Optimization

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Math for CS, Fall 2023

References

The contents of this document are taken mainly from the follow sources:

- Kevin P. Murphy. Probabilistic Machine Learning: An Introduction. [1]

[1] https://probml.github.io/pml-book/book1.html

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Introduction

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- The term **objective function** refers to a function we want to maximize or minimize.
- An algorithm to find an optimum of an objective function is a **solver**.

Local versus global optimization

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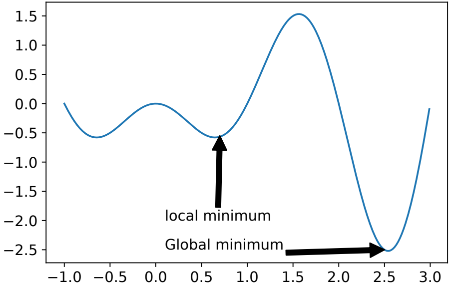
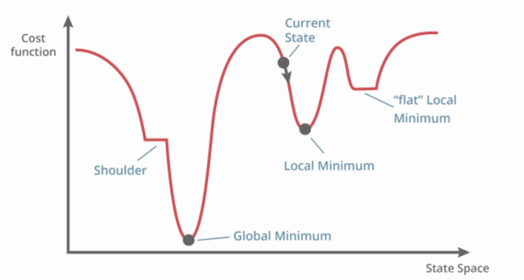
- In general, finding global optima is computationally intractable. We will try to find a local optimum.
- For continuous problem, a local optimum is a point $\boldsymbol{\theta}^*$ which has lower (or equal) cost than "nearby" points.

$$\exists \delta > 0, \forall \boldsymbol{\theta} \in \Theta, \quad \texttt{s.t.}\ \|\boldsymbol{\theta} - \boldsymbol{\theta}^*\| < \delta,\ \mathcal{L}(\boldsymbol{\theta}^*) \leq \mathcal{L}(\boldsymbol{\theta}) \tag{2}$$



Local versus global optimization

- A local minimum could be surrounded by other local minima with the same objective value; this is known as a **flat local minimum**.



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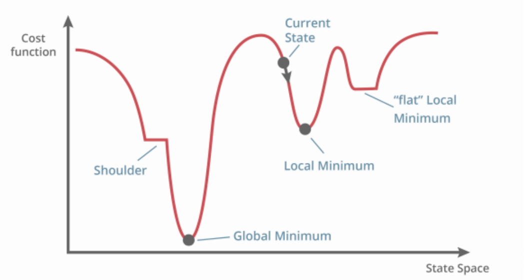

- A point is said to be a **strict local minimum** if its cost is strictly lower than those of neighboring points.

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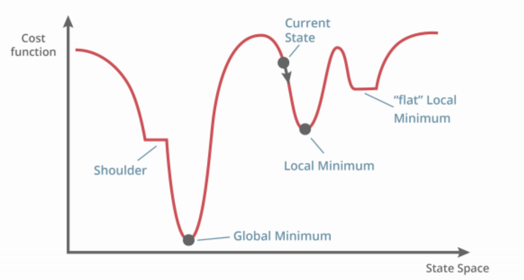

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- We can define a (strict) **local maximum** analogously.

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- Consider a scalar-argument function $f : \mathbb{R} \to \mathbb{R}$. Its **derivative** at a point a is the quantity

$$f'(x) \triangleq \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

assuming the limit exists.

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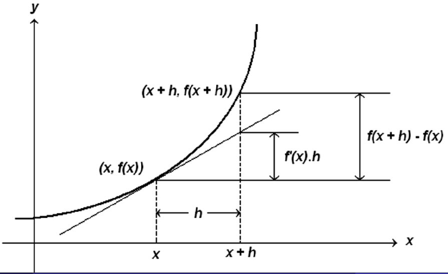
assuming the limit exists.
- This measures how quickly the output changes when we move a small distance in the input space away from x (i.e., the "rate of change").



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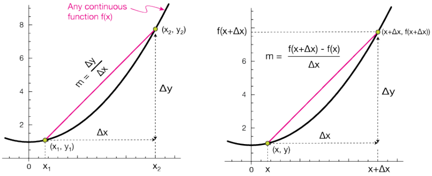
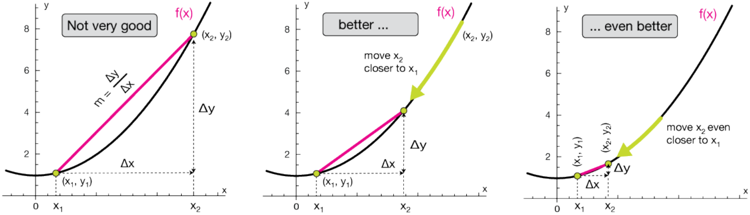


- $f'(x)$ can be seen as the slope of the tangent line at $f(x)$

$$f(x + \Delta x) \approx f(x) + f'(x)\Delta x$$

for small Δx.



Derivatives

- We can compute a **finite difference** approximation to the derivative by using a finite step size h

$$
\begin{aligned}
f'(x) &= \underbrace{\lim_{h\to 0} \frac{f(x+h)-f(x)}{h}}_{\text{forward difference}} \\
&= \underbrace{\lim_{h\to 0} \frac{f(x+h/2)-f(x-h/2)}{h}}_{\text{central difference}} \\
&= \underbrace{\lim_{h\to 0} \frac{f(x)-f(x-h)}{h}}_{\text{backward difference}}
\end{aligned}
$$

- The smaller the step size h, the better the estimate.

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- We can use **Leibniz notation**, if we denote the function by $y = f(x)$, and its derivative by $\frac{dy}{dx}$ or $\frac{d}{dx}f(x)$.
- To denote the evaluation of the derivative at a point a, we write $\left.\frac{df}{dx}\right|_{x=a}$.

Gradients

- We extend the notion of derivatives to handle vector-argument functions, $f:\ \mathbb{R}^n \to \mathbb{R}$, by defining the **partial derivative** of f with respect to x_i to be

$$\frac{\partial f}{\partial x_i} = \lim_{h\to 0} \frac{f(\boldsymbol{x} + h\boldsymbol{e}_i) - f(\boldsymbol{x})}{h}$$

  where $\boldsymbol{e}_i$ is the i'th unit vector, $\boldsymbol{e}_i = (0, \ldots, 1, \ldots, 0)$ with the i'th element $=$ 1 and all the other elements are 0.

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- The **gradient** of f at a point $\boldsymbol{x}$ is the vector of its partial derivatives

$$\boldsymbol{g} = \frac{\partial f}{\partial \boldsymbol{x}} = \nabla f = \begin{pmatrix} \frac{\partial f}{\partial x_1} \\ \vdots \\ \frac{\partial f}{\partial x_n} \end{pmatrix} = \frac{\partial f}{\partial x_1}\boldsymbol{e}_1 + \ldots + \frac{\partial f}{\partial x_n}\boldsymbol{e}_n$$

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- To emphasize the point at which the gradient is evaluated, we write

$$\boldsymbol{g}(\boldsymbol{x}^*) \triangleq \left.\frac{\partial f}{\partial \boldsymbol{x}}\right|_{\boldsymbol{x}^*}$$

Gradients

- Example:

$$f(x_1, x_2) = x_1^2 + x_1 x_2 + 3x_2^2$$

$$\nabla f(x_1, x_2) = \begin{pmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{pmatrix} = \begin{pmatrix} 2x_1 + x_2 \\ x_1 + 6x_2 \end{pmatrix}$$

- The nabla operator ∇ maps a function $f : \mathbb{R}^n \to \mathbb{R}$ to another function $\boldsymbol{g} : \mathbb{R}^n \to \mathbb{R}^n$.
- Since $\boldsymbol{g}()$ is a vector-valued function, it is known as a vector field.

Directional derivative

- The **directional derivative** measures how much the function $f: \mathbb{R}^n \to \mathbb{R}$ changes along a direction $\boldsymbol{v}$ in space.

$$D_{\boldsymbol{v}} f(\boldsymbol{x}) = \lim_{h \to 0} \frac{f(\boldsymbol{x} + h\boldsymbol{v}) - f(\boldsymbol{x})}{h}$$

- We can approximate this numerically using 2 function calls to f, regardless of n.
- By contrast, a numerical approximation to the standard gradient vector takes $n + 1$ calls (or $2n$ if using central differences).
- The directional derivative along $\boldsymbol{v}$ is the scalar product of the gradient $\boldsymbol{g}$ and the vector $\boldsymbol{v}$:

$$D_{\boldsymbol{v}} f(\boldsymbol{x}) = \nabla f(\boldsymbol{x}) \cdot \boldsymbol{v}$$

Directional derivative

Example: Let $f(x, y) = x^2 y$. Find the derivative of f in the direction (1,2) at the point (3,2).

- The gradient $\nabla f(x, y)$ is:

$$\nabla f(x, y) = \begin{pmatrix} \frac{\partial f}{\partial x} \\ \frac{\partial f}{\partial y} \end{pmatrix} = \begin{pmatrix} 2xy \\ x^2 \end{pmatrix}$$

$$\nabla f(3, 2) = \begin{pmatrix} 12 \\ 9 \end{pmatrix} = 12 \begin{pmatrix} 1 \\ 0 \end{pmatrix} + 9 \begin{pmatrix} 0 \\ 1 \end{pmatrix} = 12\boldsymbol{e}_1 + 9\boldsymbol{e}_2$$

- Let $\boldsymbol{u} = u_1\boldsymbol{e}_1 + u_2\boldsymbol{e}_2$ be a unit vector. The derivative of f in the direction of $\boldsymbol{u}$ at (3,2) is:

$$\begin{aligned} D_{\boldsymbol{u}} f(3, 2) &= \nabla f(3, 2) \cdot \boldsymbol{u} \\ &= (12\boldsymbol{e}_1 + 9\boldsymbol{e}_2) \cdot (u_1\boldsymbol{e}_1 + u_2\boldsymbol{e}_2) \\ &= 12u_1 + 9u_2 \end{aligned}$$

Directional derivative

Example (cont.)

- The unit vector in the direction of vector (1,2) is:

$$\boldsymbol{u} = \frac{(1,2)}{\|(1,2)\|} = \frac{(1,2)}{\sqrt{1^2+2^2}} = \frac{(1,2)}{\sqrt{5}} = (1/\sqrt{5}, 2/\sqrt{5})$$

- The directional derivative at (3,2) in the direction of (1,2) is:

$$\begin{aligned} D_{\boldsymbol{u}} f(3,2) &= 12u_1 + 9u_2 \\ &= \frac{12}{\sqrt{5}} + \frac{18}{\sqrt{5}} = \frac{30}{\sqrt{5}} \end{aligned}$$

- We normalize vector (1,2) so that the directional derivative is independent of its magnitude and depending only on its direction.

Directional derivative

Example 2: Let $f(x, y) = x^2y$. Find the derivative of f in the direction of (2,1) at the point (3,2).

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- The unit vector in the direction of (2,1) is:

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- The directional derivative of f at (3,2) in the direction of (2,1) is:

$$\begin{aligned} D_{\boldsymbol{u}} f(3,2) &= 12u_1 + 9u_2 \\ &= \frac{24}{\sqrt{5}} + \frac{9}{\sqrt{5}} = \frac{33}{\sqrt{5}} \end{aligned}$$

Directional derivative

Questions:

- At a point $\boldsymbol{a}$, in which direction $\boldsymbol{u}$ is the directional derivative $D_{\boldsymbol{u}} f(\boldsymbol{a})$ maximal?
- What is the directional derivative in that direction $D_{\boldsymbol{u}} f(\boldsymbol{a}) =?$

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The relationship between the gradient and the directional derivative:

$$\begin{aligned} D_{\boldsymbol{u}} f(\boldsymbol{a}) &= \nabla f(\boldsymbol{a}) \cdot \boldsymbol{u} \\ &= \|\nabla f(\boldsymbol{a})\| \|\boldsymbol{u}\| \cos\theta \quad [\theta \text{ is the angle between } \boldsymbol{u} \text{ and the gradient.}] \\ &= \|\nabla f(\boldsymbol{a})\| \cos\theta \quad [\boldsymbol{u} \text{ is a unit vector.}] \end{aligned}$$

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The maximal value of $D_{\boldsymbol{u}}f(\boldsymbol{a})$ occurs when $\boldsymbol{u}$ and $\nabla f(\boldsymbol{a})$ point in the same direction (i.e., $\theta = 0$).

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$$

- When $\theta = 0$, the directional derivative $D_{\boldsymbol{u}} f(\boldsymbol{a}) = \|\nabla f(\boldsymbol{a})\|$.
- When $\theta = \pi$, the directional derivative $D_{\boldsymbol{u}} f(\boldsymbol{a}) = -\|\nabla f(\boldsymbol{a})\|$.
- For what value of θ is $D_{\boldsymbol{u}} f(\boldsymbol{a}) = 0$?

Jacobian

- Consider a function that maps a vector to another vector, $\boldsymbol{f}: \mathbb{R}^n \to \mathbb{R}^m$. The **Jacobian matrix** of this function is an $m \times n$ matrix of partial derivatives:

$$\boldsymbol{J}_{\boldsymbol{f}}(\boldsymbol{x}) = \frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}^\mathsf{T}} \triangleq \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_m}{\partial x_1} & \cdots & \frac{\partial f_m}{\partial x_n} \end{pmatrix} = \begin{pmatrix} \nabla f_1(\boldsymbol{x})^\mathsf{T} \\ \vdots \\ \nabla f_m(\boldsymbol{x})^\mathsf{T} \end{pmatrix}$$

- We layout the results in the same orientation as the output $\boldsymbol{f}$. This is called the numerator layout of the Jacobian formulation.

Hessian

- For a function $f : \mathbb{R}^n \to \mathbb{R}$ that is twice differentiable, the **Hessian matrix** is the (symmetric) $n \times n$ matrix of second partial derivatives

$$\boldsymbol{H}_f = \frac{\partial^2 f}{\partial \boldsymbol{x}^2} = \nabla^2 f = \begin{pmatrix} \frac{\partial^2 f}{\partial x_1^2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{pmatrix}$$

- The Hessian is the Jacobian of the gradient.

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Example: Find the Hessian of $f(x, y) = x^2y + y^2x$ at the point (1,1).

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- Second, compute the Hessian (i.e., second-order partial derivatives):

$$\boldsymbol{H}_f(x, y) = \begin{pmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x \partial y} \\ \frac{\partial^2 f}{\partial y \partial x} & \frac{\partial^2 f}{\partial y^2} \end{pmatrix} = \begin{pmatrix} 2y & 2x + 2y \\ 2x + 2y & 2x \end{pmatrix}$$

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- Finally, evaluate the Hessian matrix at the point (1,1):

$$\boldsymbol{H}_f(1,1) = \begin{pmatrix} 2 & 4 \\ 4 & 2 \end{pmatrix}$$

Geometric meaning

- If we follow the direction $\boldsymbol{d}$ from $\boldsymbol{x}$, we can define a uni-dimensional function $g(\alpha)$:

$$g(\alpha) = f(\boldsymbol{x} + \alpha \boldsymbol{d})$$
$$g'(\alpha) = \boldsymbol{d}^{\mathsf{T}} \nabla f(\boldsymbol{x} + \alpha \boldsymbol{d})$$
$$g''(\alpha) = \boldsymbol{d}^{\mathsf{T}} \nabla^2 f(\boldsymbol{x} + \alpha \boldsymbol{d}) \boldsymbol{d}$$

- Interpretation

$$g'(0) = \boldsymbol{d}^{\mathsf{T}} \nabla f(\boldsymbol{x}) \quad \texttt{[directional derivative]}$$
$$g''(0) = \boldsymbol{d}^{\mathsf{T}} \nabla^2 f(\boldsymbol{x}) \boldsymbol{d} \quad \texttt{[directional curvature]}$$

- If $g''(0)$ is non-negative with a certain $\boldsymbol{d}$: f is convex in direction $\boldsymbol{d}$.
- If $g''(0)$ is non-negative for all $\boldsymbol{d}$: $\nabla^2 f(\boldsymbol{x})$ is positive semidefinite $\rightarrow f$ is convex at $\boldsymbol{x}$.

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Definitions

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- positive semidefinite $(A \succeq 0)$ if $\boldsymbol{x}^\mathsf{T} A\boldsymbol{x} \geq 0$ for all $\boldsymbol{x}$,
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- The expression $\boldsymbol{x}^\mathsf{T} A \boldsymbol{x}$ is a function of $\boldsymbol{x}$ called the quadratic form associated to A. (It's made up of terms like x_i^2 and $x_i x_j$.)
- We make these definitions for a symmetric matrix A, i.e., $A^\mathsf{T} = A$.
- Hessian matrices are symmetric.

Diagonal matrices

For a diagonal matrix

$$D = \begin{bmatrix} d_1 & 0 & \dots & 0 \\ 0 & d_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \vdots & d_n \end{bmatrix}$$

the quadratic form

$$\boldsymbol{x}^\mathsf{T} D\boldsymbol{x} = \begin{bmatrix} x_1 & x_2 & \dots & x_n \end{bmatrix} \begin{bmatrix} d_1 & 0 & \dots & 0 \\ 0 & d_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \vdots & d_n \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$

is just $d_1x_1^2 + d_2x_2^2 + \ldots + d_nx_n^2$.

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- If $d_1, \ldots, d_n$ are all nonnegative, then $d_1 x_1^2 + d_2 x_2^2 + \ldots + d_n x_n^2$ must be nonnegative for any $\boldsymbol{x}$, so $D \succeq 0$: D is positive semidefinite.

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- So, $\boldsymbol{H}_f(x, y) \succ 0$ for all $(x, y) \in \mathbb{R}^2$. $\boldsymbol{H}_f(x, y)$ is positive definite.

Positive definiteness and eigenvalues

- For an $n \times n$ matrix A, if a nonzero vector $\boldsymbol{x} \in \mathbb{R}^n$ satisfies

$$A\boldsymbol{x} = \lambda\boldsymbol{x}$$

  for some scalar $\lambda \in \mathbb{R}$, we call λ an eigenvalue of A and $\boldsymbol{x}$ its associated eigenvector.

- If A is an $n \times n$ symmetric matrix, then it can be factored as

$$A = Q^{\mathsf{T}}\Lambda Q = Q^{\mathsf{T}} \begin{bmatrix} \lambda_1 & 0 & \dots & 0 \\ 0 & \lambda_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \vdots & \lambda_n \end{bmatrix} Q$$

  where $\lambda_1, \dots, \lambda_n$ are the eigenvalues of A and the columns of Q are the corresponding eigenvectors.

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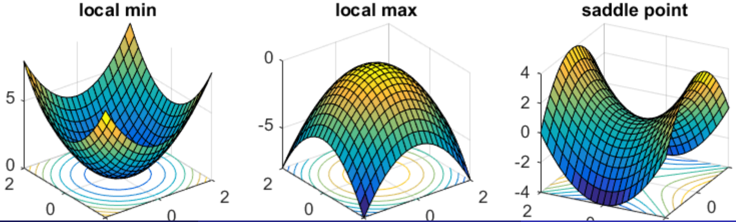
   - Why a zero gradient is not sufficient?
   - The stationary point could be a local minimum, local maximum, or **saddle** point.



Global optimizers

- We classify a stationary point of a function $f : \mathbb{R}^n \to \mathbb{R}$ as a global minimizer if the Hessian matrix of f is positive semidefinite **everywhere**,
- and as a global maximizer if the Hessian matrix is negative semidefinite everywhere.
- If the Hessian matrix is positive definite, or negative definite, the minimizer and maximizer (respectively) is strict.

Example

Let $f(x_1, x_2) = (x_1^2 + x_2^2 - 1)^2 + (x_2^2 - 1)^2$.

- The gradient is $\nabla f(\boldsymbol{x}) = 4 \begin{pmatrix} (x_1^2 + x_2^2 - 1)x_1 \\ (x_1^2 + x_2^2 - 1)x_2 + (x_2^2 - 1)x_2 \end{pmatrix}$

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- Since $\nabla^2 f(0,0) = 4 \begin{pmatrix} -1 & 0 \\ 0 & -2 \end{pmatrix} \prec 0$, it follows that (0,0) is a strict local maximum point.

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- The Hessian is $\nabla^2 f(\boldsymbol{x}) = 4 \begin{pmatrix} 3x_1^2 + x_2^2 - 1 & 2x_1x_2 \\ 2x_1x_2 & x_1^2 + 6x_2^2 - 2 \end{pmatrix}$
- Since $\nabla^2 f(0,0) = 4 \begin{pmatrix} -1 & 0 \\ 0 & -2 \end{pmatrix} \prec 0$, it follows that (0,0) is a strict local maximum point.
- By the fact that $f(x_1, 0) = (x_1^2 - 1)^2 + 1 \to \infty$ as $x_1 \to \infty$, the function is not bounded above, and thus (0,0) is not a global maximum point.

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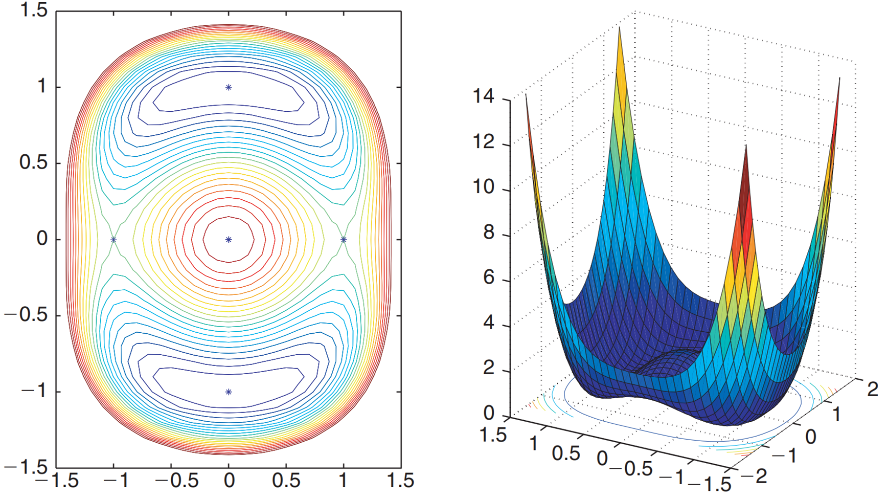
- Because there are two global minimum points, they are **nonstrict** global minima, but they are **strict** local minimum points, since each has a neighborhood in which it is the unique minimizer.

Example



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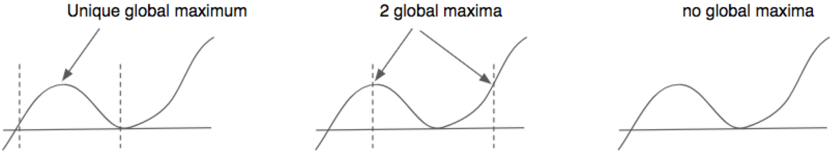

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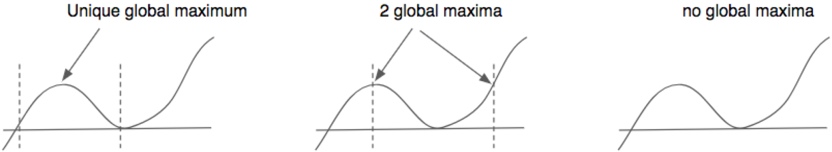

- The task of finding any point (regardless of its cost) in the feasible set is called **feasibility problem**.

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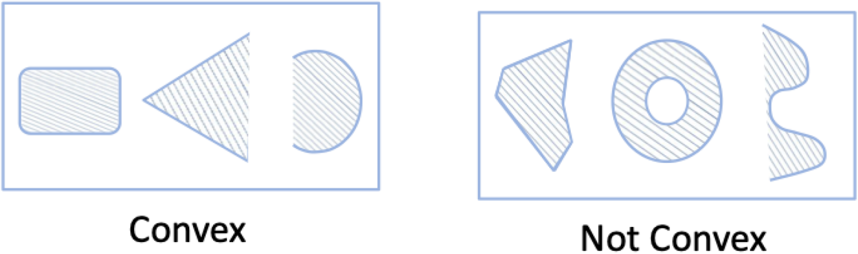
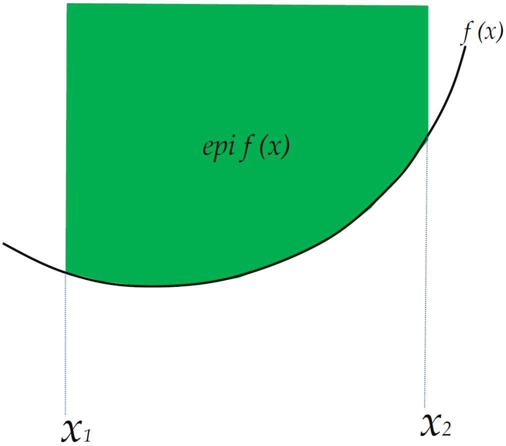
- If we draw a line from $\boldsymbol{x}$ to $\boldsymbol{x}'$, all points on the line lie inside the set.



Convex functions

- f is a **convex function** if its **epigraph** (the set of points above the function) defines a convex set.



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- $f(\boldsymbol{x})$ is called a convex function if it is defined on a convex set, and if, for any $\boldsymbol{x}, \boldsymbol{y} \in \mathcal{S}$, and for any $0 \leq \lambda \leq 1$, we have:

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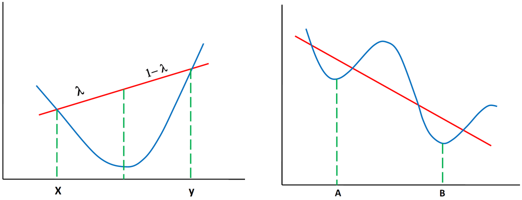

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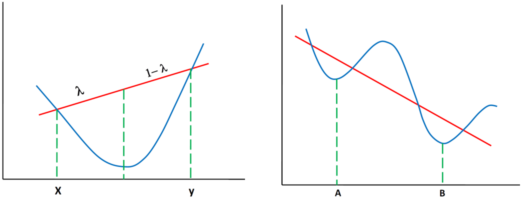

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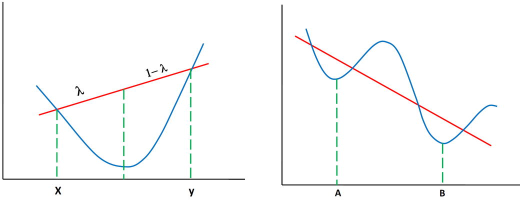

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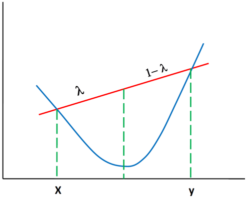

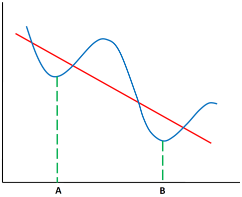

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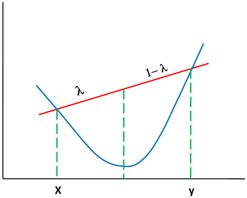

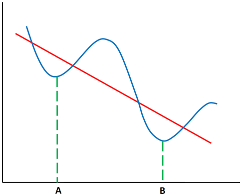

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- Some examples of $1d$ convex functions: x^2, e^{ax}, $-\log(x)$, $x^a(a>1, x>0)$, $|x|^a(a \geq 1)$, $x \log x (x > 0)$.

Convex functions

Theorem

Suppose $f: \mathbb{R}^n \to \mathbb{R}$ *is twice differentiable over its domain. Then* f *is convex iff* $\boldsymbol{H} = \nabla^2 f(\boldsymbol{x})$ *is positive semi-definite for all* $\boldsymbol{x} \in \mathtt{dom}(f)$*. Furthermore,* f *is strictly convex if* $\boldsymbol{H}$ *is positive definite.*

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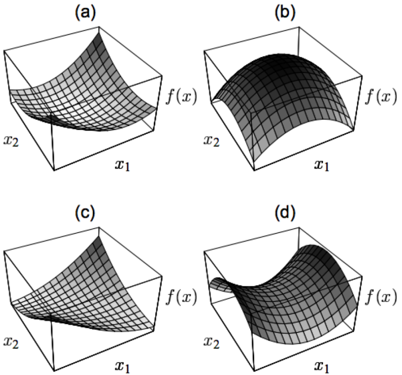
- Intuitively, a convex function is shaped like a bowl.

Convex functions



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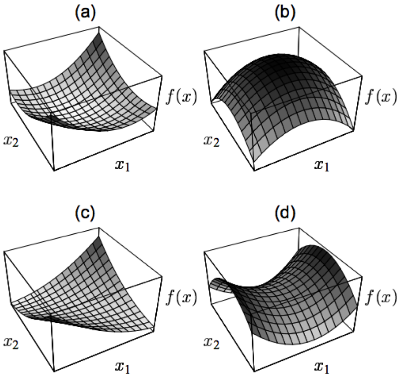

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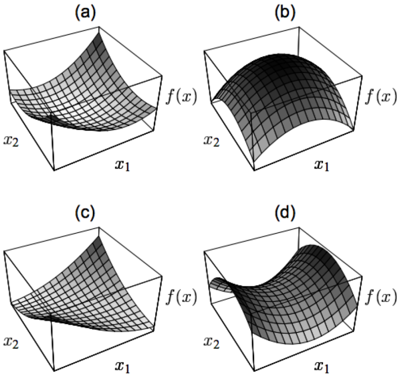

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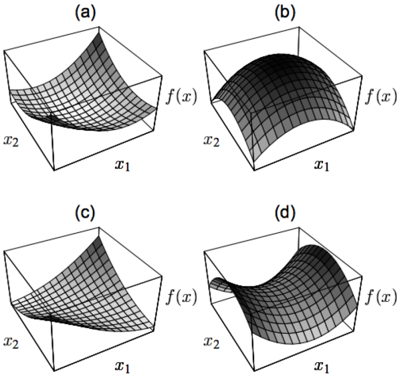

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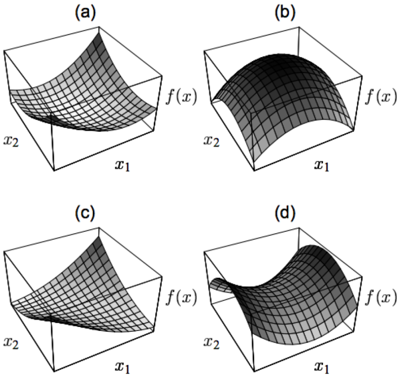

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$$\boldsymbol{g}_t \triangleq \nabla \mathcal{L}(\boldsymbol{\theta})|_{\boldsymbol{\theta}_t} = \nabla \mathcal{L}(\boldsymbol{\theta}_t) = \boldsymbol{g}(\boldsymbol{\theta}_t)$$

  points in the direction of maximal increase in f, so the negative gradient is a descent direction.

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- Any direction $\boldsymbol{d}$ is also a descent direction if the angle θ between $\boldsymbol{d}$ and $-\boldsymbol{g}_t$ is less than 90 degrees and satisfies

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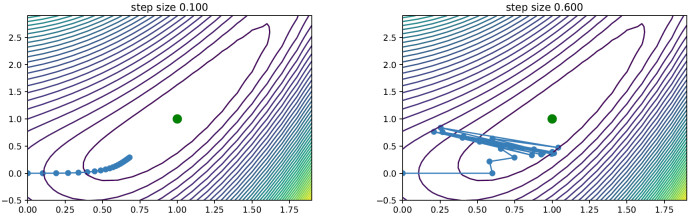
- The sequence of step sizes $\{\rho_t\}$ is called the **learning rate schedule**.
- The simplest method is to use constant step size, $\rho_t = \rho$.
- However, if it is too large, the method may fail to converge. If it is too small, the function will converge but very slowly.
- Example:

$$\mathcal{L}(\boldsymbol{\theta}) = 0.5(\theta_1^2 - \theta_2)^2 + 0.5(\theta_1 - 1)^2$$

- Pick our descent direction $\boldsymbol{d}_t = -\boldsymbol{g}_t$. Consider $\rho_t = 0.1$ vs $\rho_t = 0.6$:



- The **optimal step size** can be found by finding the value that maximally decreases the objective along the chosen direction by solving the $1d$ minimization problem

$$\rho_t = \operatorname*{argmin}_{\rho>0} \phi_t(\rho) = \operatorname*{argmin}_{\rho>0} \mathcal{L}(\boldsymbol{\theta}_t + \rho \boldsymbol{d}_t)$$

- This is **line search**: we are searching along the line defined by $\boldsymbol{d}_t$.
- $\phi_t(\rho) = \mathcal{L}(\boldsymbol{\theta}_t + \rho \boldsymbol{d}_t)$ is a convex function of an affine function of ρ, for fixed $\boldsymbol{\theta}_t$ and $\boldsymbol{d}$.
- If the loss is convex, this subproblem is also convex.

- Example, consider the quadratic loss

$$\mathcal{L}(\boldsymbol{\theta}) = \frac{1}{2}\boldsymbol{\theta}^\top \boldsymbol{A}\boldsymbol{\theta} + \boldsymbol{b}^\top \boldsymbol{\theta} + c$$

- Compute the derivatives of $\phi(\rho) = \mathcal{L}(\boldsymbol{\theta} + \rho \boldsymbol{d})$ gives

$$\begin{aligned} \frac{d\phi(\rho)}{d\rho} &= \frac{d}{d\rho}\left[\frac{1}{2}(\boldsymbol{\theta} + \rho\boldsymbol{d})^\top \boldsymbol{A}(\boldsymbol{\theta} + \rho\boldsymbol{d}) + \boldsymbol{b}^\top(\boldsymbol{\theta} + \rho\boldsymbol{d}) + c\right] \\ &= \boldsymbol{d}^\top \boldsymbol{A}(\boldsymbol{\theta} + \rho\boldsymbol{d}) + \boldsymbol{d}^\top \boldsymbol{b} \\ &= \boldsymbol{d}^\top(\boldsymbol{A}\boldsymbol{\theta} + \boldsymbol{b}) + \rho \boldsymbol{d}^\top \boldsymbol{A}\boldsymbol{d} \end{aligned}$$

- Solving for $\frac{d\phi(\rho)}{d\rho} = 0$ gives

$$\rho = -\frac{\boldsymbol{d}^\top(\boldsymbol{A}\boldsymbol{\theta} + \boldsymbol{b})}{\boldsymbol{d}^\top \boldsymbol{A}\boldsymbol{d}}$$

- This is **exact line search**. There are several methods, such as **Armijo backtracking method**, that try to ensure reduction in the objective function without spending too much time trying to solve this subproblem precisely.