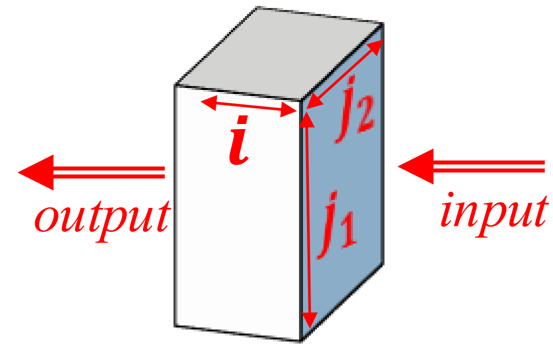
Tensors

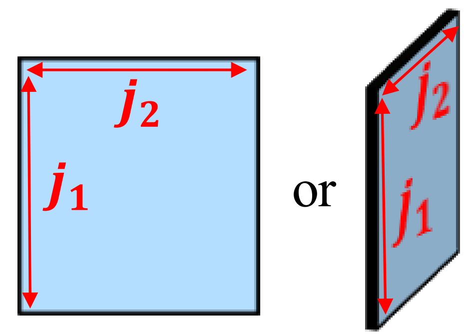
- Contravariant and covariant tensors
- Einstein notation
- Interpretation

What is a Tensor?

- It is the generalization of a:
  - Matrix operator for >2 dimensions



  - Vector data to >1 dimension

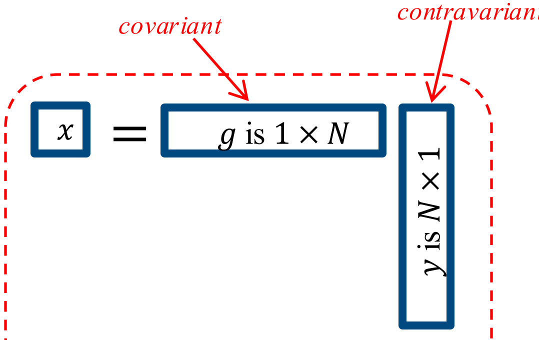


- Why do we need it?
  - Came out of differential geometry.
  - Was used by Albert Einstein to formulate the theory of General Relativity.
  - It's useful for many problems, including Deep NNs.

Contravariant and Covariant Vectors

$$x = gy$$

- Contravariant vectors:
  - "Column Vectors" that represent data
  - Vectors that describe the position of something
  - y^j for $0 \leq j < N$ and $x \in \Re$
- Covariant vector:
  - "Row vectors" that operate on data
  - Gradient vectors
  - g_j for $0 \leq j < N$



Picture of multiplication

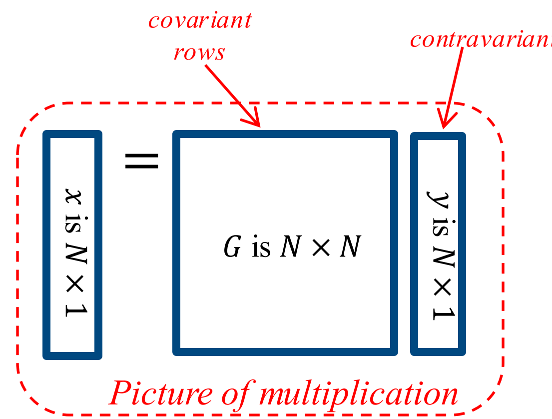
- Einstein notation

$$x = g_j\, y^j = \sum_{j=0}^{N-1} g_j\, y^j$$

  - Leave out the sum to make notation cleaner
  - Always sum over any two indices that appear twice

Vector-Matrix Products as Tensors

$$x = Gy$$



- Rank 1 Contravariant vectors:
  - y^j for $0 \le j < N_y$
  - x^j for $0 \le j < N_x$
- Rank 2 tensor (i.e., matrix):
  - $G^i{}_j$ for $0 \le i < N_x$ and $0 \le j < N_y$
  - There is a gradient for each component x^i
- Einstein notation

$$x^i = G^i{}_j\, y^j = \sum_{j=0}^{N_y - 1} G^i{}_j\, y^j$$

  - Leave out the sum to make notation cleaner
  - Always sum over any two indices that appear twice

Tensor Products

- Einstein notation

Sum over pairs of indices

$$x^{i_1,i_2} = G^{i_1,i_2}{}_{\boxed{j_1,j_2}}\, y^{\boxed{j_1,j_2}}$$

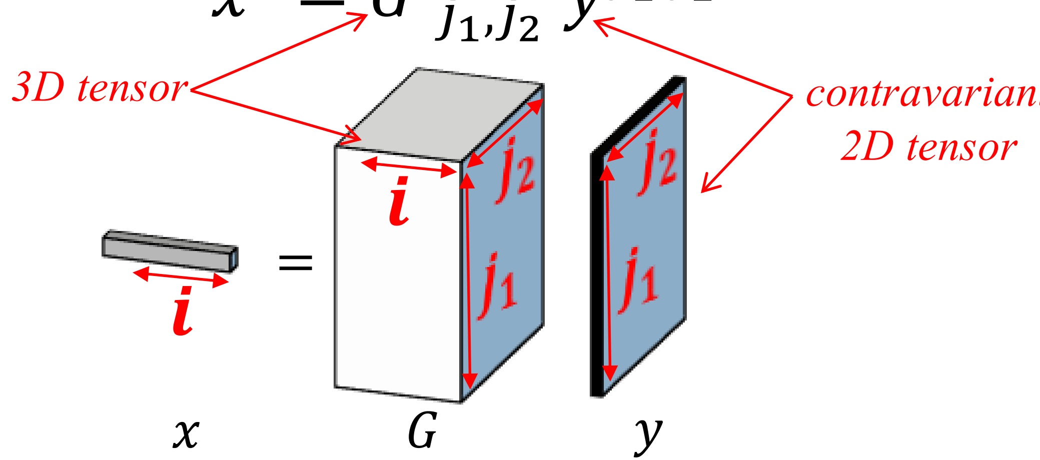
- 2-D Contravariant Tensors:
  - y^{j_1,j_2} for $0 \le j_1, j_2 < N_y$
  - x^{i_1,i_2} for $0 \le i_1, i_2 < N_x$

- 4-D Tensor:
  - $G^{i_1,i_2}{}_{j_1,j_2}$ for $0 \le i_1, i_2 < N_x$ and $0 \le j_1, j_2 < N_y$
  - G is known as a tensor
    - 2D covariant input
    - 2D contravariant output

Picture of a Tensor Product

- For example, if we have

$$x^i = G^i{}_{j_1,j_2}\, y^{j_1,j_2}$$



  – Tensor 3-D tensor G has

    Input: 2D image indexed by (j_1, j_2)

    Output: 1D vector indexed by i

  – General idea: $G \in \Re^{N_o \times N_i}$

Some Useful Definitions

- Delta functions:

$$\delta^i{}_j = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}$$

  - So then we have that

$$G^k{}_j = G^k{}_i \, \delta^i{}_j$$

- Gradient w.r.t. vector

$$\nabla_y (Ay) = A$$

  - In tensor notation, we have that

$$\left[\nabla_y (Ay)\right]^i{}_j = A^i{}_j$$

- Gradient w.r.t. matrix

$$\nabla_A (Ay) = ??$$

  - First, it must have 1 output dimension and 2 input dimensions. So we have that

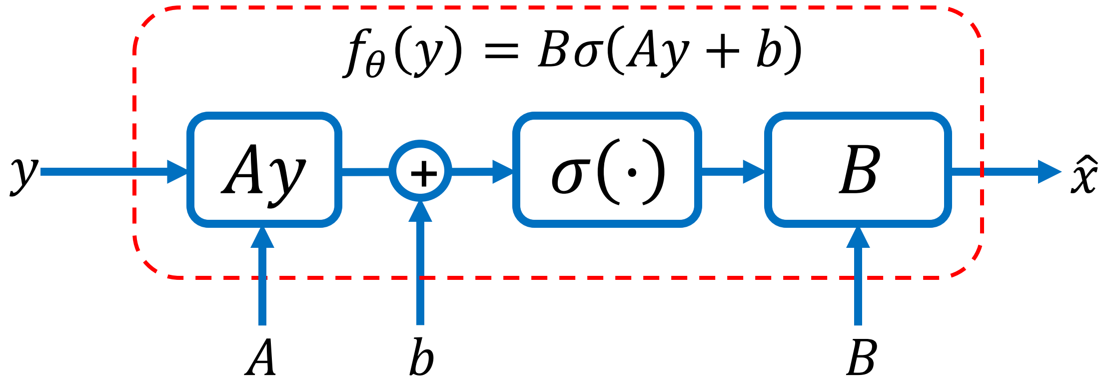
$$[\nabla_A (Ay)]^i{}_{j_1, j_2} = \delta^i{}_{j_1} y^{j_2}$$

GD for Single Layer NN

- Structure of the Gradient
- Gradients for NN parameters
- Updates for NN parameters

Gradient Direction for Single Layer NN

- Single layer NN:



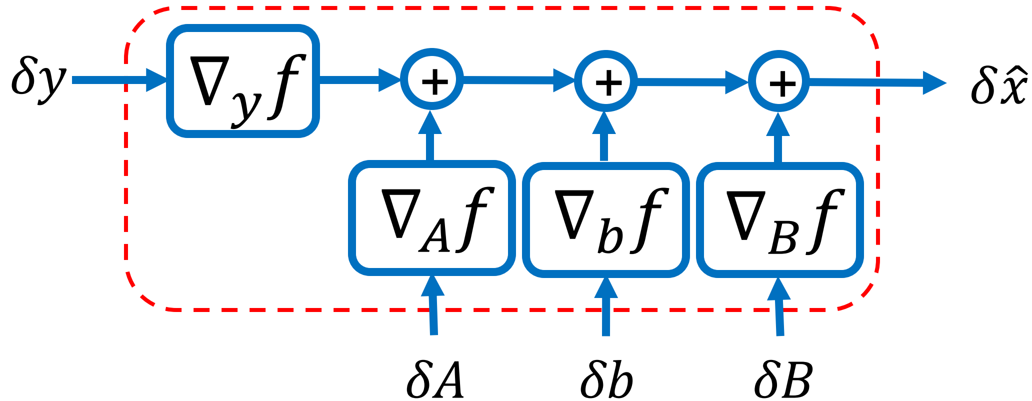
  - We will need gradient w.r.t the parameters $\theta = (A, b, B)$:

$$\nabla_\theta f_\theta(y) = \left[\nabla_A f_{(A,b,B)}(y), \nabla_b f_{(A,b,B)}(y), \nabla_B f_{(A,b,B)}(y)\right]$$

  - Later, we will also need:

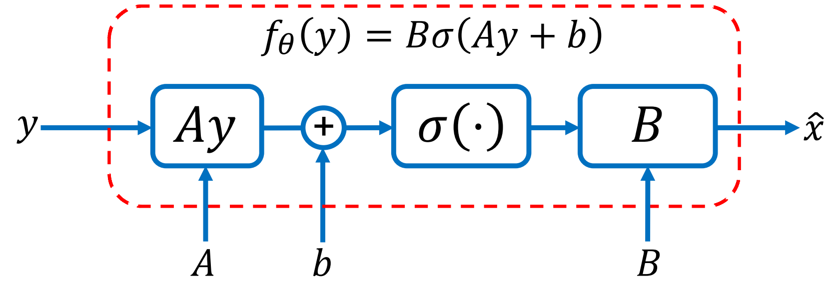
$$\nabla_y f_\theta(y)$$

Gradient Structure for Single Layer NN



- Single layer NN:
  - Parameters are $\theta = (A, b, B)$
  - We will need the parameter gradients:
    $$\nabla_\theta f_\theta(y) = \left[\nabla_A f_{(A,b,B)}(y), \nabla_b f_{(A,b,B)}(y), \nabla_B f_{(A,b,B)}(y)\right]$$
  - And the input gradient:
    $$\nabla_y f_\theta(y)$$

Gradient w.r.t. y



- For this case,

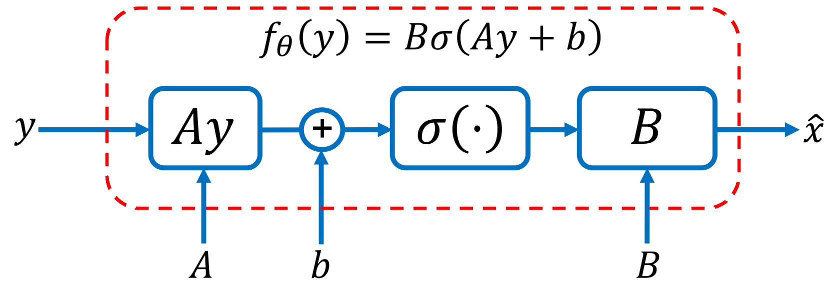
$$\nabla_y f = \nabla_y f_\theta(y) = \nabla_y B[\sigma(Ay + b)]$$
$$= B[\nabla\sigma(Ay + b)]A$$

  – Using Einstein notation

$$\boxed{[\nabla_y f]^i{}_j = B^i{}_{i_1}[\nabla\sigma]^{i_1}{}_{i_2}A^{i_2}{}_j}$$

This is a matrix or 2-D tensor

Gradient w.r.t. A



- For this case,

$$\nabla_A f = B\,[\nabla\sigma(Ay + b)]\,\boxed{\nabla_A(Ay)}$$

This is a tensor!

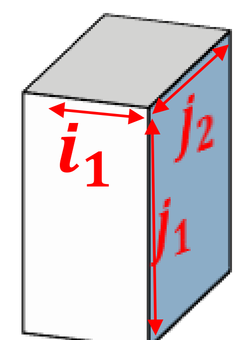
  – Using Einstein notation, since

$$[\nabla_A(Ay)]^i{}_{j_1,j_2} = \delta^i{}_{j_1} y^{j_2}$$

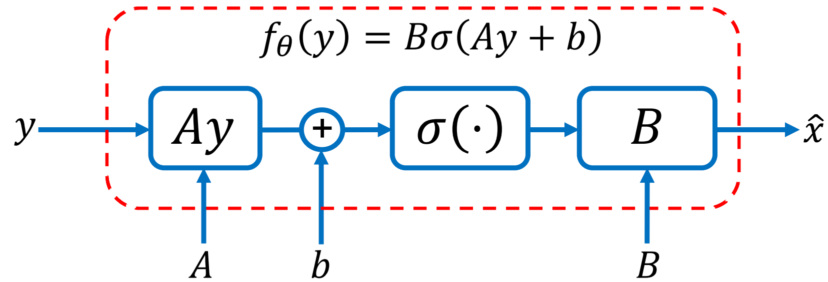
  – Then

$$\begin{aligned}[\nabla_A f]^{i_1}{}_{j_1,j_2} &= B^{i_1}{}_{i_2}[\nabla\sigma]^{i_2}{}_{i_3}[\nabla_A(Ay)]^{i_3}{}_{j_1,j_2} \\ &= B^{i_1}{}_{i_2}[\nabla\sigma]^{i_2}{}_{i_3}\delta^{i_3}{}_{j_1} y^{j_2}\end{aligned}$$

$$\boxed{[\nabla_A f]^{i_1}{}_{j_1,j_2} = B^{i_1}{}_{i_2}[\nabla\sigma]^{i_2}{}_{j_1}\, y^{j_2}}$$



Gradient w.r.t. b



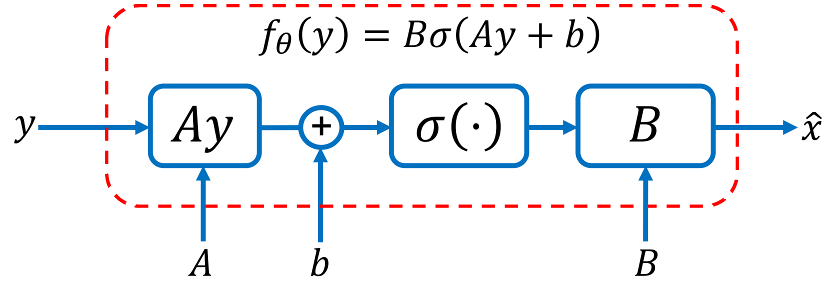
- For this case,

$$\nabla_b f = B\,[\nabla\sigma(Ay+b)]\,\nabla_b(Ay+b)$$
$$= B\,[\nabla\sigma]I = B\,\nabla\sigma$$

  – Using Einstein notation,

$$\boxed{[\nabla_b f]^{i_1}{}_{j_1} = B^{i_1}{}_{i_2}[\nabla\sigma]^{i_2}{}_{j_1}}$$

Gradient w.r.t. *B*



- For this case,

$$\nabla_B f = \boxed{\nabla_B(B\sigma)}$$

This is a tensor!

  – Using Einstein notation, since

$$[\nabla_B(B\sigma)]^i{}_{j_1,j_2} = \delta^i{}_{j_1}\sigma^{j_2}$$

  – We have that

$$\boxed{[\nabla_B f]^{i_1}{}_{j_1,j_2} = \delta^{i_1}{}_{j_1}\sigma^{j_2}}$$

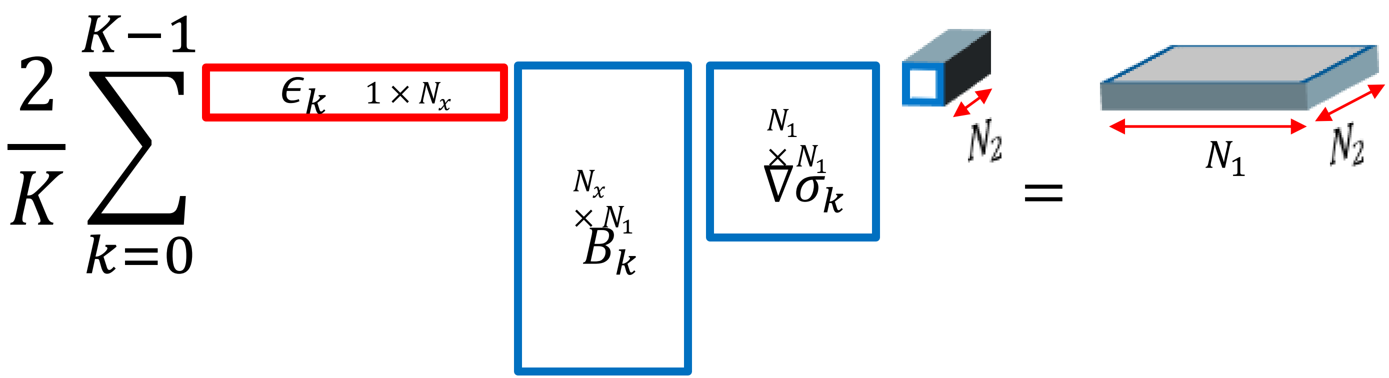
Update Direction for A

Gradient step:

$$A \leftarrow A + \alpha d^t$$

where d is given by

$$d_{j_1,j_2} = -\nabla_A L(\theta) = \frac{2}{K}\sum_{k=0}^{K-1} \epsilon_{k,i_1}\, B^{i_1}{}_{i_2} [\nabla\sigma_k]^{i_2}{}_{j_1}\, y_k{}^{j_2}$$



For efficiency, computation goes this way!

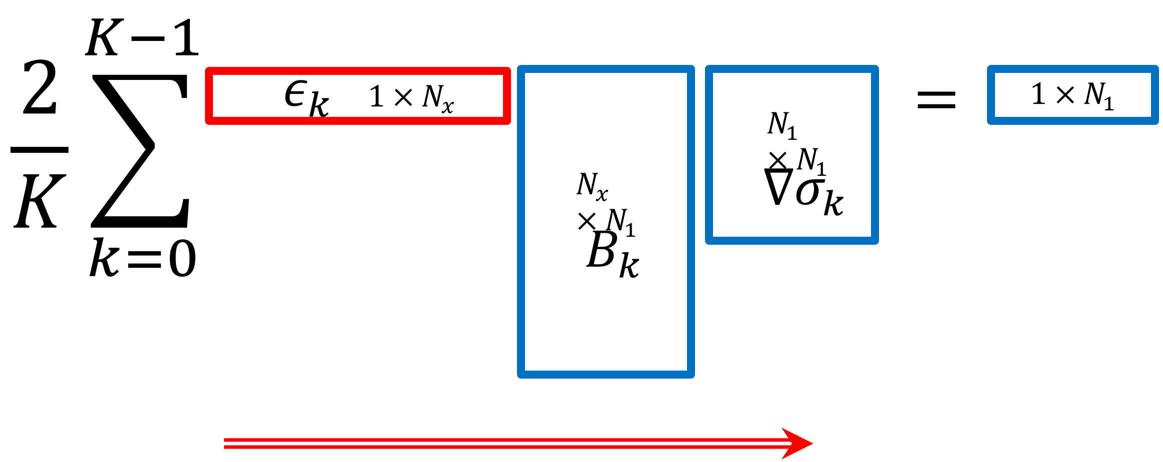
Update Direction for *b*

Gradient step:

$$b \leftarrow b + \alpha d^t$$

where d is given by

$$d_{j_1} = -\nabla_b L(\theta) = \frac{2}{K} \sum_{k=0}^{K-1} \epsilon_{k,i_1} \, B^{i_1}{}_{i_2} [\nabla \sigma_k]^{i_2}{}_{j_1}$$



For efficiency, computation goes this way!

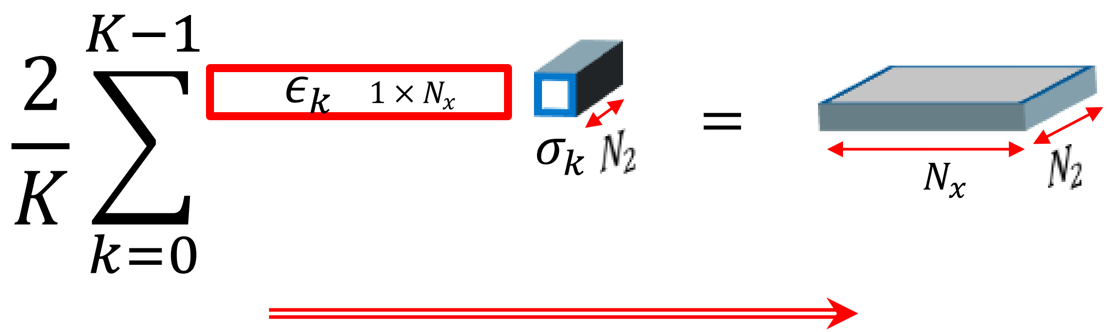
Update Direction for B

Gradient step:

$$B \leftarrow B + \alpha d^t$$

where d is given by

$$d_{j_1,j_2} = -\nabla_B L(\theta) = \frac{2}{K}\sum_{k=0}^{K-1} \epsilon_{k,j_1} \sigma_k{}^{j_2}$$



For efficiency, computation goes this way!

Local and Global Minima

- Open and Closed Sets
- Convex Sets and Functions
- Properties of Convex Functions
- Local Minimum, Saddle Points, and Global Minima
- Optimization Theorems

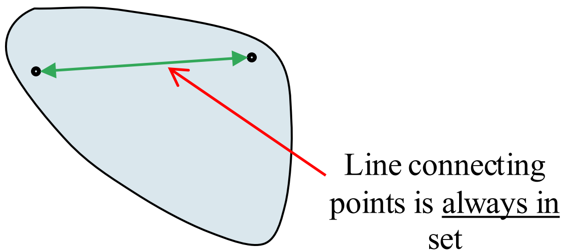
Open and Closed Sets

- Define:
  - $\mathcal{A} \subset \Re^N$
  - Open ball of radius ϵ is $B(r, \epsilon) = \{r \in \Re^N : \|r - r_o\| < \epsilon\}$.
- A set $\mathcal{A}$ is open if
  - At every point, there is an open ball contained in $\mathcal{A}$.
  - $\forall r \in \mathcal{A},\ \exists \epsilon > 0$ s.t. $B(r, \epsilon) \subset \mathcal{A}$.
- A set $\mathcal{A}$ is closed if $\mathcal{A}^c = \Re^N - \mathcal{A}$ is open.
- A set $\mathcal{A}$ is compact if it is closed and bounded.
- Facts:
  - $\Re^N$ is both open and closed, but it is not compact.
  - If $\mathcal{A}$ is compact, then every sequence in $\mathcal{A}$ has a limit point in $\mathcal{A}$.

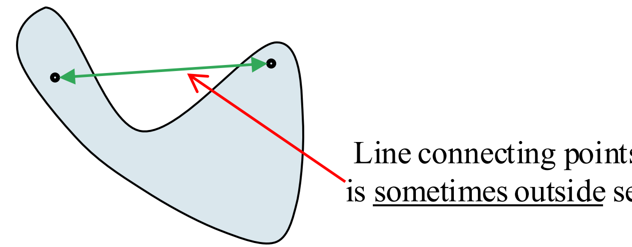
Convexity Sets

- A set $\mathcal{A}$ is convex if

  $\forall \lambda \in (0,1), \forall s, r \in \mathcal{A}$, then $\lambda r + (1-\lambda) s \in \mathcal{A}$



Convex Set



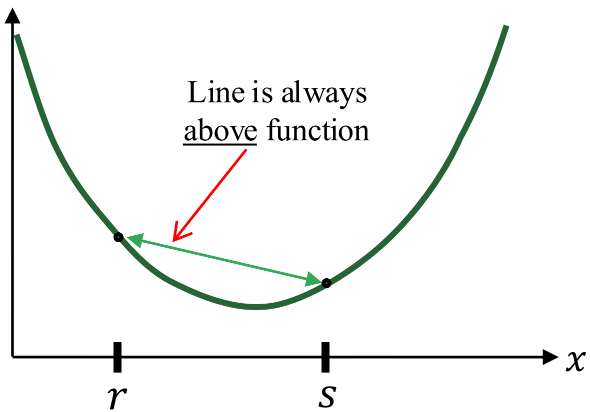
Nonconvex Set

- Properties:
  - The intersection of convex sets is convex

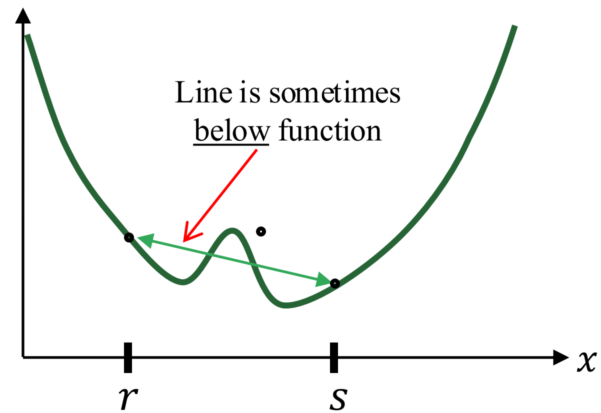
Convexity Functions

- Let $f: \mathcal{A} \rightarrow \Re$ where $\mathcal{A}$ is a convex set. Then we say that f is a convex function if

$$\forall \lambda \in (0,1), \forall s, r \in \mathcal{A}, \quad \text{then } f(\lambda r + (1-\lambda)s) \leq \lambda f(r) + (1-\lambda) f(s)$$



Convex Function



Nonconvex Function

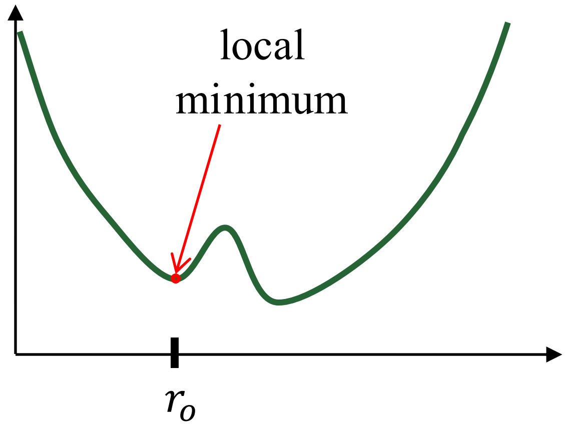
- Properties:
  - The sums of convex functions is convex
  - The maximum of a set of convex functions is convex
  - If $f(y)$ is convex, then $f(Ay)$ is also convex.
  - $f(y)$ is concave if $-f(y)$ is convex.
  - $f(y) = Ay + b$ is both convex and concave

Properties of Convex Functions

- Valuable properties of convex functions
  - The sums of convex functions is convex.
    - Let $f(x) = \sum_n f_n(x)$. If $f_n(x)$ are convex, then $f(x)$ is convex.
  - The maximum of a set of convex functions is convex.
    - Let $f(x) = \max_n f_n(x)$. If $f_n(x)$ are convex, then $f(x)$ is convex.
  - The second derivative of a convex function is positive.
    - Let $f(y)$ have two continuous derivatives, and let $H_{i,j}(y) = \frac{\partial^2 f}{\partial y_i \partial y_j}$ be the Hessian of f at y. Then $f(y)$ is convex if and only if $H(y)$ is non-negative definite for all y.
  - A convex function of a linear transform is convex.
    - If $f(y)$ is convex, then $f(Ay)$ is also convex.
  - An affine transform is both convex and concave.
    - $f(y) = Ay + b$ is both convex and concave.
  - A function is concave if its negative is convex.
    - $f(y)$ is concave if $-f(y)$ is convex.

Local Minimum

- Let $f: \mathcal{A} \to \Re$ where $\mathcal{A} \subset \Re^N$.
  - We say that $r_o \in \mathcal{A}$ is a local minimum of f if there $\exists \epsilon > 0$ s.t. $\forall\, r \in \mathcal{A} \cap B(r, \epsilon)$, $f(r) \geq f(r_o)$.

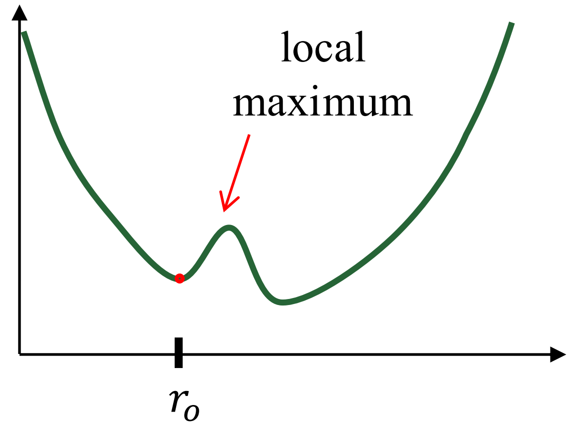


- Necessary condition for local minima:
  - Let f be continuously differentiable and let r_o be a local minimum, then $\nabla f(r_o) = 0$.

r_o a local minimum $\Rightarrow$ $\nabla f(r_o) = 0$

Local Maximum

- Let $f: \mathcal{A} \rightarrow \Re$ where $\mathcal{A} \subset \Re^N$.
  - We say that $r_o \in \mathcal{A}$ is a local minimum of f if there $\exists \epsilon > 0$ s.t. $\forall\, r \in \mathcal{A} \cap B(r, \epsilon)$, $f(r) \leq f(r_o)$.

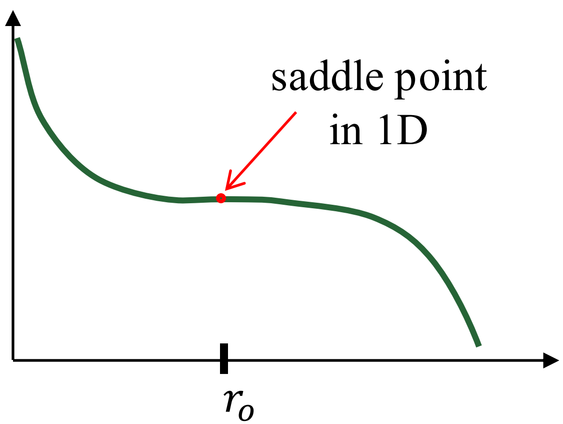


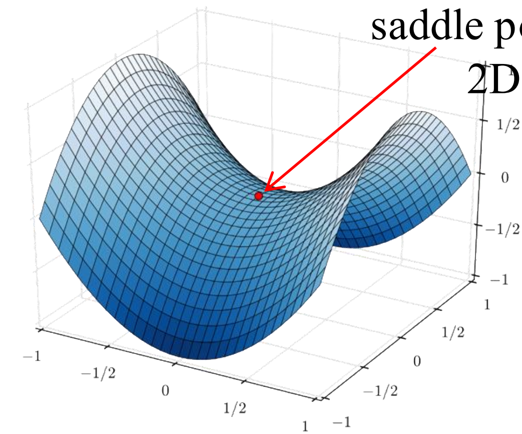
- Necessary condition for local maximum:
  - Let f be continuously differentiable and let r_o be a local minimum, then $\nabla f(r_o) = 0$.

r_o a local maximum $\Rightarrow$ $\nabla f(r_o) = 0$

Saddle Point

- Let $f: \mathcal{A} \rightarrow \Re$ where $\mathcal{A} \subset \Re^N$ be a continuously differentiable function.
  - We say that $r_o \in \mathcal{A}$ is a saddle point of f if $\nabla f(r_o) = 0$ and r_o is not a local minimum or maximum.





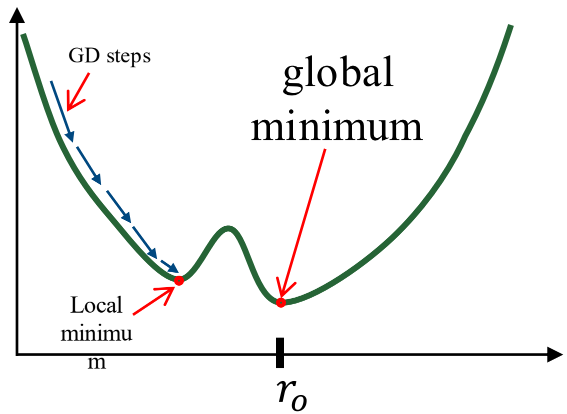
Graph of $f(x) = x_1^2 - x_2^2$

  - Saddle points can cause more problems than you might think.

*Shared from Wikipedia

Global Minimum

- Let $f: \mathcal{A} \rightarrow \Re$ where $\mathcal{A} \subset \Re^N$.
  - We say that $r_o \in \mathcal{A}$ is a global minimum of f if $\forall\, r \in \mathcal{A}$, $f(r) \geq f(r_o)$.



- Comments:
  - In general, finding global minimum is difficult.
  - Gradient descent optimization typically becomes trapped in local minima.

Optimization Theorems

- Let $f: \mathcal{A} \rightarrow \Re$ where $\mathcal{A} \subset \Re^N$.
  - If f is continuous and $\mathcal{A}$ is compact, then f takes on a global minimum in $\mathcal{A}$.
  - If f is convex on $\mathcal{A}$, then any local minimum is a global minimum.
  - If f is continuously differentiable and convex on $\mathcal{A}$, then $\nabla f(r_o) = 0$ implies that $r_o \in \mathcal{A}$ is a global minimum of f.

- Important facts:
  - Global minimum may not be unique.
  - If $\mathcal{A}$ is closed but not bounded, then it may not take on a global minimum.
  - Generally speaking, gradient descent algorithms converge to the global minimum of continuously differentiable convex functions.
  - Most interesting functions in ML are not convex!