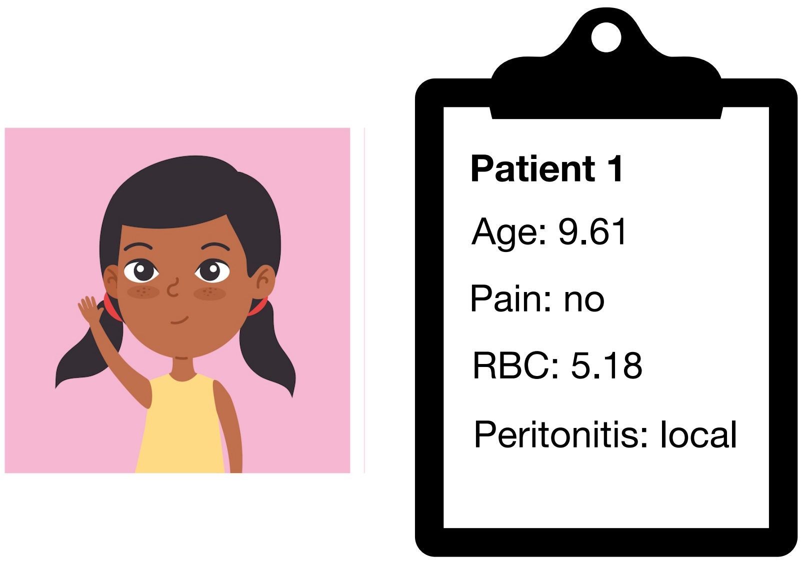
Linear regression, gradient descent & maximum likelihood

Setup

Example: Appendicitis diagnosis

Input



Patient

Neural network

Prediction

Appendicitis?

Yes / **No**

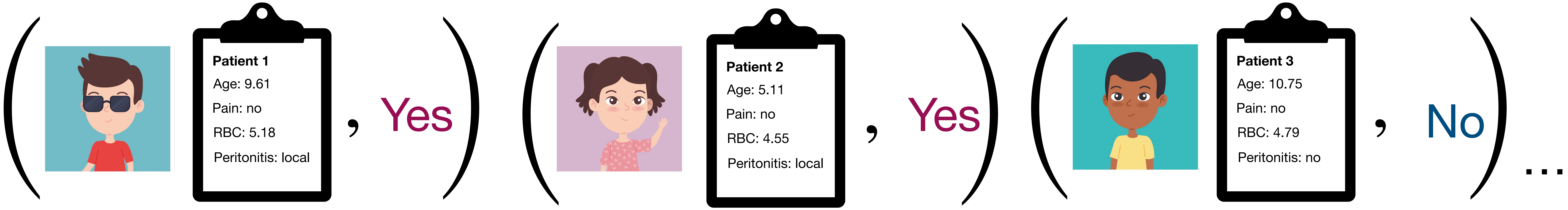
Some notation:

$$\text{Input: } \mathbf{x} \xrightarrow[\textit{predict}]{} \text{Output: } y, \qquad y = f(\mathbf{x})$$

Prediction *function*

Dataset

Set of known inputs and outputs

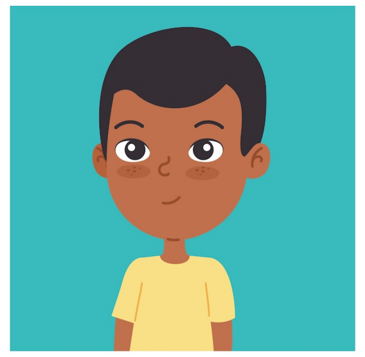


Some notation:

$$\mathcal{D} = \{(\mathbf{x}_1, y_1),\ (\mathbf{x}_2, y_2),\ \ldots\ (\mathbf{x}_N, y_N)\}$$

Dataset

Set of known inputs and outputs

( **Patient 1** Age: 9.61 Pain: no RBC: 5.18 Peritonitis: local , Yes) ( **Patient 2** Age: 5.11 Pain: no RBC: 4.55 Peritonitis: local , Yes) ( **Patient 3** Age: 10.75 Pain: no RBC: 4.79 Peritonitis: no , No) ...

Input table

Patients with abdominal pain

	Age	Appendix Size	Migratory Pain	RBC Count	RBC Urine	Peritonitis
0	9.61	9.0	no	5.18	high	local
1	5.11	7.0	no	4.55	medium	local
2	10.75	5.0	no	4.79	none	no
3	10.51	9.0	no	5.03	none	local
4	7.3	6.2	yes	4.64	low	no
5	15.21	8.5	yes	4.62	low	no
6	15.83	12.0	yes	4.33	high	no
7	9.58	7.0	yes	5.04	low	generalized
8	10.37	5.5	no	4.8	none	no
9	16.66	9.0	yes	5.31	none	no
10	14.52	4.5	yes	4.9	none	no
11	10.74	9.0	no	5.66	none	local
12	12.41	3.7	no	5.49	none	no
13	6.67	3.5	no	5.27	none	no
14	14.36	9.0	yes	4.84	low	local
15	9.04	5.3	yes	4.92	low	no
16	12.43	12.0	yes	4.62	none	generalized

Output table

Diagnosis

	Diagnosis
0	appendicitis
1	no appendicitis
2	no appendicitis
3	no appendicitis
4	appendicitis
5	no appendicitis
6	no appendicitis
7	no appendicitis
8	no appendicitis
9	appendicitis
10	appendicitis
11	no appendicitis
12	no appendicitis
13	no appendicitis
14	appendicitis
15	no appendicitis
16	appendicitis

Mathematical abstraction

As table

Patients with abdominal pain

	Age	Appendix Size	Height	Weight	RBC Count	Temperature	WBC Count
0	16.66	9.0	174.0	65.0	5.31	36.6	6.6
1	10.74	9.0	146.0	57.5	5.66	37.3	10.2
2	9.04	5.3	134.0	29.4	4.92	36.0	5.1
[illegible]	[illegible]	5.0	155.0	54.5	4.79	37.7	10.3
[illegible]	[illegible]	6.2	123.0	23.5	4.64	37.4	21.1
5	5.11	7.0	116.0	22.0	4.55	40.2	19.4
6	14.36	9.0	163.0	50.0	4.84	37.5	14.3
7	9.61	9.0	140.0	29.2	5.18	38.7	14.3
8	15.83	12.0	153.0	59.0	4.33	36.7	12.8
9	9.58	7.0	132.0	24.7	5.04	38.4	13.5
10	10.37	5.5	156.0	39.0	4.8	37.4	5.6
11	14.52	4.5	181.0	55.0	4.9	37.0	9.0
12	12.41	3.7	150.5	42.5	5.49	37.2	9.1
13	6.67	3.5	124.0	38.5	5.27	39.6	16.8
14	15.21	8.5	155.0	85.0	4.62	36.8	12.4
15	12.43	12.0	157.0	46.0	4.62	37.1	16.4
16	10.51	9.0	134.5	27.0	5.03	37.4	12.8

Observation

Feature

As matrix

Observation

$$
\mathbf{X} = \underbrace{\begin{bmatrix}
16.66 & 9.0 & 174.0 & 65.0 & 5.31 & 36.6 & 6.6 \\
10.74 & 9.0 & 146.0 & 57.5 & 5.66 & 37.3 & 10.2 \\
9.04 & 5.3 & 134.0 & 29.4 & 4.92 & 36.0 & 5.1 \\
10.75 & 5.0 & 155.0 & 54.5 & 4.79 & 37.7 & 10.3 \\
7.3 & 6.2 & 123.0 & 23.5 & 4.64 & 37.4 & 21.1 \\
5.11 & 7.0 & 116.0 & 22.0 & 4.55 & 40.2 & 19.4 \\
14.36 & 9.0 & 163.0 & 50.0 & 4.84 & 37.5 & 14.3 \\
9.61 & 9.0 & 140.0 & 29.2 & 5.18 & 38.7 & 14.3 \\
15.83 & 12.0 & 153.0 & 59.0 & 4.33 & 36.7 & 12.8 \\
9.58 & 7.0 & 132.0 & 24.7 & 5.04 & 38.4 & 13.5 \\
10.37 & 5.5 & 156.0 & 39.0 & 4.8 & 37.4 & 5.6 \\
14.52 & 4.5 & 181.0 & 55.0 & 4.9 & 37.0 & 9.0 \\
12.41 & 3.7 & 150.5 & 42.5 & 5.49 & 37.2 & 9.1 \\
6.67 & 3.5 & 124.0 & 38.5 & 5.27 & 39.6 & 16.8 \\
15.21 & 8.5 & 155.0 & 85.0 & 4.62 & 36.8 & 12.4 \\
12.43 & 12.0 & 157.0 & 46.0 & 4.62 & 37.1 & 16.4 \\
10.51 & 9.0 & 134.5 & 27.0 & 5.03 & 37.4 & 12.8
\end{bmatrix}}_{d \text{ (features)}} \left.\vphantom{\begin{bmatrix}1\\1\\1\\1\\1\\1\\1\\1\\1\\1\\1\\1\\1\\1\\1\\1\\1\end{bmatrix}}\right\} N \text{ (Obs.)}
$$

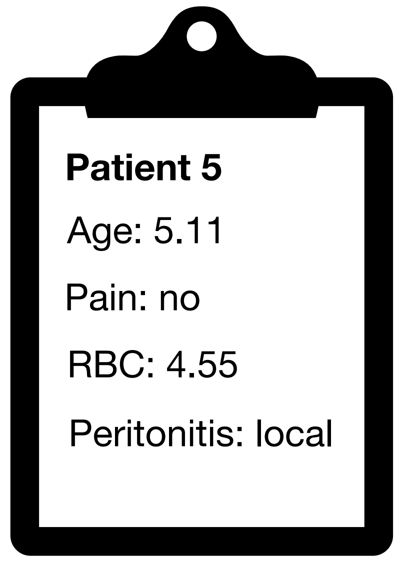
Feature

N x d Matrix: $\mathbf{X} \in \mathbb{R}^{N \times d}$

Mathematical abstraction

Labels become a vector

(



, Yes)

Output table

Diagnosis

	Diagnosis
0	appendicitis
1	no appendicitis
2	no appendicitis
3	no appendicitis
4	appendicitis
5	no appendicitis
6	no appendicitis
7	no appendicitis
8	no appendicitis
9	appendicitis
10	appendicitis
11	no appendicitis
12	no appendicitis
13	no appendicitis
14	appendicitis
15	no appendicitis
16	appendicitis

Converted

Diagnosis

	Diagnosis
0	1
1	0
2	0
3	0
4	1
5	0
6	0
7	0
8	0
9	1
10	0
11	0
12	0
13	0
14	1
15	0
16	1

$$\mathbf{y} = \left.\begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ \boxed{1} \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 1 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 1 \end{bmatrix}\right\} N$$

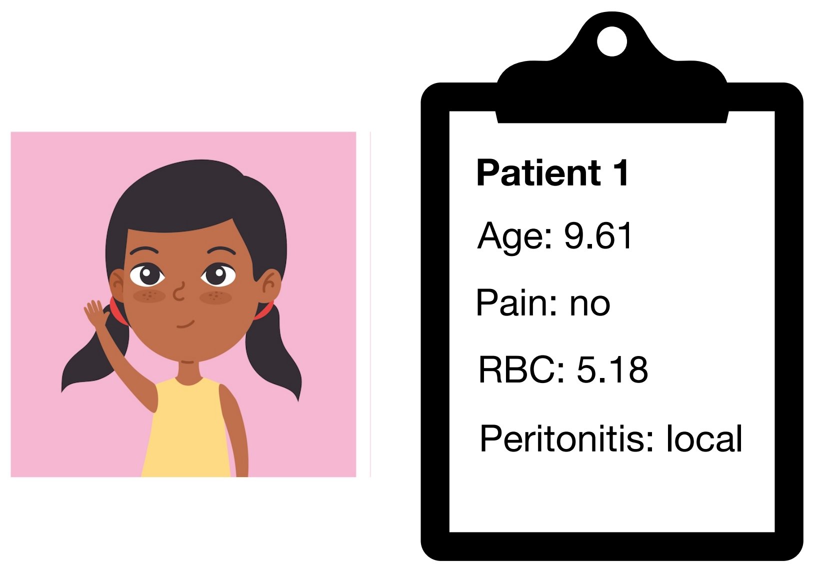
(Obs.)

$$y_5 = 1$$

Index (Obs.)

Quantitative outputs: *Regression*

Input



Patient

Neural network

Prediction
(*Regression*)

Length of hospital stay

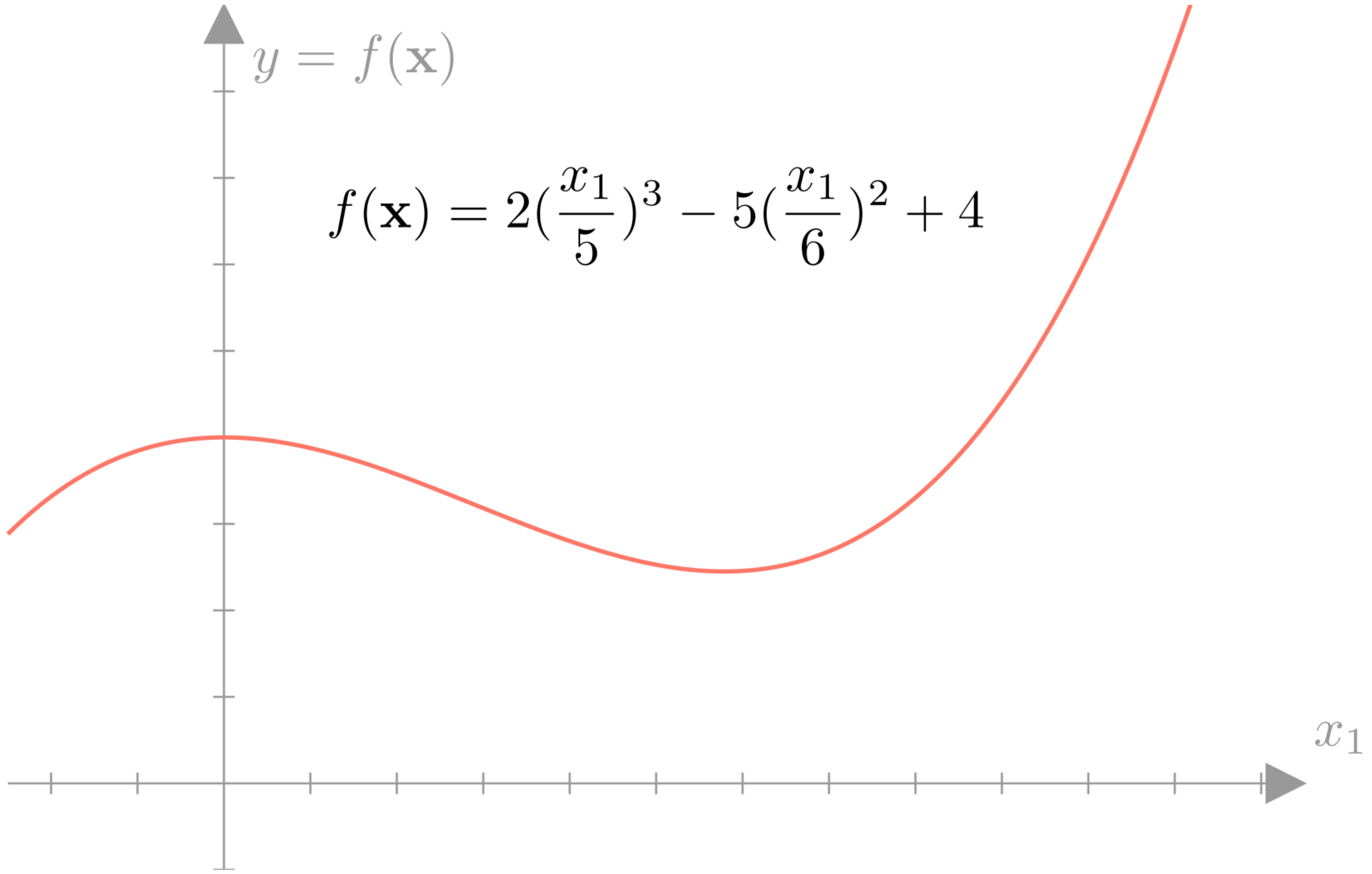
24hrs? 36hrs? …

$$\mathcal{D} = \{(\mathbf{x}_1, y_1),\ (\mathbf{x}_2, y_2),\ \ldots\ (\mathbf{x}_N, y_N)\}$$

Output domain: $y \in \mathbb{R}$

$$\text{Input: } \mathbf{x} \xrightarrow[predict]{} \text{Output: } y, \quad y = f(\mathbf{x})$$

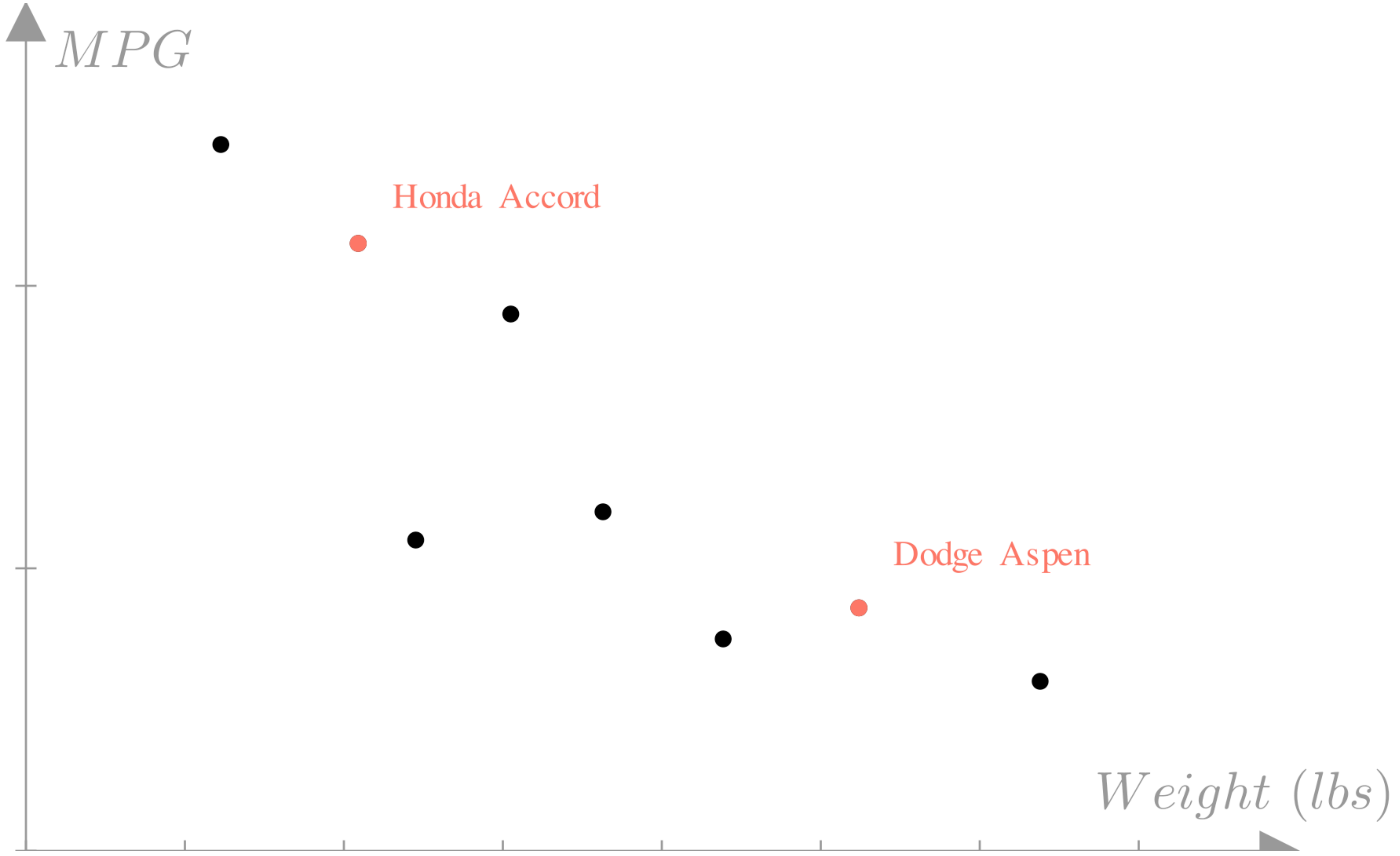
Prediction *function*



$$\text{Honda Accord:} \begin{bmatrix} \text{Weight:} & \text{2500 lbs} \\ \text{Horsepower:} & \text{123 HP} \\ \text{Displacement:} & \text{2.4 L} \\ \text{0-60mph:} & \text{7.8 Sec} \end{bmatrix} \longrightarrow \text{MPG: 33mpg}$$

$$\text{Dodge Aspen:} \begin{bmatrix} \text{Weight:} & \text{3800 lbs} \\ \text{Horsepower:} & \text{155 HP} \\ \text{Displacement:} & \text{3.2 L} \\ \text{0-60mph:} & \text{6.8 Sec} \end{bmatrix} \longrightarrow \text{MPG: 21mpg}$$

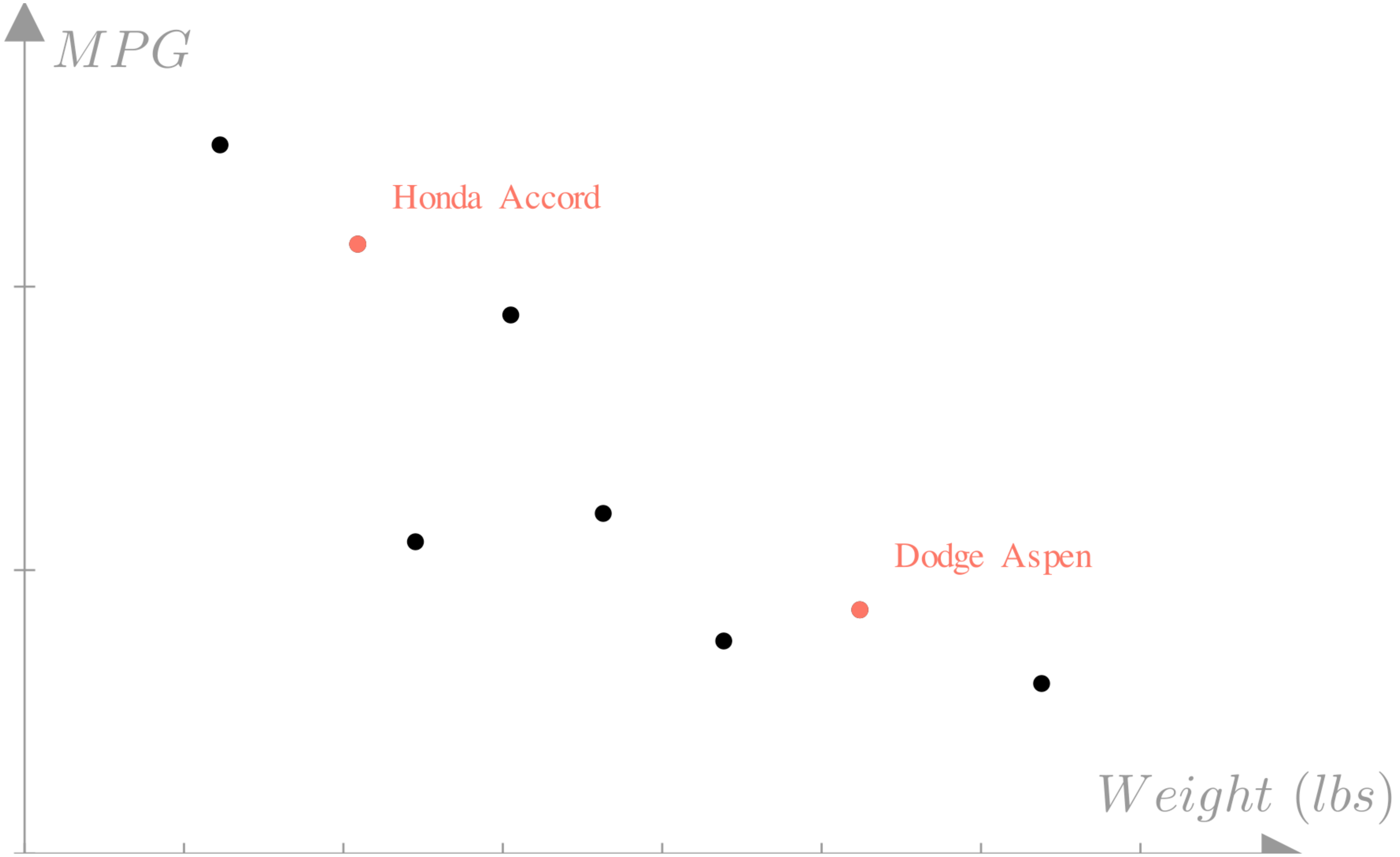
$$\vdots \quad \vdots$$

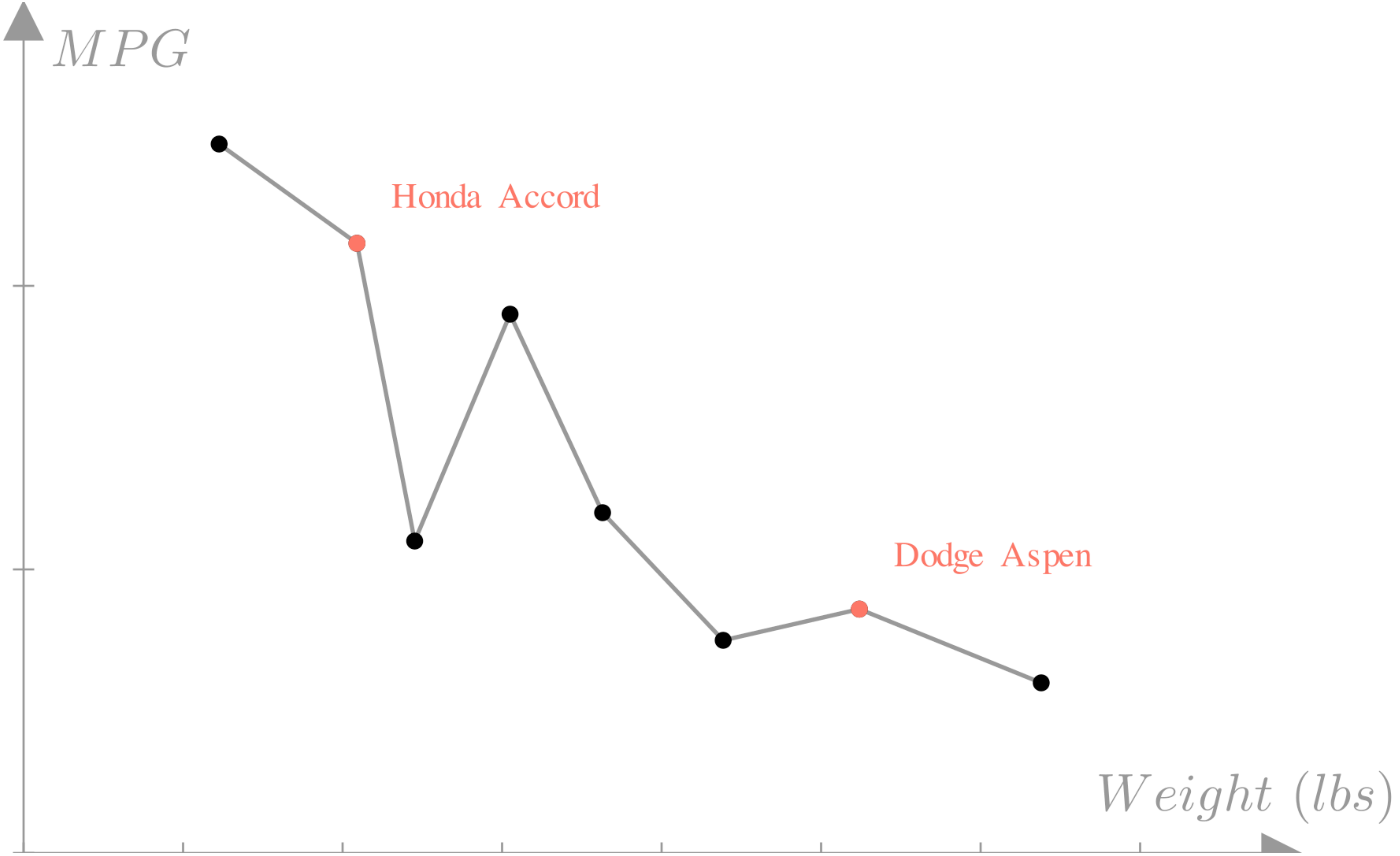


Dataset: $\mathcal{D} = \{(\mathbf{x}_i,\ y_i) \text{ for } i \in 1 \dots N\}$

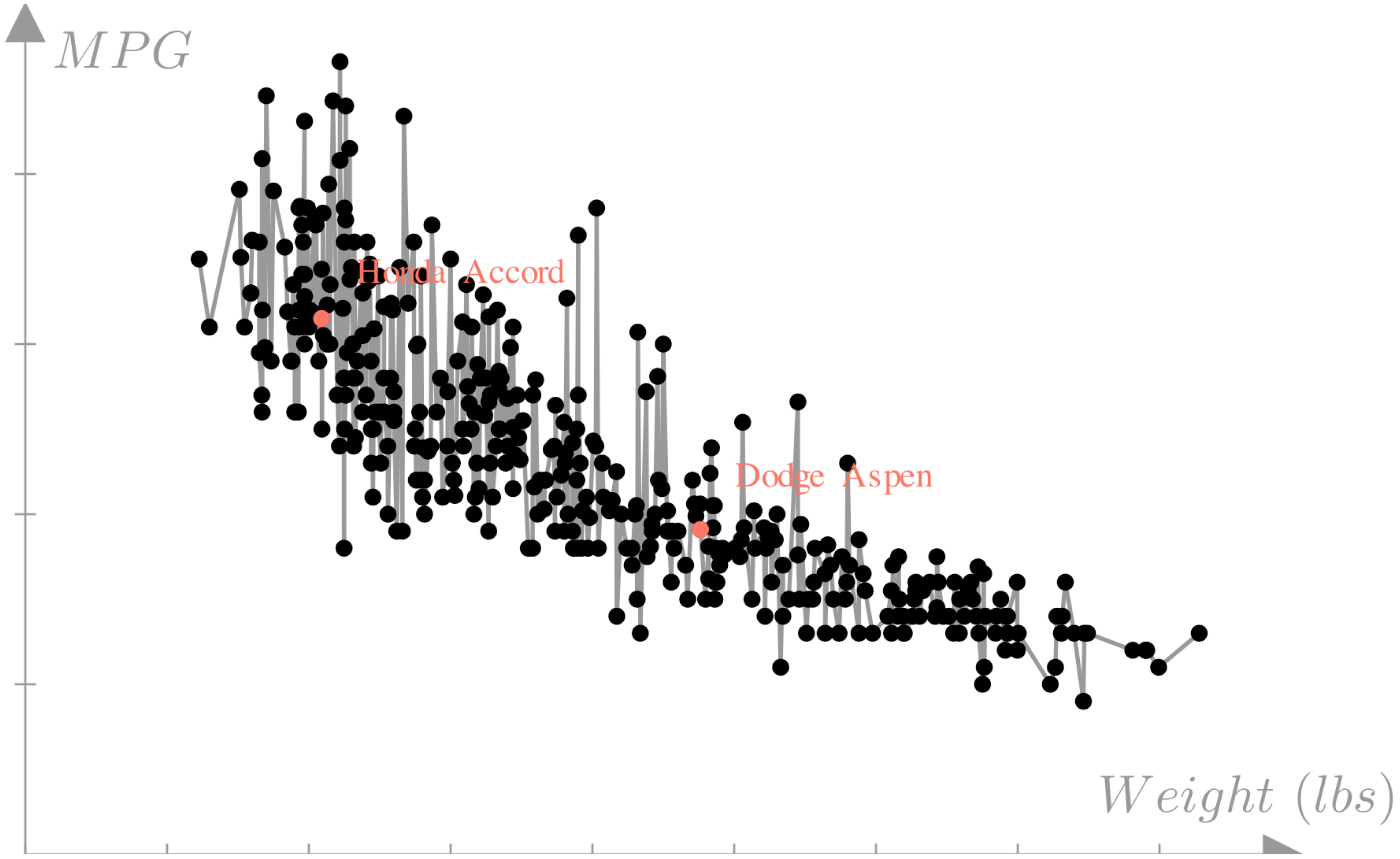
$$\text{mpg} = f(\text{weight},\ \text{horsepower}\dots)$$

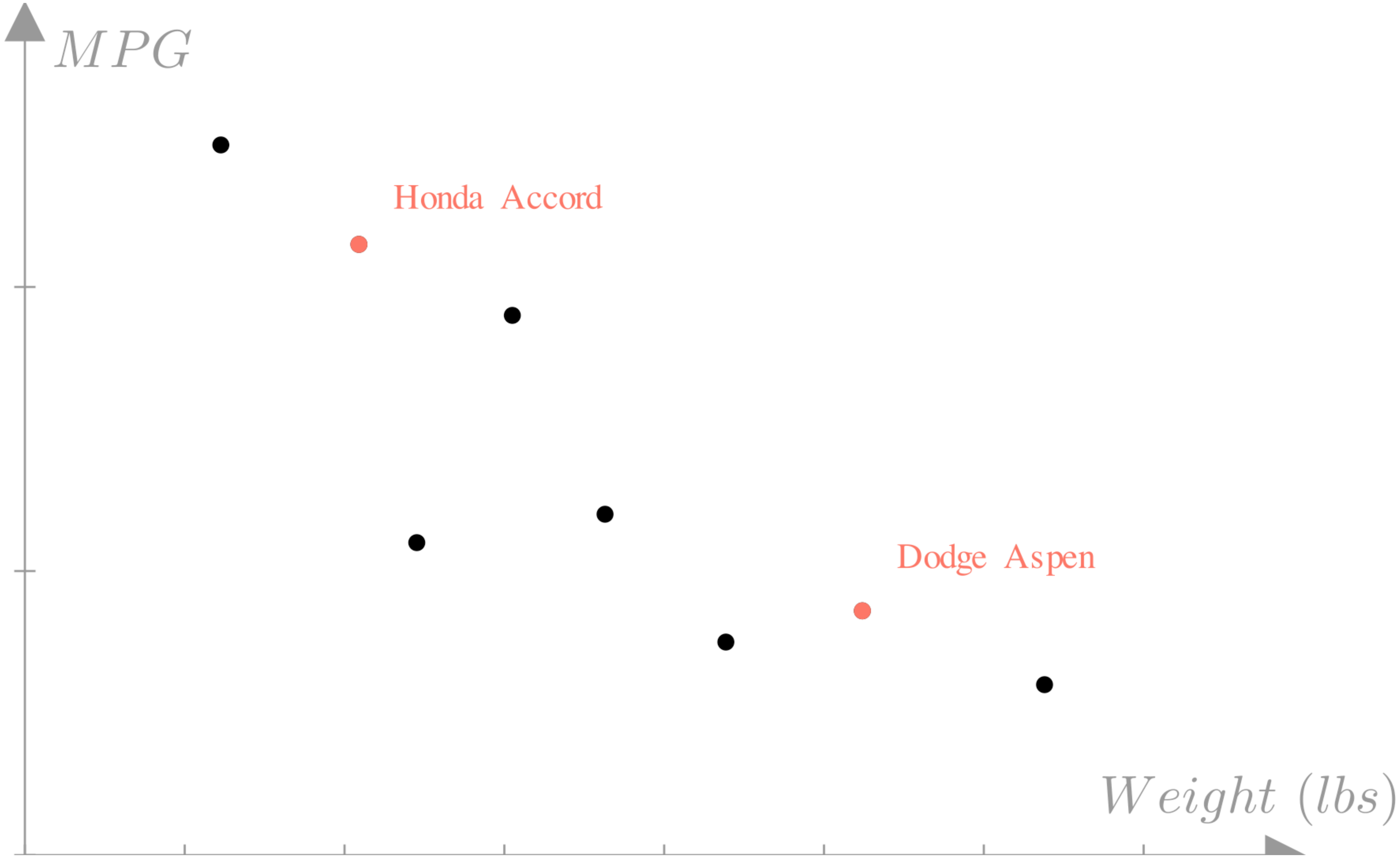
$$\text{Input: } \mathbf{x}_i = \begin{bmatrix} \text{Weight} \\ \text{Horsepower} \\ \text{Displacement} \\ \text{0-60mph} \end{bmatrix}, \quad \text{Output: } y_i = MPG$$





MPG
Honda Accord
Dodge Aspen
Weight (lbs)


MPG
Honda Accord
Dodge Aspen
Weight (lbs)



MPG
Honda Accord
Dodge Aspen
$Weight\ (lbs)$

A *linear function* is any function f where the following conditions always hold:

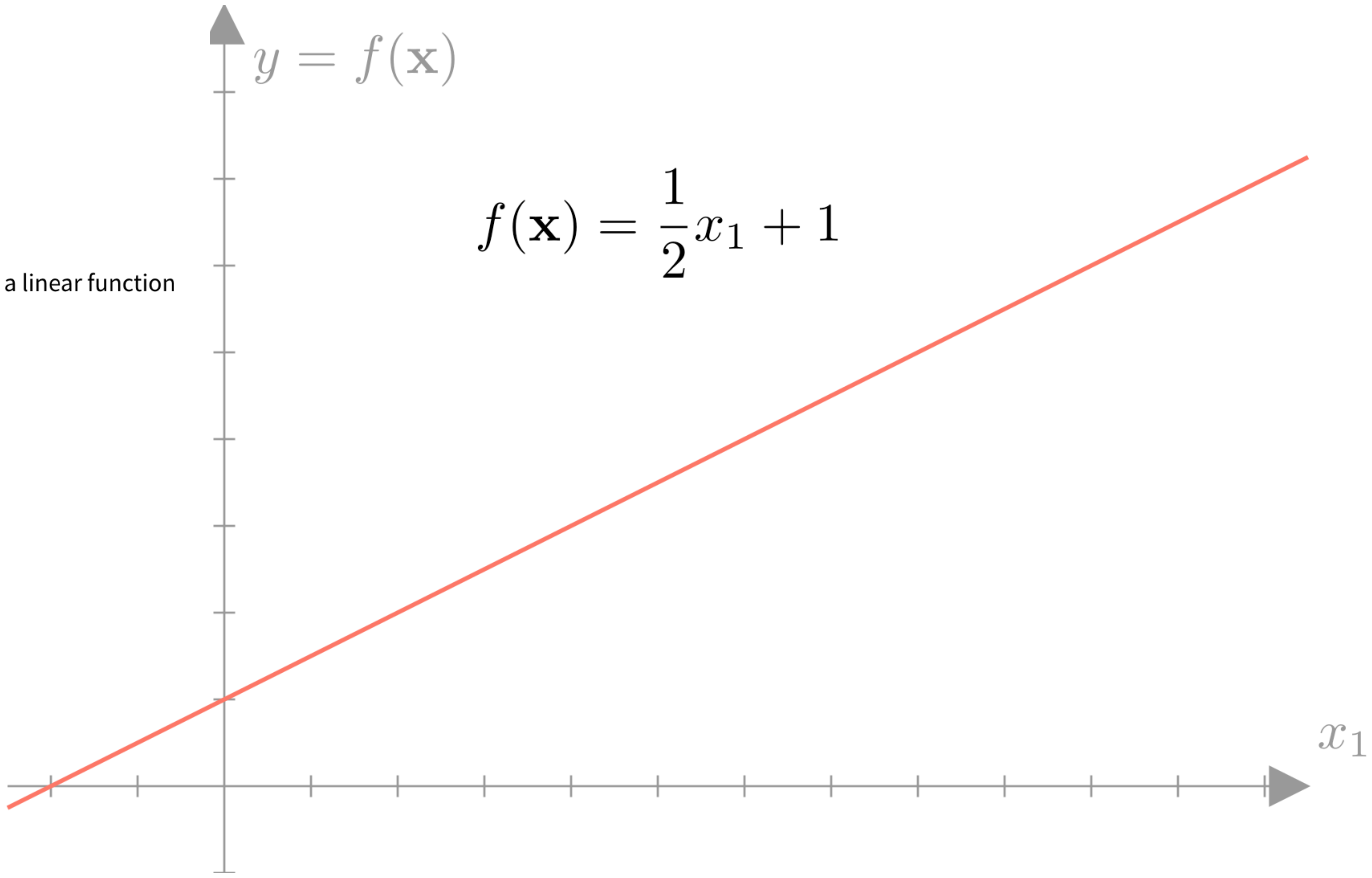
$$f(\mathbf{x} + \mathbf{y}) = f(\mathbf{x}) + f(\mathbf{y})$$

and

$$f(a\mathbf{x}) = af(\mathbf{x})$$

For a linear function, the output can be defined as a weighted sum of the inputs. In other words a linear function of a vector can always be written as:

$$f(\mathbf{x}) = \sum_{i=1}^{n} x_i w_i$$

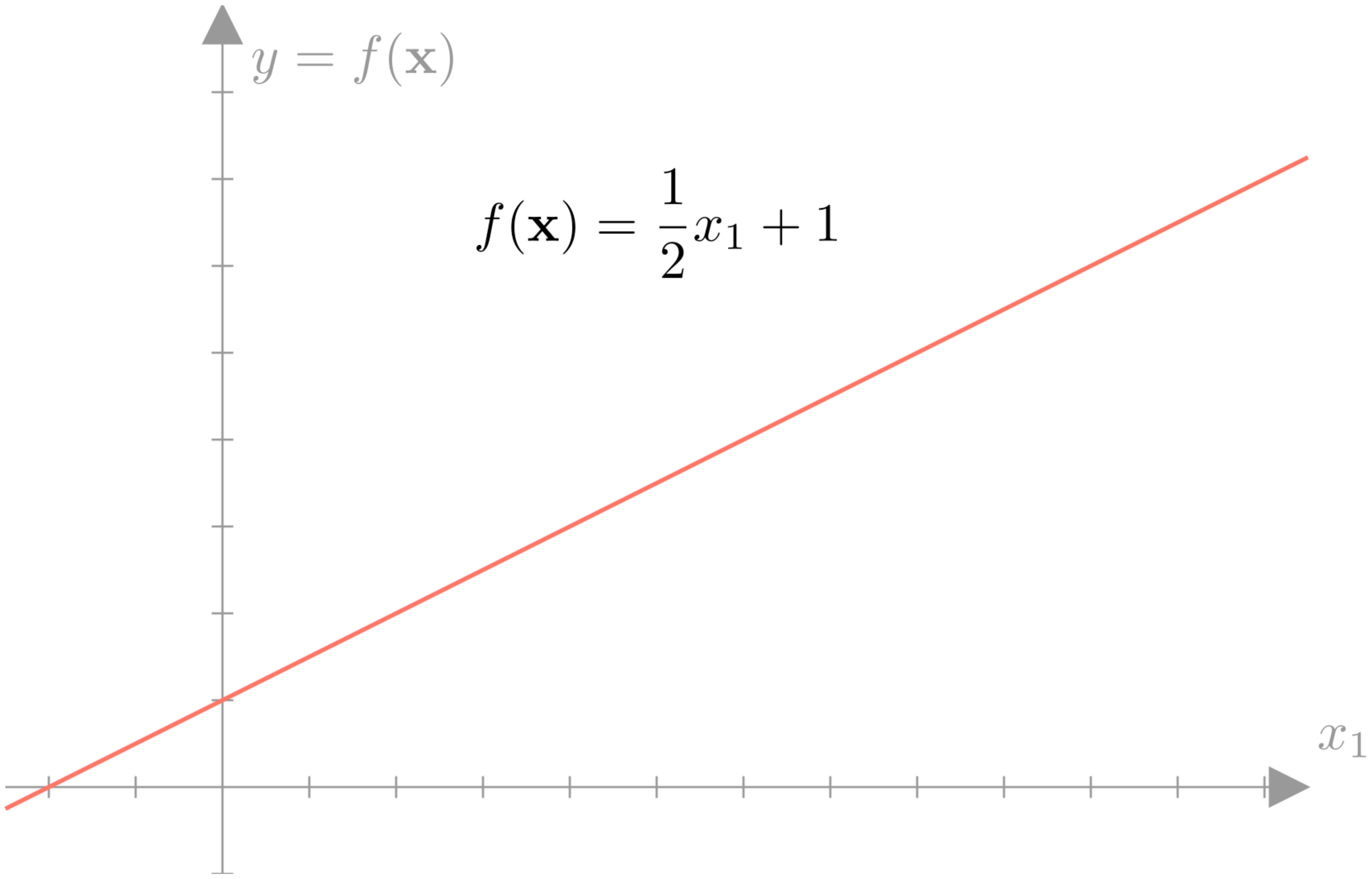


We can add an offset b to create an *affine* function:

$$f(\mathbf{x}) = \sum_{i=1}^{n} x_i w_i + b$$

In numpy we can easily write a function of this form:

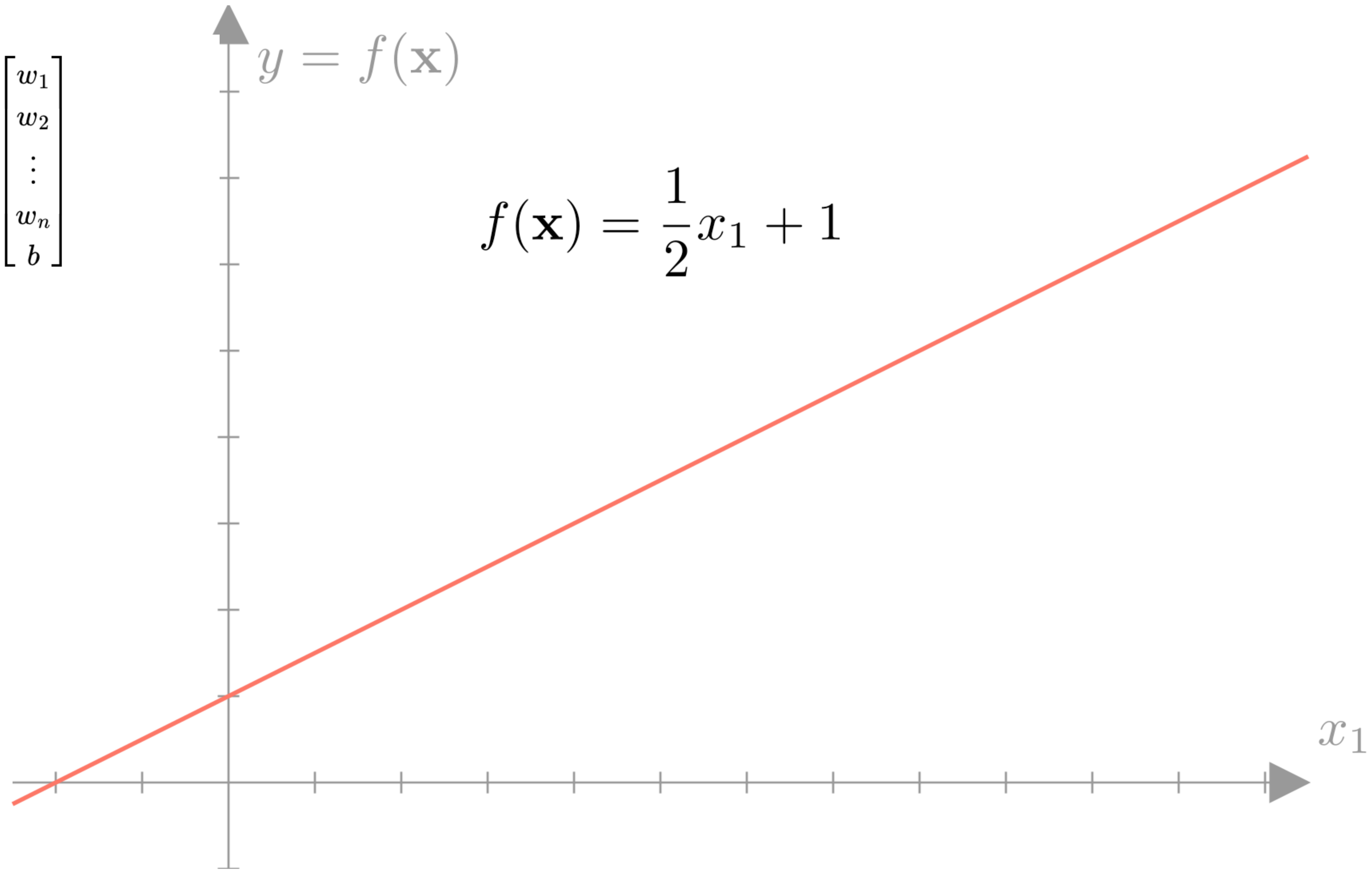
```
def f(x):
    w = np.array([-0.6, -0.2])
    b = -1
    return np.dot(x, w) + b
```

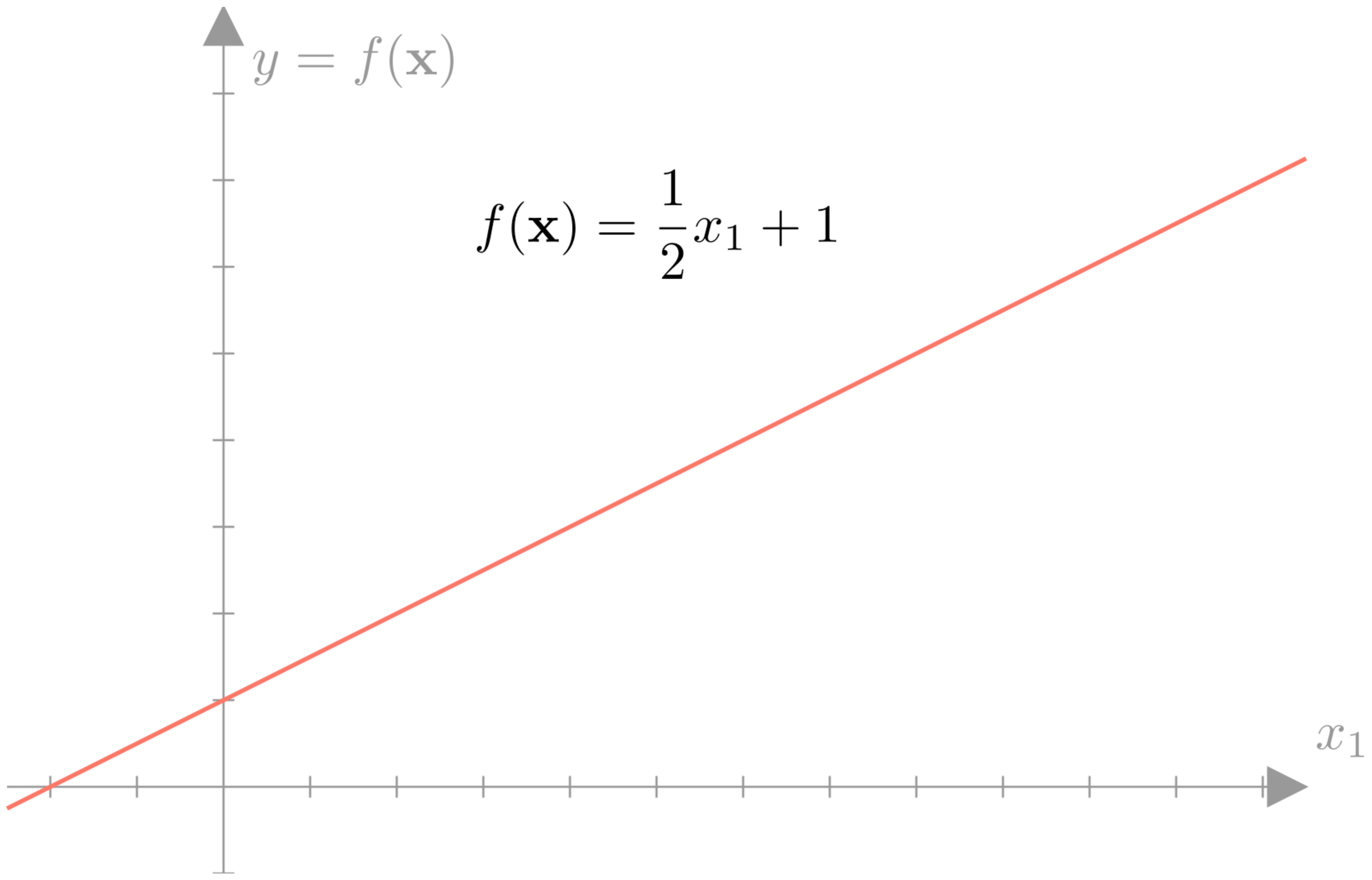


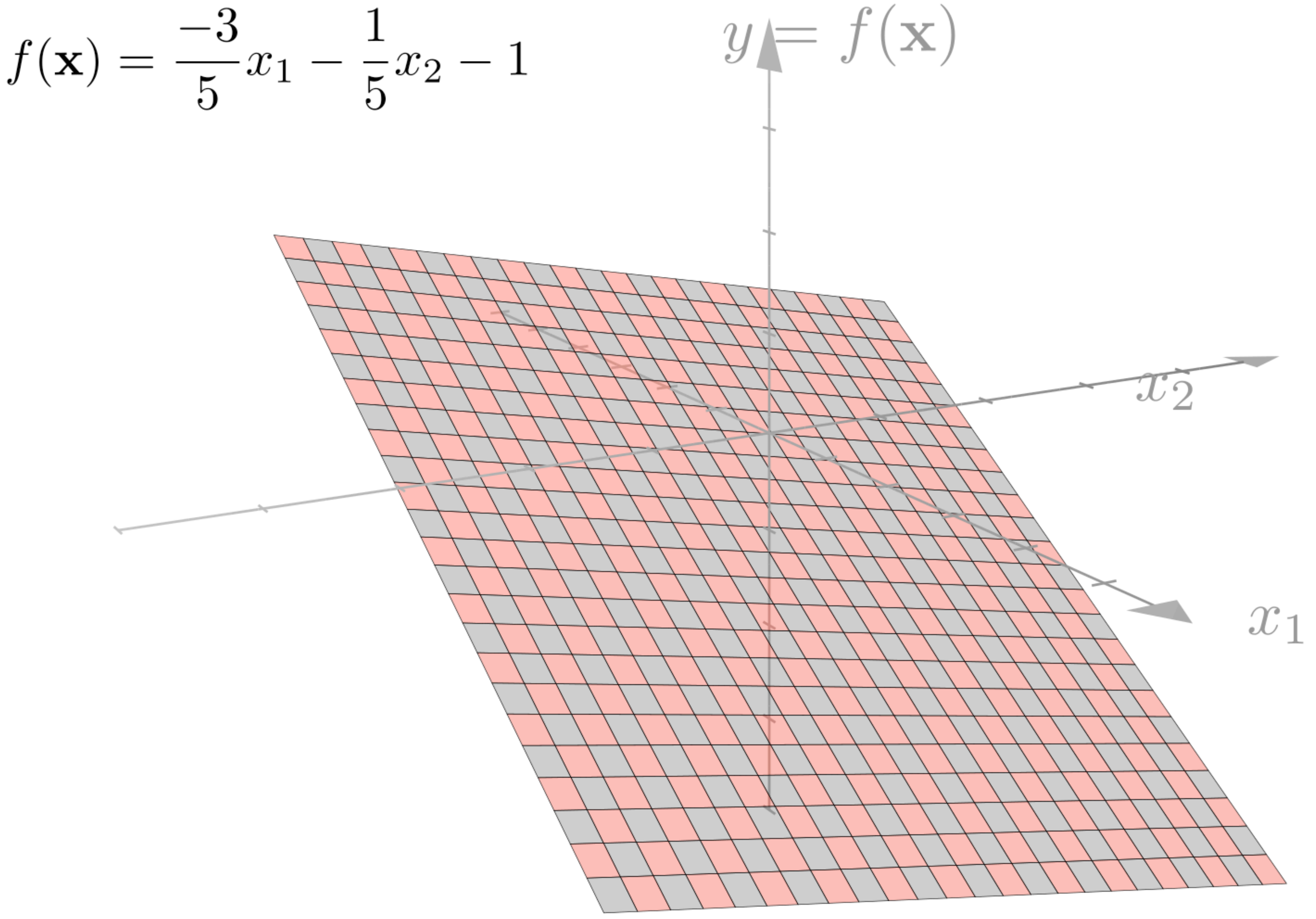
$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \longrightarrow \mathbf{x}_{aug} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \\ 1 \end{bmatrix} \quad \text{and} \quad \mathbf{w} = \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \end{bmatrix} \longrightarrow \mathbf{w}_{aug} = \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \\ b \end{bmatrix}$$

We can easily see then that using this notation:

$$f(\mathbf{x}) = \mathbf{x}^T\mathbf{w} + b = \mathbf{x}_{aug}^T\mathbf{w}_{aug}$$




$y = f(\mathbf{x})$
$f(\mathbf{x}) = \frac{1}{2}x_1 + 1$
x_1


$f(\mathbf{x}) = \frac{-3}{5}x_1 - \frac{1}{5}x_2 - 1$
$y = f(\mathbf{x})$
x_2
x_1

Linear regression is the approach of modeling an unknown function with a linear function. From our discussion of linear functions, we know that this means that we will make predictions using a function of the form:

$$f(\mathbf{x}) = \mathbf{x}^T\mathbf{w} = \sum_{i=1}^{n} x_i w_i$$

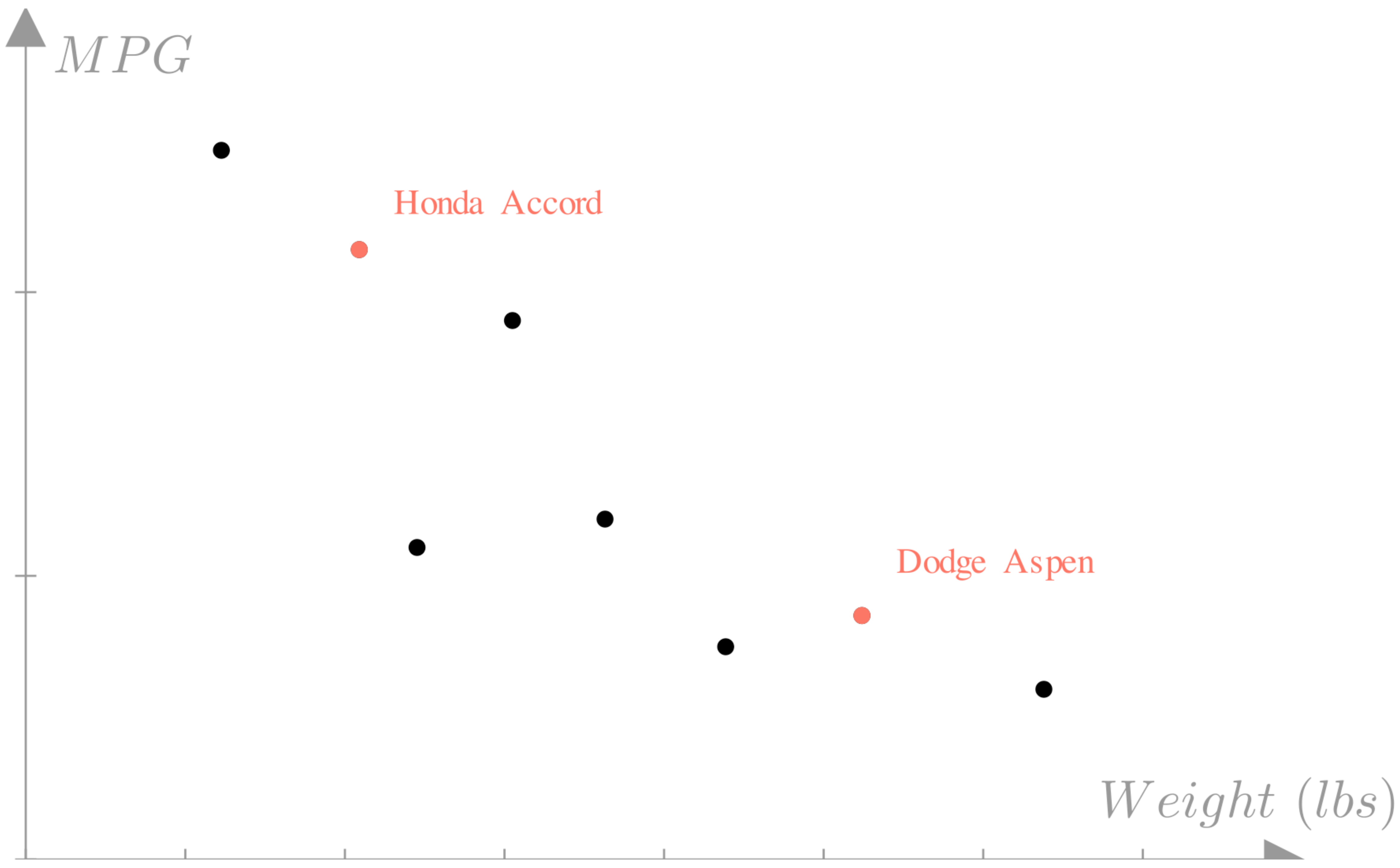
Meaning that the output will be a weighted sum of the *features* of the input. In the case of our car example, we will make predictions as:

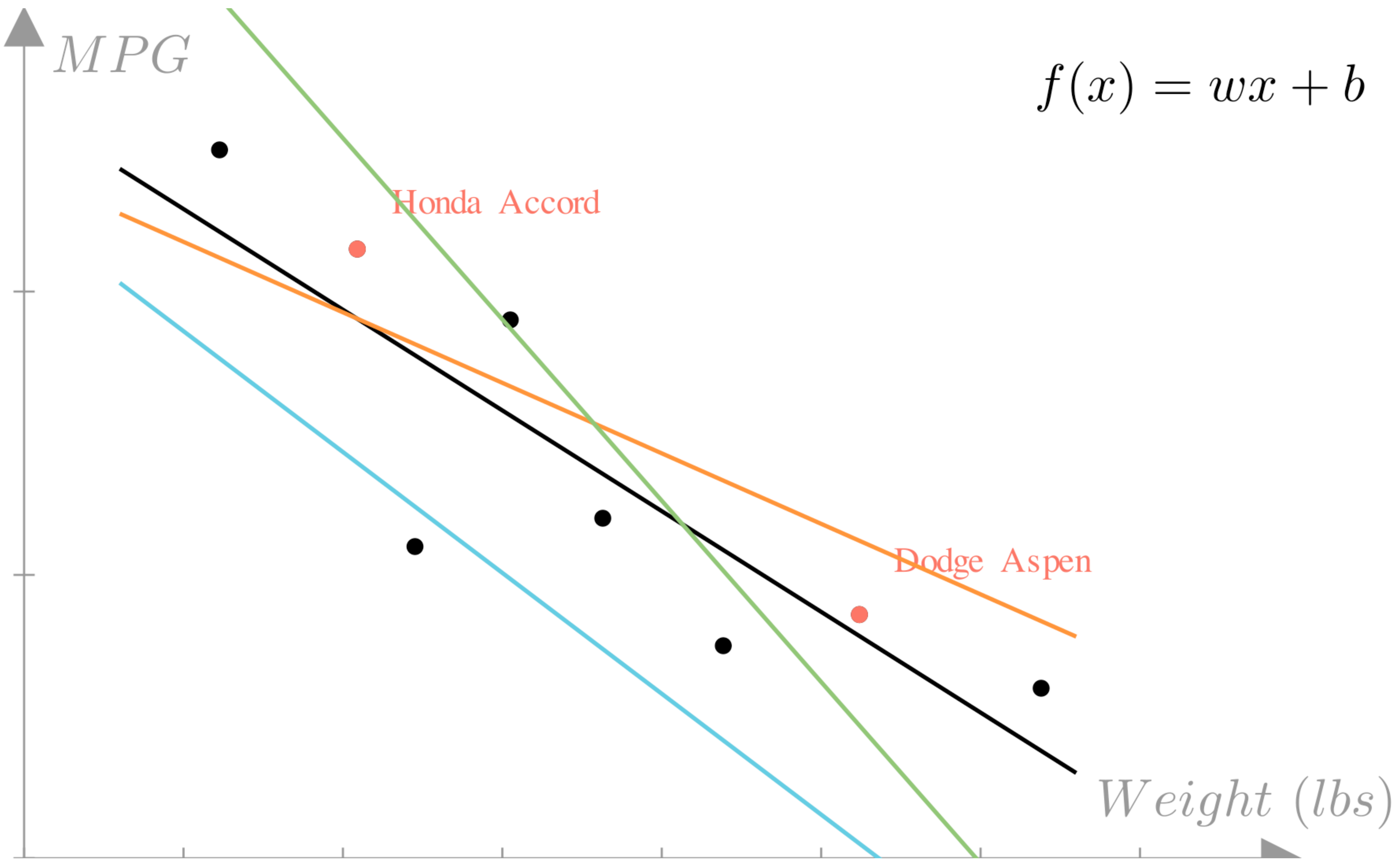
$$\text{Predicted MPG} = f(\mathbf{x}) =$$

$$(\text{weight})w_1 + (\text{horsepower})w_2 + (\text{displacement})w_3 + (\text{0-60mph})w_4 + b$$

Or in matrix notation:

$$f(\mathbf{x}) = \begin{bmatrix} \text{Weight} \\ \text{Horsepower} \\ \text{Displacement} \\ \text{0-60mph} \\ 1 \end{bmatrix} \cdot \begin{bmatrix} w_1 \\ w_2 \\ w_3 \\ w_4 \\ b \end{bmatrix}$$





MPG
$f(x) = wx + b$
Honda Accord
Dodge Aspen
$Weight\ (lbs)$

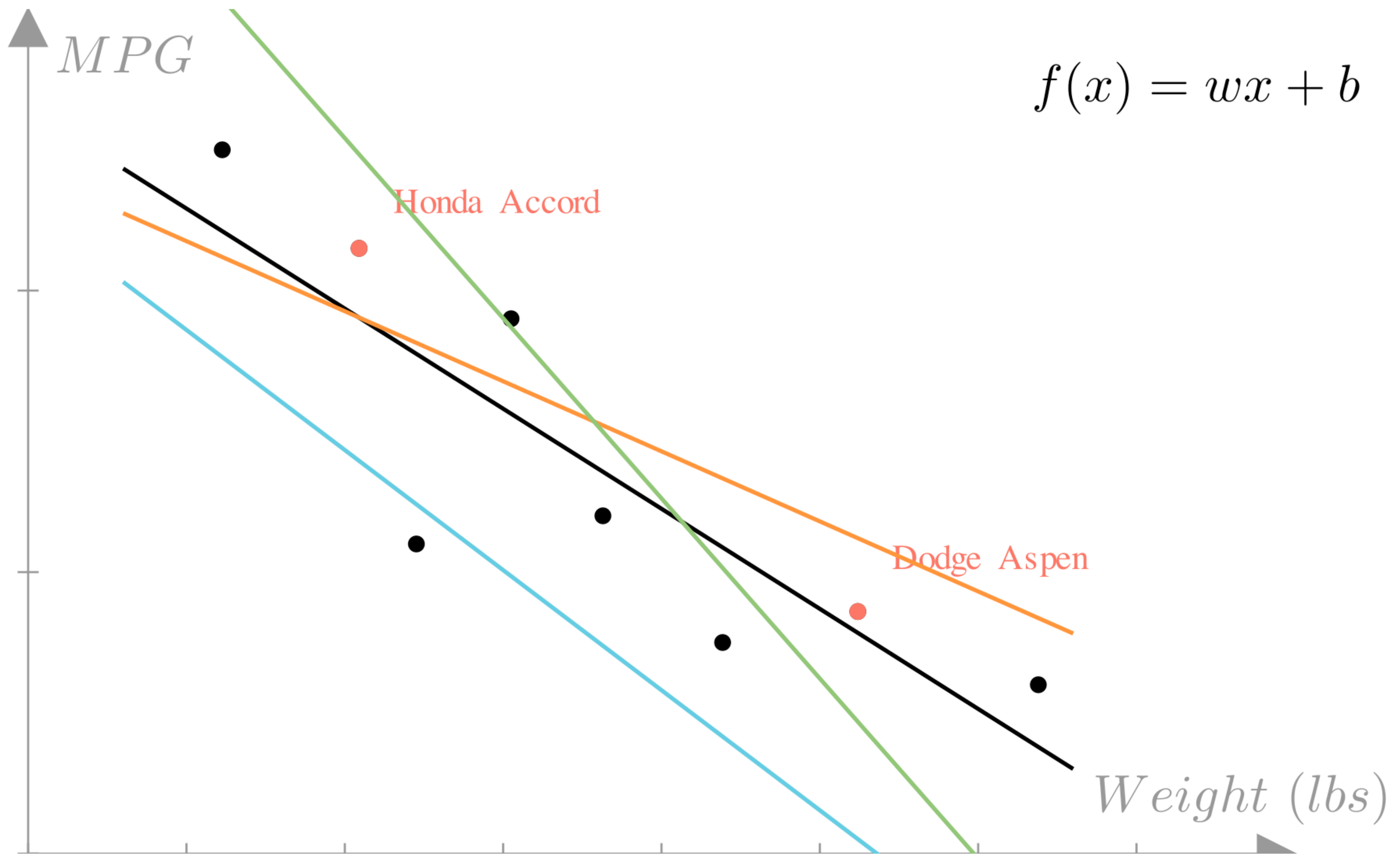
$$f(\mathbf{x}) = \sum_{i=1}^{n} x_i w_i + b$$

We typically refer to $\mathbf{w}$ specifically as the **weight vector** (or weights) and b as the **bias**. To summarize:

$$\textbf{Affine function: } f(\mathbf{x}) = \mathbf{x}^T\mathbf{w} + b, \quad \textbf{Parameters:} \quad \big(\text{Weights: } \mathbf{w},\ \text{Bias: } b\big)$$

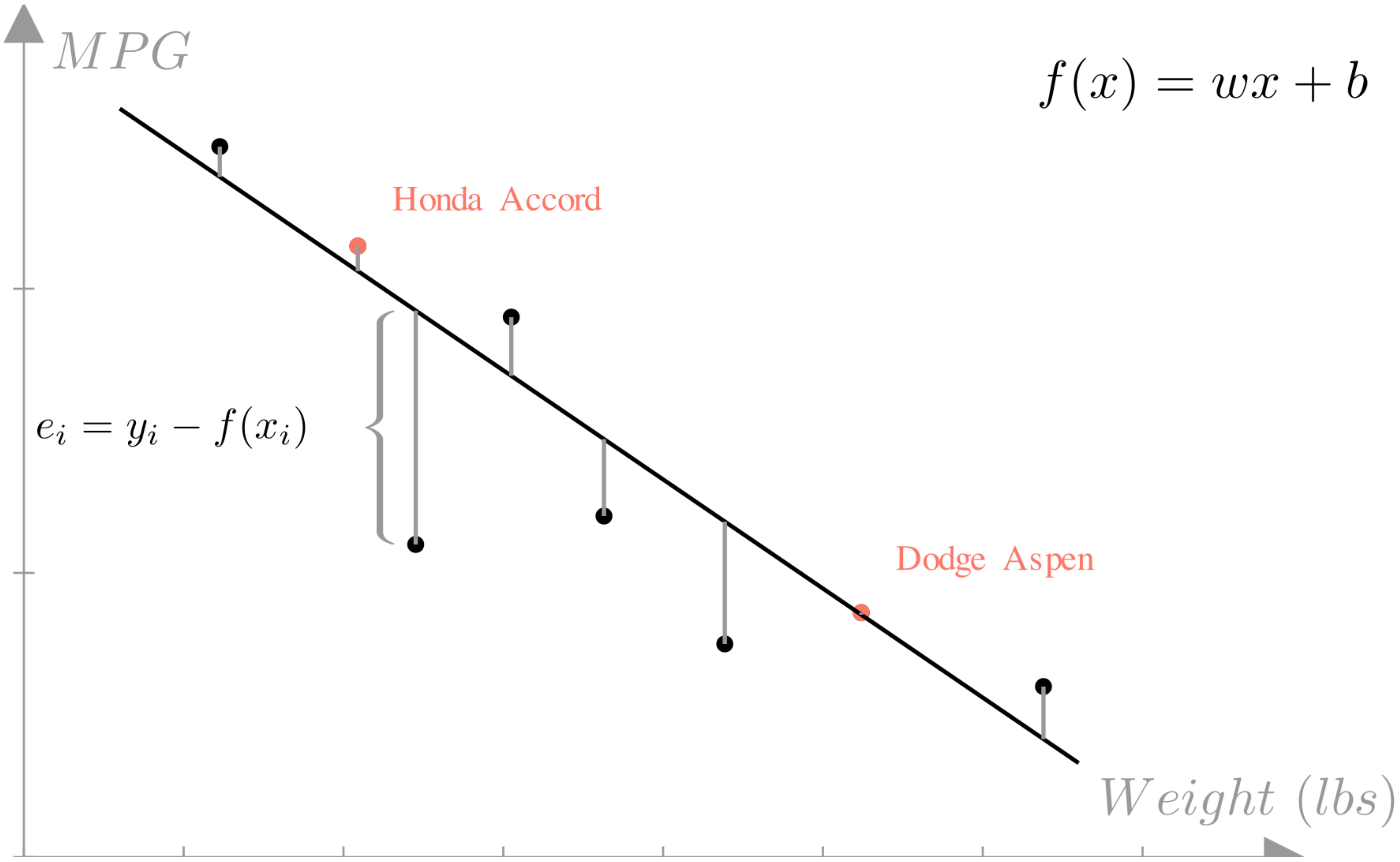
```
class Regression:
    def __init__(self, weights):
        self.weights = weights

    def predict(self, x):
        return np.dot(x, self.weights)
```



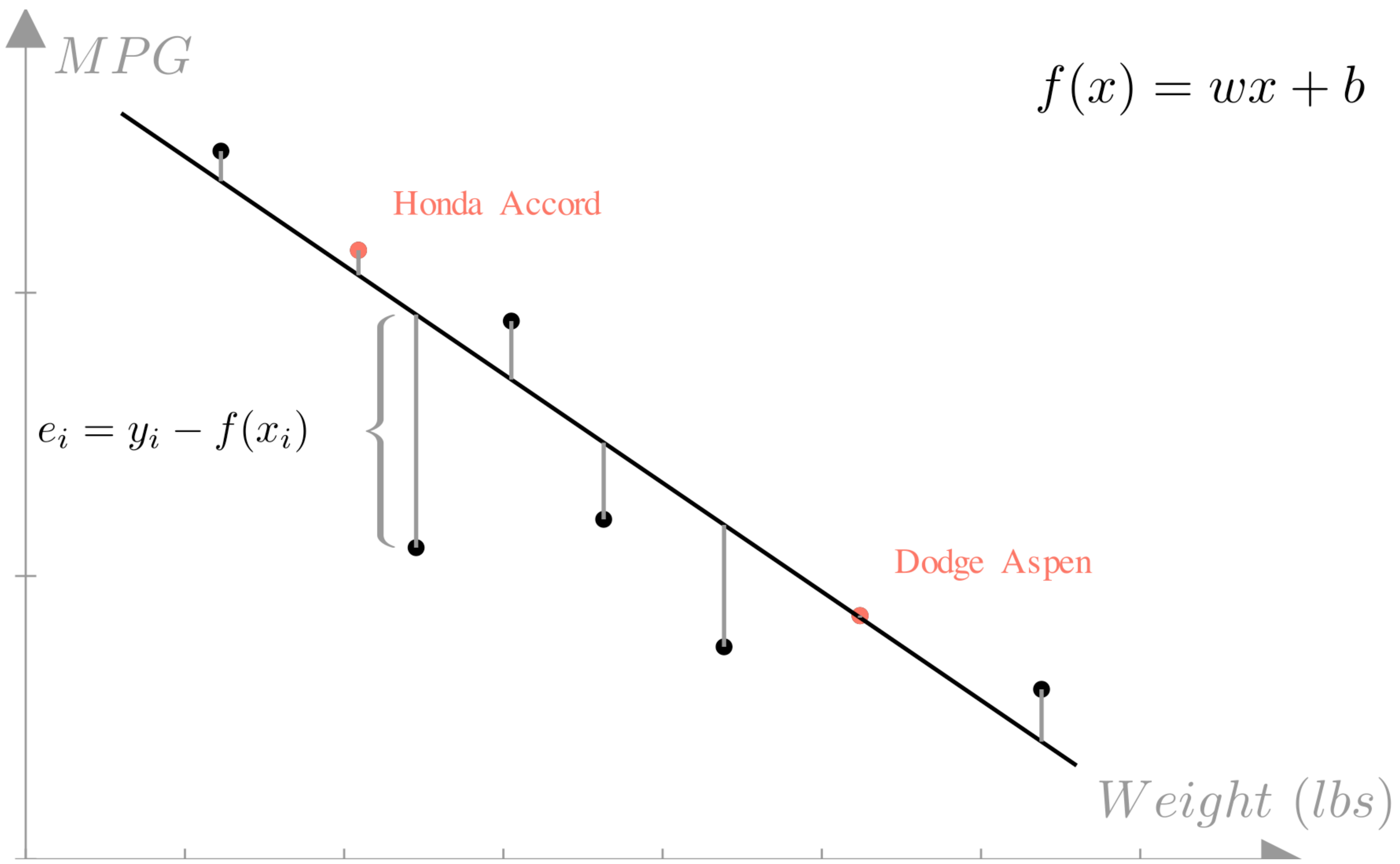
The **residual** or **error** of a prediction is the difference between the prediction and the true output:

$$e_i = y_i - f(\mathbf{x}_i)$$



$$\mathcal{D} = \{(\mathbf{x}_1, y_1),\ (\mathbf{x}_2, y_2),\ \dots\ (\mathbf{x}_N, y_N)\}$$

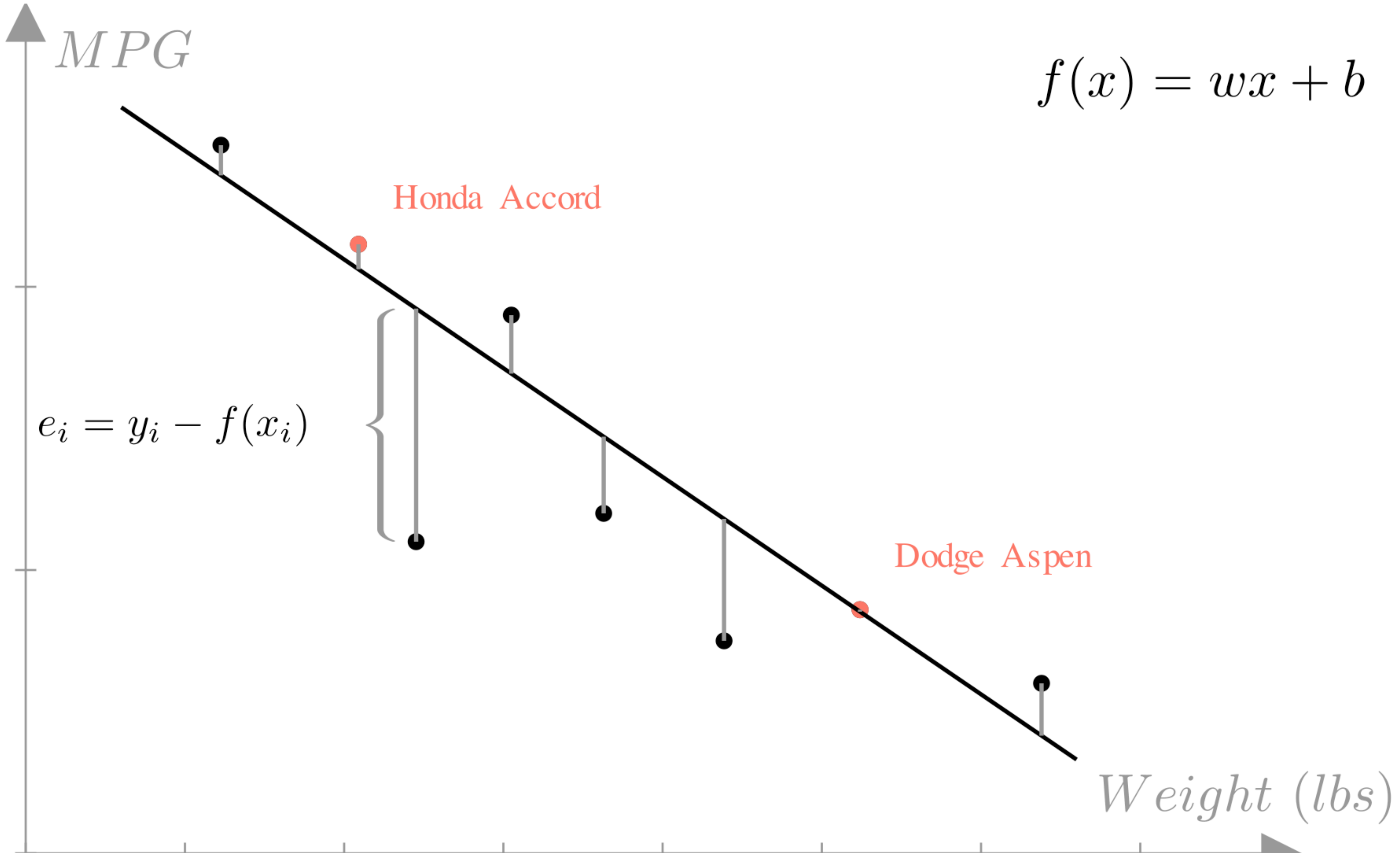
$$MSE = \frac{1}{N}\sum_{i=1}^{N}(f(\mathbf{x}_i) - y_i)^2 = \frac{1}{N}\sum_{i=1}^{N}(\mathbf{x}_i^T\mathbf{w} - y_i)^2$$



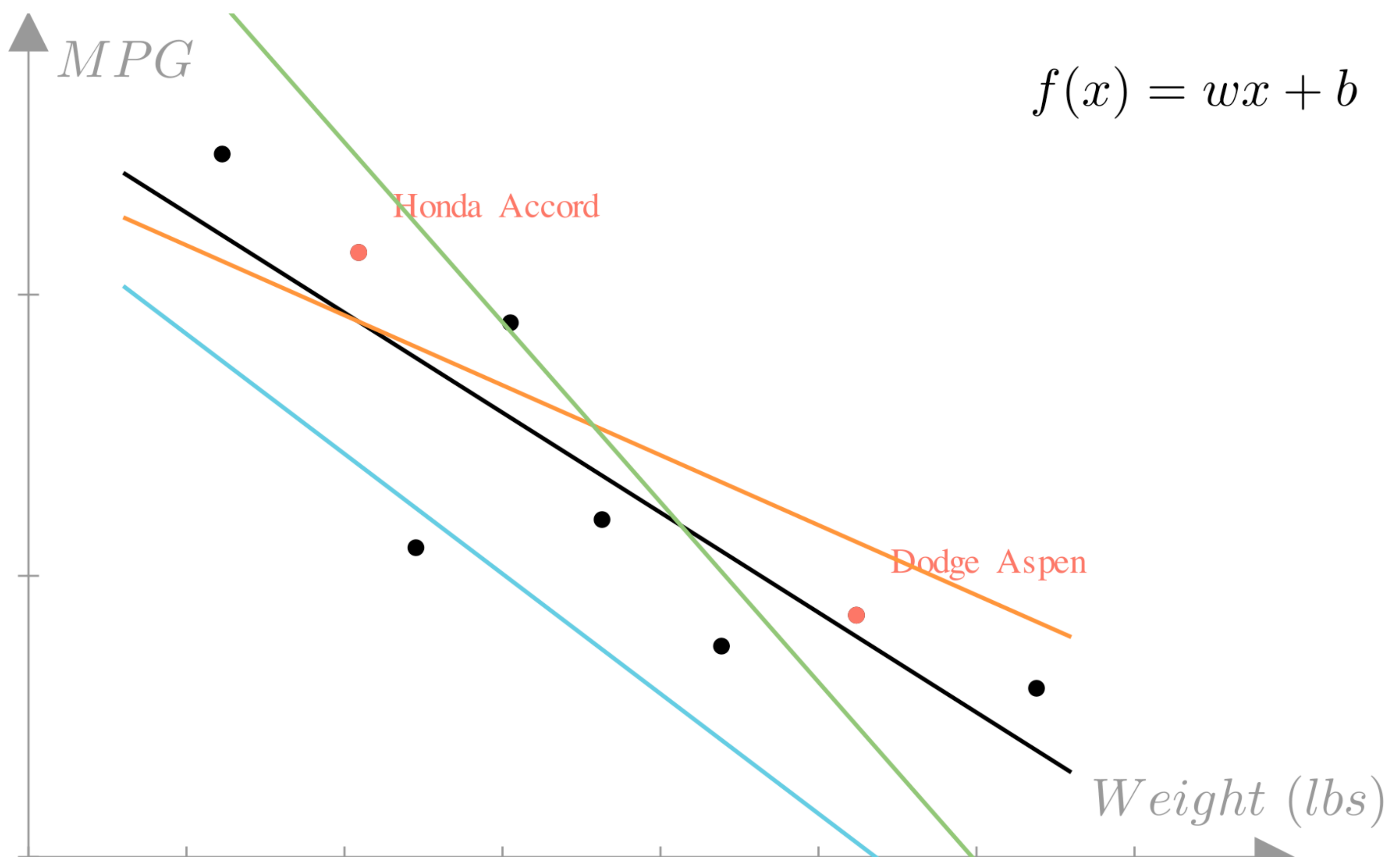
$$\mathcal{D} = \{(\mathbf{x}_1, y_1),\ (\mathbf{x}_2, y_2),\ \ldots\ (\mathbf{x}_N, y_N)\}$$

$$\mathbf{X} = \begin{bmatrix} \mathbf{x}_1^T \\ \mathbf{x}_2^T \\ \vdots \\ \mathbf{x}_N^T \end{bmatrix} = \begin{bmatrix} x_{11} & x_{12} & \ldots & x_{1n} \\ x_{21} & x_{22} & \ldots & x_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ x_{N1} & x_{N2} & \ldots & x_{Nn} \end{bmatrix}, \quad \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}$$

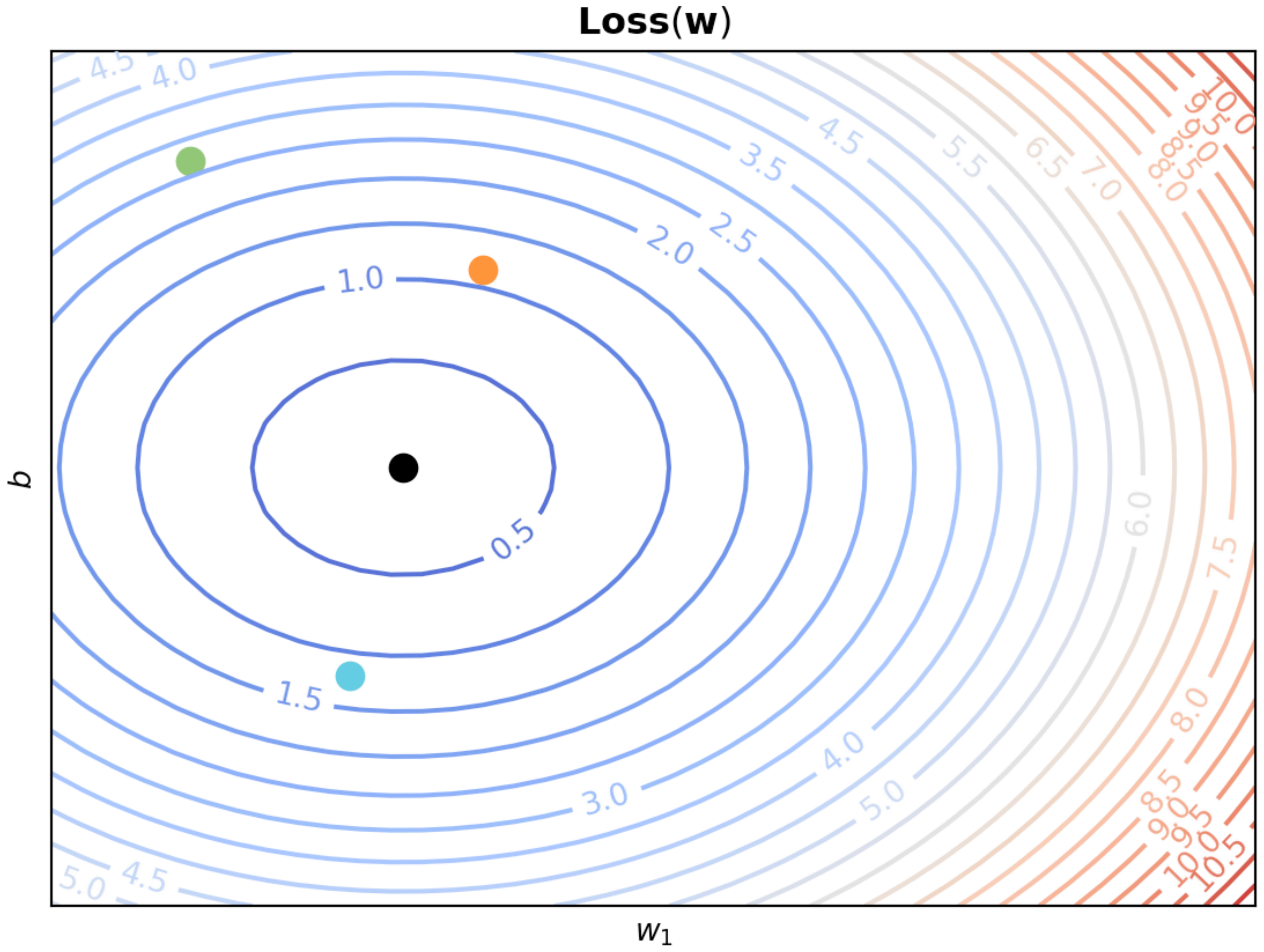
$$MSE(\mathbf{w}, \mathbf{X}, \mathbf{y}) = \frac{1}{N} \sum_{i=1}^{N} (\mathbf{x}_i^T \mathbf{w} - y_i)^2$$



$$\mathbf{Loss}(\mathbf{w}) = MSE(\mathbf{w}, \mathbf{X}, \mathbf{y}) = \frac{1}{N}\sum_{i=1}^{N}(\mathbf{x}_i^T\mathbf{w} - y_i)^2$$

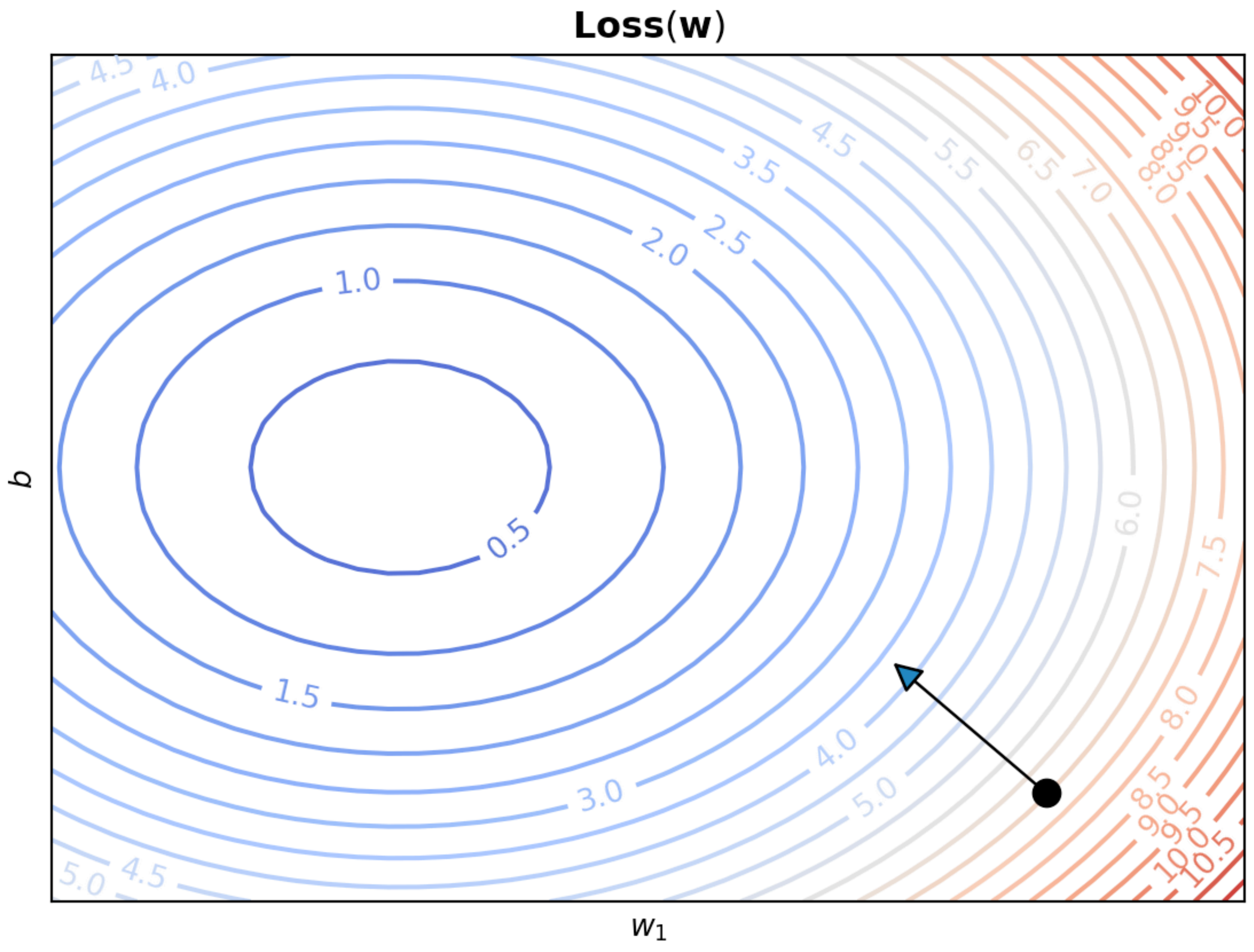


$$\mathbf{w}^* = \underset{\mathbf{w}}{\text{argmin}}\ \mathbf{Loss}(\mathbf{w}) = \underset{\mathbf{w}}{\text{argmin}}\frac{1}{N}\sum_{i=1}^{N}(\mathbf{x}_i^T\mathbf{w} - y_i)^2$$



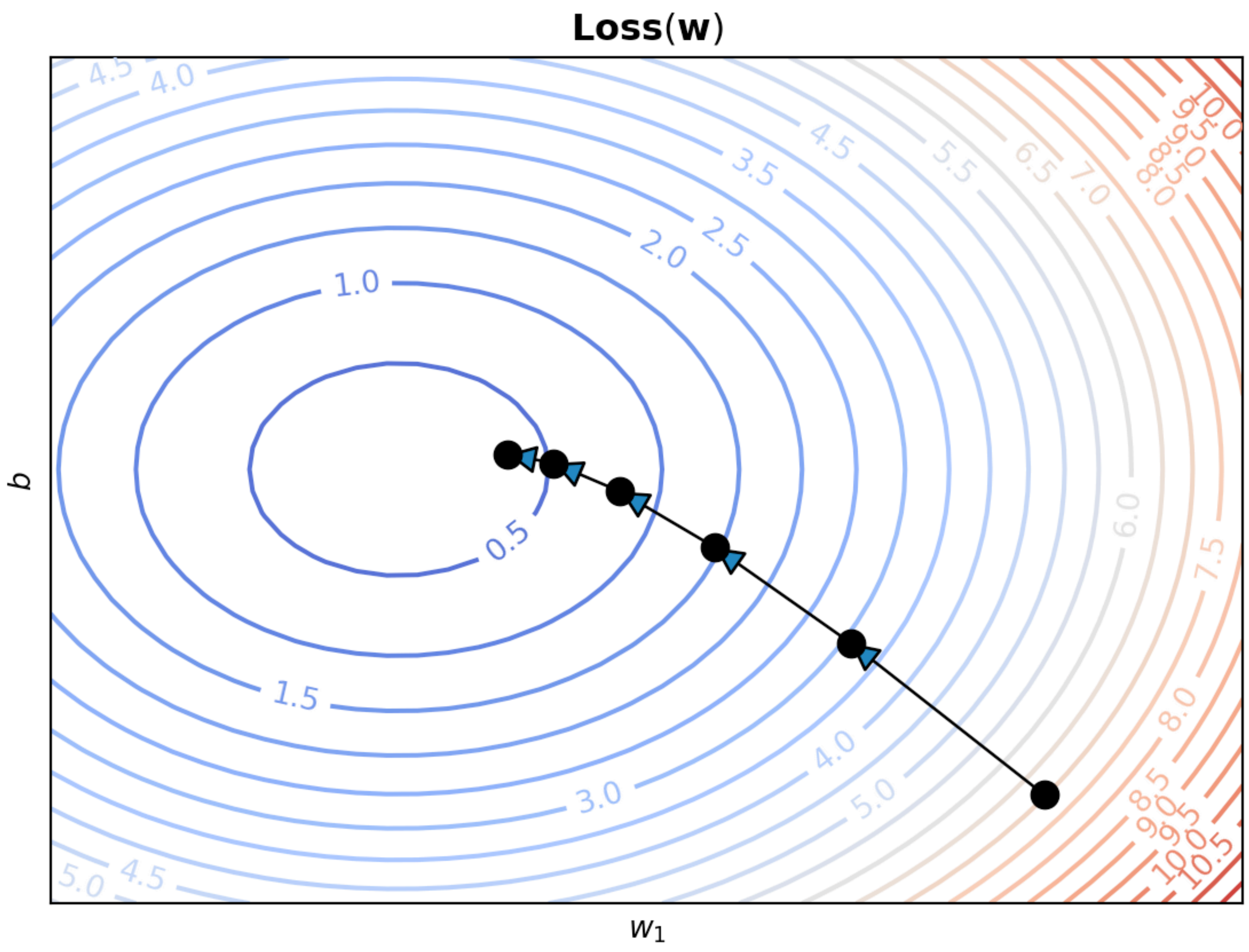
$$\text{Find: } \mathbf{w}^* = \underset{\mathbf{w}}{\operatorname{argmin}}\ f(\mathbf{w})$$

$$\mathbf{w}^{(1)} \leftarrow \mathbf{w}^{(0)} + \mathbf{g}$$



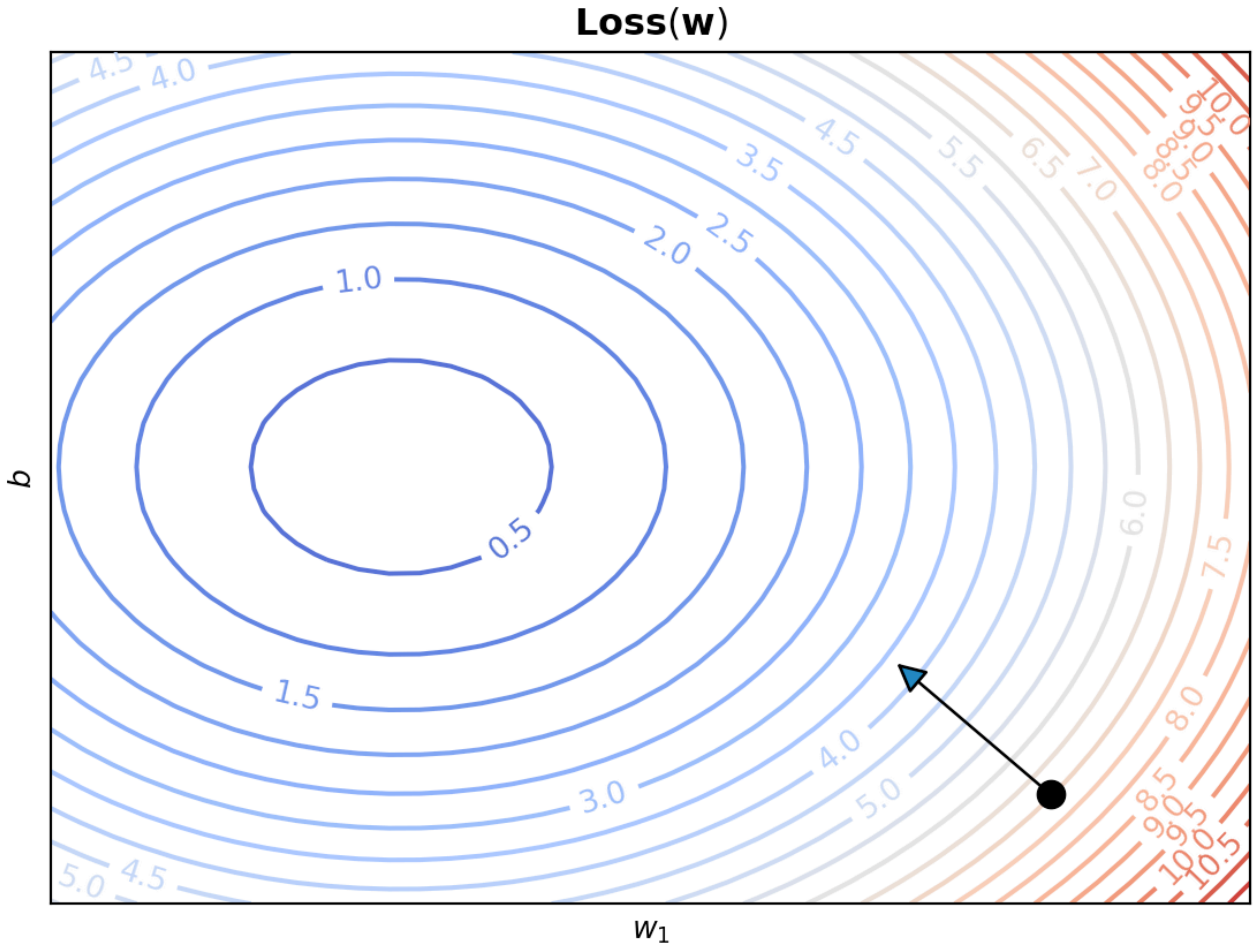
$$\text{Find: } \mathbf{w}^* = \underset{\mathbf{w}}{\operatorname{argmin}}\ f(\mathbf{w})$$

$$\mathbf{w}^{(1)} \leftarrow \mathbf{w}^{(0)} + \mathbf{g}$$



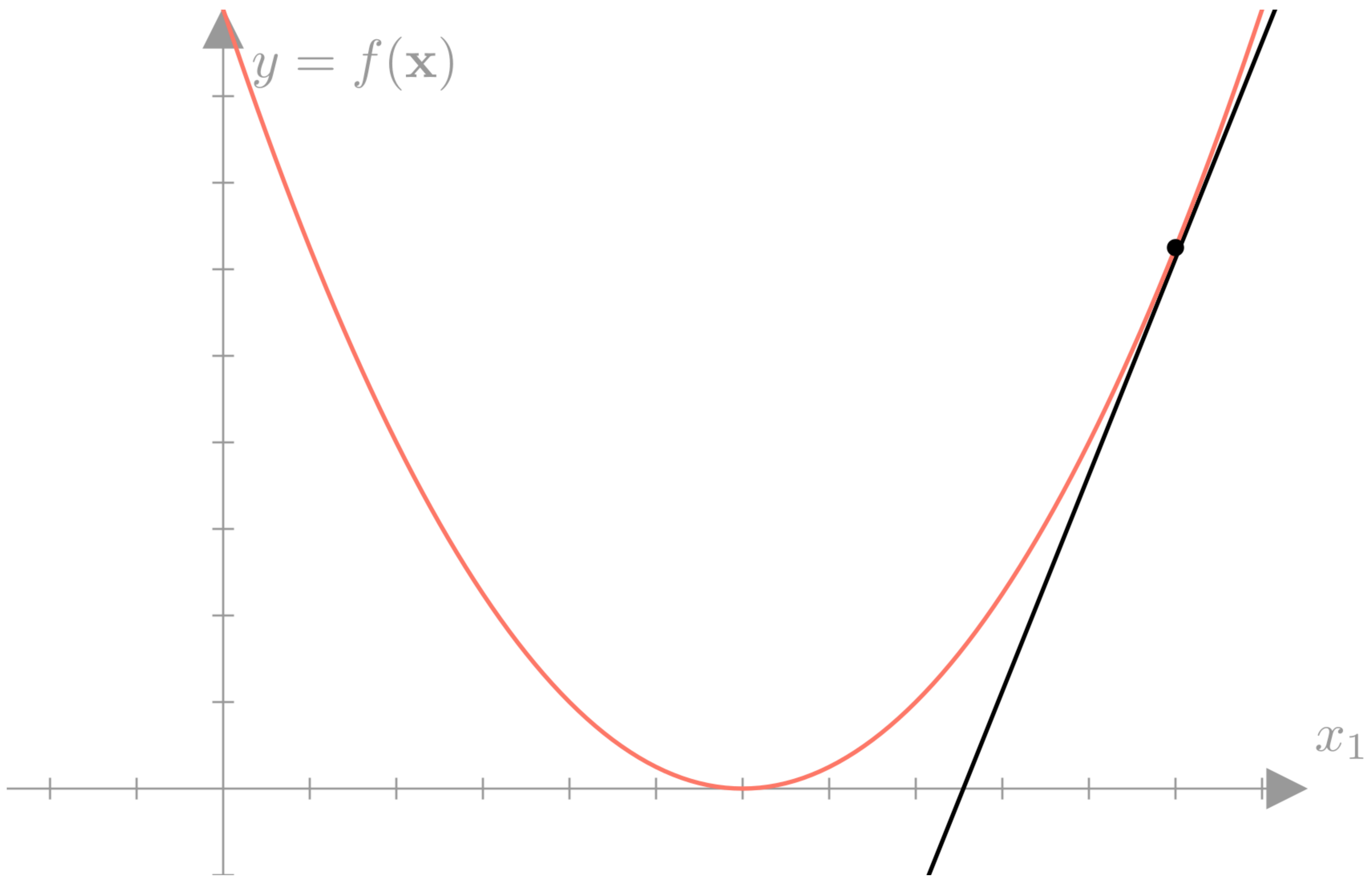
$$\text{Find: } \mathbf{w}^* = \underset{\mathbf{w}}{\operatorname{argmin}} \; f(\mathbf{w})$$

$$\mathbf{w}^{(1)} \leftarrow \mathbf{w}^{(0)} - \nabla f(\mathbf{w}^{(0)})$$



Find: $\mathbf{w}^* = \underset{\mathbf{w}}{\operatorname{argmin}}\, f(\mathbf{w})$

$$\mathbf{w}^{(1)} \leftarrow \mathbf{w}^{(0)} + \mathbf{g}$$



The **gradient** of a vector-input function is a vector such that each element is the partial derivative of the function with respect to the corresponding element of the input vector. We'll use the same notation as derivatives for gradients.

$$\frac{df}{d\mathbf{x}} = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \\ \frac{\partial f}{\partial x_3} \\ \vdots \end{bmatrix}$$

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \qquad \frac{\partial}{\partial x_1}\mathbf{x}^T\mathbf{x} =$$

The **gradient** of a vector-input function is a vector such that each element is the partial derivative of the function with respect to the corresponding element of the input vector. We'll use the same notation as derivatives for gradients.

$$\frac{df}{d\mathbf{x}} = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \\ \frac{\partial f}{\partial x_3} \\ \vdots \end{bmatrix}$$

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \qquad \frac{\partial}{\partial x_1}\mathbf{x}^T\mathbf{x} =$$

$$\frac{d}{d\mathbf{x}}\mathbf{x}^T\mathbf{x} =$$

The **gradient** of a vector-input function is a vector such that each element is the partial derivative of the function with respect to the corresponding element of the input vector. We'll use the same notation as derivatives for gradients.

$$\frac{df}{d\mathbf{x}} = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \\ \frac{\partial f}{\partial x_3} \\ \vdots \end{bmatrix}$$

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \qquad \frac{\partial}{\partial x_1} f(\mathbf{x}^T\mathbf{x}) =$$

$$\frac{d}{d\mathbf{x}} f(\mathbf{x}^T\mathbf{x}) =$$

The **gradient** of a vector-input function is a vector such that each element is the partial derivative of the function with respect to the corresponding element of the input vector. We'll use the same notation as derivatives for gradients.

$$\frac{df}{d\mathbf{x}} = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \\ \frac{\partial f}{\partial x_3} \\ \vdots \end{bmatrix}$$

$$\frac{\partial}{\partial x} \sum f(x) = \sum \frac{\partial}{\partial x} f(x)$$

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \qquad \frac{\partial}{\partial x_1} \sum_{i=1}^{3} f(x_i) =$$

The **gradient** of a vector-input function is a vector such that each element is the partial derivative of the function with respect to the corresponding element of the input vector. We'll use the same notation as derivatives for gradients.

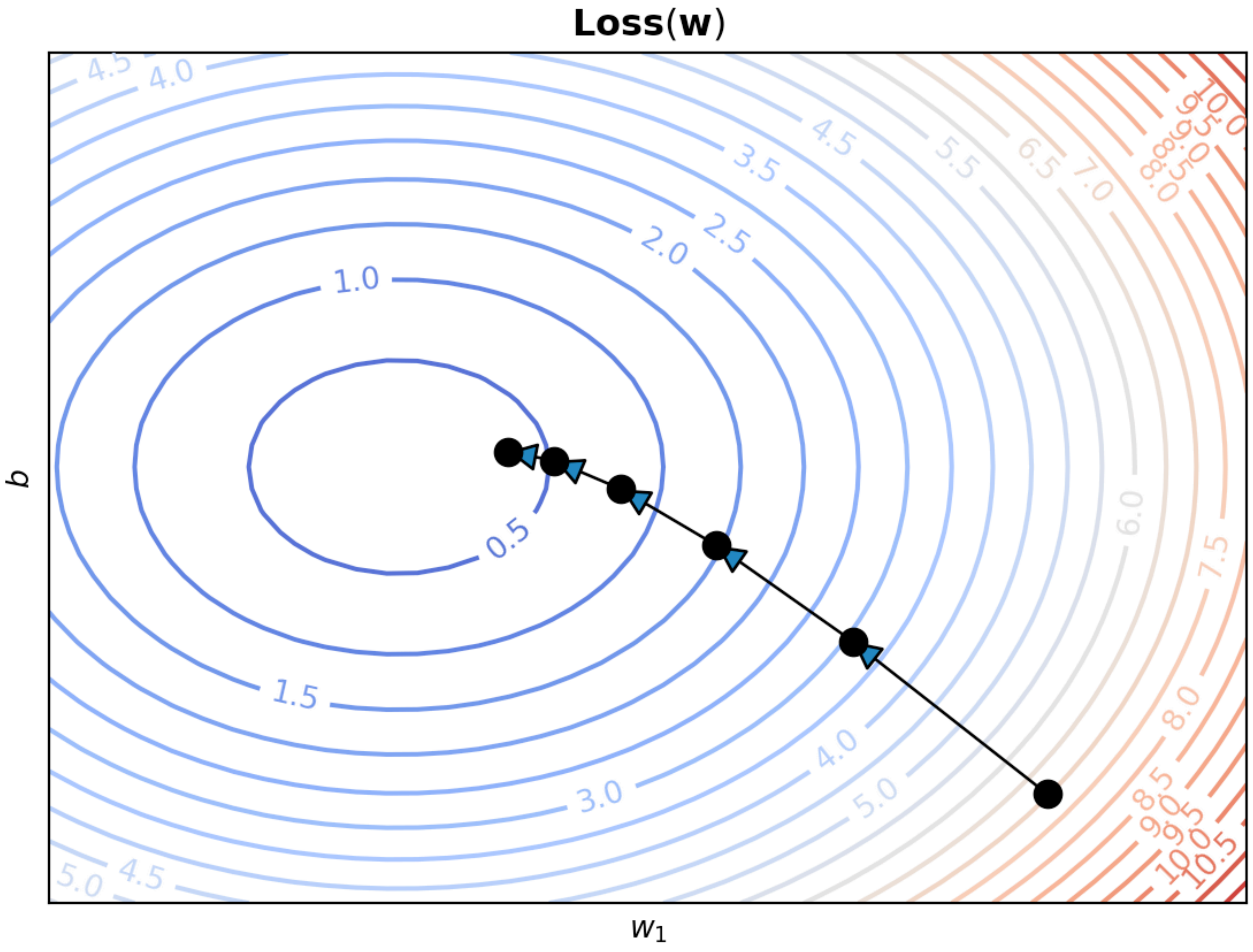
$$\frac{df}{d\mathbf{x}} = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \\ \frac{\partial f}{\partial x_3} \\ \vdots \end{bmatrix}$$

$$\frac{df}{d\mathbf{x}} = \nabla f(\mathbf{x})$$

$$\frac{df}{d\mathbf{x}} = \nabla_{\mathbf{x}} f(\mathbf{x}, \mathbf{y}), \quad \frac{df}{d\mathbf{y}} = \nabla_{\mathbf{y}} f(\mathbf{x}, \mathbf{y})$$

$$\text{Find: } \mathbf{w}^* = \underset{\mathbf{w}}{\operatorname{argmin}} \; f(\mathbf{w})$$

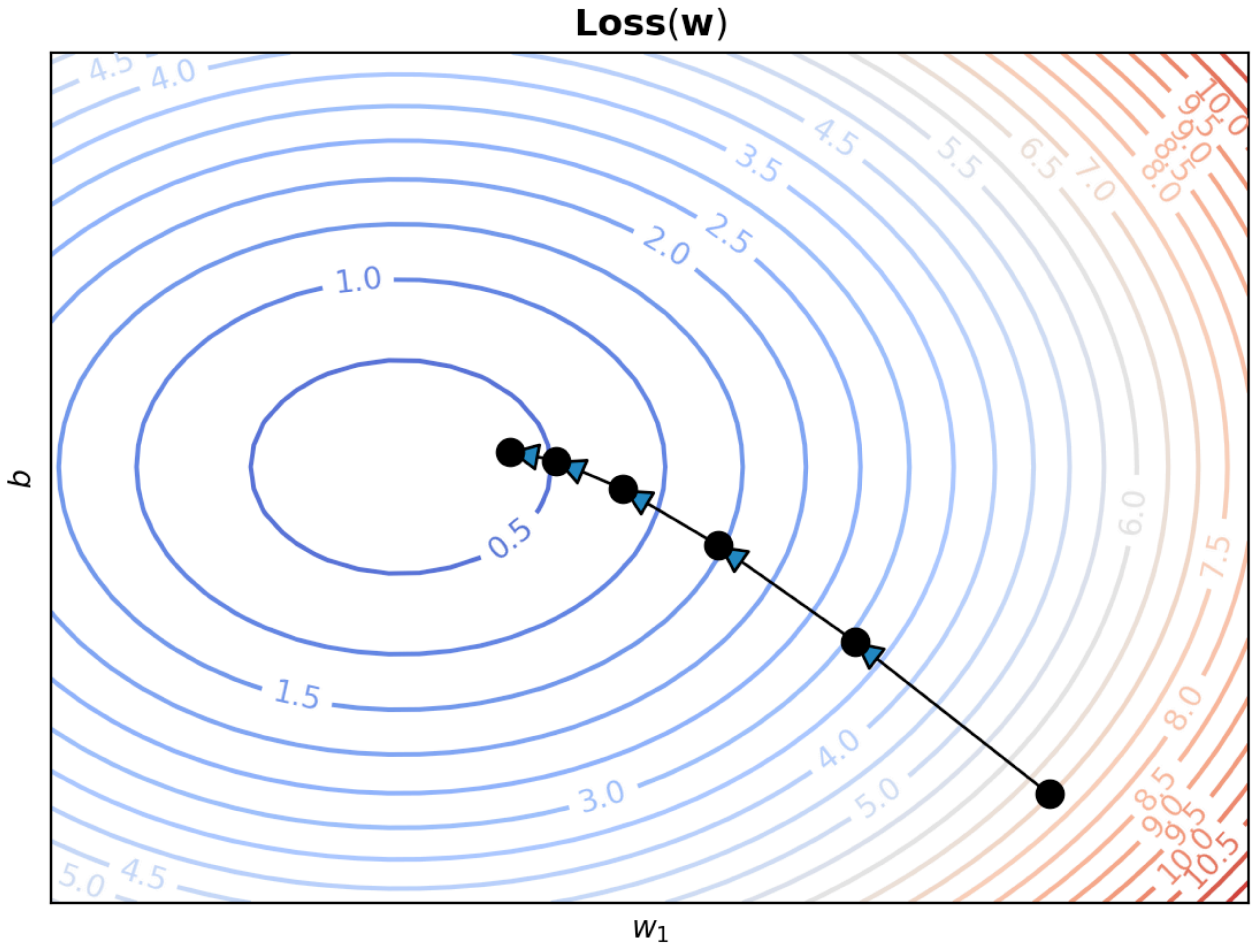
$$\text{For } i \text{ in } 1,\ldots,\text{T}: \quad \mathbf{w}^{(i+1)} \leftarrow \mathbf{w}^{(i)} - \nabla f(\mathbf{w}^{(i)})$$



$$\nabla_{\mathbf{w}} \mathbf{MSE}(\mathbf{w}, \mathbf{X}, \mathbf{y}) = \frac{d}{d\mathbf{w}} \left(\frac{1}{N} \sum_{i=1}^{N} (\mathbf{x}_i^T \mathbf{w} - y_i)^2 \right)$$

$$\text{Find: } \mathbf{w}^* = \underset{\mathbf{w}}{\operatorname{argmin}} \; f(\mathbf{w})$$

For i in 1,...,T : $\quad \mathbf{w}^{(i+1)} \leftarrow \mathbf{w}^{(i)} - \nabla f(\mathbf{w}^{(i)})$



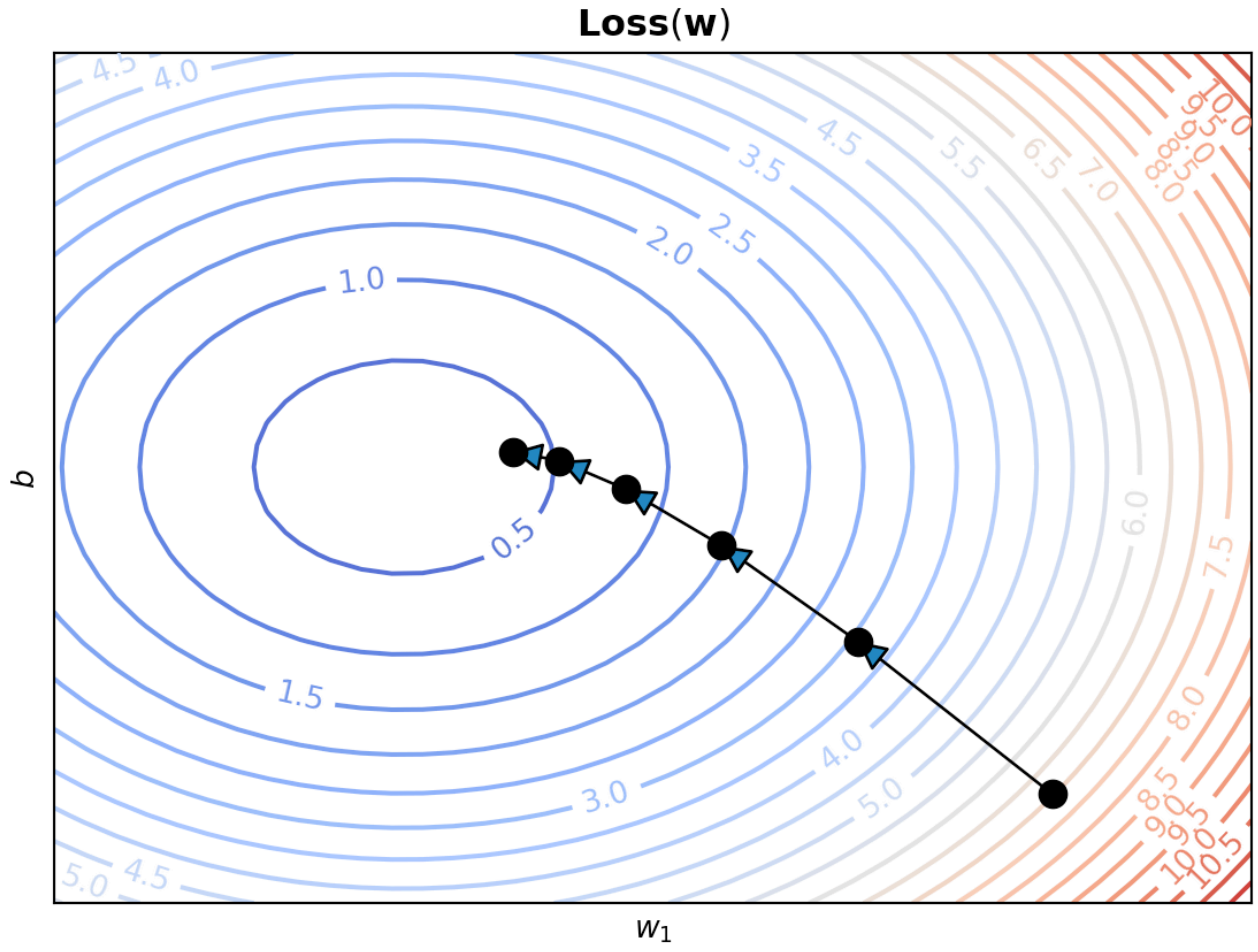
Recall that it's minimum value $\mathbf{w}^*$, a function f *must* have a gradient of $\mathbf{0}$.

$$\nabla f(\mathbf{w}^*) = \mathbf{0}$$

It follows that:

$$\mathbf{w}^* = \mathbf{w}^* - \nabla f(\mathbf{w}^*)$$

$$\text{While } \nabla f(\mathbf{w}^{(i)}) \neq \mathbf{0}: \quad \mathbf{w}^{(i+1)} \leftarrow \mathbf{w}^{(i)} - \nabla f(\mathbf{w}^{(i)})$$

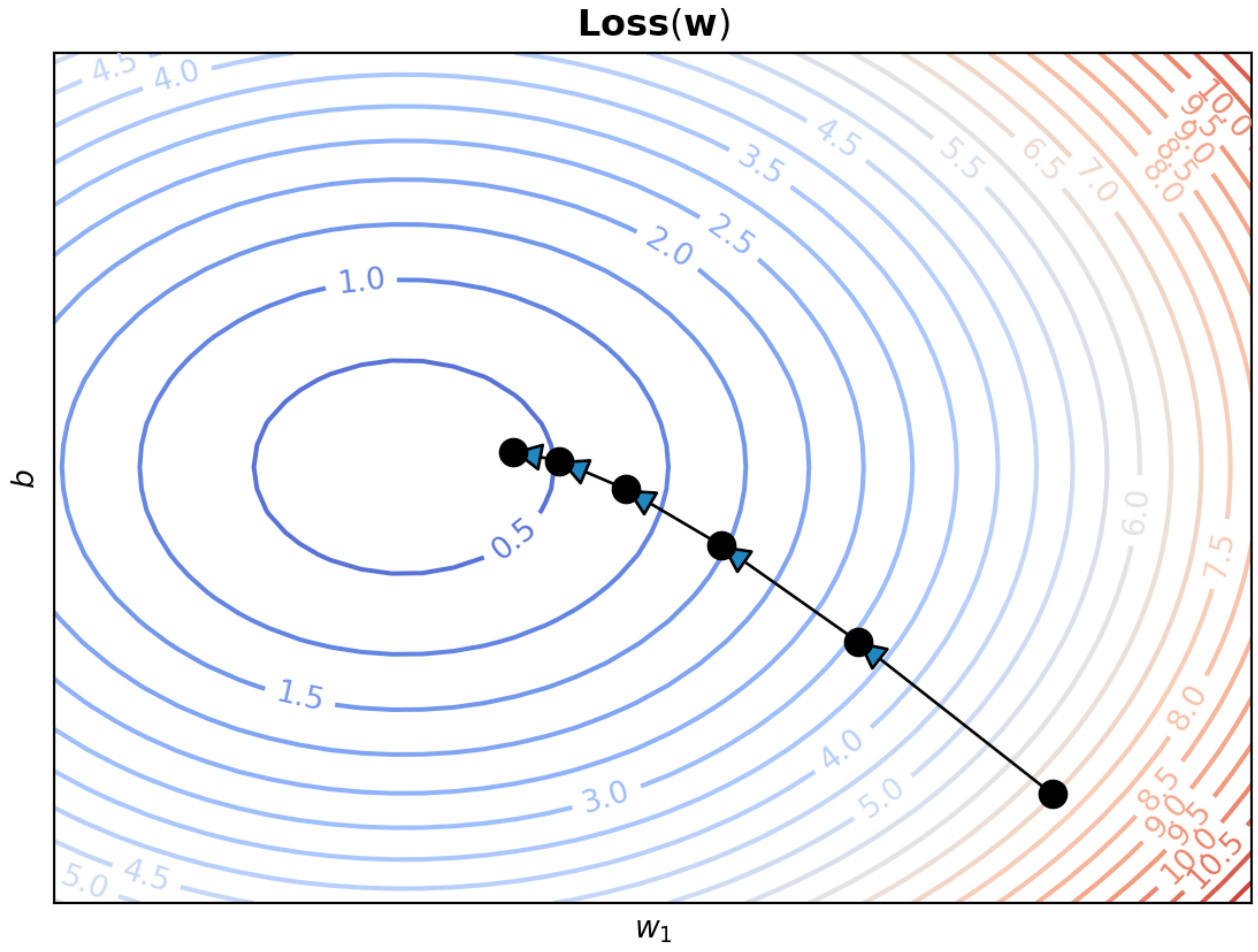


Recall that it's minimum value $\mathbf{w}^*$, a function f *must* have a gradient of $\mathbf{0}$.

$$\nabla f(\mathbf{w}^*) = \mathbf{0}$$

It follows that:

$$\mathbf{w}^* = \mathbf{w}^* - \nabla f(\mathbf{w}^*)$$



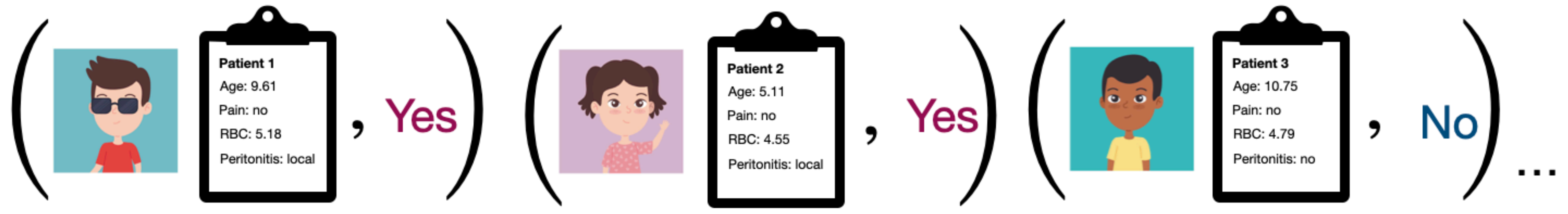
$$\text{While } ||\nabla f(\mathbf{w}^{(i)})||_2 > \epsilon: \quad \mathbf{w}^{(i+1)} \leftarrow \mathbf{w}^{(i)} - \nabla f(\mathbf{w}^{(i)})$$

$$\|\mathbf{x}\|_2 = \sqrt{\sum_{i=1}^{n} x_i^2}$$

Recap

Dataset

Set of known inputs and outputs



Input table

Patients with abdominal pain

	Age	Appendix Size	Migratory Pain	RBC Count	RBC Urine	Peritonitis
0	9.61	9.0	no	5.18	high	local
1	5.11	7.0	no	4.55	medium	local
2	10.75	5.0	no	4.79	none	no
3	10.51	9.0	no	5.03	none	local
4	7.3	6.2	yes	4.64	low	no
5	15.21	8.5	yes	4.62	low	no
6	15.83	12.0	yes	4.33	high	no
7	9.58	7.0	yes	5.04	low	generalized
8	10.37	5.5	no	4.8	none	no
9	16.66	9.0	yes	5.31	none	no
10	14.52	4.5	yes	4.9	none	no
11	10.74	9.0	no	5.66	none	local
12	12.41	3.7	no	5.49	none	no
13	6.67	3.5	no	5.27	none	no
14	14.36	9.0	yes	4.84	low	local
15	9.04	5.3	yes	4.92	low	no
16	12.43	12.0	yes	4.62	none	generalized

Output table

Diagnosis

	Diagnosis
0	appendicitis
1	no appendicitis
2	no appendicitis
3	no appendicitis
4	appendicitis
5	no appendicitis
6	no appendicitis
7	no appendicitis
8	no appendicitis
9	appendicitis
10	appendicitis
11	no appendicitis
12	no appendicitis
13	no appendicitis
14	appendicitis
15	no appendicitis
16	appendicitis

Abstraction

$$\mathcal{D} = \{(\mathbf{x}_1, y_1),\ (\mathbf{x}_2, y_2),\ \dots\ (\mathbf{x}_N, y_N)\}$$

$$\mathbf{X} = \begin{bmatrix} \mathbf{x}_1^T \\ \mathbf{x}_2^T \\ \vdots \\ \mathbf{x}_N^T \end{bmatrix} = \begin{bmatrix} x_{11} & x_{12} & \dots & x_{1n} \\ x_{21} & x_{22} & \dots & x_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ x_{N1} & x_{N2} & \dots & x_{Nn} \end{bmatrix}, \quad \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}$$

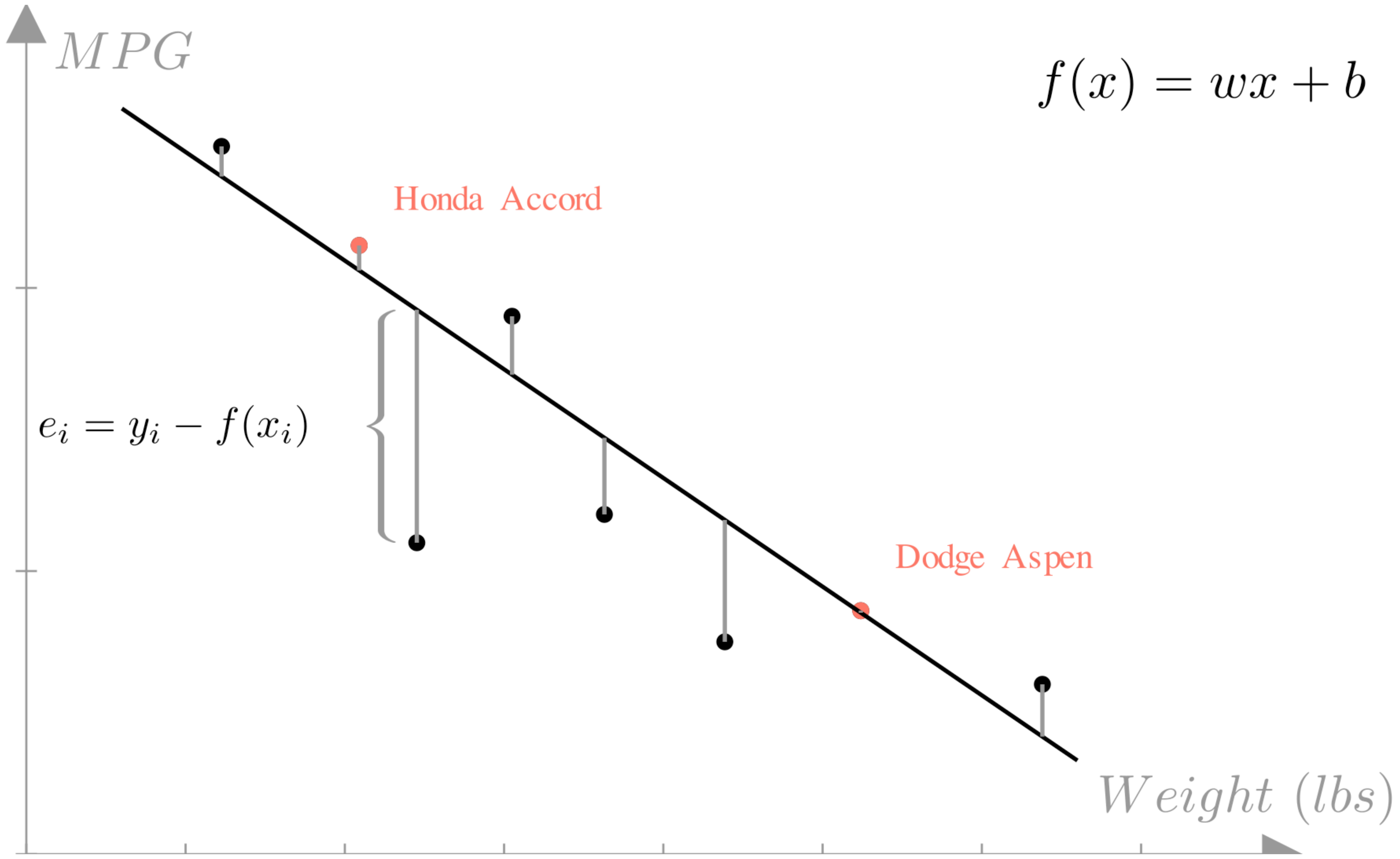
Linear (affine) prediction function

$$\text{Input: } \mathbf{x} \underset{predict}{\longrightarrow} \text{ Output: } y, \quad y = f(\mathbf{x})$$

$$f(\mathbf{x}) = \sum_{i=1}^{n} x_i w_i + b$$

We typically refer to $\mathbf{w}$ specifically as the **weight vector** (or weights) and b as the **bias**. To summarize:

$$\textbf{Affine function: } f(\mathbf{x}) = \mathbf{x}^T\mathbf{w} + b, \quad \textbf{Parameters:} \quad (\text{Weights: } \mathbf{w}, \text{ Bias: } b)$$



$$\mathcal{D} = \{(\mathbf{x}_1, y_1),\ (\mathbf{x}_2, y_2),\ \ldots\ (\mathbf{x}_N, y_N)\}$$

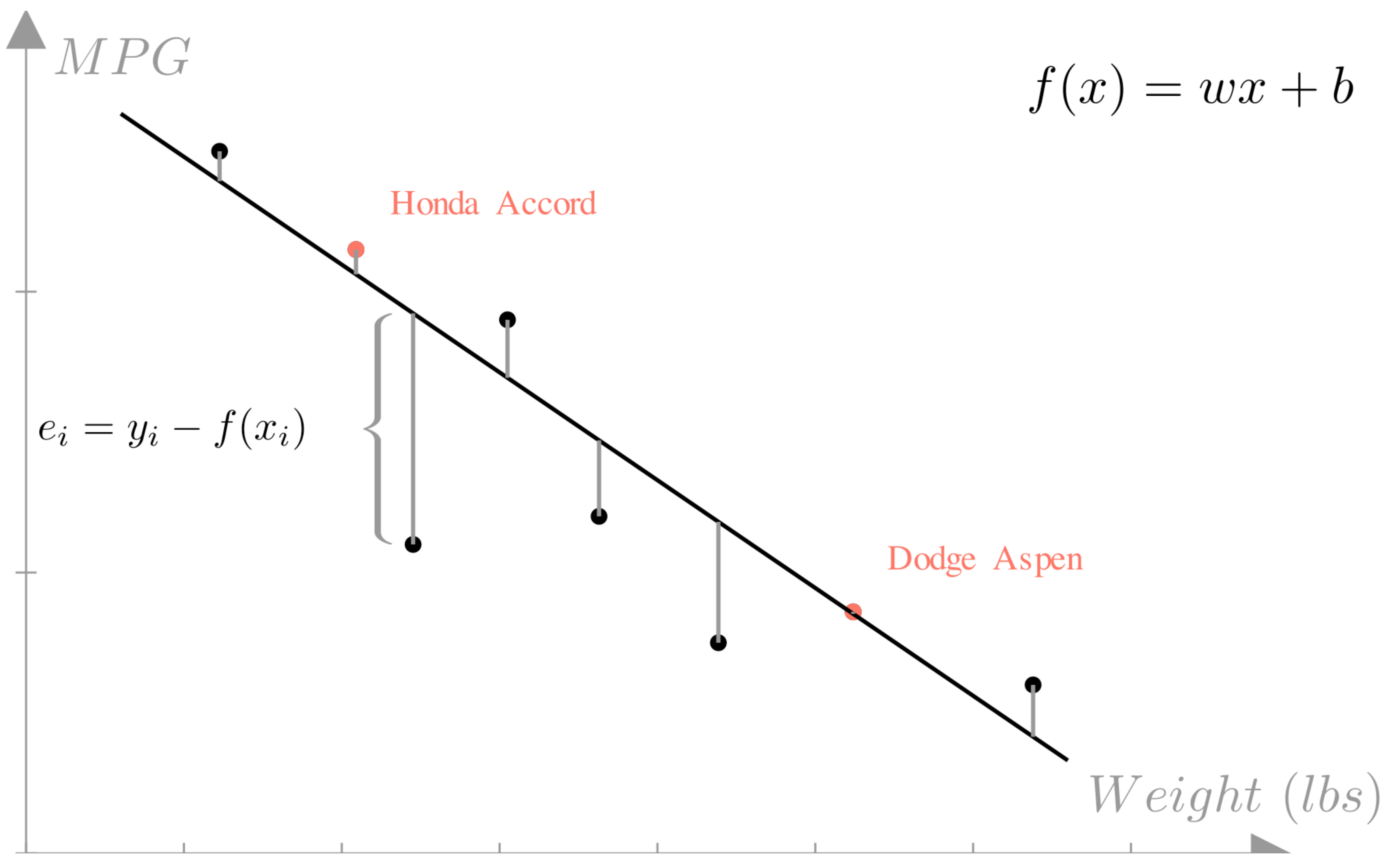
Linear (affine) prediction function

$$\text{Input: } \mathbf{x} \underset{predict}{\longrightarrow} \text{ Output: } y, \quad y = f(\mathbf{x})$$

$$f(\mathbf{x}) = \sum_{i=1}^{n} x_i w_i + b$$

We typically refer to $\mathbf{w}$ specifically as the **weight vector** (or weights) and b as the **bias**. To summarize:

$$\textbf{Affine function: } f(\mathbf{x}) = \mathbf{x}^T\mathbf{w} + b, \quad \textbf{Parameters: } \quad (\text{Weights: } \mathbf{w}, \ \text{Bias: } b)$$



$$\mathcal{D} = \{(\mathbf{x}_1, y_1), \ (\mathbf{x}_2, y_2), \ \dots \ (\mathbf{x}_N, y_N)\}$$

Augmenting inputs trick

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \longrightarrow \mathbf{x}_{aug} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \\ 1 \end{bmatrix} \quad \text{and} \quad \mathbf{w} = \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \end{bmatrix} \longrightarrow \mathbf{w}_{aug} = \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \\ b \end{bmatrix}$$

We can easily see then that using this notation:

$$f(\mathbf{x}) = \mathbf{x}^T\mathbf{w} + b = \mathbf{x}_{aug}^T \mathbf{w}_{aug}$$

Linear (affine) prediction function

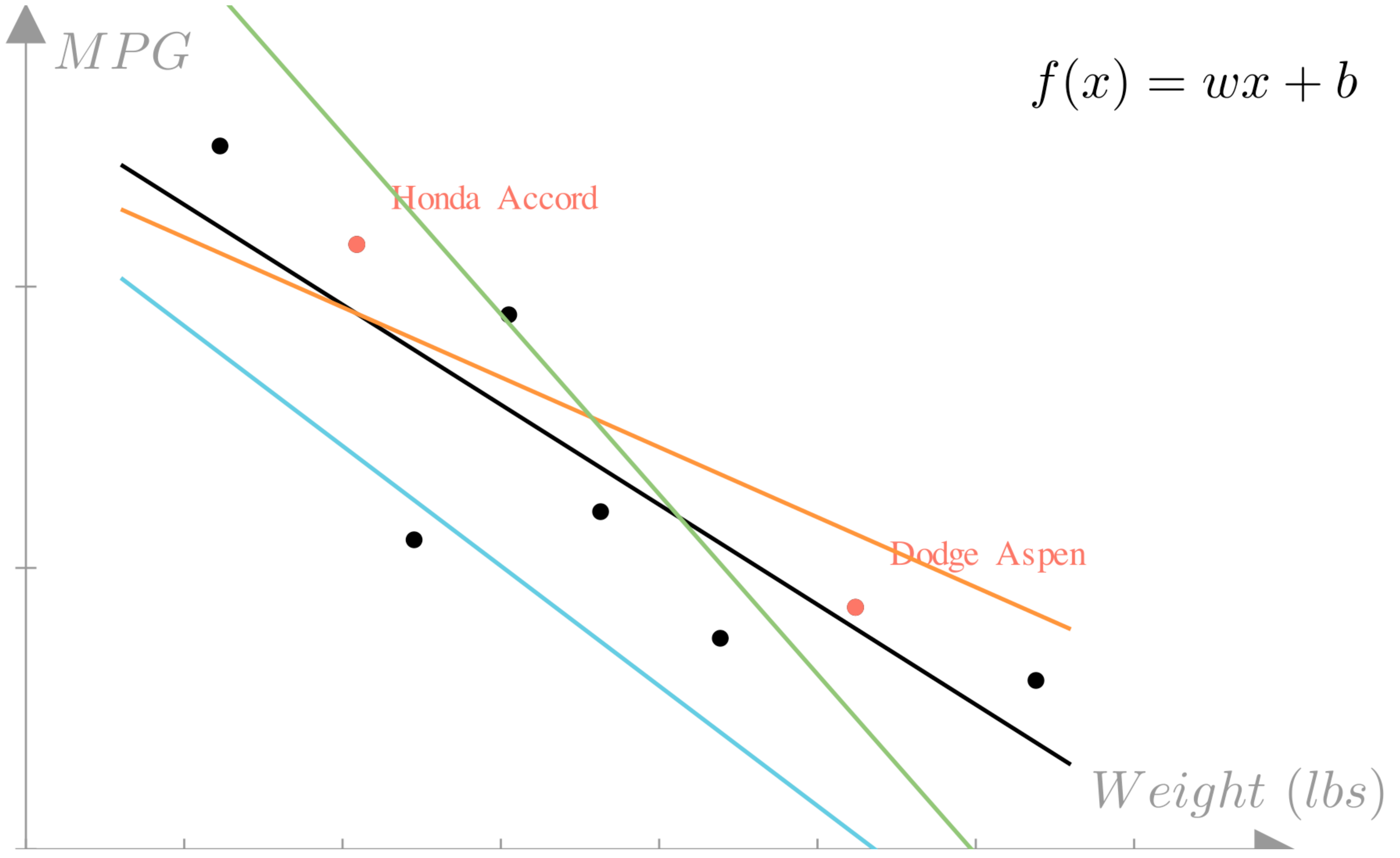
$$\text{Input: } \mathbf{x} \underset{predict}{\longrightarrow} \text{ Output: } y, \quad y = f(\mathbf{x})$$

$$f(\mathbf{x}) = \sum_{i=1}^{n} x_i w_i + b$$

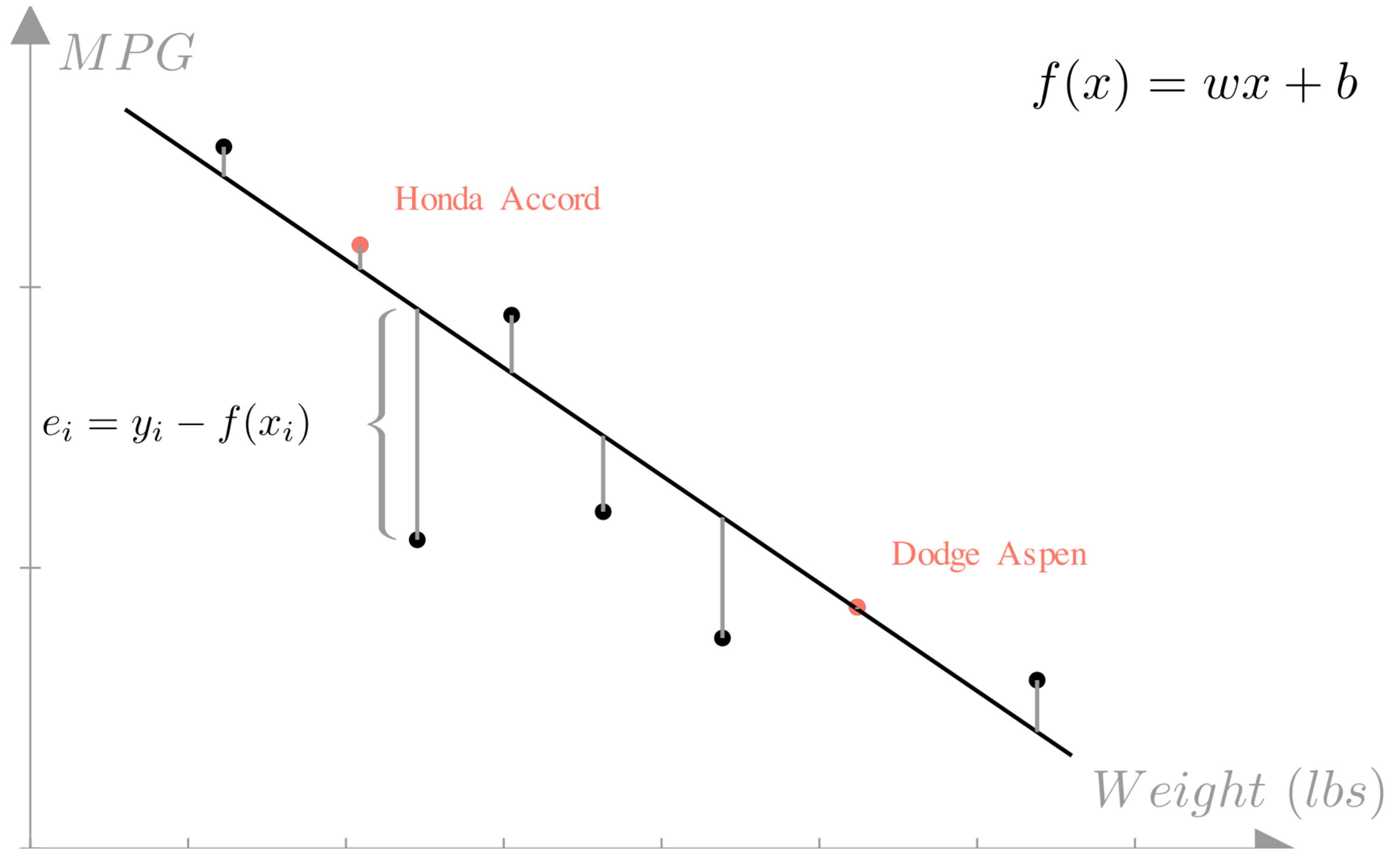
We typically refer to $\mathbf{w}$ specifically as the **weight vector** (or weights) and b as the **bias**. To summarize:

$$\textbf{Affine function: } f(\mathbf{x}) = \mathbf{x}^T\mathbf{w} + b, \quad \textbf{Parameters:} \quad (\text{Weights: } \mathbf{w},\ \text{Bias: } b)$$

How to choose a function?



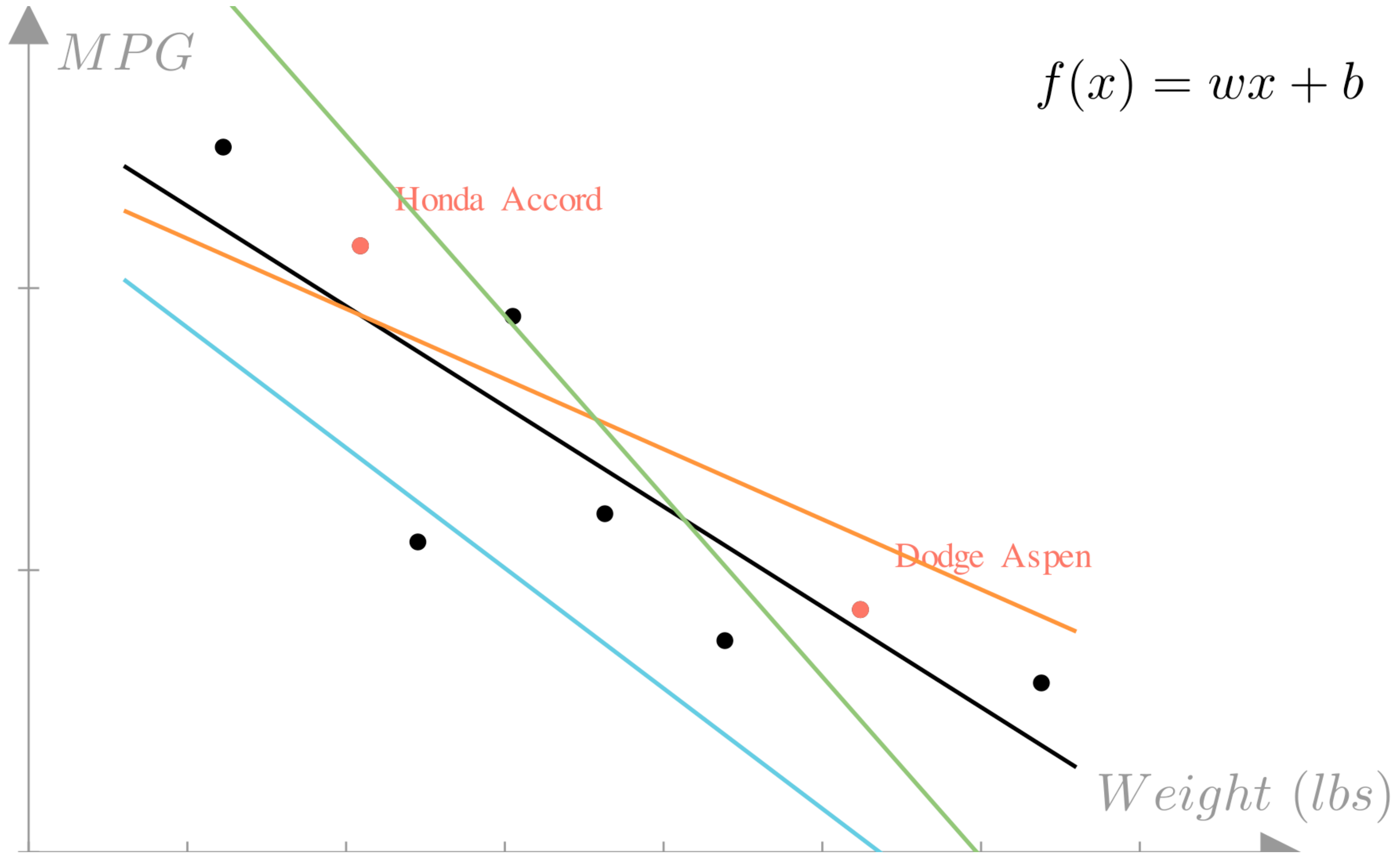
Residuals measure error

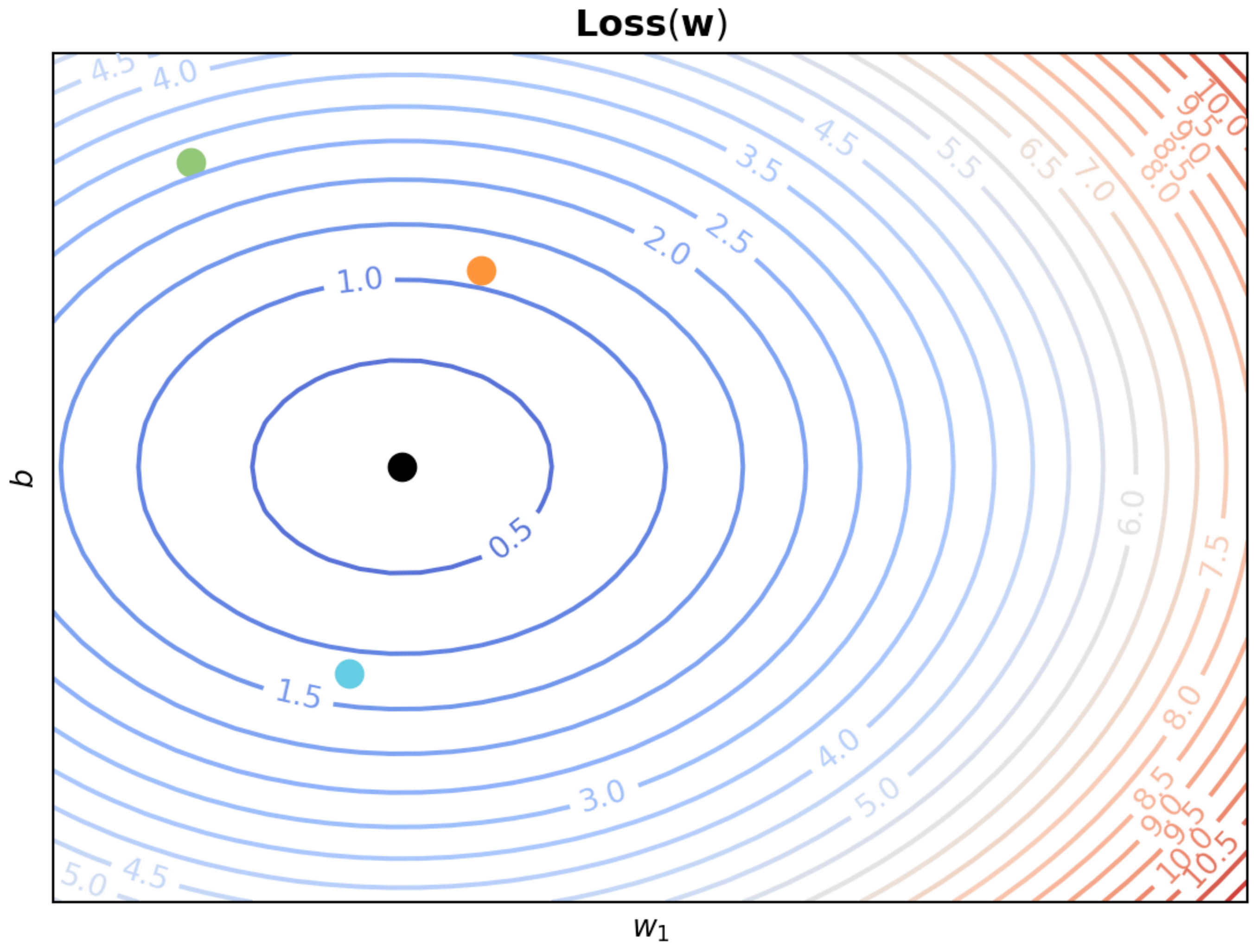


MSE loss minimizes squared residuals

$$\mathbf{Loss}(\mathbf{w}) = MSE(\mathbf{w}, \mathbf{X}, \mathbf{y}) = \frac{1}{N}\sum_{i=1}^{N}(\mathbf{x}_i^T\mathbf{w} - y_i)^2$$

Loss is a *function* of *parameters*





Find parameters that minimize loss:

$$\mathbf{w}^* = \underset{\mathbf{w}}{\operatorname{argmin}}\ \mathbf{Loss}(\mathbf{w}) = \underset{\mathbf{w}}{\operatorname{argmin}} \frac{1}{N}\sum_{i=1}^{N}(\mathbf{x}_i^T\mathbf{w} - y_i)^2$$

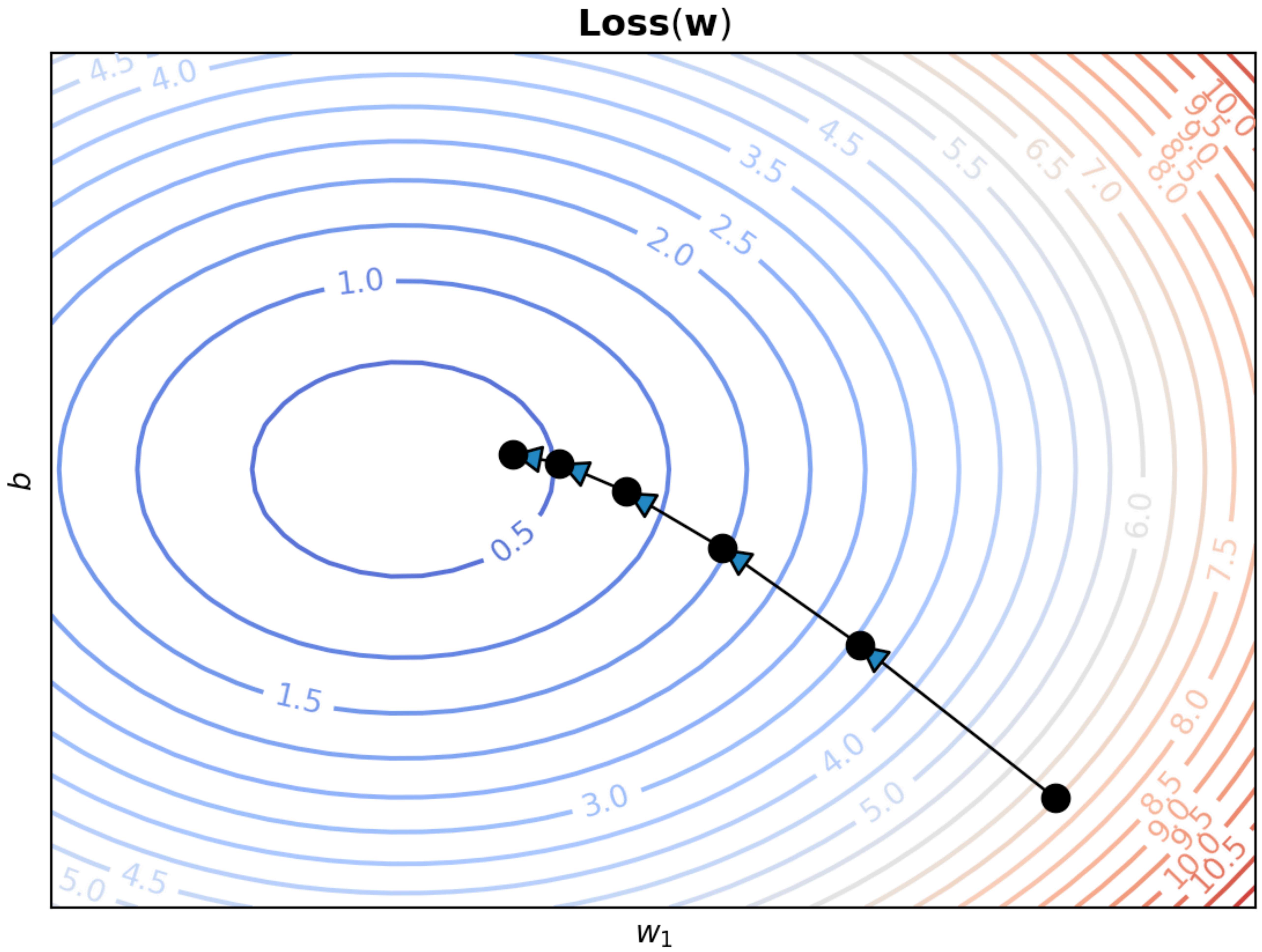
Gradient descent: start with random guess, then *update* in direction of steepest descent (gradient)

$$\text{Find: } \mathbf{w}^* = \underset{\mathbf{w}}{\operatorname{argmin}}\, f(\mathbf{w})$$

$$\text{For } i \text{ in } 1,\ldots,\mathrm{T}: \quad \mathbf{w}^{(i+1)} \leftarrow \mathbf{w}^{(i)} - \nabla f(\mathbf{w}^{(i)})$$

Gradient: *vector* of partial derivatives

$$\frac{df}{d\mathbf{x}} = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \\ \frac{\partial f}{\partial x_3} \\ \vdots \end{bmatrix} = \nabla f(\mathbf{x})$$



Calculus with vectors is similar to calculus with scalars!

$$\nabla_{\mathbf{w}} \mathbf{MSE}(\mathbf{w}, \mathbf{X}, \mathbf{y}) = \frac{d}{d\mathbf{w}} \left(\frac{1}{N} \sum_{i=1}^{N} (\mathbf{x}_i^T \mathbf{w} - y_i)^2 \right)$$

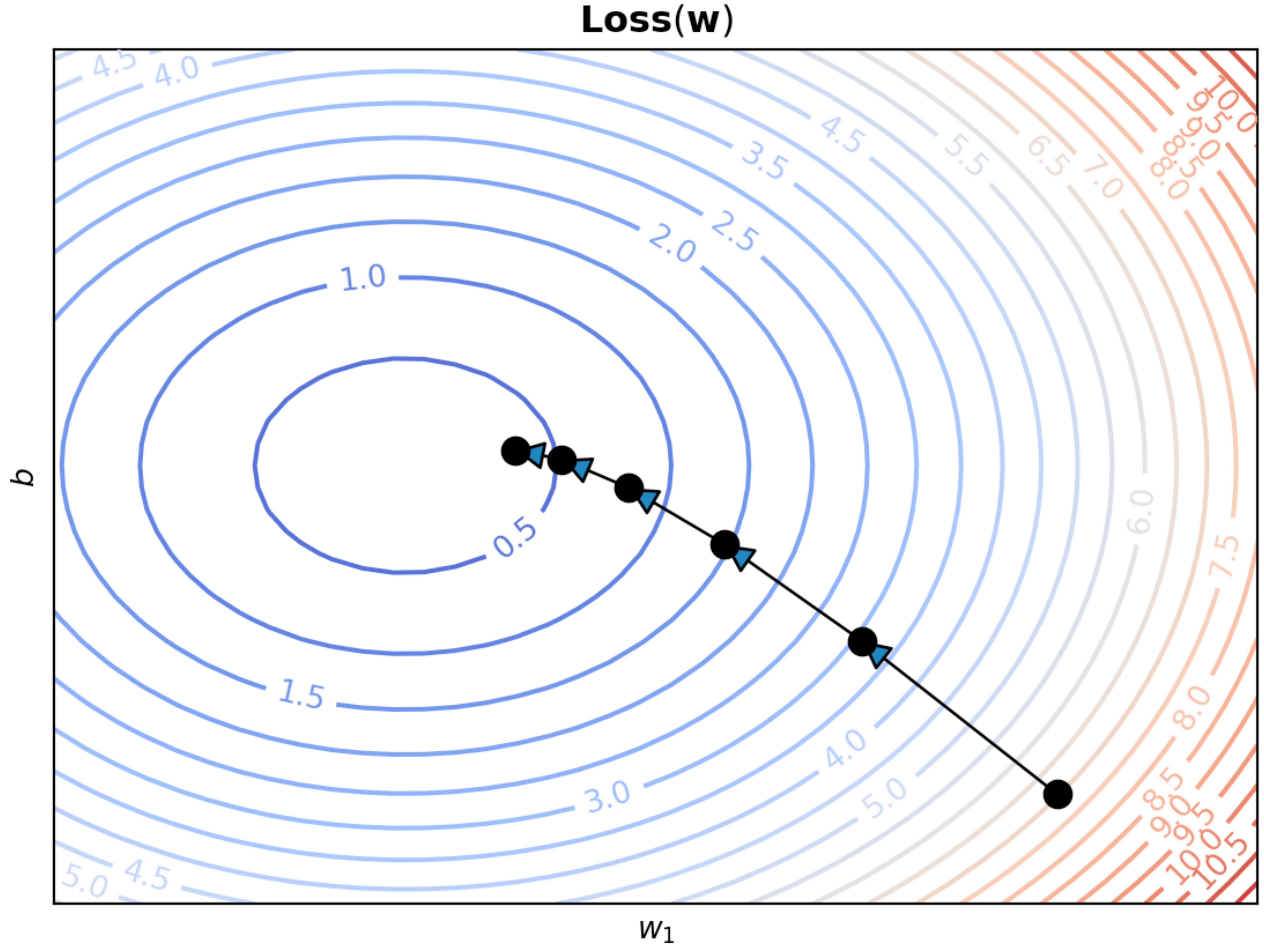
$$= \frac{2}{N} \sum_{i=1}^{N} (\mathbf{x}_i^T \mathbf{w} - y_i) \mathbf{x}_i$$

Can verify rules by taking individual partial derivatives

$$\frac{\partial}{\partial x_1} \mathbf{x}^T \mathbf{x} =$$

$$\frac{\partial}{\partial x_1} \sum_{i=1}^{n} x_i x_i = \frac{\partial}{\partial x_1} (x_1^2 + x_2^2 + x_3^2)$$

$$= \frac{\partial}{\partial x_1} x_1^2 = 2x_1$$



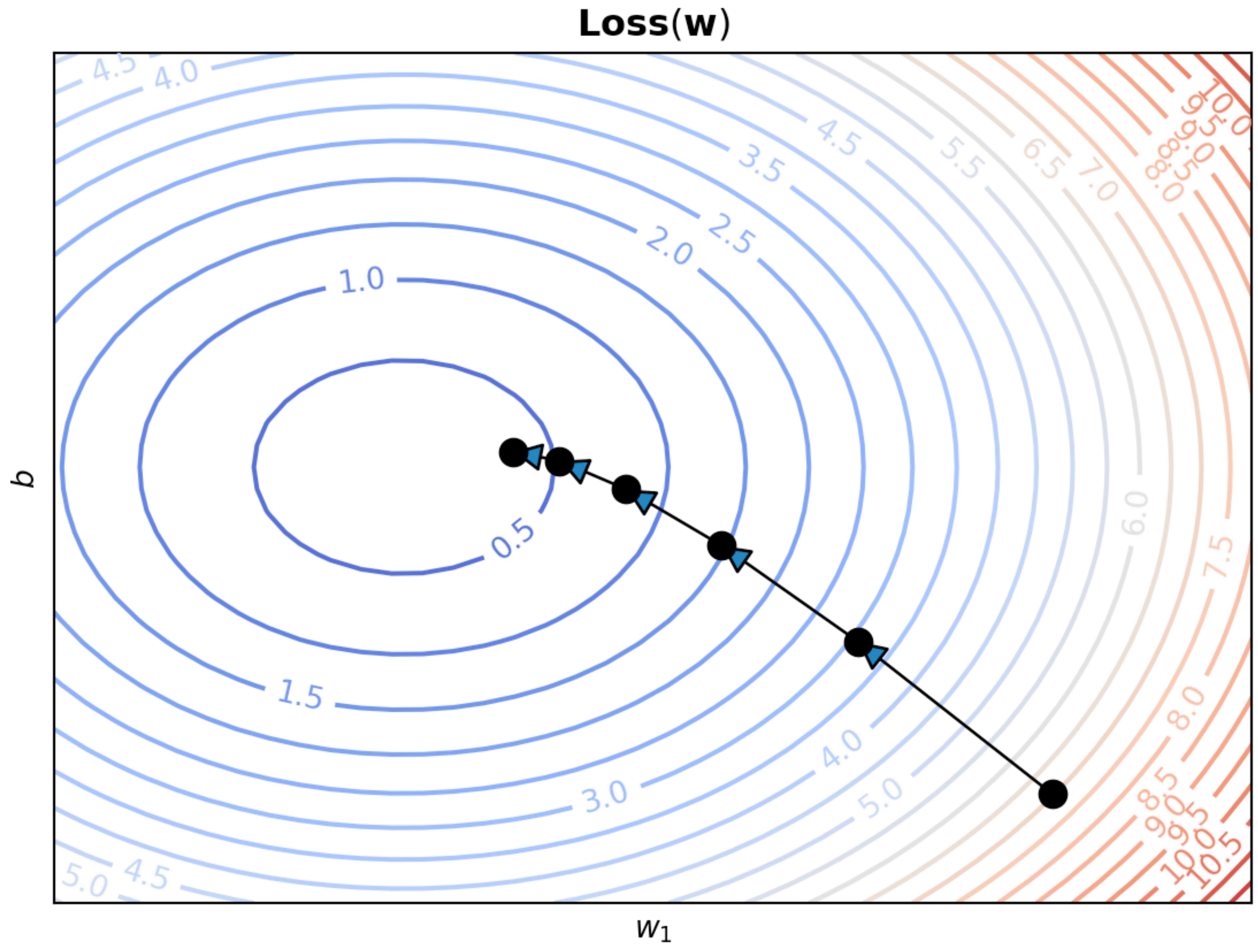
Problems with gradient descent

Recall that it's minimum value $\mathbf{w}^*$, a function f *must* have a gradient of $\mathbf{0}$.

$$\nabla f(\mathbf{w}^*) = \mathbf{0}$$

It follows that:

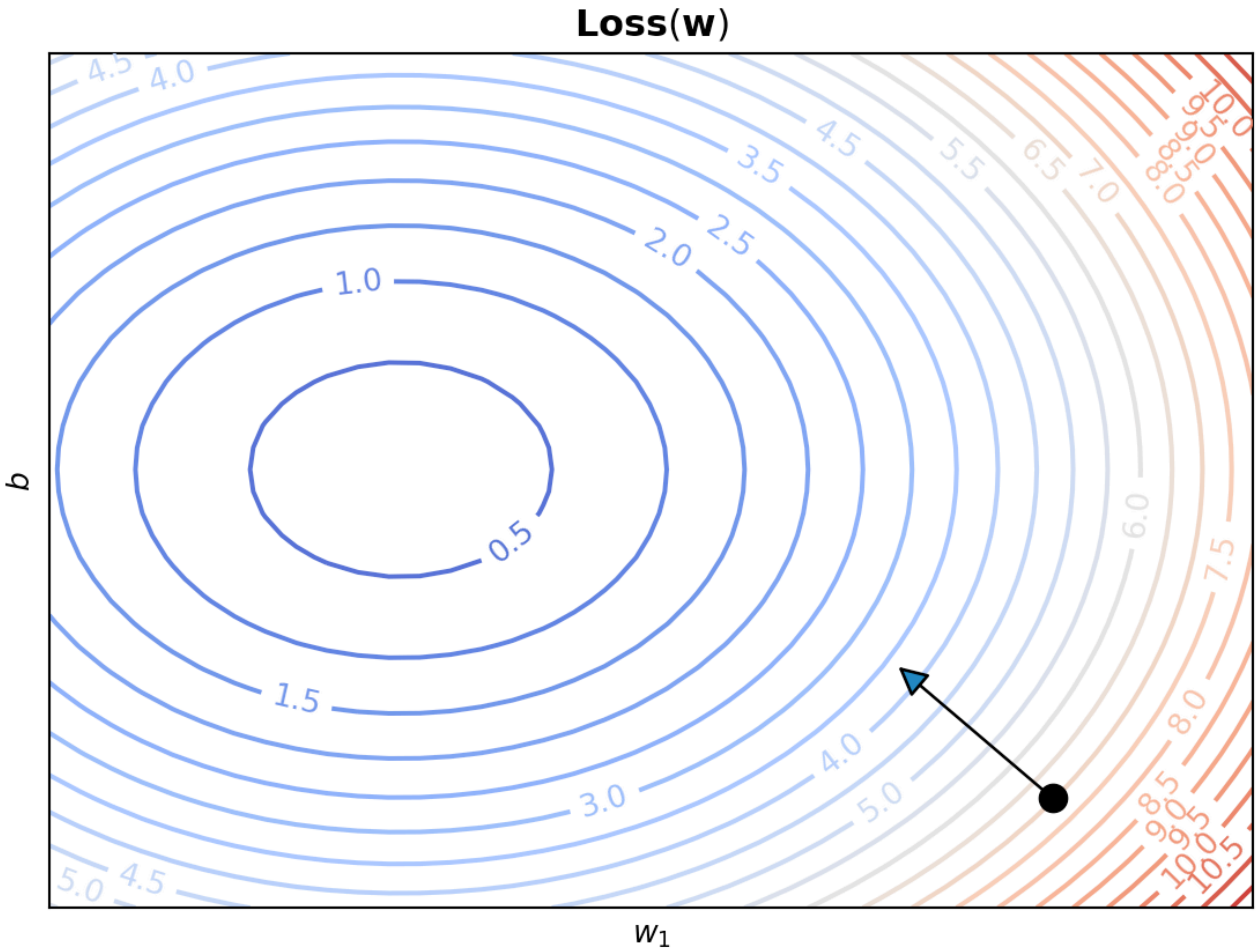
$$\mathbf{w}^* = \mathbf{w}^* - \nabla f(\mathbf{w}^*)$$



$$\text{While } ||\nabla f(\mathbf{w}^{(i)})||_2 > \epsilon : \quad \mathbf{w}^{(i+1)} \leftarrow \mathbf{w}^{(i)} - \nabla f(\mathbf{w}^{(i)})$$

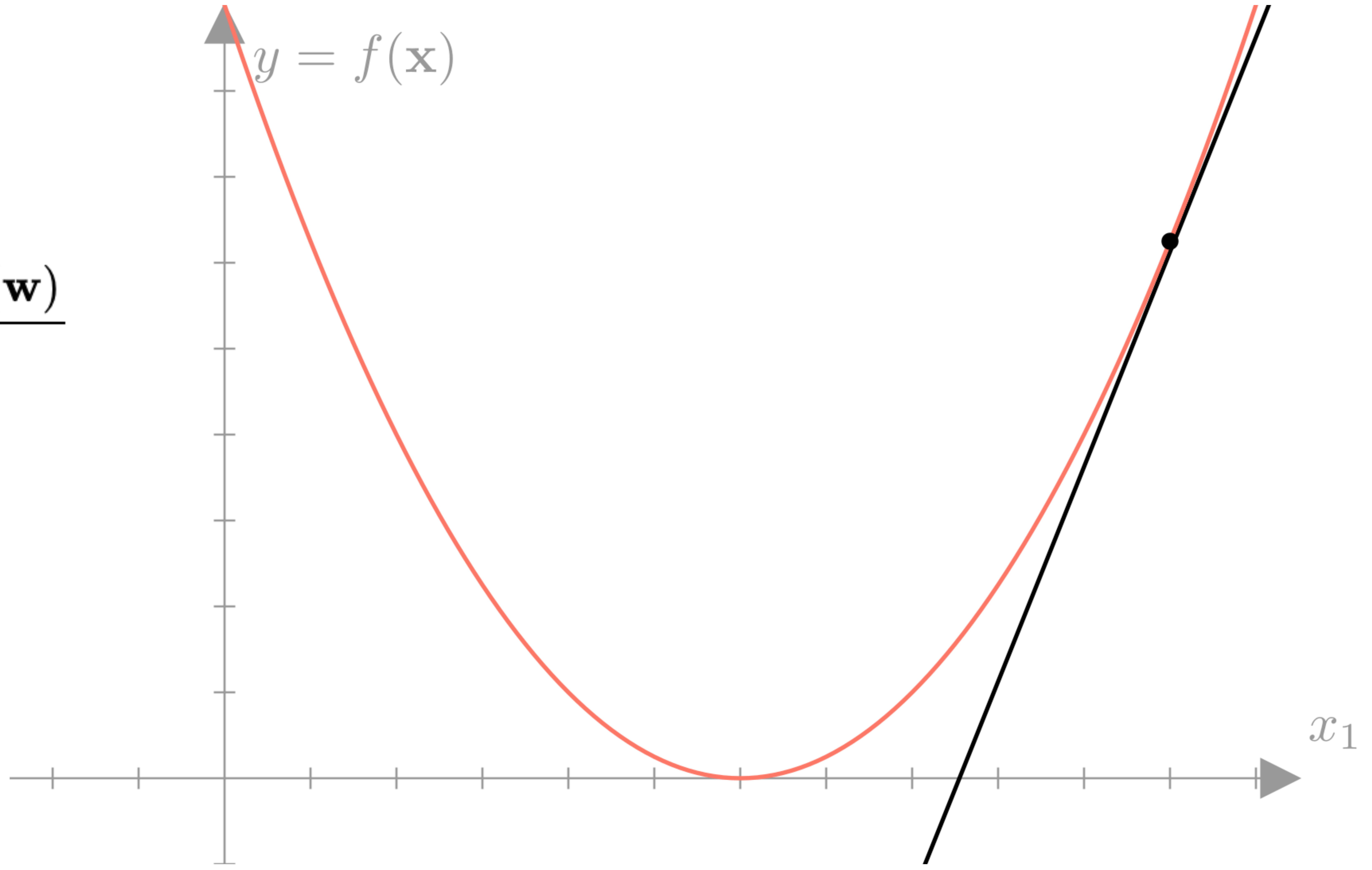
$$\|\mathbf{x}\|_2 = \sqrt{\sum_{i=1}^{n} x_i^2}$$

How big a step to take?

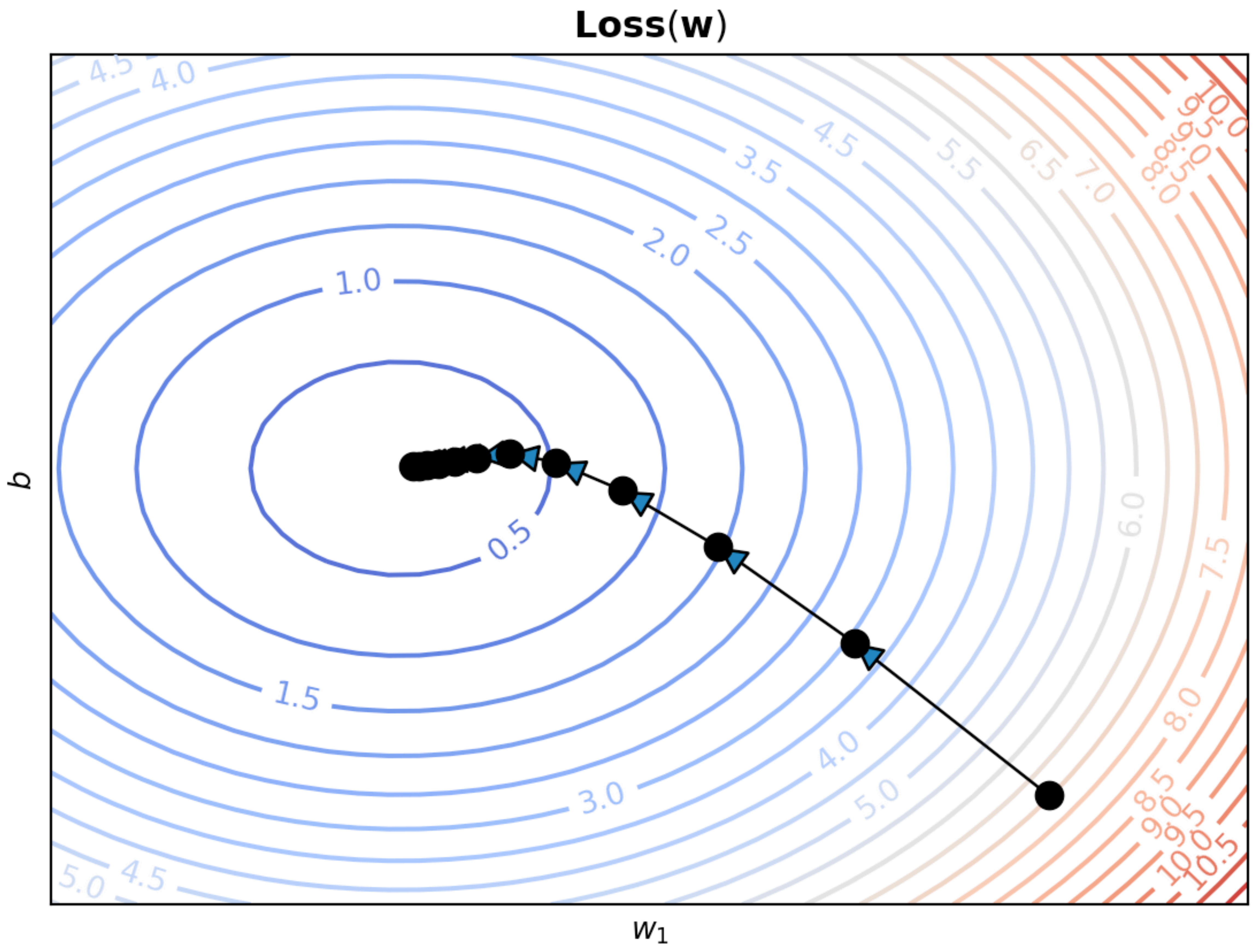


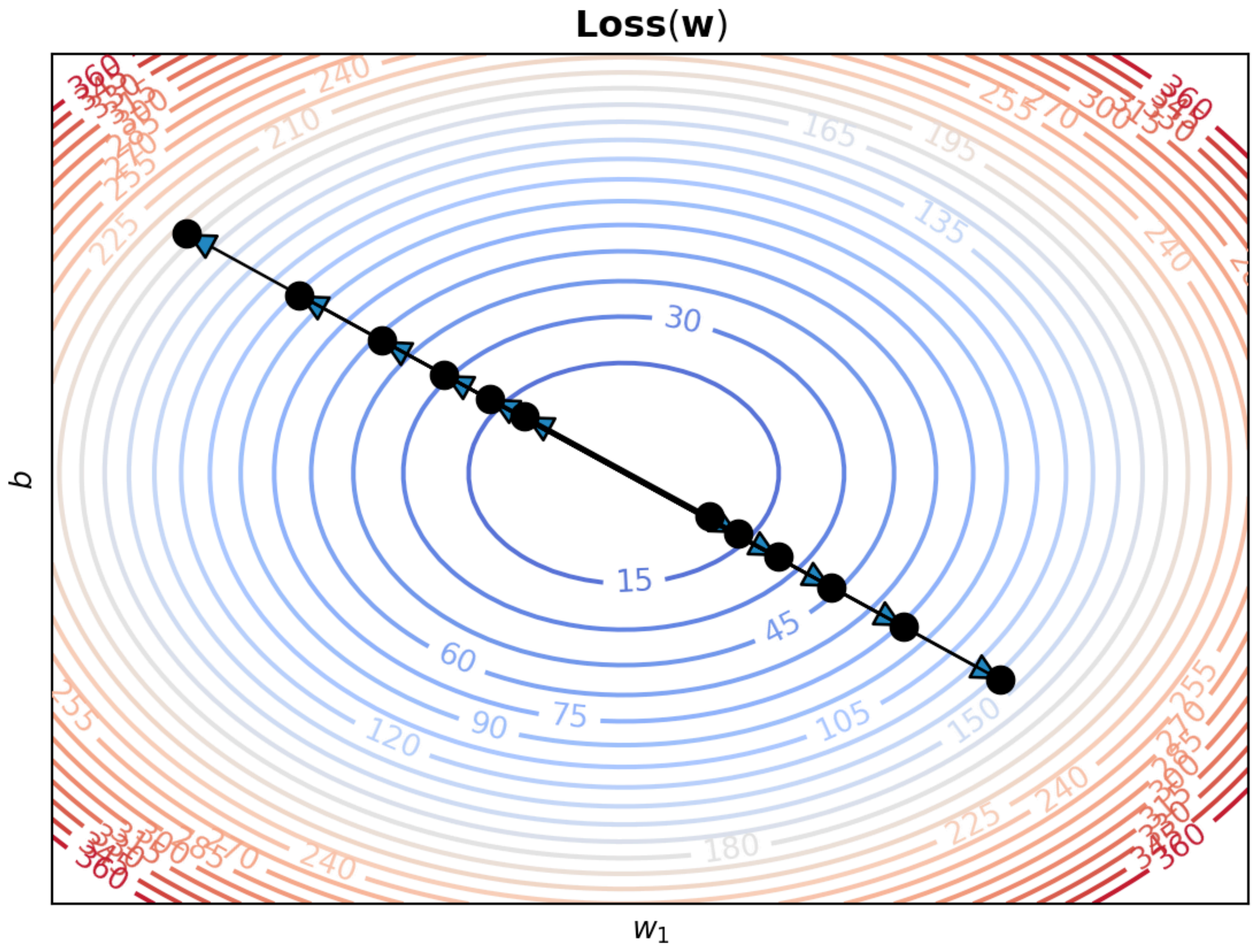
Gradient/derivative gives a *linear approximation of function*

$$\frac{df}{d\mathbf{w}} = \lim_{\gamma \to 0} \max_{\|\epsilon\|_2 < \gamma} \frac{f(\mathbf{w} + \epsilon) - f(\mathbf{w})}{\|\epsilon\|_2}$$



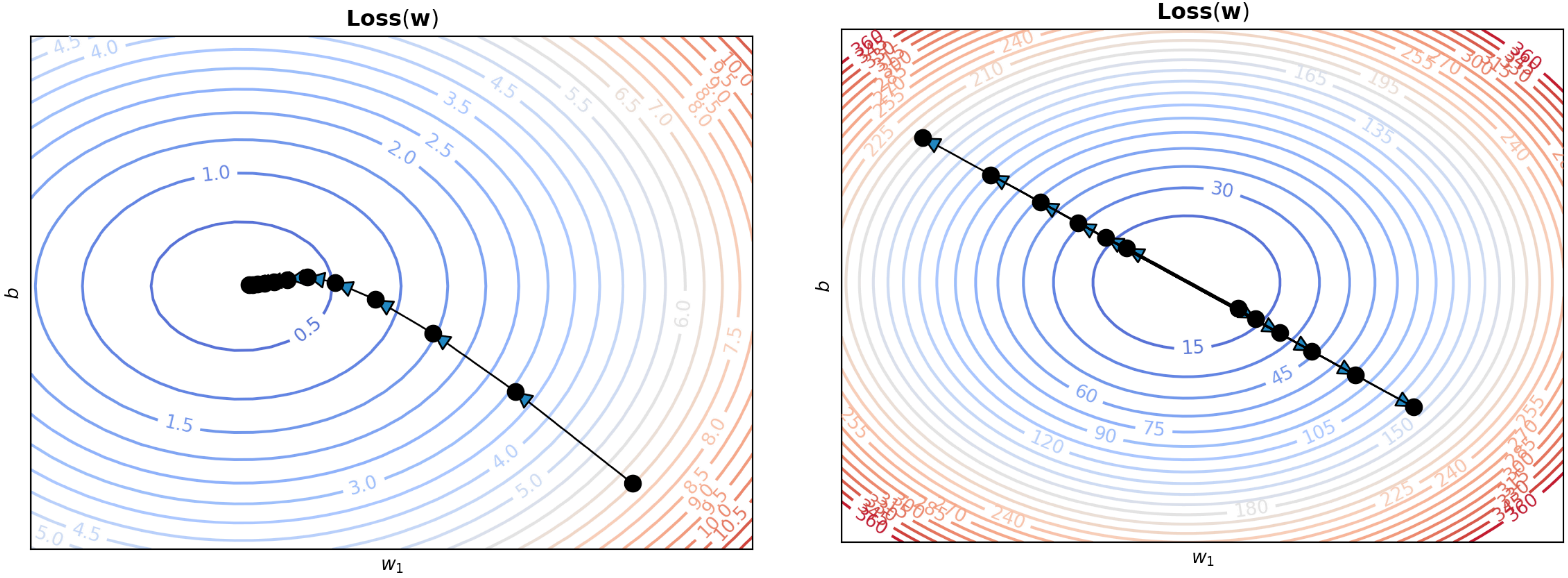
Gradients too big/too small





Step size!

$$\mathbf{w}^{(i+1)} \leftarrow \mathbf{w}^{(i)} - \alpha \nabla f(\mathbf{w}^{(i)})$$



Back to MSE

$$\nabla_{\mathbf{w}} \mathbf{MSE}(\mathbf{w}, \mathbf{X}, \mathbf{y}) = \frac{d}{d\mathbf{w}} \left(\frac{1}{N} \sum_{i=1}^{N} (\mathbf{x}_i^T \mathbf{w} - y_i)^2 \right)$$

$$= \frac{2}{N} \sum_{i=1}^{N} (\mathbf{x}_i^T \mathbf{w} - y_i) \mathbf{x}_i$$

With this gradient our gradient descent update becomes:

$$\mathbf{w}^{(i+1)} \longleftarrow \mathbf{w}^{(i)} - \alpha \left(\frac{2}{N} \right) \sum_{i=1}^{N} (\mathbf{x}_i^T \mathbf{w}^{(i)} - y_i) \mathbf{x}_i$$

Caveat

$$\nabla_{\mathbf{w}}\mathbf{MSE}(\mathbf{w},\mathbf{X},\mathbf{y}) = \frac{d}{d\mathbf{w}}\left(\frac{1}{N}\sum_{i=1}^{N}(\mathbf{x}_i^T\mathbf{w} - y_i)^2\right)$$

$$= \frac{2}{N}\sum_{i=1}^{N}(\mathbf{x}_i^T\mathbf{w} - y_i)\mathbf{x}_i$$

We know that at the minimum, the gradient must be $\mathbf{0}$, so the following condition must hold:

$$\mathbf{0} = \left(\frac{2}{N}\right)\sum_{i=1}^{N}(\mathbf{x}_i^T\mathbf{w} - y_i)\mathbf{x}_i$$

$$\left(\sum_{i=1}^{N}\mathbf{x}_i\mathbf{x}_i^T\right)^{-1}\left(\sum_{i=1}^{N}y_i\mathbf{x}_i\right) = \mathbf{w}^*$$

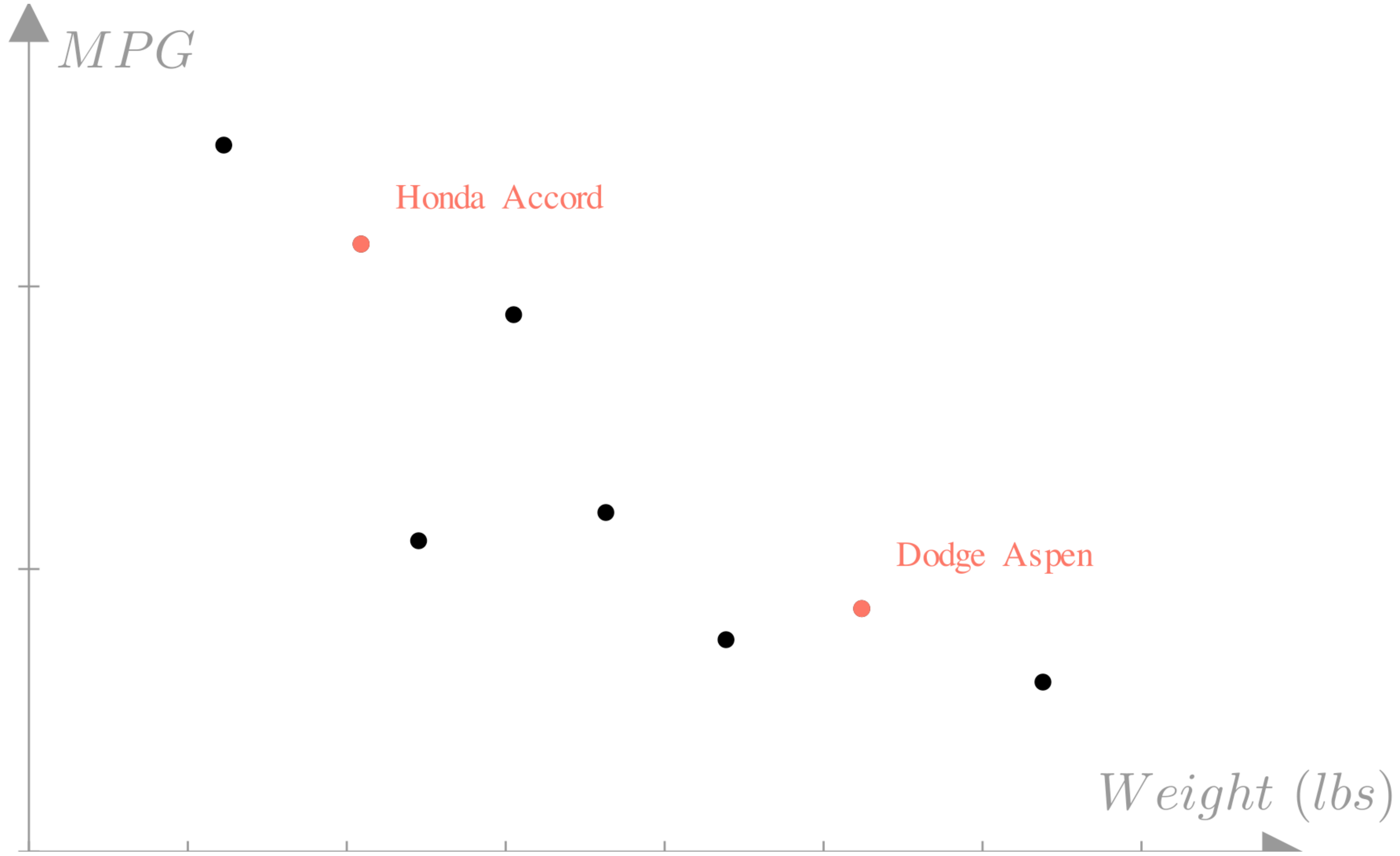
$$\mathbf{w}^* = \left(\mathbf{X}^T\mathbf{X}\right)^{-1}(\mathbf{y}\mathbf{X})$$

Predictions are inexact

$$\text{Input: } \mathbf{x}_i = \begin{bmatrix} \text{Weight} \\ \text{Horsepower} \\ \text{Displacement} \\ \text{0-60mph} \end{bmatrix}, \quad \text{Output: } y_i = MPG$$

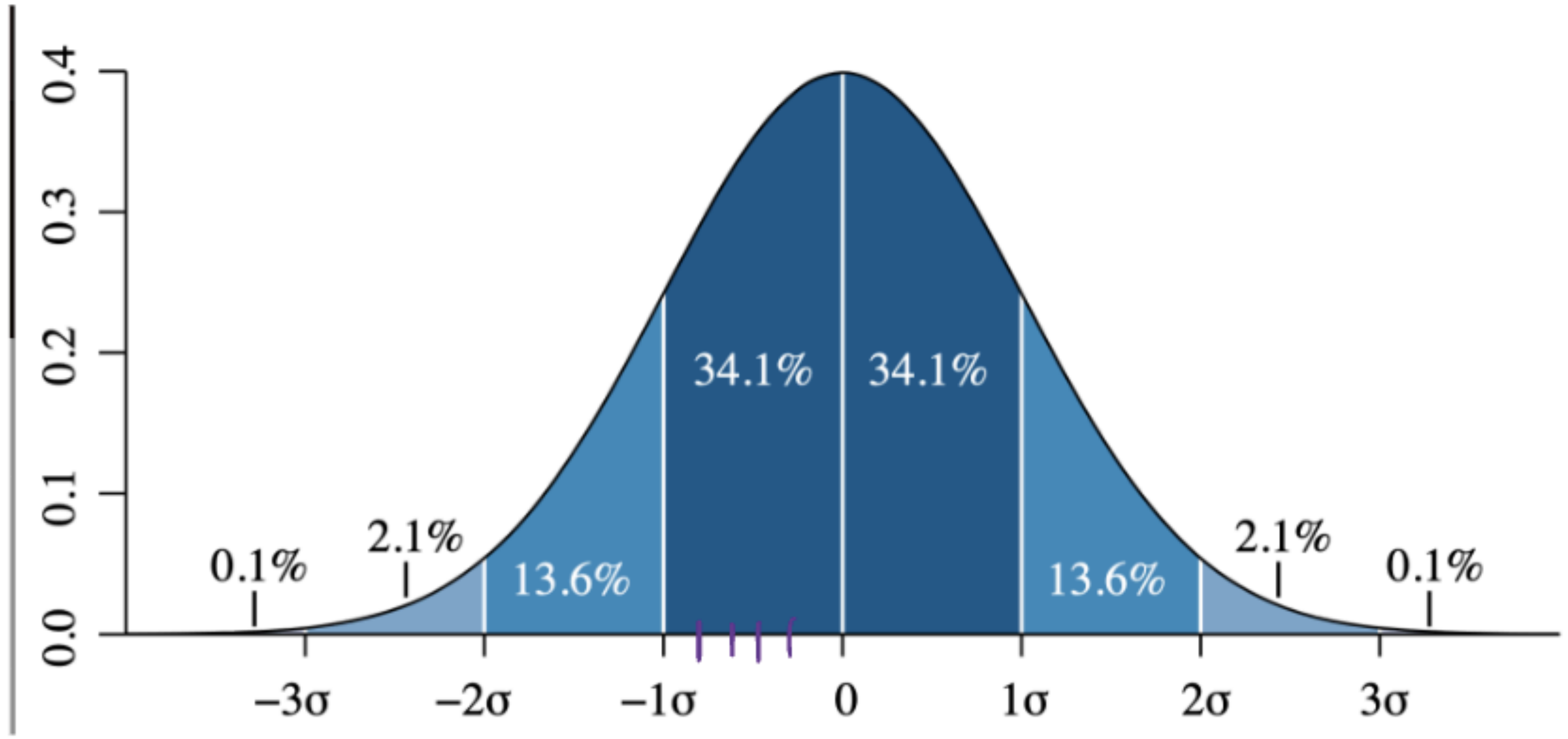
$$\text{Predicted MPG} = f(\mathbf{x}) =$$

$$(\text{weight})w_1 + (\text{horsepower})w_2 + (\text{displacement})w_3 + (\text{0-60mph})w_4$$



$$p(y) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(- \frac{1}{2\sigma^2} (y - \mu)^2 \right)$$

Normal distribution

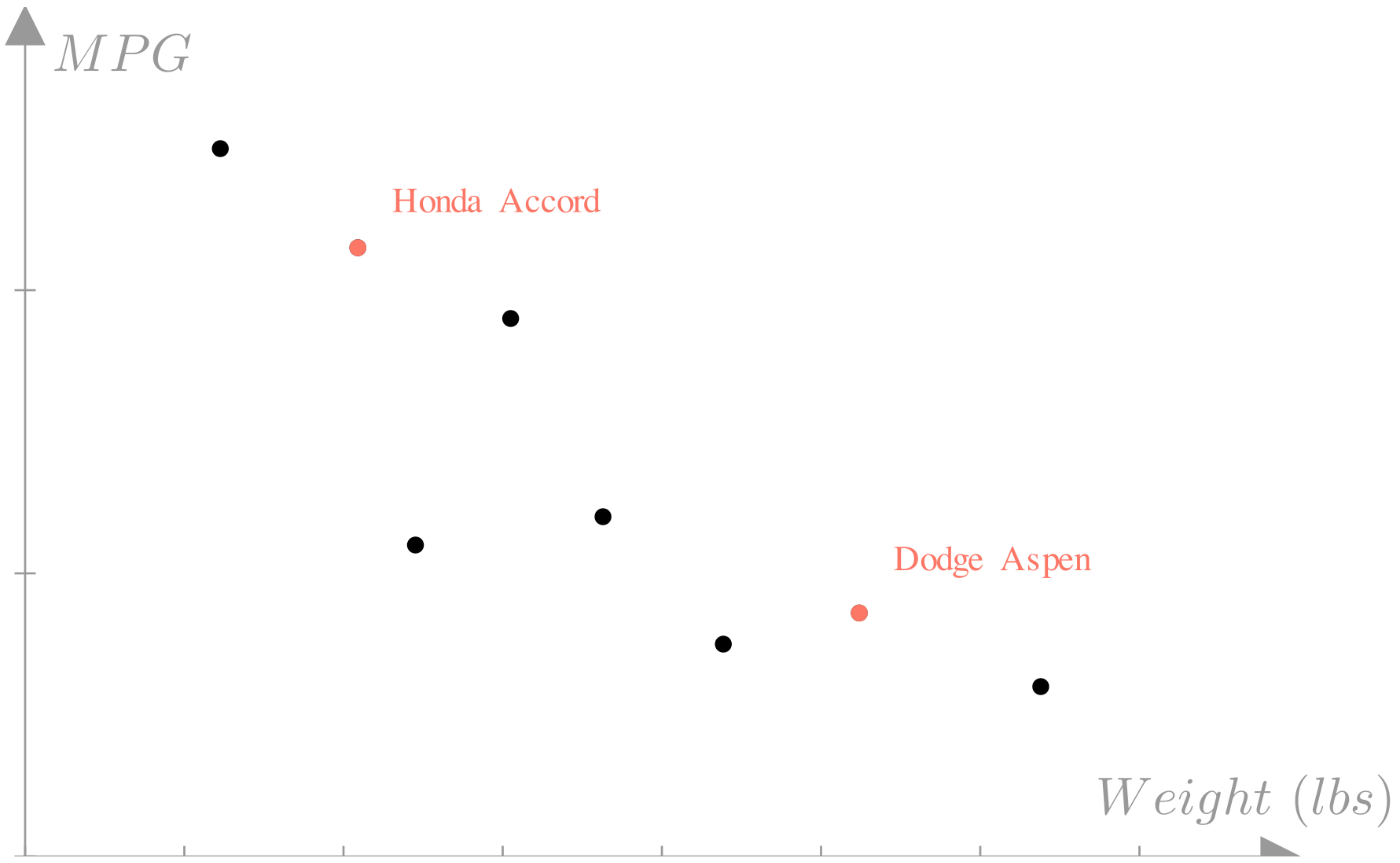


Normal distribution

$$p(y) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2\sigma^2}(y-\mu)^2 \right)$$

Linear regression predicts mean!

$$y_i \sim \mathcal{N}\left(\mathbf{x}_i^T \mathbf{w},\ \sigma^2\right)$$



Normal distribution

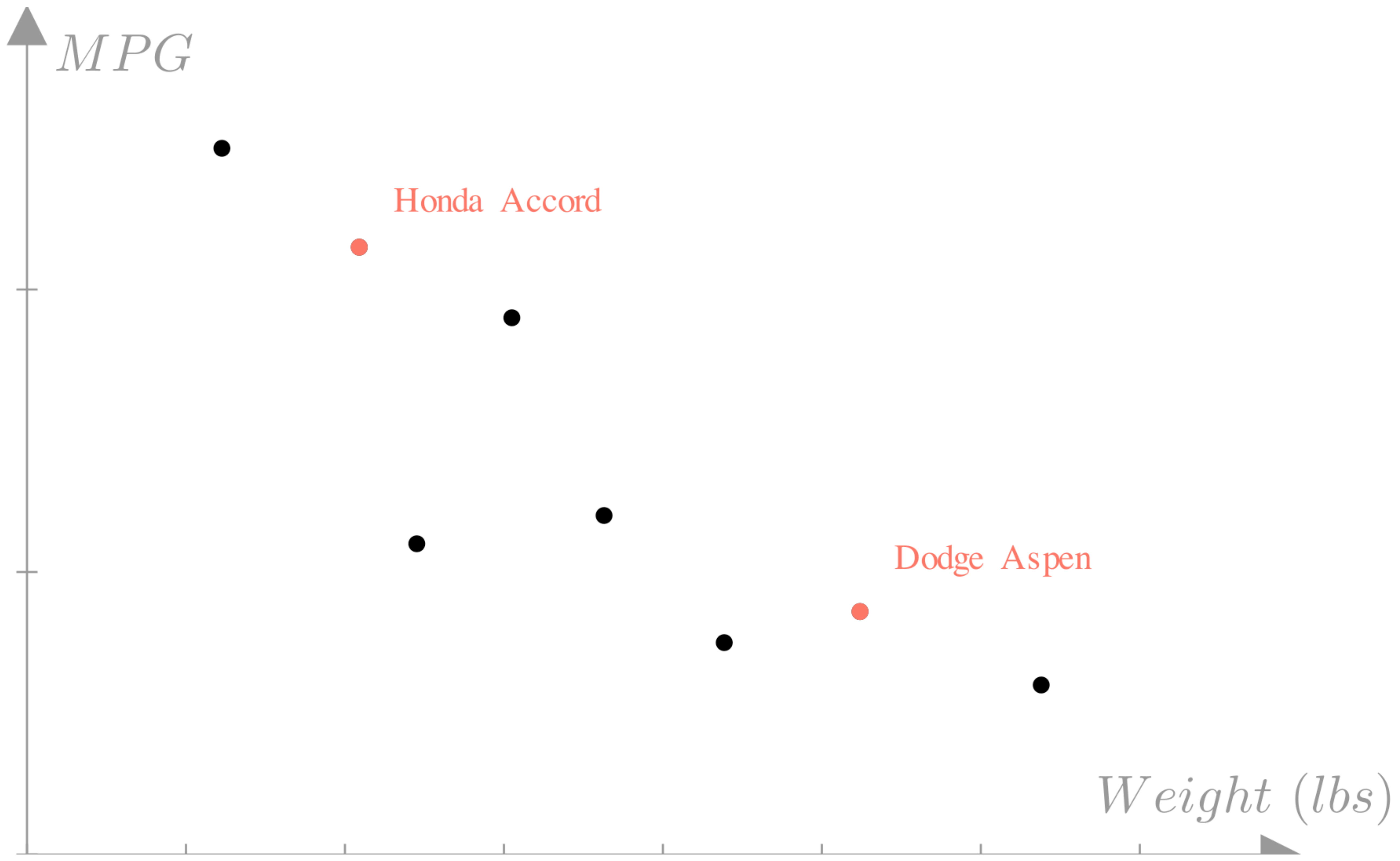
$$p(y) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2\sigma^2}(y-\mu)^2\right)$$

Linear regression predicts mean!

$$y_i \sim \mathcal{N}\left(\mathbf{x}_i^T \mathbf{w},\ \sigma^2\right)$$

Conditional probability of observation

$$p(y_i \mid \mathbf{x}_i, \mathbf{w}) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2\sigma^2}(y_i - \mathbf{x}_i^T \mathbf{w})^2\right)$$



Model labels

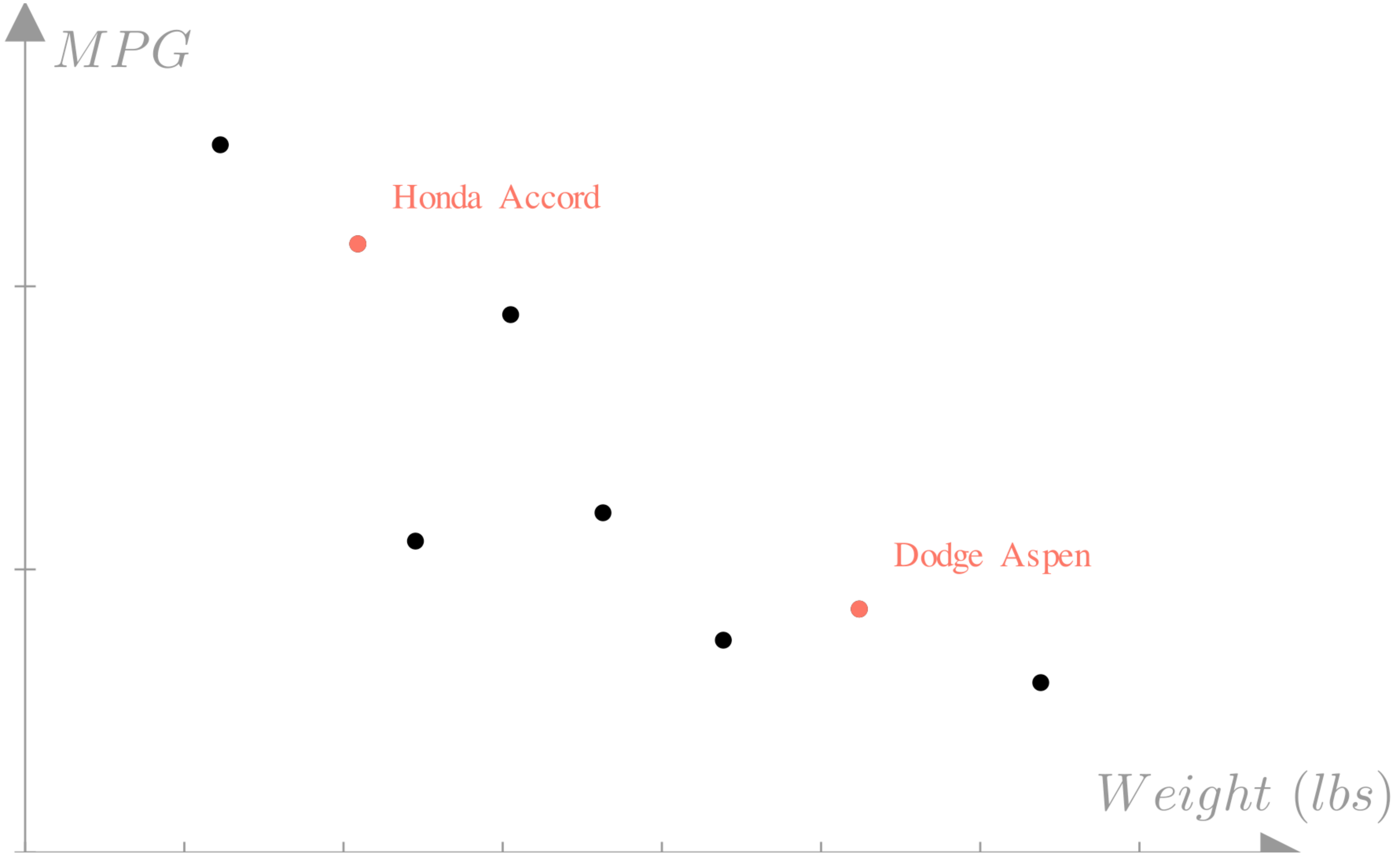
$$y_i \sim \mathcal{N}\left(\mathbf{x}_i^T \mathbf{w},\ \sigma^2\right)$$

$$p(y_i \mid \mathbf{x}_i, \mathbf{w}) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2\sigma^2}(y_i - \mathbf{x}_i^T\mathbf{w})^2\right)$$

Model residuals

$$e_i \sim \mathcal{N}\left(\mathbf{x}_i^T \mathbf{w} - y_i,\ \sigma^2\right)$$

$$p(e_i \mid \mathbf{x}_i, \mathbf{w}) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2\sigma^2}(y_i - \mathbf{x}_i^T\mathbf{w})^2\right)$$

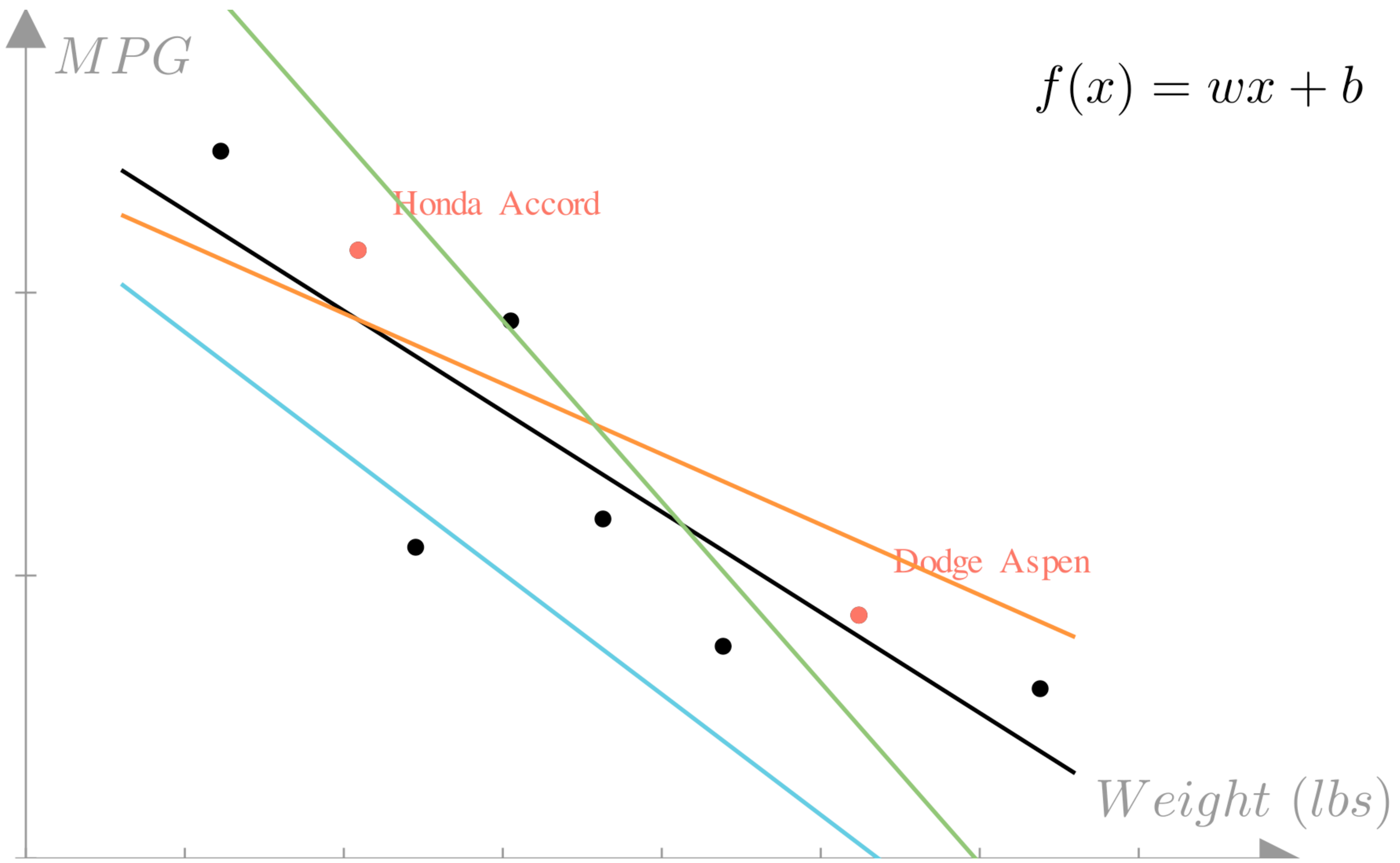


"Normal" linear regression model

$$y_i \sim \mathcal{N}\left(\mathbf{x}_i^T \mathbf{w},\ \sigma^2\right)$$

$$p(y_i \mid \mathbf{x}_i, \mathbf{w}) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2\sigma^2}(y_i - \mathbf{x}_i^T \mathbf{w})^2\right)$$

Loss function?



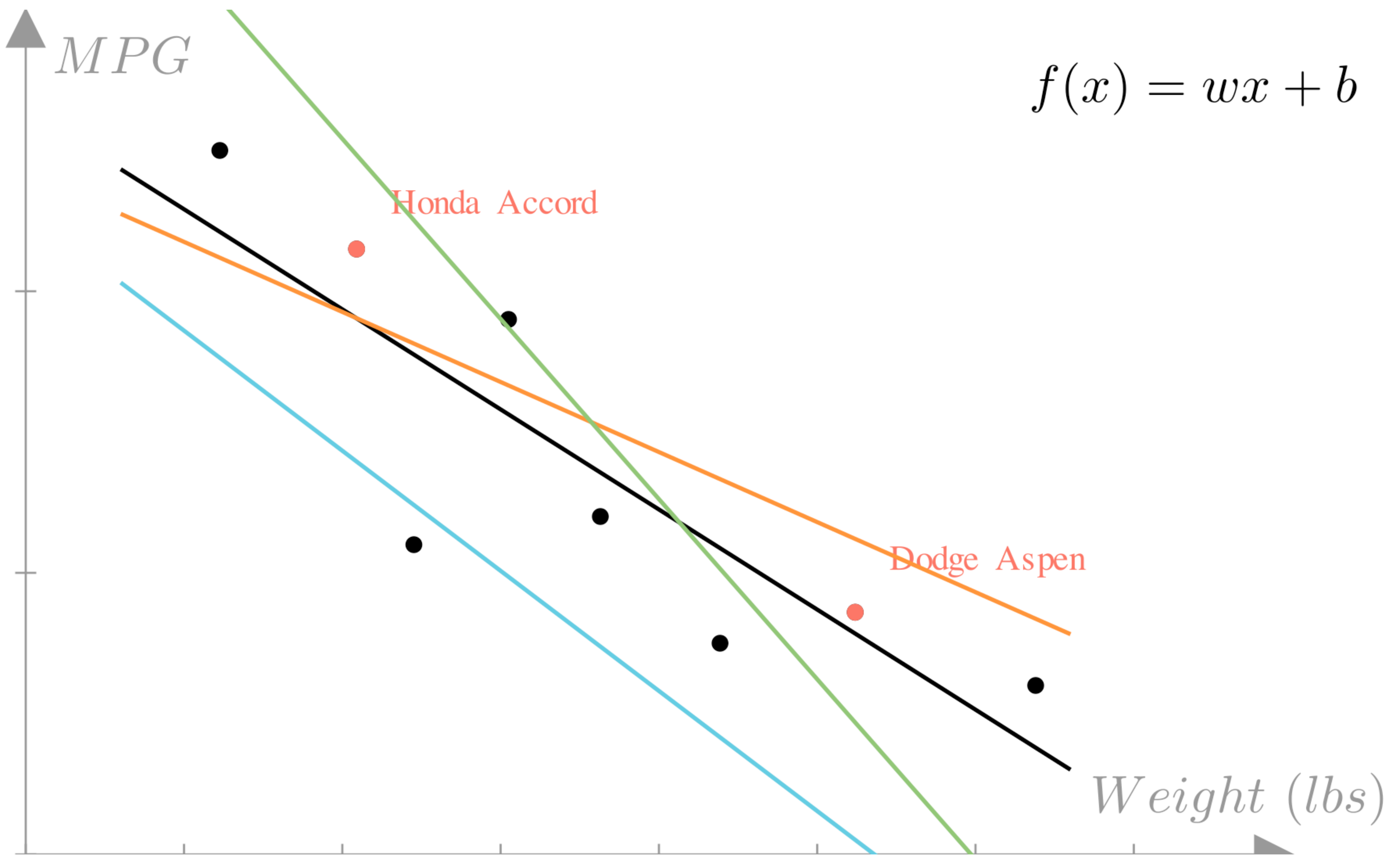
"Normal" linear regression model

$$y_i \sim \mathcal{N}\left(\mathbf{x}_i^T\mathbf{w},\ \sigma^2\right)$$

$$p(y_i \mid \mathbf{x}_i, \mathbf{w}) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(- \frac{1}{2\sigma^2}(y_i - \mathbf{x}_i^T\mathbf{w})^2 \right)$$

Loss function?

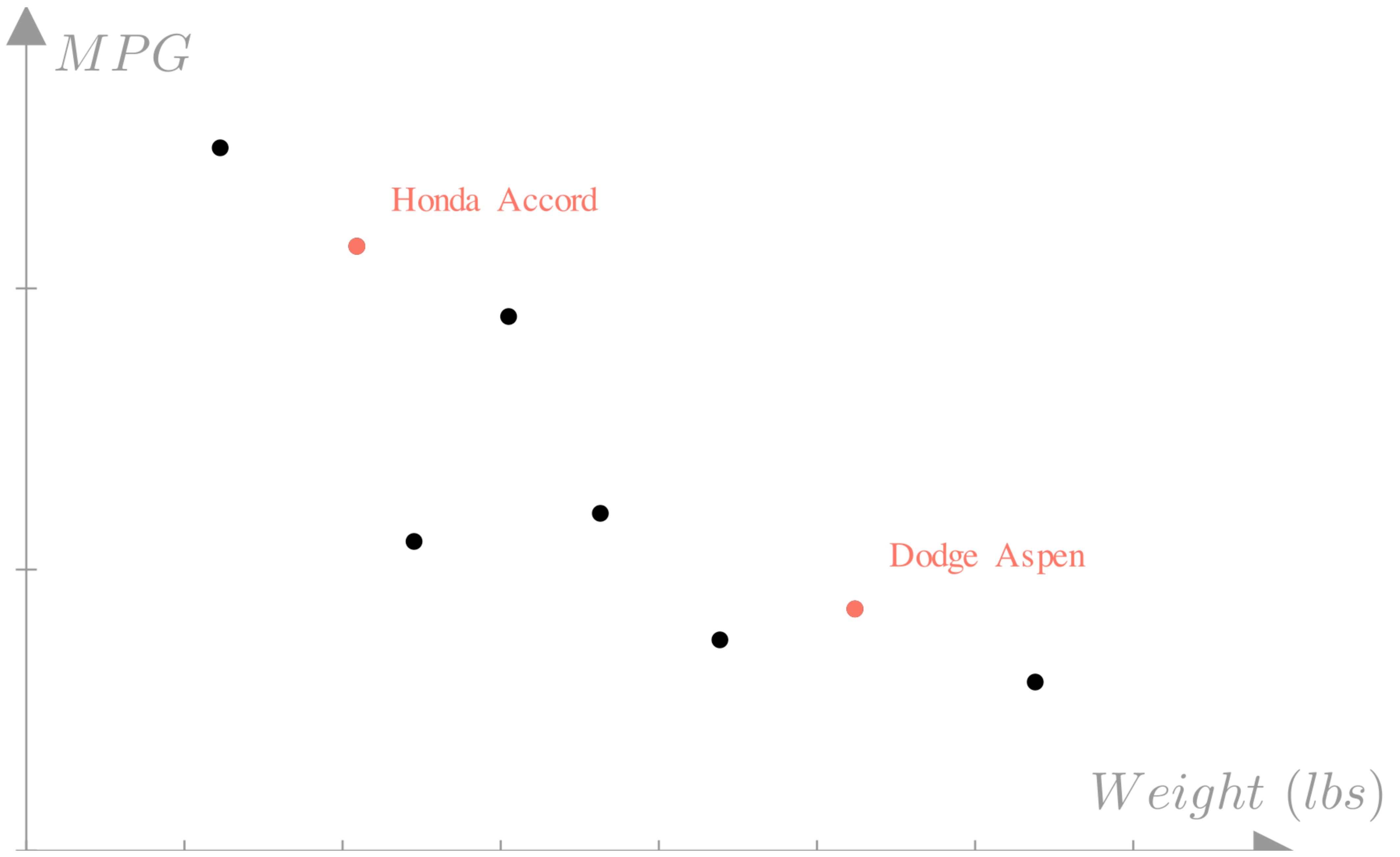
Goal: Maximize probability



$$\mathbf{w}^* = \underset{\mathbf{w}}{\operatorname{argmax}}\, p(\mathbf{y} \mid \mathbf{X}, \mathbf{w}) = \underset{\mathbf{w}}{\operatorname{argmax}}\, p(y_1, \ldots, y_N \mid \mathbf{x}_1, \ldots, \mathbf{x}_N, \mathbf{w})$$

$$\mathbf{w}^* = \underset{\mathbf{w}}{\operatorname{argmax}}\, p(\mathbf{y} \mid \mathbf{X}, \mathbf{w}) = \underset{\mathbf{w}}{\operatorname{argmax}}\, p(y_1, \ldots, y_N \mid \mathbf{x}_1, \ldots, \mathbf{x}_N, \mathbf{w})$$

$$p(y_i \mid \mathbf{x}_i, \mathbf{w}) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2\sigma^2}(y_i - \mathbf{x}_i^T\mathbf{w})^2 \right)$$



$$p(y_1, \ldots, y_N \mid \mathbf{x}_1, \ldots, \mathbf{x}_N, \mathbf{w}) = \prod_{i=1}^{N} p(y_i \mid \mathbf{x}_i, \mathbf{w})$$

$$\underset{\mathbf{w}}{\operatorname{argmax}} \prod_{i=1}^{N} p(y_i \mid \mathbf{x}_i, \mathbf{w}) = \underset{\mathbf{w}}{\operatorname{argmin}} -\sum_{i=1}^{N} \log p(y_i \mid \mathbf{x}_i, \mathbf{w}) = \mathbf{NLL}(\mathbf{w}, \mathbf{X}, \mathbf{y})$$

$$\mathbf{NLL}(\mathbf{w}, \mathbf{X}, \mathbf{y}) = -\sum_{i=1}^{N} \log\left[\frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2\sigma^2}(y_i - \mathbf{x}_i^T \mathbf{w})^2\right)\right]$$

$$\nabla_{\mathbf{w}}\mathbf{NLL}(\mathbf{w},\mathbf{X},\mathbf{y}) = \frac{d}{d\mathbf{w}}\left(\frac{1}{2\sigma^2}\sum_{i=1}^{N}(y_i - \mathbf{x}_i^T\mathbf{w})^2 + N\log\sigma\sqrt{2\pi}\right)$$

$$\underset{\mathbf{w}}{\operatorname{argmin}}\, MSE(\mathbf{w}, \mathbf{X}, \mathbf{y}) = \underset{\mathbf{w}}{\operatorname{argmin}}\, \mathbf{NLL}(\mathbf{w}, \mathbf{X}, \mathbf{y})$$