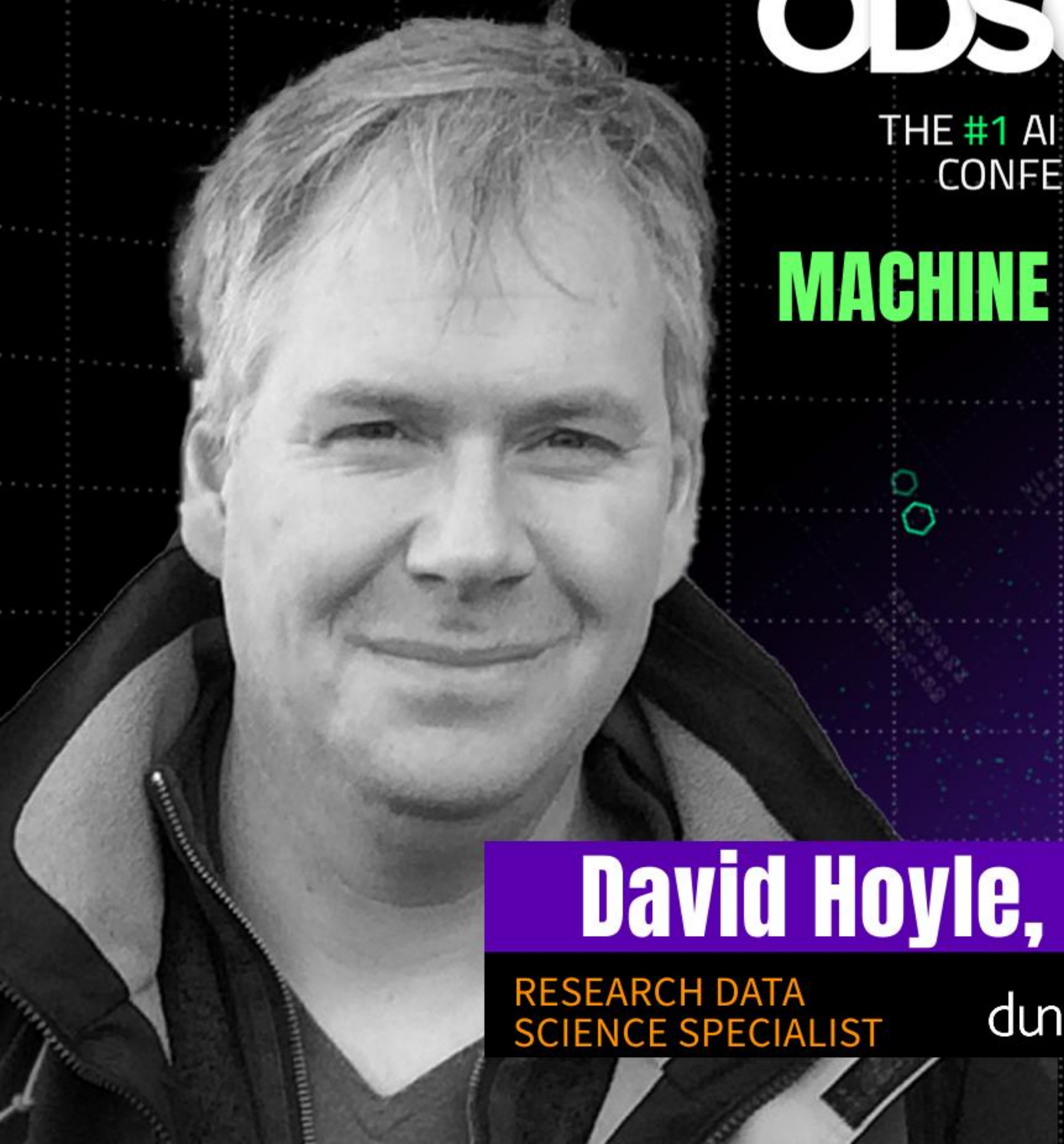
ODSC AI

THE #1 AI TRAINING CONFERENCE

MACHINE LEARNING

SAN FRANCISCO | OCT 28-30

INTRODUCTION TO MATH FOR DATA SCIENCE



David Hoyle, PhD

RESEARCH DATA SCIENCE SPECIALIST

dunnhumby

Outline

All material available at GitHub repository
https://github.com/dchoyle/ODSCWest2025_MathBootcamp

Lesson 1: The basics

1. Differential calculus
2. Vectors
3. Matrices

Lesson 2: Putting it altogether

1. Linear models
2. OLS regression
3. Gradient descent

Lesson 1

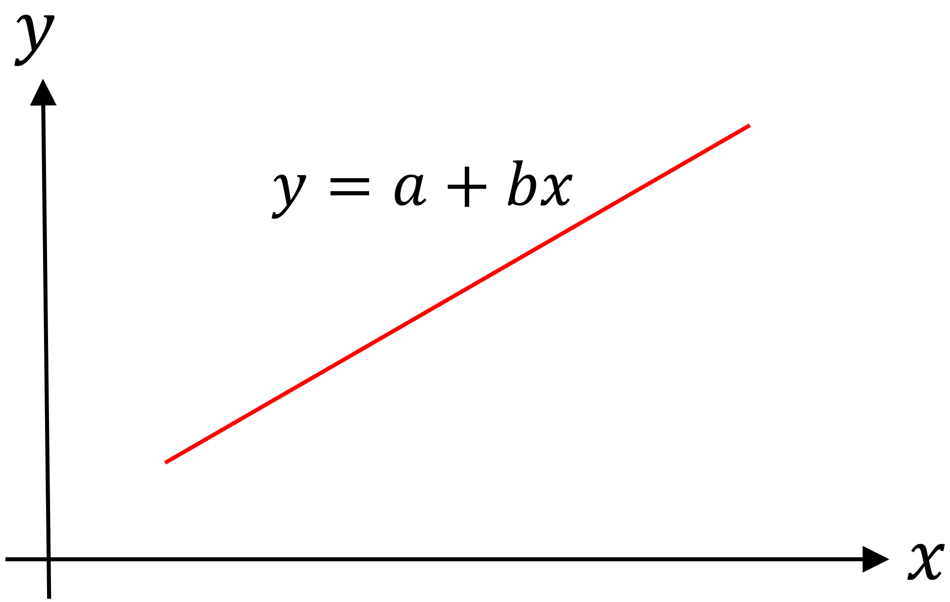
The basics

Differential calculus

– where we learn how fast things change

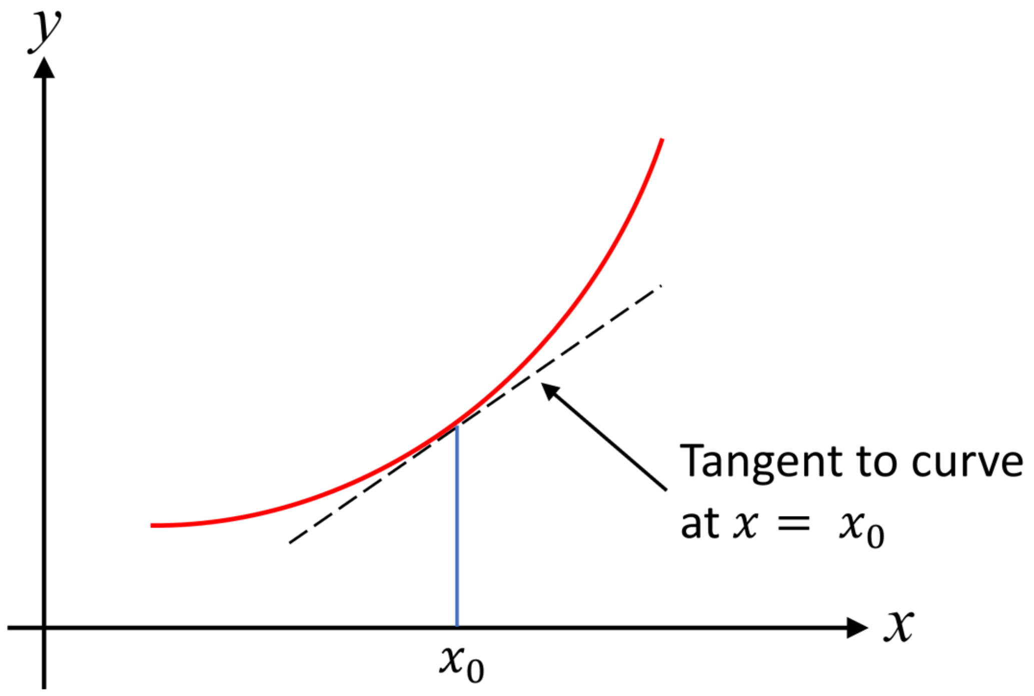
Recap: A straight line

- A straight line is a function of the form $y = a + bx$
- The parameter b is the gradient of the straight line. It tells us how fast y is increasing with respect to x



Differential calculus – working out how fast functions change

- The curve is a function, $y(x)$, of x



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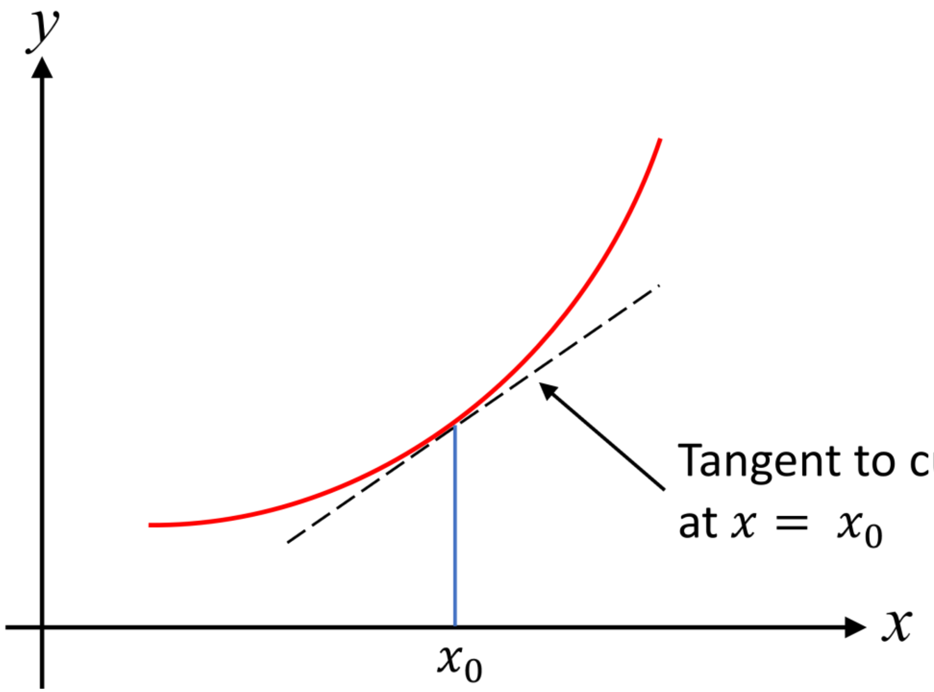

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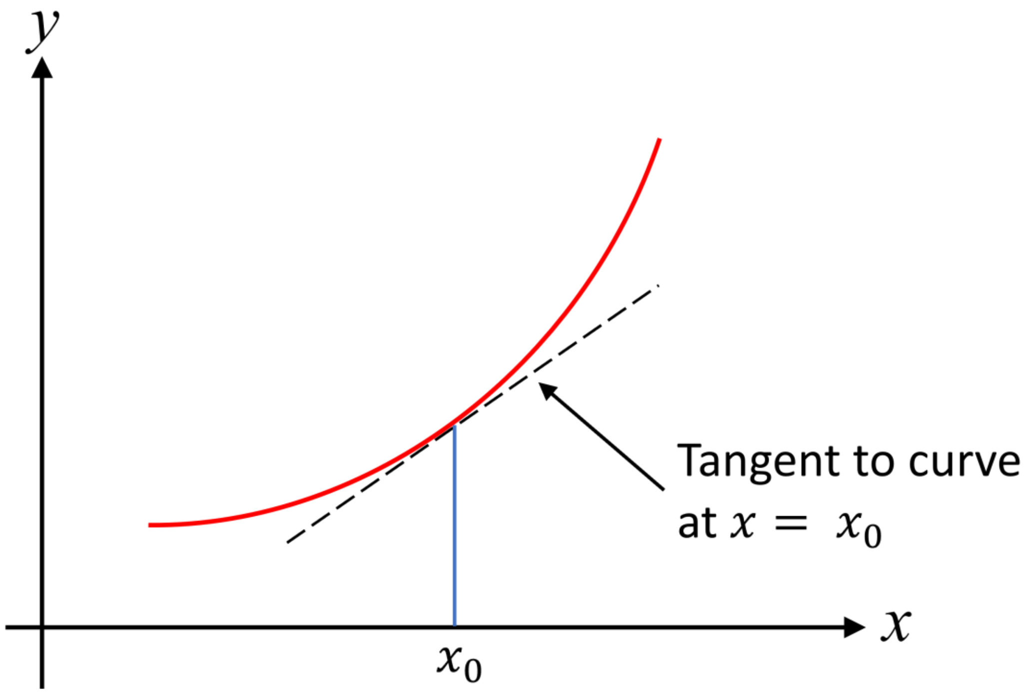
$$\frac{dy}{dx}$$



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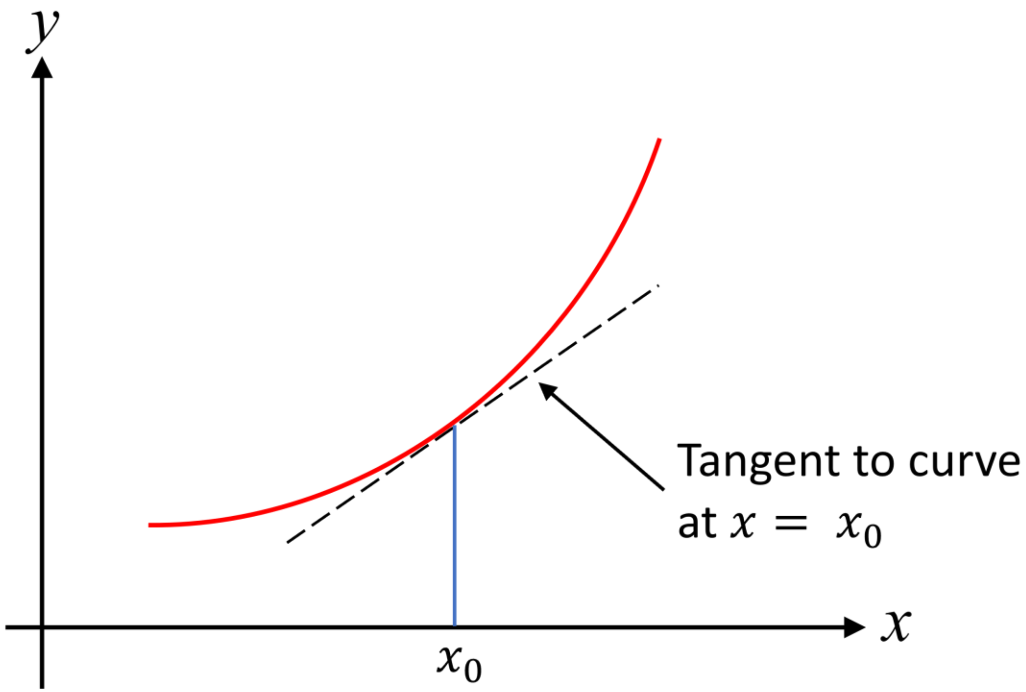

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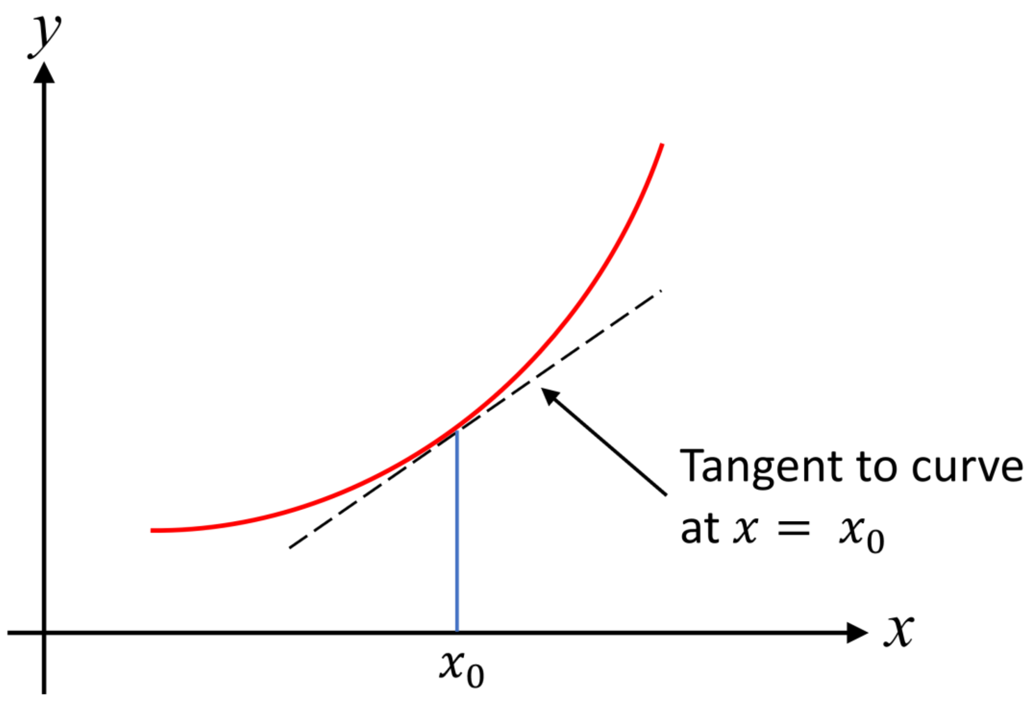
- The derivative tells us how fast y is changing at x



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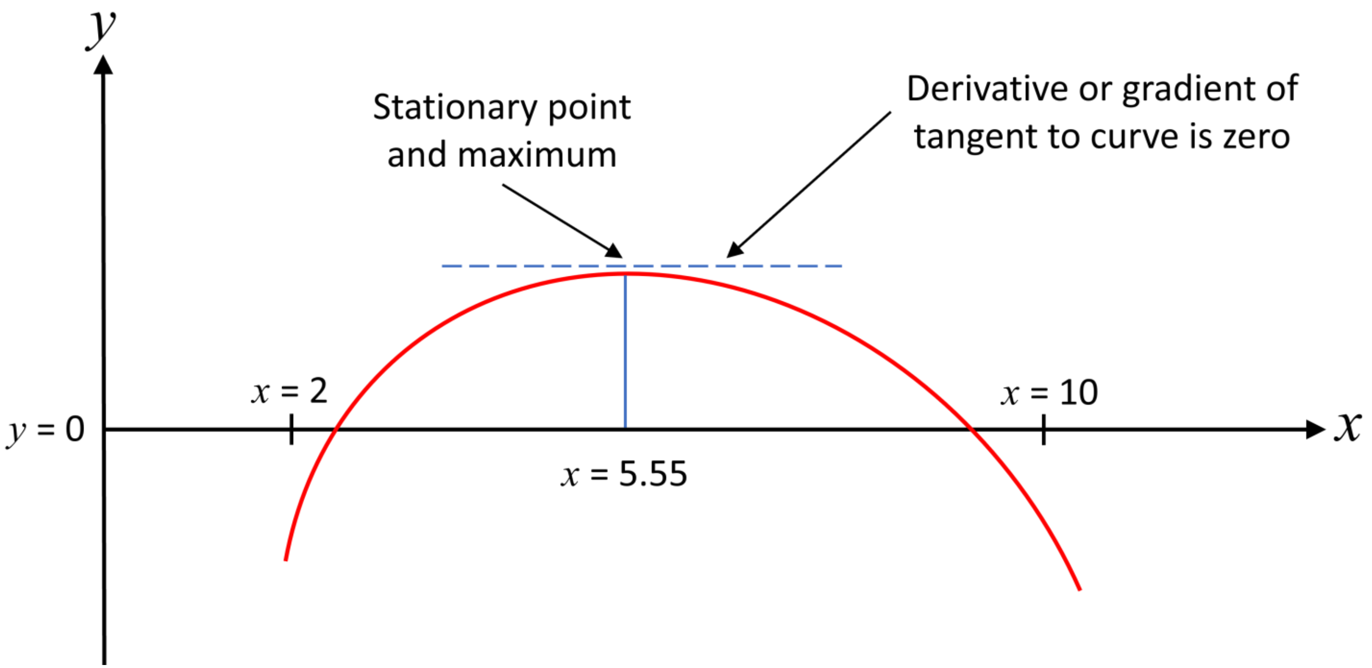
- The n^{th} derivative of $y(x)$ is written using the symbol $\frac{d^ny}{dx^n}$

Finding the maximum or minimum of a function

- Function on the right has a clear maximum
- At the maximum the derivative is zero



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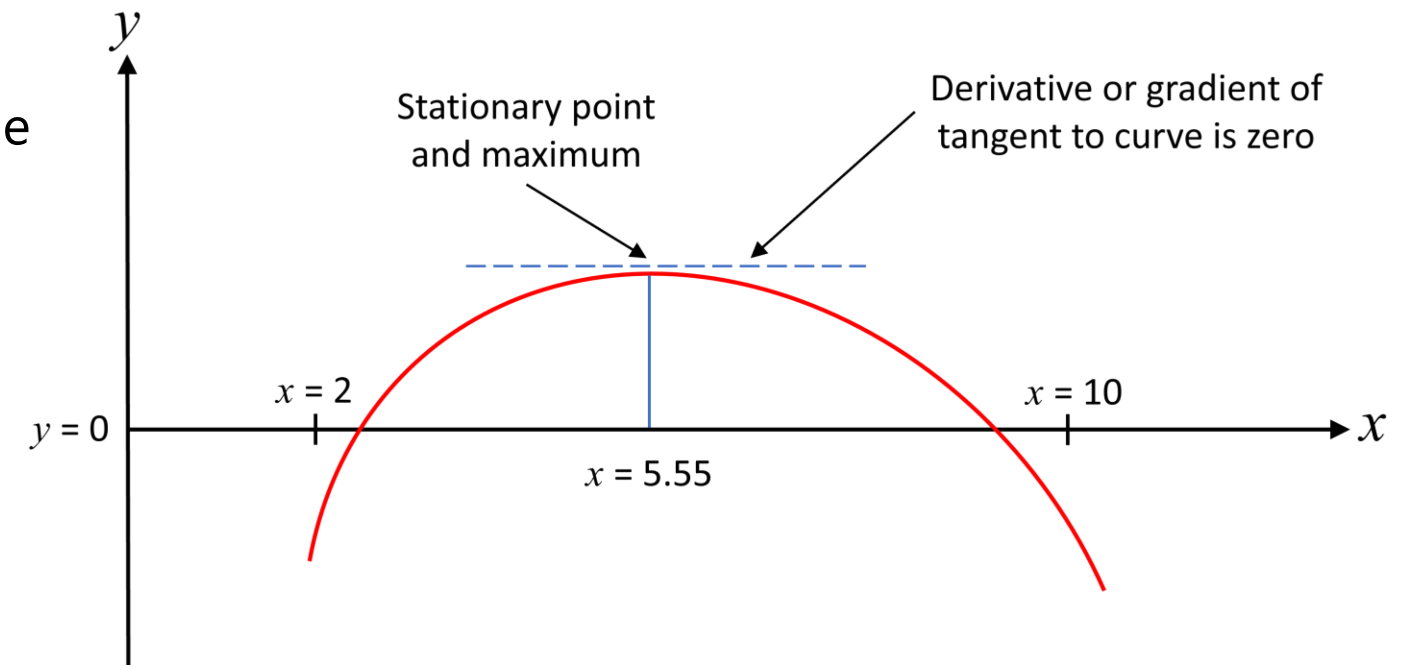

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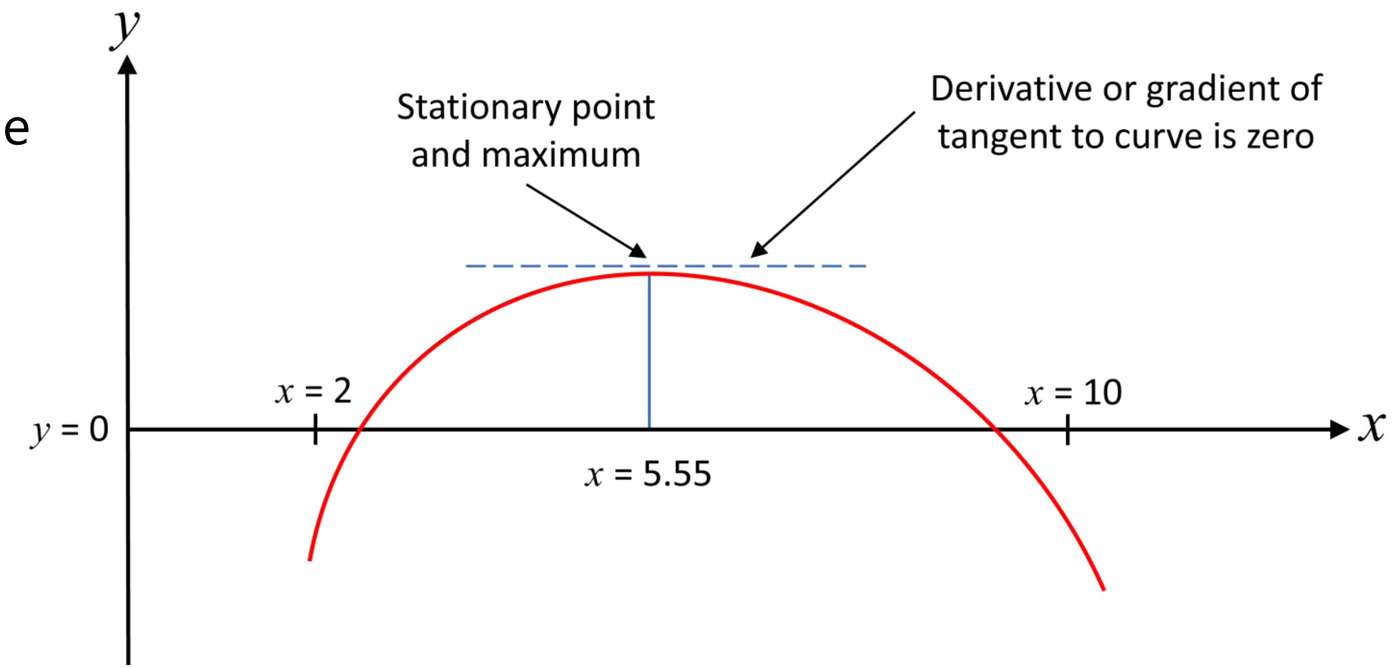

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- We call this a stationary point – because the rate of change of the function is zero
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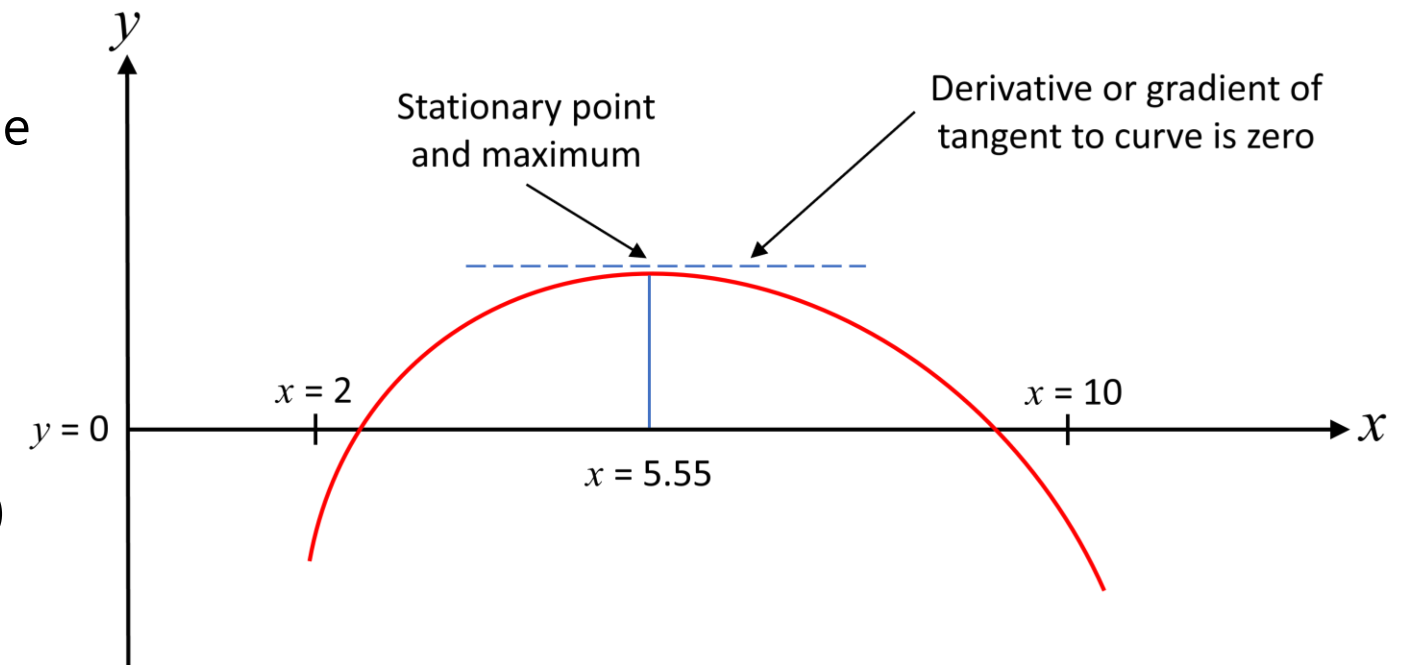
- We can use calculus to find the (stationary) maxima of a function by solving the equation below,

$$\frac{dy}{dx} = 0$$



Simple example of locating a stationary point

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- Solving $\frac{dy}{dx} = 0$ gives $-8x + 12 = 0 \implies x = \frac{12}{8} = 1.5$
- So, the function has a stationary point at $x = 1.5$

Distinguishing maxima from minima

- Minima and maxima are both stationary points
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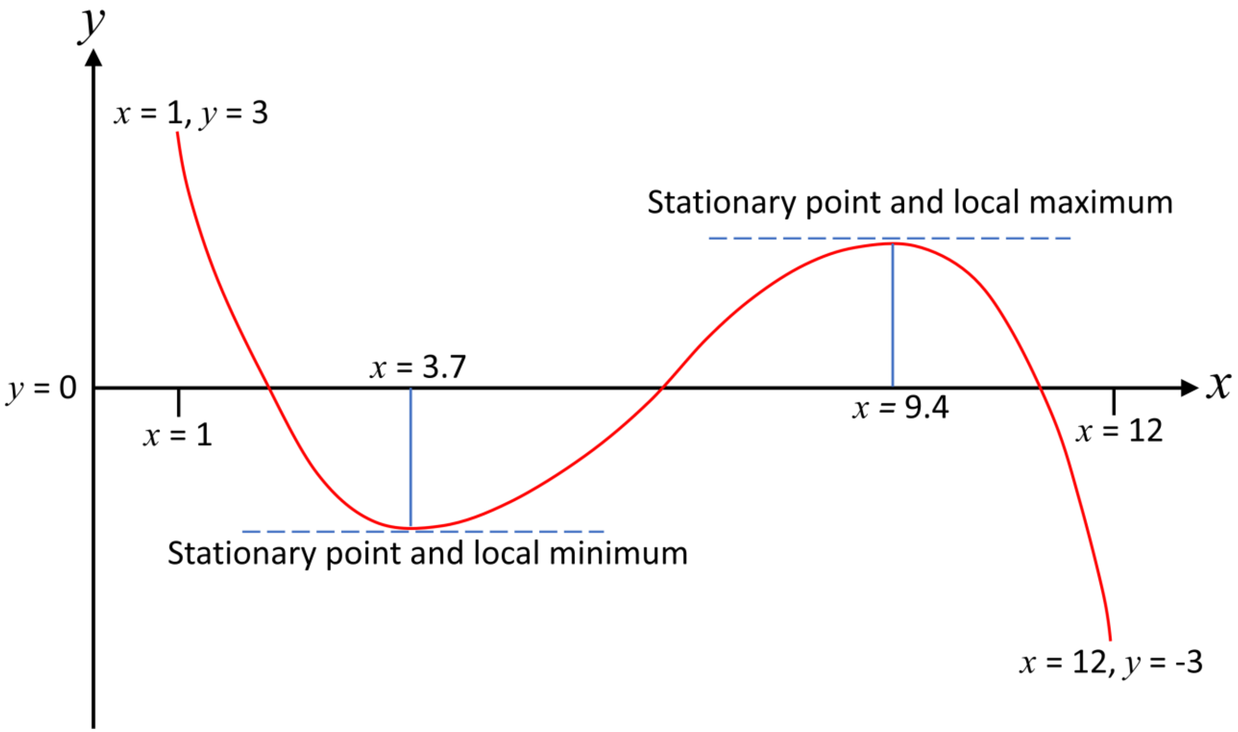

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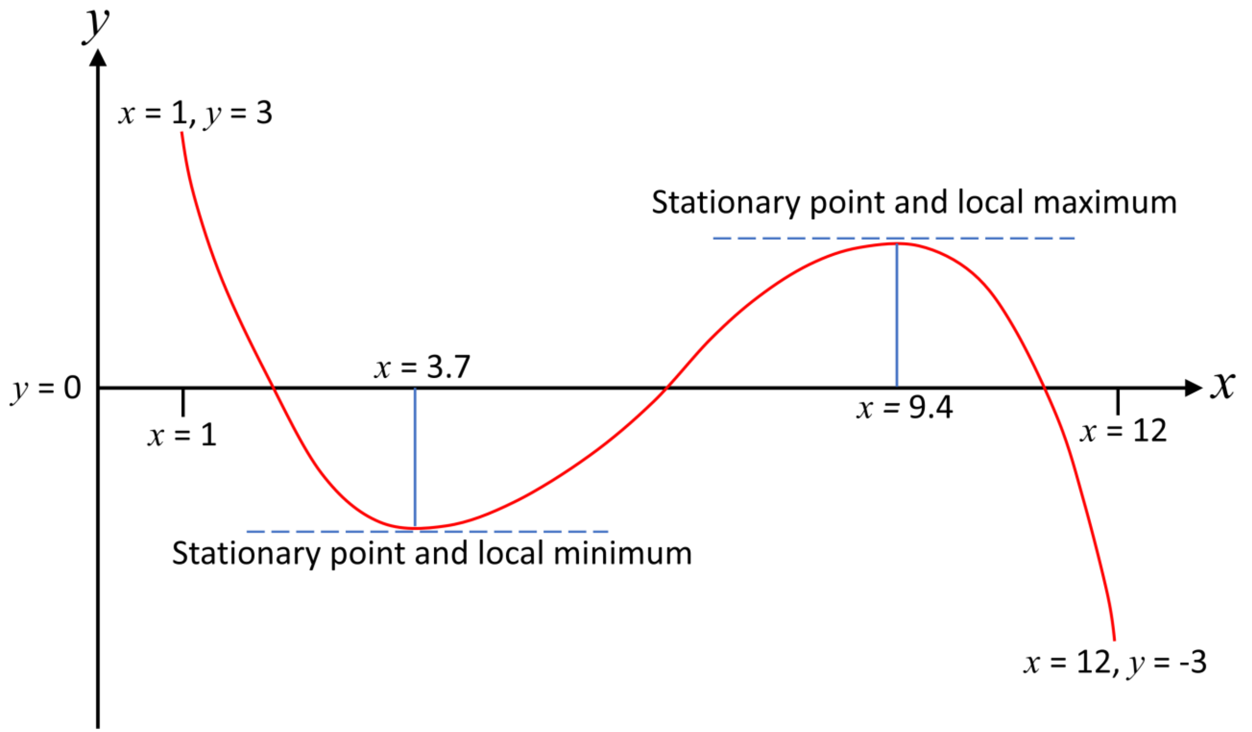

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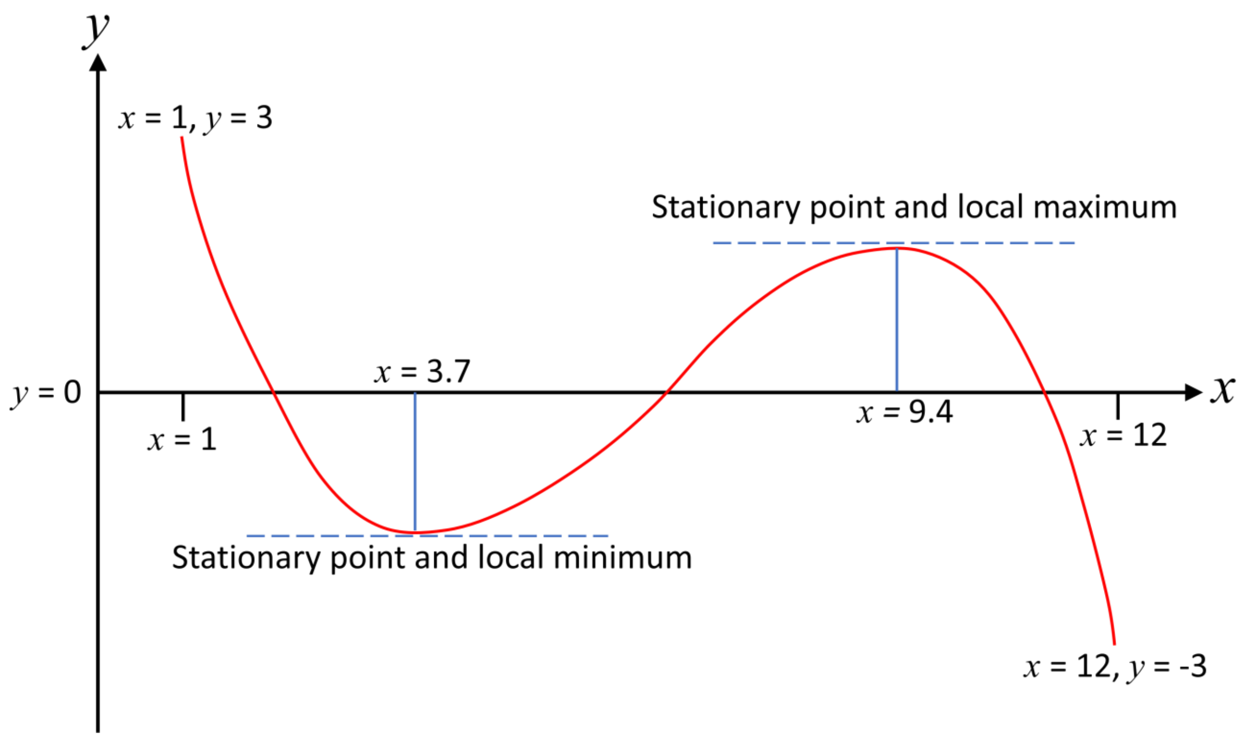
- So $\frac{d^2y}{dx^2} < 0$ at a maximum stationary point
- And $\frac{d^2y}{dx^2} > 0$ at a minimum stationary point



Distinguishing maxima from minima

Summary:

- We find stationary points of $y(x)$ by solving $\frac{dy}{dx} = 0$
- If $\frac{d^2y}{dx^2} < 0$ at a stationary point then the stationary point is a maximum, possibly local
- If $\frac{d^2y}{dx^2} > 0$ at a stationary point then the stationary point is a minimum, possibly local

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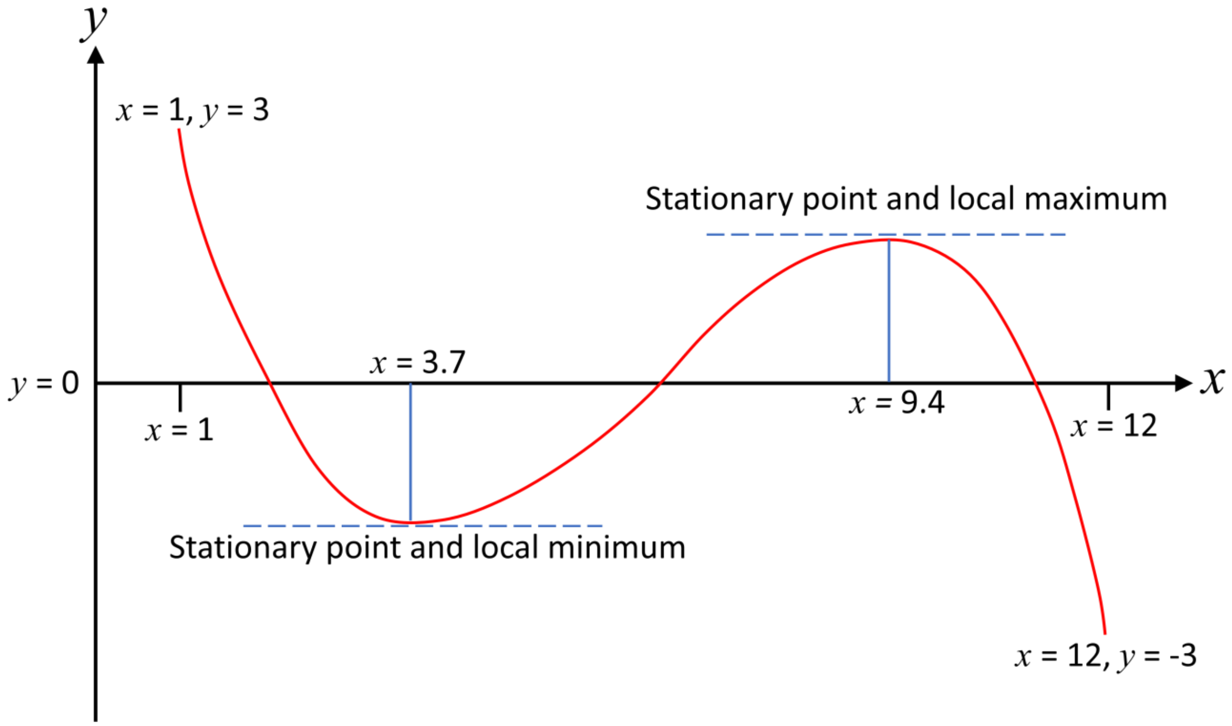
- So, $\frac{d^2y}{dx^2} < 0$ at the stationary point $\Rightarrow$ stationary point is a maximum

Maxima that is not a stationary point

- In the range $x \in [1,12]$, the global maximum value of y is $y = 3$

- This global maximum is at the left-hand edge. It is not a stationary point.



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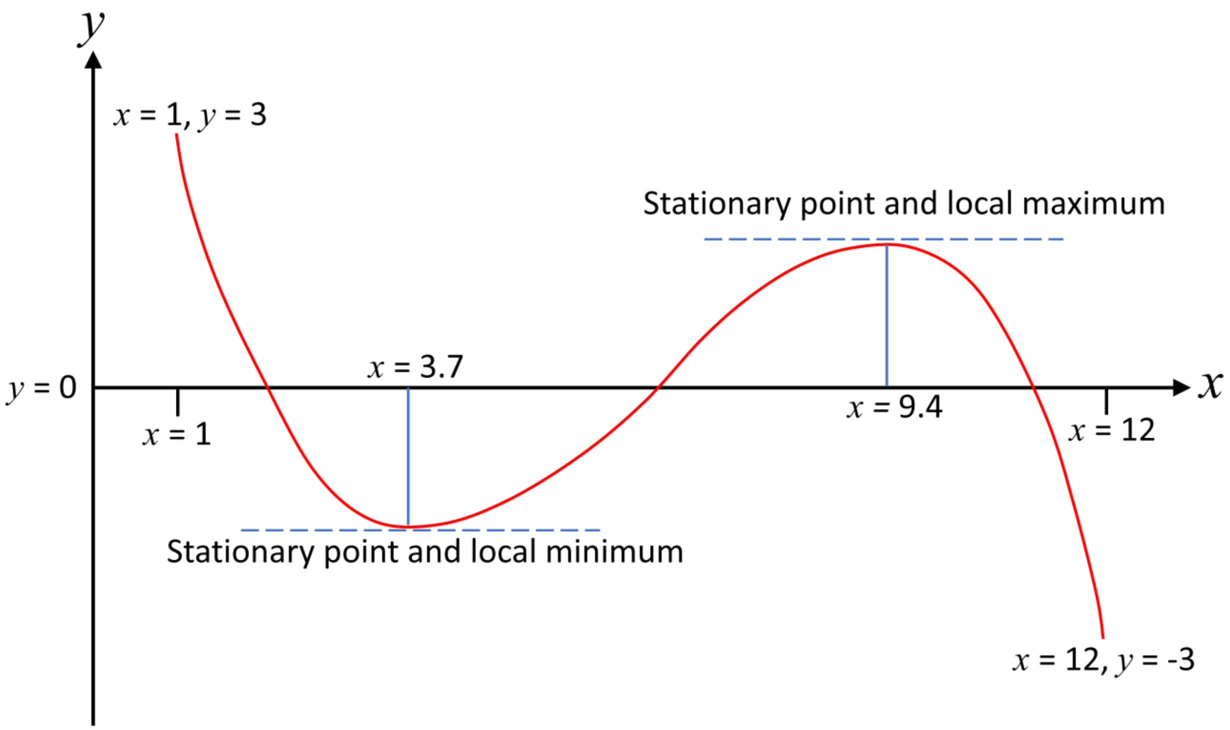

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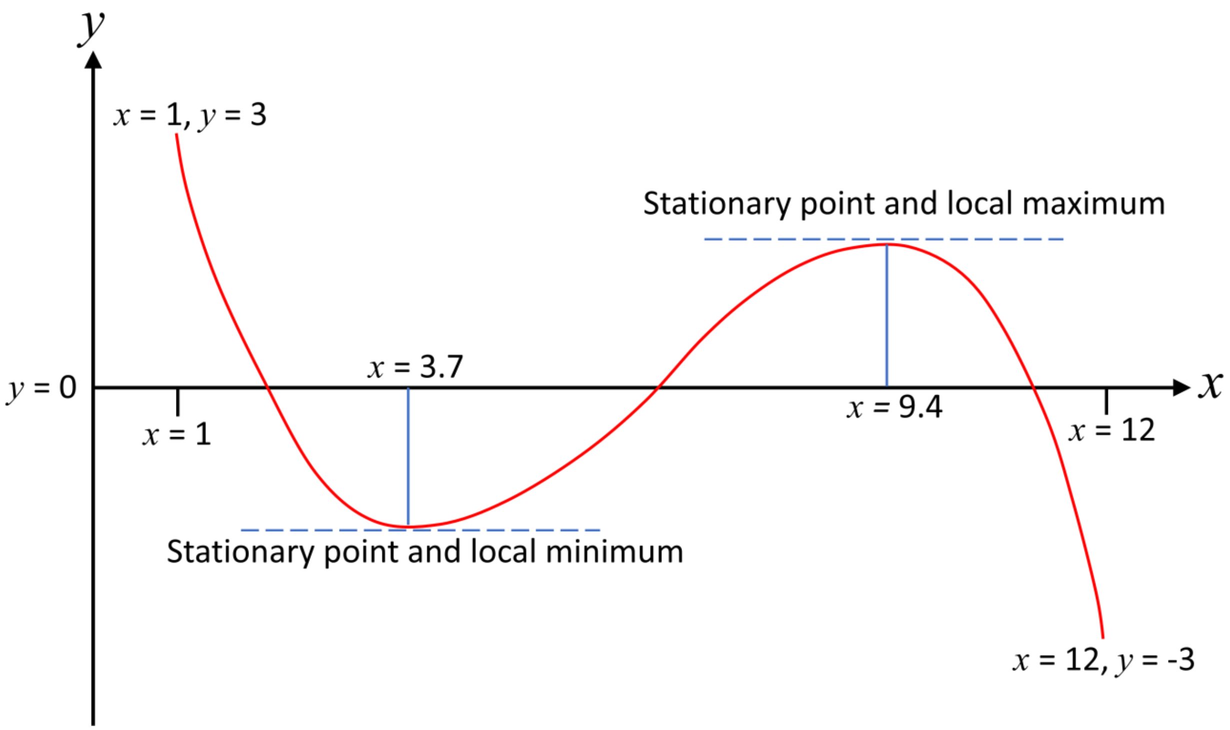
- But the global maximum doesn't have to be a stationary point. If it isn't a stationary point it has to be on the boundary of the region



Vectors

– where we learn to represent data

Data as vectors

- We think of data values $x_1, x_2, \ldots, x_d$ as being a d-dimensional row vector

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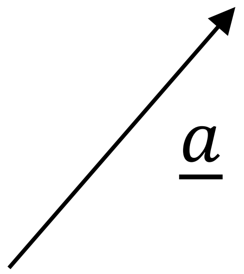

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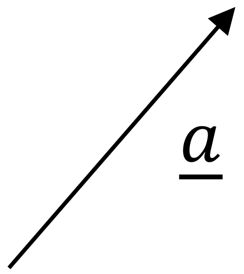
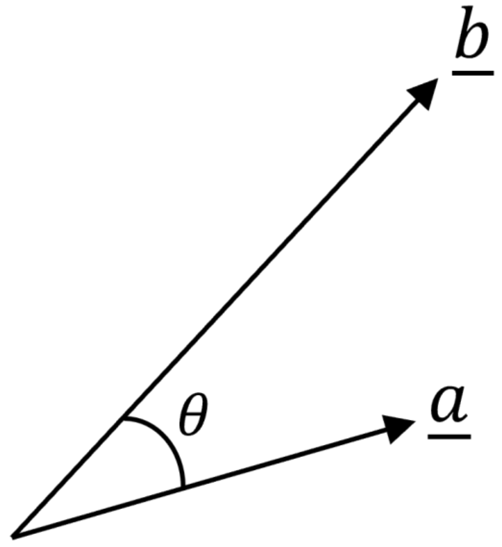


- We can also use a column vector to represent the data $\underline{a} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_d \end{pmatrix}$

Operations on vectors: Inner product

- We often want to compare vectors

- Cosine similarity: $\cos\theta = \frac{\underline{a}\cdot\underline{b}}{|\underline{a}||\underline{b}|}$



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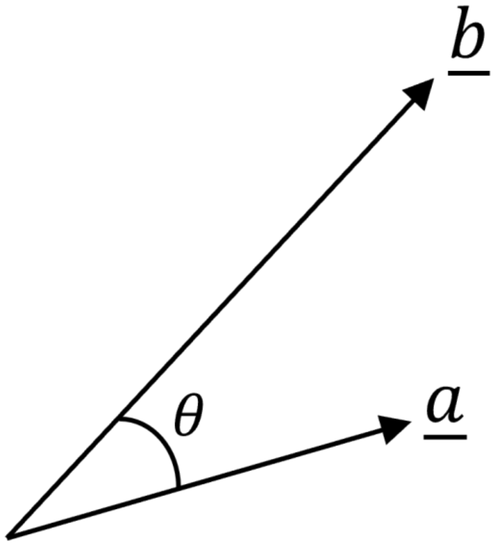
- $\underline{b} \cdot \underline{a} = \underline{a} \cdot \underline{b}$



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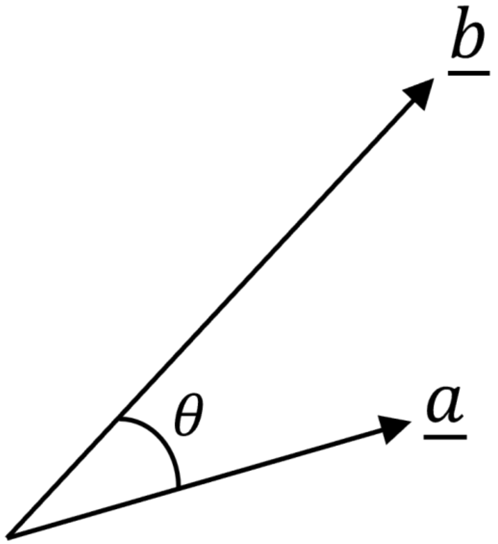
- $\underline{b}\cdot\underline{a} = \underline{a}\cdot\underline{b}$
- Inner product takes two 1-dimensionional objects (vectors) and returns a scalar (a 0-dimensional object)



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- $\underline{a} \otimes \underline{b}$ not necessarily the same as $\underline{b} \otimes \underline{a}$

Python code examples

- Open up the Jupyter notebook Lesson1.ipynb in the github repository

https://github.com/dchoyle/ODSCWest2025_MathBootcamp/

Matrices

– where we learn to transform data

Matrix elements

- A matrix is a 2D object, a 2D-array

$$\underline{\underline{M}} = \begin{pmatrix} 7 & 3 & 2 & 5 \\ 1 & -2 & -1 & 6 \\ 1 & -9 & 14 & 0 \end{pmatrix}$$

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- A d-dimensional column vector is a $d \times 1$ matrix
- A d-dimensional row vector is a $1 \times d$ matrix

Matrix operations: Transpose

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- E.g. $\underline{\underline{A}} = \begin{pmatrix} 1 & 0 & 7 \\ 2 & 3 & 1 \\ 3 & 9 & 0 \end{pmatrix} \Longrightarrow \underline{\underline{A}}^{\top} = \begin{pmatrix} 1 & 2 & 3 \\ 0 & 3 & 9 \\ 7 & 1 & 0 \end{pmatrix}$

Matrix multiplication

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- Matrix element $C_{ij} = \sum_{k=1}^{K} A_{ik} B_{kj}$
- The matrix sizes obey a simple relation

common dimension

$$\begin{array}{ccccc} M \times N & & M \times K & & K \times N \\ \text{Matrix } \underline{\underline{C}} & = & \text{Matrix } \underline{\underline{A}} & \times & \text{Matrix } \underline{\underline{B}} \end{array}$$

Inner product as a matrix multiplication

Row vector | Column vector

$$\begin{pmatrix} a_1 & a_2 & \dots & a_d \end{pmatrix} \times \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_d \end{pmatrix} = \sum_{i=1}^{d} a_i b_i$$

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$$= \underline{a}^{\top}\underline{b} \;\Rightarrow\; \underline{a} \cdot \underline{b} = \underline{b}^{\top}\underline{a}$$

Inner product as a matrix multiplication

Row vector

Column vector

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$$\underline{a} \otimes \underline{b} = \underline{a}\,\underline{b}^{\top}$$

Matrix multiplication as a series of inner products

$$\underline{\underline{A}}\,\underline{\underline{B}} = \begin{array}{c} \underline{A}_1 \rightarrow \\ \\ \\ \underline{A}_M \rightarrow \end{array} \begin{pmatrix} A_{11} & A_{12} & \cdots & A_{1K} \\ A_{21} & A_{22} & \cdots & A_{2K} \\ \vdots & \vdots & \ddots & \vdots \\ A_{M1} & A_{M2} & \cdots & A_{MK} \end{pmatrix} \times \begin{array}{c} \begin{array}{cccc} & \underline{B}_2 & & \underline{B}_N \\ & \downarrow & & \downarrow \end{array} \\ \begin{pmatrix} B_{11} & B_{12} & \cdots & B_{1N} \\ B_{21} & B_{22} & \cdots & B_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ B_{K1} & B_{K2} & \cdots & B_{KN} \end{pmatrix} \end{array}$$

$$= \begin{pmatrix} \underline{A}_1^\top \underline{B}_1 & \underline{A}_1^\top \underline{B}_2 & \cdots & \underline{A}_1^\top \underline{B}_N \\ \underline{A}_2^\top \underline{B}_1 & \underline{A}_2^\top \underline{B}_2 & \cdots & \underline{A}_2^\top \underline{B}_N \\ \vdots & \vdots & \ddots & \vdots \\ \underline{A}_M^\top \underline{B}_1 & \underline{A}_M^\top \underline{B}_2 & \cdots & \underline{A}_M^\top \underline{B}_N \end{pmatrix}$$

i, j element of $\underline{\underline{A}}\,\underline{\underline{B}}$ is the inner product between i^{th} row of $\underline{\underline{A}}$ and j^{th} column of $\underline{\underline{B}}$

Python examples 1

- Open up the Jupyter notebook Lesson1.ipynb in the github repository

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What a matrix does

- Multiplying a vector by a matrix gives us another vector

$$\underline{\underline{A}}\,\underline{b} = \begin{pmatrix} A_{11} & \cdots & A_{1N} \\ \vdots & \ddots & \vdots \\ A_{M1} & \cdots & A_{MN} \end{pmatrix} \times \begin{pmatrix} b_1 \\ \vdots \\ b_N \end{pmatrix} = \begin{pmatrix} A_{11}b_1 + A_{12}b_2 + \cdots + A_{1N}b_N \\ \vdots \\ A_{M1}b_1 + A_{M2}b_2 + \cdots + A_{MN}b_N \end{pmatrix}$$

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- So, matrices transform vectors. A matrix represents a transformation

- The components of the new vector on the RHS are linear combinations of the components of the old vector. So, a matrix represents a linear transformation

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- $\underline{\underline{I}}_d$ is a $d \times d$ square matrix. In fact $\underline{\underline{I}}_d = \begin{pmatrix} 1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 1 \end{pmatrix}$ $\quad I_{ij} = \begin{cases} 1 \text{ if } i = j \\ 0 \text{ if } i \neq j \end{cases}$

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- The inverse of the square $d \times d$ matrix $\underline{\underline{A}}$ is a matrix denoted by $\underline{\underline{A}}^{-1}$ that satisfies,

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- We can use Python functions to calculate $\underline{\underline{A}}^{-1}$

Python examples 2

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Lesson 2

Putting it altogether

Linear models

– where we learn how to make simple predictions

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$$= (x_{i0}, x_{i1}, x_{i2}, \dots, x_{id})\underline{\beta} = \underline{x}_i^\top \underline{\beta} = \underline{\beta}^\top \underline{x}_i$$

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- The vector of all our predictions is $\underline{\hat{y}} = \begin{pmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \vdots \\ \hat{y}_N \end{pmatrix} = \underline{\underline{X}}\,\underline{\beta}$

$$N \times (d+1)$$

$$\underline{\underline{X}} = \begin{pmatrix} 1 & x_{11} & \cdots & x_{1d} \\ 1 & x_{21} & & x_{2d} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_{N1} & \cdots & x_{Nd} \end{pmatrix}$$

How to train a linear model

- The observed (ground-truth) values are $\underline{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{pmatrix}$
- What is a good choice for the model parameters $\underline{\beta}$?

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- The observed (ground-truth) values are $\underline{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{pmatrix}$
- What is a good choice for the model parameters $\underline{\beta}$?
- The difference between model predictions and ground-truth values is a vector,

$$\underline{y} - \underline{\hat{y}} = \begin{pmatrix} y_1 - \hat{y}_1 \\ y_2 - \hat{y}_2 \\ \vdots \\ y_N - \hat{y}_N \end{pmatrix} = \begin{pmatrix} r_1 \\ r_2 \\ \vdots \\ r_N \end{pmatrix} = \underline{r}$$

- A good choice of parameters will make $\sum_{i=1}^{N} r_i^2$ as small as possible

OLS regression

– where we learn how to train linear models

How to train a linear model: OLS regression

- Minimizing $\sum_{i=1}^{N} r_i^2$ with respect to $\underline{\beta}$ is called Ordinary Least Squares (OLS) regression

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- The equations we have to solve are,

$$\sum_{i=1}^{N} \left(y_i - \underline{\beta}^\top \underline{x}_i\right) x_{ij} = 0 \quad \text{for} \quad j = 0,1,2,\ldots,d$$

How to train a linear model: OLS regression

- Again, we can write the equations in more succinct form using vectors and matrices ,

$$\underline{\underline{X}}^{\top}\underline{y} - \underline{\underline{X}}^{\top}\underline{\underline{X}}\,\underline{\beta} = \underline{0}$$

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$\underline{\underline{X}}^{\top}\underline{\underline{X}}$ is a $(d+1) \times (d+1)$ square matrix. It has an inverse.

How to train a linear model: OLS regression

- Apply the inverse matrix to both sides of the equation

$$\left(\underline{\underline{X}}^{\top}\underline{\underline{X}}\right)^{-1}\left(\underline{\underline{X}}^{\top}\underline{\underline{X}}\right)\underline{\beta} = \left(\underline{\underline{X}}^{\top}\underline{\underline{X}}\right)^{-1}\underline{\underline{X}}^{\top}\underline{y}$$

$$\underline{\beta} = \left(\underline{\underline{X}}^{\top}\underline{\underline{X}}\right)^{-1}\underline{\underline{X}}^{\top}\underline{y}$$

- We get a closed form expression for the OLS parameter estimates of our linear model

OLS: Python Examples

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Gradient descent

– where we learn how to use derivatives to train any model

OLS Recap

- Why did we get a simple closed-form expression for $\underline{\beta}$?
  1. Our minimum condition was linear in $\underline{\beta}$, so we could use linear algebra
  2. Our minimum condition was linear in $\underline{\beta}$ because our starting loss-function, $\sum_i r_i^2$, that was quadratic in the model parameters

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- A: Yes, using gradient descent

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- For OLS regression we had $l(y, \hat{y}) = (y - \hat{y})^2$

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- The optimal value of β solves the equation $\frac{d\text{Risk}}{d\beta} = 0$
- The current gradient value of tells us which direction we need to move β

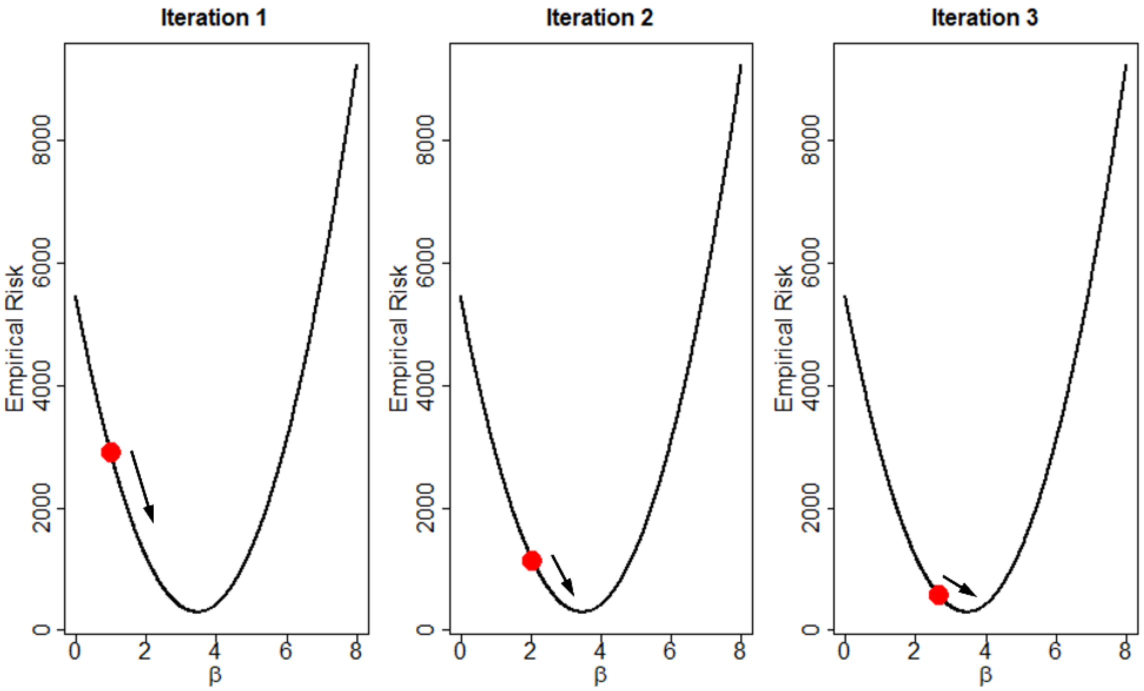
$$\frac{d\text{Risk}}{d\beta} > 0 \quad \Longrightarrow \text{ Risk is increasing } \quad \Longrightarrow \text{ Should decrease } \beta$$

$$\frac{d\text{Risk}}{d\beta} < 0 \quad \Longrightarrow \text{ Risk is decreasing } \quad \Longrightarrow \text{ Should increase } \beta$$

Gradient descent

- This produces a learning update rule
  $\beta \leftarrow \beta - \eta \dfrac{d\mathrm{Risk}}{d\beta}$

- This is "gradient descent"



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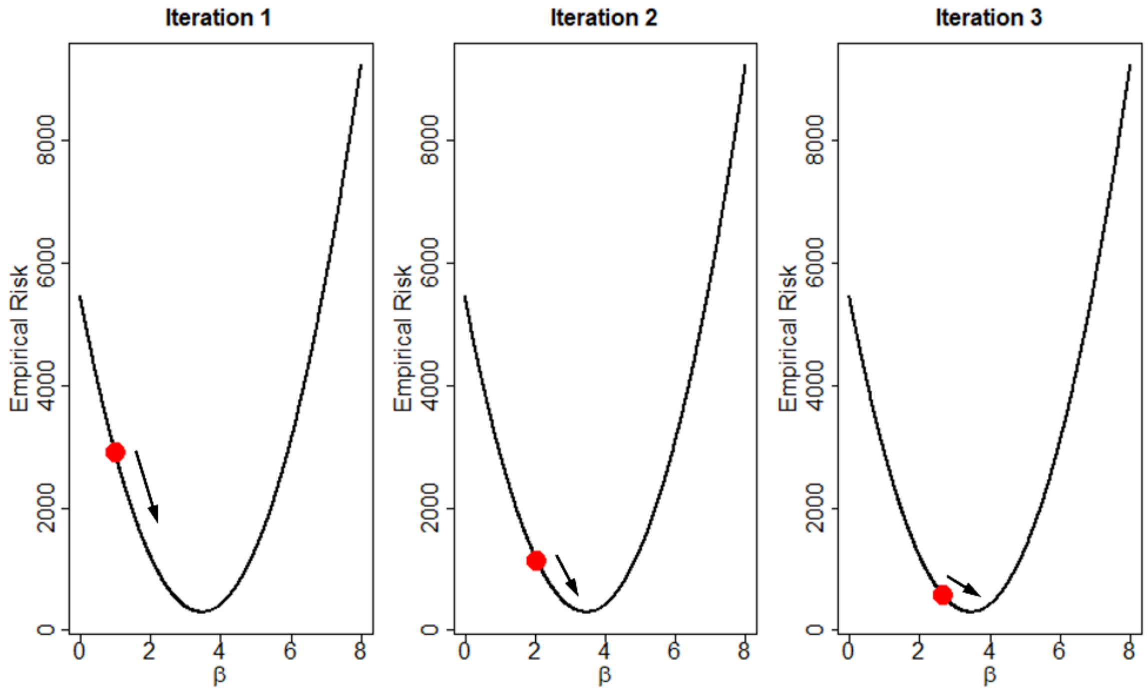

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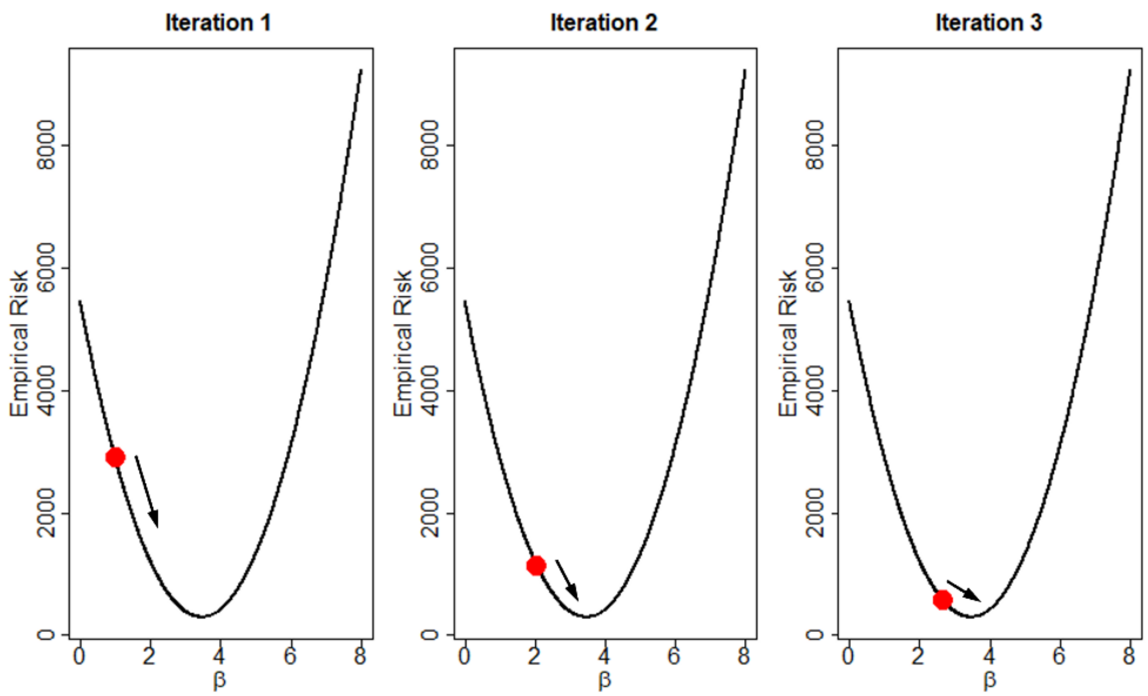
- Advanced algorithms use an adaptive learning rate



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Thank you for listening

Questions?

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