

DSC 140A

Probabilistic Modeling & Machine Learning

Lecture 8 | Part 1

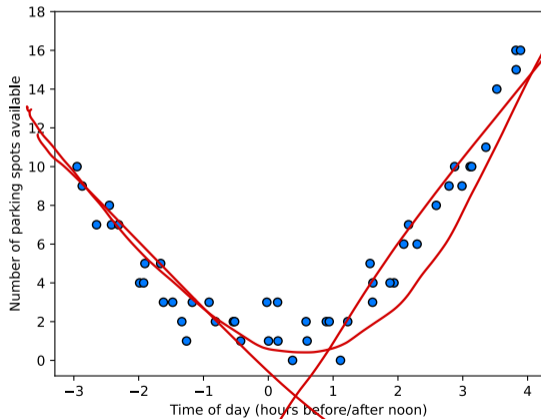
Feature Maps

Problem

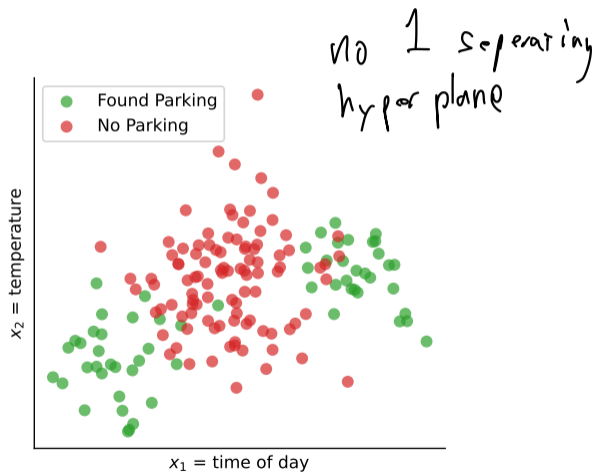
- ▶ Patterns in real world data are often **non-linear**.
- ▶ But we only know how to train **linear predictors**.

$$H(\underline{x}) = \underline{w} \cdot \text{aug}(\underline{x})$$
$$= w_0 + w_1 x_1 + w_2 x_2 + \dots$$

Example: Regression



Example: Classification



Today

- ▶ **Solution:** non-linear **feature maps**.
- ▶ Will allow us to:
 - ▶ fit complex, non-linear patterns;
 - ▶ while still using linear models (least squares, SVM, ...)
- ▶ But we'll need to be careful about **overfitting**.

Feature Map

"data features"

"modeling features"

- ▶ A **feature map** $\phi : \mathbb{R}^d \rightarrow \mathbb{R}^k$ is a function that takes in a d -dimensional vector and outputs a k -dimensional feature vector.
- ▶ I.e., it creates new features from the old ones.
 - ▶ Maybe in a non-linear way.

Example

- Define $\vec{\phi} : \mathbb{R}^2 \rightarrow \mathbb{R}^5$ as:

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

Handwritten annotations:
- "linear" written above x_1 and x_2 .
- "nonlinear" written above $x_1^2, x_2^2, x_1 x_2$ with a checkmark.
- Circles around x_1 and x_2 in the input, and around x_1 and x_2 in the output.
- A bracket under the last three terms of the output vector.

- If $\vec{x} = (2, 3)^T$, then:

$$\begin{aligned}\vec{\phi}(\vec{x}) &= (2, 3, 2^2, 3^2, 2 \times 3)^T \\ &= (2, 3, 4, 9, 6)^T\end{aligned}$$

Basis Functions

- ▶ A **basis function** is a function $\phi_i : \mathbb{R}^d \rightarrow \mathbb{R}$.
- ▶ It takes in an old feature vector and outputs a single new feature.
- ▶ We can think of a feature map $\vec{\phi} : \mathbb{R}^d \rightarrow \mathbb{R}^k$ as being made up of k basis functions.

$$\vec{\phi}(\vec{x}) = (\underbrace{\phi_1(\vec{x})}_{\text{wavy}}, \underbrace{\phi_2(\vec{x})}_{\text{wavy}}, \dots, \underbrace{\phi_k(\vec{x})}_{\text{wavy}})^T$$

Example

- ▶ Let $\vec{\phi} : \mathbb{R}^2 \rightarrow \mathbb{R}^5$ be defined as:

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

- ▶ The corresponding basis functions are:

$$\longrightarrow \phi_1(x_1, x_2) = x_1$$

$$\longleftarrow \phi_2(x_1, x_2) = x_2$$

$$\longrightarrow \phi_3(x_1, x_2) = x_1^2$$

$$\longrightarrow \phi_4(x_1, x_2) = x_2^2$$

$$\longrightarrow \phi_5(x_1, x_2) = x_1 x_2$$

A New Data Set

- ▶ Say we have a training set with d features:

$$(\vec{x}^{(1)}, y_1), \dots, (\vec{x}^{(n)}, y_n)$$

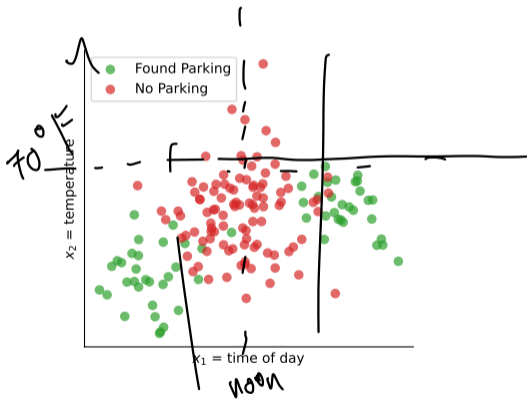
- ▶ A feature map $\vec{\phi} : \mathbb{R}^d \rightarrow \mathbb{R}^k$ gives us a **new** training set with k features:

$$(\vec{\phi}(\vec{x}^{(1)}), y_1), \dots, (\vec{\phi}(\vec{x}^{(n)}), y_n)$$

Why?

- ▶ A (good) feature map can turn **non-linear** patterns in the old data into **linear patterns** in the new data.

Example: Parking Classification

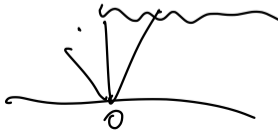


▶ Original features:

$$\vec{x} = (\text{time}, \text{temp.})^T$$

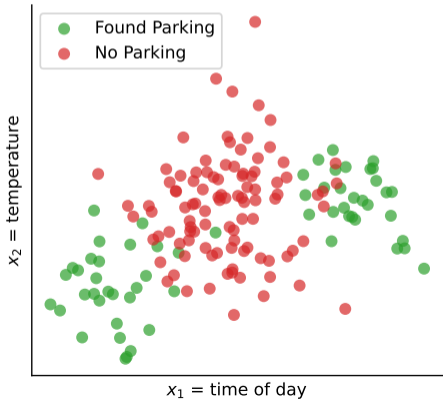
▶ Feature map:

$$\vec{\phi}(\vec{x}) = (|\text{time} - \text{Noon}|, |\text{temp.} - 70|)^T$$

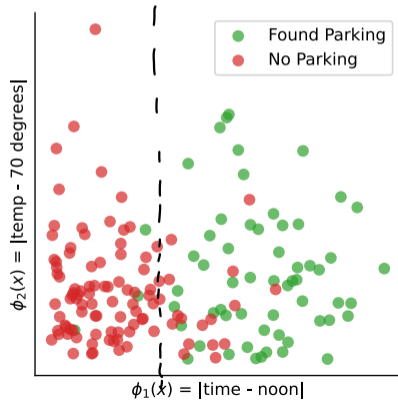


Example: Parking Classification

Input Space



Feature Space



Exercise

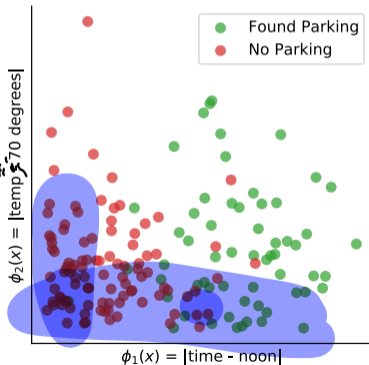
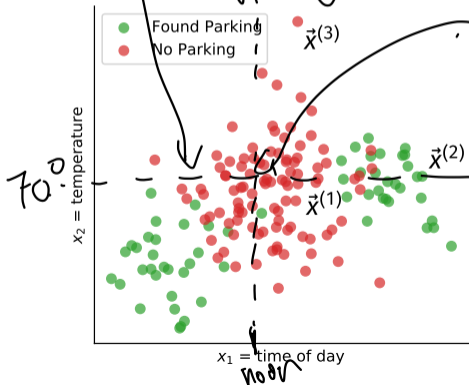
(Approximately) where do $\vec{x}^{(1)}$, $\vec{x}^{(2)}$, and $\vec{x}^{(3)}$ get mapped to in feature space?

new
coordinate
axes

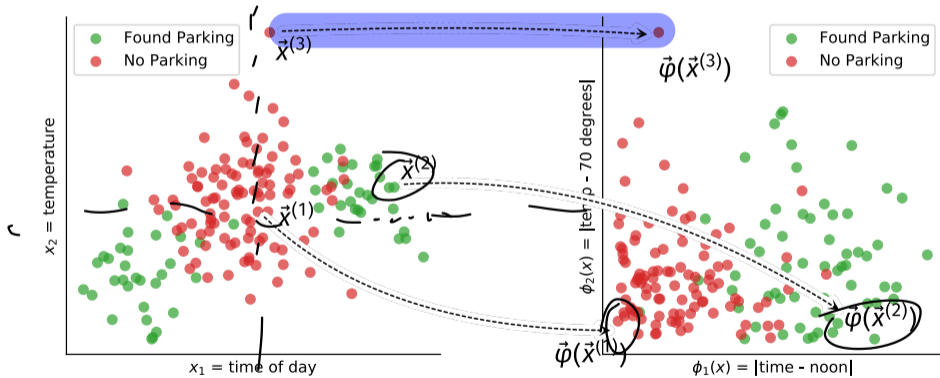
reflection

new
origin

reflection



Solution



Idea

- ▶ Feature maps turned **non-linear** patterns in input space into **linear** patterns in feature space.
- ▶ **Idea:** train a linear model in feature space.

Procedure: Learning with Feature Maps

- ▶ First, pick a feature map $\vec{\phi} : \mathbb{R}^d \rightarrow \mathbb{R}^k$.
(could be identity)
- ▶ **To train:**
 - ▶ Given training set $(\vec{x}^{(1)}, y_1), \dots, (\vec{x}^{(n)}, y_n)$. $\underline{\phi(x)} = \underline{x}$
 - 1. Map each $\vec{x}^{(i)}$ to feature space, creating a new data set $(\vec{\phi}(\vec{x}^{(1)}), y_1), \dots, (\vec{\phi}(\vec{x}^{(n)}), y_n)$.
 - 2. Train linear model (least squares, SVM, perceptron...) on the new data in feature space to get \vec{w}^* .
- ▶ **To predict:** *still need to select loss*
 - ▶ Given new input \vec{x} .
 - 1. Map \vec{x} to feature space: $\vec{\phi}(\vec{x})$.
 - 2. Predict $H(\vec{x}; \vec{w}^*) = \vec{w}^* \cdot \text{Aug}(\vec{\phi}(\vec{x}))$.

new step

$$d = 2 \quad k = 5$$

Exercise

Suppose the original feature vectors are in \mathbb{R}^2 and the feature map is defined as

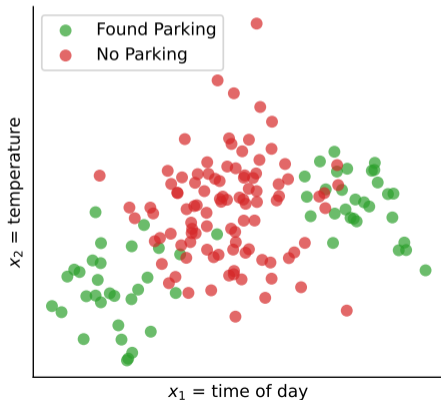
$$\vec{\phi}(x_1, x_2) = (x_1, x_2, x_1^2, x_2^2, x_1 x_2)^T$$

We train an SVM in feature space. What is the dimensionality of \vec{w}^* ? = 6

$$H(x) = w_0 + w_1 \phi_1(x) + w_2 \phi_2(x) + \dots$$

Example: Least Squares

- ▶ Let's train a least squares classifier using a feature map.



Step 1: Pick a Feature Map

- ▶ In the input space, we have features (x_1, x_2) .

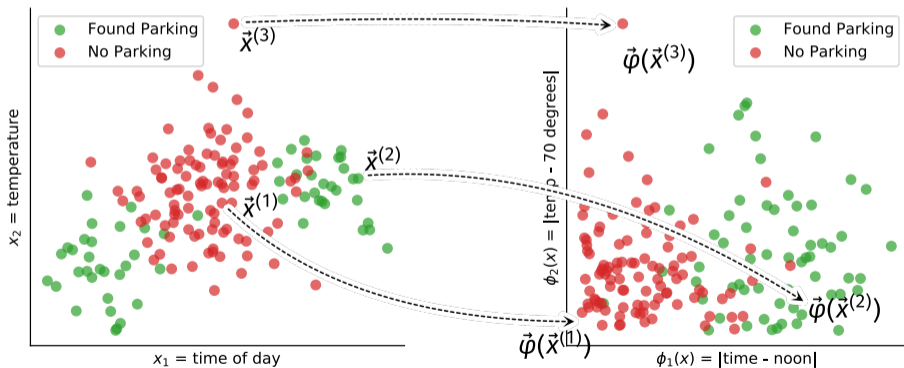
$$x_1 = \text{time}, \quad x_2 = \text{temperature}.$$

- ▶ We'll use the same feature map as before:

$$\vec{\phi}(x_1, x_2) = (|x_1 - 12|, |x_2 - 70|)^T$$

Step 2(a): Map to Feature Space

- ▶ Map every data point to feature space.



Step 2(b): Train in Feature Space

- ▶ Recall: we train a least squares classifier in **input space** by computing:

$$R = \frac{1}{n} \sum_{i=1}^n (y_i - \underline{w} \cdot \text{aug}(\vec{x}_i))^2 \quad \vec{w}^* = (\vec{X}^T \vec{X})^{-1} \vec{X}^T \vec{y}$$
$$= \frac{1}{n} \|\vec{y} - \underline{X} \underline{w}\|_2^2$$

- ▶ Here, X is the (augmented) ($n \times d$) design matrix:

$$X = \begin{pmatrix} \text{Aug}(\vec{x}^{(1)})^T \longrightarrow \\ \text{Aug}(\vec{x}^{(2)})^T \longrightarrow \\ \vdots \\ \text{Aug}(\vec{x}^{(n)})^T \longrightarrow \end{pmatrix} = \begin{pmatrix} 1 & x_1^{(1)} & x_2^{(1)} \\ 1 & x_1^{(2)} & x_2^{(2)} \\ \vdots & \vdots & \vdots \\ 1 & x_1^{(n)} & x_2^{(n)} \end{pmatrix}$$

Step 2(b): Train in Feature Space

$$\phi_0(x) = 1$$

- ▶ In feature space, our feature vectors are

$$\vec{\phi}(\vec{x}^{(1)}), \dots, \vec{\phi}(\vec{x}^{(n)}). \quad \underline{\phi} = (\phi_0(x), \phi_1(x), \dots)$$

phi

- ▶ So the design matrix becomes the $(n \times \overset{k+1}{\cancel{k}})$ matrix:

$$\Phi = \begin{pmatrix} \vec{\phi}(\vec{x}^{(1)})^T \longrightarrow \\ \vec{\phi}(\vec{x}^{(2)})^T \longrightarrow \\ \vdots \\ \vec{\phi}(\vec{x}^{(n)})^T \longrightarrow \end{pmatrix} = \begin{pmatrix} 1 & |x_1^{(1)} - 12| & |x_2^{(1)} - 70| \\ 1 & |x_1^{(2)} - 12| & |x_2^{(2)} - 70| \\ \vdots & \vdots & \vdots \\ 1 & |x_1^{(n)} - 12| & |x_2^{(n)} - 70| \end{pmatrix}$$

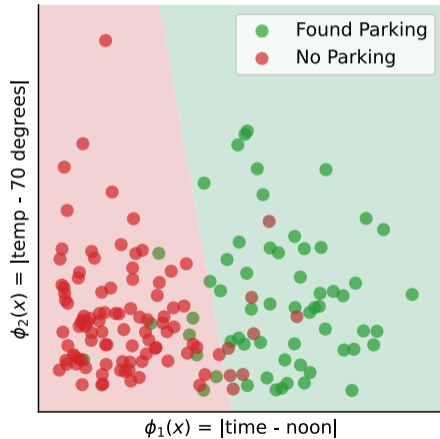
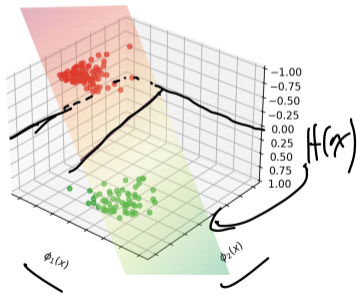
Step 2(b): Train in Feature Space

- ▶ The least squares solution in feature space is:

$$\vec{w}^* = (\Phi^T \Phi)^{-1} \Phi^T \vec{y}$$

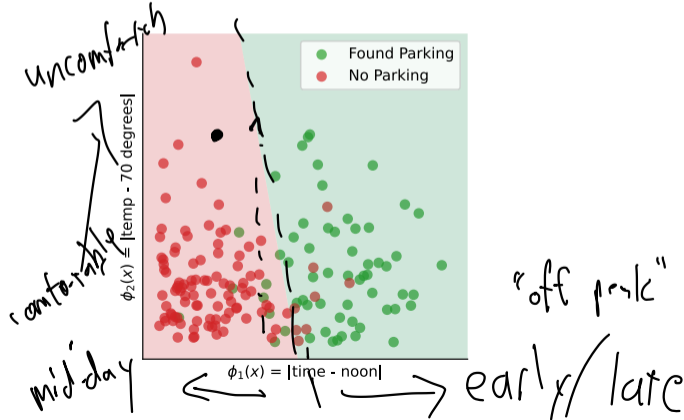
"Phi"

Solution in Feature Space



Step 3: Predict

- ▶ Given a new example \vec{x} in input space:
 1. Map \vec{x} to feature space: $\vec{\phi}(\vec{x})$.
 2. Predict $\text{sign}(\vec{w}^* \cdot \text{Aug}(\vec{\phi}(\vec{x})))$.



$$\phi_1(\mathbf{x}) = |x_1 - 12| = |10 - 12| = 2$$
$$\phi_2(\mathbf{x}) = |x_2 - 70| = |65 - 70| = 5$$

$$H(\mathbf{x}) = w_0 + w_1 \phi_1(\mathbf{x}) + w_2 \phi_2(\mathbf{x})$$
$$= 3 + (-1) \cdot 2 + 2 \cdot 5 = 3 - 2 + 10 = 11 > 0$$

\Rightarrow Yes!

Exercise

Let $\vec{\phi}(x_1, x_2) = (|x_1 - 12|, |x_2 - 70|)^T$. Suppose we train a least squares classifier in feature space and find $\vec{w}^* = (3, -1, 2)^T \leftarrow (w_0, w_1, w_2)$

Given a new point $\vec{x} = (10, 65)^T$ in input space, what is the prediction, $H(\vec{x})$?

The Prediction Function(s)

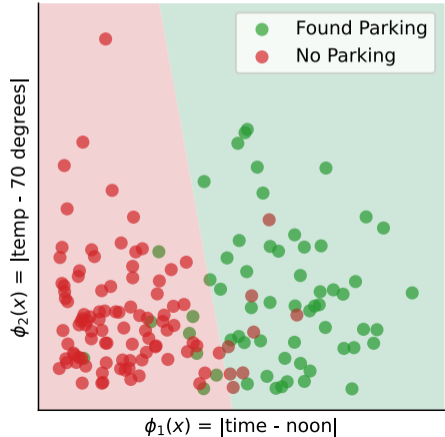
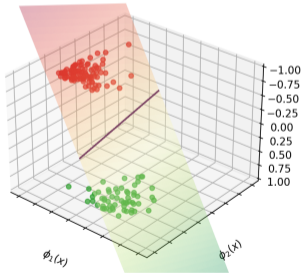
- ▶ There are, in a sense, **two** prediction functions to consider.
- ▶ First, the prediction function in feature space:

$$\begin{aligned}H_{\phi}(\vec{z}) &= \vec{w} \cdot \text{Aug}(\vec{z}) \\ &= w_0 + w_1 z_1 + w_2 z_2 + \dots + w_k z_k\end{aligned}$$

- ▶ This function takes in a vector \vec{z} that is already in feature space. \Rightarrow linear in " \vec{z} "

H_ϕ in Feature Space

$$H_\phi(\vec{Z}) = W_0 + W_1 Z_1 + W_2 Z_2$$



The Prediction Function

- ▶ There is also the prediction function $H(\vec{x})$ that takes in vectors in input space.

$$\begin{aligned}H(\vec{x}) &= H_{\phi}(\vec{\phi}(\vec{x})) \\ &= \vec{w} \cdot \text{Aug}(\vec{\phi}(\vec{x})) \\ &= w_0 + w_1\phi_1(\vec{x}) + w_2\phi_2(\vec{x}) + \dots + w_k\phi_k(\vec{x})\end{aligned}$$

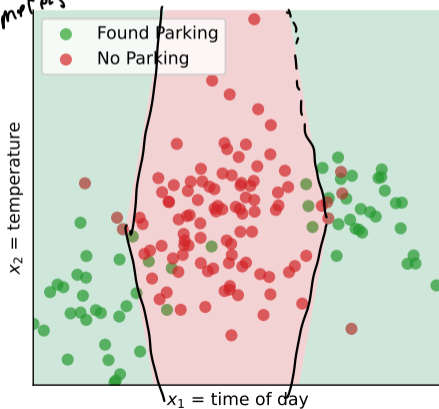
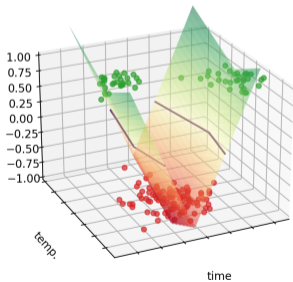
- ▶ When plotted, this function will look **non-linear**.

in \underline{x}

H in Input Space

$$H(\vec{x}) = w_0 + w_1 |x_1 - 12| + w_2 |x_2 - 70|$$

"linear in parameters"



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Probabilistic Modeling & Machine Learning

Lecture 8 | Part 2

Example: Non-Linear Regression

Non-Linear Regression

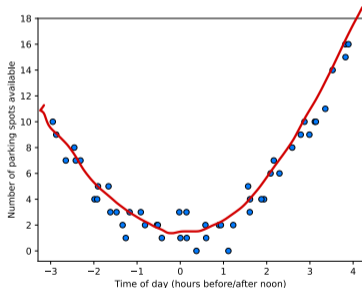
- ▶ With a feature map $\vec{\phi}(\vec{x}) = (\phi_1(\vec{x}), \dots, \phi_k(\vec{x}))^T$, our prediction function becomes:

$$H(\vec{x}) = w_0 + w_1\phi_1(\vec{x}) + w_2\phi_2(\vec{x}) + \dots + w_k\phi_k(\vec{x})$$

- ▶ In other words, we're not constrained to only fitting straight lines/planes:

$$H(x) = w_0 + w_1x$$

Example: Parking Regression



- ▶ Data looks like a quadratic function.
- ▶ Idea: fit a function of the form:

$$H(t) = w_0 + w_1 t + w_2 t^2$$

$$x \Rightarrow \begin{aligned} \phi_0(x) &= 1 \\ \phi_1(x) &= x \\ \phi_2(x) &= x^2 \end{aligned}$$

Exercise

Suppose we wish to fit a function of the form $H(t) = w_0 + w_1 t + w_2 t^2$ to the data.

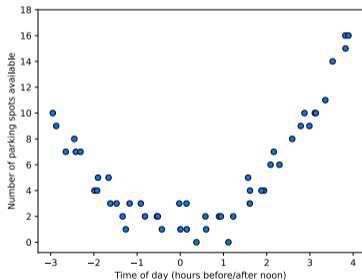
What feature map $\vec{\phi}$ should we use to get this form of prediction function?

Answer

- ▶ Use $\vec{\phi}(t) = (t, t^2)^T$.
- ▶ Then the prediction function is:

$$\begin{aligned} H(t) &= \vec{w} \cdot \text{Aug}(\vec{\phi}(t)) \\ &= (w_0, w_1, w_2) \cdot (1, t, t^2)^T \\ &= w_0 + w_1 t + w_2 t^2 \end{aligned}$$

Example: Parking Regression



- ▶ Original features:

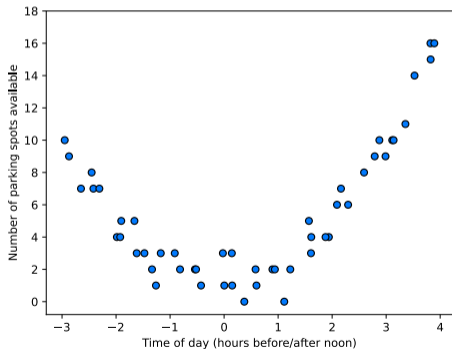
$$\vec{x} = (\text{time})^T$$

- ▶ Feature map:

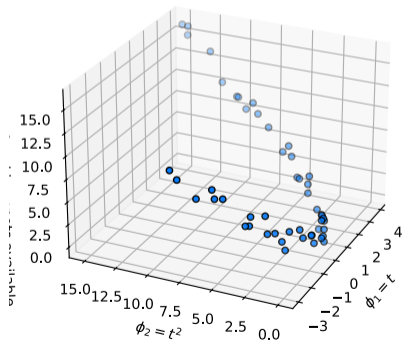
$$\vec{\phi}(\vec{x}) = (\text{time}, \text{time}^2)^T$$

Example: Parking Regression

Input Space



Feature Space



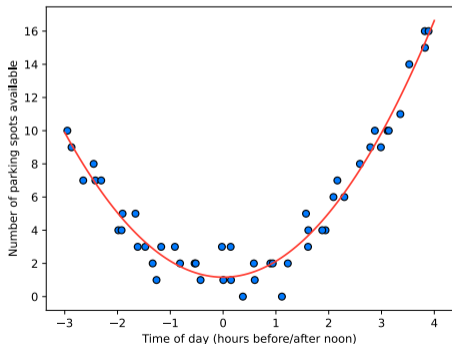
Least Squares

- ▶ After mapping to feature space, we fit a plane with least squares.
- ▶ The design matrix becomes:

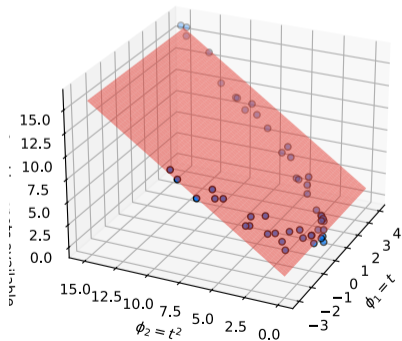
$$\Phi = \begin{pmatrix} \text{Aug}(t^{(1)})^T \longrightarrow \\ \text{Aug}(t^{(2)})^T \longrightarrow \\ \vdots \\ \text{Aug}(t^{(n)})^T \longrightarrow \end{pmatrix} = \begin{pmatrix} 1 & t^{(1)} & (t^{(1)})^2 \\ 1 & t^{(2)} & (t^{(2)})^2 \\ \vdots & \vdots & \vdots \\ 1 & t^{(n)} & (t^{(n)})^2 \end{pmatrix}$$

Example: Parking Regression

Input Space



Feature Space



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Probabilistic Modeling & Machine Learning

Lecture 8 | Part 3

ERM with Feature Maps

Learning with Feature Maps

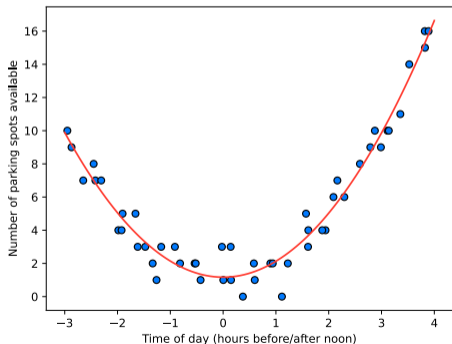
- ▶ We've developed a procedure for fitting non-linear patterns with linear models.
 - ▶ Map to feature space, learn there.
- ▶ Is this the “best” approach?

Empirical Risk Minimization

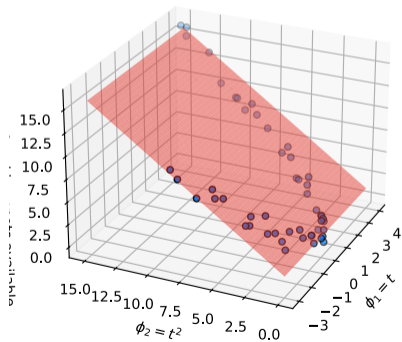
- ▶ Step 1: choose a **hypothesis class**
 - ▶ Functions of the form $H(\vec{x}) = \vec{w} \cdot \text{Aug}(\vec{\phi}(\vec{x}))$.
- ▶ Step 2: choose a **loss function**
 - ▶ Square loss, perceptron loss, hinge loss, etc.
- ▶ Step 3: find H minimizing **empirical risk**
 - ▶ Do we get the same H if we train in feature space?

Example: Parking Regression

Input Space



Feature Space



Yes

- ▶ The H_ϕ that minimizes risk in feature space is the same as the H that minimizes risk in input space.
 - ▶ As long as H is a linear function of the **parameters**.

Argument

- ▶ Take, for example, square loss.
- ▶ The risk is:

$$R(\vec{w}) = \frac{1}{n} \sum_{i=1}^n (y_i - \vec{w} \cdot \text{Aug}(\vec{\phi}(\vec{x}^{(i)})))^2$$

- ▶ Minimizer is $\vec{w}^* = (\Phi^T \Phi)^{-1} \Phi^T \vec{y}$.

In General

- ▶ Assume prediction function is of the form:

$$H(\vec{X}) = w_0 + w_1\phi_1(\vec{X}) + w_2\phi_2(\vec{X}) + \dots + w_k\phi_k(\vec{X})$$

- ▶ To find \vec{w} that minimizes risk:
 - ▶ Map data to feature space;
 - ▶ Train a linear model in feature space.
- ▶ Works for least squares, perceptron, SVM, etc.

Takeaway

- ▶ The “linear” in “linear prediction function” refers to the **parameters**, not the features!
- ▶ We can fit any function of the form:

$$H(x) = w_1\phi_1(x) + w_2\phi_2(x) + \dots + w_k\phi_k(x)$$

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Probabilistic Modeling & Machine Learning

Lecture 8 | Part 4

Gaussian Radial Basis Functions

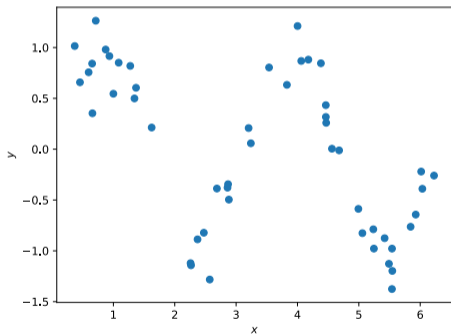
General Basis Functions

- ▶ We can fit any function of the form:

$$H(x) = w_1\phi_1(x) + w_2\phi_2(x) + \dots + w_k\phi_k(x)$$

- ▶ Before: we chose ϕ_j carefully based on the problem.
- ▶ Is there an easier way?
 - ▶ Are there basis functions that work well for many problems?

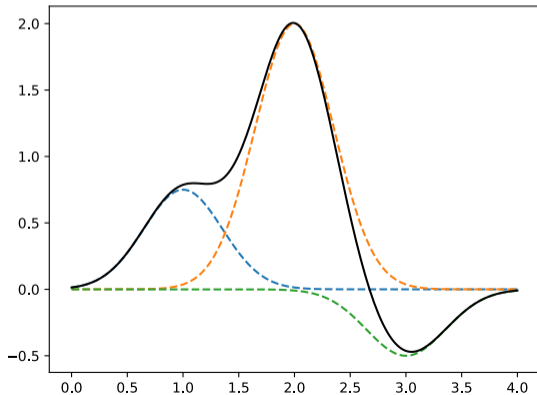
Example



- ▶ Suppose we want to fit a function H to this data.
- ▶ Locally, each part of the curve looks like a “bump”.
- ▶ **Idea:** let H be a sum of bumps.

A Sum of Bumps

$$H(x) = w_1 \text{bump}_1(x) + w_2 \text{bump}_2(x) + w_3 \text{bump}_3(x)$$



Gaussian Basis Functions

- ▶ One way to make a bump: a **Gaussian**

$$\phi_i(x) = \exp\left(-\frac{(x - \mu_i)^2}{\sigma_i^2}\right)$$

- ▶ Must specify¹ **center** μ_i and **width** σ_i for each Gaussian basis function.

¹You pick these; they are not learned!

Exercise

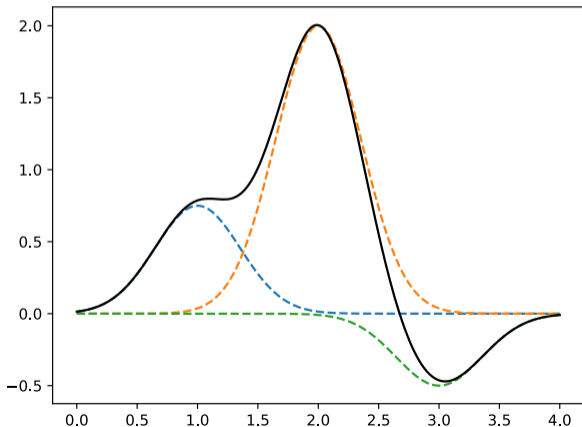
Suppose we have a Gaussian of the form:

$$\phi(x) = \exp\left(-\frac{(x-2)^2}{3}\right)$$

What is the value of $\phi(2)$? What is the value of $\phi(100)$, approximately?

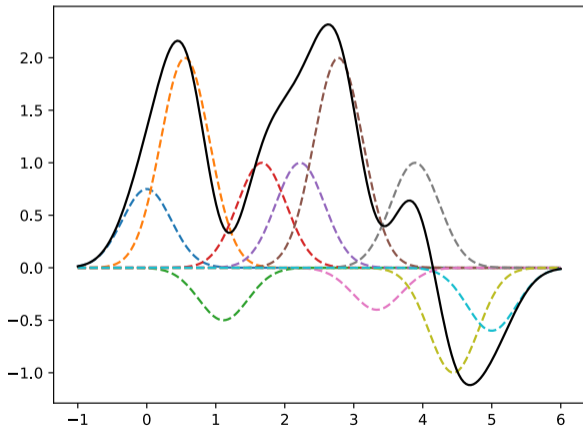
Example: $k = 3$

- ▶ A function of the form: $H(x) = w_1\phi_1(x) + w_2\phi_2(x) + w_3\phi_3(x)$, using 3 Gaussian basis functions.



Example: $k = 10$

- The more basis functions, the more complex H can be.

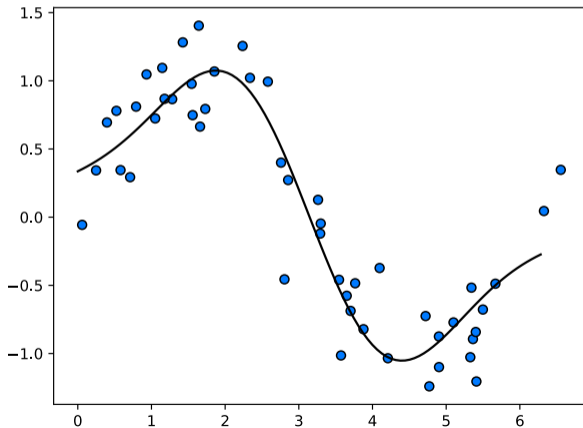


Procedure: Learning with Gaussian Basis Functions

1. Pick number and location of Gaussians.
 - ▶ μ_1, \dots, μ_k and $\sigma_1, \dots, \sigma_k$.
2. Make k basis functions:
 - ▶ $\phi_i(x) = \exp\left(-\frac{(x-\mu_i)^2}{\sigma_i^2}\right)$.
3. Map data to feature space and train a linear model as before.

Demo: Sinusoidal Data

- ▶ Fit curve to 50 noisy data points.
- ▶ Use $k = 4$ Gaussian basis functions.



Demo: Sinusoidal Data

- ▶ Fit curve to 50 noisy data points.
- ▶ Use $k = 50$ Gaussian basis functions. → **overfitting**

