Week 2: Linear Models

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COMP0088 Introduction to Machine Learning • UCL Computer Science • Autumn 2024

Admin

- Pulse surveys!
- Triage?

Week 2 Recap

This One Weird Trick

$$\boldsymbol{\theta}^{\star} = \underset{\boldsymbol{\theta}}{\operatorname{argmin}}\, L\left(\mathbf{f}, \boldsymbol{\theta}, \{\mathbf{X}[, \mathbf{Y}]\}\right)$$

$$\mathbf{w}^\star = \underset{\mathbf{w}}{\operatorname{argmin}}\, L(\mathbf{f}, \mathbf{w}, \{\mathbf{X}[, \mathbf{Y}]\})$$

$$\mathbf{w}^{\star} = \underset{\mathbf{w}}{\operatorname{argmin}}\, L(\mathbf{f}, \mathbf{w}, \{\mathbf{X}, \mathbf{Y}\})$$

$$\mathbf{w}^\star = \underset{\mathbf{w}}{\operatorname{argmin}}\, L(\mathbf{f}, \mathbf{w}, \mathbf{X}, \mathbf{y})$$

$$\mathbf{w}^\star = \underset{\mathbf{w}}{\operatorname{argmin}}\, L(\mathbf{w}, \mathbf{X}, \mathbf{y})$$

↓ Feature dimensions ↓

$$\mathbf{X} = \begin{bmatrix} \mathbf{x}_1^\top \\ \mathbf{x}_2^\top \\ \vdots \\ \mathbf{x}_n^\top \end{bmatrix} = \begin{bmatrix} x_{1,1} & x_{1,2} & \cdots & x_{1,d} \\ x_{1,1} & x_{1,2} & \cdots & x_{1,d} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n,1} & x_{n,2} & \cdots & x_{n,d} \end{bmatrix}$$

↑ Samples ↑

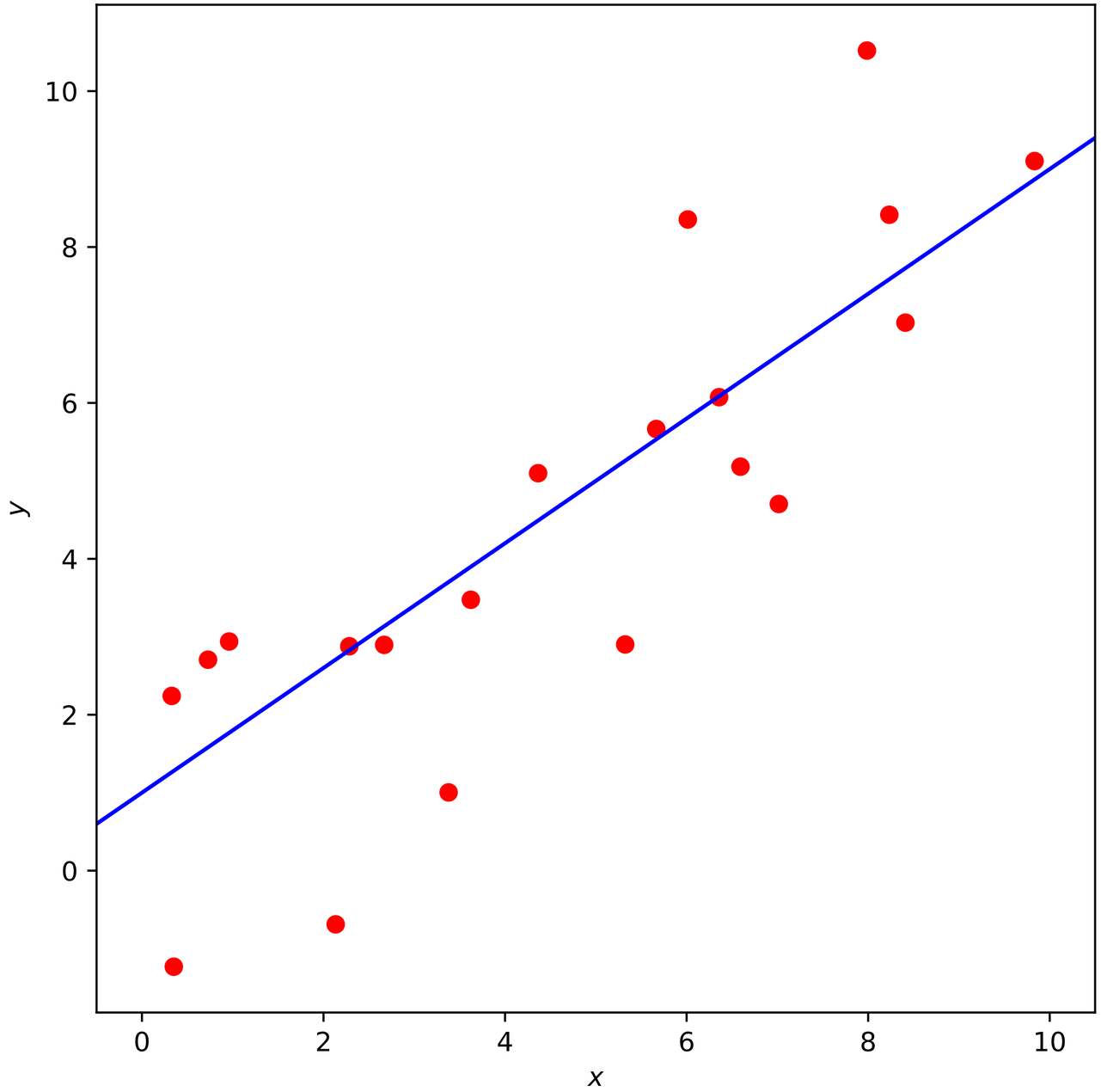
“Design Matrix”

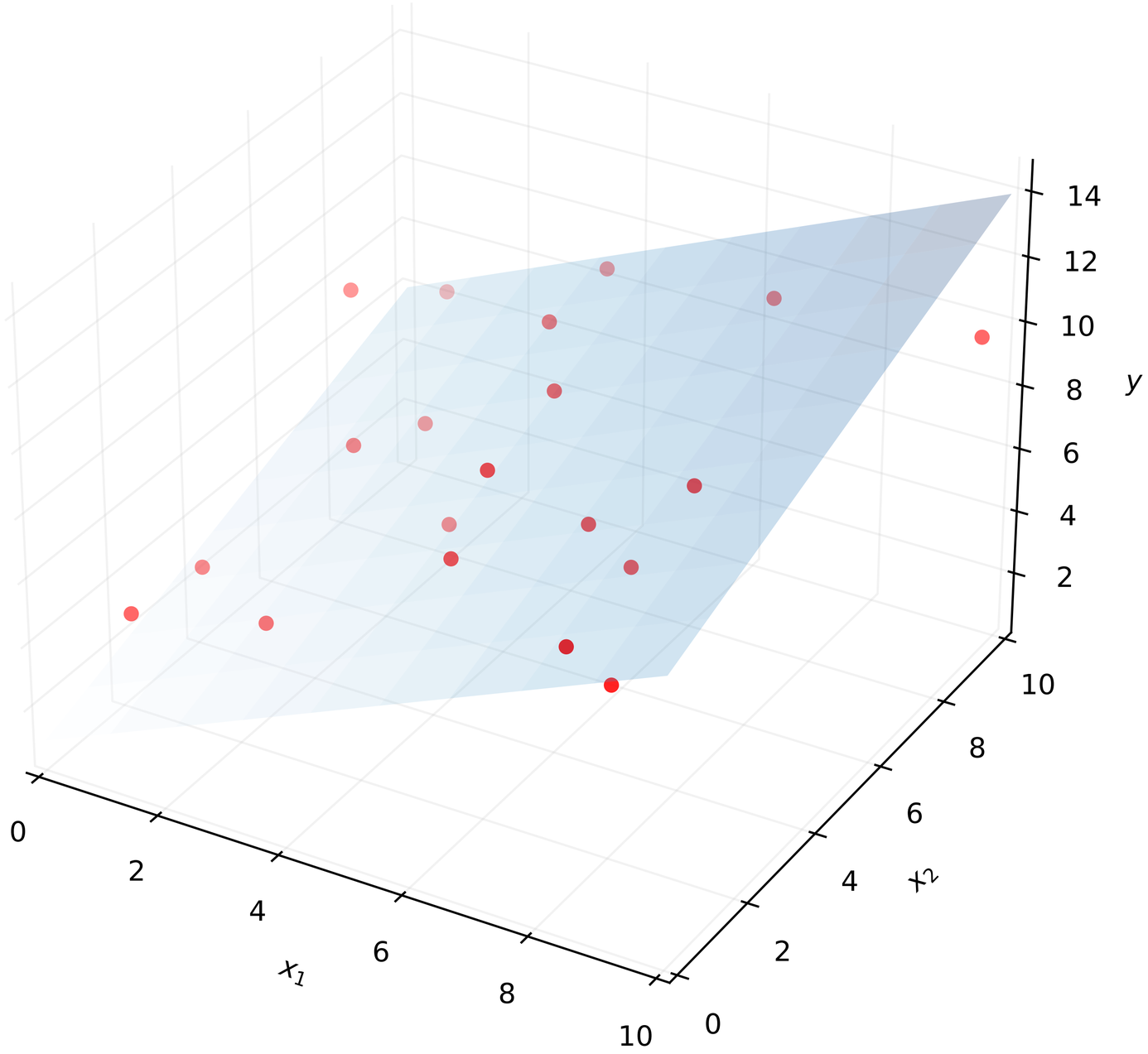
Meerkats

#	Age	Weight	Sex	Captive	...
1	11.8	815	1	0	
2	9.7	672	1	0	
3	8.9	446	1	0	
4	10.8	761	0	0	
5	8.3	1035	0	1	
6	11.7	930	1	1	
7	8.5	1027	0	1	
8	7.6	1234	0	1	
9	15.5	1461	0	1	
10	8.8	720	1	0	
11	12.8	1223	0	1	
12	7.7	711	1	0	
13	7.2	526			

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} \qquad \mathbf{w} = \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_d \end{bmatrix}$$

$$\hat{\mathbf{y}} == \mathbf{X}\mathbf{w}$$


10
8
6
4
2
0
y
0
2
4
6
8
10
x


14
12
10
8
6
4
2
y
0
2
4
6
8
10
x_1
0
2
4
6
8
10
x_2

Linear models are the best models!

$$\hat{\mathbf{y}} == \mathbf{X}\mathbf{w}$$

Comprehensible

Interpretable

Tractable

Versatile

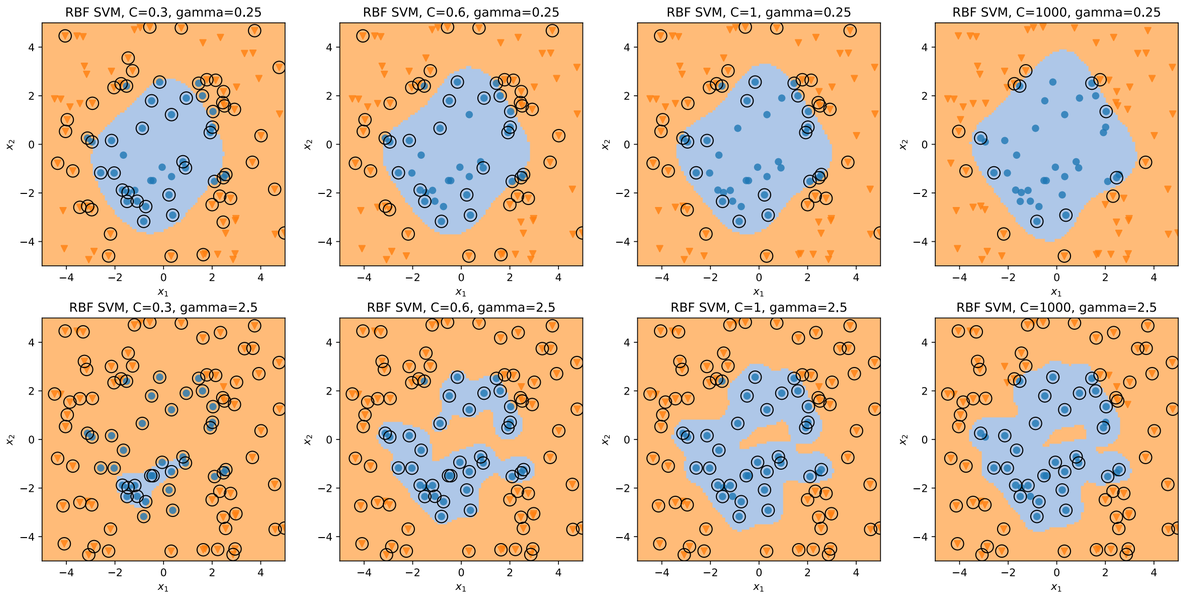
$$\mathbf{w} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

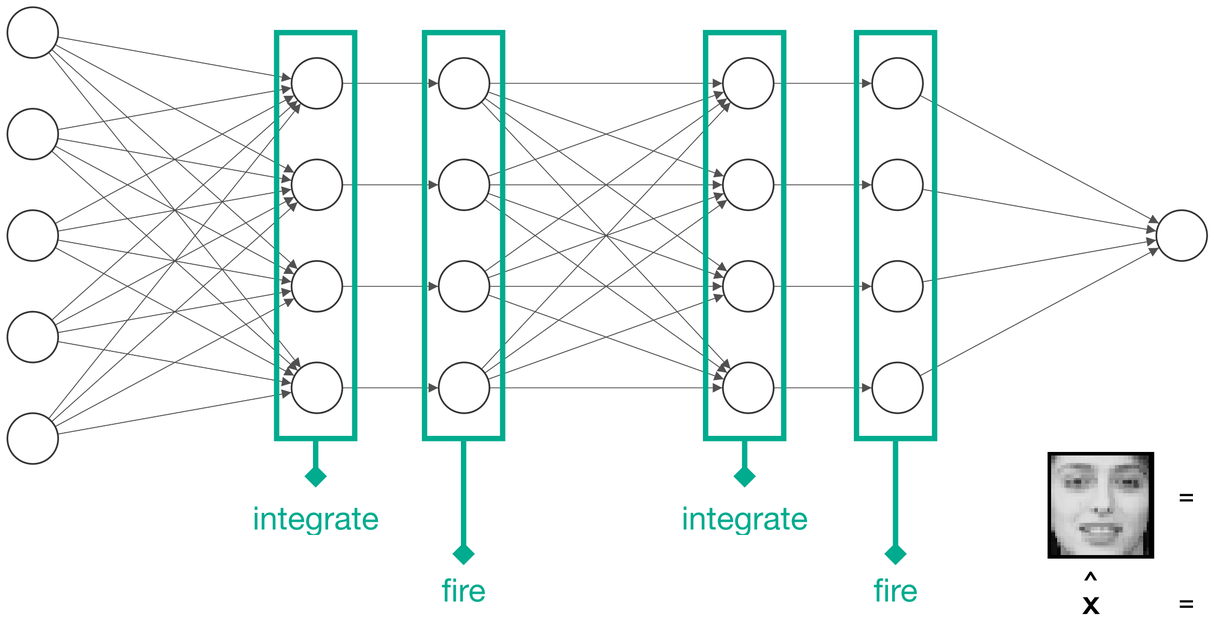
$$\mathbf{w} = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$$

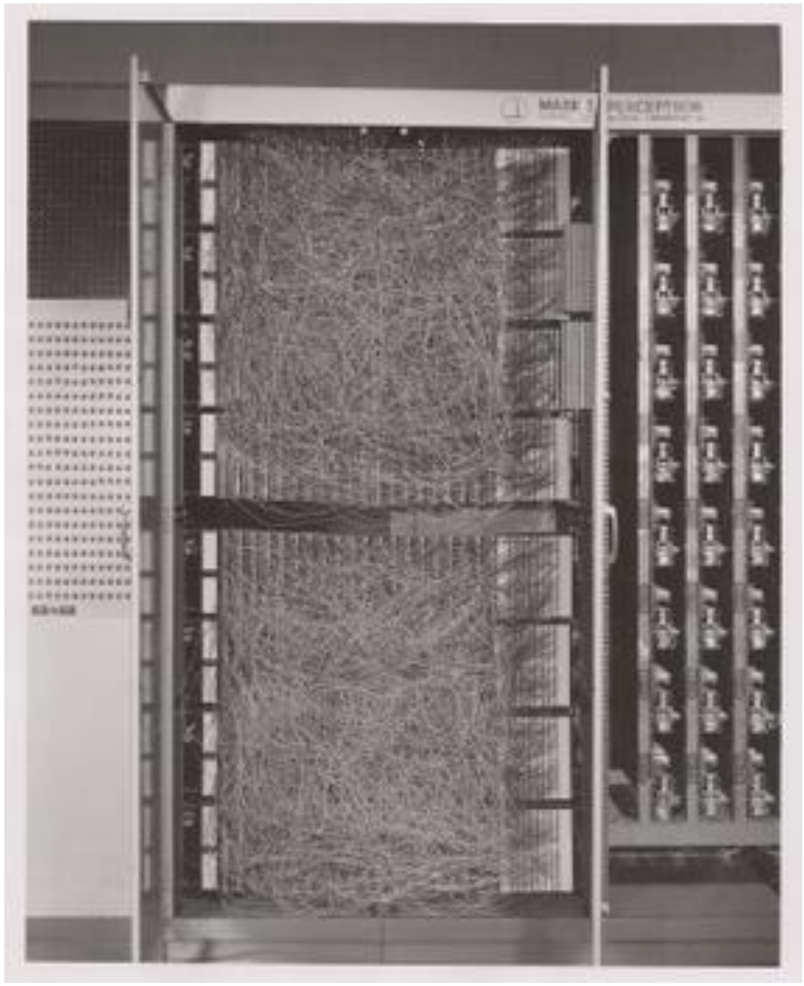
$$\mathbf{w} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$$

$$\mathbf{w} = \begin{bmatrix} 0.25 \\ 0.25 \\ 0.25 \\ 0.25 \end{bmatrix}$$

$$\mathbf{w} = \begin{bmatrix} ? \\ ? \\ ? \\ ? \\ ? \end{bmatrix}$$







$\hat{x} = \mu + w_1u_1+w_2u_2+w_3u_3+w_4u_4+ \ldots$

$$\mathbf{w}^\star = \underset{\mathbf{w}}{\operatorname{argmin}}\, L(\mathbf{w}, \mathbf{X}, \mathbf{y})$$

$$\mathbf{w}^\star = \underset{\mathbf{w}}{\operatorname{argmin}} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2$$

$$\mathbf{X}^\top \mathbf{X} \mathbf{w}^\star = \mathbf{X}^\top \mathbf{y}$$

$$\mathbf{w}^\star = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}$$

“Normal Equations”

$$(\mathbf{X}^\mathsf{T}\mathbf{X} + \lambda\mathbf{I})\mathbf{w}^\star = \mathbf{X}^\mathsf{T}\mathbf{y}$$

$$\mathbf{w}^\star = (\mathbf{X}^\mathsf{T}\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^\mathsf{T}\mathbf{y}$$

“Revised Normal Equations”

$$(\mathbf{X}^\mathsf{T}\mathbf{X} + \lambda\mathbf{I})\mathbf{w}^\star = \mathbf{X}^\mathsf{T}\mathbf{y}$$

$$\mathbf{w}^\star = (\mathbf{X}^\mathsf{T}\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^\mathsf{T}\mathbf{y}$$

“Revised Normal Equations”

#1

$$\mathbf{y} == \mathbf{f}(\mathbf{x}, \boldsymbol{\theta})$$

$$\mathbf{y} == \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x})$$

$$\boldsymbol{\theta}^{\star} = \underset{\boldsymbol{\theta}}{\operatorname{argmin}}\, L\left(\mathbf{f}, \boldsymbol{\theta}, \left\{\mathbf{X}\left[, \mathbf{Y}\right]\right\}\right)$$

$$\boldsymbol{\theta}^{\star} = \underset{\boldsymbol{\theta}}{\operatorname{argmin}}\ L_{\mathbf{f},\mathbf{X},\mathbf{Y}}(\boldsymbol{\theta})$$

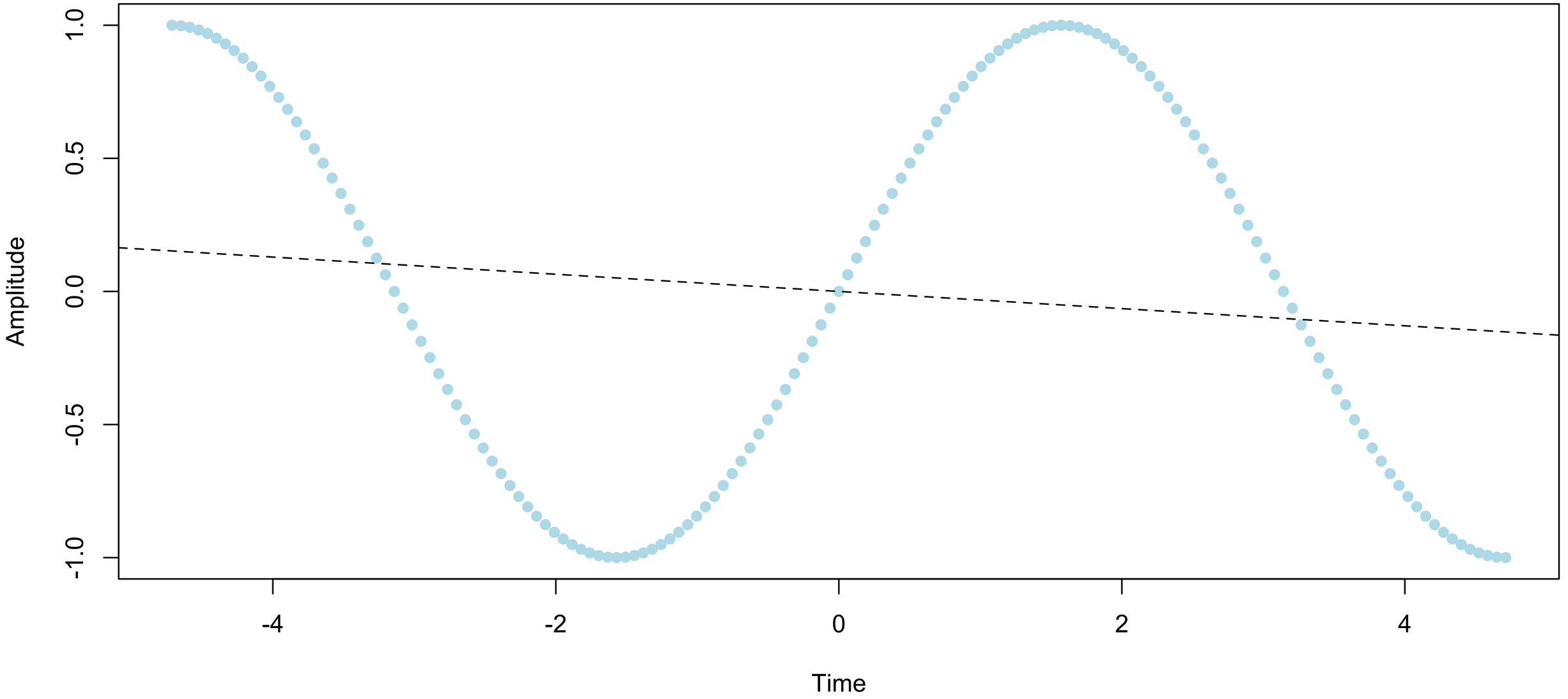
$$P(\mathbf{y}|\mathbf{x};\boldsymbol{\theta}) = f(\mathbf{x},\mathbf{y},\boldsymbol{\theta})$$

$$L(\boldsymbol{\theta}) = f(\mathbf{x}, \mathbf{y}, \boldsymbol{\theta})$$

$$\boldsymbol{\theta}^{\star} = \underset{\boldsymbol{\theta}}{\operatorname{argmax}}\ L_{\mathbf{f},\mathbf{X},\mathbf{Y}}(\boldsymbol{\theta})$$

training ≠ test

Given the training set, loss (or likelihood) is solely a function of the parameters


Amplitude
1.0
0.5
0.0
-0.5
-1.0
-4
-2
0
2
4
Time

Don’t fit a straight line to curvy data

#2

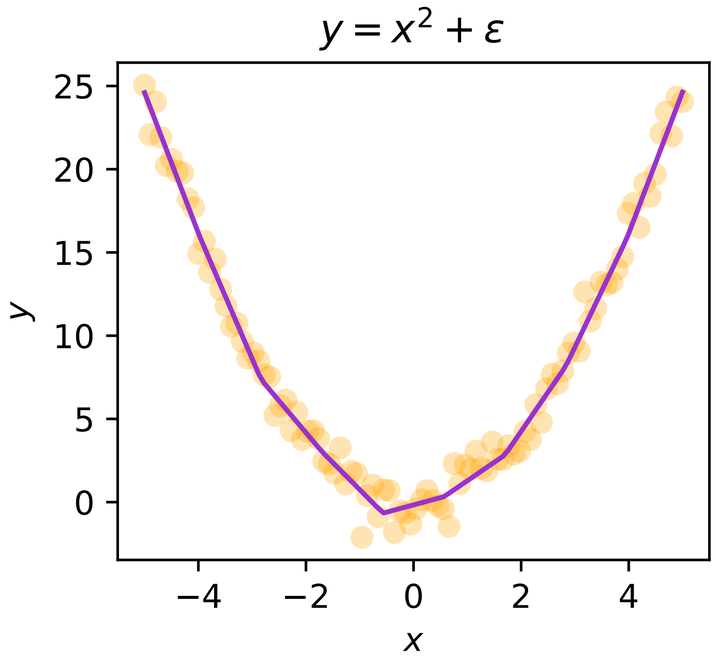
$$\hat{y} = \sum_{i}^{k} w_i h_i(\mathbf{x}) = \mathbf{h}(\mathbf{x}) \cdot \mathbf{w} = \mathbf{x}' \cdot \mathbf{w}$$

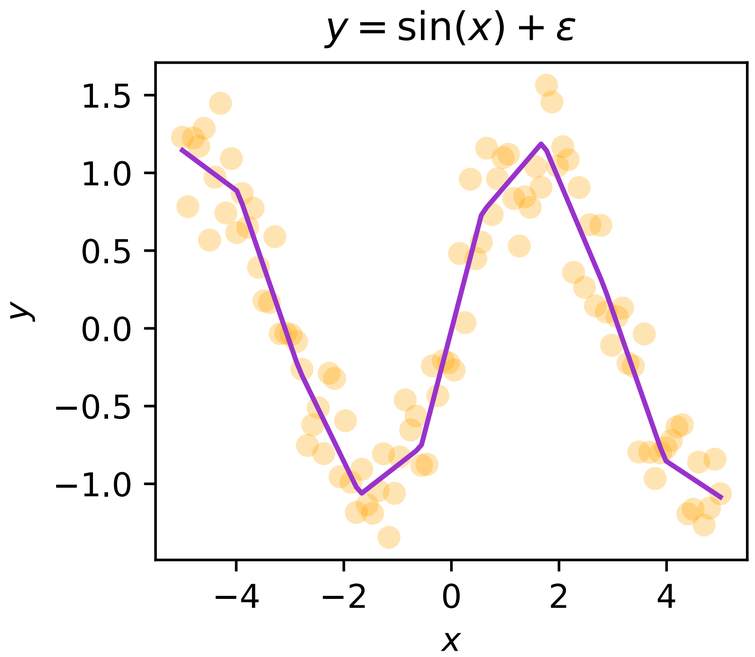
$$\mathbf{x}' = \mathbf{h}(\mathbf{x}) = [\, h_1(\mathbf{x}), h_2(\mathbf{x}), \ldots, h_k(\mathbf{x}) \,]$$

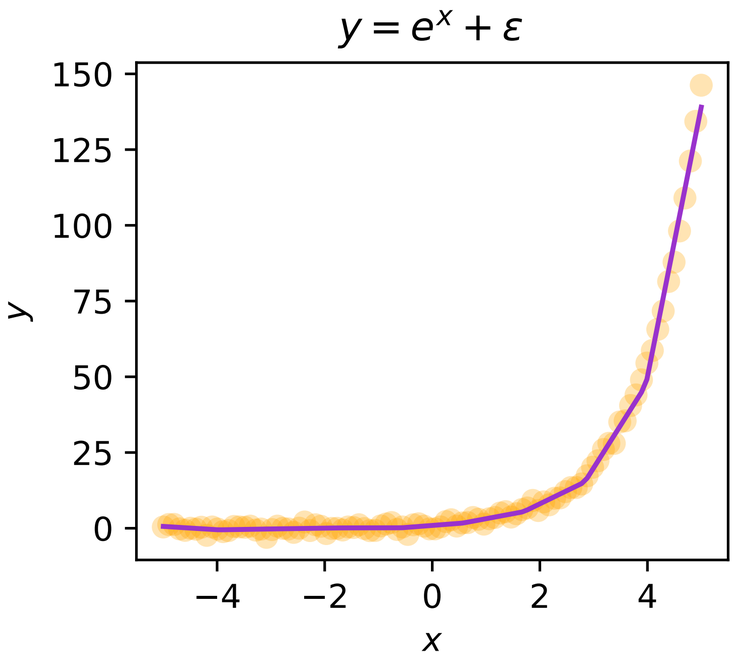
$$h_1(x) = 1$$

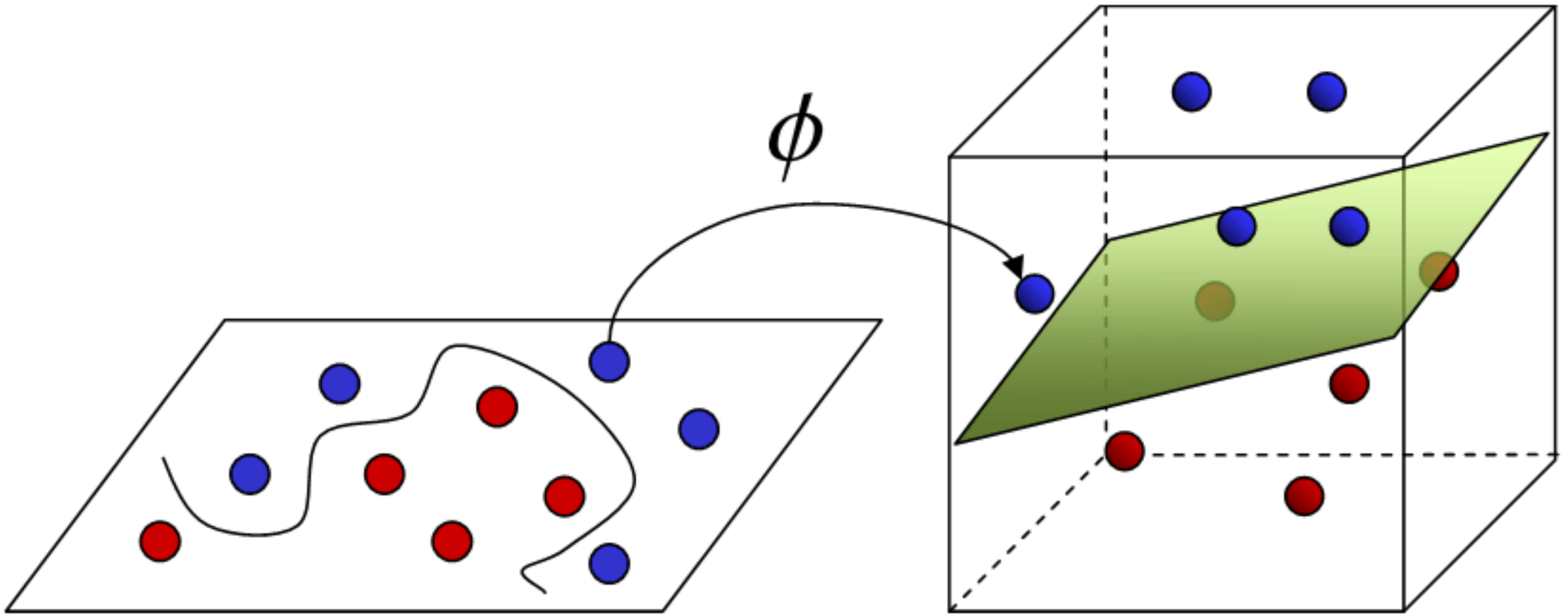
$$h_2(x) = x$$

$$h_{i+2}(x) = \max(0, x - t_i), \qquad i \in \{1, 2, \ldots, m\}$$








ϕ
a) Input Space
b) Feature Space

#3


DEFEND THE CHILDREN OF THE
POOR & PVNISH THE WRONGDOER

$$L(\mathbf{X}, \mathbf{y}; \boldsymbol{\theta}) = D(f_{\boldsymbol{\theta}}(\mathbf{X}, \mathbf{y}), \mathbf{y}) + \lambda P(\boldsymbol{\theta})$$

$$L(\mathbf{X}, \mathbf{y}; \mathbf{w}) = \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2 + \lambda P(\mathbf{w})$$

$$P(\mathbf{w}) = \|\mathbf{w}\|^2$$

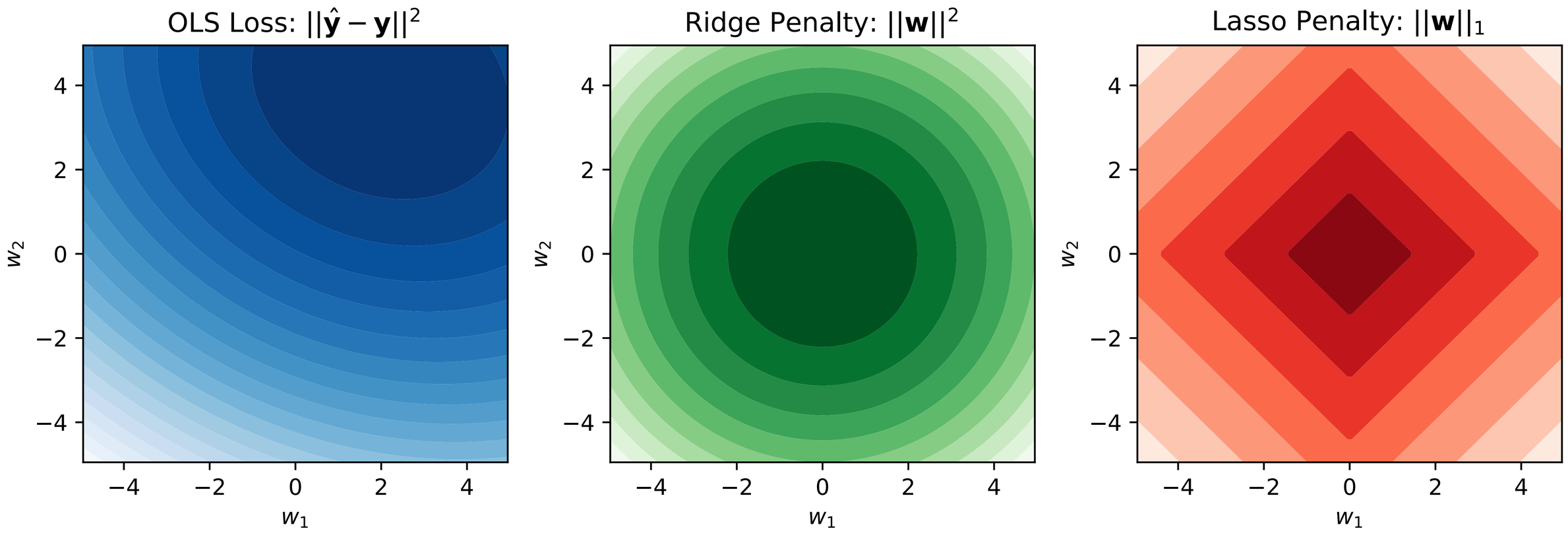
$$\mathbf{w}^\star = \underset{\mathbf{w}}{\operatorname{argmin}} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2 + \lambda \|\mathbf{w}\|^2$$

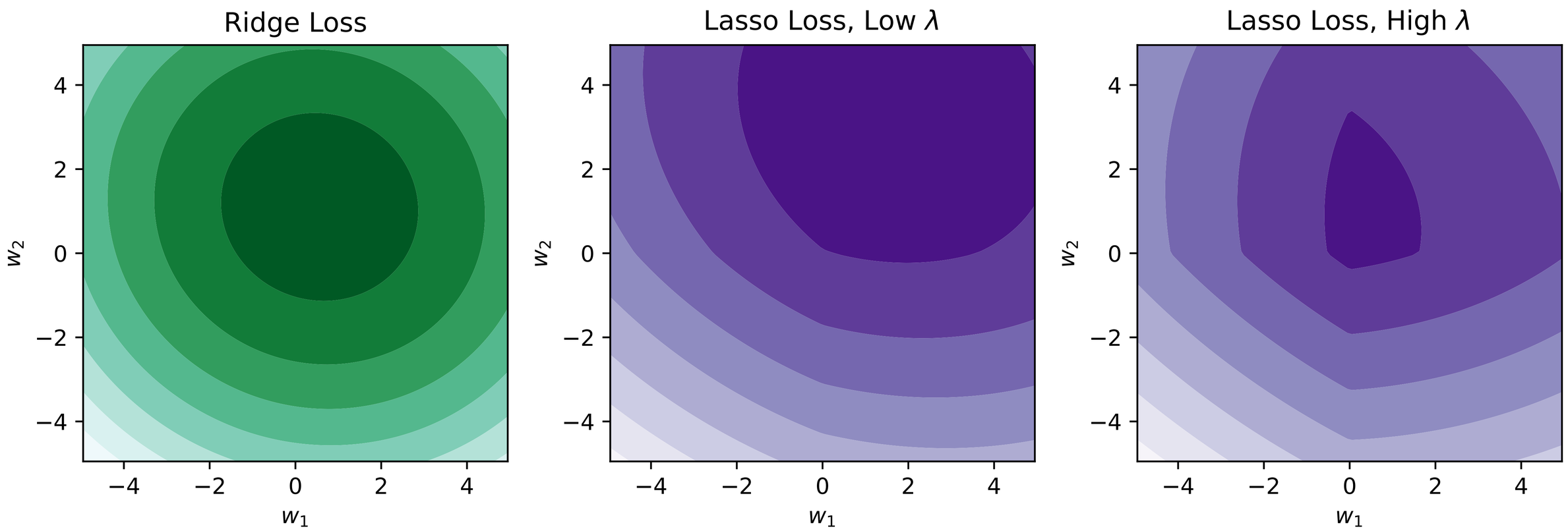
“Ridge Regression”

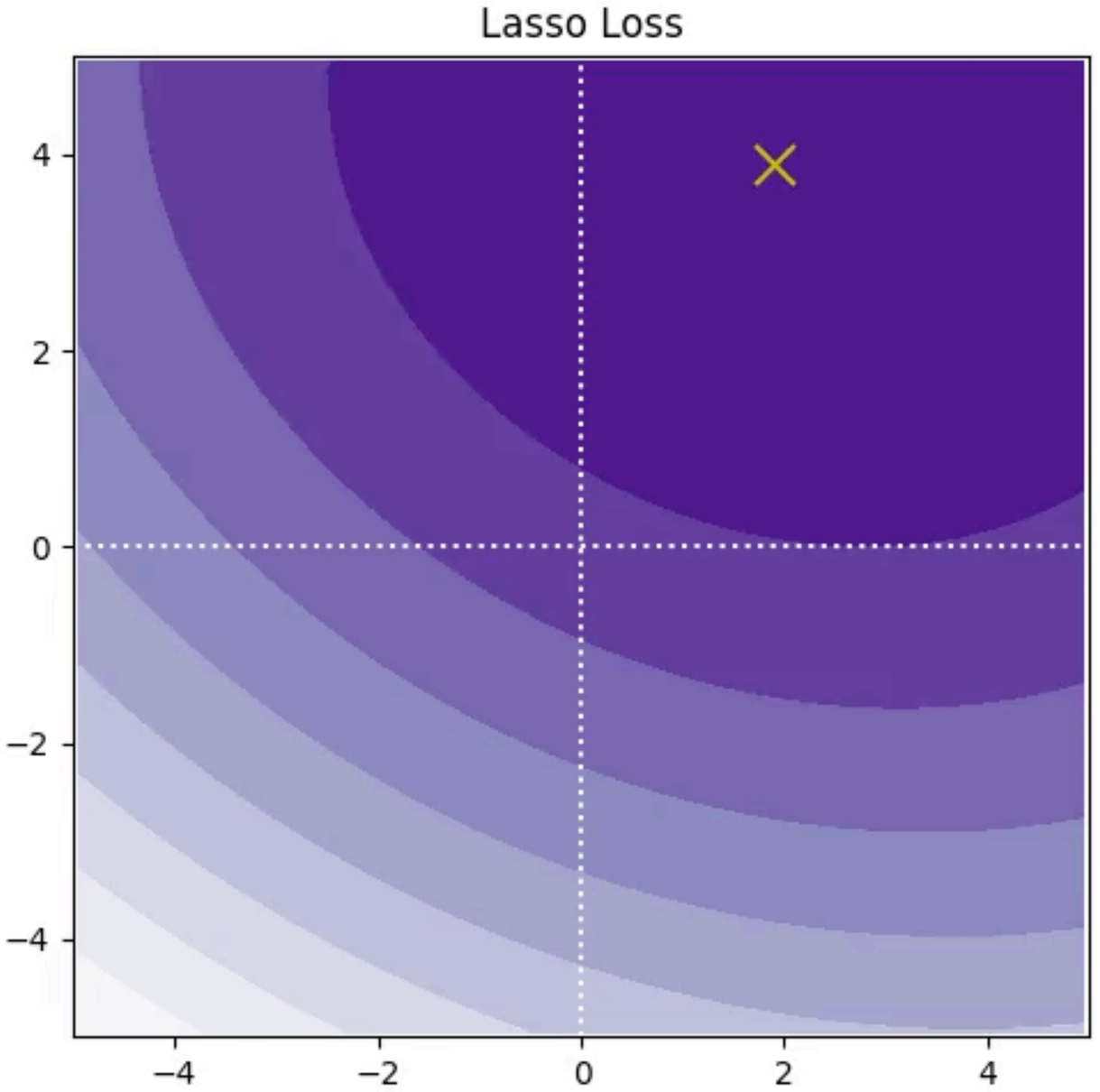
$$P(\mathbf{w}) = \|\mathbf{w}\|_1$$

$$\mathbf{w}^\star = \underset{\mathbf{w}}{\operatorname{argmin}} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2 + \lambda\|\mathbf{w}\|_1$$

“Lasso”


OLS Loss: $||\hat{\mathbf{y}} - \mathbf{y}||^2$
Ridge Penalty: $||\mathbf{w}||^2$
Lasso Penalty: $||\mathbf{w}||_1$
w_1
w_2
4
2
0
−2
−4


Ridge Loss
Lasso Loss, Low λ
Lasso Loss, High λ
w2
w1
4
2
0
−2
−4
−4
−2
0
2
4


Lasso Loss
4
2
0
−2
−4
−4
−2
0
2
4

Anonymous User

[Q+A] Clarification from Lectures: Feature Contributions and Correlation

18 hours ago

Hello,

I have a question regarding a point made in the beginning of Lecture 2.5, "Overfitting and Regularization".

In the Friday Q&A, could you clarify the following statement:

"Models may be prone to overfitting in various ways, but one common theme is to offset contributions from different features with large opposing weights, amplifying random differences for marginal loss improvements",

and also mention why "Especially when features are correlated". Thanks!

$$\mathbf{w}^\star = \underset{\mathbf{w}}{\operatorname{argmin}} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2 + \lambda \|\mathbf{w}\|^2$$

$$\mathbf{w}^\star = \underset{\mathbf{w}}{\operatorname{argmin}} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2 + \lambda \|\mathbf{w}\|_1$$

#4

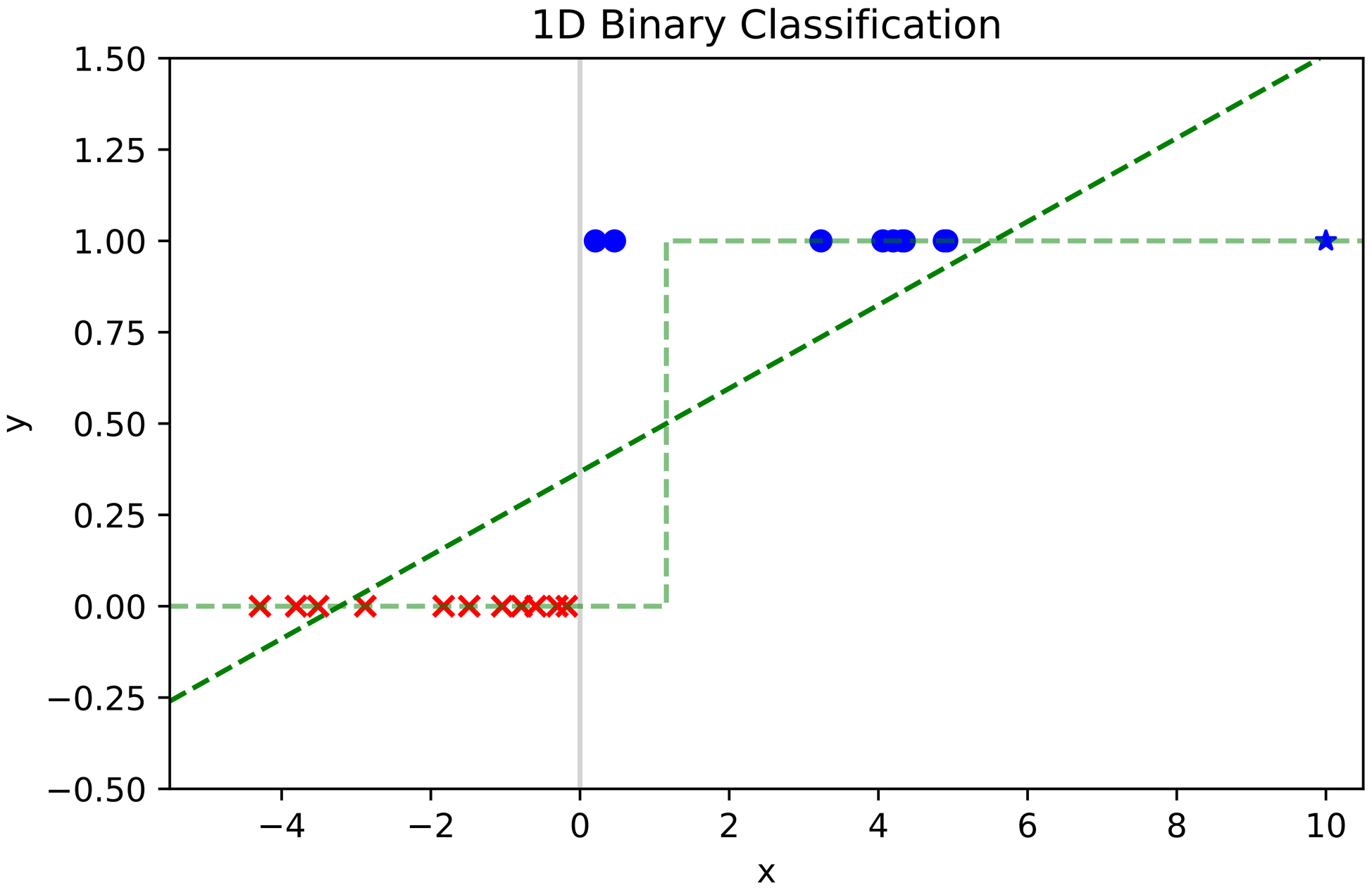
$$\mathbf{w} \leftarrow \mathbf{w} - \alpha \nabla_{\mathbf{w}} L(\mathbf{f}, \mathbf{X}, \mathbf{y}, \mathbf{w})$$

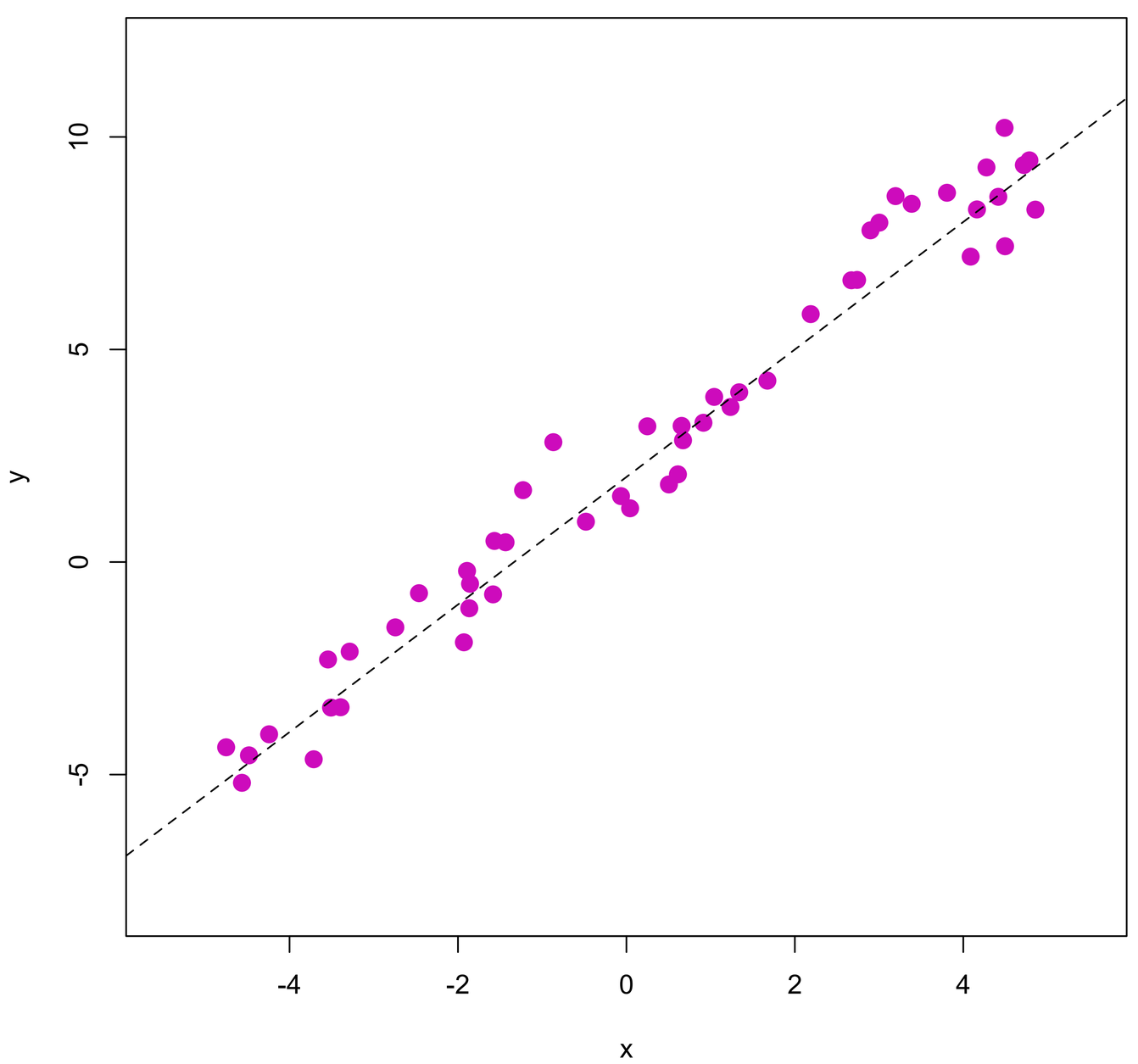
“Gradient Descent”

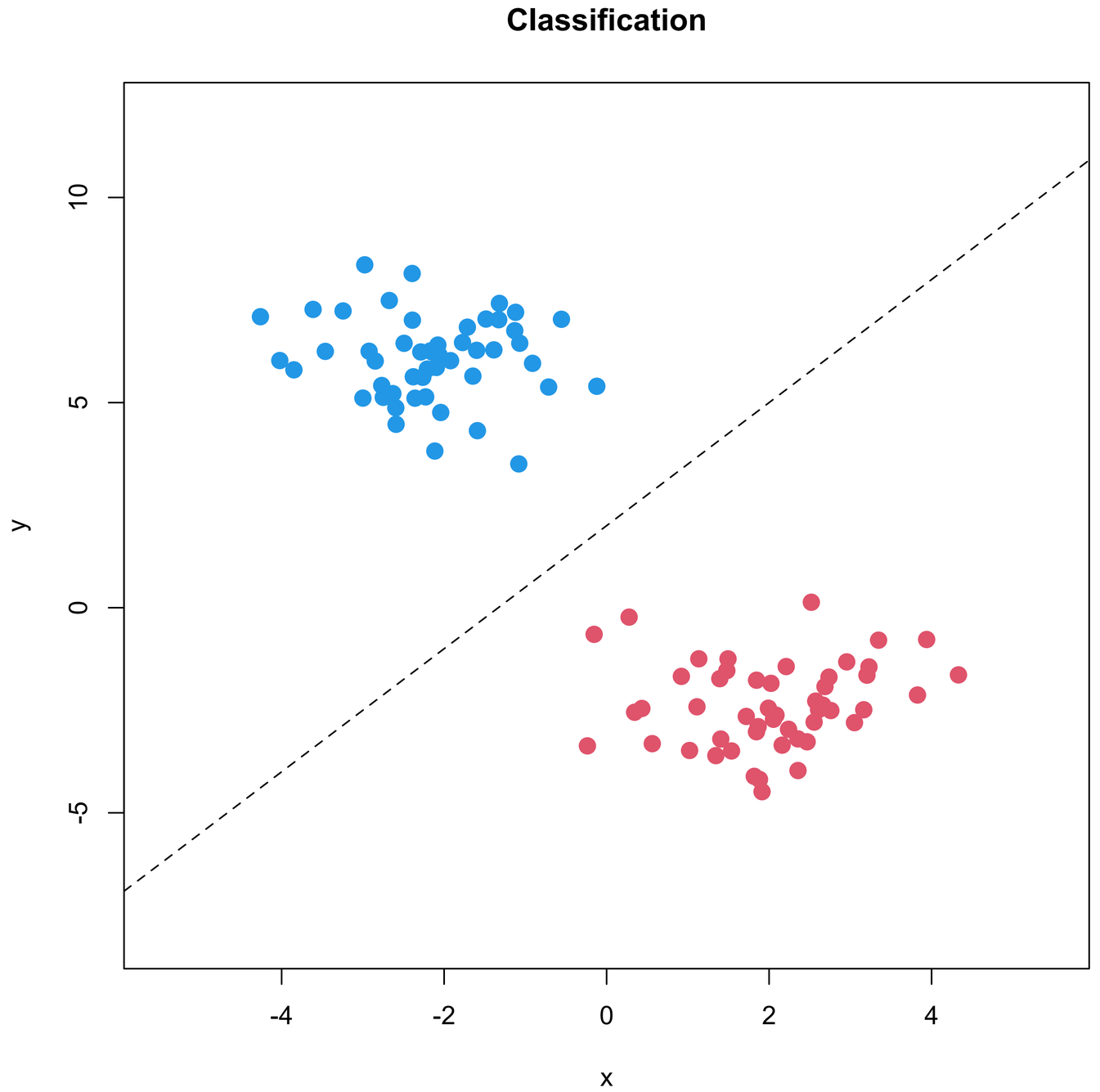
$$\mathbf{w} \leftarrow \mathbf{w} - \alpha \nabla_{\mathbf{w}} L(\mathbf{f}, \mathbf{x}, y, \mathbf{w})$$

“Stochastic Gradient Descent”

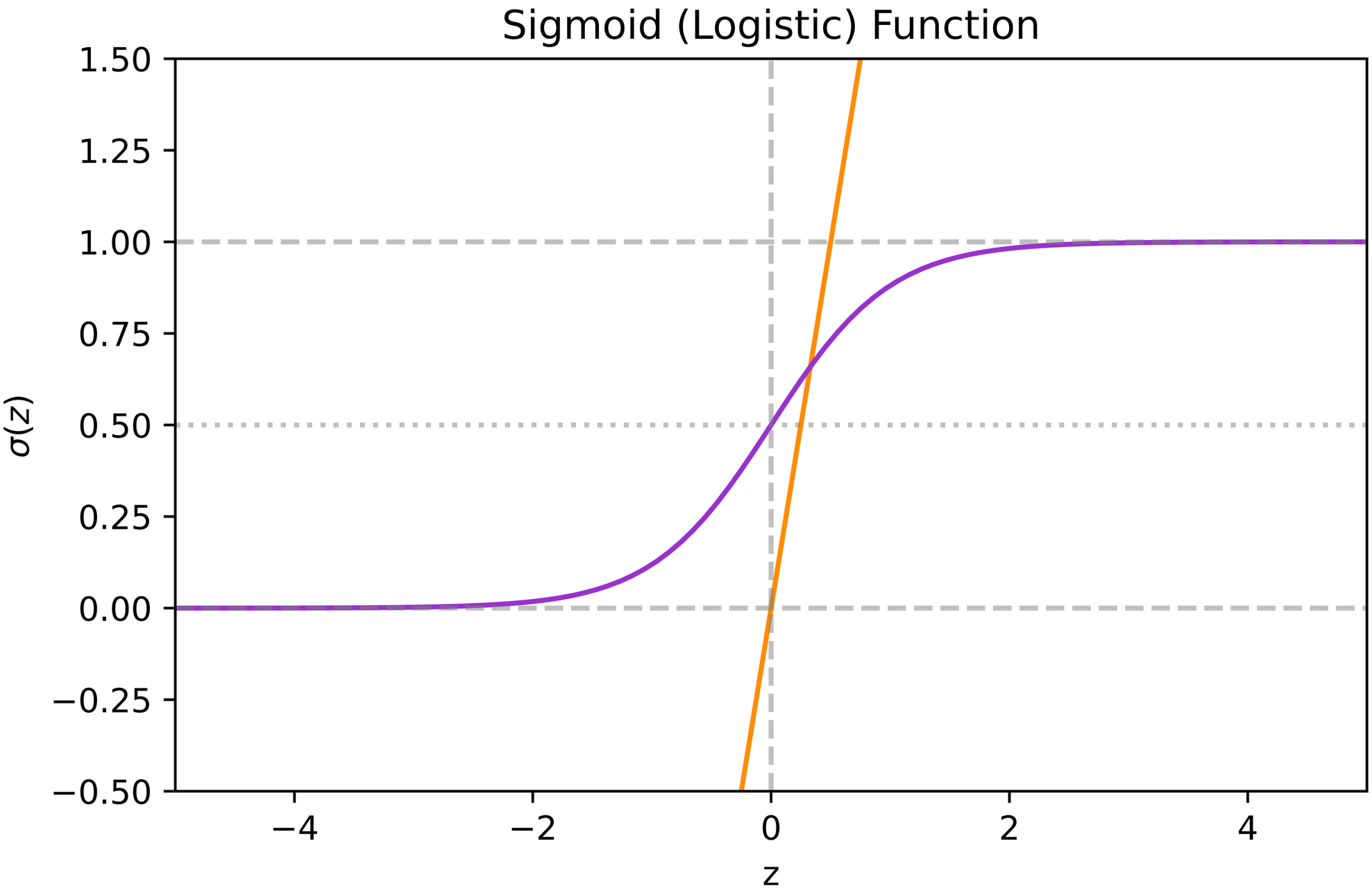
#5


1D Binary Classification
1.50
1.25
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
y
−4
−2
0
2
4
6
8
10
x

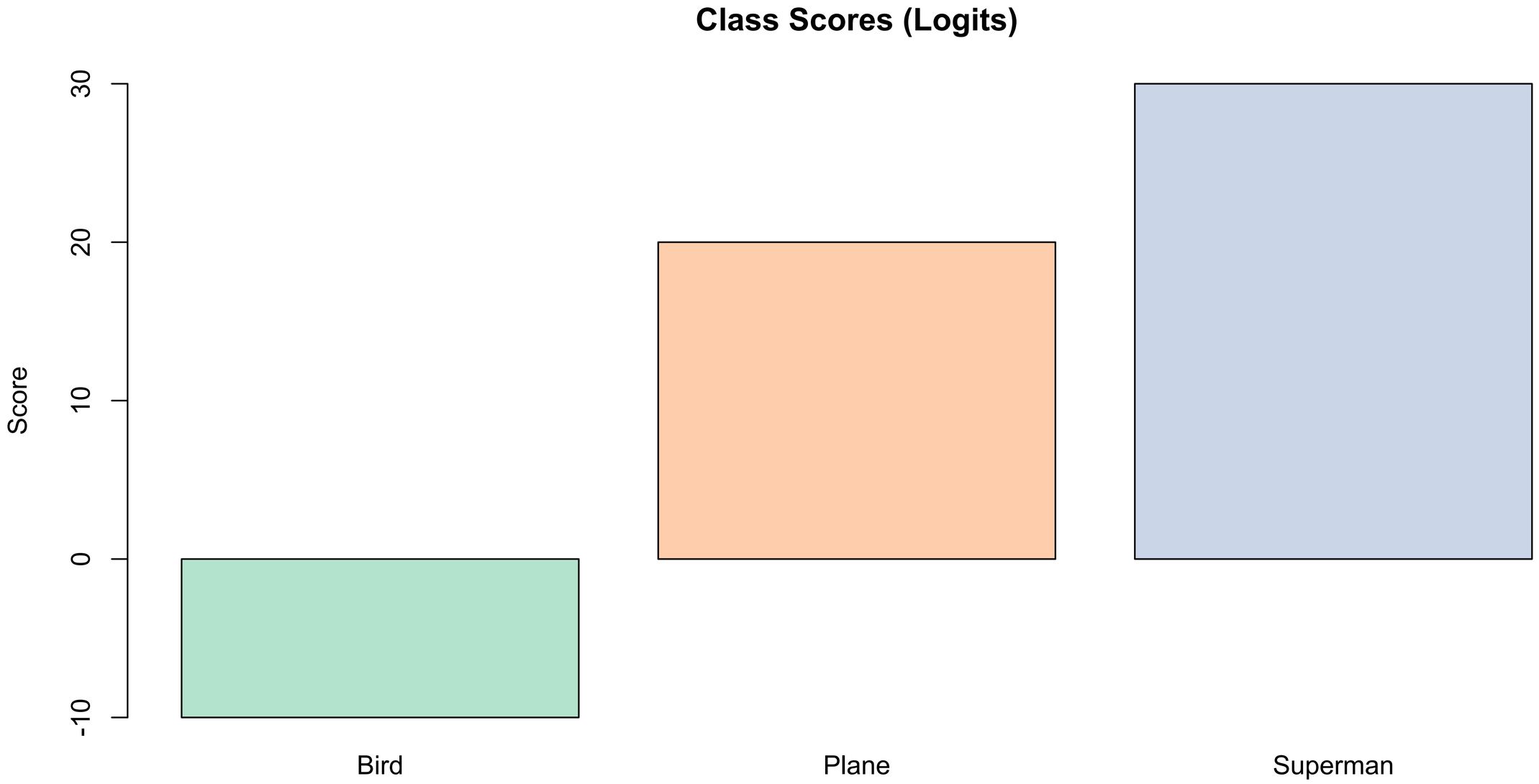

Regression
y
x
10
5
0
-5
-4
-2
0
2
4

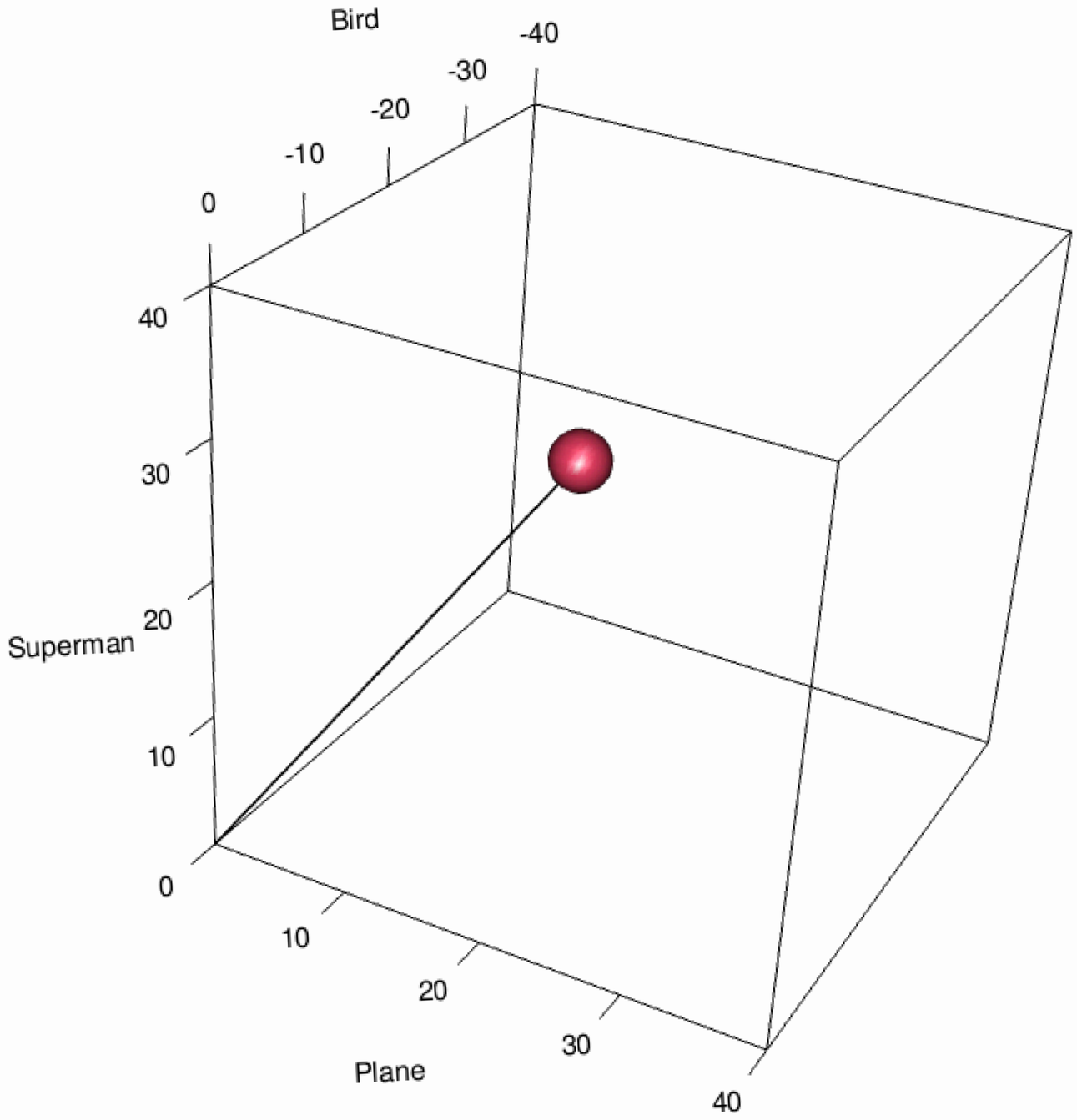

Classification
y
10
5
0
-5
-4
-2
0
2
4
x

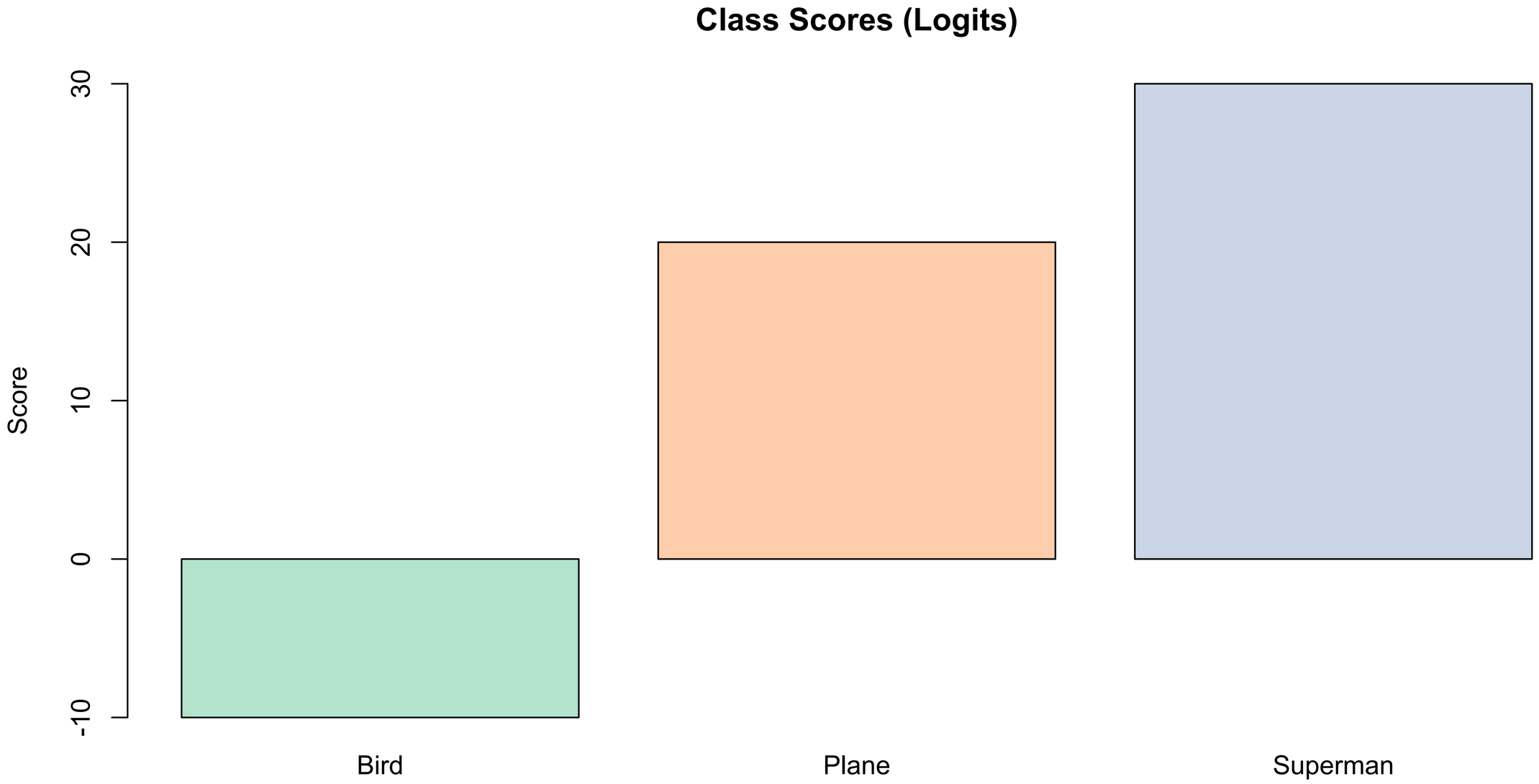
$$\sigma(z) = \frac{1}{1 + e^{-z}}$$


Sigmoid (Logistic) Function
1.50
1.25
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
σ(z)
−4
−2
0
2
4
z

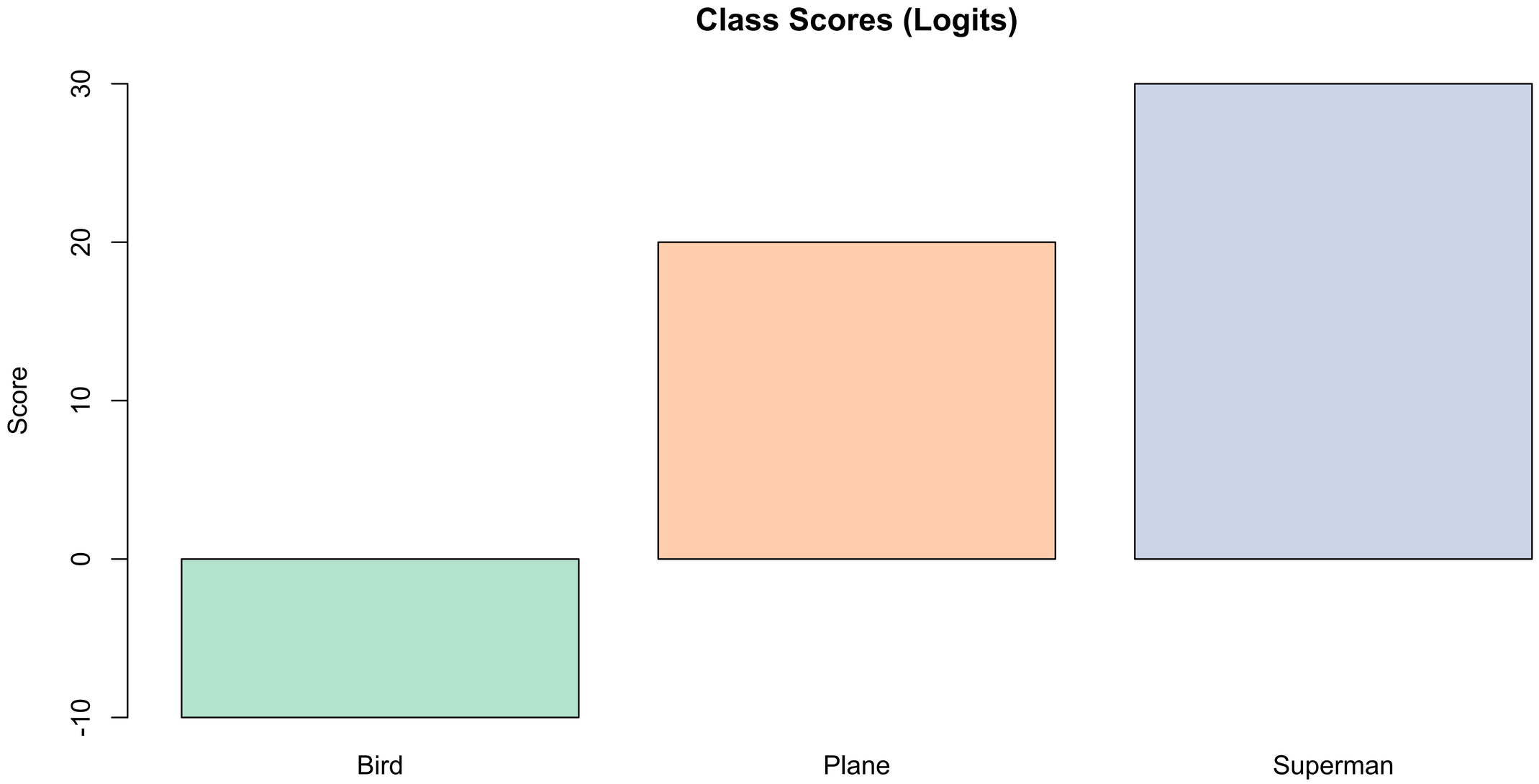
$$
\begin{aligned}
\nabla_{\mathbf{w}} l &= \mathbf{X}^{\top}(\mathbf{y} - \hat{\mathbf{y}}) \\
&= \mathbf{X}^{\top}(\mathbf{y} - \sigma(\mathbf{X}\mathbf{w})) \\
&= \mathbf{X}^{\top}\left(\mathbf{y} - \frac{1}{1 + e^{-\mathbf{X}\mathbf{w}}}\right)
\end{aligned}
$$

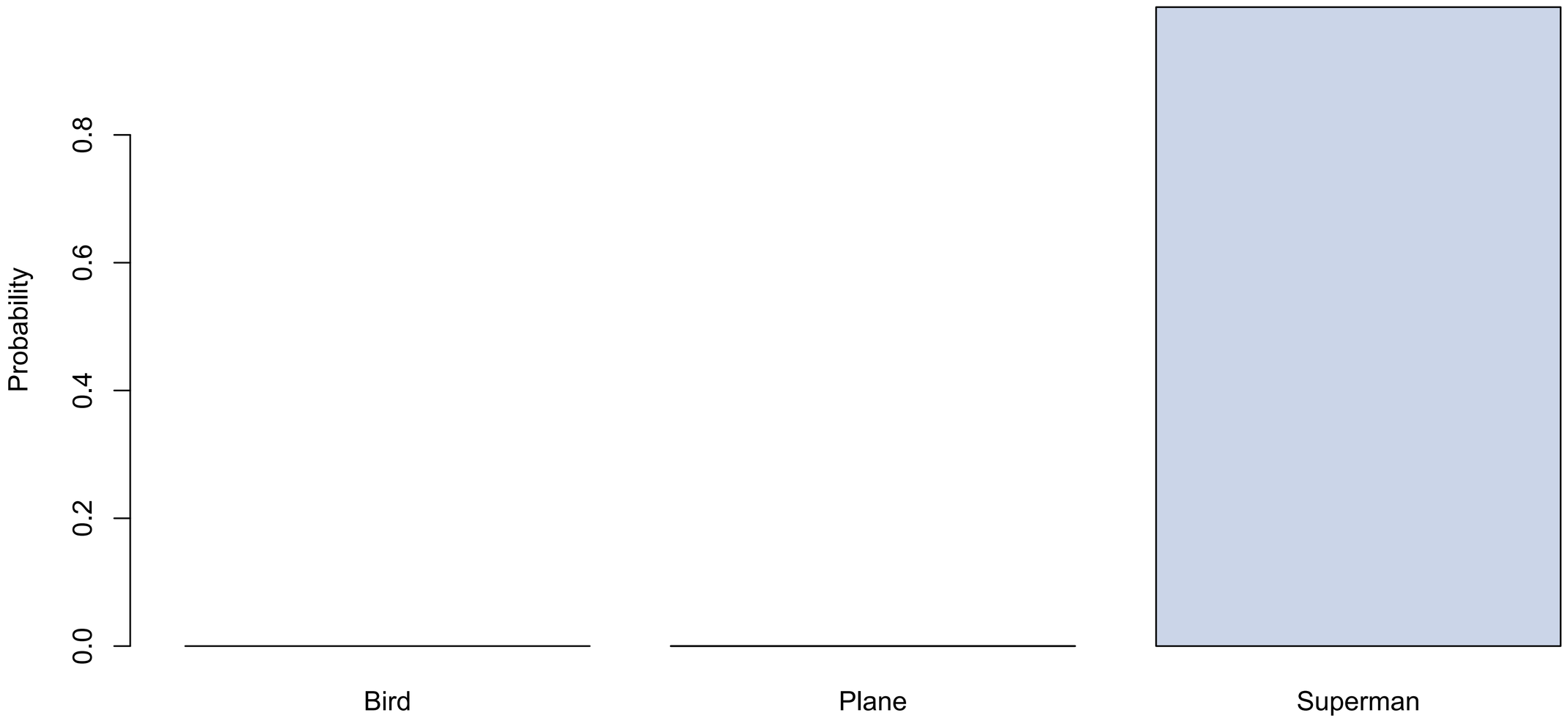

Class Scores (Logits)
Score
30
20
10
0
-10
Bird
Plane
Superman


Bird
-40
-30
-20
-10
0
40
30
20
Superman
10
0
10
20
30
40
Plane


Class Scores (Logits)
Score
30
20
10
0
-10
Bird
Plane
Superman

$$\varsigma(\mathbf{z}) = \frac{e^{\mathbf{z}}}{\sum e^{\mathbf{z}}}$$


Class Scores (Logits)
Score
30
20
10
0
-10
Bird
Plane
Superman


Class Probabilities
Probability
0.0
0.2
0.4
0.6
0.8
Bird
Plane
Superman

$$\nabla_{\mathbf{W}} L = \mathbf{X}^{\top}(\hat{\mathbf{Y}} - \mathbf{Y})$$

Questions?

Next week: Non-Parametric Models