma^2}$$

An Interpretation

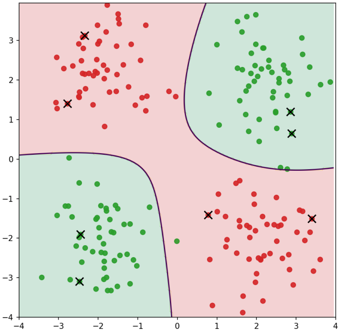
- Basis function φ_i makes a "bump" in surface of H
- w_i adjusts the "prominance" of this bump

Decision Boundary

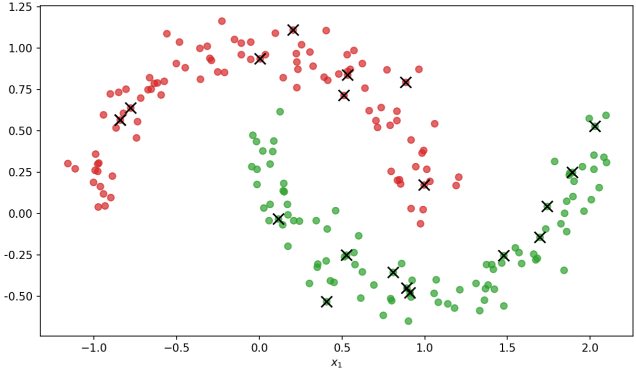


More Features

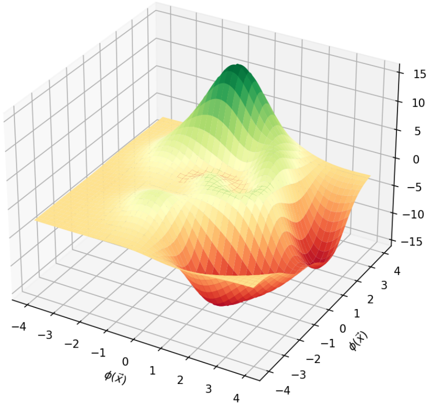
- By increasing number of basis functions, we can make more complex decision surfaces.



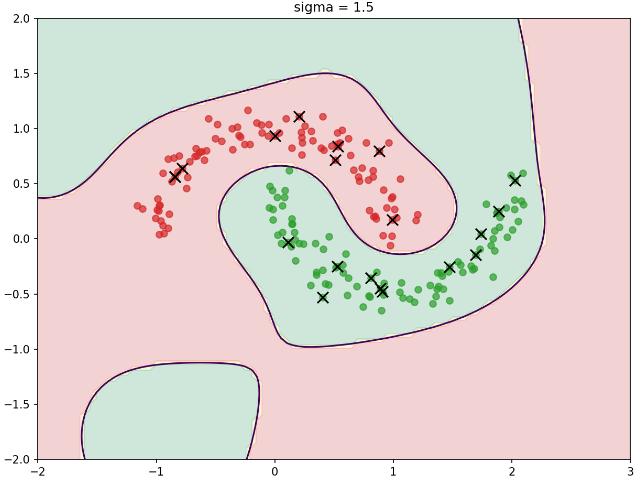
Another Example



Prediction Surface



Decision Boundary



Radial Basis Functions

- Gaussians are examples of **radial basis functions**.
- Each basis function has a **center**, $\vec{c}$.
- Value depends only on distance from center:

$$\varphi(\vec{x}; \vec{c}) = f(\|\vec{x} - \vec{c}\|)$$

Another Radial Basis Function

- **Multiquadric**: $\varphi(\vec{x};\vec{c}) = \sqrt{\sigma^2 + \|\vec{x} - \vec{c}\|}/\sigma$

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Representation Learning

Lecture 20 | Part 4

Radial Basis Function Networks

Recap

1. Choose basis functions, $\varphi_1, \dots, \varphi_{d'}$

2. Transform data to new representation:

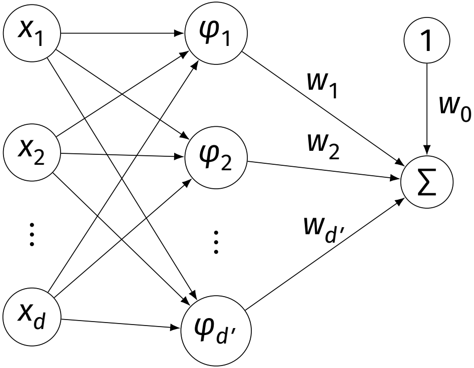
$$\vec{x} \mapsto (\varphi_1(\vec{x}), \varphi_2(\vec{x}), \dots, \varphi_{d'}(\vec{x}))^T$$

3. Train a linear classifier in this new space:

$$H(\vec{x}) = w_0 + w_1 \varphi_1(\vec{x}) + w_2 \varphi_2(\vec{x}) + \dots + w_{d'} \varphi_{d'}(\vec{x})$$

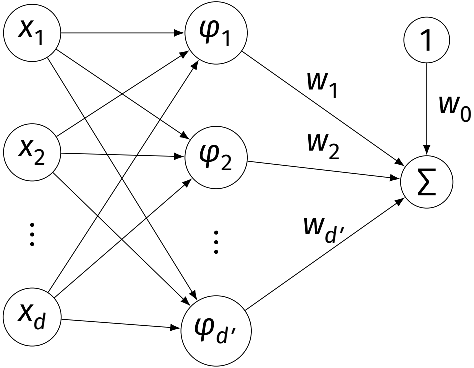
The Model

- The φ are **basis functions**.



$$H(\vec{x}) = w_0 + w_1\varphi_1(\vec{x}) + w_2\varphi_2(\vec{x})$$

Radial Basis Function Networks



If the basis functions are **radial basis functions**, we call this a **radial basis function (RBF) network**.

Training

- An RBF network has these parameters:
  - the parameters of each individual basis function:
    - $\vec{\mu}_i$ (the center)
    - possibly others (e.g., σ)
  - w_i: the weights associated to each “new” feature

- How do we choose the parameters?

First Idea

- We can include all parameters in one big cost function, optimize.
- The cost function will generally be **complicated, non-convex** and thus **hard to optimize**.

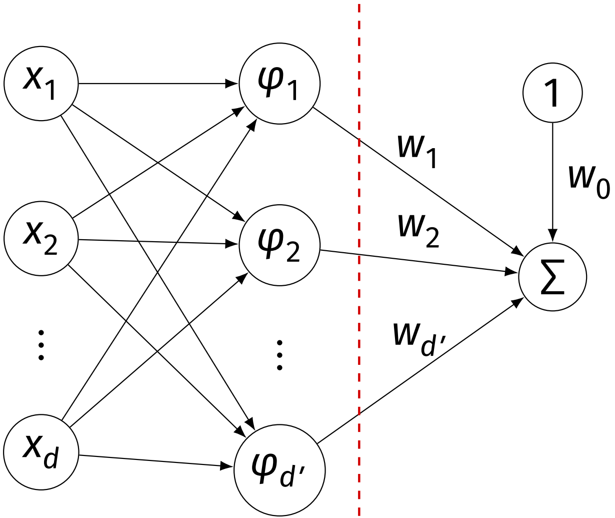
Another Idea

- Break the process into two steps:

1. Find the parameters of the RBFs *somehow*.
    - Some optimization procedure, clustering, randomly, ...
2. Having fixed those parameters, optimize the w's.

- **Linear; easier to optimize.**

Training



x_1
x_2
$\vdots$
x_d
φ_1
φ_2
$\vdots$
$\varphi_{d'}$
w_1
w_2
$w_{d'}$
1
w_0
Σ

Training an RBF Network

1. Choose the form of the RBF, how many.
   - E.g., k Gaussian RBFs, $\varphi_1, \ldots, \varphi_k$.

2. Pick the parameters of the RBFs *somehow*.

3. Create new data set by mapping
   $\vec{x} \mapsto (\varphi_1(\vec{x}), \ldots, \varphi_k(\vec{x}))^T$

4. Train a linear predictor H_f on new data set
   - That is, in feature space.

Making Predictions

1. Given a point $\vec{x}$, map it to feature space: $\vec{x} \mapsto (\varphi_1(\vec{x}), \ldots, \varphi_k(\vec{x}))^T$

2. Evaluate the trained linear predictor H_f in feature space

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Representation Learning

Lecture 20 | Part 5

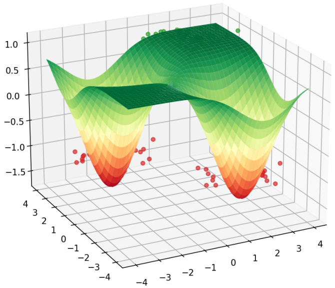
Choosing RBF Locations

Recap

- We map data to a new representation by first choosing **basis functions**.
- Radial Basis Functions (RBFs), such as Gaussians, are a popular choice.
- Requires choosing **center** for each basis function.

Prediction Function

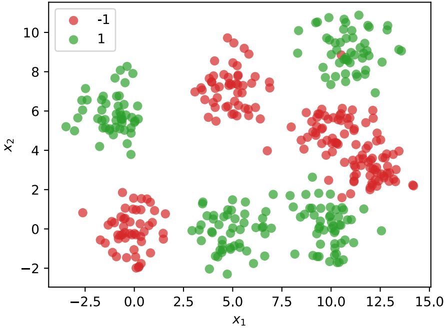
- Our prediction function H is a surface that is made up of Gaussian "bumps".



$$H(\vec{x}) = w_0 + w_1 e^{-\|\vec{x}-\vec{\mu}_1\|^2/\sigma^2} + w_2 e^{-\|\vec{x}-\vec{\mu}_2\|^2/\sigma^2}$$

Choosing Centers

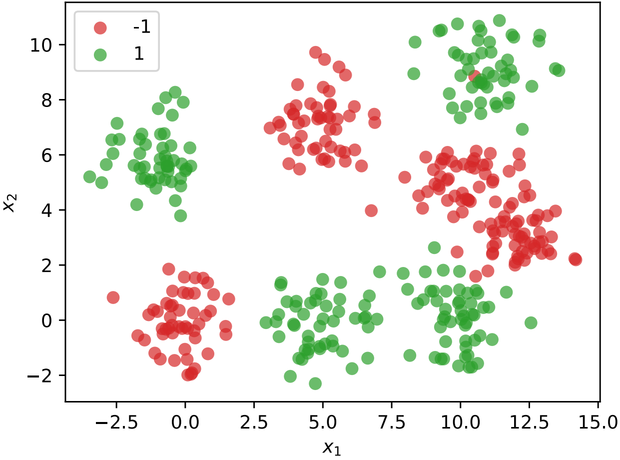
- Place the centers where the value of the prediction function should be controlled.
- Intuitively: place centers where the data is.



Approaches

1. Every data point as a center
2. Randomly choose centers
3. Clustering

Approach #1: Every Data Point as a Center



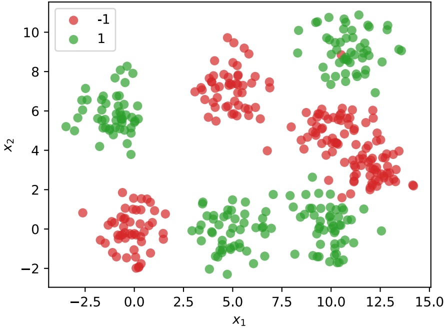
Dimensionality

- We'll have n basis functions – one for each point.
- That means we'll have n features.
- Each feature vector $\vec{\phi}(\vec{x}) \in \mathbb{R}^n$.

$$\vec{\phi}(\vec{x}) = (\phi_1(\vec{x}), \phi_2(\vec{x}), \ldots, \phi_n(\vec{x}))^T$$

Problems

- This causes problems.
- First: more likely to **overfit**.
- Second: computationally expensive

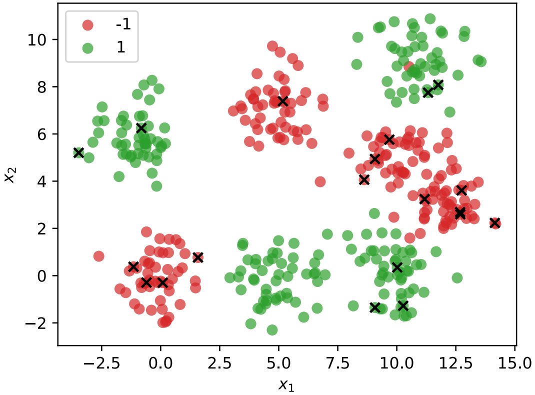


Computational Cost

- Suppose feature matrix X is $n \times d$
  - n points in d dimensions
- Time complexity of solving $X^T X \vec{w} = X^T \vec{y}$ is $\Theta(nd^2)$
- Usually $d \ll n$. But if $d = n$, this is $\Theta(n^3)$.
- Not great! If $n \approx 10,000$, then takes > 10 minutes.

Approach #2: A Random Sample

- Idea: randomly choose k data points as centers.



Problem

- May undersample/oversample a region.
- More advanced sampling approaches exist.

Approach #3: Clustering

- Group data points into **clusters**.
- Cluster centers are good places for RBFs.
- For example, use k-means clustering to pick k centers.