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Introduction to Numerical Optimization:

Week 1

Data everywhere

Data science → Extracting useful info from raw data.

Uses ML Tools.

Data Engineering / Data science / Data Analyst

How to collect and store data → Making decision From that data. → Make visualisation From data.

→ Backbone of Datascience:

- Mathematics
  1. Linear Algebra
  2. Calculus
  3. Optimization.
  4. Statistics.
- Computer - Algo, Computation, Storage.

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→ Broad classification of ML prob:

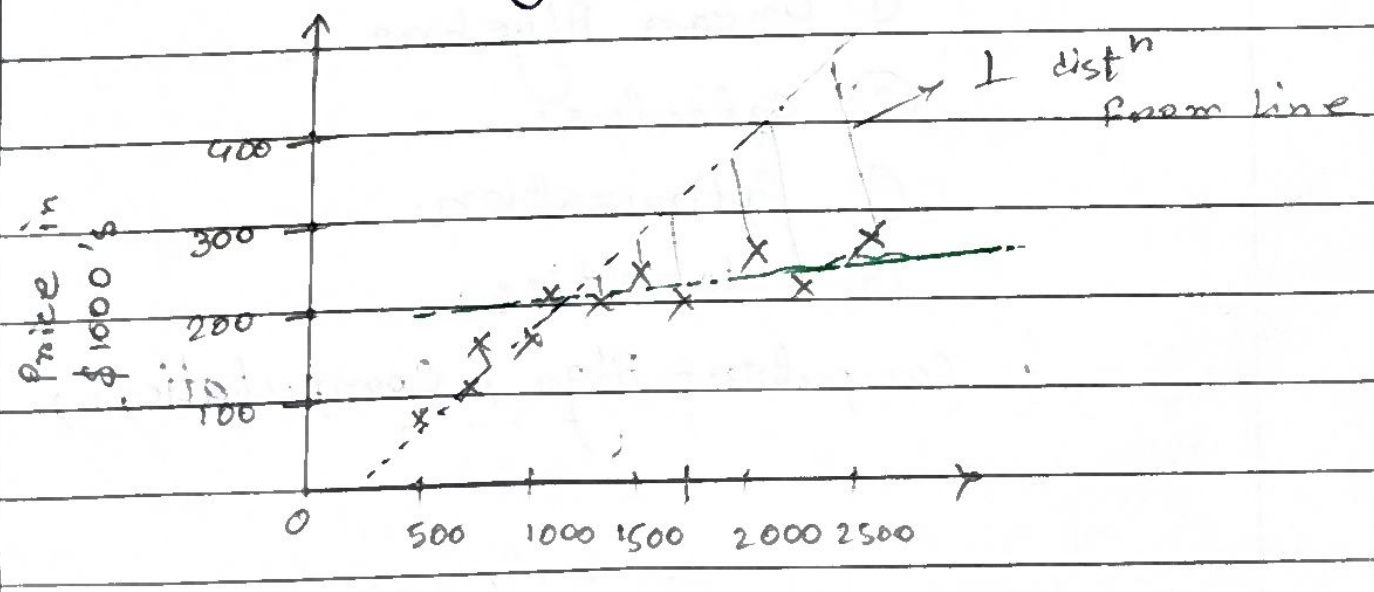
- Model fitting
- Classification.

→ Application:

- Weather Forecast
- recommendations
- Computer vision
- Pattern Recognition.

Why Optimization Matters?

- Regression Model
- Suppose a few data point $\{(x_i, y_i)\}$ have been given in the plane.



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we collect the data of some house of price and size and plot in graph.

Based on the price we predict the price or get an approx range of it.

- Suppose we guess there is a linear relation.

$$price(p) = \alpha \cdot size(s) + \beta$$

↳ similar to straight line Eq^n.

Note: This is not the absolute model to predict price. There are more model.

Different Model give different result.

There are NO unified model

There is NO unified prediction

Q. Which α and β to choose?

Bring in optimization perspective

↳ Ok, I have a model, with that model, can I pass it through all the data point

↳ Typically very unlikely

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of course, there will be error.
↳ Mathematical one

We can take 1 distn from the line and sum them up, a valid error indeed.

We can also use (Mis)feet

price = (α)(size) + β

direct correlation b/w price ↔ size.

$$\xi (\alpha(\text{size}) + \beta - \text{price})^2$$

↓

some of the term +ve and some -ve which cancle out so, we square.

- Typically we need/want least error in prediction.

- This is achieved by finding a straight line $y = \alpha x + \beta$ such that.

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$f(a,b) = \sum_{i=1}^{n} (ax_i + b - y_i)^2$ is minimized.

Concept:

- Optimising problem is typically minimising or maximising Fn of some veriables.

Observative (loss) Fn
Decision veriables (Parameters)
Constraints (optional)

minimize $f(x)$
subject to $x \in S$ and
where $f: \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\}$ is a map, $S \subseteq \mathbb{R}^n$ is a nonempty constraint set.

Eg: If we go from class to Mess and have three routes, not always the shortest route is better.
If the objective is workout. then take the longest route.

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Types of Problem:

- Unconstraint vs constraint
- Convex vs Non-convex

Unconstraint	Constraint
↓	↓
We give a model a whole playground and tell them to figure out themselves, what the patterns are	We give a model a whole playground with some directions/hint which make the model recognise patterns with our guidance

Q. Why convexity Matters? → we will look into it later

convex prob → easy prob.

non-convex prob → extreamly Heard prob.

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Example:

- Geometric problem: Given a fixed perimeter, what is the largest area that can be covered?

suppose, we take rectangle → L, B

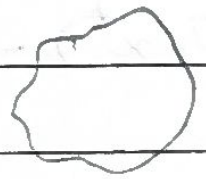
maximize $f(L,B) = L \times B$

subject to $2(L+B) = 10$

$S = \{(L,B) \in R^2 : 2(L+B) = 10\}$

a 5

→ 2(a+b)



(→ We use calculus. For the area

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Solution Concept:

Solution

↳ ~~f(x)~~

In optimization we want a point x^* such that

$f(x^*) \leq f(x)$ for all x

when it is a minimization prob.

~~x^* ⟷ Minimizer~~

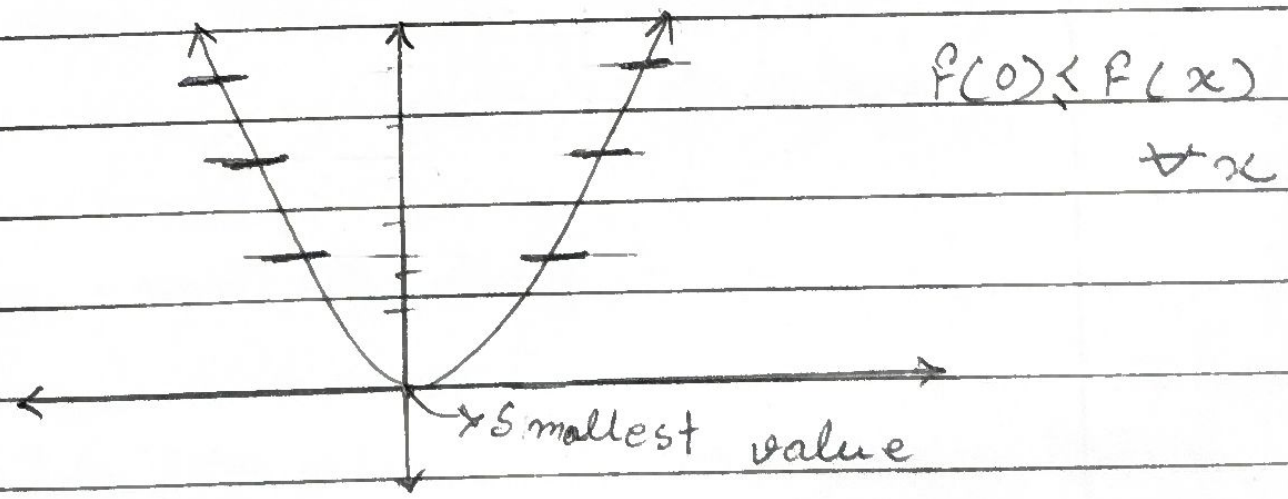
~~$f(x^*)$ ⟷ Minimum value~~

x^* → Minimizer

$F(x^*)$ → Minimum value.

Eg:

minimize $f(x) = x^2$ over $S = \mathbb{R}$



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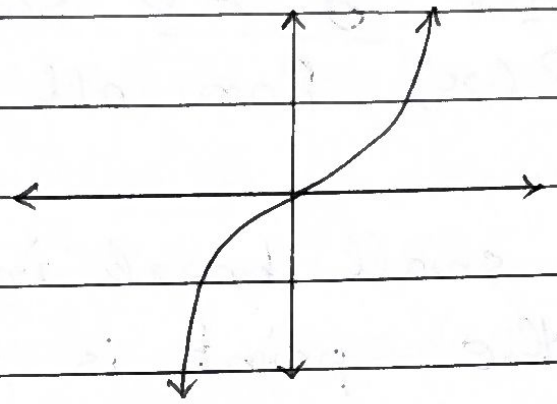
if $f(x) = x^3$



The minimum is

$-\infty$

↳ unknown

so, we say

it doesn't

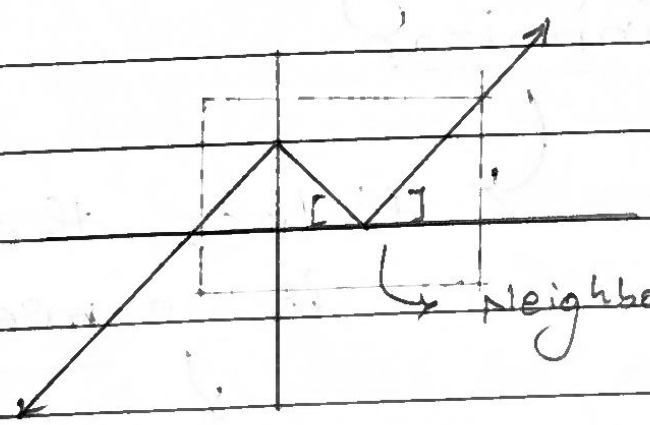
have minimize

or even maximizer

if we see other

side of the graph

$$f(x) = \begin{cases} x+2 & x \leq 0 \\ |2-x| & x \geq 0 \end{cases}$$



Here we use

Local Minimizer

$f(x) \geq f(2)$ $\forall x$ around

$\forall x \in [1, 3]$

Note: There is a slight break in in the almost continuous function.

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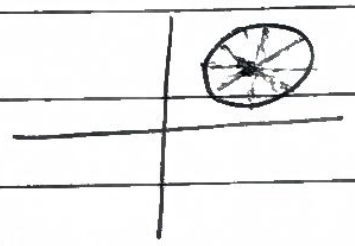
- A point $x^* \in S$ is called a local minimizer if there exist $\delta > 0$ such that $f(x^*) \leq f(x)$ For all $x \in B_\delta(x^*) \cap S$

$\delta \rightarrow$ that small break in the Function and the point is typically



Why it is ~~not~~ Important ?

→ Most of the numarical Algorithm we will study we have Local Minimizar.

↳ Unless the problem is convex problem

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convexity will gurentee that local minimizar is global minimizar

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Important thing in optimization:

- When can we say sol^n exist?

→ When there is global Minimizer, local is considered in the absence of global minimizer and presence of convexity.

- If a pt is sol^n, how do we know it?

- How to Find Sol^n? → Main Topic of this course

↓

Numarically

Lecture Takeaway: Numarical optimization

↓

Does Sol^n exist,
What kind of Sol^n (local/Global),
How to Find it Numarically?

Data Science, its Back Bone, Application, Classification:

Most ML Training prob are solve via numarical optimization of a loss fn.

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A review of Calculus and Linear Algebra

- Derivative
- $F: R \to R$, the derivative $F'(x_0) = \frac{d}{dx} F(x_0)$

$$= \lim_{t \to 0} \frac{F(x_0+t) - F(x_0)}{t}$$

- calculus of derivative.
  - $(F \pm g)'(x) = F'(x) \pm g'(x)$
  - $(Fg)'(x) = F'(x)g(x) + g'(x)F(x)$
  - $(1/g)'(x) = \frac{g'(x)}{(g(x))^2}$
- $F''(x) = (F')'(x)$

$F(x) = \sin(x)$	$F(x) = x^2$
$F'(x) = \cos(x)$	$F'(x) = 2x$
$F''(x) = -\sin(x)$	$F''(x) = 2.$

Taylor's Expansion Theorem:

- If a fn is differentiable at around point x_0

$$f(x) \approx$$

1st order derivative.

If x is ve... this is a very ... of $f(x)$

double differentiable at around

$$+ f'(x_0)(x-x_0) + \frac{1}{2} f''(x_0)(x-x_0)^2$$

$$f(x) \approx f(x_0) + f'(x_0)(x-x_0)$$

- If x is very close to x_0 this is a very good **approximater** of $f(x)$

$$f(x) \approx f(x_0) + f'(x_0)(x-x_0) + \frac{1}{2} f''(x_0)(x-x_0)^2$$

- If double derivative exist
- x is very close to x_0.

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Eg: $f(x) = e^x$, $x_0 = 0$

1st order: $e^x \approx 1 + x$

2nd order: $e^x \approx 1 + x + \frac{x^2}{2}$

Differentiability of Function of several variable:

. For a function $F: \mathbb{R}^n \to \mathbb{R}$, the partial derivative is used,

F at x with respect to x_i

fix one of the dimensions

$\mathbb{R}^2 \to$ ↑ →

$\mathbb{R}^3 \to$ ↑ →

$$\frac{\partial f}{x_i}(x) = \lim_{t \to 0} \frac{f(x + te_i) - f(x)}{t}$$

Eg: $f(x, y) = x^2 + xy + y^2$

$\frac{\partial f}{\partial x} = 2x + y.$

$\frac{\partial f}{\partial y} = x + 2y.$

$x + te_i$ is actually a vector sum.

$$\begin{bmatrix} 2 \\ 3 \end{bmatrix} + t \begin{bmatrix} 4 \\ 5 \end{bmatrix} = \begin{bmatrix} 2+4t \\ 3+5t \end{bmatrix}$$

=

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- Derivative of $F = \underbrace{\nabla F(x)}_{\text{Gradient}}$

$$= \begin{bmatrix} \frac{\partial F}{\partial x_1} \\ \vdots \\ \frac{\partial F}{\partial x_n} \end{bmatrix}$$

→ Collection of all the partial derivatives.

→ vector.

For the above Eg:

$$\nabla F(x) = \begin{bmatrix} 2x+y \\ x+2y \end{bmatrix}$$

Let,

$$\begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad \begin{bmatrix} 2 \\ 1 \end{bmatrix}$$

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- Second-order partial derivative:

$$\frac{\partial^2 f}{\partial x_i \partial x_j} = \frac{\partial}{\partial x_i}\left(\frac{\partial f}{\partial x_j}\right)$$

- Hessain matrix: all second-order partial derivatives.

$$H_f(x) = \nabla^2 f(x) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix}$$

Eg: $f(x,y) = x^2 + yx + y^2$

$$\frac{\partial^2 f}{\partial x \partial y} \Big/ \frac{\partial^2 f}{\partial x^2} \Big/ \frac{\partial^2 f}{\partial^2 y}$$

$$H(x,y) = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}$$

- A matrix is a rectangular arrangement of numbers, symbols or expressions written in rows and columns, usually enclosed with brackets.

Taylor's theorem of several Variables:

- For a function $f: \mathbb{R}^n \to \mathbb{R}$, the derivative of f at x, denoted by $\nabla f(x)$ is a vector such that.

Dot product

Some term

$$f(x+h) = f(x) + \langle \nabla f(x), h \rangle + o(\|h\|)$$

$$f(x) = f(x_0) + f'(x_0)(x - x_0)$$

$$y = \frac{(y - x_0)}{h} + x_0$$

scalar analog

Very very small term

Roughly,

$$f(x+h) \approx f(x) + \langle \nabla f(x), h \rangle$$

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- For a fn $f: R^n \rightarrow R$, the second derivative of f at x, denoted by $\nabla^2 f(x)$ is a Matrix such that,

$$f(x+h) = f(x) + \langle \nabla f(x), h \rangle + \frac{1}{2!} \langle h, \nabla^2 f(x) h \rangle + o(\|h\|^2)$$

$\langle \nabla f(x), h \rangle \rightarrow$ dot$(\nabla f(x), h)$

$\langle h, \nabla^2 f(x) h \rangle \rightarrow$ dot$(h, \nabla^2 f(x) h)$

Roughly,

$$f(x+h) \approx f(x) + \langle \nabla f(x), h \rangle + \frac{1}{2!} \langle h, \nabla^2 f(x) h \rangle$$

Note : ① This is a quadratic function.
② We need to be careful about linear fn and quadratic fn
As, they will be the function we will be frequently need data science course.

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Dot Product :

- For $u, v \in \mathbb{R}^n$: $u \cdot v = \sum_{i=1}^{n} u_i v_i$

- $u = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$, $v = \begin{bmatrix} 3 \\ 4 \end{bmatrix}$

$$u v = (1 \cdot 3) + (2 \cdot 4) = 11$$

Transpose : Flips rows and columns.

$$(A^T)_{ij} = A_{ji}$$

$$A = \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix} \quad A^T = \begin{bmatrix} 1 & 3 \\ 2 & 4 \end{bmatrix}$$

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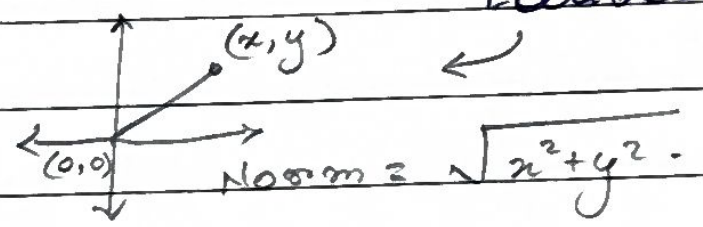
* Norm (length of a vector)

- Denoted by $\|v\|$
- For $\vec{v} = (v_1, v_2 \dots\dots, v_n)$

$$\|v\|_2 = \sqrt{v_1^2 + v_2^2 + \dots\dots + v_n}$$

↓

Euclidean Norm. or L2 Norm.



$$\|v\| = |v_1| + |v_2| + \dots\dots + |v_n|$$

- Measures the magnitude (length) of a vector.

Dot Product :

$$\|v\|_2 = \underset{1\times n \; n\times 1}{v^T v}.$$