Week 4: Linear Models Revisited

Matthew Caldwell

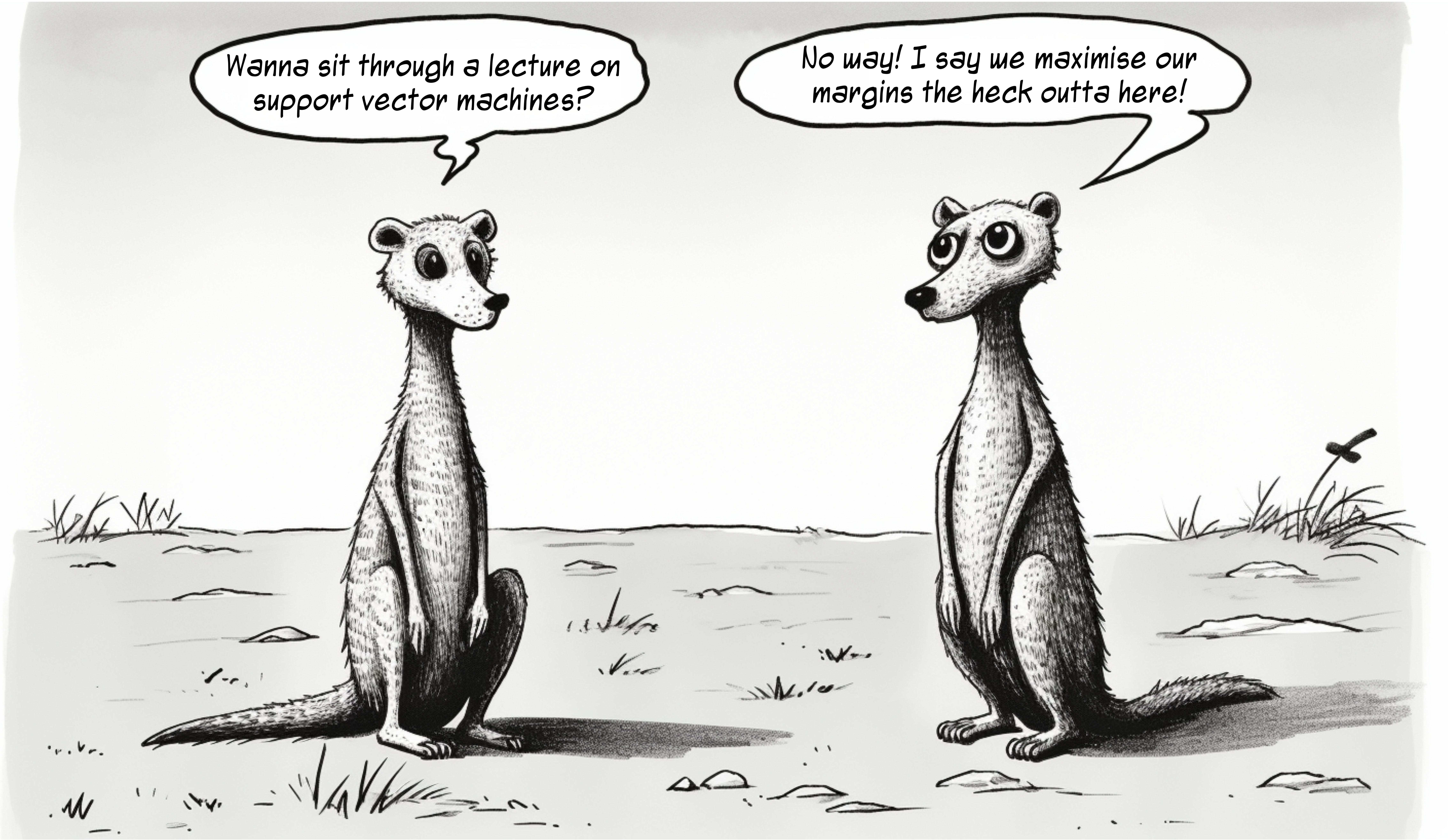
COMP0088 Introduction to Machine Learning • UCL Computer Science • Autumn 2023

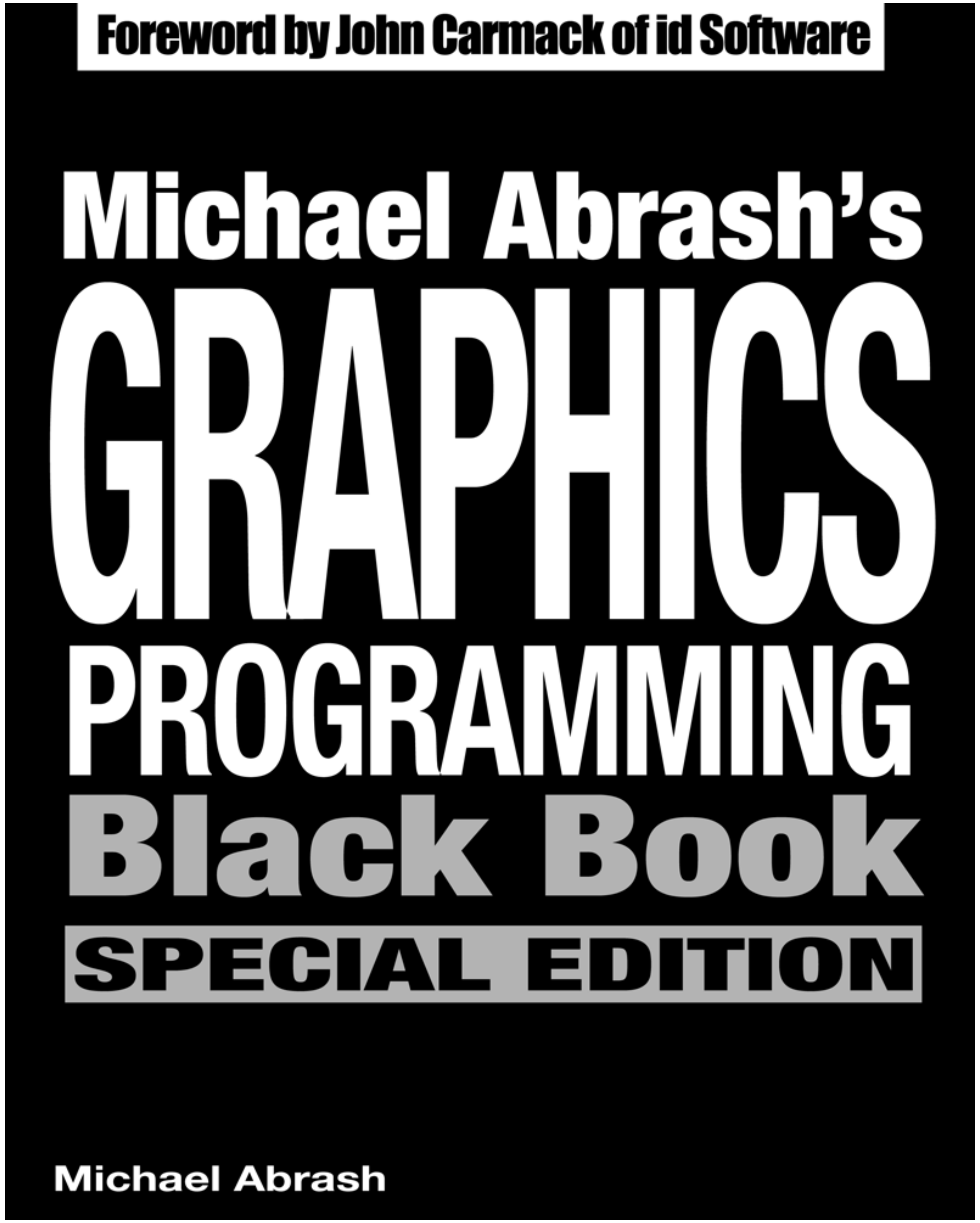
Admin

- Bartlett questionnaires
- Pulse surveys

Week 4 Recap

Joining the Dots


Wanna sit through a lecture on support vector machines?
No way! I say we maximise our margins the heck outta here!


Foreword by John Carmack of id Software
Michael Abrash's
GRAPHICS
PROGRAMMING
Black Book
SPECIAL EDITION
Michael Abrash

$$\mathbf{a} \cdot \mathbf{b} = \mathbf{a}^\mathsf{T}\mathbf{b} = \langle \mathbf{a}, \mathbf{b} \rangle = \sum_i a_i b_i$$

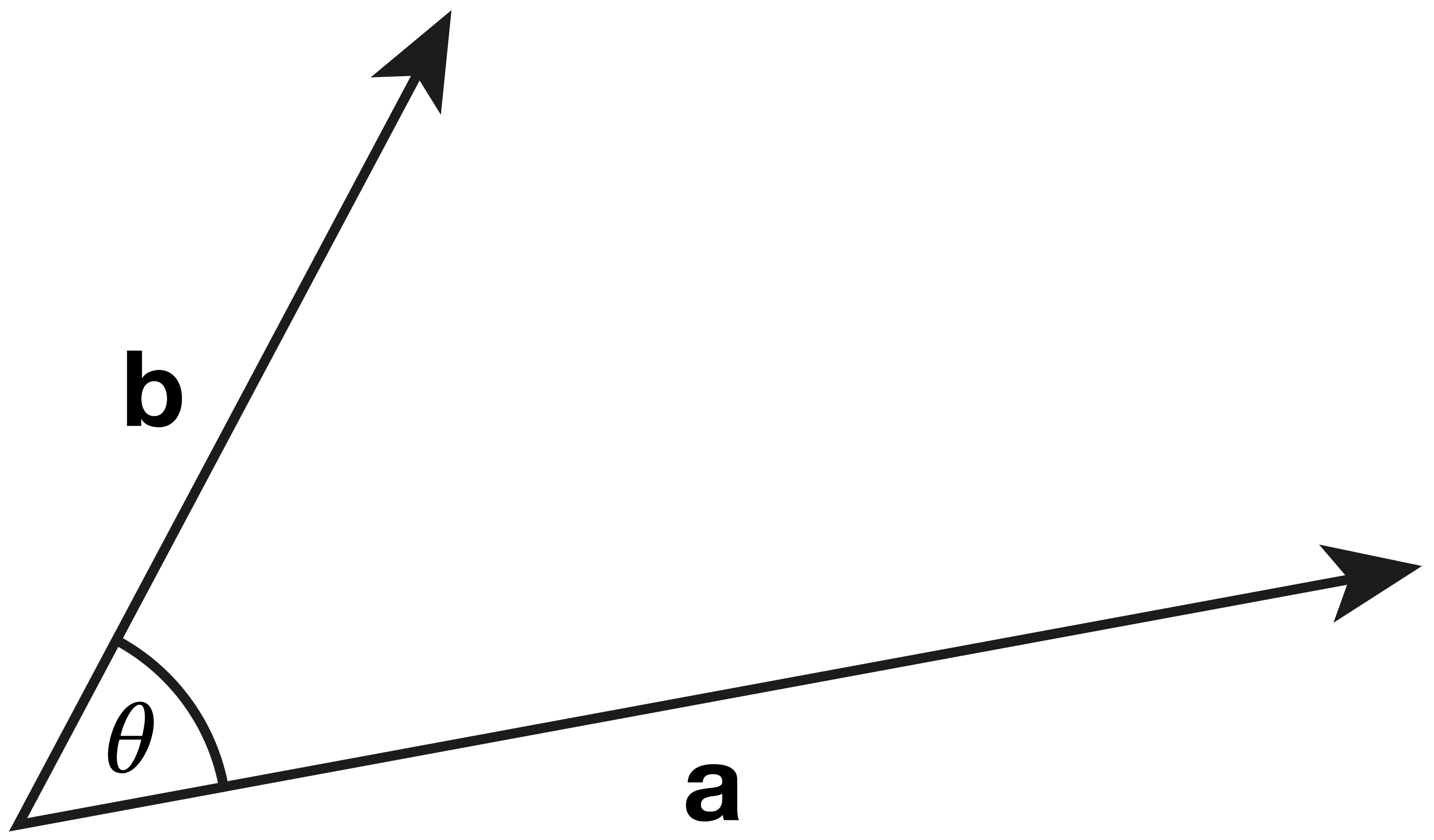
$$\mathbf{x} \cdot \mathbf{x} = \|\mathbf{x}\|^2$$

$$\mathbf{w} \cdot \mathbf{x} = w_1 x_1 + w_2 x_2 + \ldots + w_d x_d$$

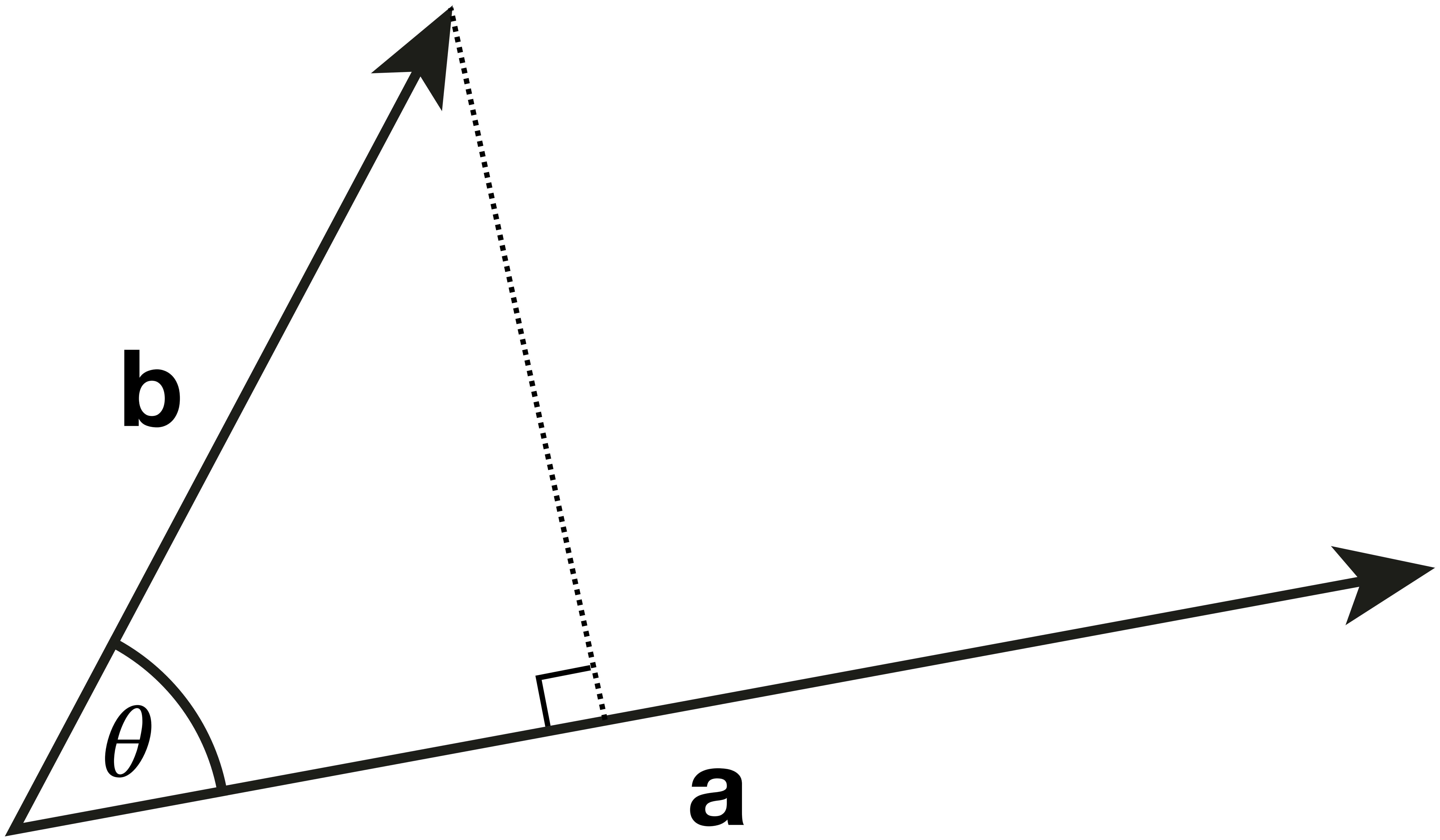
$$\mathbf{w} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \qquad \mathbf{w} = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$$

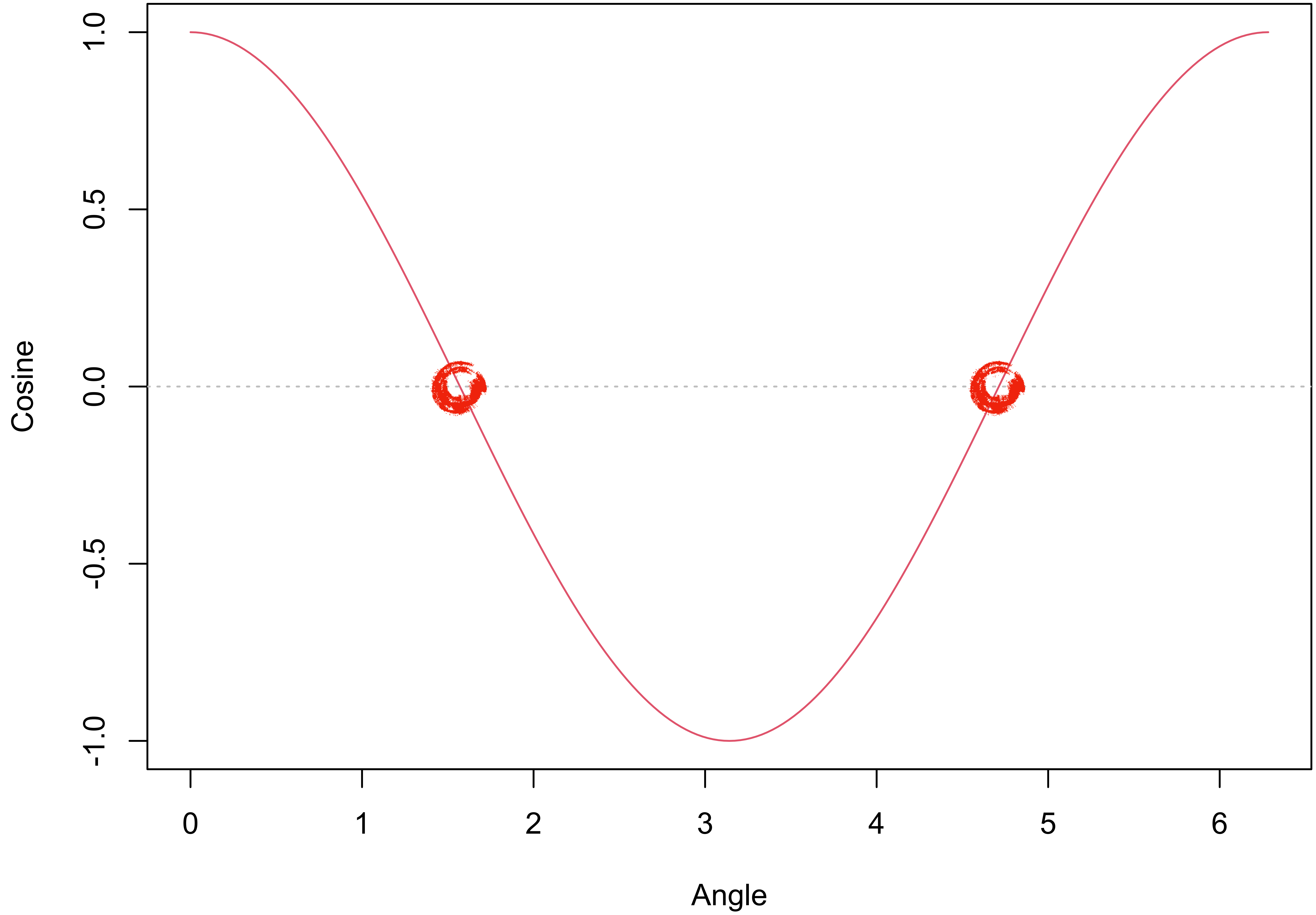
$$\mathbf{w} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} \qquad \mathbf{w} = \begin{bmatrix} 0.25 \\ 0.25 \\ 0.25 \\ 0.25 \end{bmatrix}$$

$$\mathbf{AB} = \begin{bmatrix} \mathbf{a}_1^\top \\ \mathbf{a}_2^\top \\ \vdots \\ \mathbf{a}_n^\top \end{bmatrix} \begin{bmatrix} \mathbf{b}_1 & \mathbf{b}_2 & \dots & \mathbf{b}_d \end{bmatrix} = \begin{bmatrix} \mathbf{a}_1 \cdot \mathbf{b}_1 & \mathbf{a}_1 \cdot \mathbf{b}_2 & \dots & \mathbf{a}_1 \cdot \mathbf{b}_d \\ \mathbf{a}_2 \cdot \mathbf{b}_1 & \mathbf{a}_2 \cdot \mathbf{b}_2 & \dots & \mathbf{a}_2 \cdot \mathbf{b}_d \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{a}_n \cdot \mathbf{b}_1 & \mathbf{a}_n \cdot \mathbf{b}_2 & \dots & \mathbf{a}_n \cdot \mathbf{b}_d \end{bmatrix}$$


b
θ
a

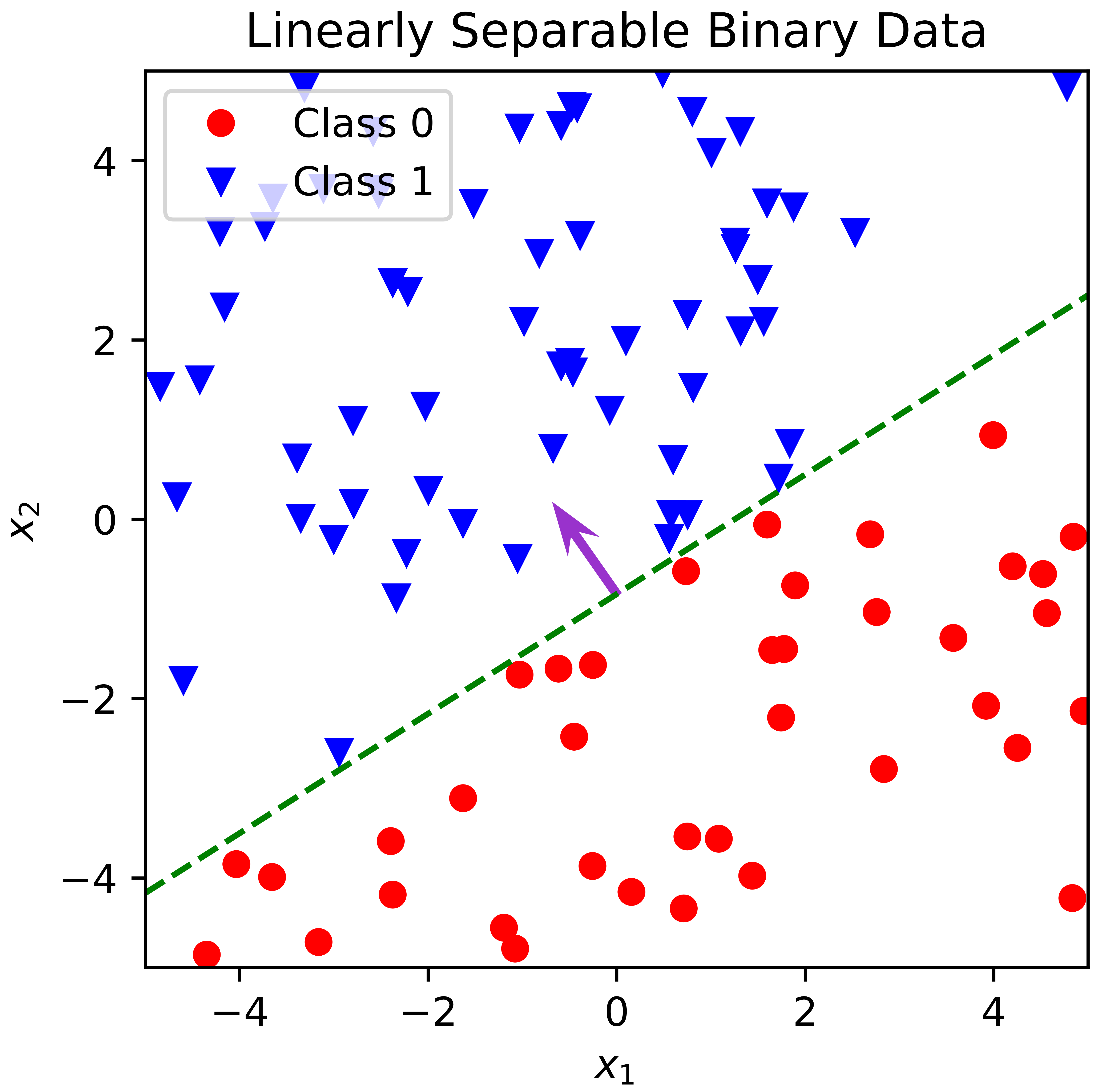
$$\mathbf{a} \cdot \mathbf{b} = |\mathbf{a}||\mathbf{b}| \cos\theta$$

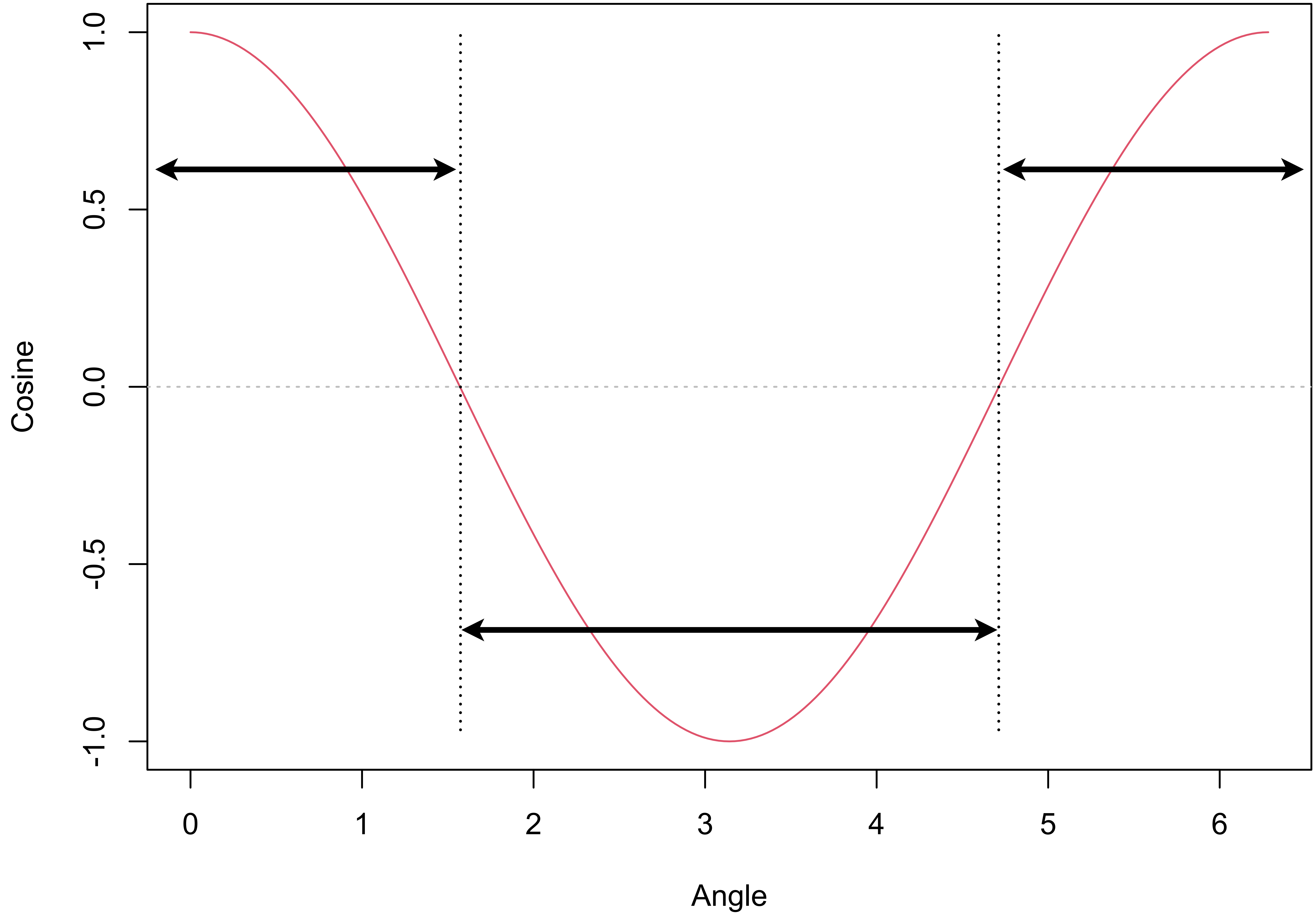

b
θ
a


1.0
0.5
0.0
-0.5
-1.0
Cosine
0
1
2
3
4
5
6
Angle

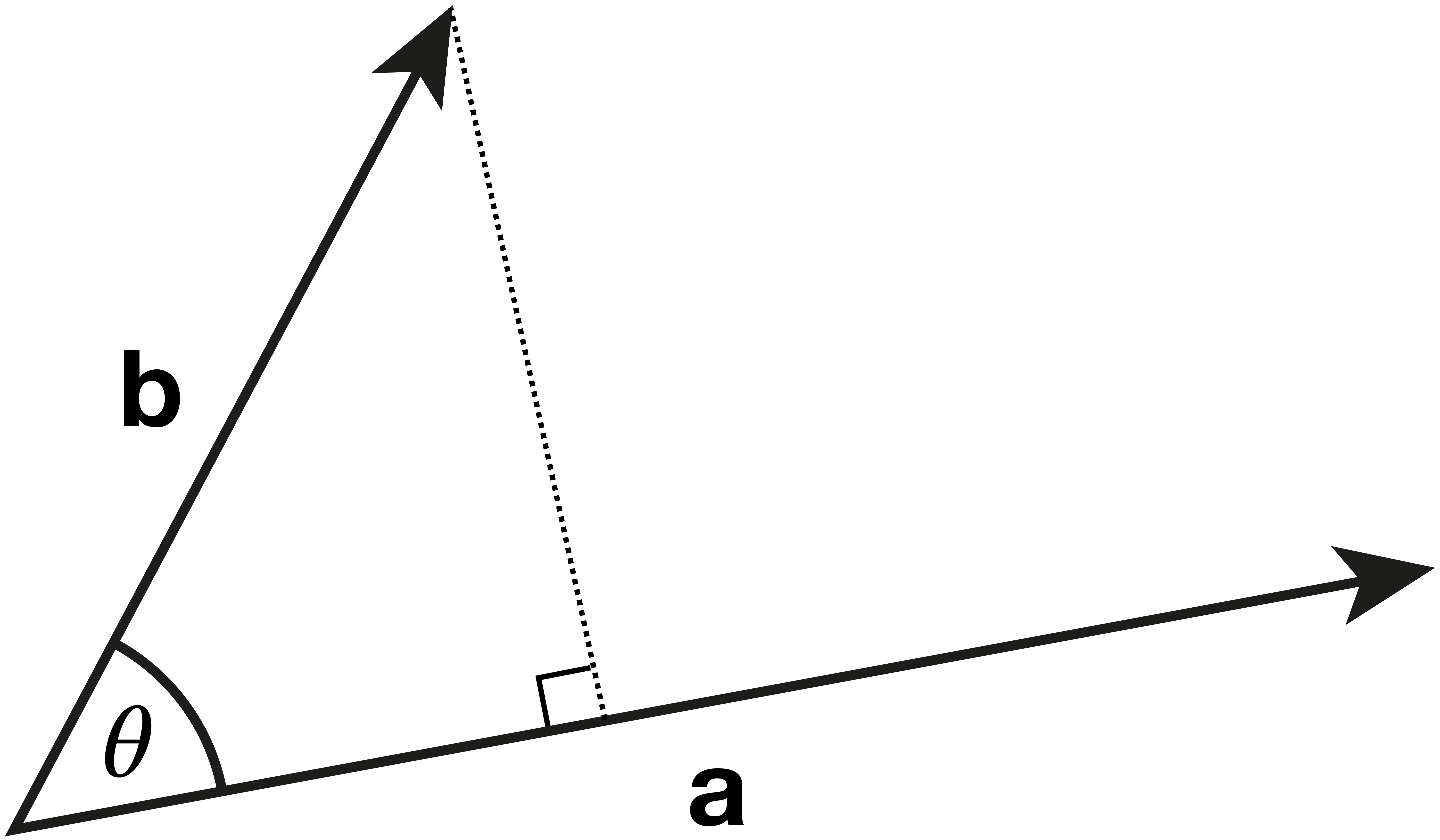
$$\mathbf{x} \cdot \mathbf{w} = 0$$

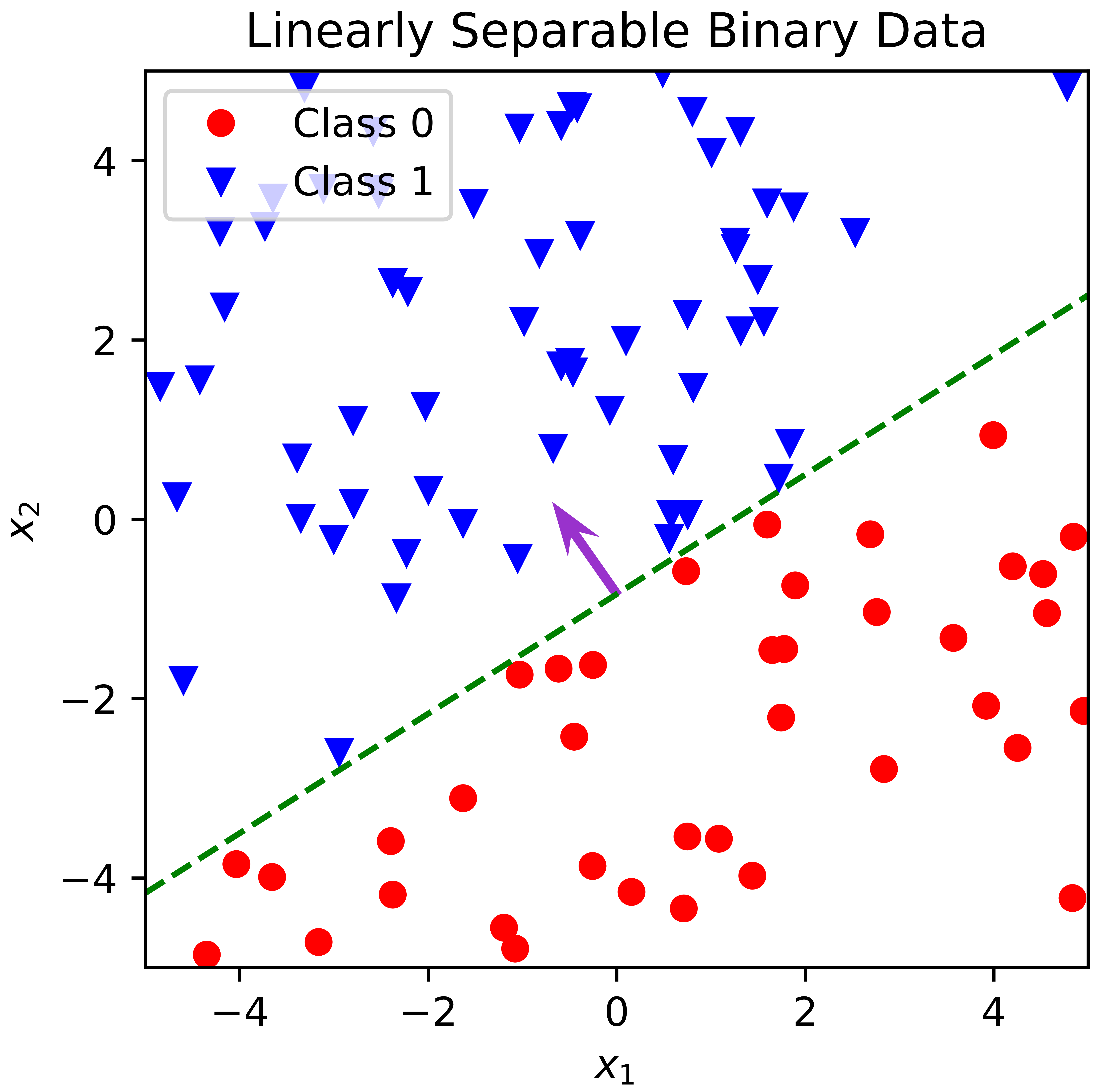
$$\implies \mathbf{x} \perp \mathbf{w}$$


Linearly Separable Binary Data
Class 0
Class 1
4
2
0
−2
−4
x_2
−4
−2
0
2
4
x_1


Cosine
1.0
0.5
0.0
-0.5
-1.0
0
1
2
3
4
5
6
Angle

$$\hat{y} = \begin{cases} 1 & \text{if } \mathbf{x} \cdot \mathbf{w} \geq 0 \\ 0 & \text{otherwise} \end{cases}$$


b
θ
a



Linearly Separable Binary Data
Class 0
Class 1
4
2
0
−2
−4
x_2
−4
−2
0
2
4
x_1

$$\mathbf{x} \cdot \mathbf{w}$$

$$\frac{\mathbf{x} \cdot \mathbf{w}}{|\mathbf{w}|}$$

$$y \in \{0, 1\}$$

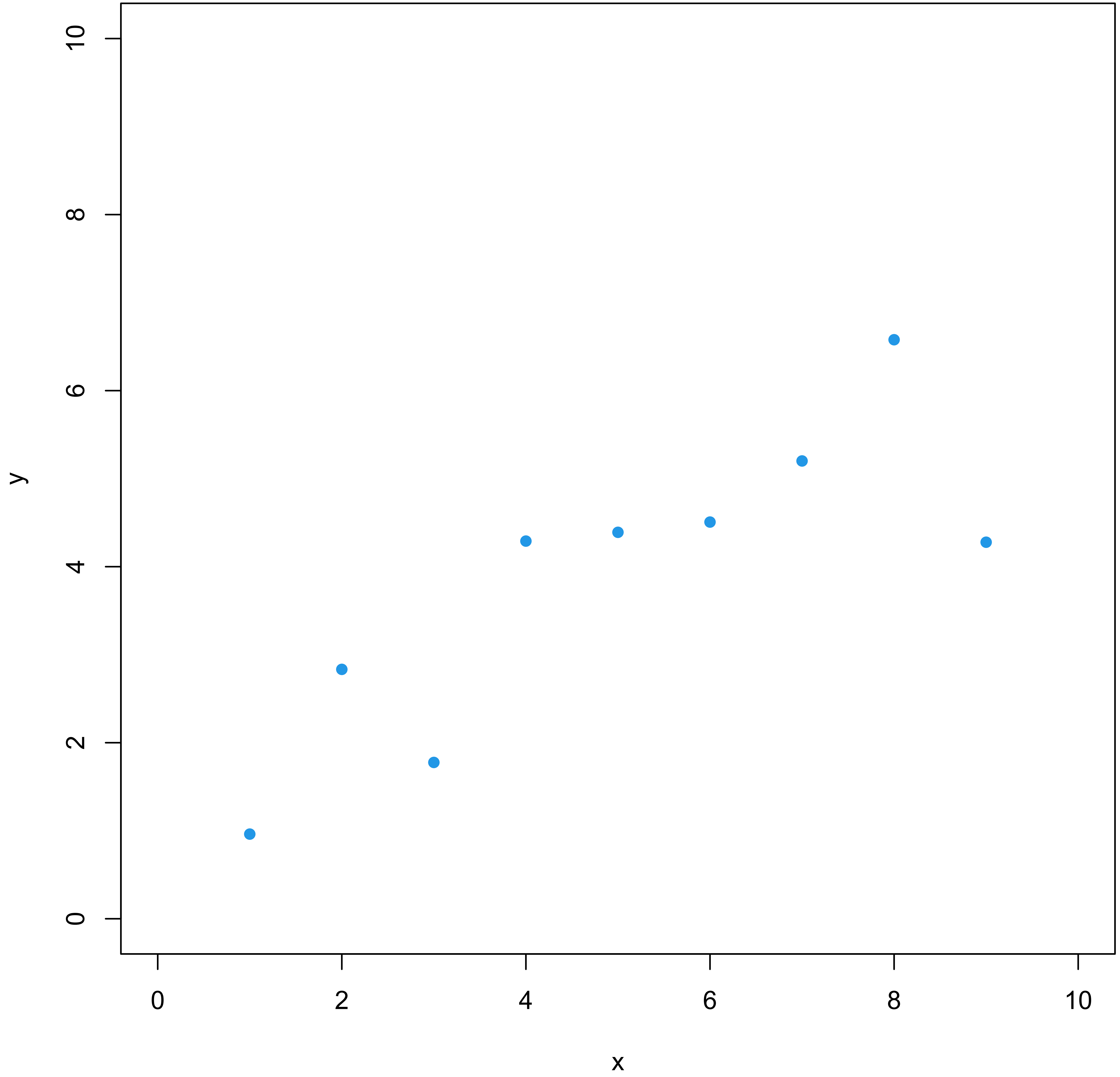
$$y \in \{-1, 1\}$$

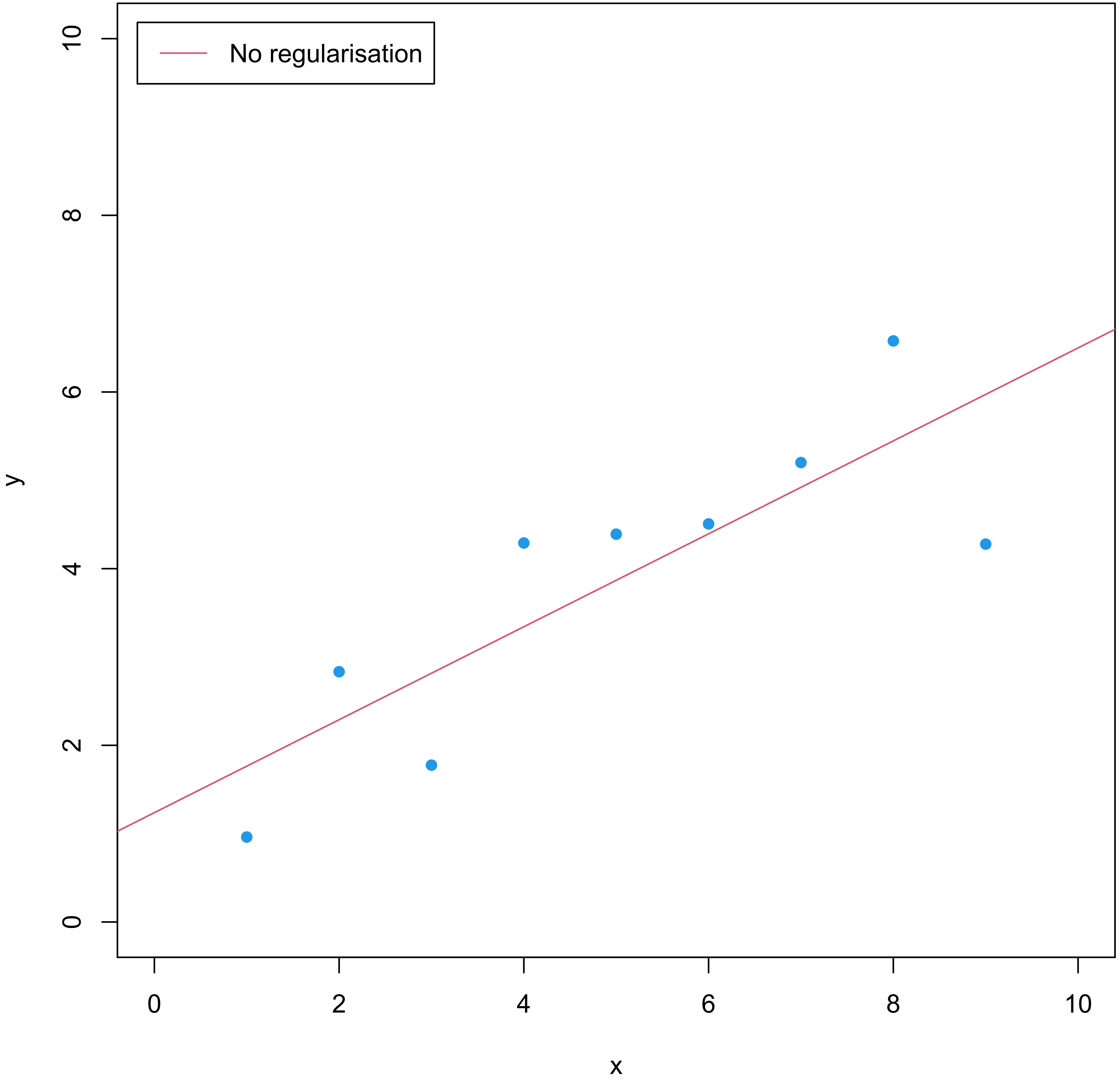
Functional Margin

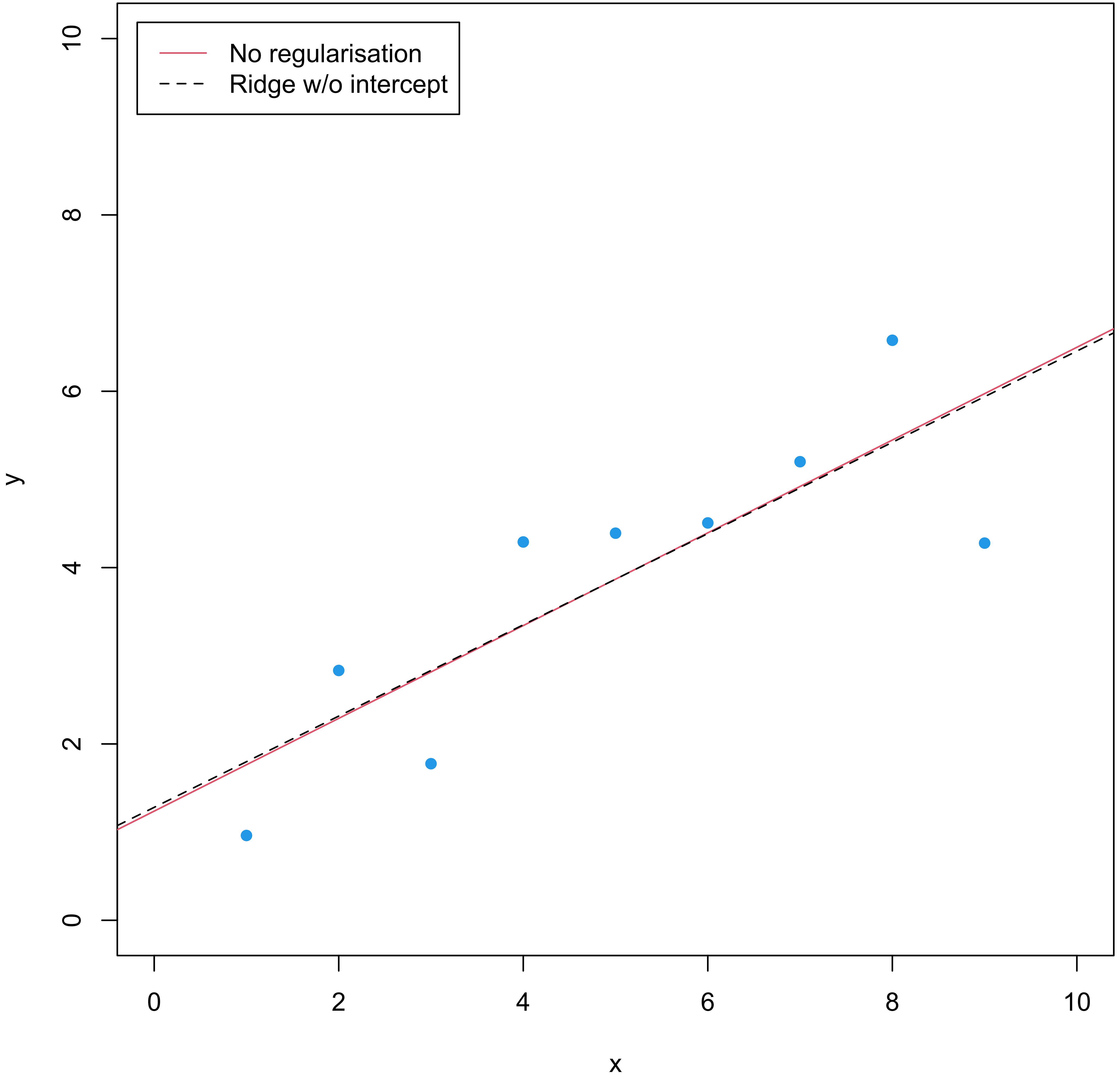
$$y\hat{y} = yf(\mathbf{x}) = y\,\mathbf{x} \cdot \mathbf{w}$$

Geometric Margin

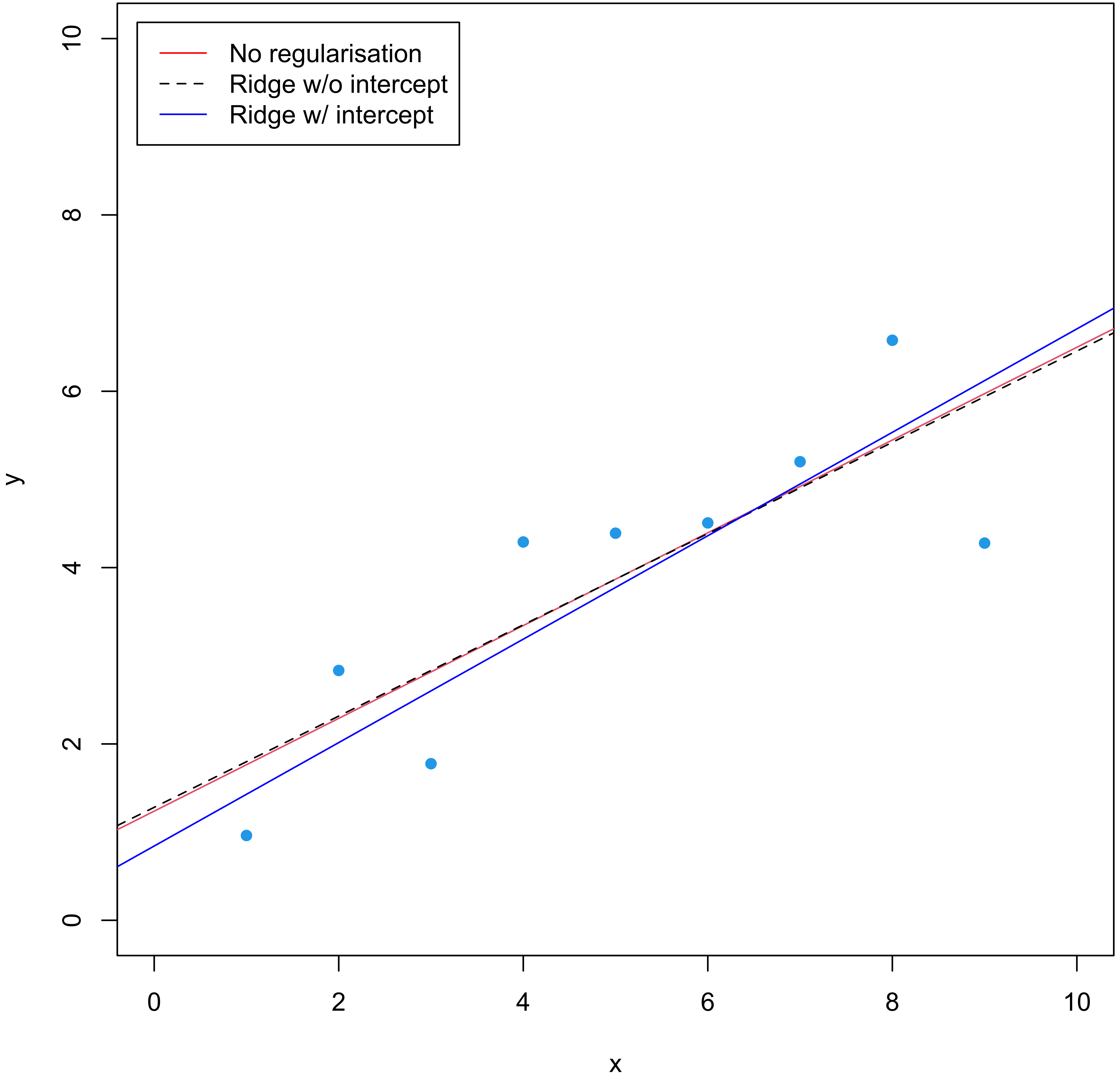
$$\frac{y\,\mathbf{x}\cdot\mathbf{w}}{|\mathbf{w}|}$$

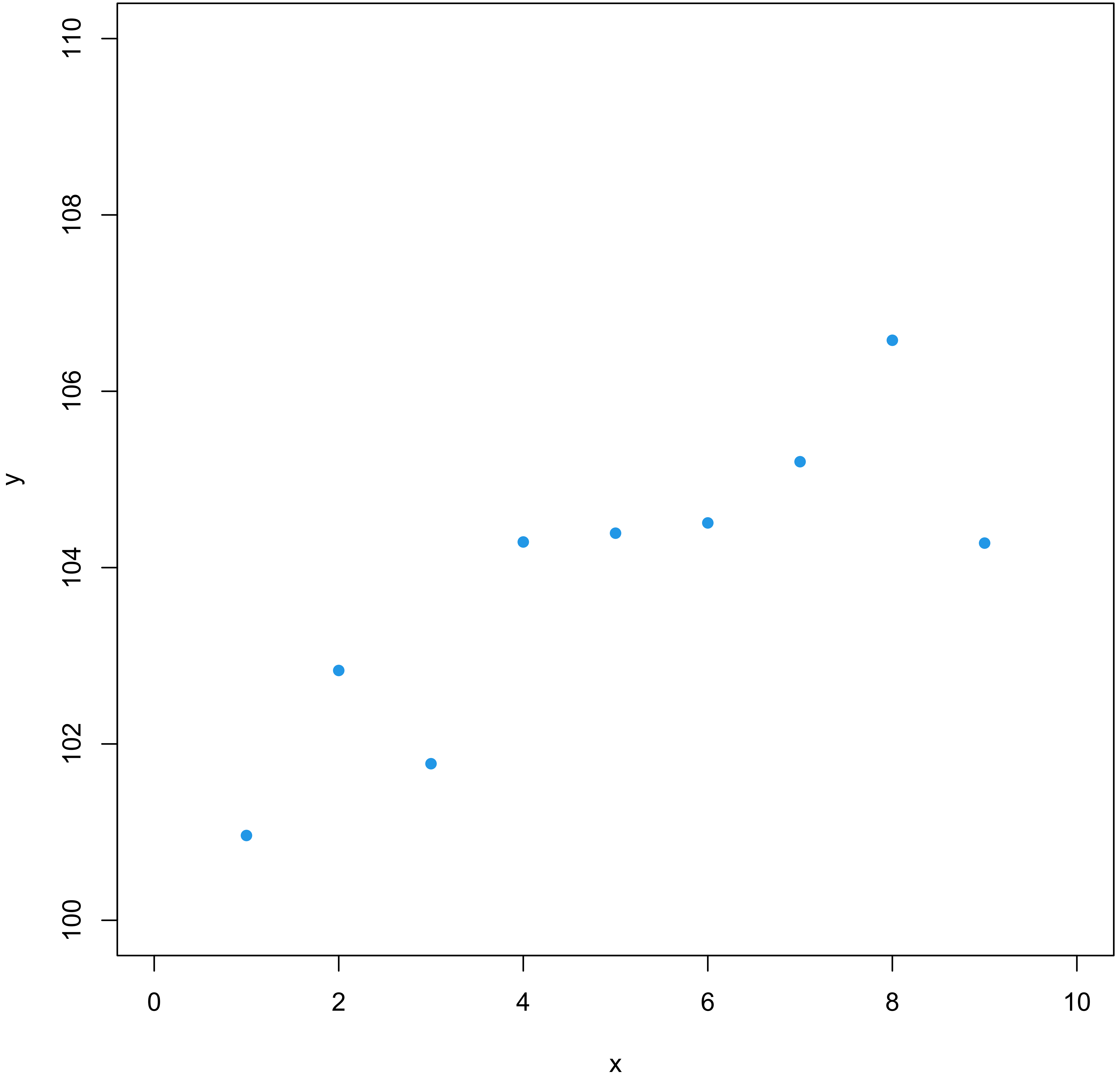

0
2
4
6
8
10
y
0
2
4
6
8
10
x


No regularisation
y
x
0
2
4
6
8
10
0
2
4
6
8
10

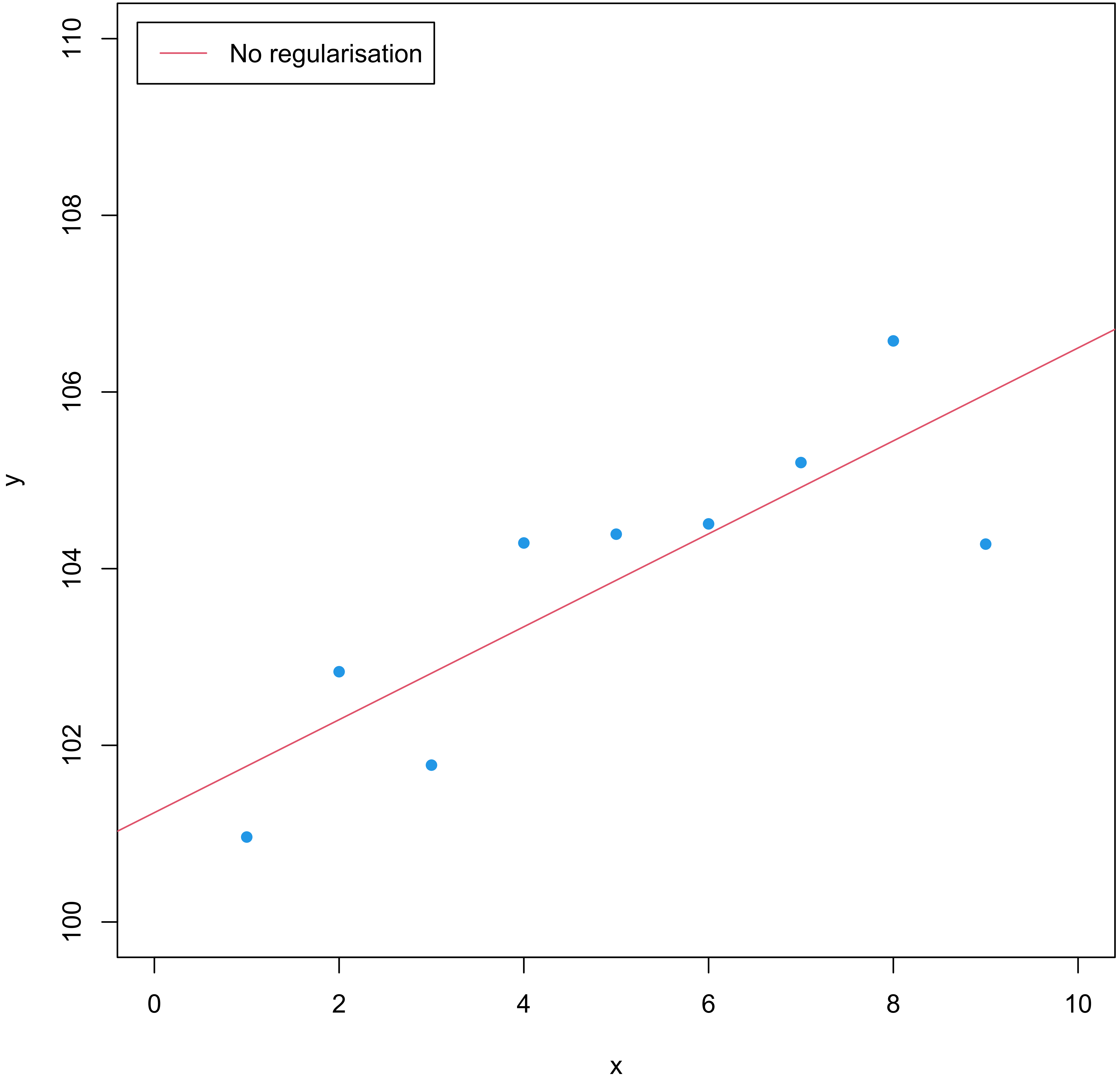


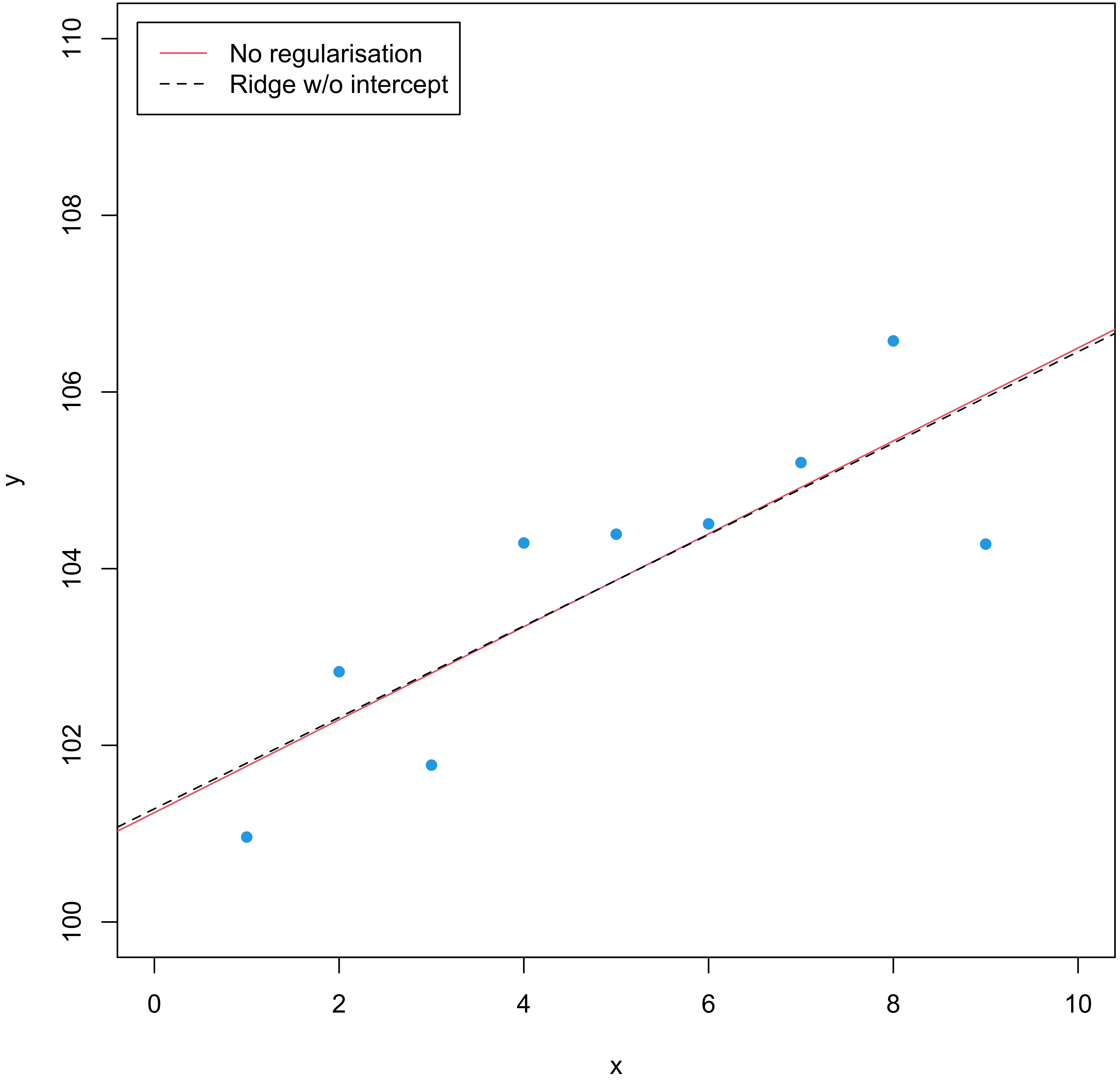
No regularisation
Ridge w/o intercept
y
x
0
2
4
6
8
10

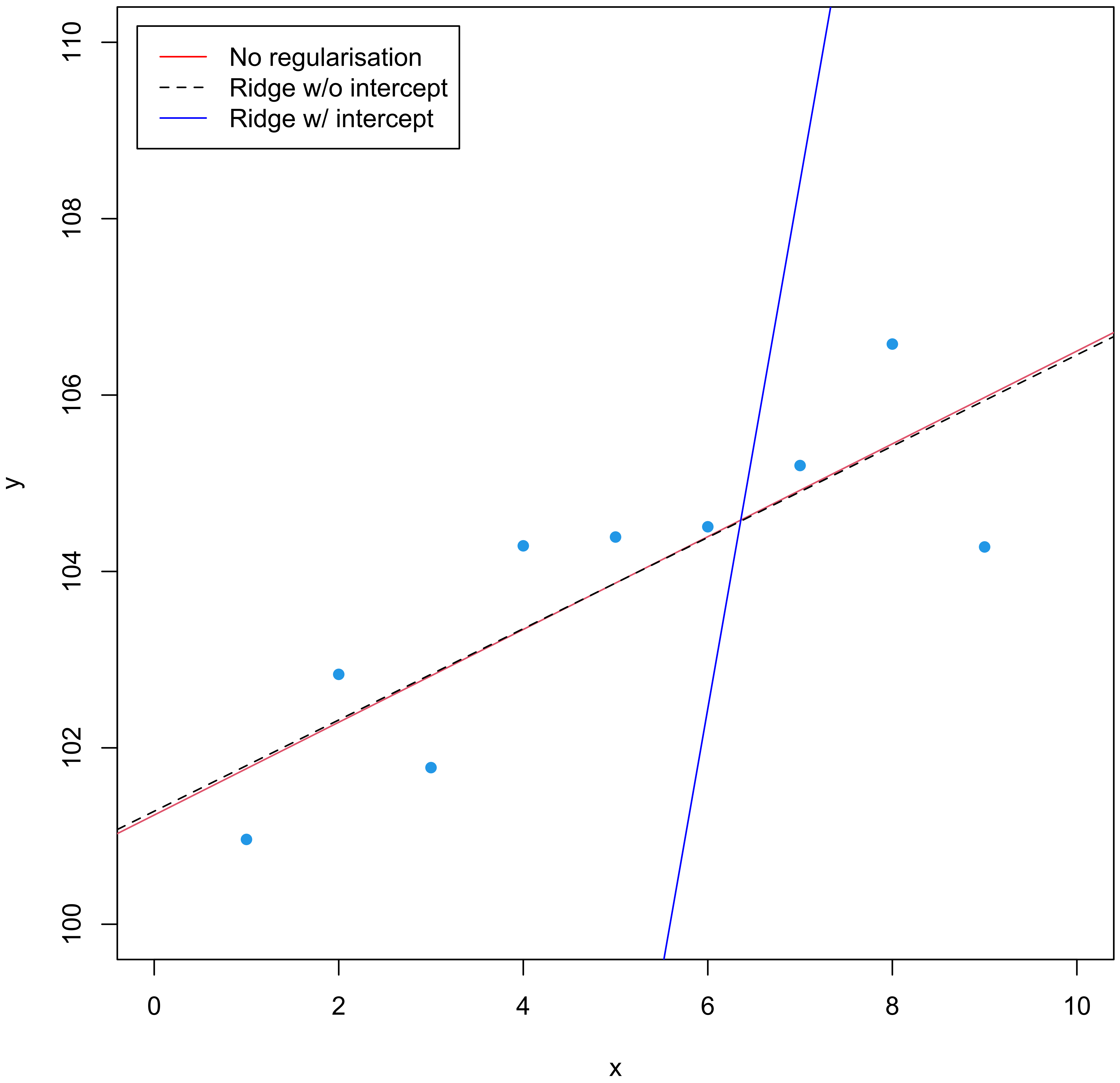

No regularisation
Ridge w/o intercept
Ridge w/ intercept
y
x
0
2
4
6
8
10
0
2
4
6
8
10

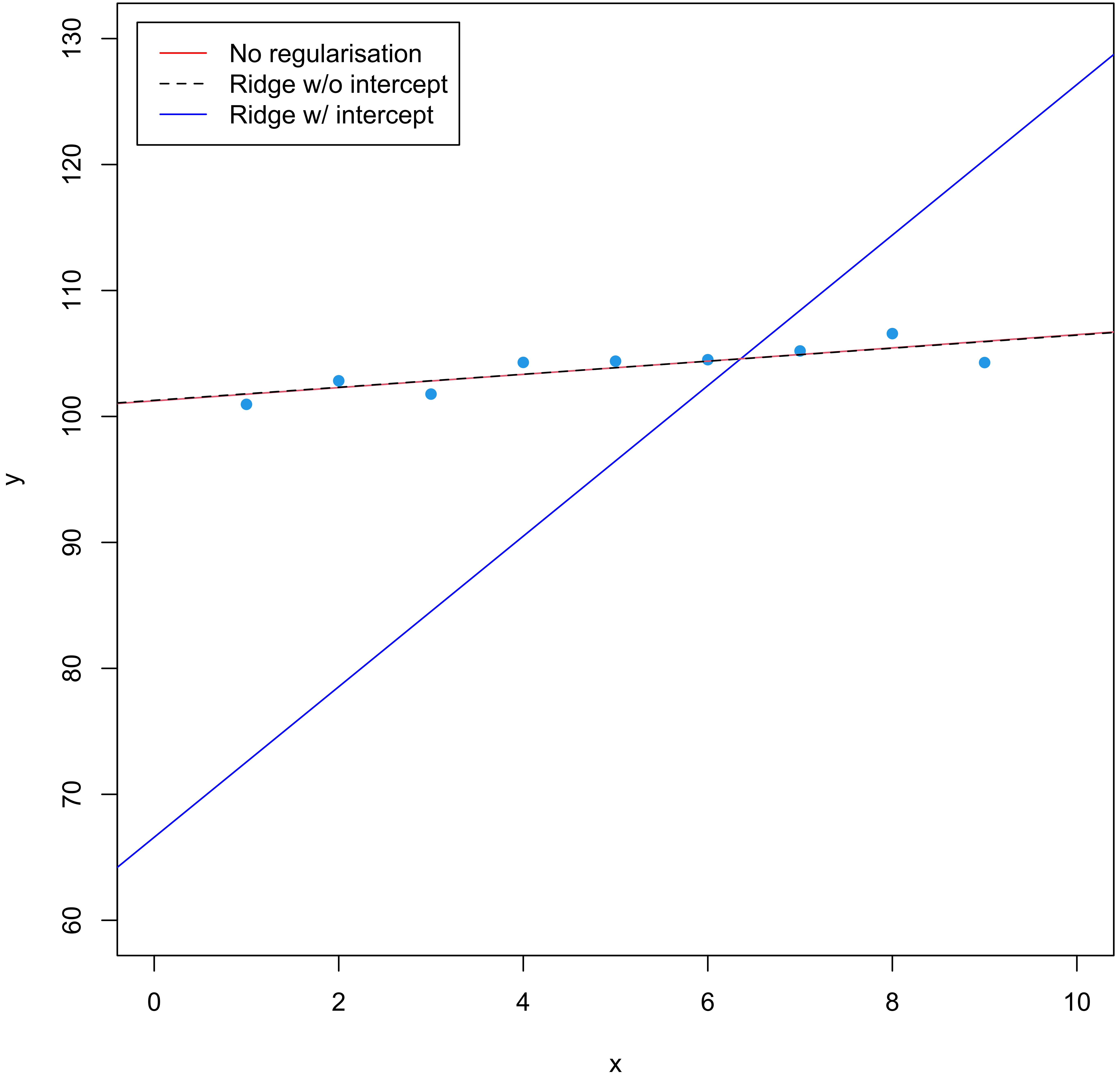


110
108
106
104
102
100
y
0
2
4
6
8
10
x

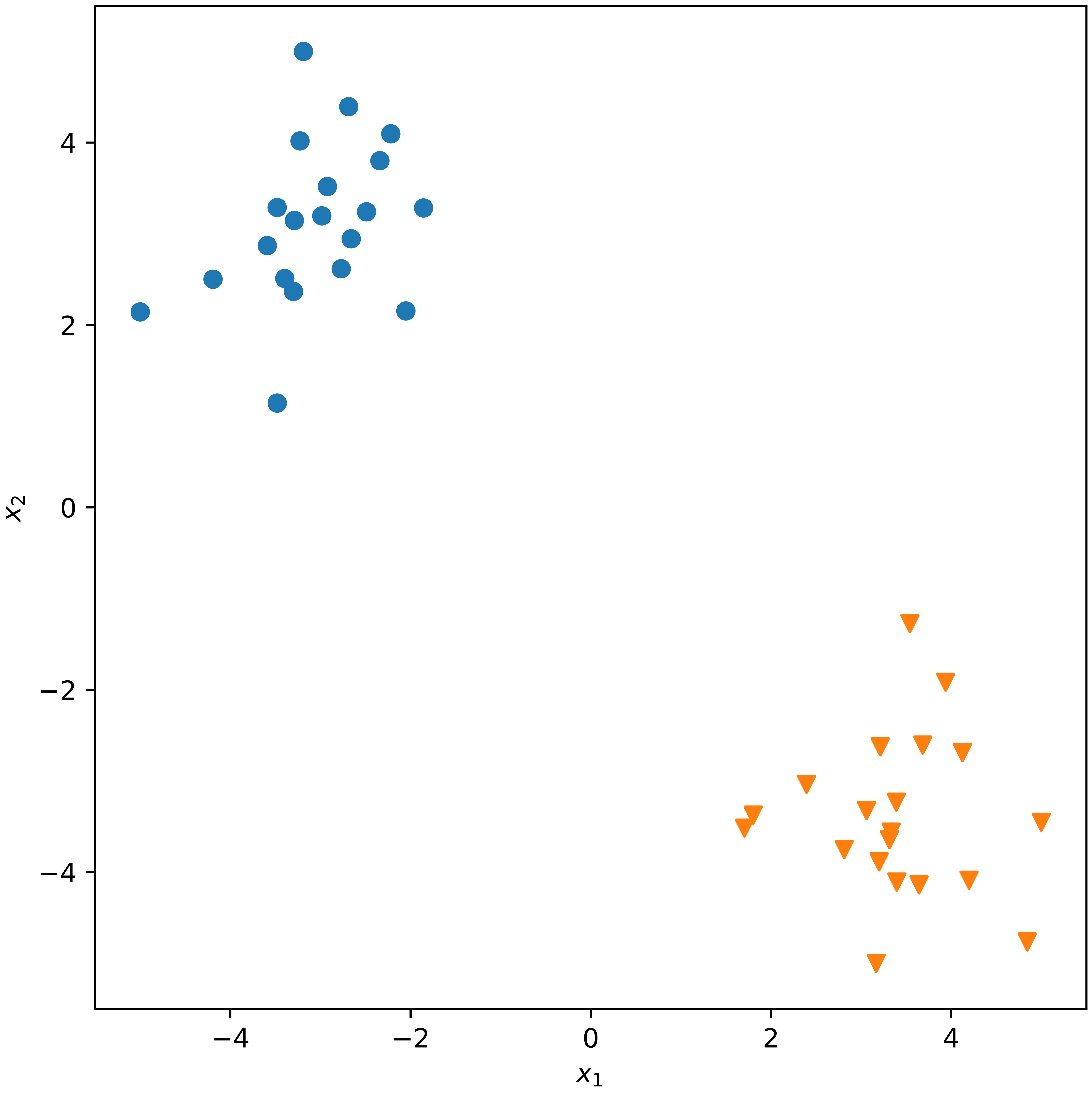

No regularisation
y
x
100
102
104
106
108
110
0
2
4
6
8
10


No regularisation
Ridge w/o intercept
110
108
106
104
102
100
y
0
2
4
6
8
10
x

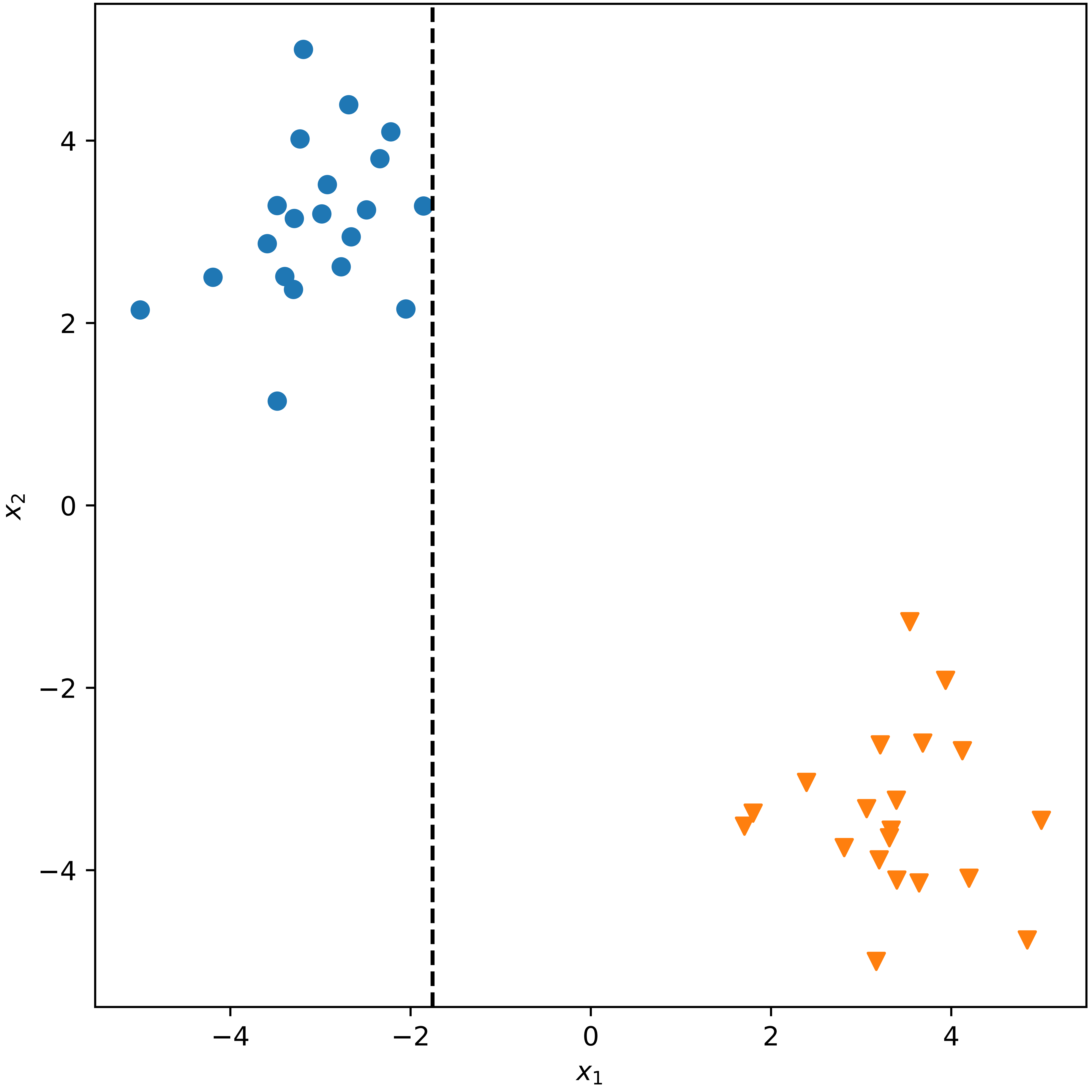

No regularisation
Ridge w/o intercept
Ridge w/ intercept
y
x
0
2
4
6
8
10
100
102
104
106
108
110

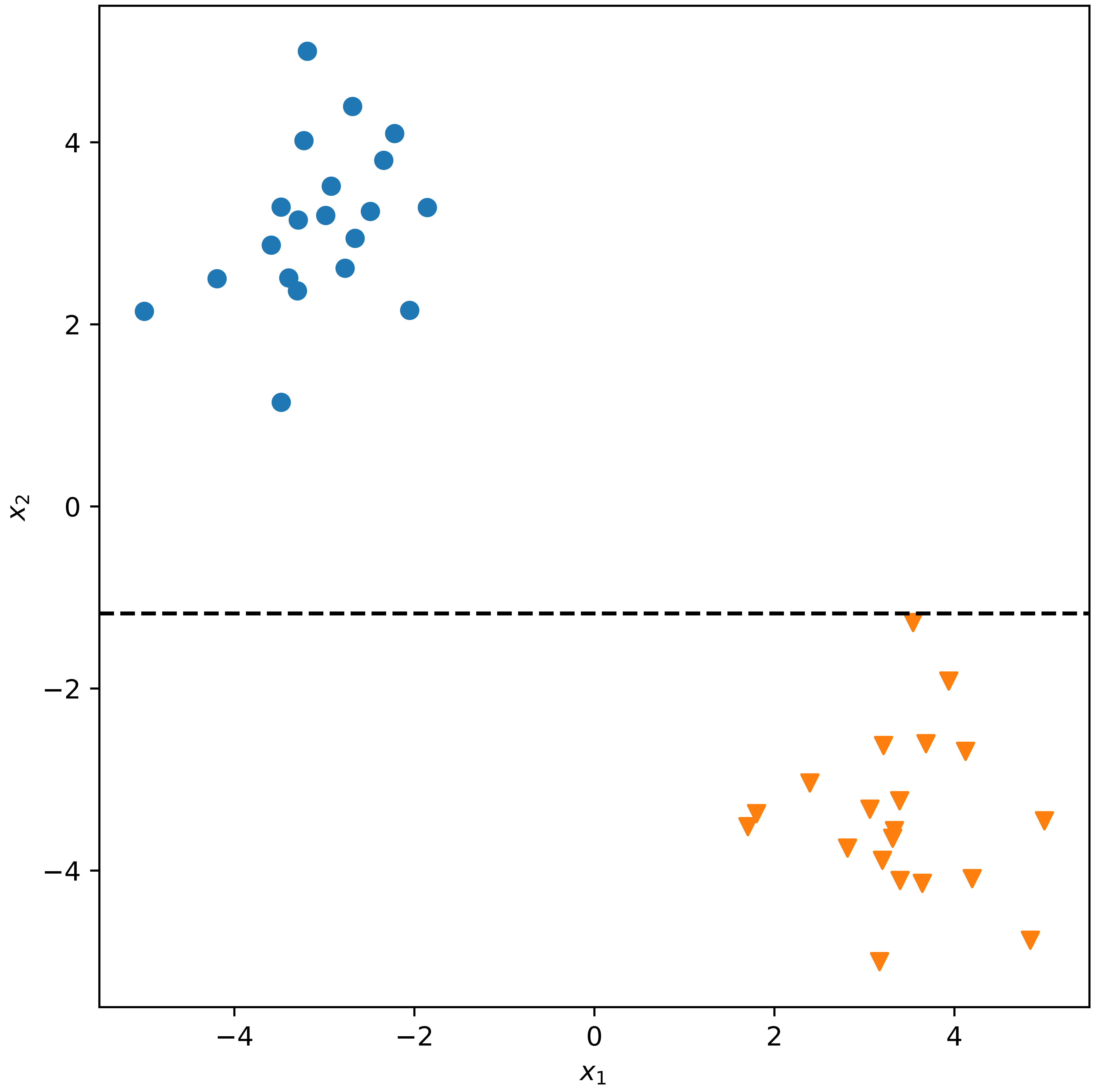

No regularisation
Ridge w/o intercept
Ridge w/ intercept
y
x
60
70
80
90
100
110
120
130
0
2
4
6
8
10

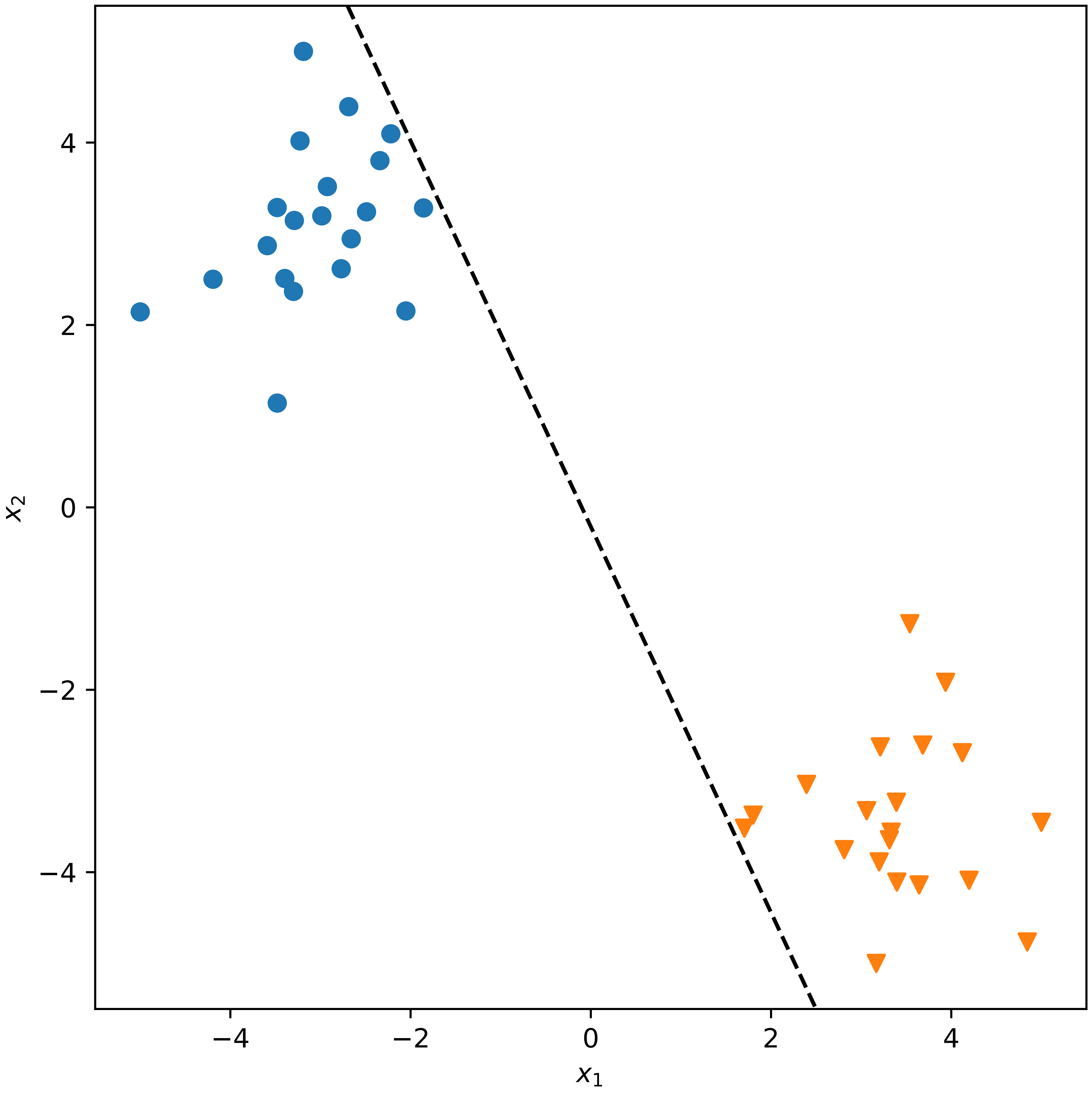
$$\hat{y} = \begin{cases} 1 & \text{if } \mathbf{x} \cdot \mathbf{w} + b \geq 0 \\ -1 & \text{otherwise} \end{cases}$$



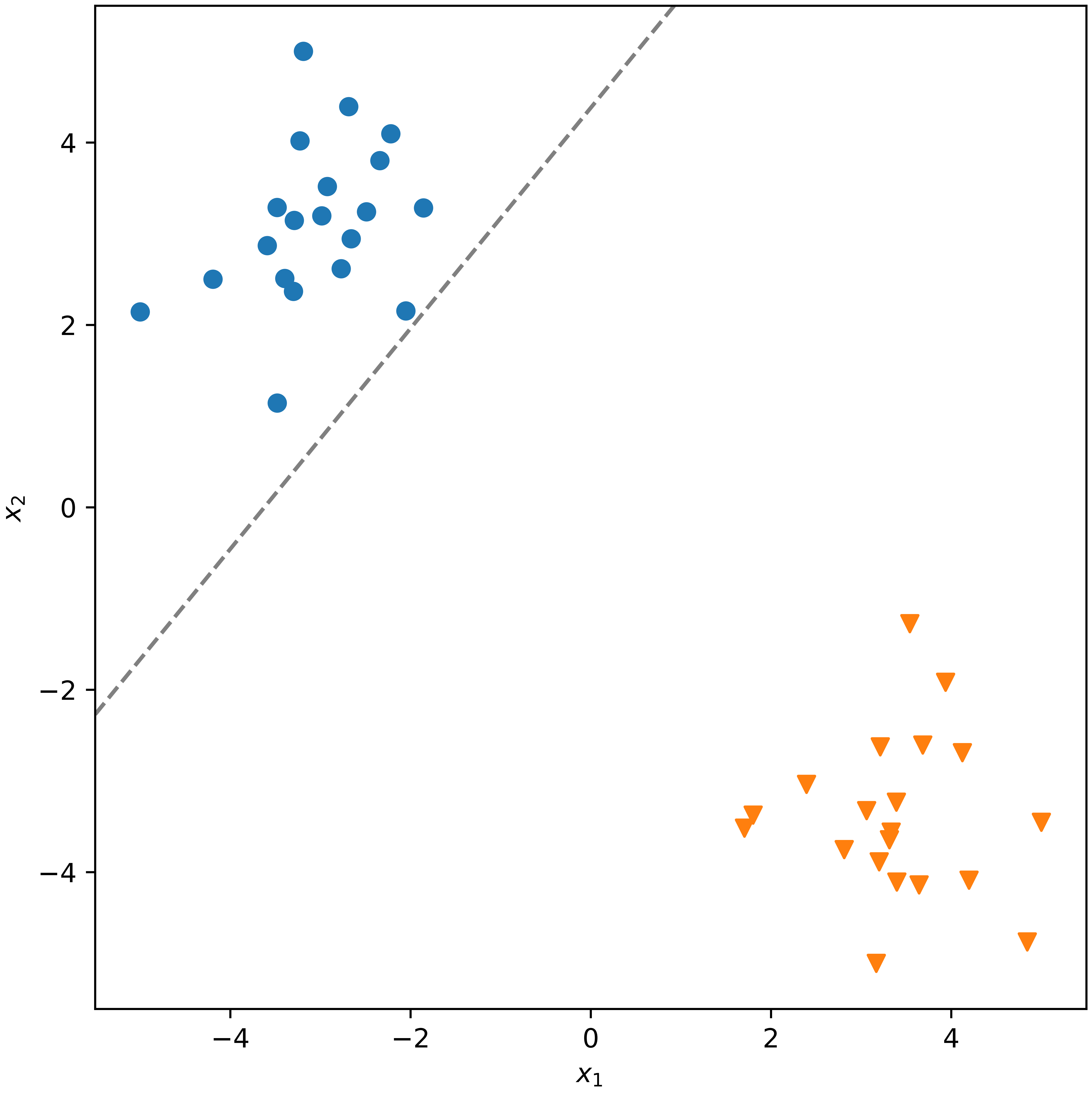
4
2
0
−2
−4
x_2
−4
−2
0
2
4
x_1


4
2
0
−2
−4
x_2
−4
−2
0
2
4
x_1

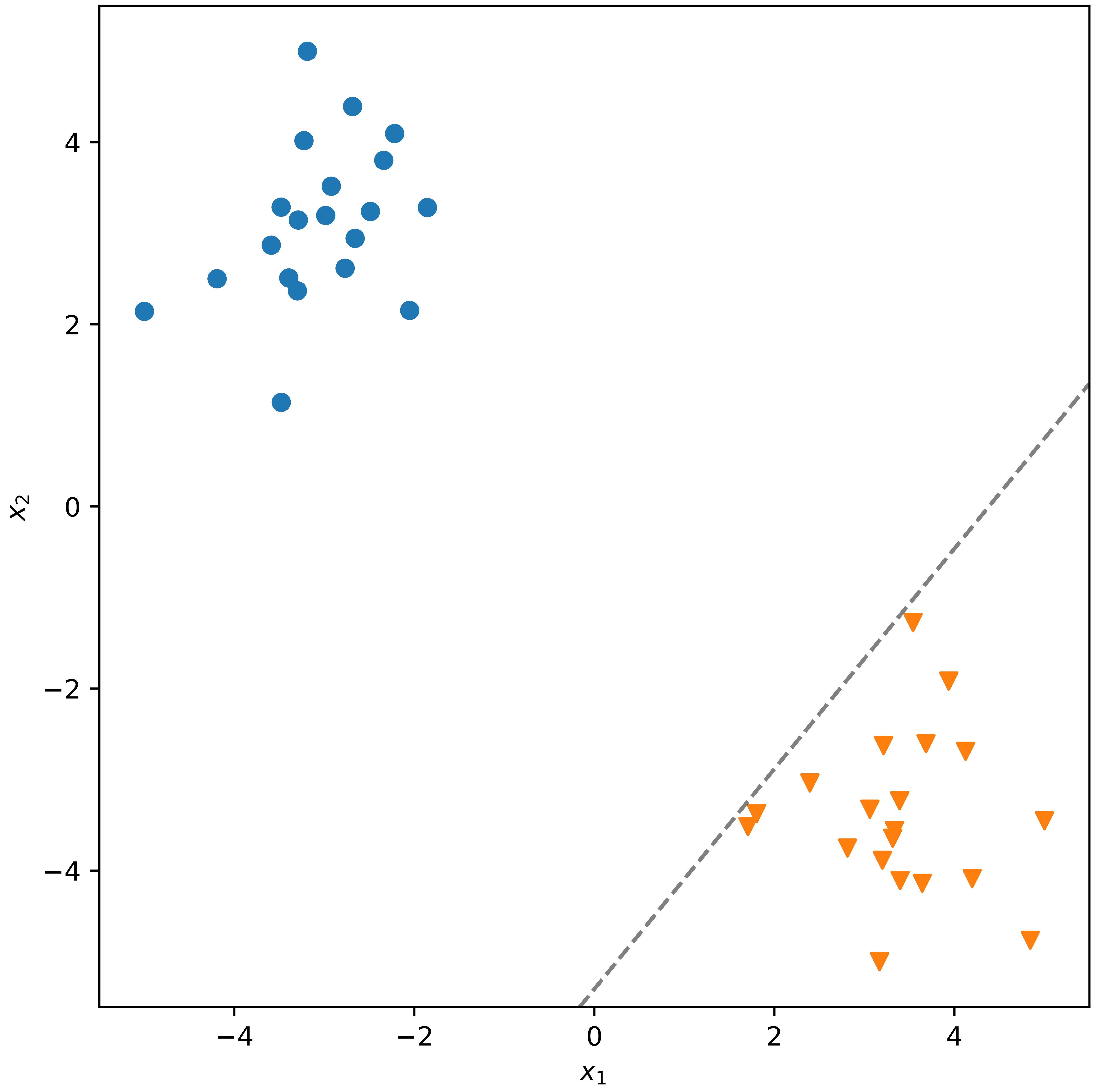

4
2
0
−2
−4
x_2
−4
−2
0
2
4
x_1



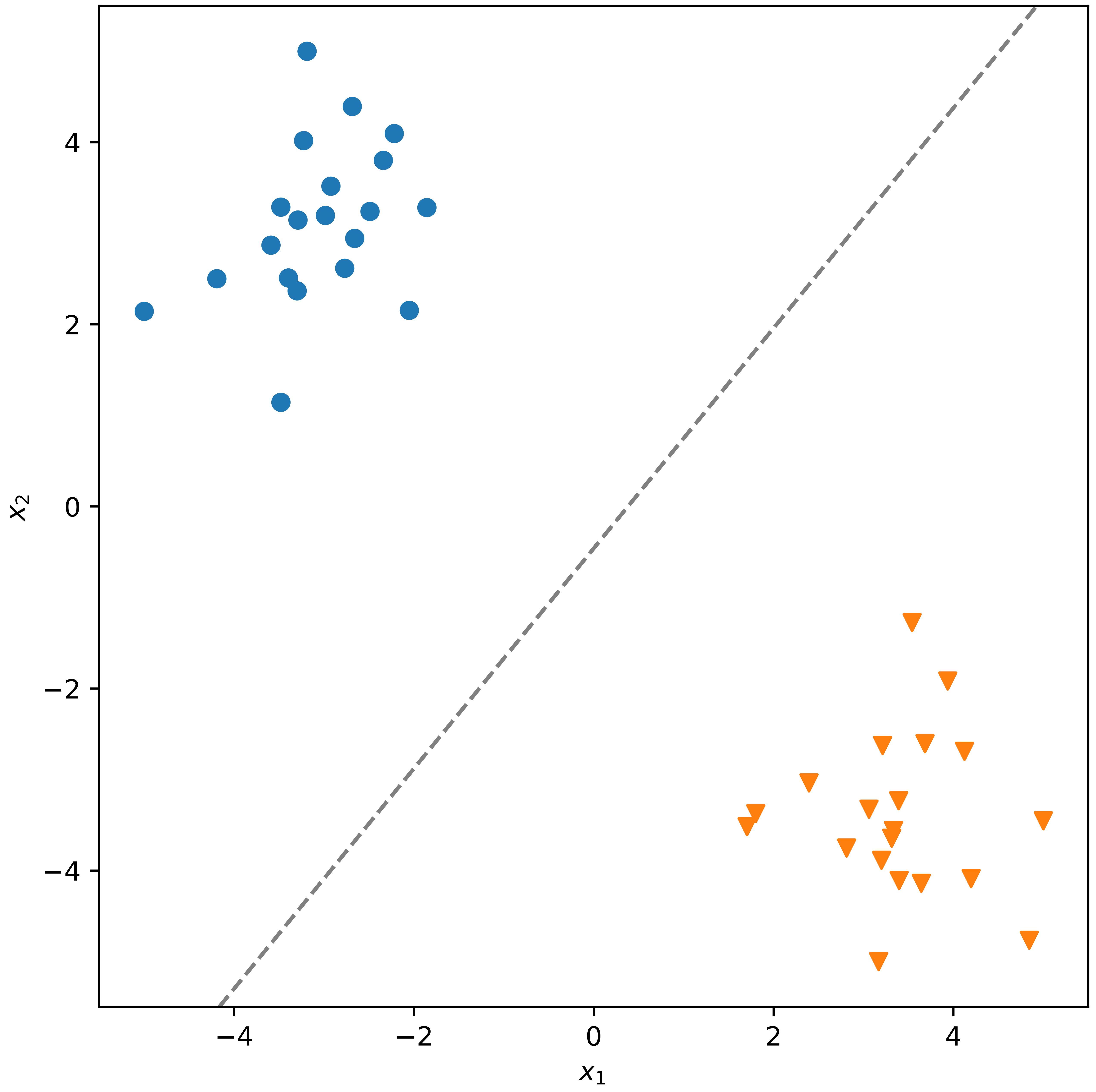
4
2
0
−2
−4
x_2
−4
−2
0
2
4
x_1



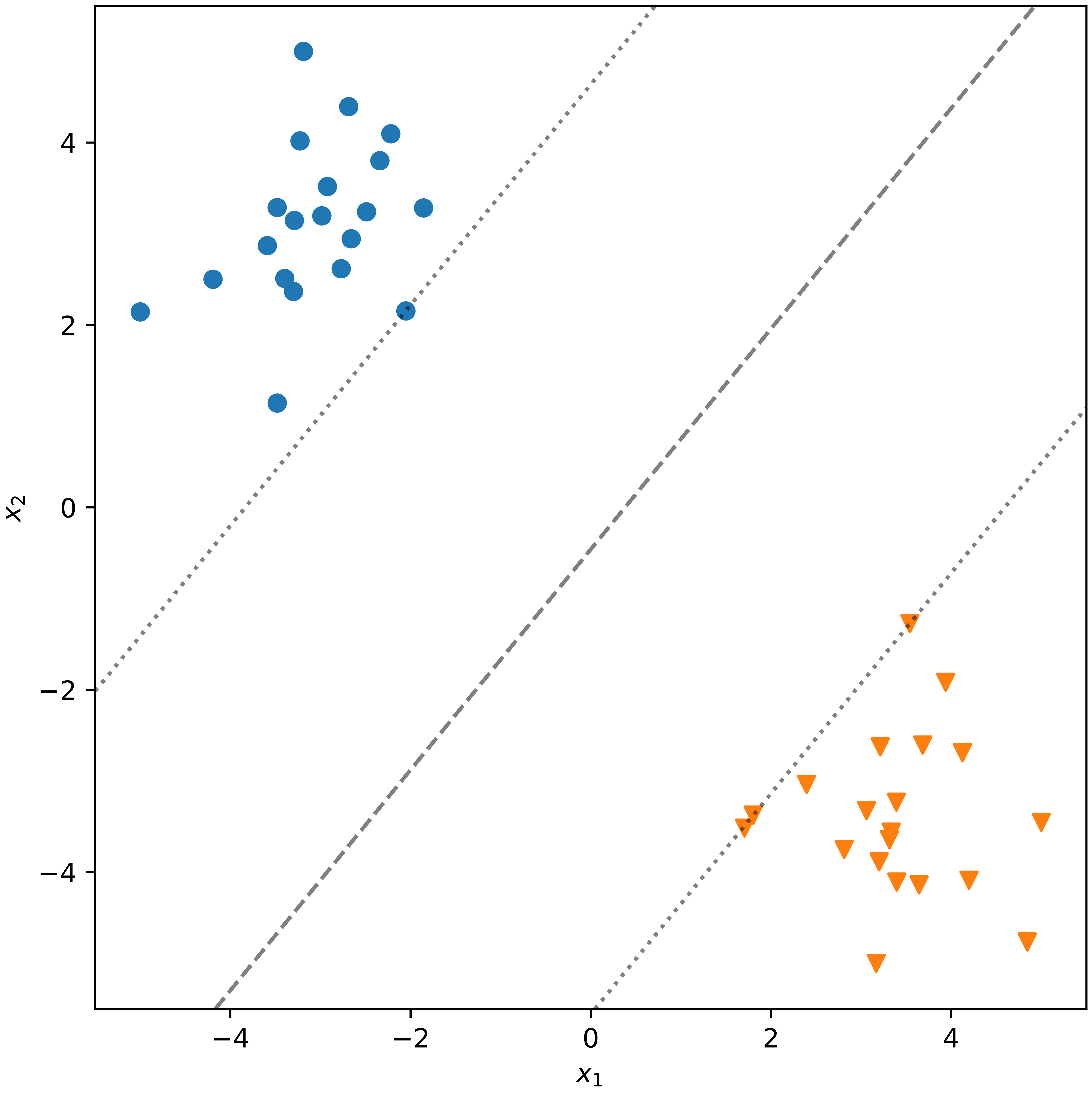
4
2
0
−2
−4
x_2
−4
−2
0
2
4
x_1



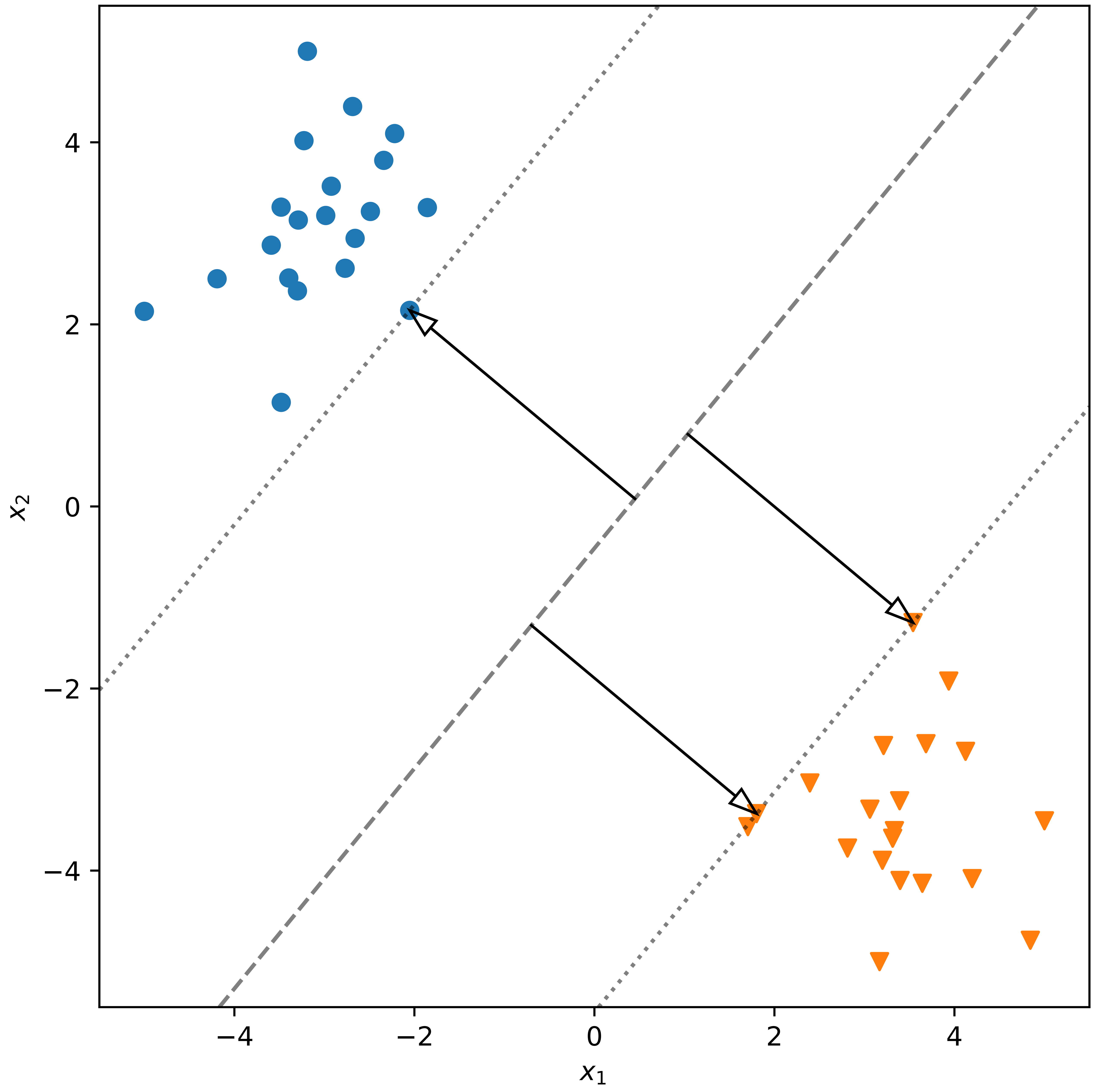
4
2
0
−2
−4
x_2
−4
−2
0
2
4
x_1



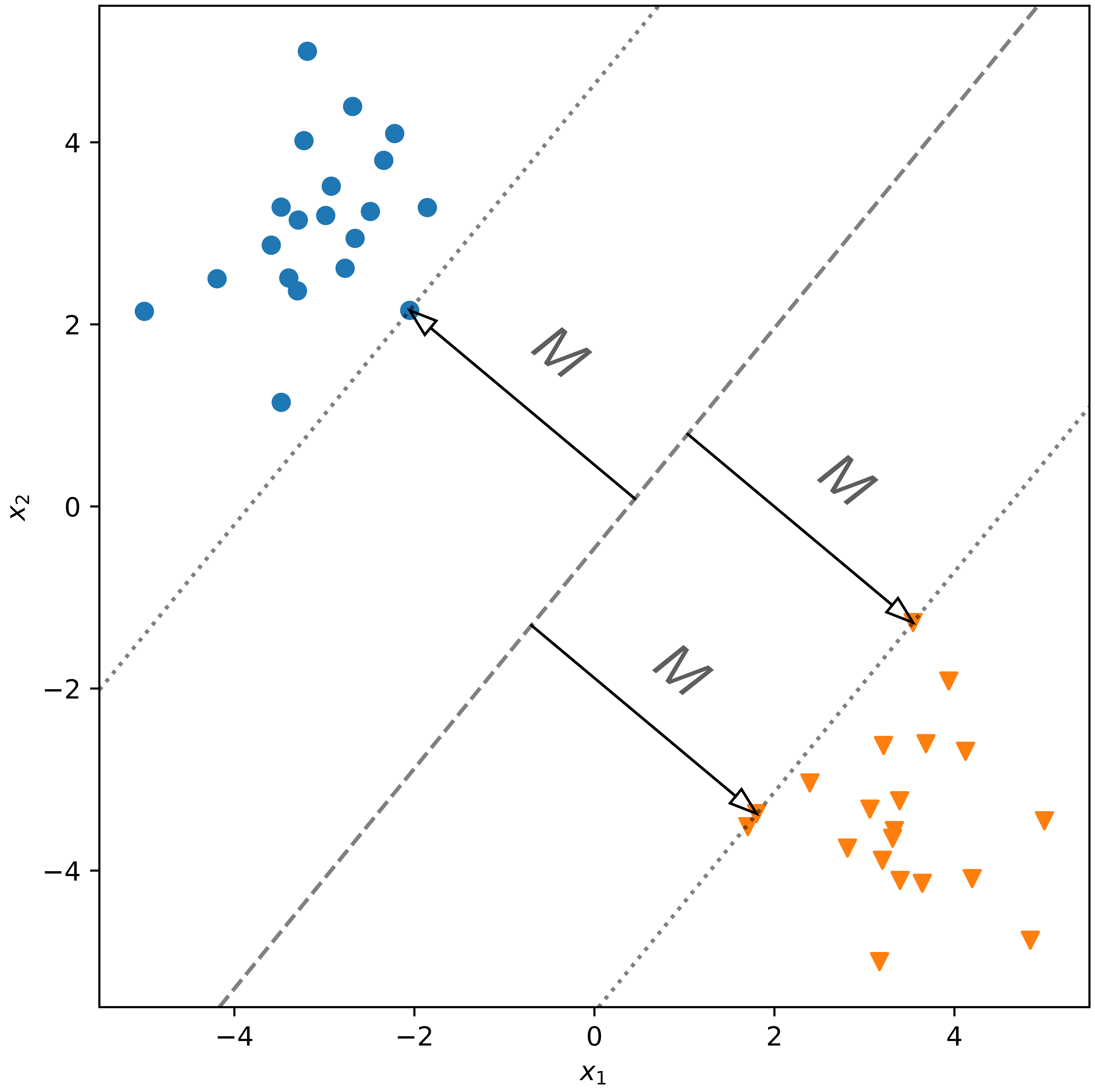
4
2
0
−2
−4
x_2
−4
−2
0
2
4
x_1



4
2
0
−2
−4
x_2
−4
−2
0
2
4
x_1



4
2
0
−2
−4
x_2
−4
−2
0
2
4
x_1



M
M
M
x_1
x_2
−4
−2
0
2
4

$$M = yf(\mathbf{x}) = y\left(\mathbf{x} \cdot \mathbf{w} + b\right)$$

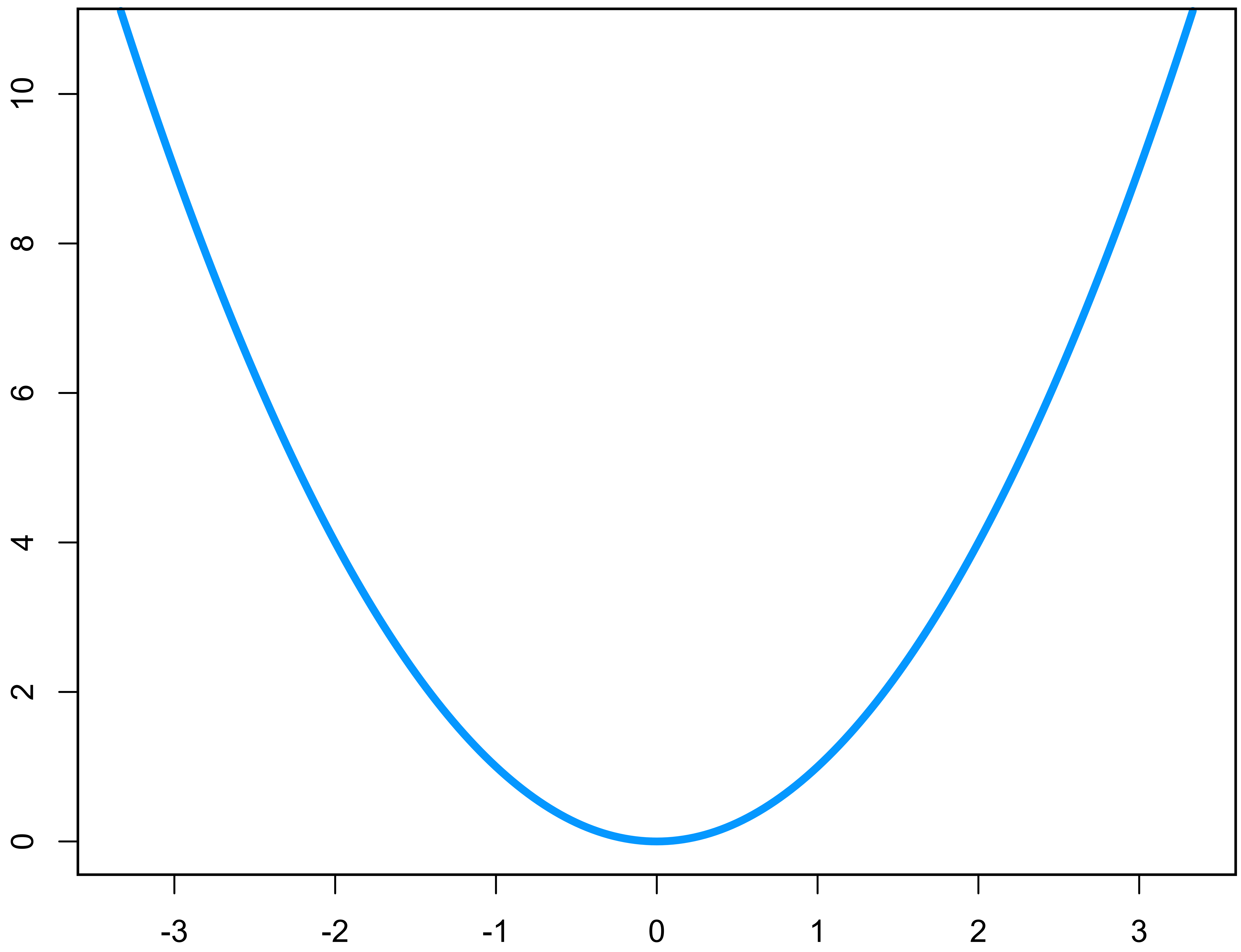
$$\|\mathbf{w}\| = 1$$

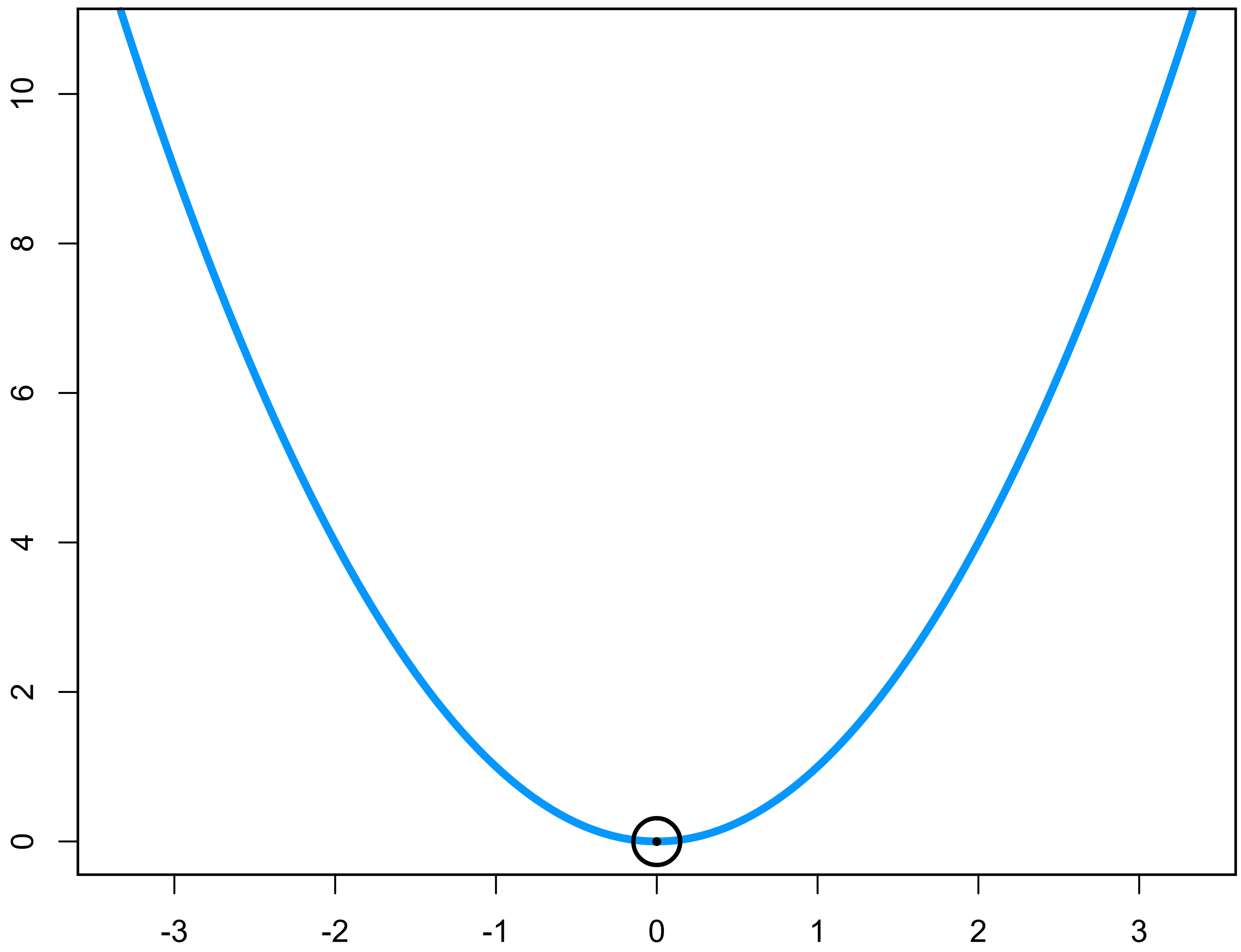
$$\underset{\mathbf{w},b}{\text{maximise}}\ M$$

subject to:

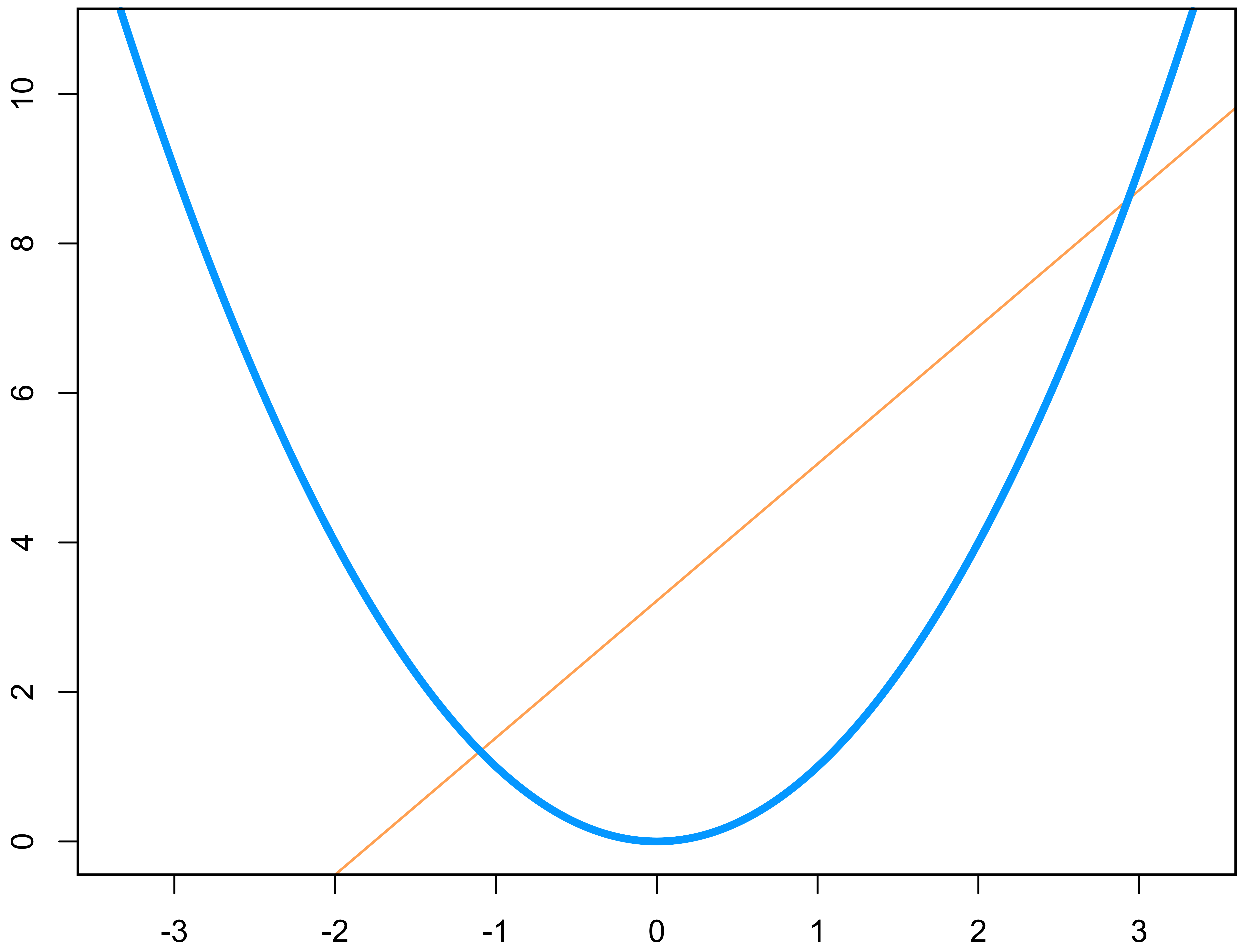
$$y_i \left(\mathbf{x}_i \cdot \mathbf{w} + b \right) \geq M$$

$$\|\mathbf{w}\| = 1$$

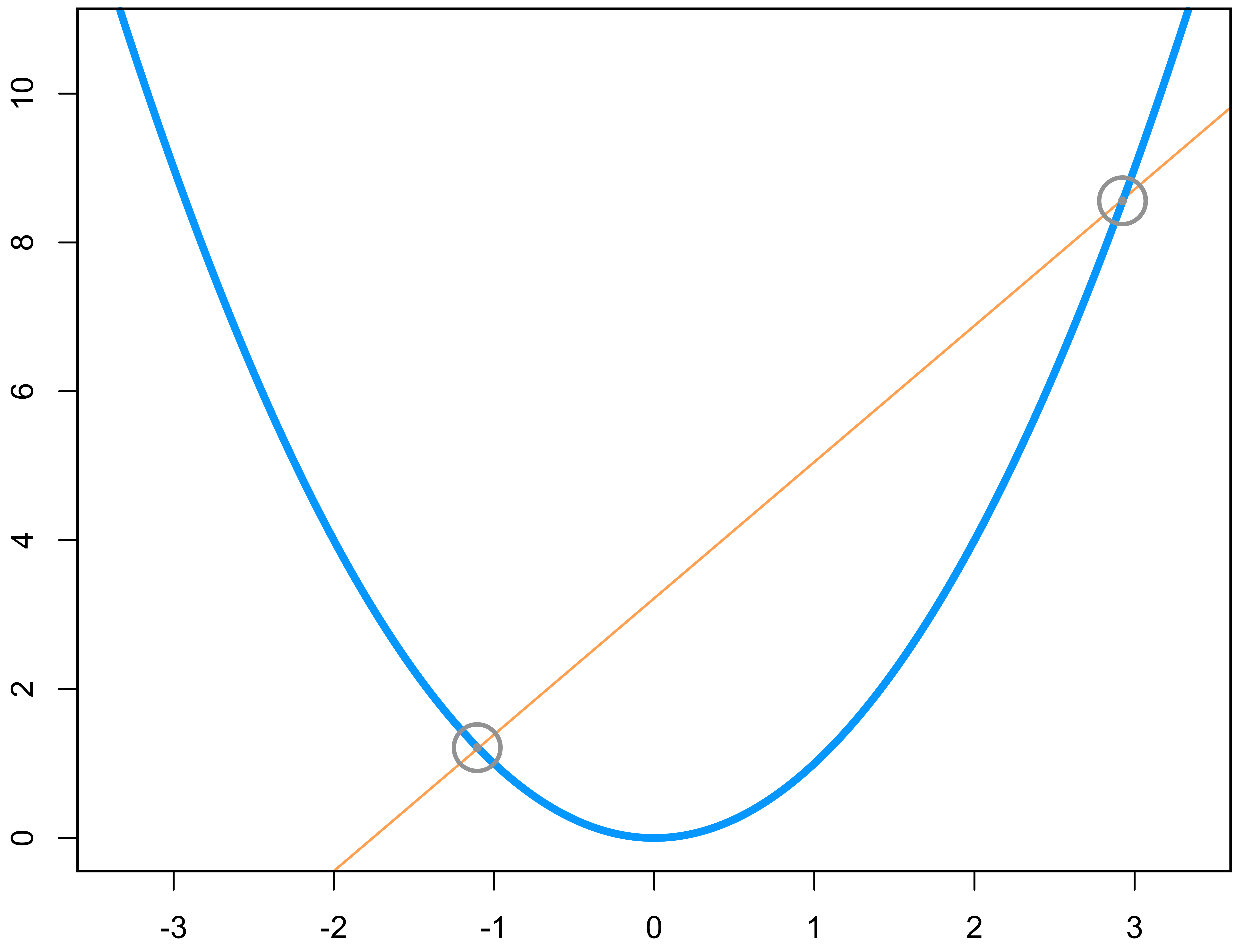

0
2
4
6
8
10
-3
-2
-1
0
1
2
3



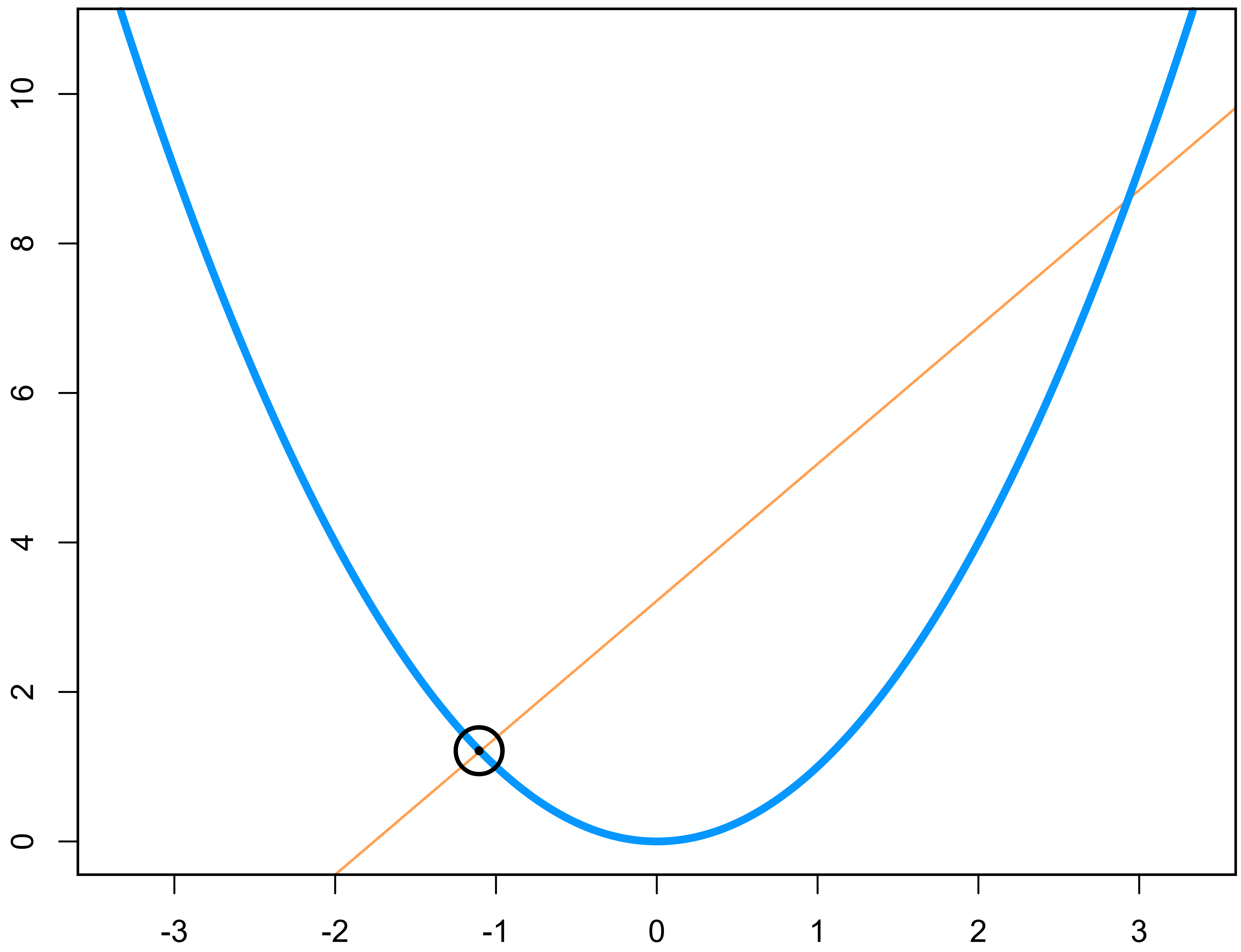
10
8
6
4
2
0
-3
-2
-1
0
1
2
3

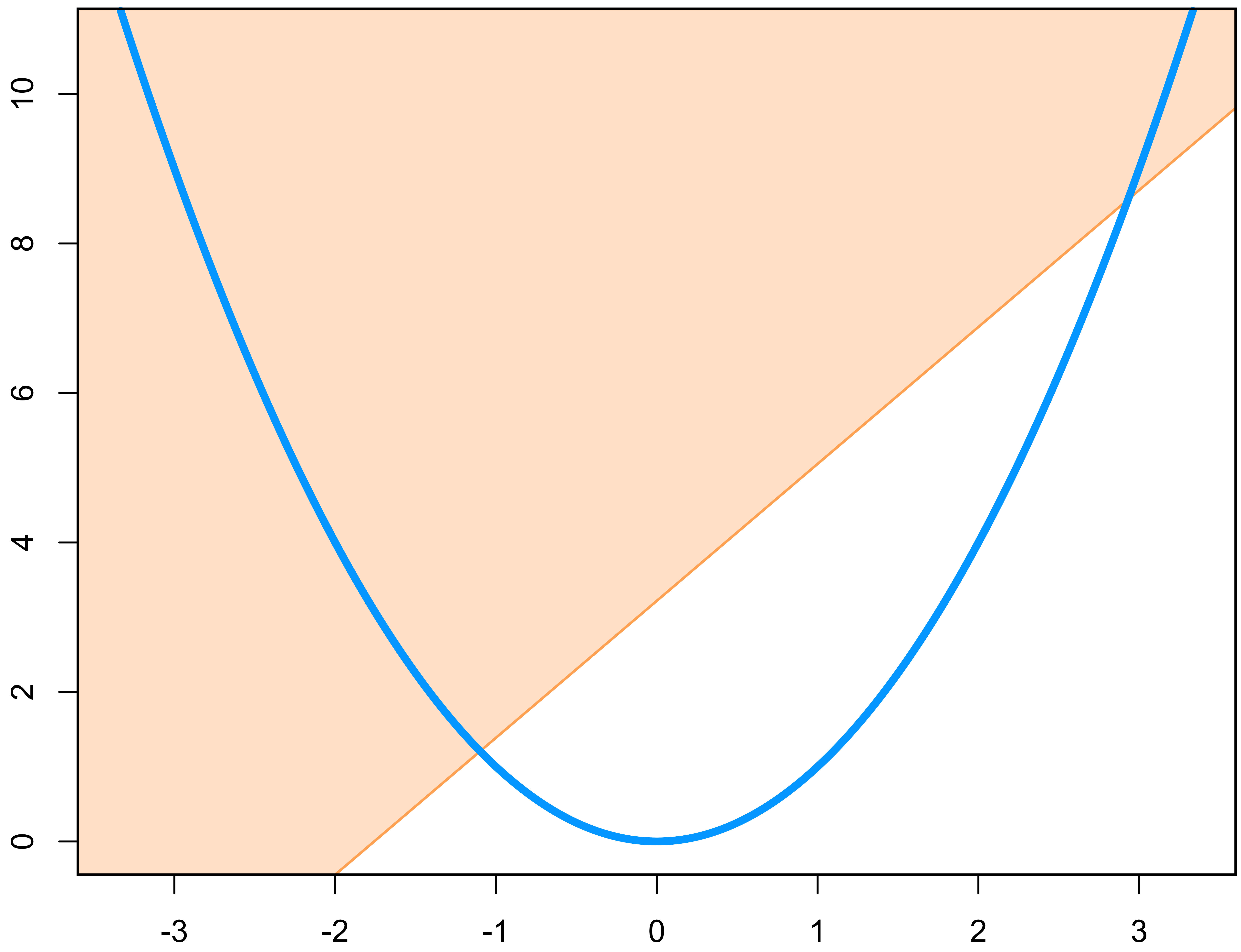


0
2
4
6
8
10
-3
-2
-1
0
1
2
3

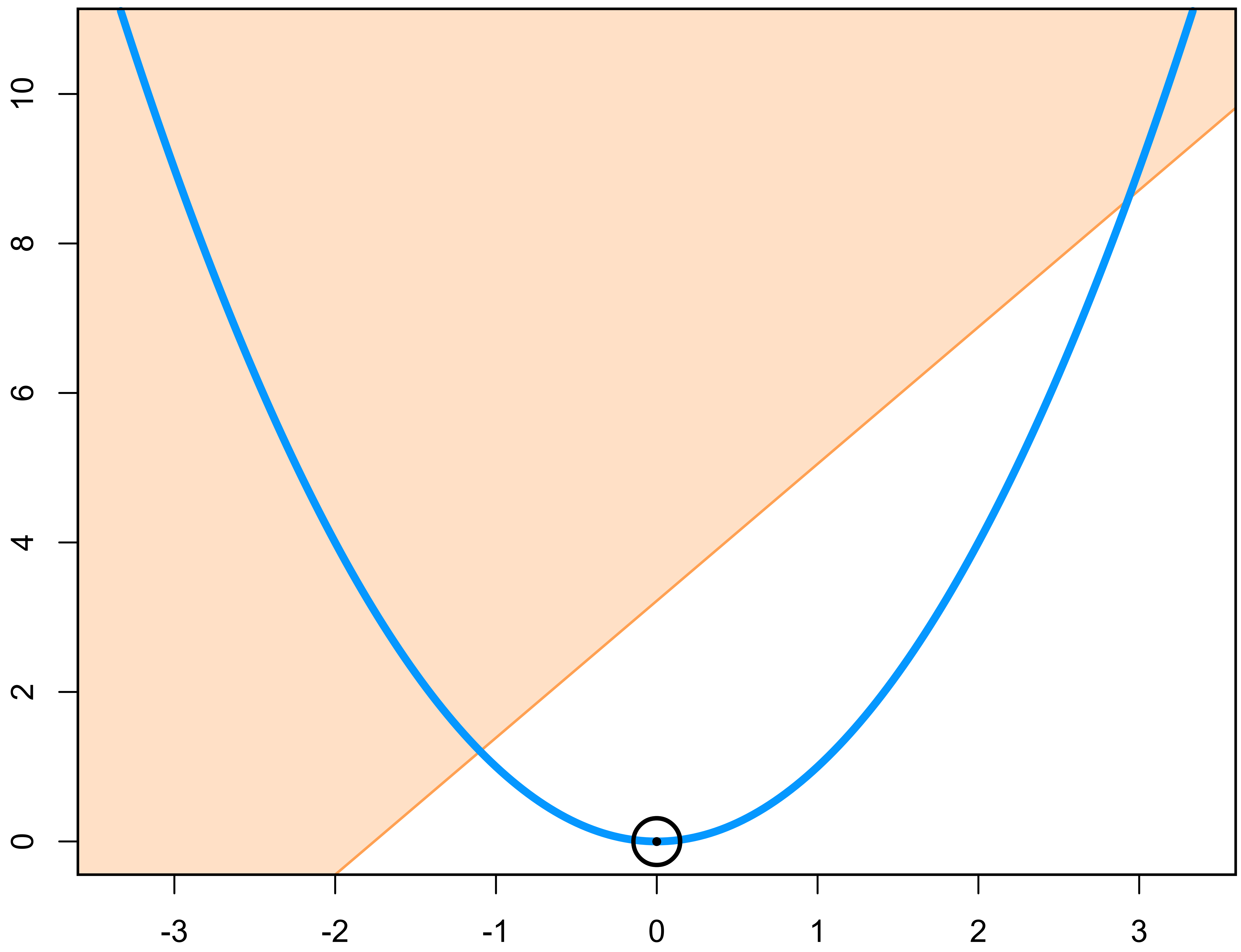


10
8
6
4
2
0
-3
-2
-1
0
1
2
3

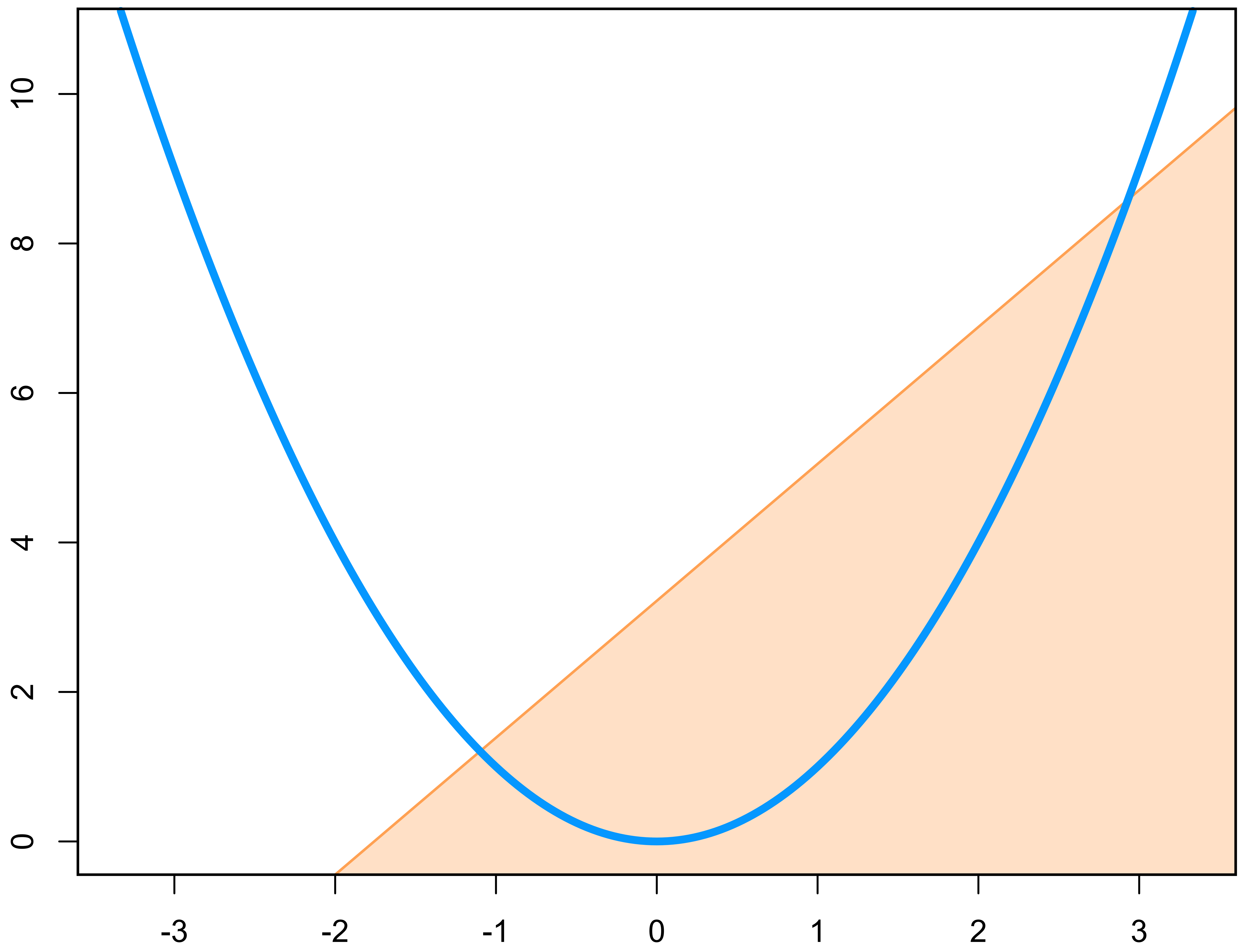

10
8
6
4
2
0
-3
-2
-1
0
1
2
3

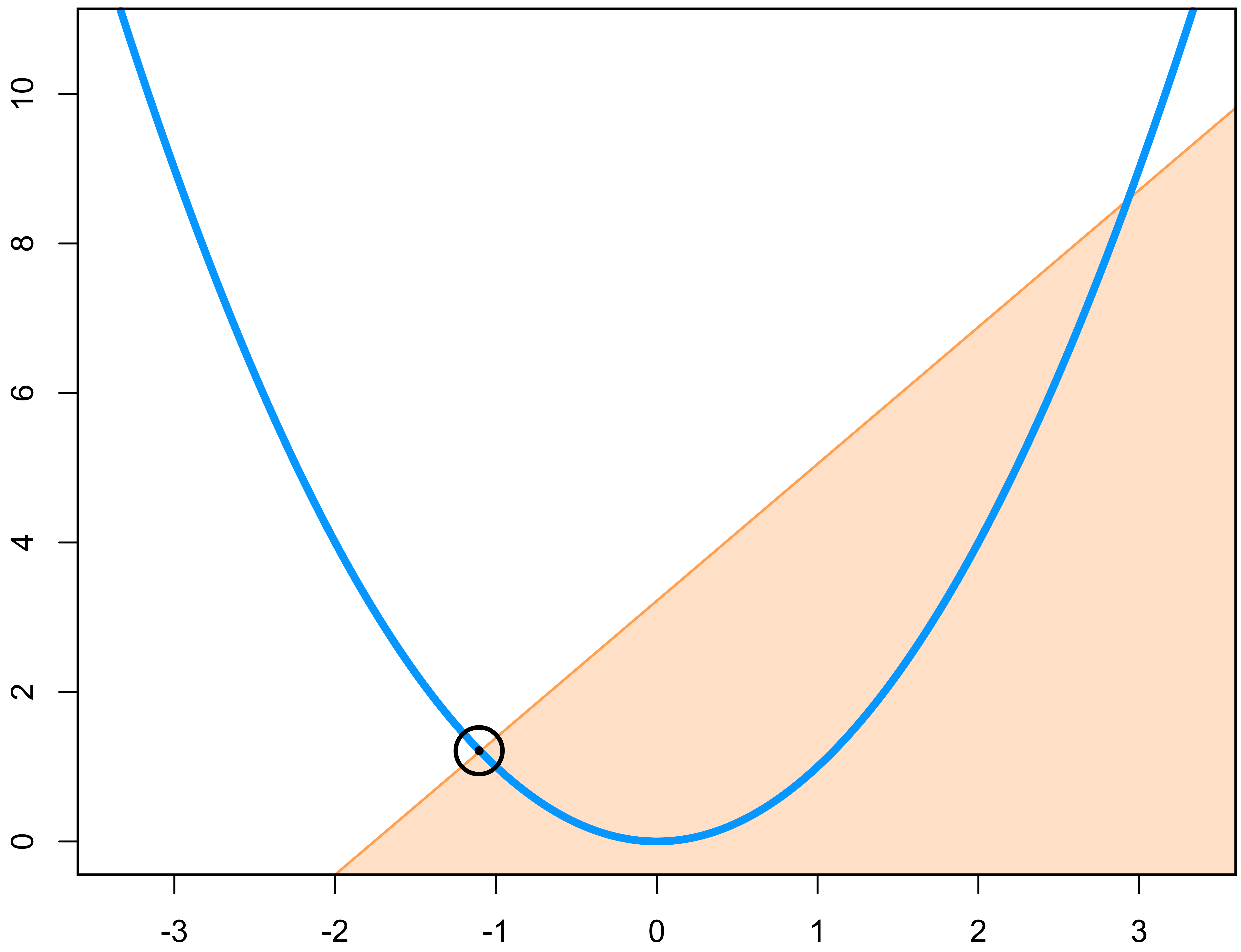


10
8
6
4
2
0
-3
-2
-1
0
1
2
3



10
8
6
4
2
0
-3
-2
-1
0
1
2
3


10
8
6
4
2
0
-3
-2
-1
0
1
2
3


10
8
6
4
2
0
-3
-2
-1
0
1
2
3

$$\underset{x}{\text{maximise}} \;\; f(x)$$

$$\text{subject to: } g(x) = 0$$

$$\mathcal{L}(x, \alpha) = f(x) - \alpha g(x)$$

$$\underset{x}{\text{maximise}} \;\; f(x)$$

$$\text{subject to: } g(x) = 0$$

$$\begin{aligned} \underset{x}{\text{maximise}} \quad & f(x) \\ \text{subject to:} \quad & g(x) \leq 0 \end{aligned}$$

$$\alpha_i g_i(x) = 0, \quad \forall i$$

Complementary Slackness

Inequality constraints are only active at equality

$$\underset{\mathbf{w},b}{\text{maximise}} \;\; M$$

subject to:

$$y_i \left(\mathbf{x}_i \cdot \mathbf{w} + b\right) \geq M$$

$$\|\mathbf{w}\| = 1$$

$$\underset{\mathbf{w},b}{\text{minimise}} \ \frac{1}{2}\|\mathbf{w}\|^2$$

$$\text{subject to: } y_i \left(\mathbf{x}_i \cdot \mathbf{w} + b\right) \geq 1$$

$$L_p = \frac{1}{2}\|\mathbf{w}\|^2 - \sum_i^n \alpha_i \left(y_i(\mathbf{x}_i \cdot \mathbf{w} + b) - 1 \right)$$

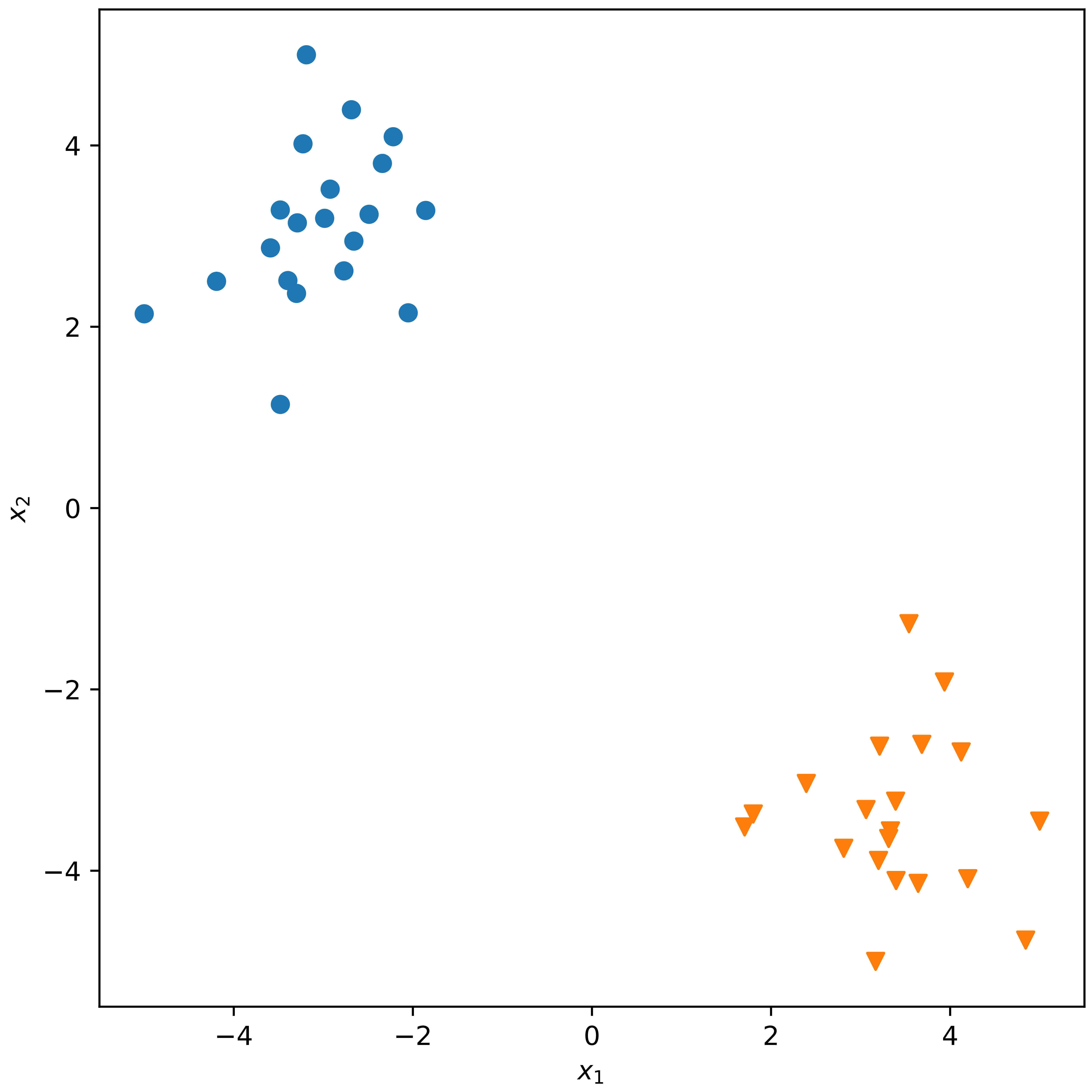
$$L_d = \sum_i^n \alpha_i - \frac{1}{2}\sum_i^n \sum_j^n \alpha_i \alpha_j y_i y_j (\mathbf{x}_i \cdot \mathbf{x}_j)$$

$$\mathbf{w} = \sum_{i}^{n} \alpha_i y_i \mathbf{x}_i$$

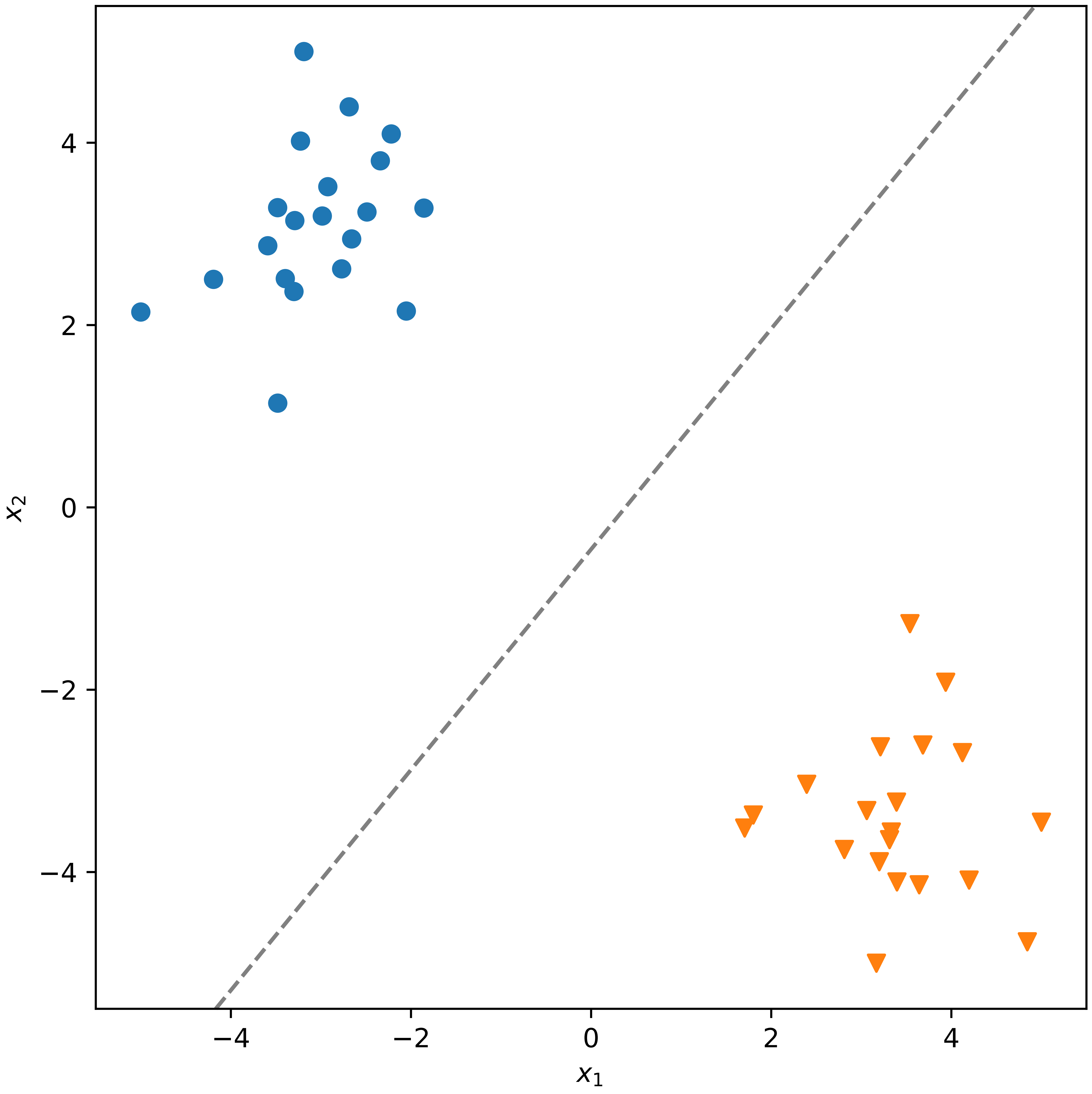
$$\alpha_i \left[y_i(\mathbf{x}_i \cdot \mathbf{w} + b) - 1 \right] = 0 \quad \forall i$$

$$\underset{\boldsymbol{\alpha}}{\text{maximise}} \quad \sum_{i}^{n} \alpha_i - \frac{1}{2} \sum_{i}^{n} \sum_{j}^{n} \alpha_i \alpha_j y_i y_j \boxed{(\mathbf{x}_i \cdot \mathbf{x}_j)}$$

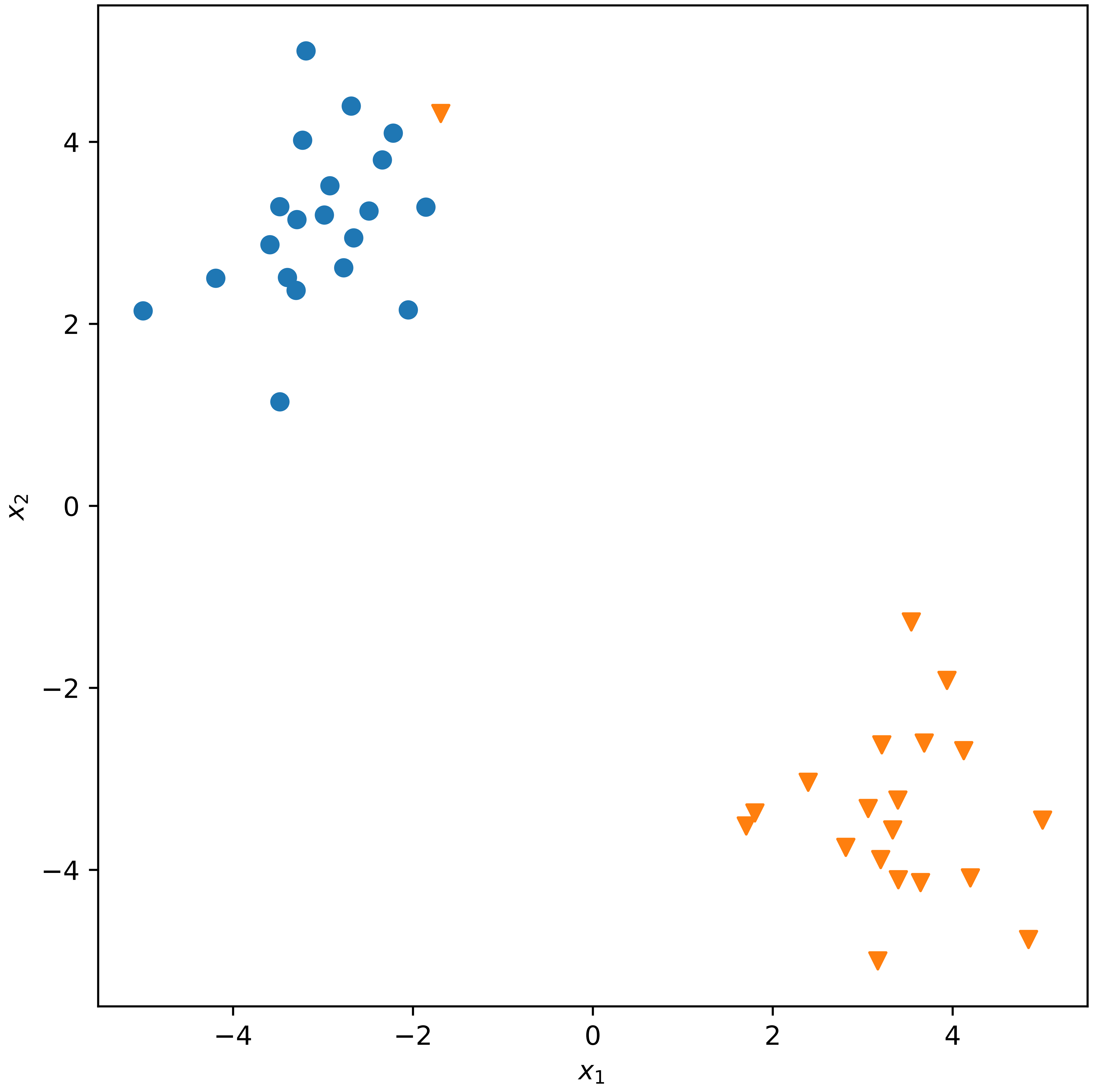
$$\hat{y} = \begin{cases} 1 & \text{if } \sum_i^n \alpha_i y_i \boxed{(\mathbf{x}_i \cdot \mathbf{x})} + b \geq 0 \\ -1 & \text{otherwise} \end{cases}$$



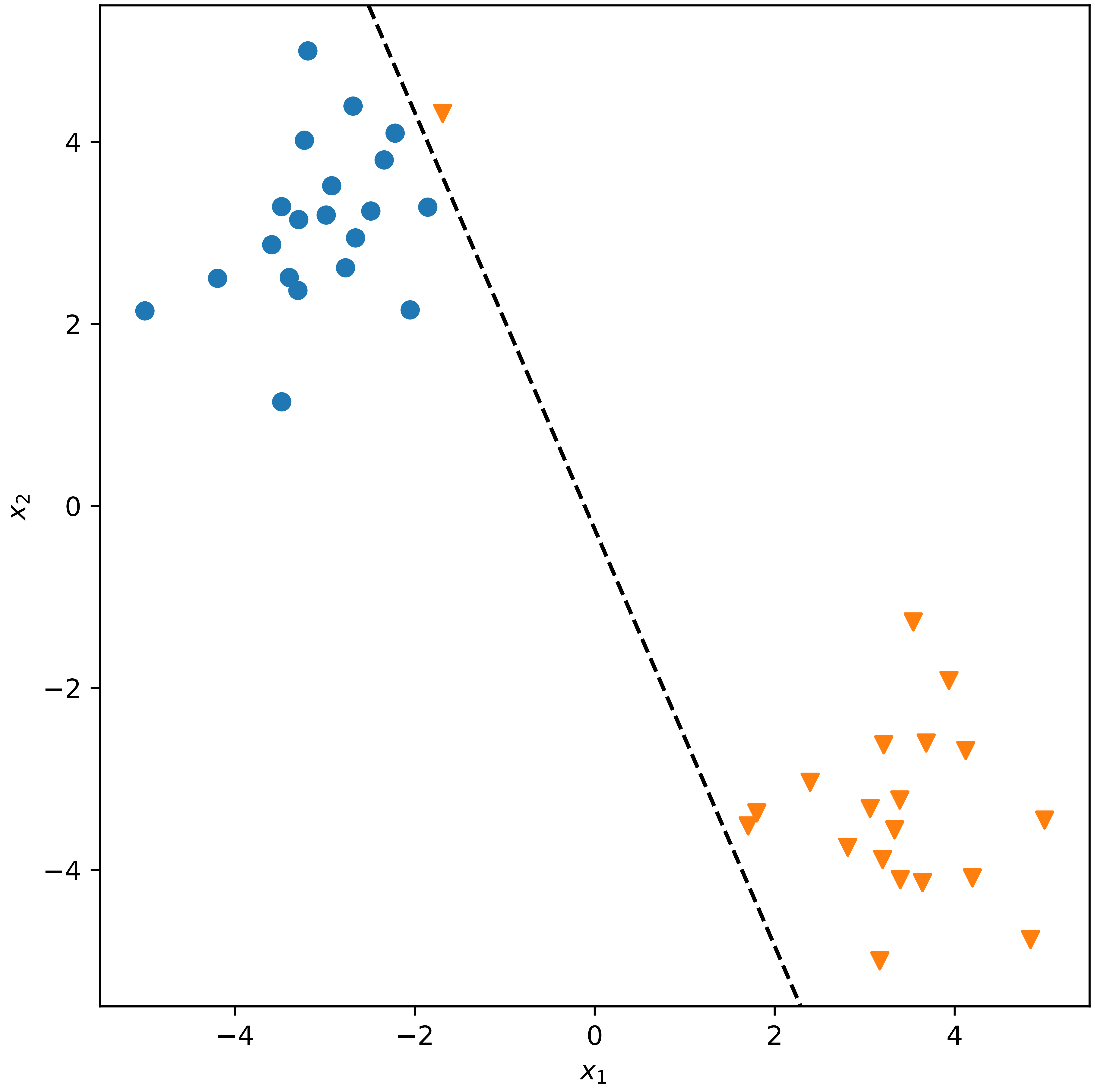
x_1
x_2
−4
−2
0
2
4



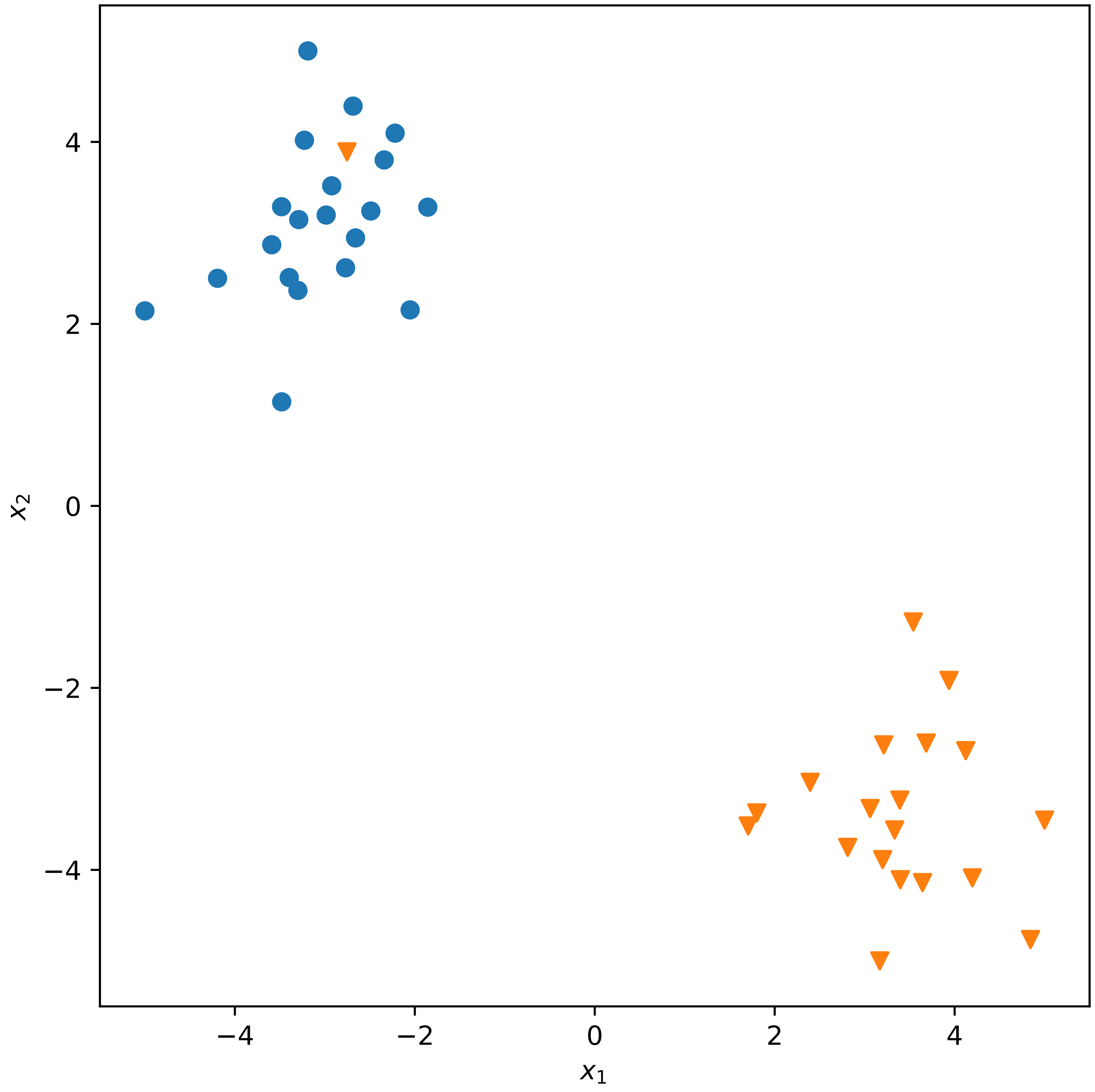
4
2
0
−2
−4
x_2
−4
−2
0
2
4
x_1



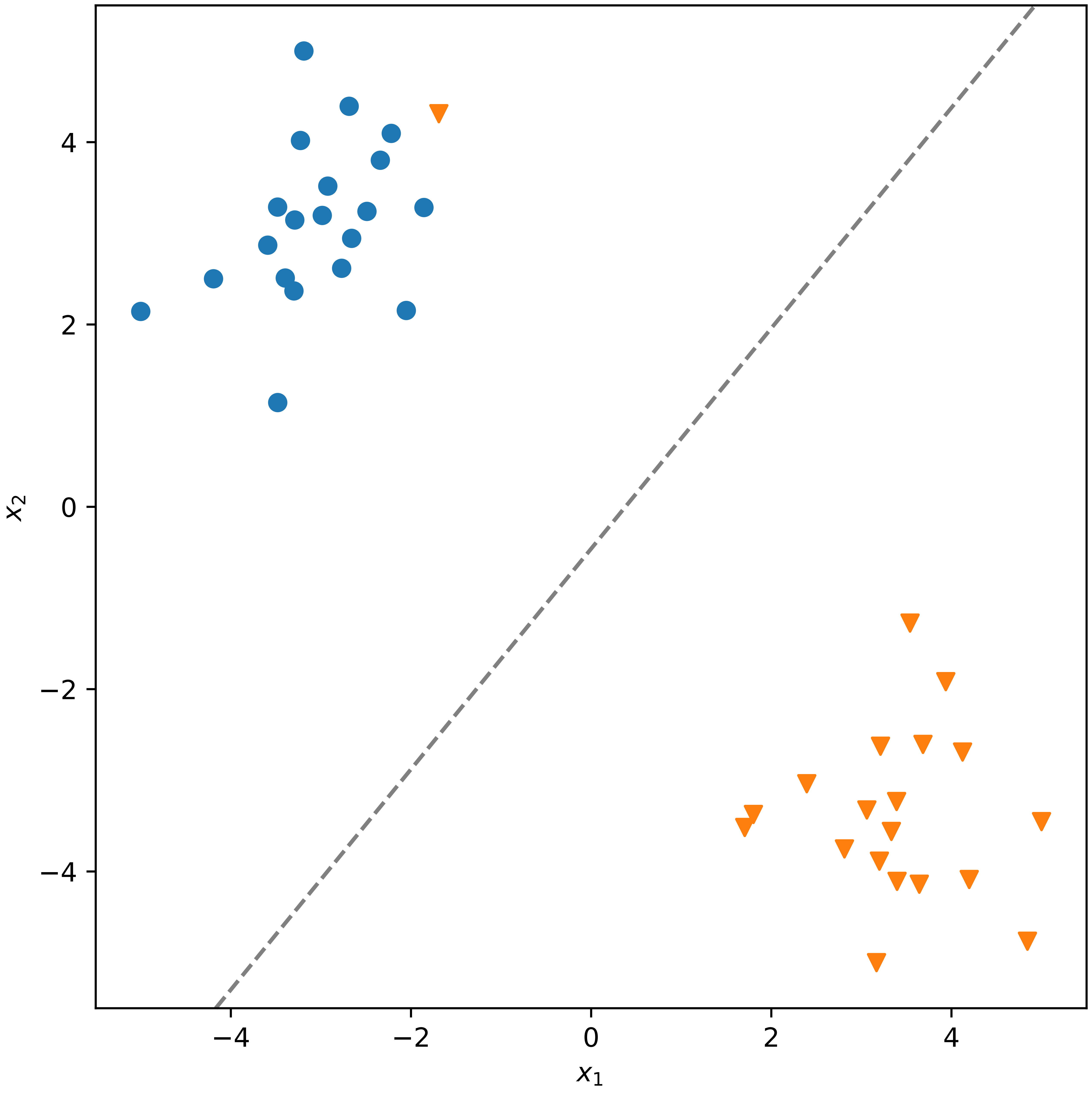
4
2
0
−2
−4
x_2
−4
−2
0
2
4
x_1



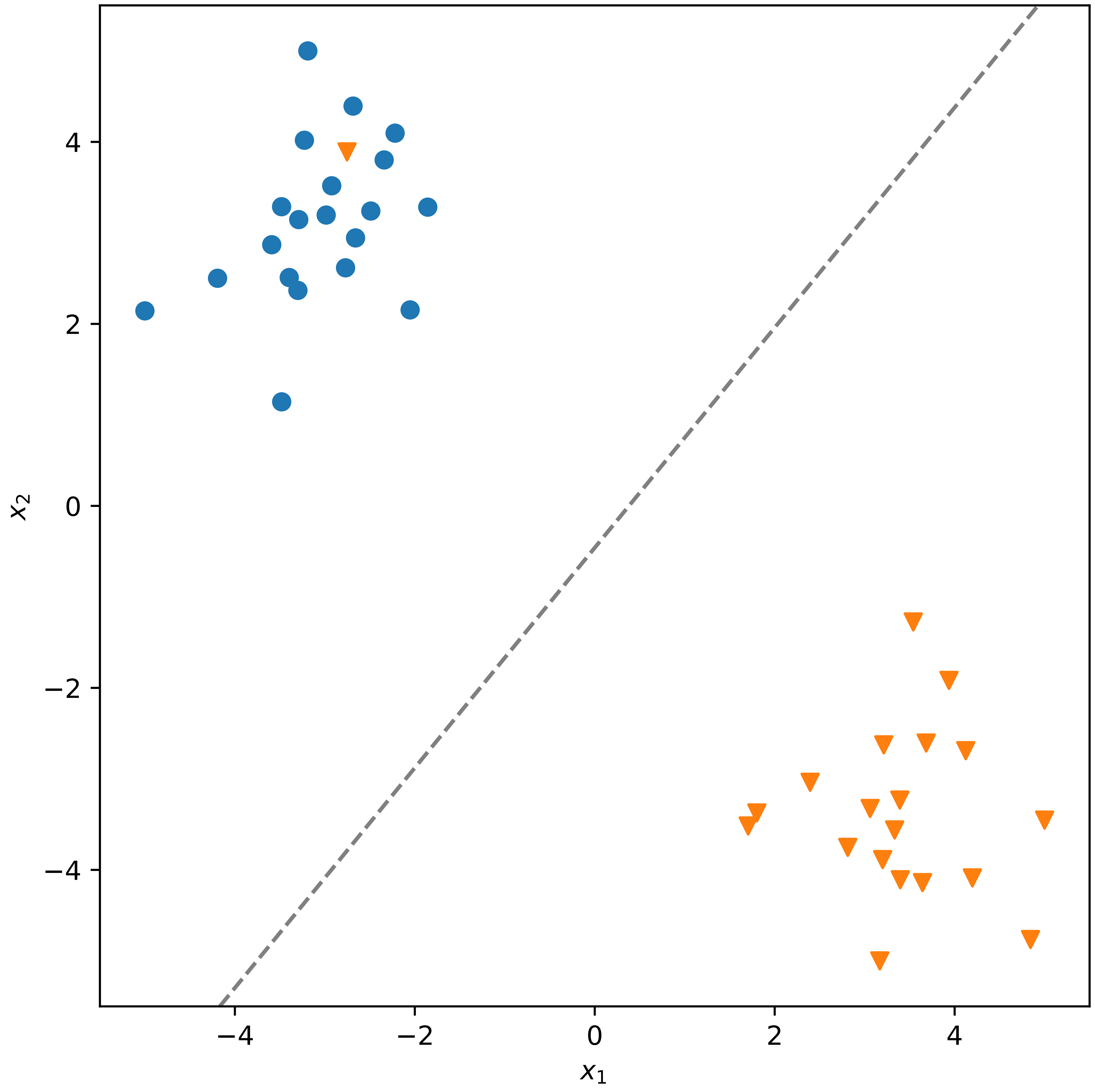
4
2
0
−2
−4
x_2
−4
−2
0
2
4
x_1



4
2
0
−2
−4
x_2
−4
−2
0
2
4
x_1



4
2
0
−2
−4
x_2
−4
−2
0
2
4
x_1



4
2
0
−2
−4
x_2
−4
−2
0
2
4
x_1

$$\underset{\mathbf{w},b,\xi}{\text{maximise}} \; M$$

subject to:

$$y_i \left(\mathbf{x}_i \cdot \mathbf{w} + b\right) \geq M(1 - \xi_i)$$

$$\|\mathbf{w}\| = 1$$

$$\xi_i \geq 0 \;\; \forall i$$

$$\sum_i \xi_i \leq \; \text{constant}$$

$$\underset{\mathbf{w},b,\xi}{\text{minimise}} \;\; \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i}^{n}\xi_i$$

subject to:

$$y_i\left(\mathbf{x}_i \cdot \mathbf{w} + b\right) \geq 1 - \xi_i$$

$$\xi_i \geq 0$$

$$L_p = \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_i^n \xi_i - \sum_i^n \alpha_i \left[y_i(\mathbf{x}_i \cdot \mathbf{w} + b) - (1 - \xi_i)\right] - \sum_i^n \mu_i \xi_i$$

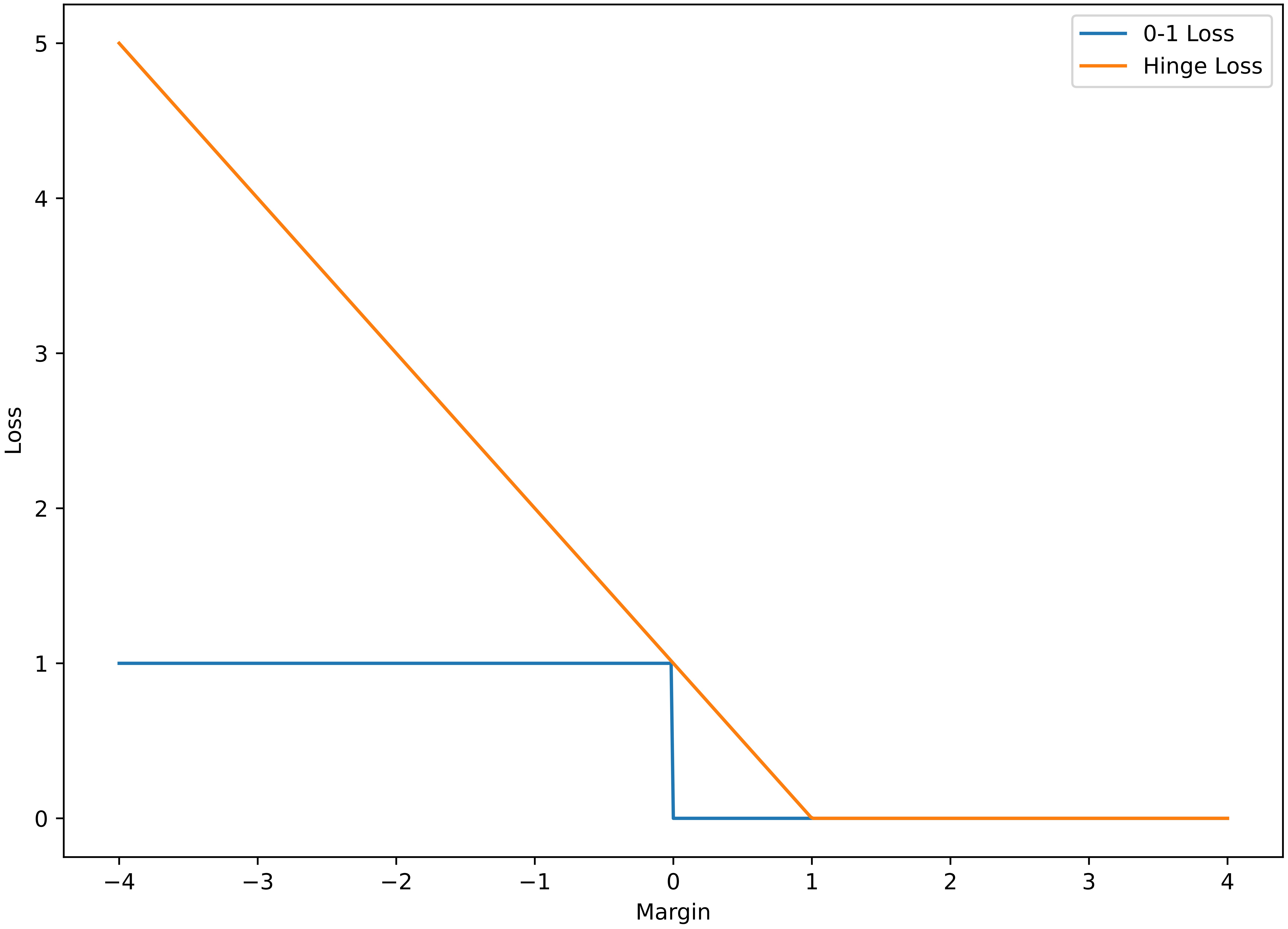
$$L_d = \sum_i^n \alpha_i - \frac{1}{2}\sum_i^n \sum_j^n \alpha_i \alpha_j y_i y_j (\mathbf{x}_i \cdot \mathbf{x}_j)$$

$$0 \leq \alpha_i \leq C$$

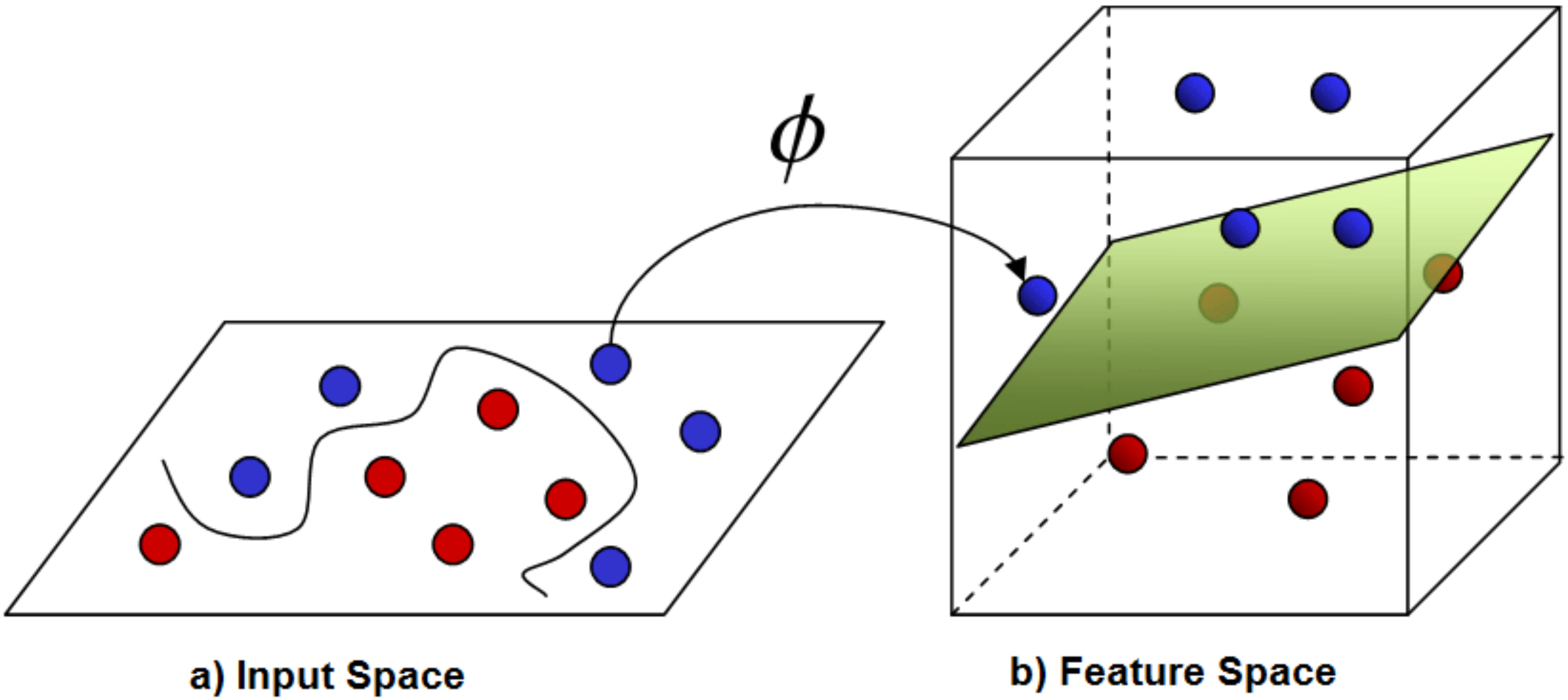
$$\alpha_i \left[y_i(\mathbf{x}_i \cdot \mathbf{w}) - (1 - \xi_i) \right] = 0$$

$$y_i(\mathbf{x}_i \cdot \mathbf{w}) - (1 - \xi_i) \geq 0$$

$$
\begin{aligned}
L(y, \mathbf{x}) &= \max(0, 1 - yf(\mathbf{x})) \\
&= \max(0, 1 - y(\mathbf{x} \cdot \mathbf{w} + b))
\end{aligned}
$$


0-1 Loss
Hinge Loss
Loss
Margin
5
4
3
2
1
0
−4
−3
−2
−1
0
1
2
3
4

This One Weird Trick



ϕ
a) Input Space
b) Feature Space

$$\mathbf{x}' = \phi(\mathbf{x})$$

$$\underset{\boldsymbol{\alpha}}{\text{maximise}} \quad \sum_{i}^{n} \alpha_i - \frac{1}{2} \sum_{i}^{n} \sum_{j}^{n} \alpha_i \alpha_j y_i y_j \boxed{(\mathbf{x}_i \cdot \mathbf{x}_j)}$$

$$\hat{y} = \begin{cases} 1 & \text{if } \sum_i^n \alpha_i y_i \boxed{(\mathbf{x}_i \cdot \mathbf{x})} + b \geq 0 \\ -1 & \text{otherwise} \end{cases}$$

$$\underset{\boldsymbol{\alpha}}{\text{maximise}} \;\; \sum_{i}^{n} \alpha_i - \frac{1}{2} \sum_{i}^{n} \sum_{j}^{n} \alpha_i \alpha_j y_i y_j (\phi(\mathbf{x}_i) \cdot \phi(\mathbf{x}_j))$$

$$\hat{y} = \begin{cases} 1 & \text{if } \sum_i^n \alpha_i y_i (\phi(\mathbf{x}_i) \cdot \phi(\mathbf{x})) + b \geq 0 \\ -1 & \text{otherwise} \end{cases}$$

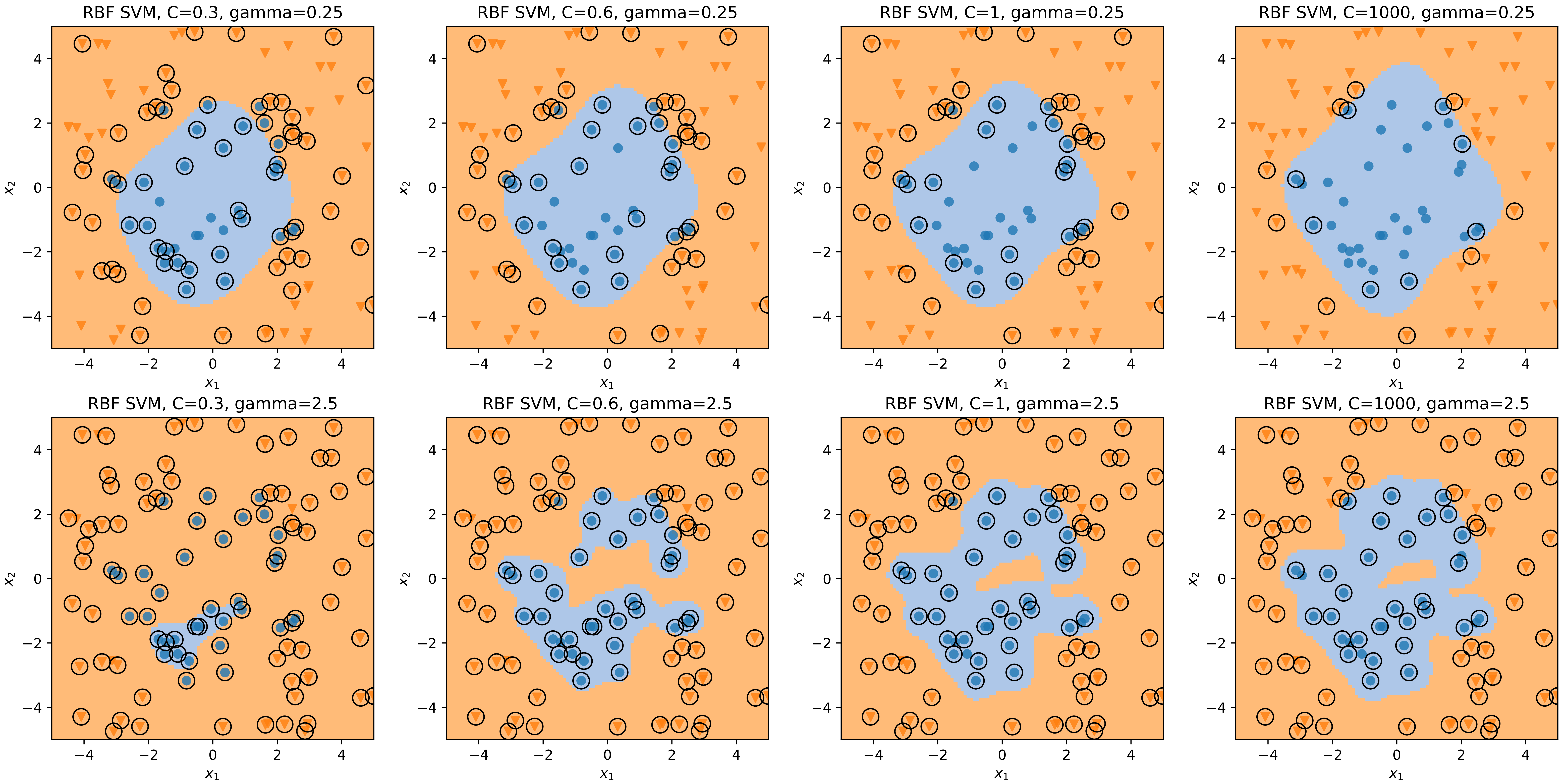
$$\phi(\mathbf{x}) \mapsto \mathbb{R}^{10,000,000}$$

$$K(\mathbf{u}, \mathbf{v}) = \phi(\mathbf{u}) \cdot \phi(\mathbf{v})$$

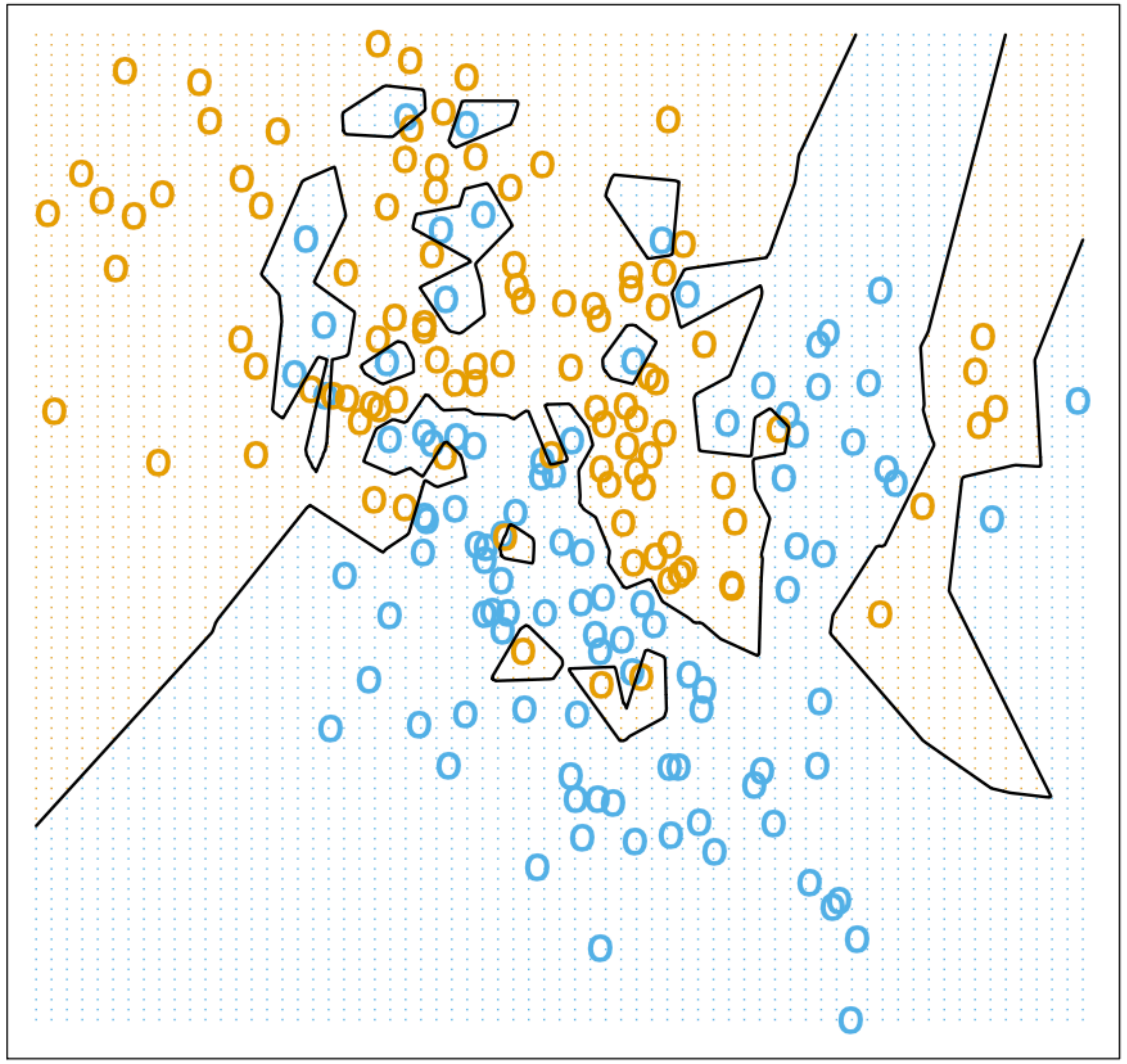
$$\underset{\boldsymbol{\alpha}}{\text{maximise}} \; \sum_{i}^{n} \alpha_i - \frac{1}{2} \sum_{i}^{n} \sum_{j}^{n} \alpha_i \alpha_j y_i y_j K(\mathbf{x}_i, \mathbf{x}_j)$$

$$\hat{y} = \begin{cases} 1 & \text{if } \sum_i^n \alpha_i y_i K(\mathbf{x}_i, \mathbf{x}) + b \geq 0 \\ -1 & \text{otherwise} \end{cases}$$

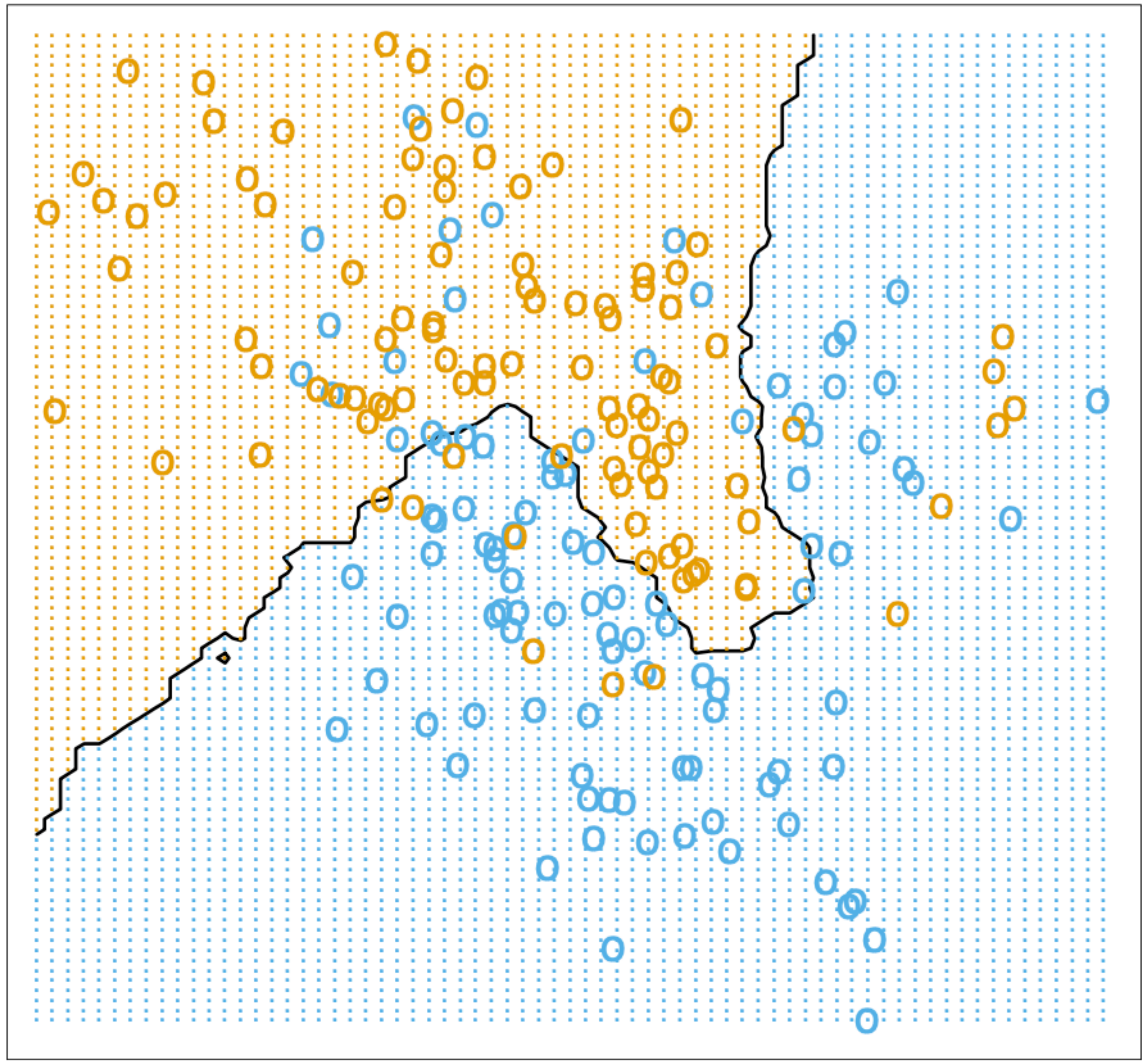
$$
\begin{aligned}
K(\mathbf{u}, \mathbf{v}) &= e^{-\gamma \|\mathbf{u} - \mathbf{v}\|^2} \\
&= e^{-\frac{\|\mathbf{u} - \mathbf{v}\|^2}{2\sigma^2}}
\end{aligned}
$$



RBF SVM, C=0.3, gamma=0.25
RBF SVM, C=0.6, gamma=0.25
RBF SVM, C=1, gamma=0.25
RBF SVM, C=1000, gamma=0.25
RBF SVM, C=0.3, gamma=2.5
RBF SVM, C=0.6, gamma=2.5
RBF SVM, C=1, gamma=2.5
RBF SVM, C=1000, gamma=2.5
x_1
x_2



k=1



k=15

$$K(\mathbf{u}, \mathbf{v}) = \phi(\mathbf{u}) \cdot \phi(\mathbf{v})$$

$$\mathbf{K} = \begin{bmatrix} K(\mathbf{x}_1, \mathbf{x}_1) & K(\mathbf{x}_1, \mathbf{x}_2) & \cdots & K(\mathbf{x}_1, \mathbf{x}_n) \\ K(\mathbf{x}_2, \mathbf{x}_1) & K(\mathbf{x}_2, \mathbf{x}_2) & \cdots & K(\mathbf{x}_2, \mathbf{x}_n) \\ \vdots & \vdots & \ddots & \vdots \\ K(\mathbf{x}_n, \mathbf{x}_1) & K(\mathbf{x}_n, \mathbf{x}_2) & \cdots & K(\mathbf{x}_n, \mathbf{x}_n) \end{bmatrix}$$

Mercer's Condition

$$K(\mathbf{u}, \mathbf{v}) = \phi(\mathbf{u}) \cdot \phi(\mathbf{v}) \iff \mathbf{K} \text{ is PSD}$$

Questions?

Next week: Neural Networks