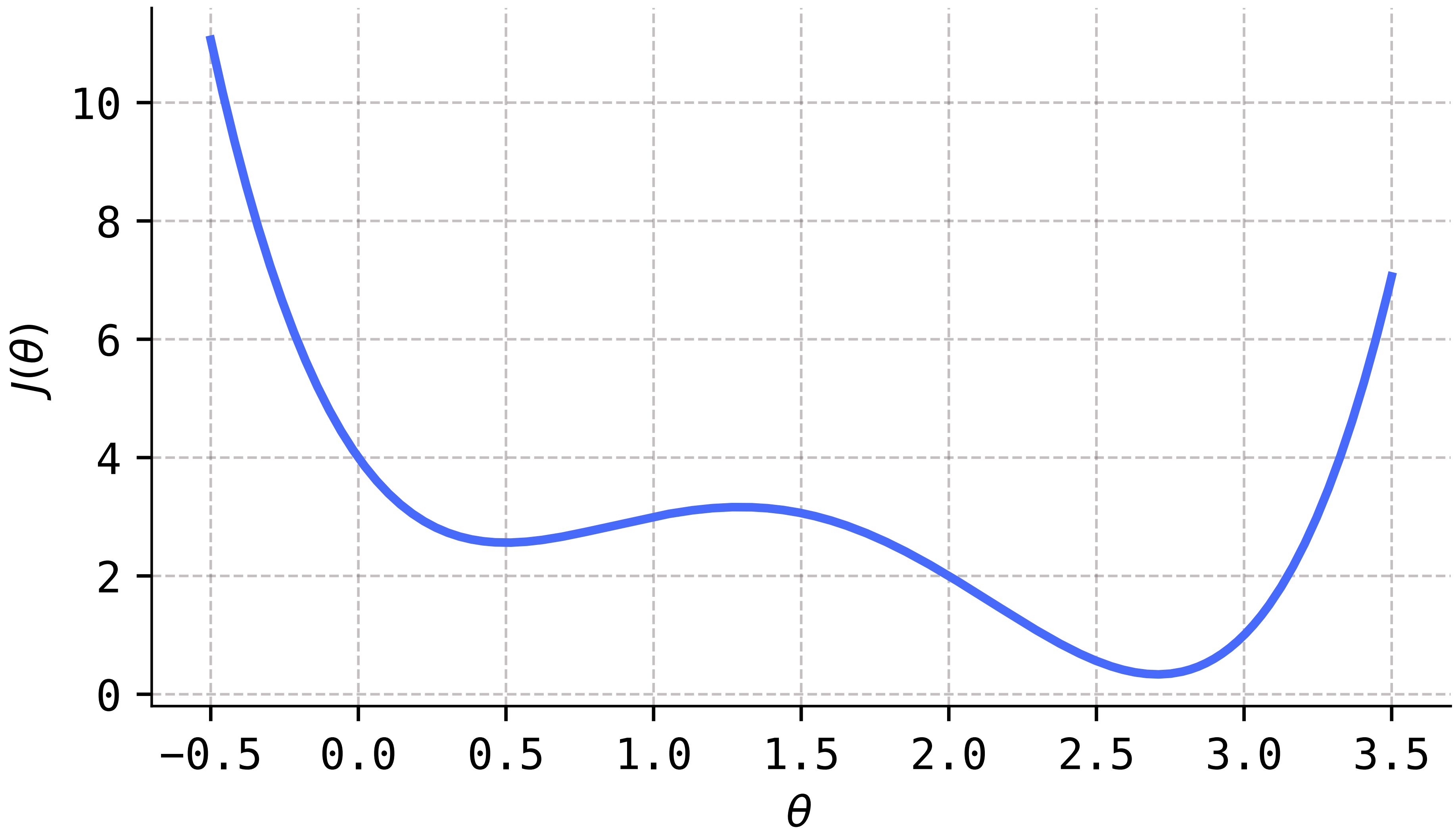
11. Optimization

11.1. Gradient descent in one variable



$J(\theta)$
10
8
6
4
2
0
−0.5
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
θ

Definition 11.1

Let $J : \mathbb{R}^n \to \mathbb{R}$ be a function. A vector $\boldsymbol{\theta}^\star$ is a *local minimizer* of $J(\boldsymbol{\theta})$ provided that

$$J(\boldsymbol{\theta}^\star) \leq J(\boldsymbol{\theta})$$

for all $\boldsymbol{\theta}$ in a neighborhood of $\boldsymbol{\theta}^\star$; if this inequality holds for *all* $\boldsymbol{\theta}$, then $\boldsymbol{\theta}^\star$ is called a *global minimizer* of $J(\boldsymbol{\theta})$. If we flip the inequality the other direction, then we obtain the definitions of *local* and *global maximizers*. Collectively, local and global minimizers and maximizers of $J(\boldsymbol{\theta})$ are called *extremizers*, and the values $J(\boldsymbol{\theta}^\star)$ of the function where $\boldsymbol{\theta}^\star$ is an extremizer are called *extrema* or *extreme values*.

Algorithm 11.1 (Single-variable gradient descent)

Input: A differentiable objective function $J : \mathbb{R} \to \mathbb{R}$, an initial guess $\theta_0 \in \mathbb{R}$ for a local minimizer $\theta^\star$, a learning rate $\alpha > 0$, and the number N of gradient steps.

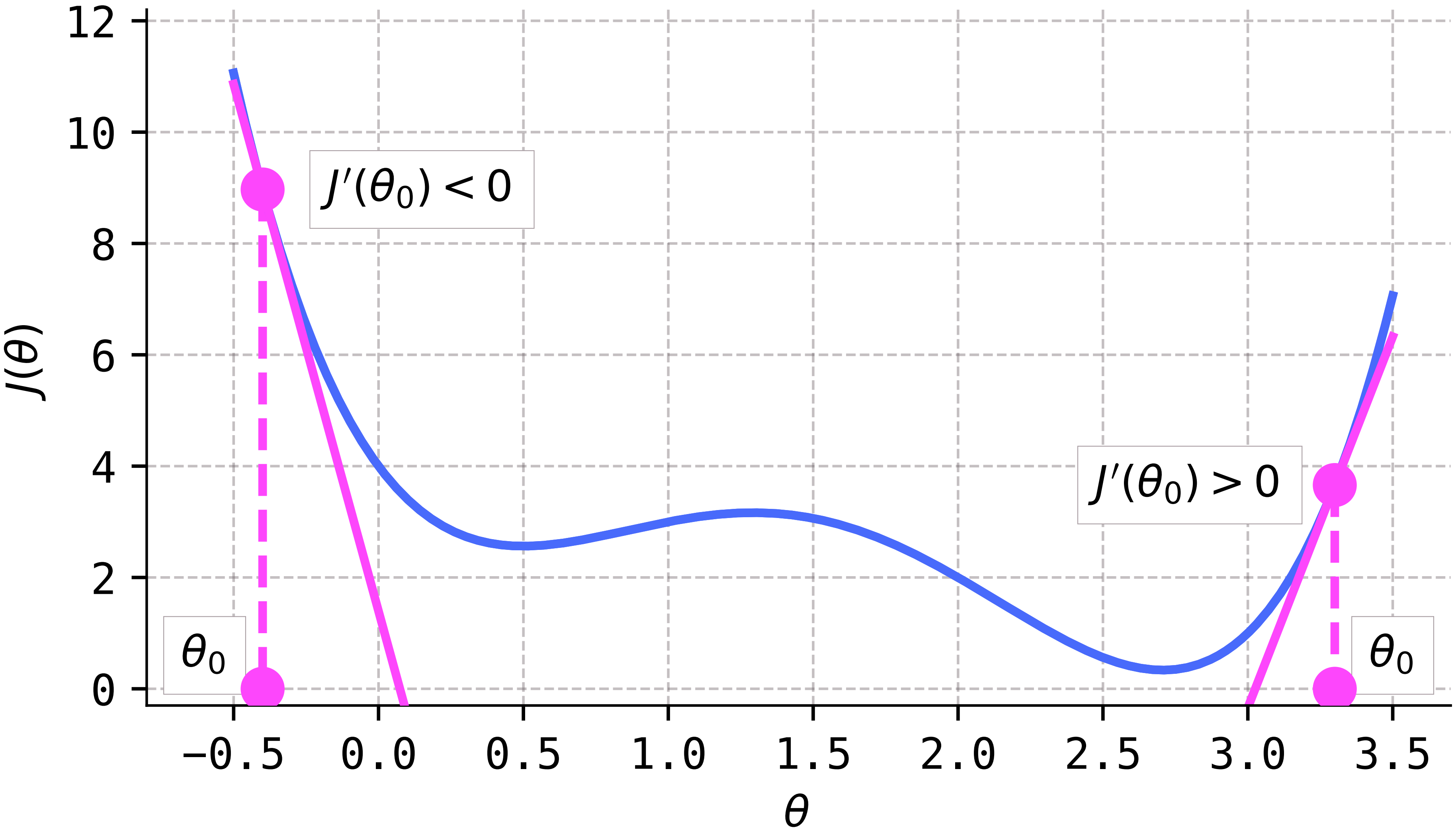
Output: An approximation to a local minimizer $\theta^\star$.

$\theta := \theta_0$

For t from 0 to $N-1$, do:

$\quad \theta := \theta - \alpha J'(\theta)$

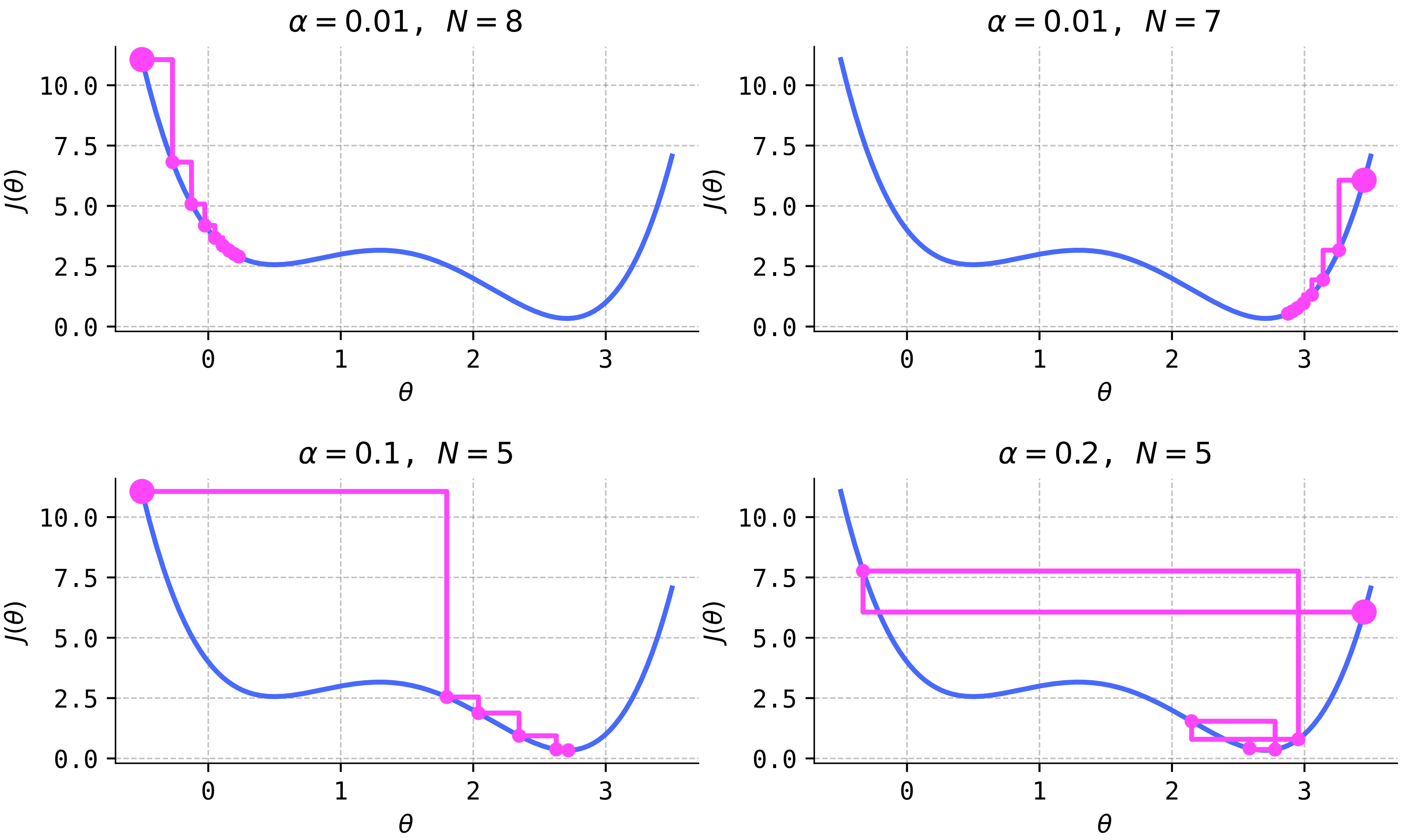
Return θ



$J'(\theta_0) < 0$
$J'(\theta_0) > 0$
θ_0
θ_0
12
10
8
6
4
2
0
$J(\theta)$
−0.5
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
θ

Observation 11.1

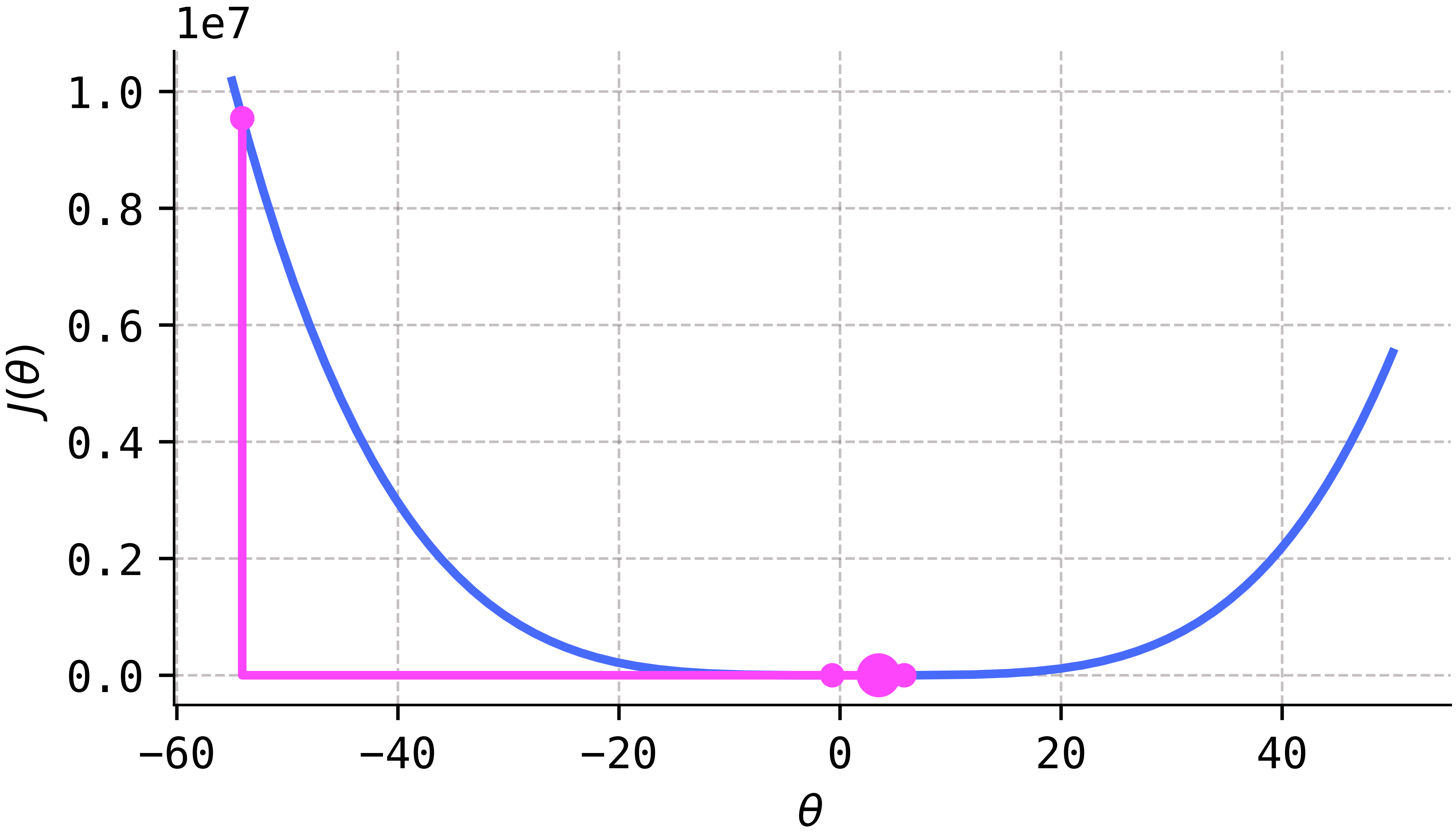
- The negative derivative $-J'(\theta)$ always “points downhill.”
- When the gradient descent algorithm works, it locates a minimizer by following the negative derivative “downhill.”



$\alpha = 0.01, \ N = 8$
$\alpha = 0.01, \ N = 7$
$\alpha = 0.1, \ N = 5$
$\alpha = 0.2, \ N = 5$
$J(\theta)$
θ
10.0
7.5
5.0
2.5
0.0
0
1
2
3

Problem Prompt

Do problem 1 on the worksheet.


1e7
1.0
0.8
0.6
0.4
0.2
0.0
$J(\theta)$
−60
−40
−20
0
20
40
θ

Problem Prompt

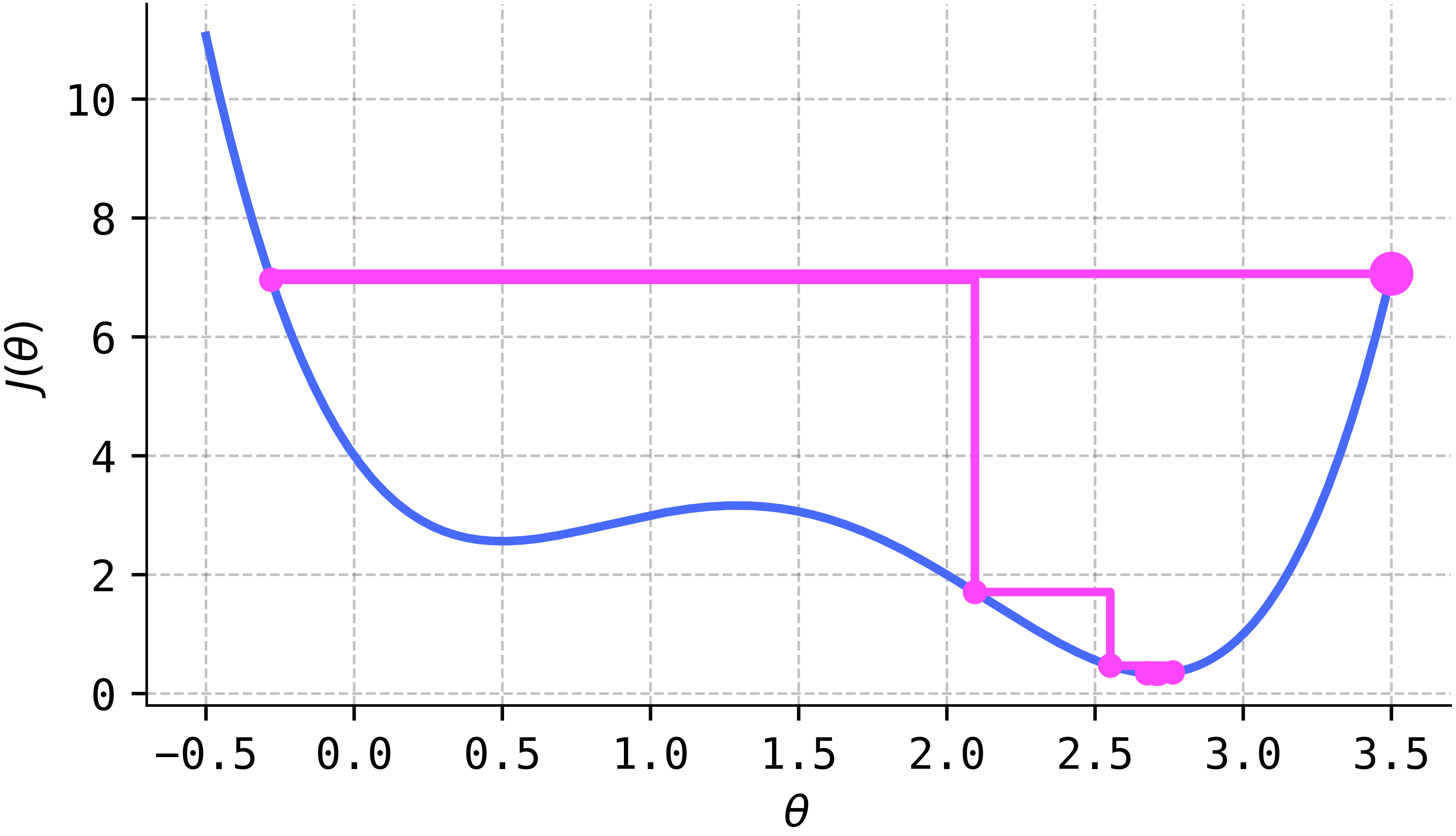
Do problems 2 and 3 on the worksheet.

Algorithm 11.2 (Single-variable gradient descent with learning rate decay)

Input: A differentiable objective function $J : \mathbb{R} \to \mathbb{R}$, an initial guess $\theta_0 \in \mathbb{R}$ for a local minimizer $\theta^\star$, a learning rate $\alpha > 0$, a decay rate $\beta \in [0, 1)$, and the number N of gradient steps.

Output: An approximation to a local minimizer $\theta^\star$.

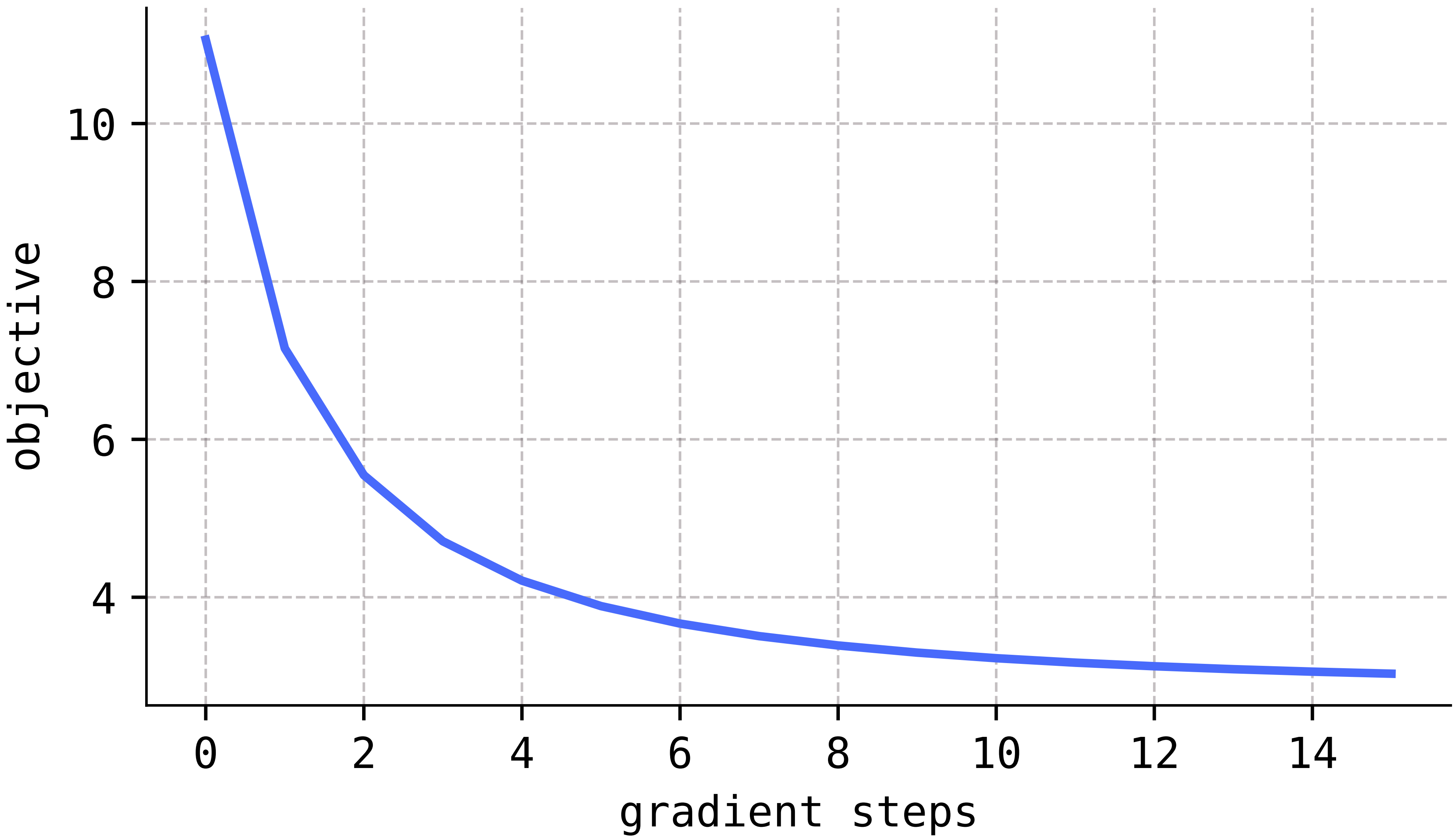
$\theta := \theta_0$
For t from 0 to $N-1$, do:
    $\theta := \theta - \alpha(1-\beta)^{t+1} J'(\theta)$
Return θ



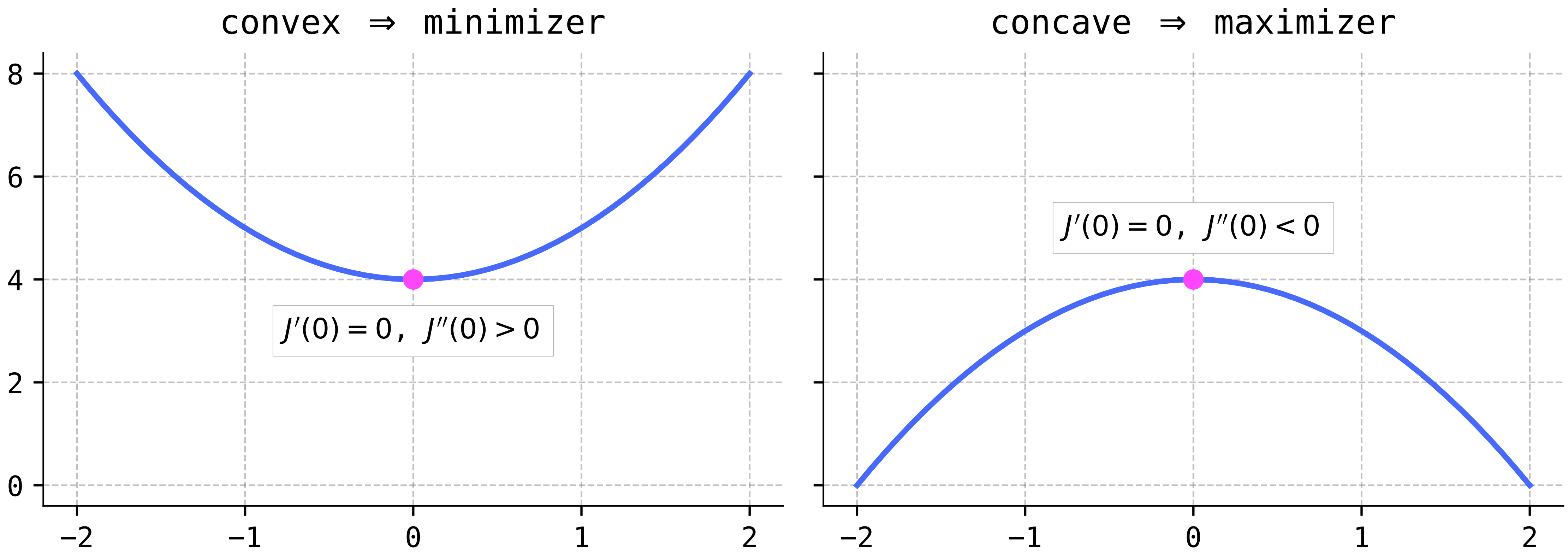
10
8
6
4
2
0
$J(\theta)$
−0.5
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
θ

Problem Prompt

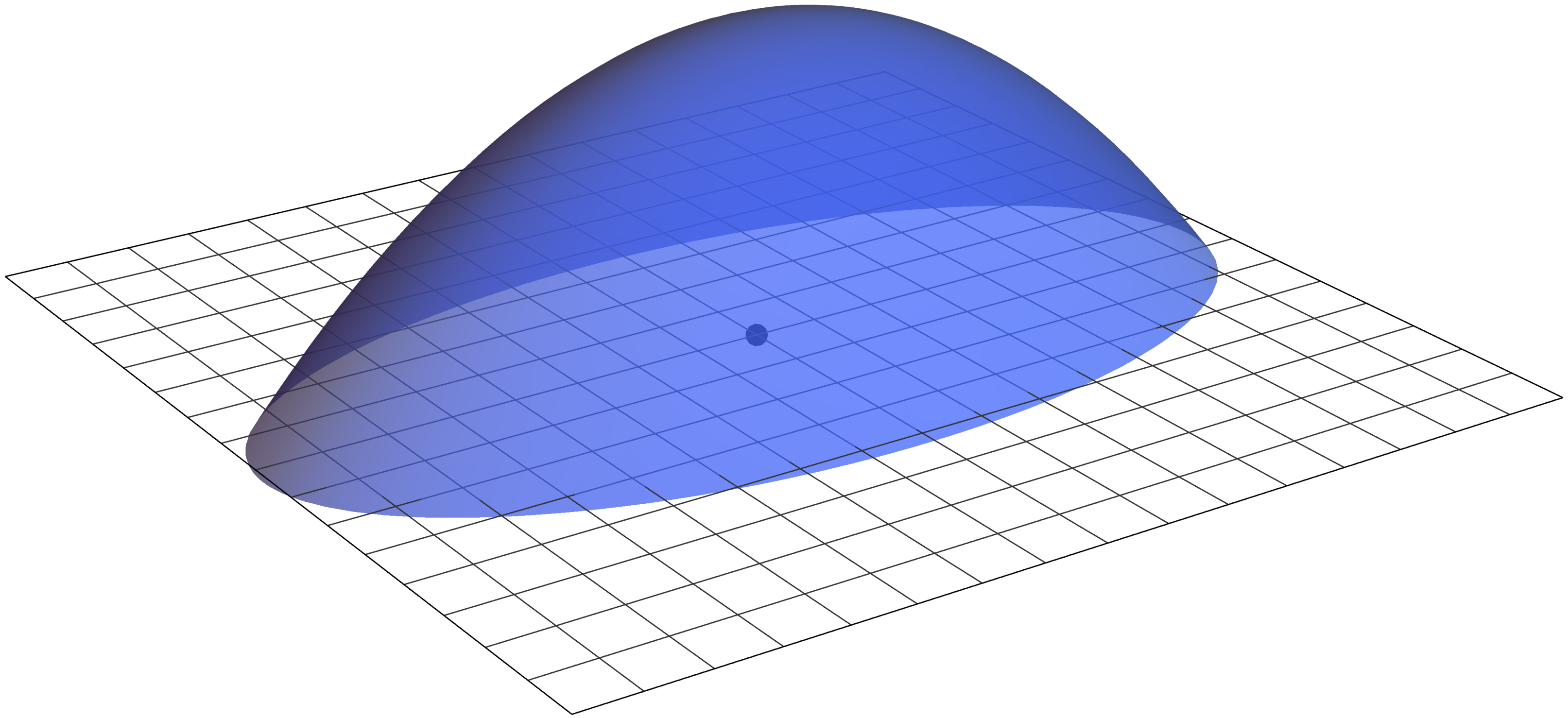
Do problem 4 on the worksheet.

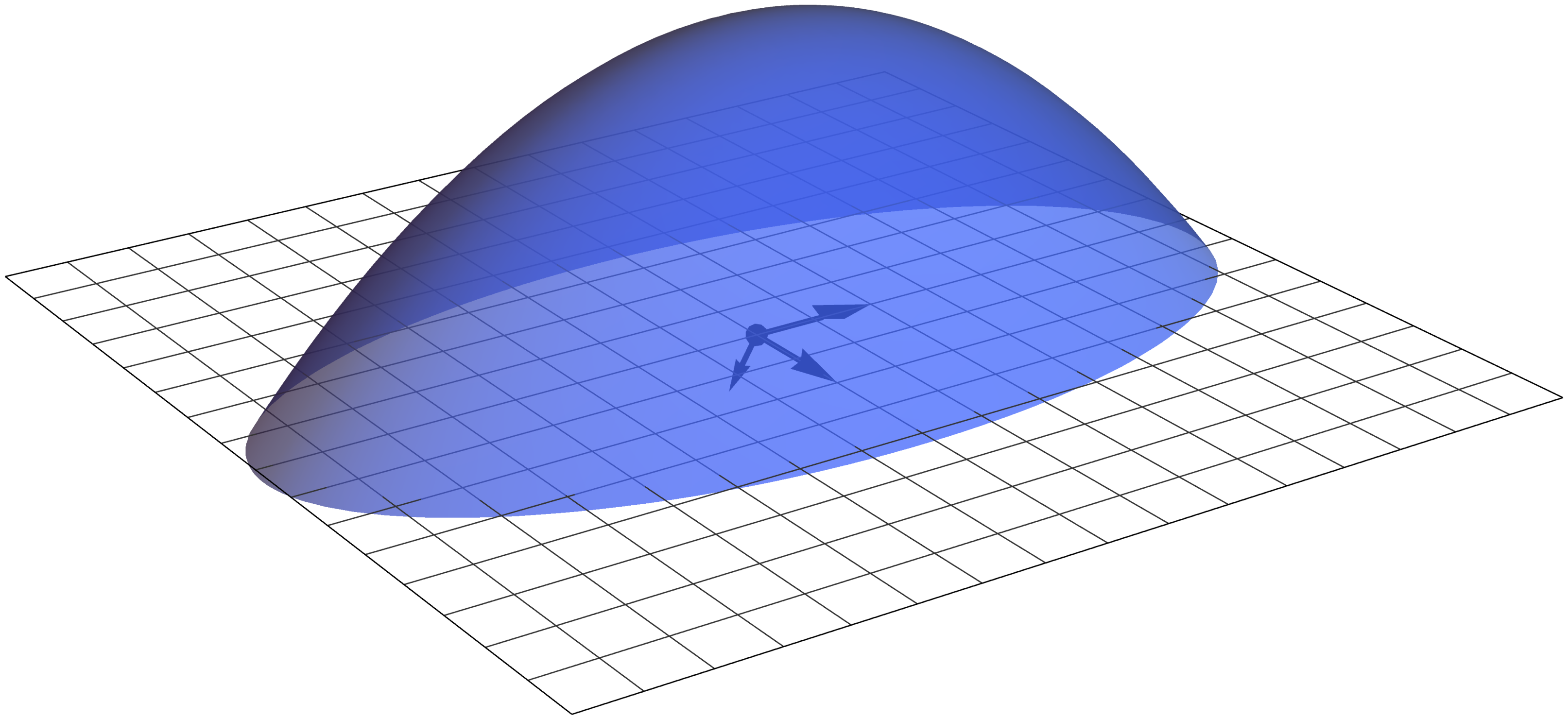

objective
gradient steps
10
8
6
4
0
2
4
6
8
10
12
14

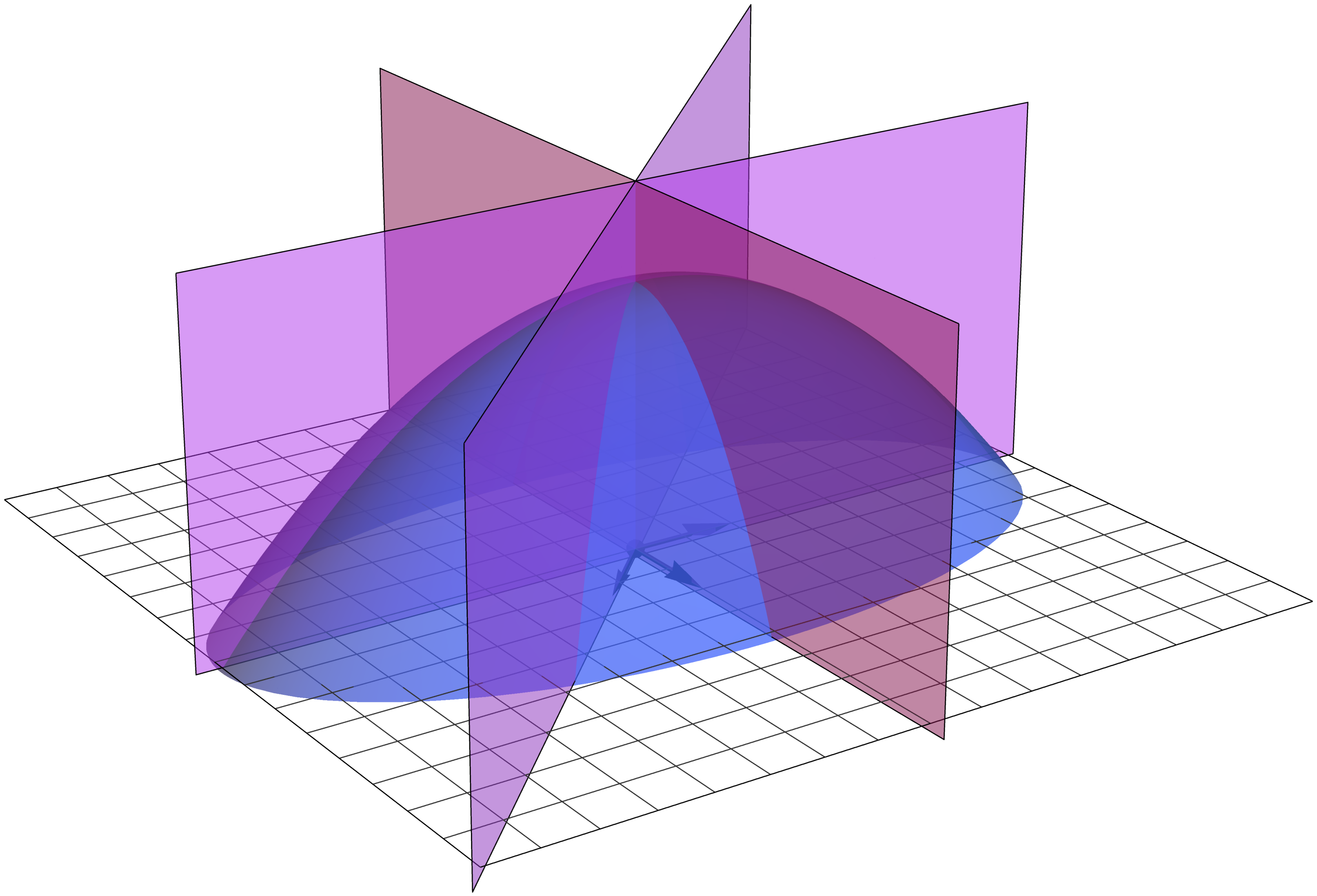
11.2. Differential geometry



convex ⇒ minimizer
$J'(0) = 0,\ J''(0) > 0$
concave ⇒ maximizer
$J'(0) = 0,\ J''(0) < 0$
8
6
4
2
0
−2
−1
0
1
2







Definition 11.2

Let $J:\mathbb{R}^n\to\mathbb{R}$ be a function of class C^2, $\boldsymbol{\theta}\in\mathbb{R}^n$ a point, and $\mathbf{v}\in\mathbb{R}^n$ a vector. We define the *directional first derivative of J at $\boldsymbol{\theta}$ in the direction* $\mathbf{v}$ to be

$$J'_{\mathbf{v}}(\boldsymbol{\theta}) \overset{\text{def}}{=} \frac{\mathrm{d}}{\mathrm{d}t}\bigg|_{t=0} J(t\mathbf{v}+\boldsymbol{\theta}),$$

while we define the *directional second derivative* to be

$$J''_{\mathbf{v}}(\boldsymbol{\theta}) \overset{\text{def}}{=} \frac{\mathrm{d}^2}{\mathrm{d}t^2}\bigg|_{t=0} J(t\mathbf{v}+\boldsymbol{\theta}).$$

In this context, the vector $\mathbf{v}$ is called the *directional vector*.

Problem Prompt

Do problem 5 on the worksheet.

Definition 11.3

Let $J : \mathbb{R}^n \to \mathbb{R}$ be a function of class C^2 and $\boldsymbol{\theta} \in \mathbb{R}^n$ a point. We define the *gradient vector* to be

$$\nabla J(\boldsymbol{\theta}) \stackrel{\text{def}}{=} \left[\frac{\partial J}{\partial \theta_i}(\boldsymbol{\theta})\right] = \begin{bmatrix} \frac{\partial J}{\partial \theta_1}(\boldsymbol{\theta}) \\ \vdots \\ \frac{\partial J}{\partial \theta_n}(\boldsymbol{\theta}) \end{bmatrix} \in \mathbb{R}^n,$$

while we define the the *Hessian matrix* to be

$$\nabla^2 J(\boldsymbol{\theta}) \stackrel{\text{def}}{=} \left[\frac{\partial^2 J}{\partial \theta_i \partial \theta_j}(\boldsymbol{\theta})\right] = \begin{bmatrix} \frac{\partial^2 J}{\partial \theta_1^2}(\boldsymbol{\theta}) & \cdots & \frac{\partial^2 J}{\partial \theta_1 \partial \theta_n}(\boldsymbol{\theta}) \\ \vdots & \ddots & \vdots \\ \frac{\partial^2 J}{\partial \theta_n \partial \theta_1}(\boldsymbol{\theta}) & \cdots & \frac{\partial^2 J}{\partial \theta_n^2}(\boldsymbol{\theta}) \end{bmatrix} \in \mathbb{R}^{n \times n}.$$

Theorem 11.1 (Slopes, curvatures, and partial derivatives)

Let $J : \mathbb{R}^n \to \mathbb{R}$ be a function of class C^2, $\boldsymbol{\theta} \in \mathbb{R}^n$ a point, and $\mathbf{v} \in \mathbb{R}^n$ a directional vector.

1. We have

$$J'_{\mathbf{v}}(\boldsymbol{\theta}) = \mathbf{v}^\intercal \nabla J(\boldsymbol{\theta}).$$

2. We have

$$J''_{\mathbf{v}}(\boldsymbol{\theta}) = \mathbf{v}^\intercal \nabla^2 J(\boldsymbol{\theta}) \mathbf{v}.$$

Problem Prompt

Do problem 6 on the worksheet.

Theorem 11.2 (Properties of gradient vectors)

Let $J:\mathbb{R}^n \to \mathbb{R}$ be a function of class C^2, $\boldsymbol{\theta} \in \mathbb{R}^n$ a point, and suppose the gradient vector $\nabla J(\boldsymbol{\theta})$ is nonzero.

1. The gradient vector $\nabla J(\boldsymbol{\theta})$ points in the direction of maximum rate of change.
2. The negative gradient vector $-\nabla J(\boldsymbol{\theta})$ points in the direction of minimum rate of change.
3. The gradient vector $\nabla J(\boldsymbol{\theta})$ is orthogonal to level surfaces.

Problem Prompt

Do problem 7 on the worksheet.

Theorem 11.3 (Second Derivative Test)

Let $J : \mathbb{R}^n \to \mathbb{R}$ be a function of class C^2 and $\boldsymbol{\theta}^\star \in \mathbb{R}^n$ a stationary point.

1. If the Hessian matrix $\nabla^2 J(\boldsymbol{\theta}^\star)$ is positive definite, then $\boldsymbol{\theta}^\star$ is a local minimizer.
2. If the Hessian matrix $\nabla^2 J(\boldsymbol{\theta}^\star)$ is negative definite, then $\boldsymbol{\theta}^\star$ is a local maximizer.

Problem Prompt

Do problem 8 on the worksheet.

Theorem 11.4 (Eigenvalues, eigenvectors, and local curvature)

Let $J : \mathbb{R}^n \to \mathbb{R}$ be a function of class C^2 and $\boldsymbol{\theta} \in \mathbb{R}^n$ a point with positive definite Hessian matrix $\nabla^2 J(\boldsymbol{\theta})$. Suppose we linearly order the eigenvalues of the Hessian matrix as

$$0 < \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n. \tag{11.8}$$

Then:

1. The directional curvature $J''_{\mathbf{v}}(\boldsymbol{\theta})$ is maximized exactly when $\mathbf{v}$ lies in the eigenspace of λ_n, in which case $J''_{\mathbf{v}}(\boldsymbol{\theta}) = \lambda_n$.
2. The directional curvature $J''_{\mathbf{v}}(\boldsymbol{\theta})$ is minimized exactly when $\mathbf{v}$ lies in the eigenspace of λ_1, in which case $J''_{\mathbf{v}}(\boldsymbol{\theta}) = \lambda_1$.

Problem Prompt

Do problem 9 on the worksheet.

Definition 11.4

Let $\mathbf{A}$ be an $n \times n$ square matrix.

1. The *spectrum* of $\mathbf{A}$, denoted $\sigma(\mathbf{A})$, is the set of eigenvalues of $\mathbf{A}$.
2. The *spectral radius* of $\mathbf{A}$, denoted $\rho(\mathbf{A})$, is given by

$$\rho(\mathbf{A}) \stackrel{\text{def}}{=} \max_{\lambda \in \sigma(\mathbf{A})} |\lambda|.$$

3. If $\mathbf{A}$ is positive definite, the *condition number* of $\mathbf{A}$, denoted $\kappa(\mathbf{A})$, is the ratio

$$\kappa(\mathbf{A}) \stackrel{\text{def}}{=} \frac{\lambda_{\max}}{\lambda_{\min}}$$

of the largest eigenvalue of $\mathbf{A}$ to the smallest.

Problem Prompt

Do problem 10 on the worksheet.