Gradient Based Optimization I

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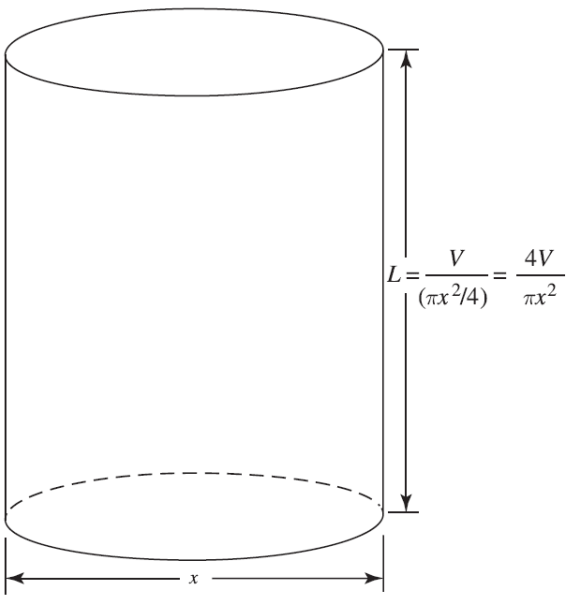
Objective

At the end of this chapter you should be able to:

- Mathematically define the optimality conditions for an unconstrained problem.
- Describe, implement, and use line-search-based methods.
- Gradient Descent based method

Unconstrained optimization problems

Determine the objective function for building a minimum cost cylinderical refrigeration tank of volume 50 m^3, if the circular ends cost \$ 10 per m^2 , the cylindrical wall costs \$6 per m^2, and it costs \$80 per m^2 to refrigerate over the useful life.



$$
\begin{aligned}
f(x, L) &= (10)(2)\left(\frac{\pi x^2}{4}\right) \\
&\quad + (6)(\pi x L) + 80\left((2)\frac{\pi x^2}{4} + \pi x L\right) \\
&= 45\pi x^2 + 86\pi x L \\
L &= \frac{(50)(4)}{\pi x^2} = \frac{200}{\pi x^2} \\
f(x) &= 45\pi x^2 + \frac{17200}{x}
\end{aligned}
$$

One problem is minimize $f(x)$ for all real x. How!

Unconstrained optimization problems

We consider unconstrained optimization problems with continuous design variables,

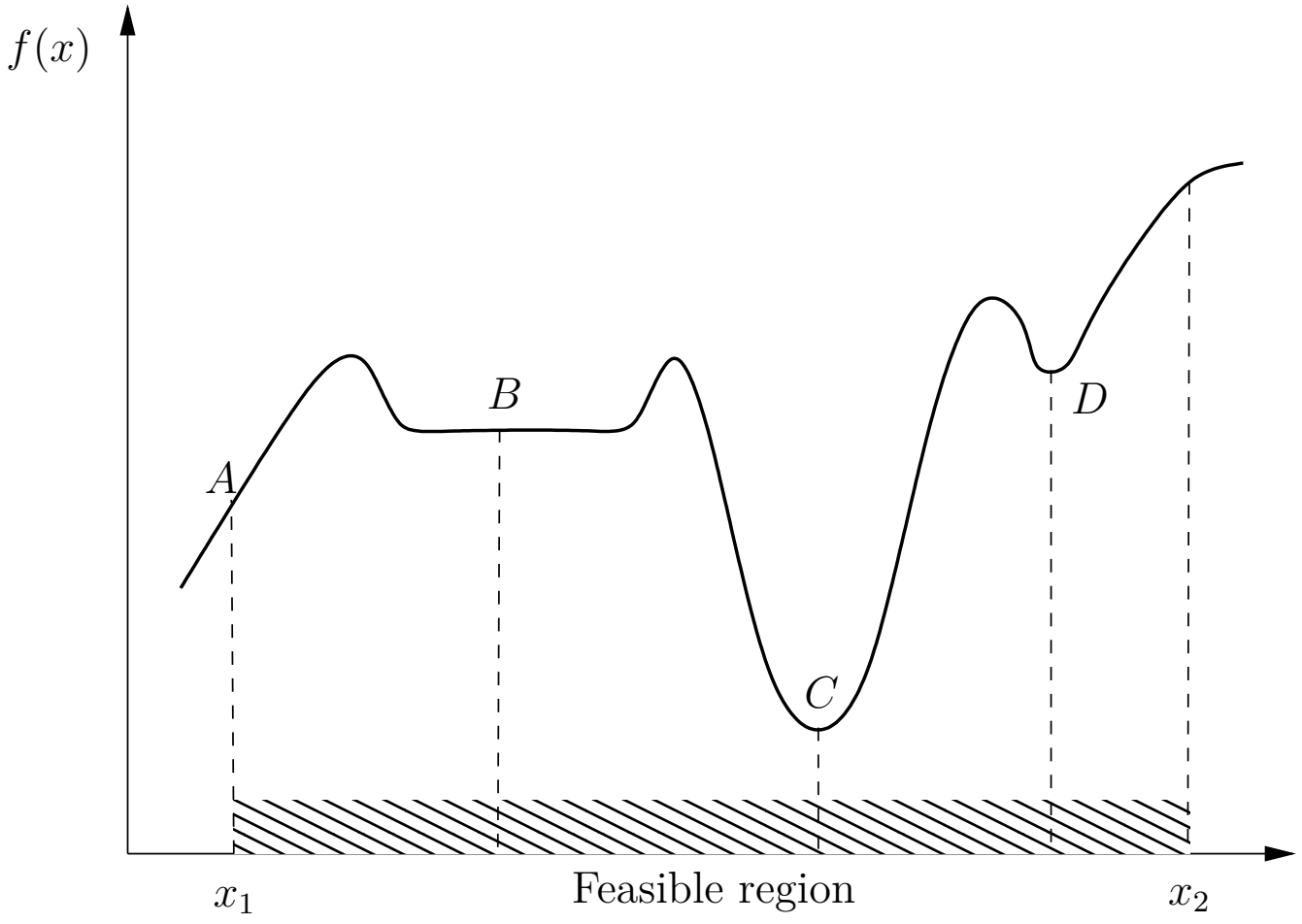
$$\underset{\mathbf{x}}{\text{minimize}}\, f(\mathbf{x}),$$

where $\mathbf{x} = [x_1, \ldots, x_n]$ is composed of the design variables that the optimization algorithm can change.

Minimum Points:

- the point $\mathbf{x}^*$ is a **weak local minimum** if there exists a $\delta > 0$ such that $f(\mathbf{x}^*) \leq f(\mathbf{x})$ for all $\mathbf{x}$ such that $|\mathbf{x} - \mathbf{x}^*| < \delta$, that is $f(\mathbf{x}^*) \leq f(\mathbf{x})$ for all $\mathbf{x}$ in a δ-neighborhood of $\mathbf{x}^*$.
- the point $\mathbf{x}^*$ is a **strong local minimum** if there exists a $\delta > 0$ such that $f(\mathbf{x}^*) < f(\mathbf{x})$ for all $\mathbf{x}$ such that $|\mathbf{x} - \mathbf{x}^*| < \delta$.
- $\mathbf{x}^*$ is a **global minimum** if $f(\mathbf{x}^*) < f(\mathbf{x})$ for all $\mathbf{x}$

Unconstrained optimization problems



Optimality Conditions

A point $\mathbf{x}^*$ is a local minimum if $f(\mathbf{x}^*) \leq f(\mathbf{x})$ for all $\mathbf{x}$ in the neighborhood of $\mathbf{x}^*$. A second-order Taylor series expansion about $\mathbf{x}^*$ for small steps of size $\mathbf{p}$ yields

$$f(\mathbf{x}^* + \mathbf{p}) = f(\mathbf{x}^*) + \nabla f(\mathbf{x}^*)^T \mathbf{p} + \frac{1}{2}\mathbf{p}^T \mathbf{H}(\mathbf{x}^*)\mathbf{p} + \dots$$
$$f(\mathbf{x}^* - \mathbf{p}) = f(\mathbf{x}^*) - \nabla f(\mathbf{x}^*)^T \mathbf{p} + \frac{1}{2}\mathbf{p}^T \mathbf{H}(\mathbf{x}^*)\mathbf{p} + \dots$$

For x^* to be an optimal point, we must have $f(\mathbf{x}^* + \mathbf{p}) \geq f(\mathbf{x}^*)$ for all $\mathbf{p}$. This implies that

$$\nabla f(\mathbf{x}^*)^T \mathbf{p} + \frac{1}{2}\mathbf{p}^T \mathbf{H}(\mathbf{x}^*)\mathbf{p} \geq 0 \text{ and } -\nabla f(\mathbf{x}^*)^T \mathbf{p} + \frac{1}{2}\mathbf{p}^T \mathbf{H}(\mathbf{x}^*)\mathbf{p} \geq 0 \qquad \forall \mathbf{p}.$$

The magnitude of $\mathbf{p}$ is small, the second term can be neglected. Therefore, we require that

$$\nabla f(\mathbf{x}^*)^T \mathbf{p} \geq 0 \text{ and } -\nabla f(\mathbf{x}^*)^T \mathbf{p} \geq 0 \implies \nabla f(\mathbf{x}^*) = 0$$

Optimality Conditions

The condition $\nabla f(\mathbf{x}^*) = 0$ is called the first-order necessary optimality condition.

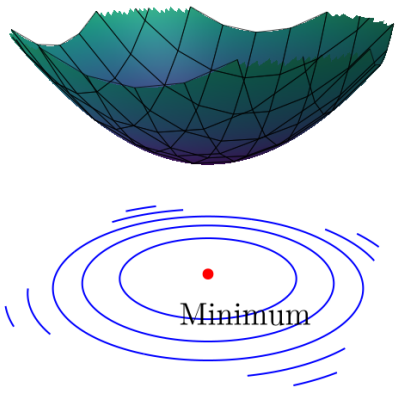
Because the gradient term has to be zero, we must satisfy the remaining term in the previous inequality, that is

$$\mathbf{p}^T \mathbf{H}(\mathbf{x}^*)\mathbf{p} \geq 0 \quad \forall \mathbf{p} \quad \text{or } \mathbf{H}(\mathbf{x}^*) \succeq 0$$

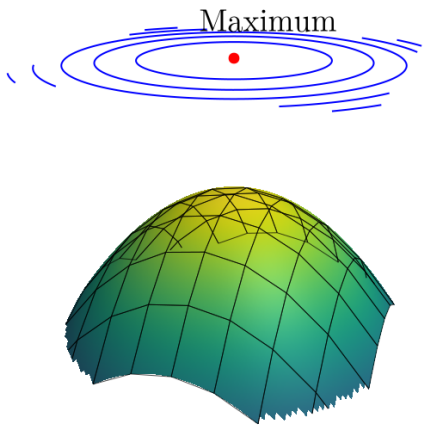
- These two conditions $\nabla f(\mathbf{x}^*) = 0$ and $\mathbf{H}(\mathbf{x}^*) \succeq 0$ are necessary conditions for a local minimum but not sufficient.
- In some direction $\mathbf{p}^T \mathbf{H}(\mathbf{x}^*)\mathbf{p}$ can be zero. We need to check the third-order term. If it is a minimum, it is a weak minimum.
- To have the sufficient optimality condition, $\mathbf{H}(\mathbf{x}^*)$ must be positive definite.

Quadratic function with different types of Hessian

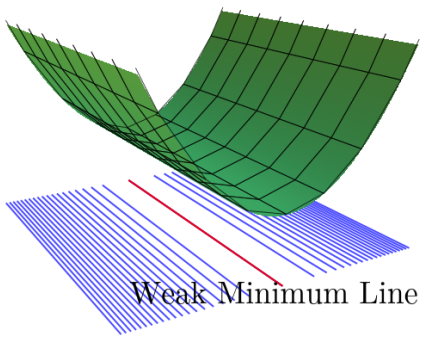
Positive Definite



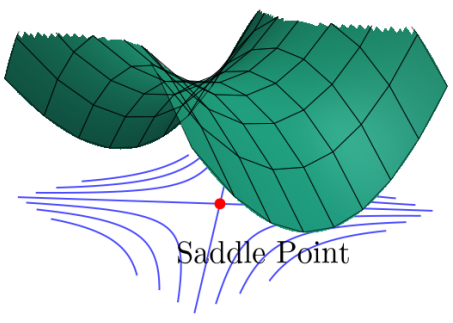
Negative Definite



Positive Semidefinite



Indefinite



Optimality Conditions: Finding minima analytically

Consider the following function of two variables:

$$f(x_1, x_2) = 0.5x_1^4 + 2x_1^3 + 1.5x_1^2 + x_2^2 - 2x_1x_2$$

Let the gradient equal to zero,

$$\nabla f(x_1, x_2) = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \\ \frac{\partial f}{\partial x_2} \end{bmatrix} = \begin{bmatrix} 2x_1^3 + 6x_1^2 + 3x_1 - 2x_2 \\ 2x_2 - 2x_1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

From the second row, we have $x_1 = x_2$. Substituting this in to the first equation yields

$$x_1 \left(2x_1^2 + 6x_1 + 1\right) = 0 \quad \Longrightarrow \quad x_1 = 0, -2.8223, -0.1771$$

The solution of this equation has three points: $x_A = (0, 0)$, $x_B = (-2.8223, -2.8223)$, and $x_C = (-0.1771, -0.1771)$. `(see ch2/optimal_condition.jl)`

Optimality Conditions: Finding minima analytically

To clarify these three points, we need to find the Hessian matrix.

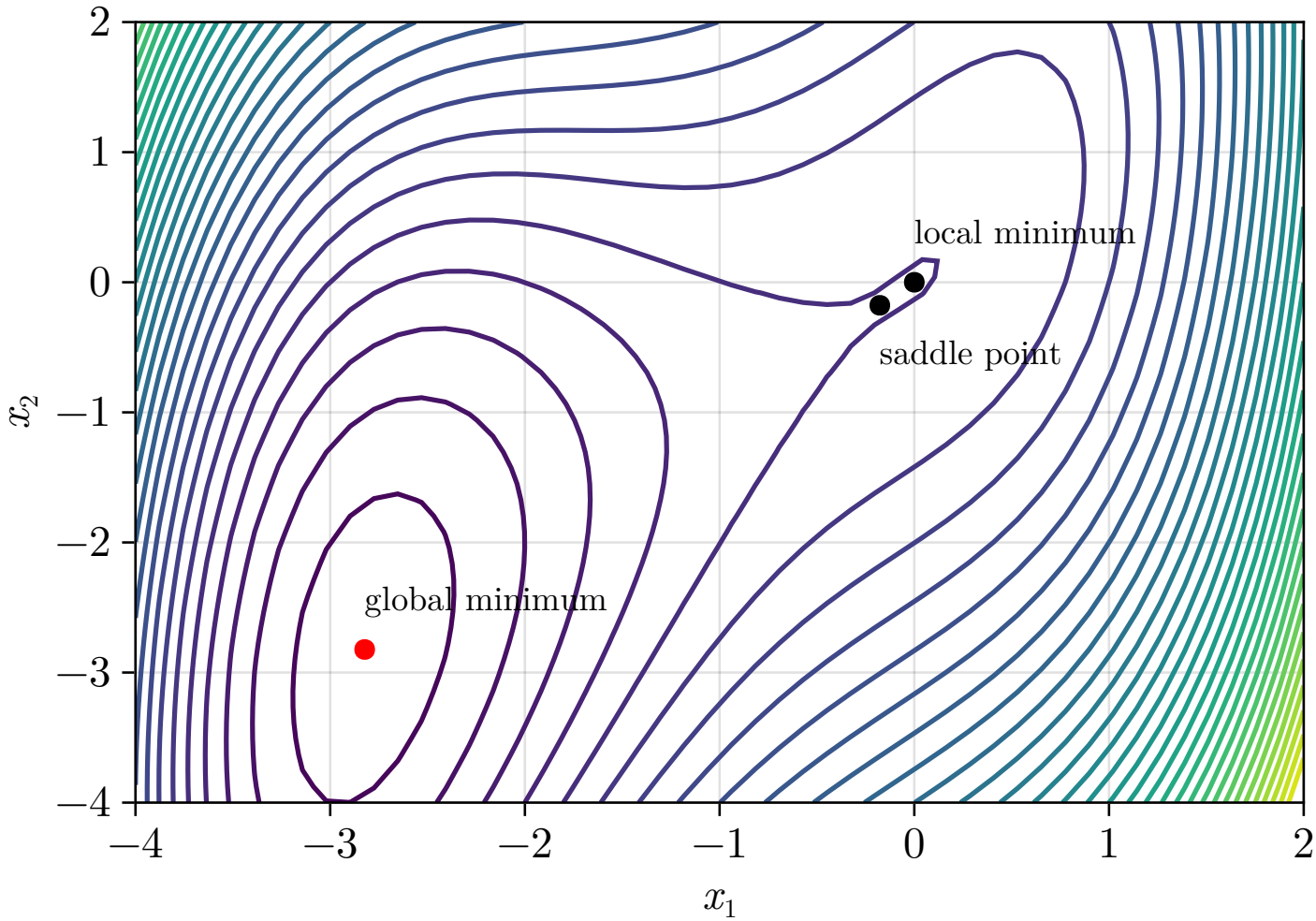
$$\mathbf{H}(x_1, x_2) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} \\ \frac{\partial^2 f}{\partial x_1 \partial x_2} & \frac{\partial^2 f}{\partial x_2^2} \end{bmatrix} = \begin{bmatrix} 6x_1^2 + 12x_1 + 3 & -2 \\ -2 & 2 \end{bmatrix}$$

For each point, we have

$$\mathbf{H}(\mathbf{x}_A) = \begin{bmatrix} 3 & -2 \\ -2 & 2 \end{bmatrix}, \qquad \mathbf{H}(\mathbf{x}_B) = \begin{bmatrix} 16.9373 & -2 \\ -2 & 2 \end{bmatrix}, \qquad \mathbf{H}(\mathbf{x}_C) = \begin{bmatrix} 1.0627 & -2 \\ -2 & 2 \end{bmatrix}$$

The eigenvalues are $\lambda_A = (0.438, 4.561)$, $\lambda_B = (1.737, 17.200)$, and $\lambda_C = (-0.523, 3.586)$, respectively. The first two eigenvalues show the evidence of the local minimum points, while the last one addresses the saddle point.

Optimality Conditions
Example: Finding minima analytically



Optimality Conditions
Example: Finding minimum analytically

We want to

$$\underset{x}{\text{minimize}} \qquad 45\pi x^2 - \frac{17200}{x}$$

We set

$$\nabla f = 90\pi x - \frac{17200}{x^2} = 0 \qquad \Longrightarrow \qquad x^3 = \frac{17200}{90\pi} = 60.833$$

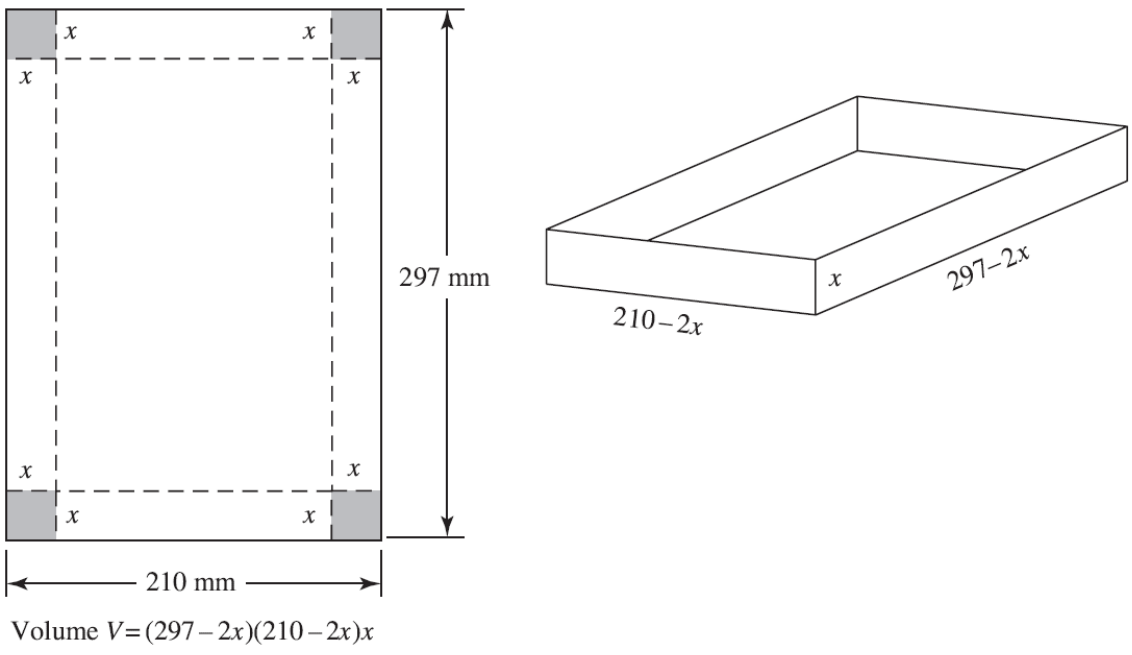
We have $x = 3.93$ m and $L = 200/(\pi x^2) = 4.12$ m.
The cost is

$$f(x^*) = 45(x^*)^2 + \frac{17200}{x^*} = 6560$$

Since $\mathbf{H}(x^*) = 90\pi + (3(17200))/(x^*)^3 = 1132.85$, it is strictly positive. Thus the solution is a strict or strong minimum.

Optimality Conditions
Example: Maximize Problem

Determine the dimensions of an open box of maximum volume that can be constructed form an A4 sheet 210 mm $\times$ 297 mm by cutting four squares of side x from the corners and folding and gluing the edges as shown in Fig.



Volume $V = (297 - 2x)(210 - 2x)x$

The problem is to

$$\underset{x}{\text{maximize}} \qquad V(x) = (297 - 2x)(210 - 2x)x = 62370x - 1014x^2 + 4x^3$$

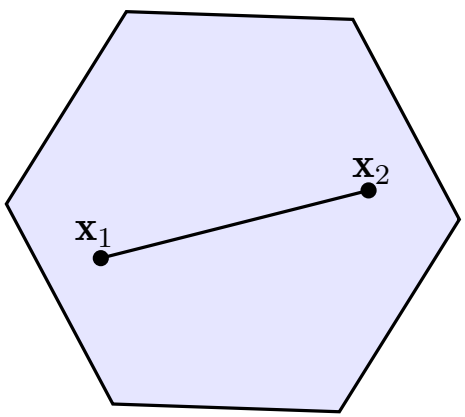
We set $f(x) = -V(x) = -62370x + 1014x^2 - 4x^3$. Setting $\nabla f(x) = 0$, we get

$$\nabla f(x) = -62370 + 2028x - 12x^2 = 0 \quad \Longrightarrow \quad x = 40.423 \text{ and } 128.577 \text{ mm.}$$

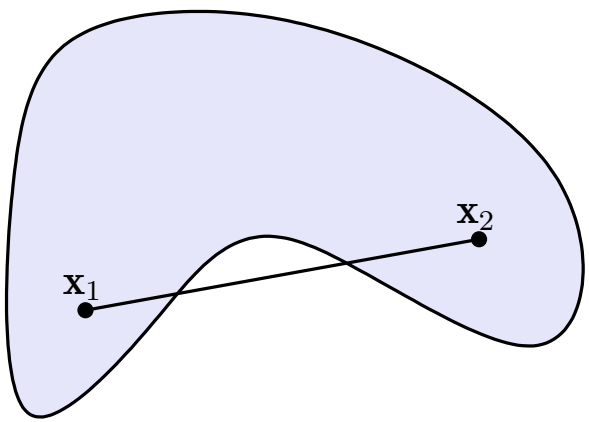
The possible solution of x is only the first one, where $x^* = 40.423$ mm. The $\mathbf{H}(x^*) = 2028 - 24x^* = 1057.848 > 0$. implies that x^* is a strict minimum of $f(x)$ or maximum of $V(x)$.
The maximum value of the box is 1128.5 cm^3.

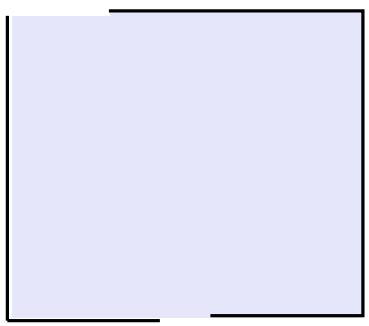
Convex Sets

- A set $\mathbb{S}$ is called a convex set if for any two points in the set, every point on the line joining the two points is in the set.
- Alternatively, the $\mathbb{S}$ is convex if for every pair of points $\mathbf{x}_1$ and $\mathbf{x}_2$ in $\mathbb{S}$, and every α such that $0 < \alpha < 1$, the point $\alpha\mathbf{x}_1 + (1-\alpha)\mathbf{x}_2$ is in $\mathbb{S}$.
- example of convex sets:
  - the set of all real numbers $\mathbb{R}$ is a convex set.
  - any closed interval of $\mathbb{R}$ is also a convex set.
  - $\mathbf{A} = \{x \in \mathbb{R} : 0 \leq x \leq 1\}$, $\mathbf{B} = \{x \in \mathbb{R} : 2 \leq x \leq 3\}$ and $\mathbb{S} = \mathbf{A} \cup \mathbf{B}$. $\mathbb{S}$ is not a convex set.



convex set





nonconvex set

Convex Functions

- A function $f(\mathbf{x})$ defined over a convex set $\mathbb{R}_c$ is said to be convex if for every pair of points $\mathbf{x}_1, \mathbf{x}_2 \in \mathbb{R}_c$ and every real number $0 \leq \alpha \leq 1$, the inequality

$$f(\alpha\mathbf{x}_1 + (1-\alpha)\mathbf{x}_2) \leq \alpha f(\mathbf{x}_1) + (1-\alpha)f(\mathbf{x}_2)$$

  hold. If $x_1 \neq x_2$ and

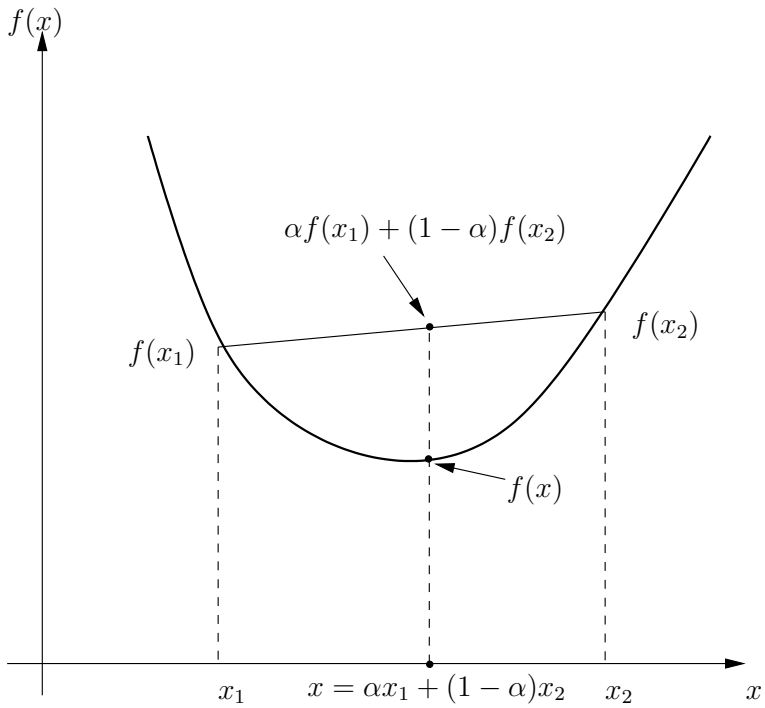
$$f(\alpha\mathbf{x}_1 + (1-\alpha)\mathbf{x}_2) < \alpha f(\mathbf{x}_1) + (1-\alpha)f(\mathbf{x}_2)$$

  then $f(\mathbf{x})$ is said to be strictly convex.

- If $\psi(\mathbf{x})$ is defined over a convex set $\mathbb{R}_c$ and $f(\mathbf{x}) = -\psi(\mathbf{x})$ is convex, then $\phi(\mathbf{x})$ is said to be concave. If $f(\mathbf{x})$ is strictly convex, $\psi(\mathbf{x})$ is strictly concave.

is located in $\mathbb{R}_c$

Properties Convex Functions



Properties of Convex Functions

- If f has continuous first derivatives then f is convex over a convex set $\mathbf{S}$ if and only if for every x and y in $\mathbf{S}$, $f(y) \geq f(x) + f'(x)(y - x)$ This means that the graph of the function lies above the tangent line drawn at point show in above figure.

Properties Convex Functions

- If f has continuous second derivatives then f is convex over a convex set $\mathbf{S}$ if and only if for every x in $\mathbf{S}$,

$$f''(x) \geq 0$$

- If $f(x^*)$ is a local minimum for a convex function f on a convex set $\mathbf{S}$, then it is also a global minimum.
- If f has continuous first derivatives on a convex set $\mathbf{S}$ and for a point x^* in $\mathbf{S}$, $f'(x^*)(y - x^*) \geq 0$ for every y in $\mathbf{S}$, then x^* is a global minimum point of f over $\mathbf{S}$.

Example: Convex Function

Prove that $f = |x|, x \in \mathbb{R}^1$, is a convex function. Using the triangular inequality $|x + y| \leq |x| + |y|$, we have, for any two real numbers x_1 and x_2 and $0 < \alpha < 1$,

$$\begin{aligned} f(\alpha x_1 + (1-\alpha)x_2) &= |\alpha x_1 + (1-\alpha)x_2| \leq \alpha|x_1| + (1-\alpha)|x_2| \\ &\leq \alpha f(x_1) + (1-\alpha)f(x_2) \end{aligned}$$

Descent Direction

Consider an unconstraint problem

$$\underset{\mathbf{x}\in\mathbb{R}^n}{\text{minimize}} \qquad f(\mathbf{x})$$

Definition: Descent Direction

A vector $\mathbf{d} \in \mathbb{R}^n$ is called a *descent direction* for f at $\mathbf{x}$ if moving a small amount in that direction decreases the function value.

$$\exists \alpha > 0 \text{ such that } f(\mathbf{x} + \alpha\mathbf{d}) < f(\mathbf{x})$$

To check the descent direction, we could use the First-order Condition. From a first-order Taylor approximation around $\mathbf{x}$:

$$f(\mathbf{x} + \alpha\mathbf{d}) \approx f(\mathbf{x}) + \alpha\nabla f(\mathbf{x})^T\mathbf{d}$$

For small $\alpha > 0$, we will have decrease if: $\nabla f(\mathbf{x})^T\mathbf{d} < 0$. This condition defines a descent direction.

Example: Steepest Descent

The most common descent direction is the *negative gradient:*

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

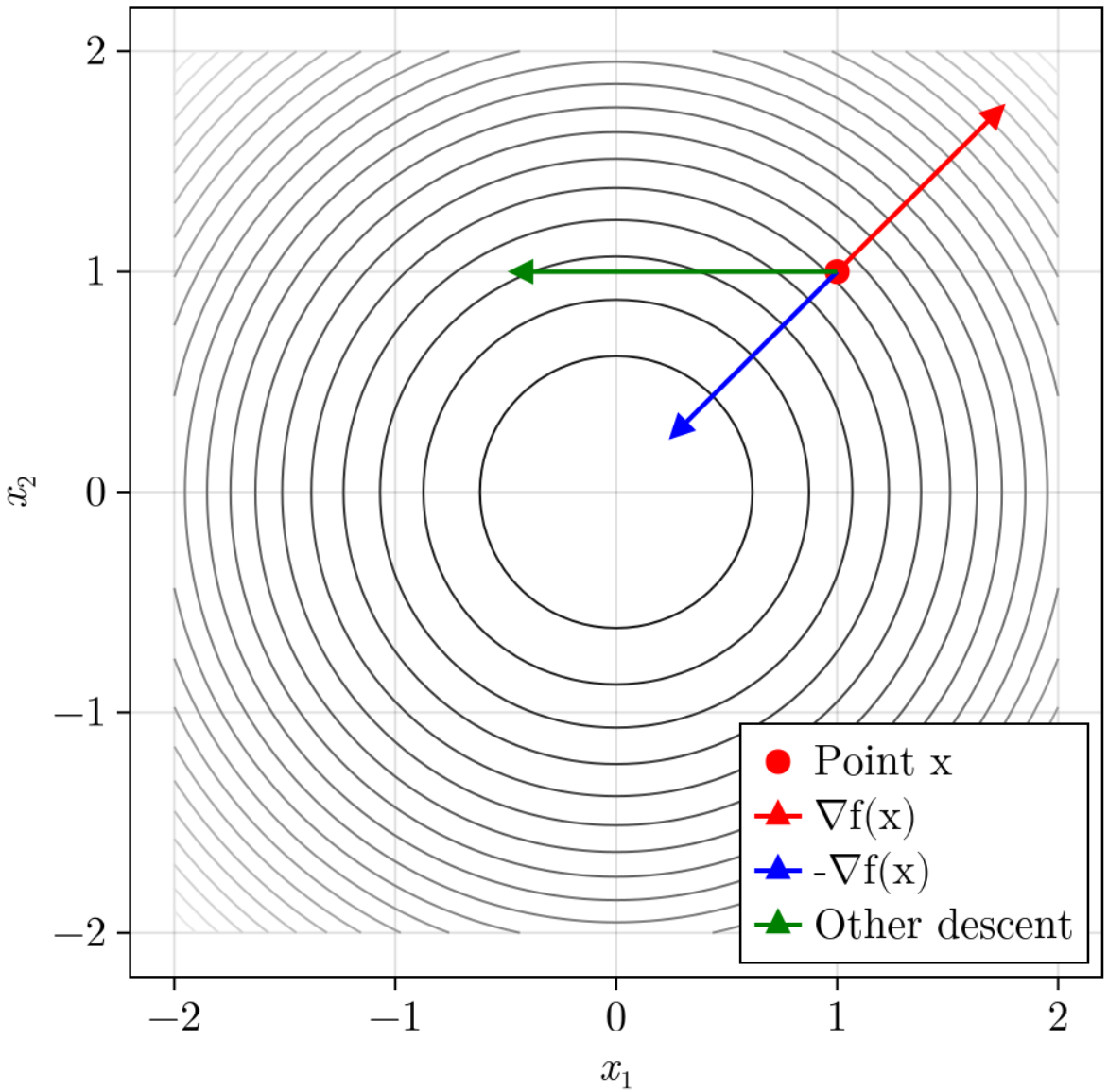
Why? Because:

$$\nabla f(\mathbf{x})^T(-\nabla f(\mathbf{x})) = -\|\nabla f(\mathbf{x})\|^2 < 0, \text{ where } \nabla f(\mathbf{x}) > 0$$

so it always guarantees descent.

- A descent direction is any vector $\mathbf{d}$ such that $\nabla f(\mathbf{x})^T\mathbf{d} < 0$
- It ensures that moving a little in direction $\mathbf{d}$ decreases $f(\mathbf{x})$
- The negative gradient $-\nabla f(\mathbf{x})$ is the steepest descent direction.

Example: Steepest Descent



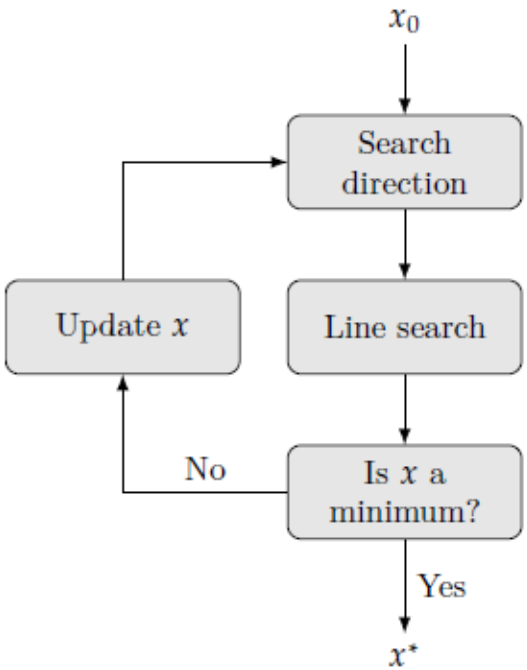
Gradient Based Optimization

A Gradient descent is one of the most popular and versatile technique in all of optimization.

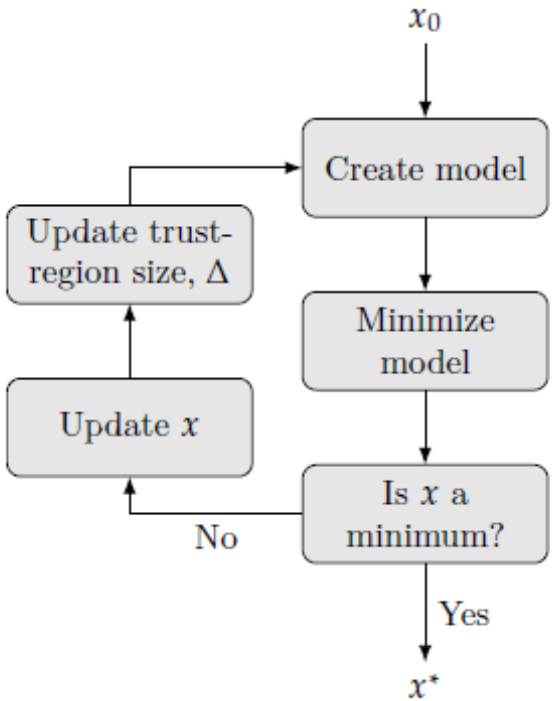
- A local minimum of a smooth, unconstrained objective function $f(\mathbf{x}$ will be a point $\mathbf{x}^*$ with zero gradient, $\nabla f(\mathbf{x}^*) = 0$, and positive semi-definite Hessian, $\nabla^2 f(\mathbf{x}^*) > 0$.
- The idea is find the point $\mathbf{x}$ where $\nabla f(\mathbf{x}) = 0$. We known as a root finding problem.
- However, in general, the function $\nabla f(x)$ is too complex to solve for its roots. We need to use iterative method to obtain a sequence of point $\mathbf{x}_k$ that eventually converge towards the local minimum $\mathbf{x}^*$:

$$f(\mathbf{x}_0) \geq f(\mathbf{x}_1) \geq f(\mathbf{x}_2) \geq \cdots \geq f(\mathbf{x}^*)$$
$$f(\mathbf{x}_{k+1}) - f(\mathbf{x}_k) < 0 \implies \mathbf{x}_{k+1} = F(\mathbf{x}_k)$$

Two Approaches to Finding and Optimum



Line search approach



Trust-region approach

Basic Concept

Consider a problem

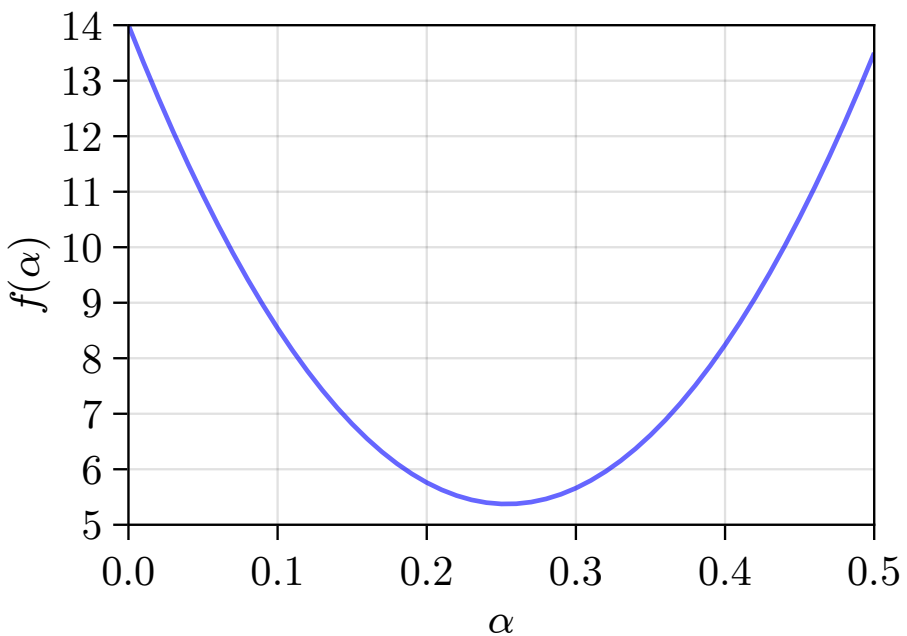
$$\underset{\mathbf{x}}{\text{minimize}} \quad f(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^n$$

- Most numerical methods require a starting design or point which we call $\mathbf{x}_0$ (initial point).
- We then determine the *direction of travel* $\mathbf{d}_0$.
- A *step size* α_0 is then determined based on minimizing f as much as possible and the design point is updated as $\mathbf{x}_1 = \mathbf{x}_0 + \alpha_0 \mathbf{d}_0$.
- The process of where to go and how far to go are repeated from $\mathbf{x}_1$ or $\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k \mathbf{d}_k$.

Basic Concept: Example

Given $f(x_1, x_2) = x_1^2 + 5x_2^2$, a point $\mathbf{x}_0 = [3\ 1]^T$, $f_0 = f(\mathbf{x}_0) = 14$.

1. Assume we already have a descent direction $\mathbf{d} = [-3\ \ -5]^T$. We need to find a step size α.
2. Construct $f(\alpha) = f(\mathbf{x}_0 + \alpha\mathbf{d})$ along the direction $\mathbf{d}$ and provide a plot of $f(\alpha)$ versus α, for $\alpha \geq 0$. We have $\mathbf{x}(\alpha) = \mathbf{x}_0 + \alpha\mathbf{d} = [3 - 3\alpha,\ 1 - 5\alpha]^T$ and $f(\alpha) = (3 - 3\alpha)^2 + 5(1 - 5\alpha)^2$.



Basic Concept : Example

2. Find the slope $df(\alpha)/d\alpha)$ at $\alpha = 0$. Verify that this equal $\nabla f(\mathbf{x}_0)^T \mathbf{d}$ (direction derivative). We have

$$\left.\frac{df(\alpha)}{d\alpha}\right|_{\alpha=0} = (-6(3-3\alpha) - 50(1-5\alpha))|_{\alpha=0} = -68$$

$$\nabla f(\mathbf{x}_0)^T \mathbf{d} = \begin{bmatrix} 2(3) & 10(1) \end{bmatrix} \begin{bmatrix} -3 \\ -5 \end{bmatrix} = -68$$

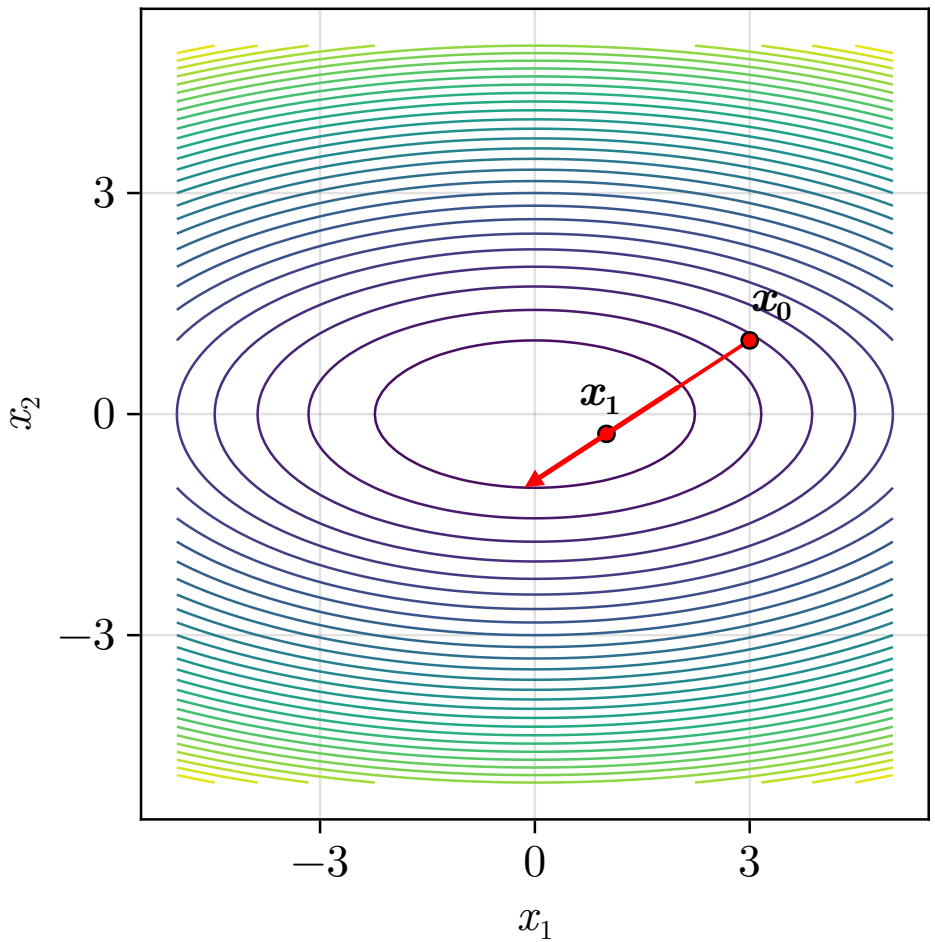
3. Minimize $f(\alpha)$ with respect to α, to obtain step size α_0. Given the corresponding new point $\mathbf{x}_1$ and value of $f_1 = f(\mathbf{x}_1)$. We have $df(\alpha)/d\alpha = 0$ or

$$\frac{df(\alpha)}{d\alpha} = -6(3-3\alpha) - 50(1-5\alpha) = 0 \Longrightarrow 268\alpha = 68 \text{ or } \alpha = 0.2537$$

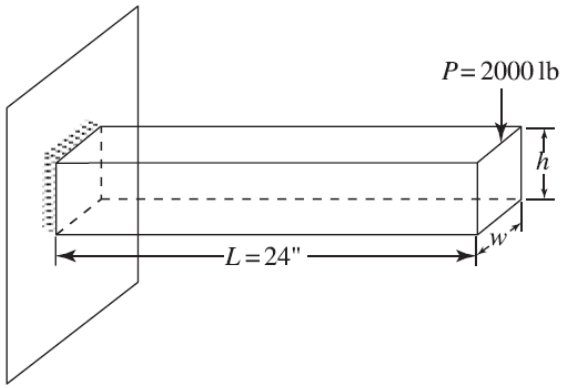
$$\mathbf{x}_1 = \begin{bmatrix} 3 \\ 1 \end{bmatrix} + \alpha_0 \begin{bmatrix} -3 \\ -5 \end{bmatrix} = \begin{bmatrix} 2.2388 \\ -0.2687 \end{bmatrix}, \; f(\mathbf{x}_1) = 5.3732, \text{ less than } f_0 = 14.$$

Basic Concept : Example

2. Provide a plot showing contours of the function, steepest descent direction x_0 and x_1.



Basic Concept : Example



We want to design the width and height of the rectangular cross-section to increase the bending stress defined by

$$\sigma_0 = \frac{6M}{wh^2}, \text{ where } M \text{ is a moment.}$$

With the initial design $\mathbf{x} = (w, h) = (1, 3)$, we have

$$\sigma_0 = \frac{6(2000 \times 24)}{1(3^2)} = 32,000\text{psi}$$

Using $\mathbf{d} = [-1/\sqrt{5} \ -2/\sqrt{5}]^T$ and $\alpha = 0.2$ we have

$$\mathbf{x}_1 = \mathbf{x}_0 + \alpha\mathbf{d} = \begin{bmatrix} 1 \\ 3 \end{bmatrix} + 0.2 \begin{bmatrix} -1/\sqrt{5} \\ -2/\sqrt{5} \end{bmatrix} = \begin{bmatrix} 0.9106 \\ 2.8211 \end{bmatrix}, \qquad \sigma_1 = 71,342 \text{ psi}$$

Gradient Descent Method

Gradient descent seeks to find a local minima of an objective function $f(\mathbf{x})$ by taking iterative steps in the negative gradient direction.

- The gradient of a function $\nabla f(\mathbf{x})$ determines the direction of locally steepest ascent, and so the negative gradient $-\nabla f(\mathbf{x})$ is the direction of locally steepest descent. The gradient algorithm is:

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \alpha \nabla f(\mathbf{x}_k)$$

  where α is the step size (learning rate)

- The method is based on a first-order Taylor series approximation of $f(\mathbf{x})$

$$f(\mathbf{x}) \approx f(\mathbf{x}_0) + \nabla f(\mathbf{x}_0)^T (\mathbf{x} - \mathbf{x}_0)$$

- There are two questions: stability and convergence of the algorithm.
- How to choose a good step size α. If α is too large, the iteration will be unstable or barely stable (overshoot the minimum, causing oscillations, or even divergence). If α is too small, the iteration will converge very slowly, making it ineffective for problems.

Gradient Descent Method: Fixed Step Size

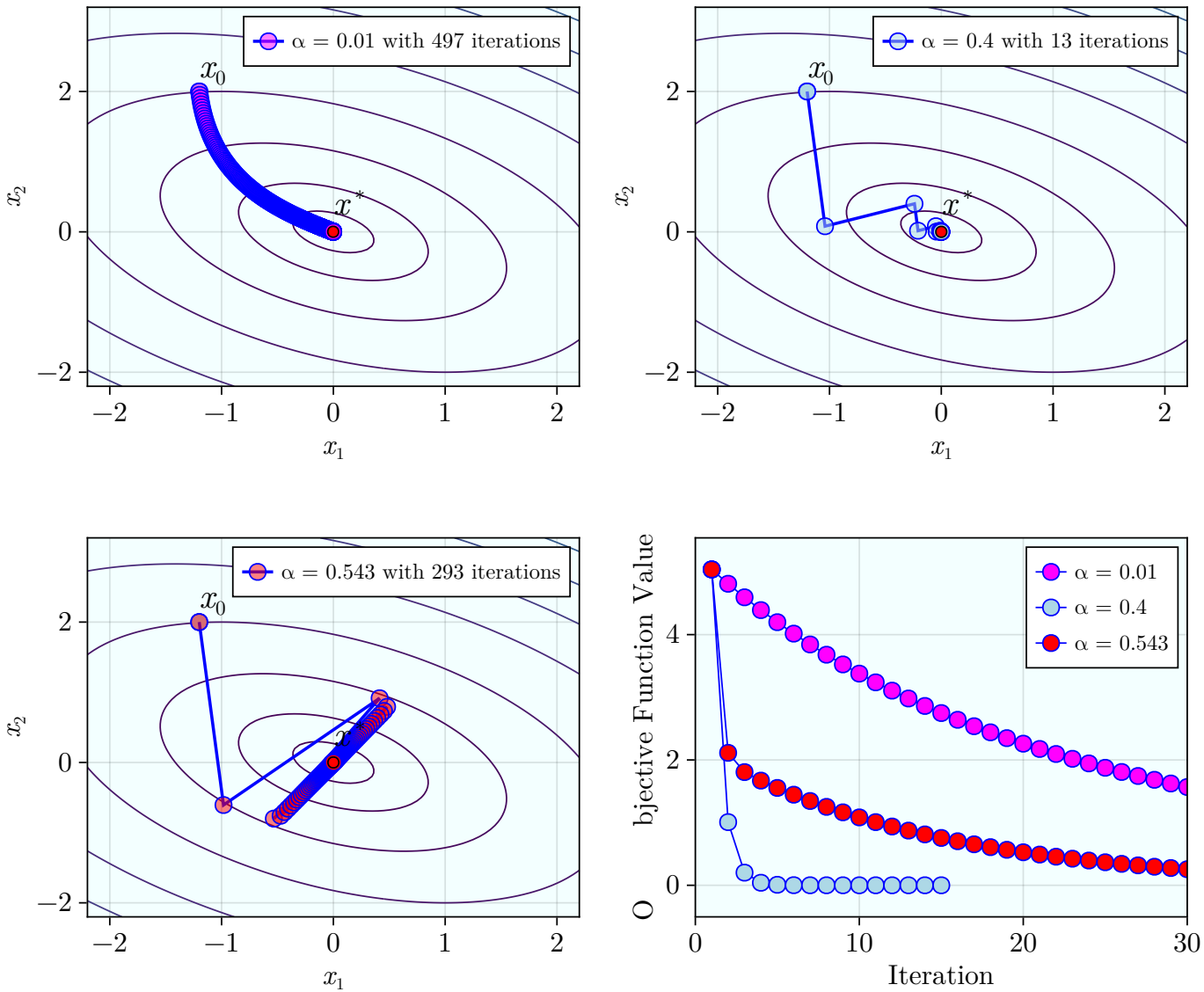
The simplest approach to determine the step-size α is fixed step size.

- A fixed step-size α is good for a convex objective function $f(\mathbf{x})$ with a well-conditioned Hessian $\nabla^2 f(\mathbf{x})$.
- We can show a simple example with quadratic objective to see the effect of the condition number of $\nabla^2 f(\mathbf{x})$ on a fixed-step gradient descent algorithm.
- Fixed-step schemes are simple, but may require tuning for adequate convergence.
- Consider an unconstrained optimization problem:

$$\underset{\mathbf{x}\in\mathbb{R}^2}{\text{minimize}} \quad \frac{1}{2}\mathbf{x}^T\mathbf{Q}\mathbf{x}, \mathbf{Q} = \begin{bmatrix} 2 & 1 \\ 1 & 3 \end{bmatrix}$$

  We will solve the problem, using the gradient descent method with $\alpha = 0.01, 0.06, 0.543$.

Gradient Descent Method: Fixed Step Size



Gradient Descent Method: Analysis

- After we have the direction vector $\mathbf{d}_k$ at the point $\mathbf{x}_k$. If we move along $\mathbf{d}_k$ the design variables and the objective function depend only on α as

$$\mathbf{x}(\alpha) = \mathbf{x}_k + \alpha \mathbf{d}_k, \qquad f(\alpha) = f(\mathbf{x}_k + \alpha \mathbf{d}_k)$$

$$\alpha_k = \underset{\alpha}{\text{arg minimize}} \; f(\mathbf{x}_k + \alpha_k \mathbf{d}_k) \quad \Longrightarrow \quad \frac{\partial f(\mathbf{x}_k + \alpha \mathbf{d}_k)}{\partial \alpha_k} = 0$$

The optimization above implies that the directional derivative equals zero:

$$\nabla f(\mathbf{x}_k + \alpha \mathbf{d}_k)^T \mathbf{d}_k = 0, \quad \mathbf{d}_{k+1} = -\nabla f(\mathbf{x}_k + \alpha \mathbf{d}_k)$$

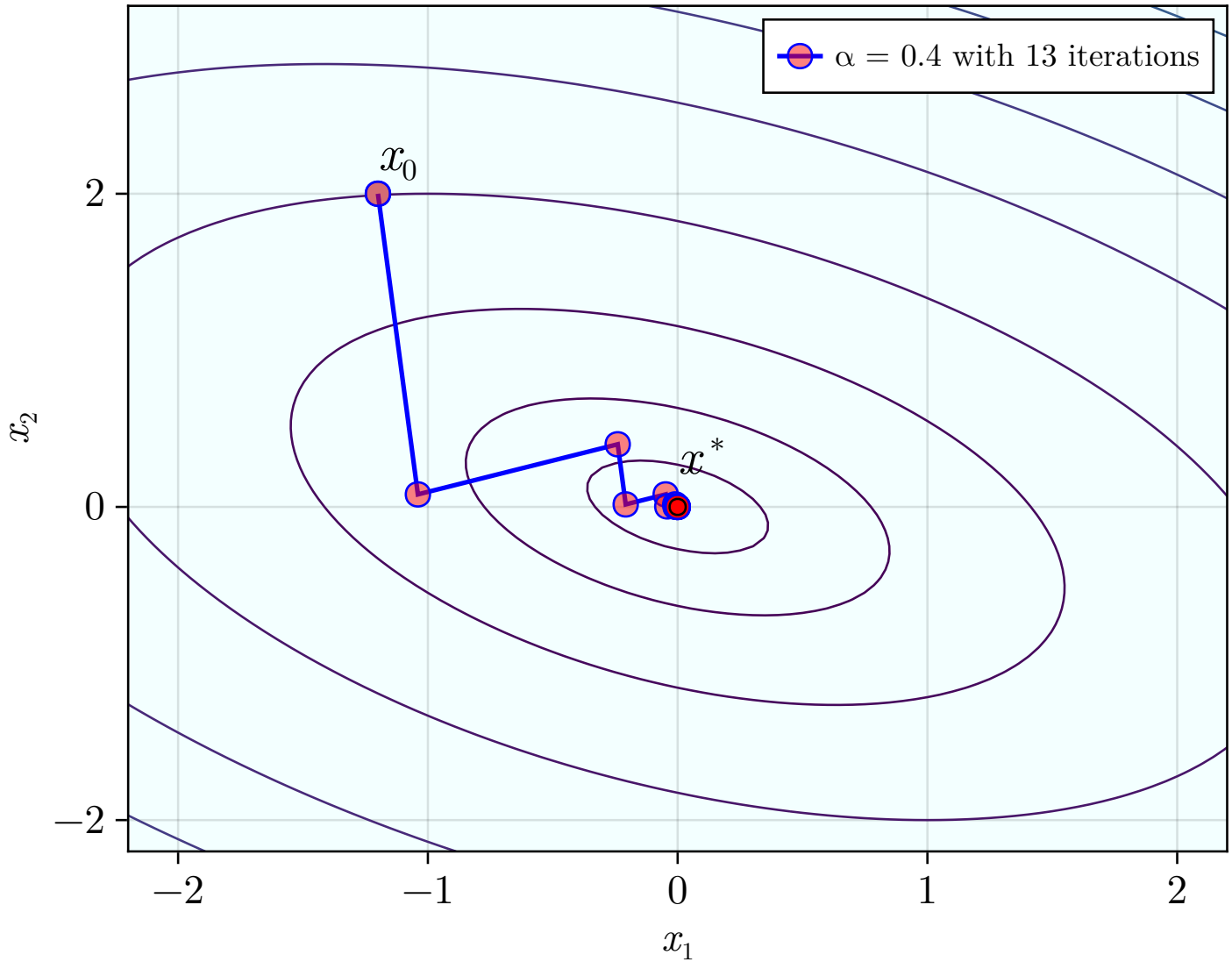
$$\mathbf{d}_{k+1}^T \mathbf{d}_k = 0, \quad \mathbf{d}_{k+1} \text{ and } \mathbf{d}_k \text{ are orthogonal. (source of zig-zags)}$$

- In the steepest descent method, the direction vector is $-\nabla f(\mathbf{x}_k)$ resulting in the slope at the current point $\alpha = 0$ being

$$\left. \frac{df(\alpha)}{d\alpha} \right|_{\alpha=0} = \nabla f(\mathbf{x}_k)^T (-\nabla f(\mathbf{x}_k)) = -\|\nabla f(\mathbf{x}_k)\|^2 < 0$$

Implying a move in a downhill direction.

Gradient Descent Method: Zig-Zags



The Steepest Descent Method: Stoping Criteria

- Starting from an initial point, we determine a direction vector and a step size, and obtain a new point as $\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k \mathbf{d}_k$.
- The question is to know when to stop the iterative process. We have two stop criteria to discuss here.
- **First** Befor performing the step-size, the necessary condition for optimality is checked:

$$\|\nabla f(\mathbf{x}_k)\| \leq \varepsilon_G,$$

  where ϵ_G is a tolerance on the gradient and is supplied by the user. This indicates you are near a stationary point.
- **Second:** We check the successive reductions in f as a criterion for stopping.

$$|f(\mathbf{x}_{k+1}) - f(\mathbf{x}_k)| \leq \varepsilon_A + \varepsilon_R |f(\mathbf{x}_k)|$$

  where $\varepsilon_A =$ absolute tolerance on the change in function value and $\varepsilon_R =$ relative tolerance. Only if the condition is satisfied for two consecutive iterations is the descent process stopped.

Gradient Descent Method: Fixed Step Size

Steepest Descent

Require: $\mathbf{x}_0, \varepsilon_G, \varepsilon_A, \varepsilon_R$

$k = 0$, N = max_number

while $k < N$ **do**

Compute $\nabla f(\mathbf{x}_k)$

if $\|\nabla f(x_k)\| \leq \varepsilon_G$ **then**

Stop

else if then

$\mathbf{d}_k = -\nabla f(\mathbf{x}_k)$

end if

$\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k \mathbf{d}_k$,

if $|f(\mathbf{x}_{k+1}) - f(\mathbf{x}_k)| \leq \varepsilon_A + \varepsilon_R |f(\mathbf{x}_k)|$ **then**

Stop

else

$k = k + 1$, $\mathbf{x}_k = \mathbf{x}_{k+1}$

end if

end while

Gradient Descent Method: Convergence

Definition: Lipschitz continuity

A function f is Lipschitz continuous with Lipschitz constant L if

$$|f(\mathbf{x}_1) - f(\mathbf{x}_2)| \leq L\|\mathbf{x}_1 - \mathbf{x}_2\| \quad \forall \mathbf{x}_1, \mathbf{x}_2$$

- If $f(\mathbf{x})$ is convex and Lipschitz continuous with Lipschitz constant L , then gradient descent with a step size $\alpha = 1/L$ is

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \frac{1}{L}\nabla f(\mathbf{x}_k)$$

- achieves the sublinear rate

$$f(\mathbf{x}_k) - f(\mathbf{x}^*) \leq \frac{L}{2k}\|\mathbf{x}_0 - \mathbf{x}^*\|^2, \quad k \geq 1$$

  Thus the convergence rate is $\mathcal{O}(1/k)$, i.e., sublinear in k. (the rate is slower than $\mathcal{O}(k)$)

Gradient Descent Method: Convergence

- If $f(\mathbf{x})$ is strongly convex, the convergence rate is improved. A function is called strongly convex if

$$f(\mathbf{y}) \geq f(\mathbf{x}) + \nabla f(\mathbf{x})^T(\mathbf{y}-\mathbf{x}) + \frac{\mu}{2}\|\mathbf{y}-\mathbf{x}\|^2, \qquad \mathbf{x},\mathbf{y} \in \mathbb{R}^2, \mu > 0$$

  In this case, the convergence rate is:

$$f(\mathbf{x}_k) = f(\mathbf{x}^*) \leq \frac{L}{2}\left(1-\frac{\mu}{L}\right)^k \|\mathbf{x}_0 - \mathbf{x}^*\|^2$$

Gradient Descent Method: Stability

- Consider a quadratic function $f(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T\mathbf{Q}\mathbf{x}$, where $\mathbf{Q} \in \mathbb{R}^{n\times n}$ is a symmetric positive definite matrix. The gradient is

$$\nabla f(\mathbf{x}) = \mathbf{Q}\mathbf{x} \quad \Longrightarrow \quad \mathbf{x}_{k+1} = \mathbf{x}_k - \alpha\mathbf{Q}\mathbf{x}_k = (\mathbf{I} - \alpha\mathbf{Q})\mathbf{x}_k$$

- Then the update rule is simply a discrete-time linear system is

$$\mathbf{x}_{k+1} = (\mathbf{I} - \alpha\mathbf{Q})\mathbf{x}_k = \mathbf{T}^{-1}(\mathbf{I} - \alpha\mathbf{Q})\mathbf{T} = \mathbf{I} - \alpha\mathbf{D}$$

- If $\mathbf{I} - \alpha\mathbf{D}$ is diagonal, then the eigenvalues of it is $1 - \alpha\lambda_i$. From the linear discrete-time system theory, the system is stable if $|1 - \alpha\lambda_i| < 1 \quad \forall i$. This may be rewritten as

$$-1 < 1 - \alpha\lambda_i < 1 \quad \Longrightarrow \quad -2 < -\alpha\lambda_i < 0 \quad \Longrightarrow 0 < \alpha < \frac{2}{\lambda_{\text{max}}}$$

Gradient Descent Method: Optimal Step Size

Now we want to determine an optimal step-size α for fastest convergence of the gradient descent algorithm.

- The optimal step size for gradient descent with a quadratic objective function is determined by the spectral radius of $(\mathbf{I} - \alpha\mathbf{Q})$, which is hte largest absolute eigenvalue:

$$\rho\left(\mathbf{I} - \alpha\mathbf{Q}\right) = \max_i |1 - \alpha\lambda_i|.$$

- To minimize the convergence rate, we choose α such that $\rho\left(\mathbf{I} - \alpha\mathbf{Q}\right)$ is as small as possible. (To get the largest α.)
- We set the optimal value at

$$|1 - \alpha\lambda_{\text{min}}| = |1 - \alpha\lambda_{\text{max}}| \implies 1 - \alpha^*\lambda_{\text{min}} = -(1 - \alpha^*\lambda_{\text{max}})$$

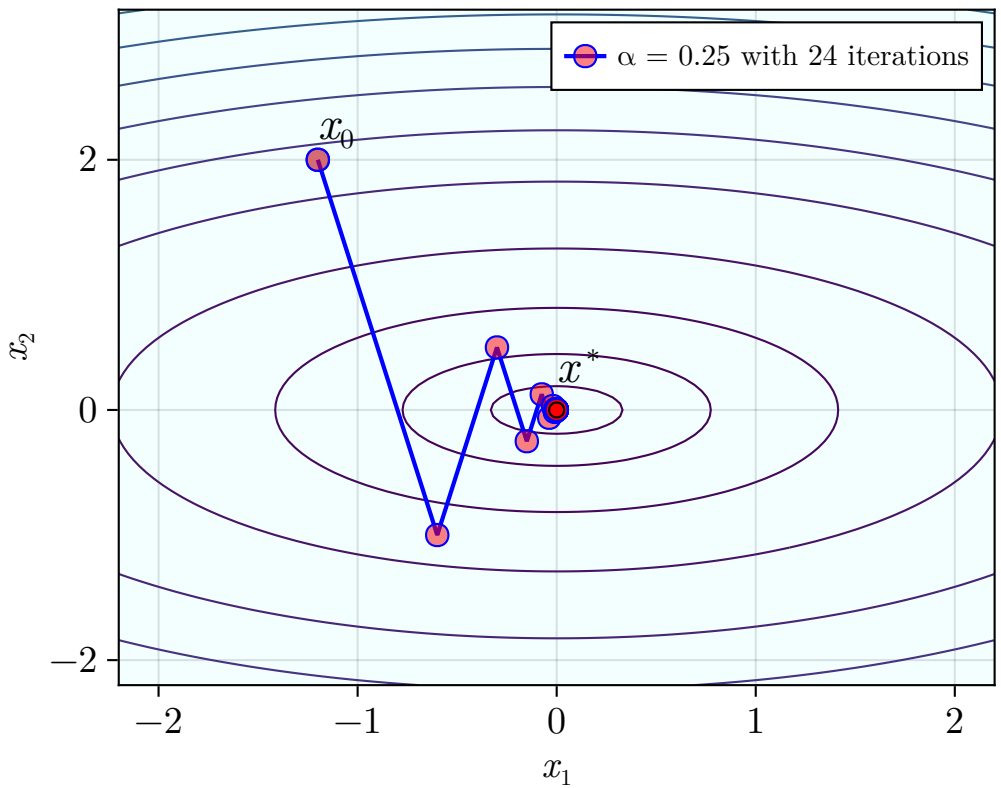
$$\alpha^* = \frac{2}{\lambda_{\text{min}} + \lambda_{\text{max}}}$$

- The best possible performance is limited by the ratio of eigenvalues

$$\kappa = \frac{\lambda_{\text{max}}}{\lambda_{\text{min}}}$$

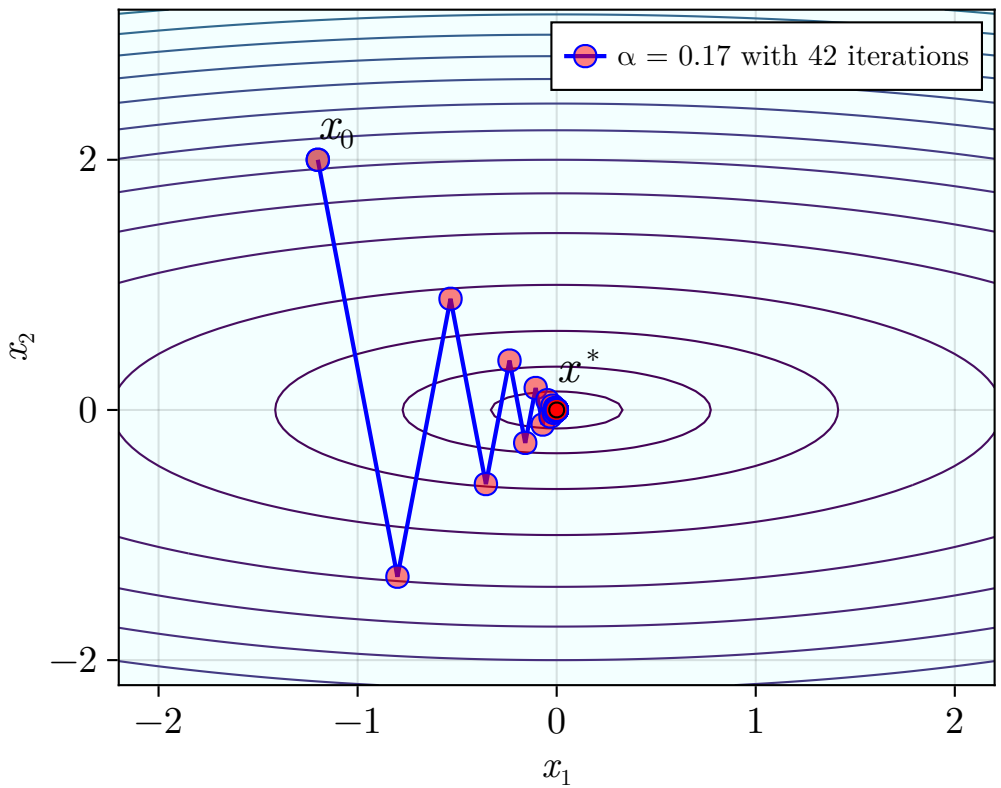
Gradient Descent Method: Optimal Step Size

$f(\mathbf{x}) = \frac{1}{2} x^T \begin{bmatrix} 2 & 0 \\ 0 & 2\gamma \end{bmatrix} x, \gamma = 3$. The Hessian $\nabla^2 f(\mathbf{x})$ is $\begin{bmatrix} 2 & 0 \\ 0 & 6 \end{bmatrix}$, then $\alpha = \frac{2}{8} = 0.25$



Gradient Descent Method: Optimal Step Size

$f(\mathbf{x}) = \frac{1}{2} x^T \begin{bmatrix} 2 & 0 \\ 0 & 2\gamma \end{bmatrix} x, \gamma = 5$. The Hessian $\nabla^2 f(\mathbf{x})$ is $\begin{bmatrix} 2 & 0 \\ 0 & 10 \end{bmatrix}$, then $\alpha = \frac{2}{12} = 0.167$



Gradient Descent Method: Optimal Step Size

Julia Code:

```
function gradient_descent(f,  f, x0; α=0.1, ε_G=1e-6, N=100)
    xgra = zeros(length(x0), N)
    xgra[:, 1] = x0

    for i in 2:N
        xgra[:, i] = xgra[:, i-1] - α *  f(xgra[:, i-1])
        if norm( f(xgra[:, i])) <= ε_G
            return xgra[:, 1:i]
        end
    end
    return xgra
end
#-------------------------------------------------
f(x) = x[1]^2 + 2x[2]^2
 f(x) = [2x[1], 4x[2]]
x0 = [1.0, 1.0]

result = gradient_descent(f,  f, x0)
```

Gradient Descent Method: Optimal Step Size

Matlab Code:

```
f = @(x1, x2) [x1; x2]' *[2 0; 0 2*2]*[x1; x2];   % gamma = 2
gf = matlabFunction(gradient(f(x1,x2),[x1,x2]));

N = 2000; X = zeros(N,2); EG = 1e-10; EA = 1e-10; ER = 1e-10; th0 = 1e-5;

X(1,:) = x0;
for k = 2:N
    % first criteria
    if norm(gf(x0(1), x0(2))) <= EG
        break;
    end
    % transpose to make a column vector
    alpha = 0.3
    % new point
    x0 = x0 - alpha*gf(x0(1), x0(2)))';
    X(k,:) = x0;

    % check second criteria
    nX = abs(fobj(X(k,:)) - fobj(X(k-1,:)));
    if  nX < EA + ER * abs(fobj(X(k-1,:)))
        break;
    end
end
```

Reference

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2. Alexander Mitsos, "*Applied Numerical Optimization*," Lecture Note RWTH AACHEN University
3. Ashok D. Belegundu, Tirupathi R. Chandrupatla, "Optimization Concepts and Applications in Engineering," Cambridge University Press, 2019