Introduction to Data Science and Machine Learning

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Summary

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  - **Computer Science**: How to program a computer to solve problems?

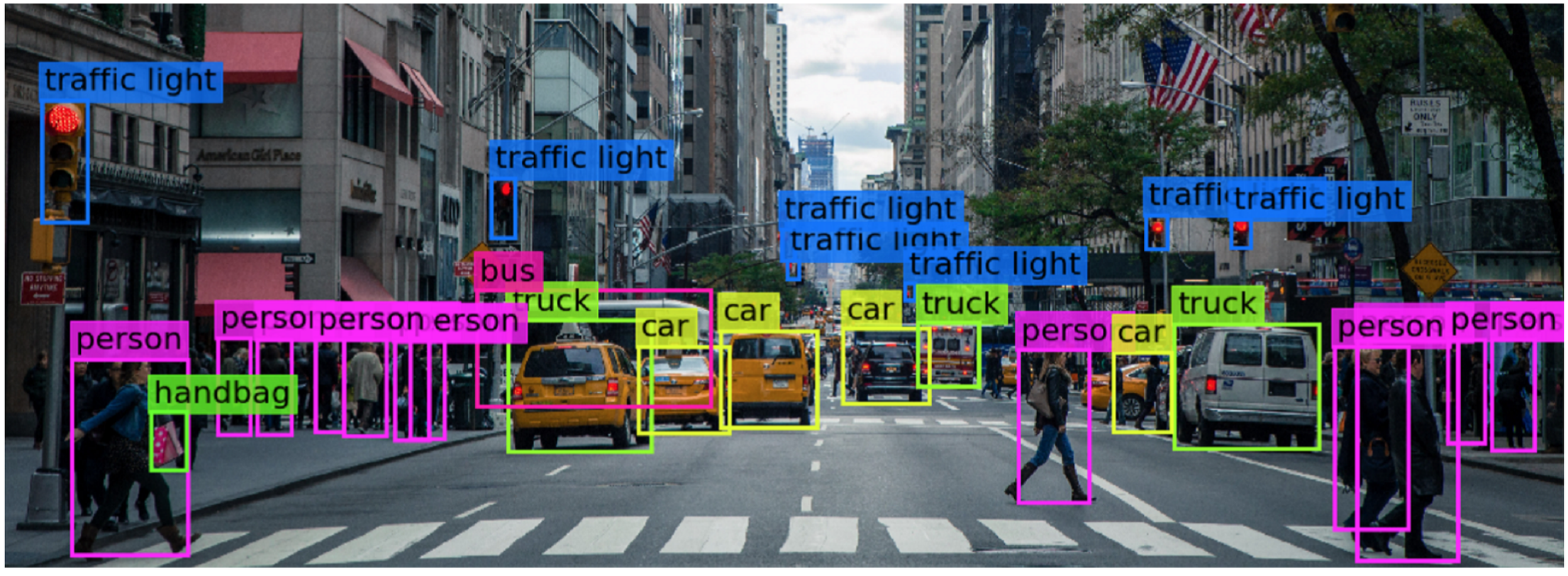
  - **Statistics**: How to extract knowledge from data?

Machine Learning is everywhere

- Computer Vision
- Robotics
- Autonomous vehicles
- Natural language processing, Speech recognition
- Search engines
- Recommender systems
- Medical diagnosis
- Etc.

Computer vision

- Object recognition / scene labeling



Robotics

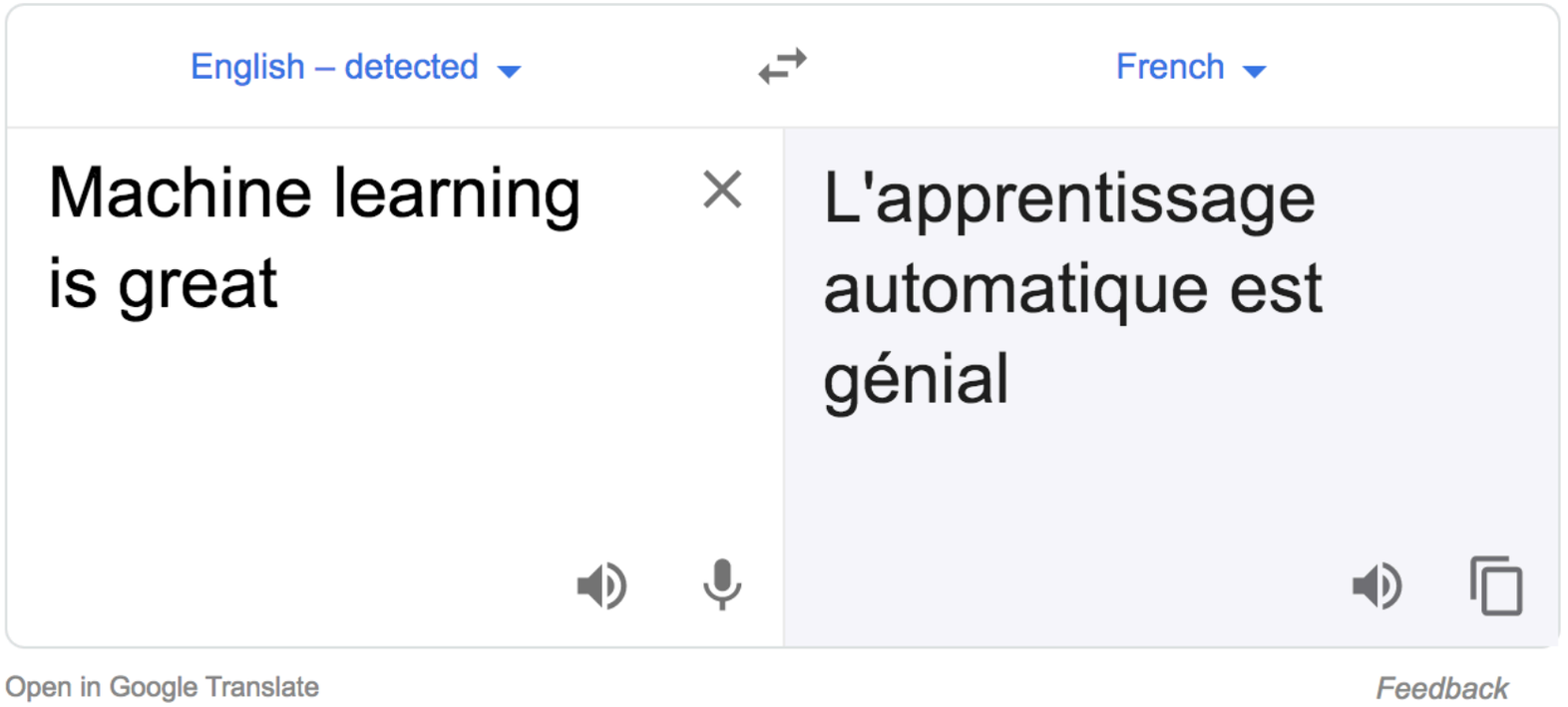
- Tasks automation

Autonomous vehicles

- Autonomous driving

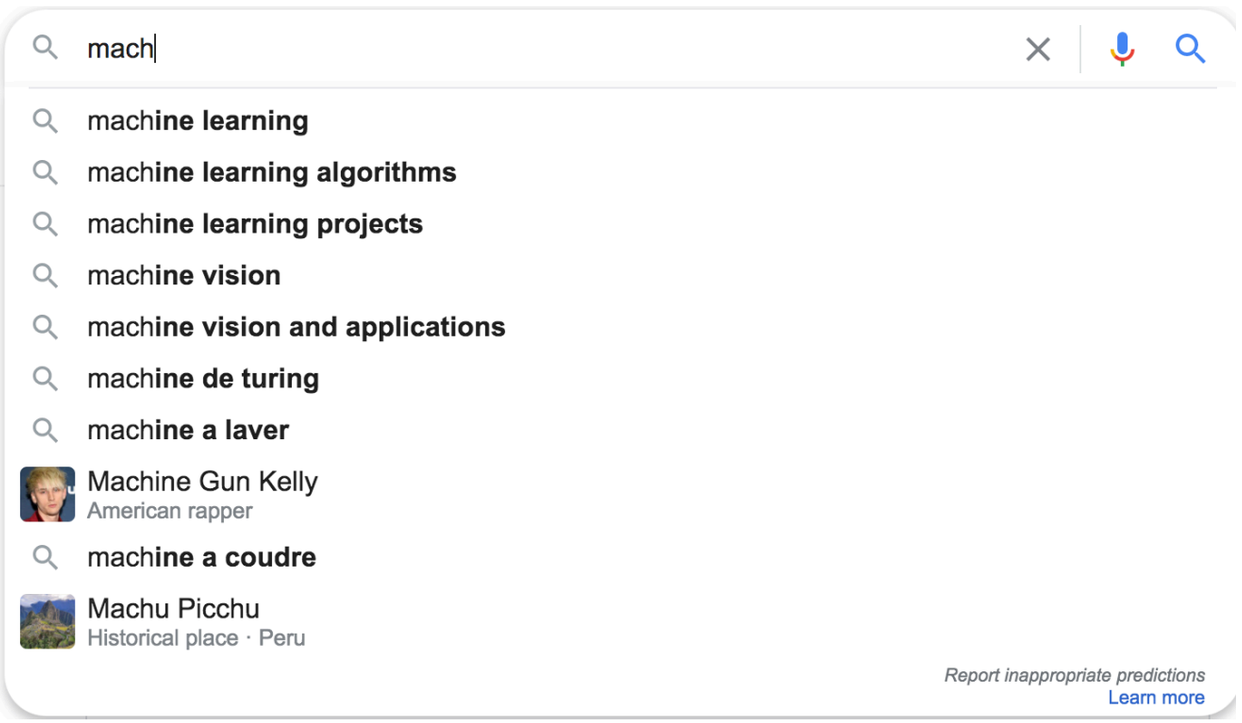
Natural language processing

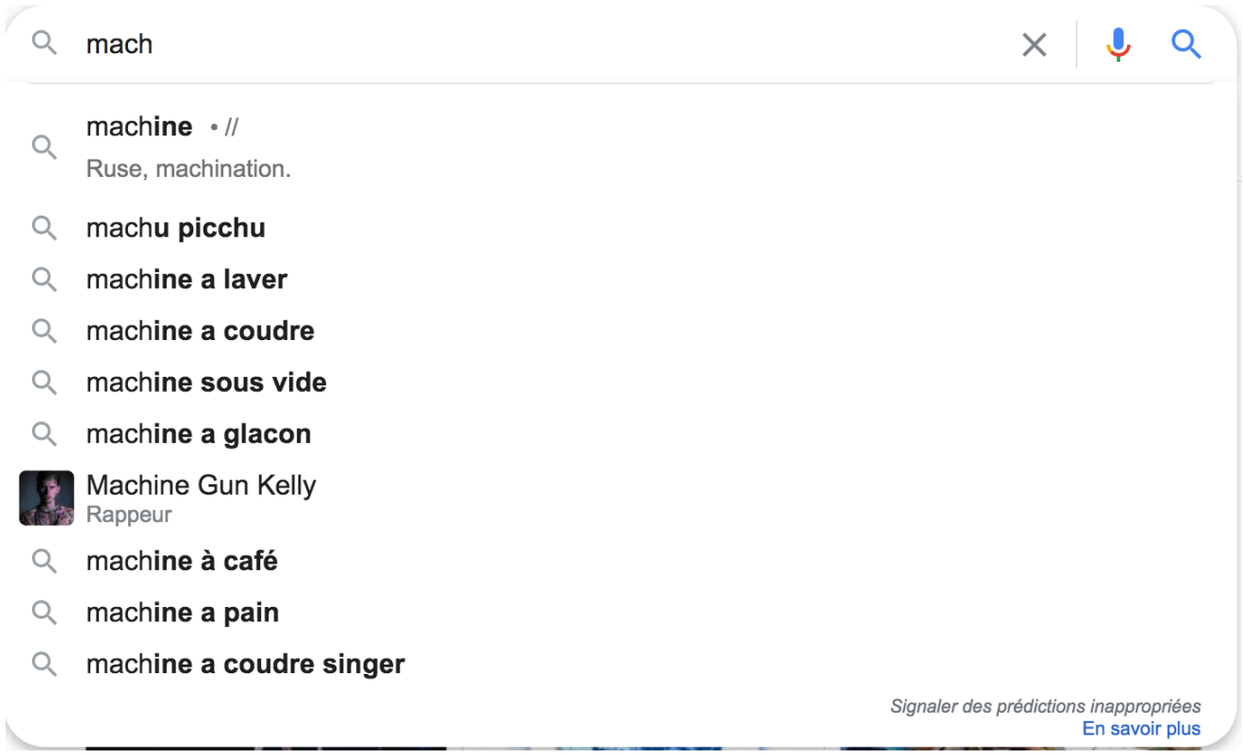
- Machine translation



Search engines

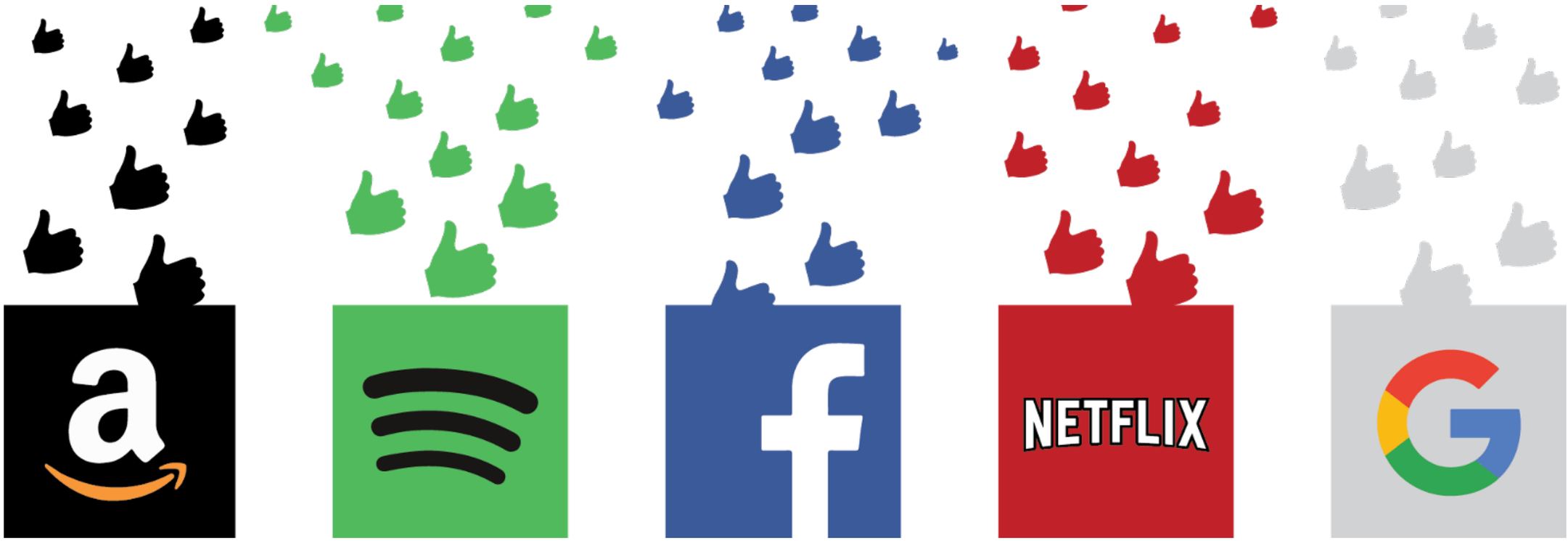
- Search engines optimization





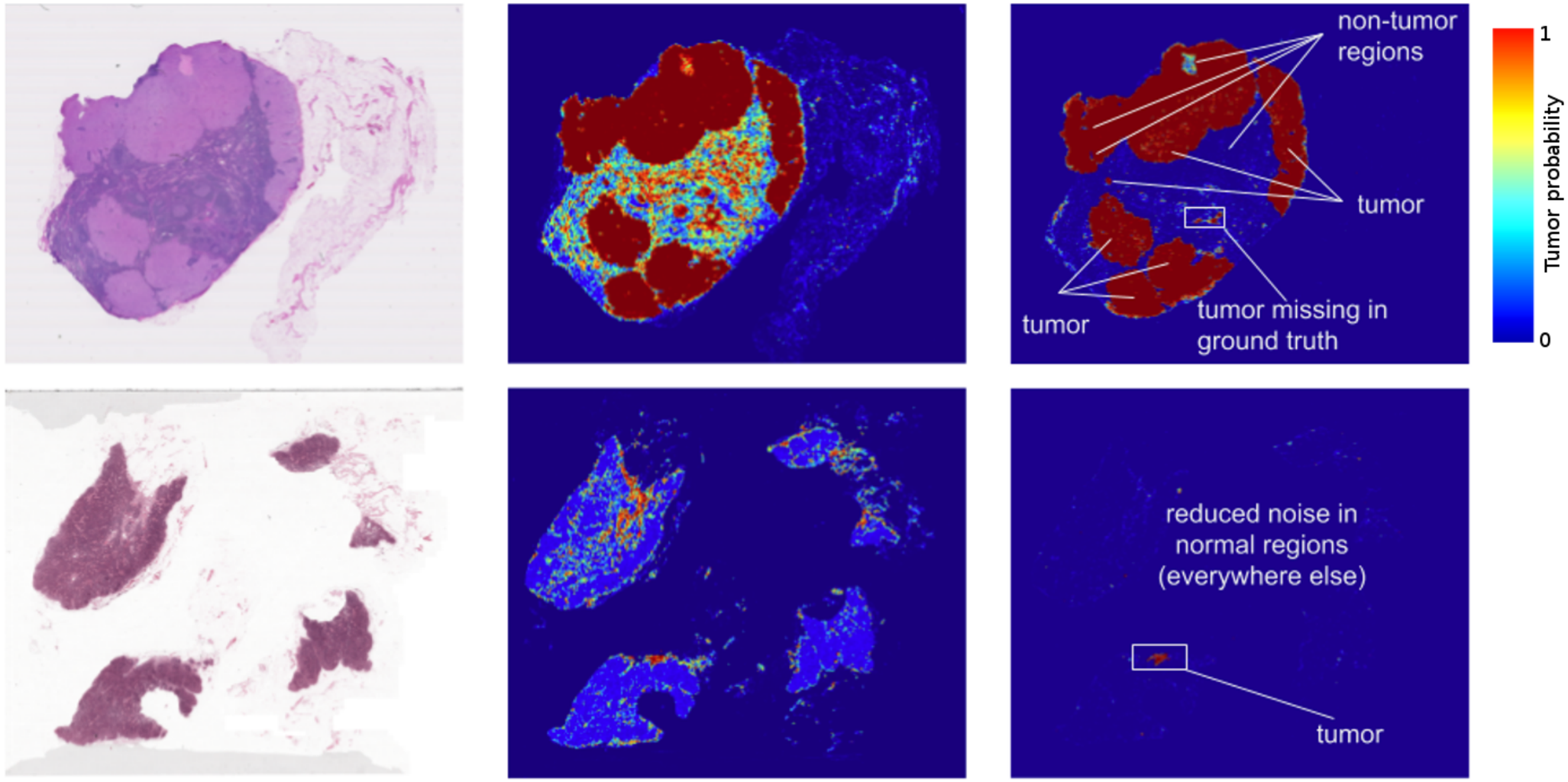
Recommender systems

- Recommender systems optimization



Medical diagnosis

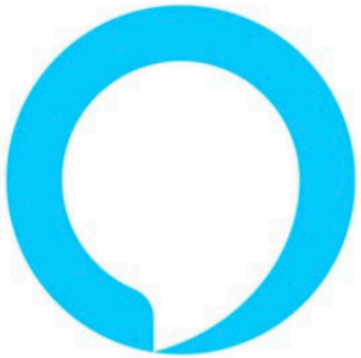
- Cancer detection



Speech recognition

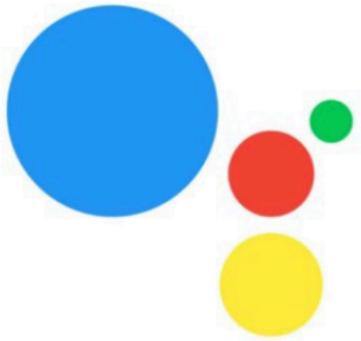
- Voice assistants

"Hey Cortana"



"Hey Alexa"

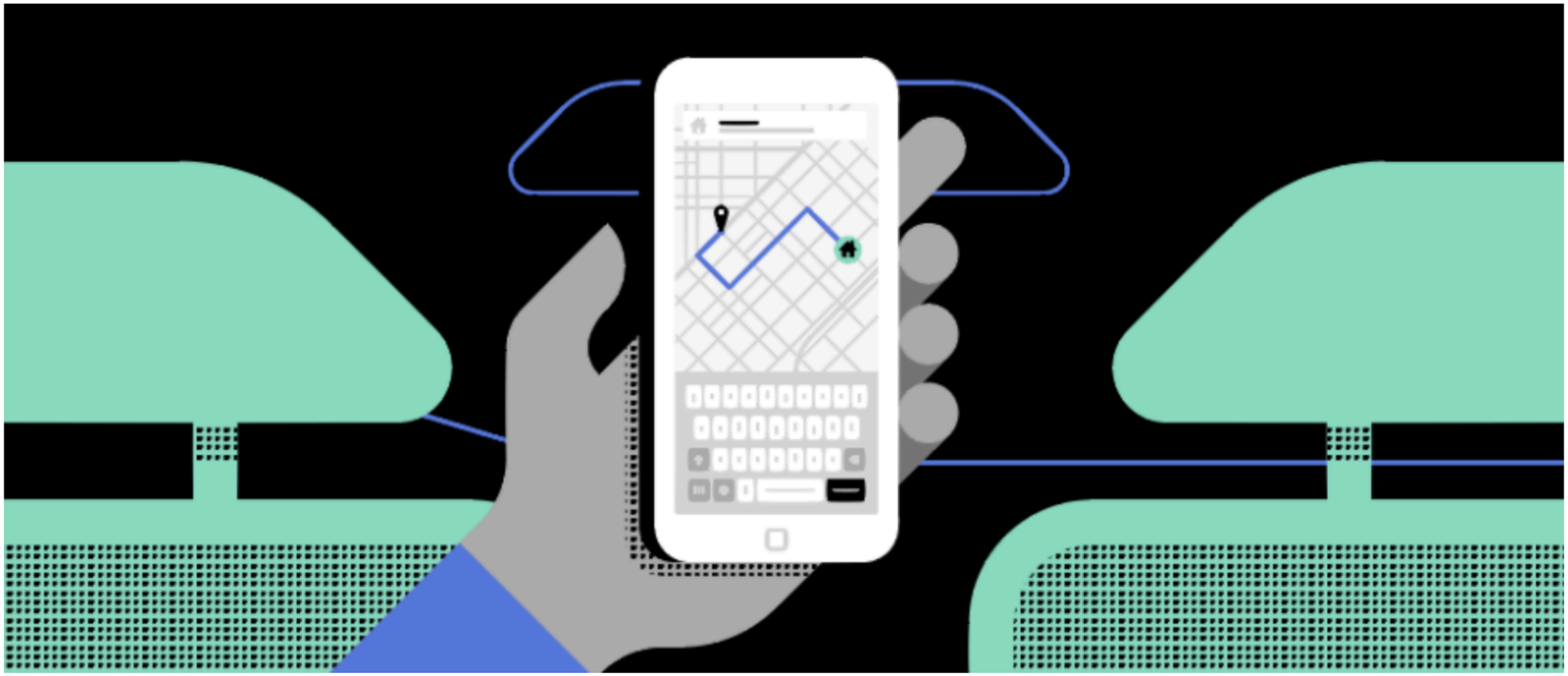
"Hey Siri"



"Hey Google"

Pricing

- Dynamic pricing in Travel



Fraud detection

- Fraudulent banking operations

Main Types of Machine Learning

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- Supervised Learning
  - Classification
  - Regression
  - Ranking

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- The algorithm is given a **set of labeled training data** (x_1,y_1), (x_2,y_2), … , (x_N,y_N), i.e observations of (input,output)

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- The objective is to correctly **predict unseen** test cases and **understand** which inputs **affect** the outcome and how

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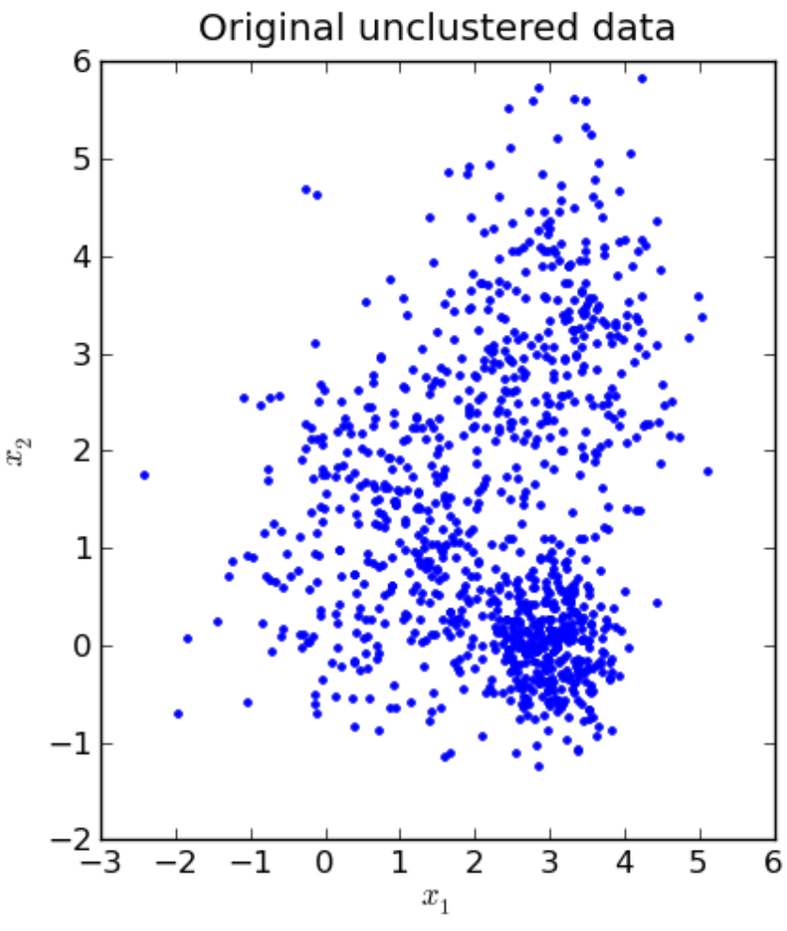
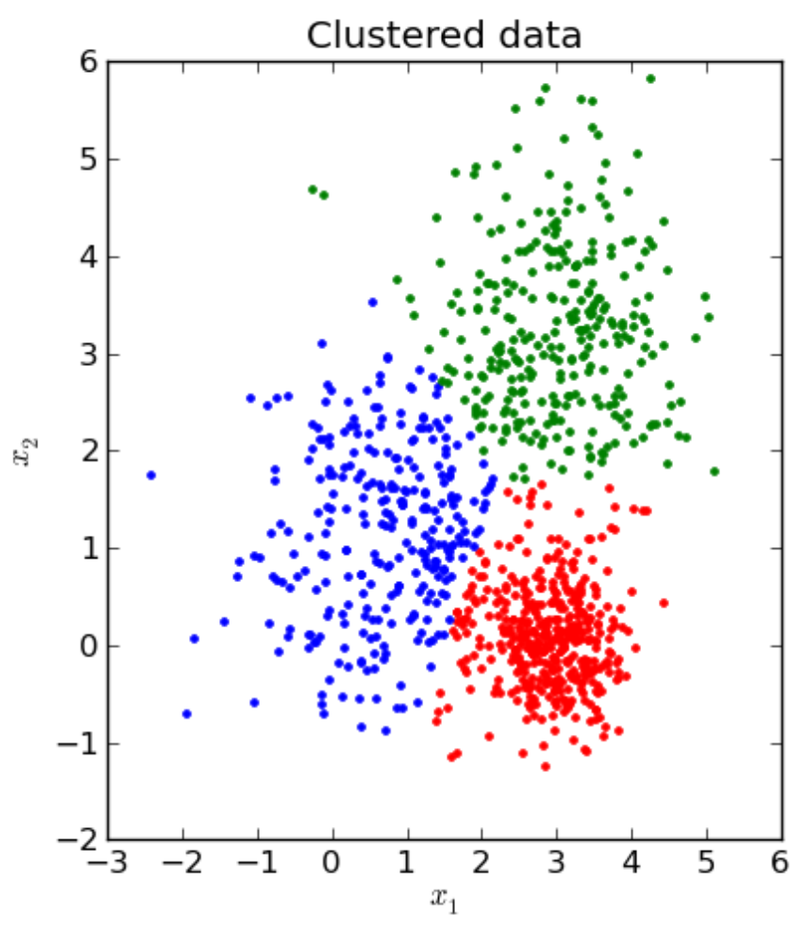
  - Find combinations of features with the most variation (e.g dimensionality reduction)

Unsupervised Learning

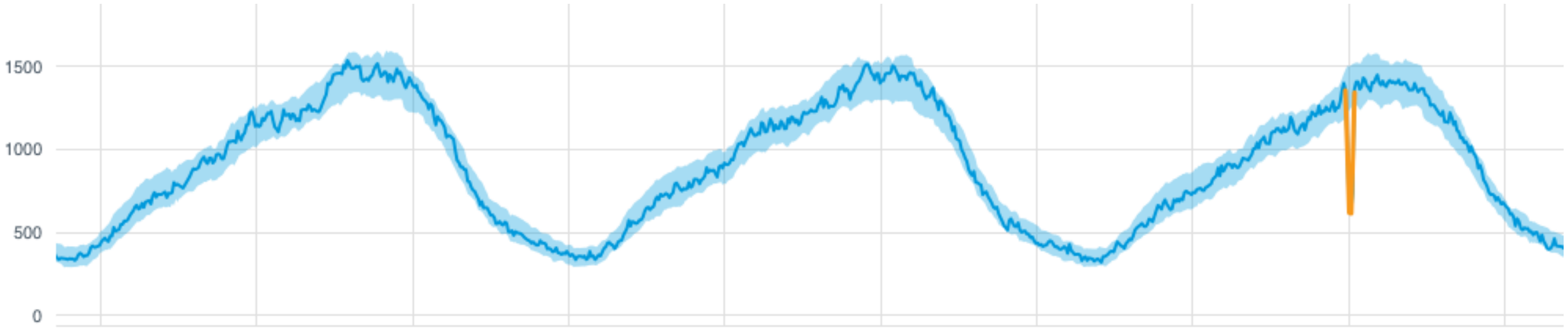
- Clustering





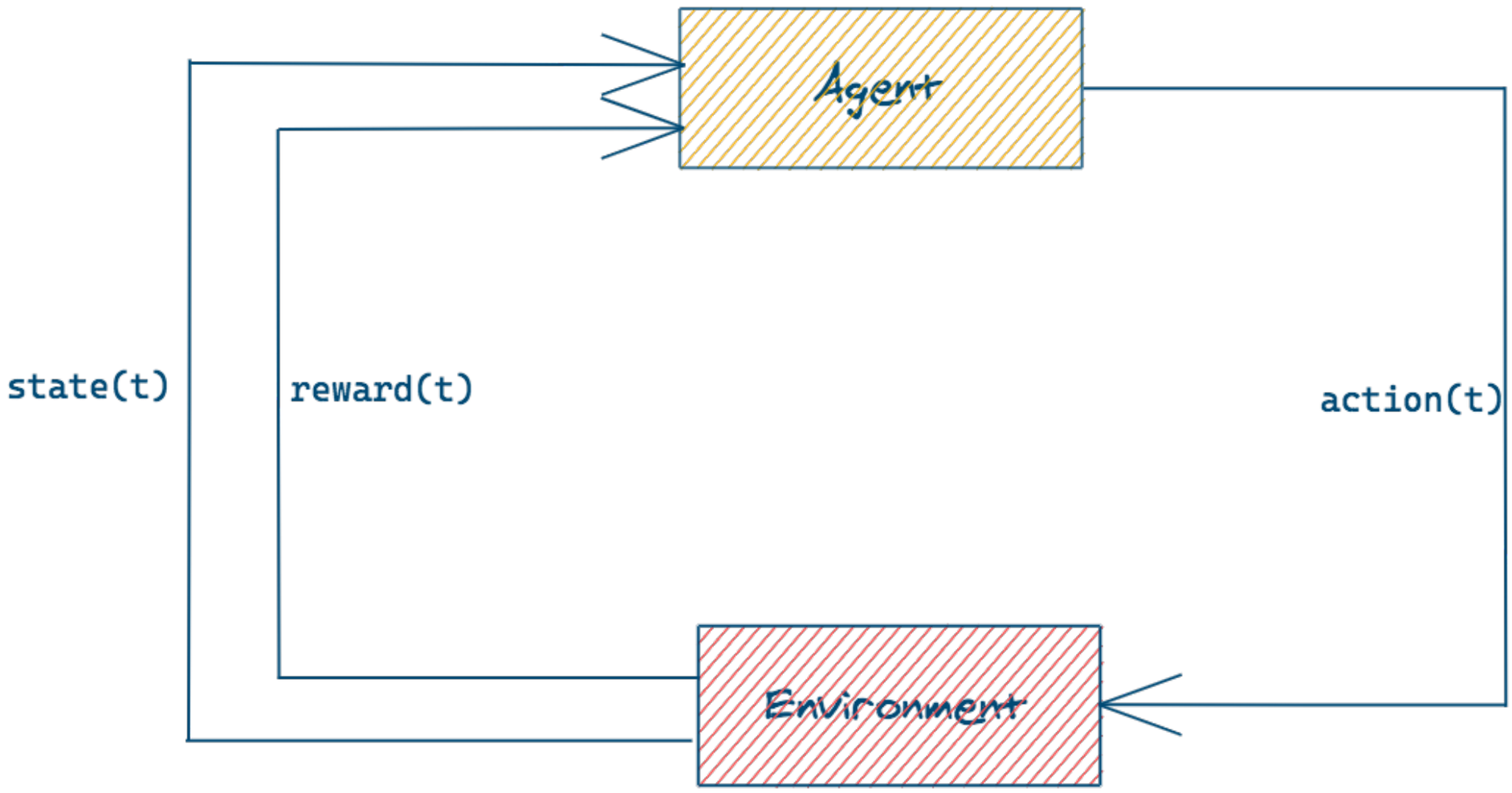
Unsupervised Learning

- Anomaly detection



Reinforcement Learning

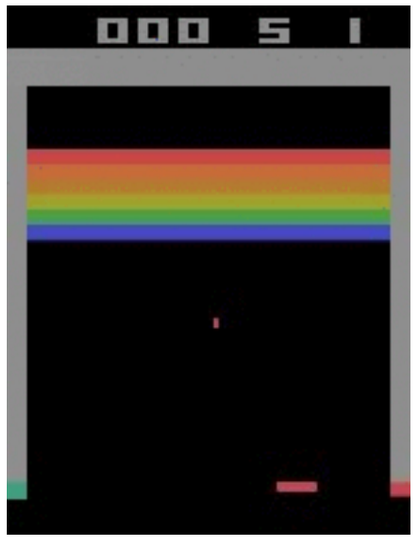
- Algorithms used to train software agents to take actions in an environment in order to maximize a given reward



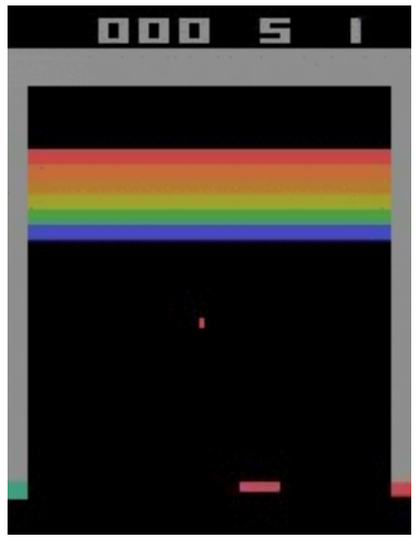
Reinforcement Learning examples

- The ATARI benchmark

Initial attempt



After 30 mins



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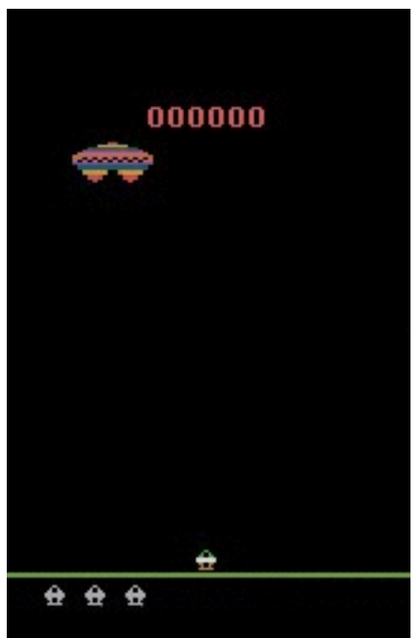

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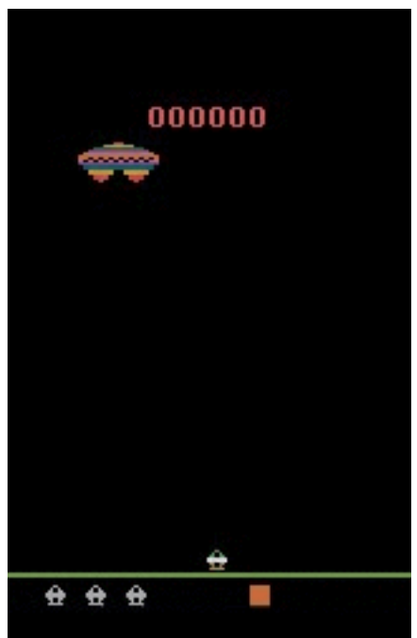

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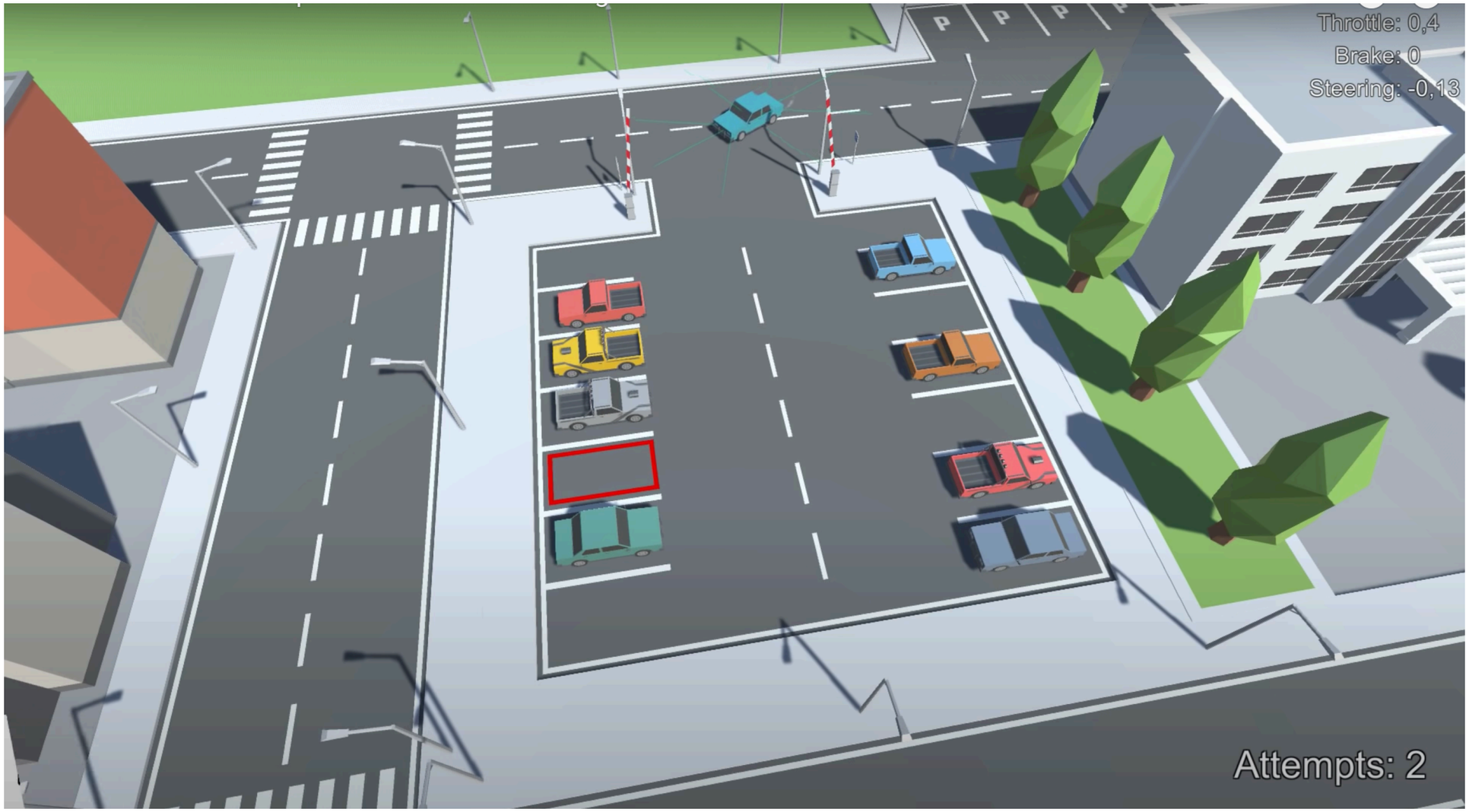
Reinforcement Learning examples

- Learning to park



Generalized Linear Models

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  - **Regression**: predicting quantitative outputs

  - **Classification**: predicting qualitative outputs

- Both can be viewed as a **function approximation task**

First approach: Ordinary Least Squares

- Given a vector of inputs $X^T = (X_1, X_2, \ldots, X_n)$ we predict the output Y via the model

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- **Least Squares** approach: pick $\hat{\beta}$ so as the **minimize** the residual sum of squares

$$RSS(\beta) = \sum_{i=1}^{N} (y_i - x_i^T \beta)^2 = (y - X\beta)^T (y - X\beta)$$

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- This is the **analytical** solution to the minimum least squares

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  - Computing $(X^T X)$ can be **very expensive** for big datasets
  - Matrix inversion to get $(X^T X)^{-1}$ is a **very expensive** and **numerically unstable** operation (e.g: in case of collinearity)
- We need to find a **numerical alternative** solution

Gradient Descent

- Remember: The **goal** is to find the **set of parameters** β to **minimize** a given **cost function** (numerical optimization task)

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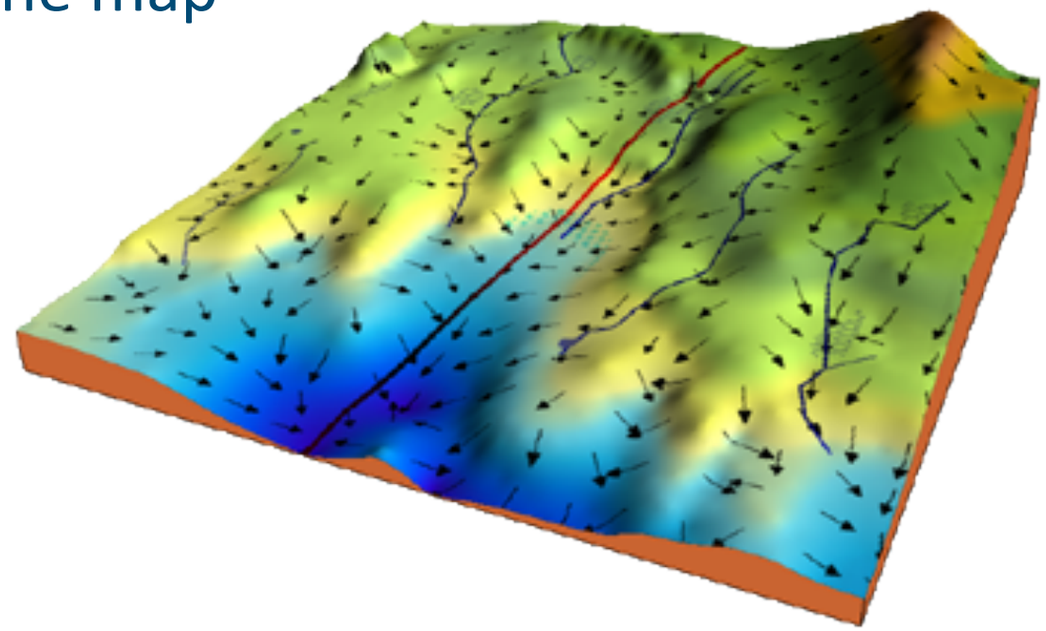
- It is a first-order **iterative optimization algorithm** for finding a local **minimum** of a **differentiable** function
- At each iteration, we take a step proportional to the negative of the gradient of the function

Gradient Descent analogy

- Imagine you're on the **top** of a mountain and you want to reach the **lowest** point of the map



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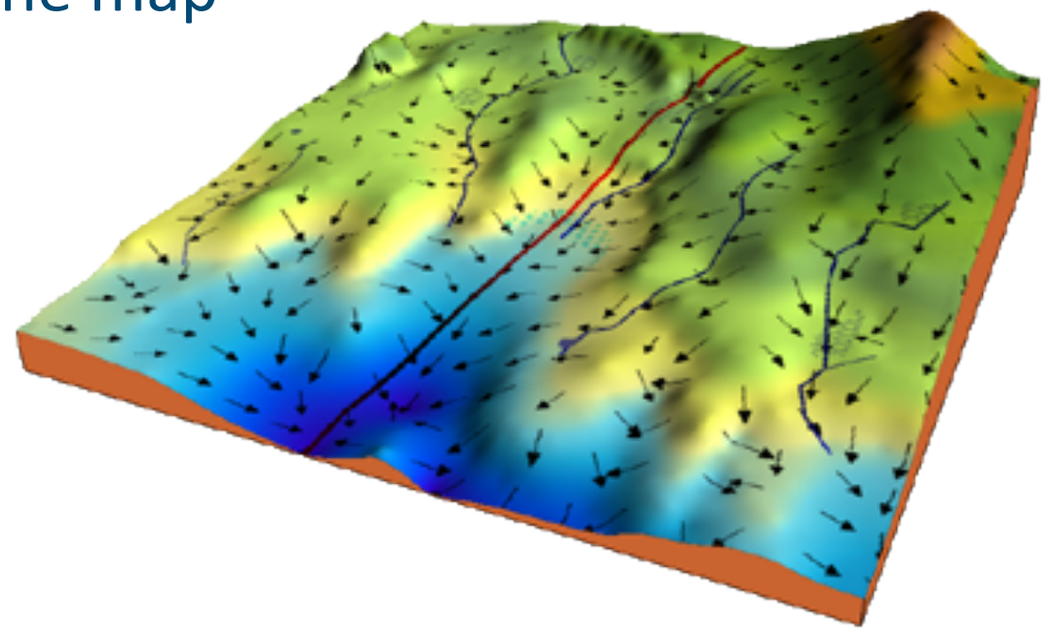

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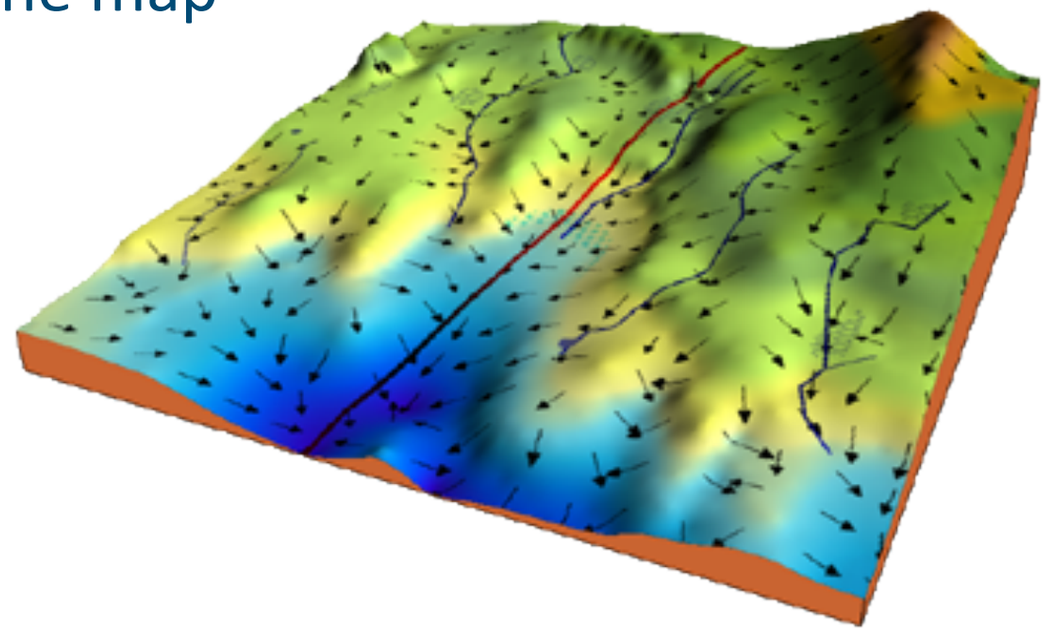

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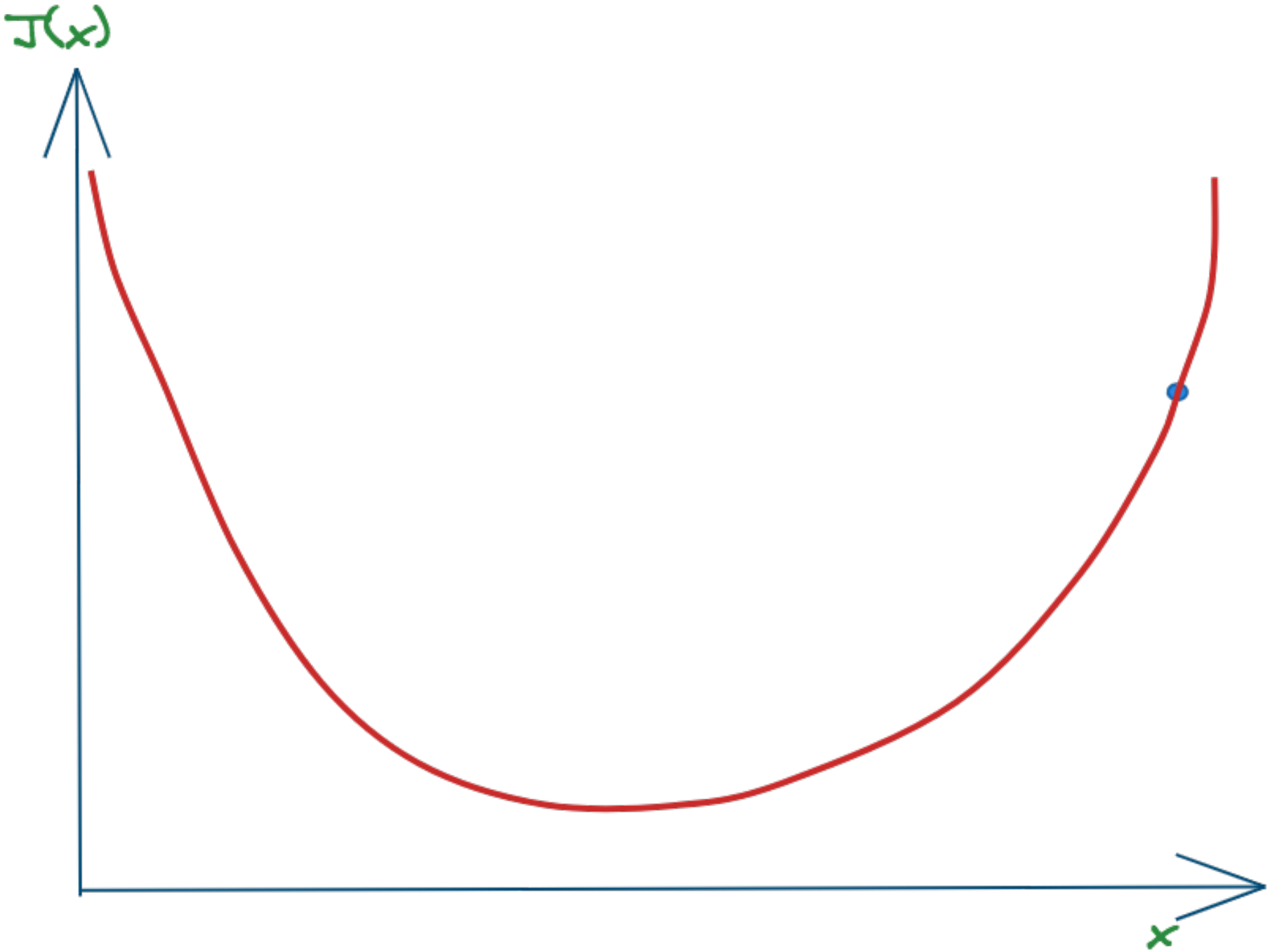
- The idea is to **iteratively** take the direction of the **steepest descent** until you can no longer move downhill (local minimum)

Gradient Descent intuition



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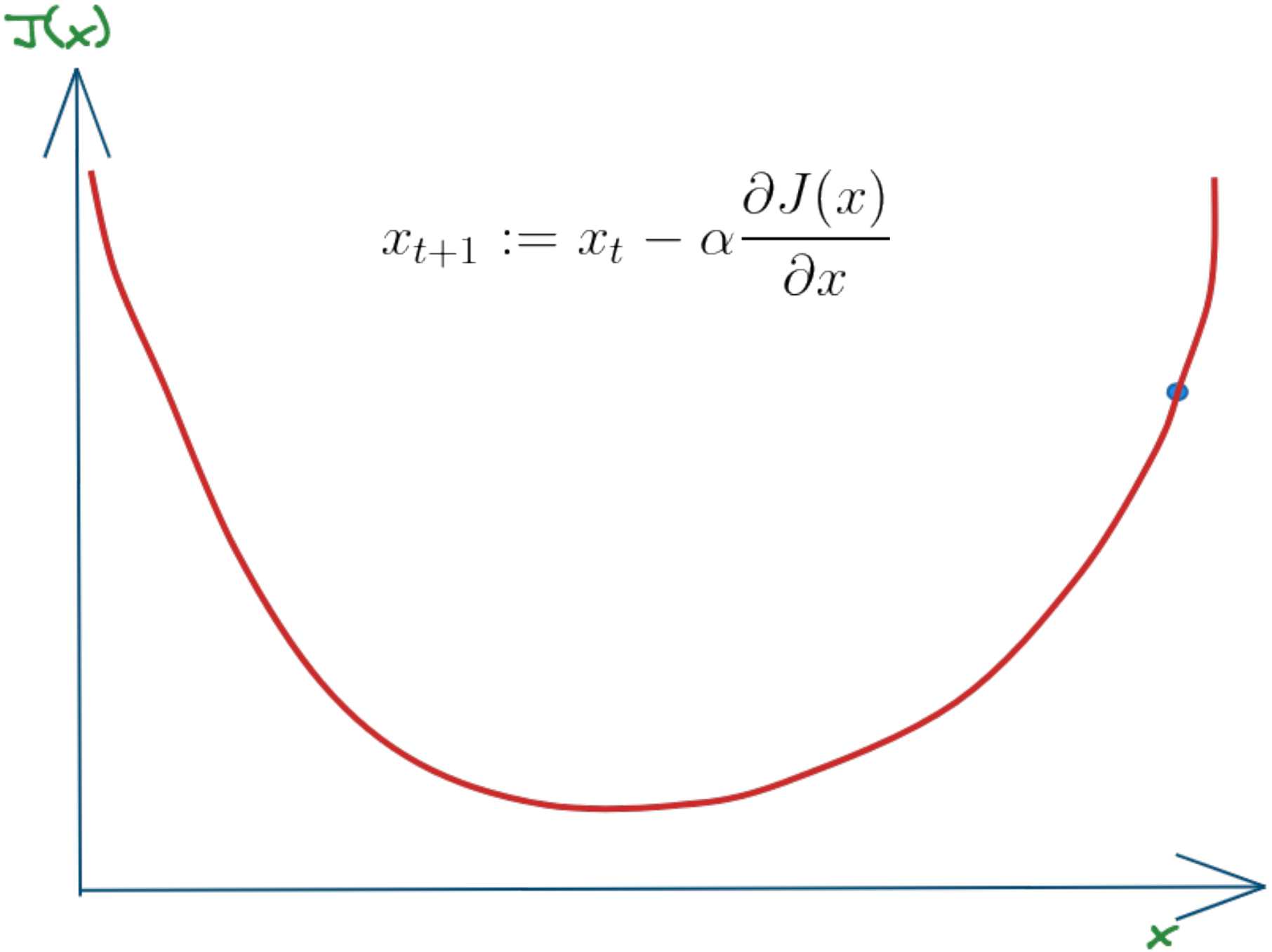

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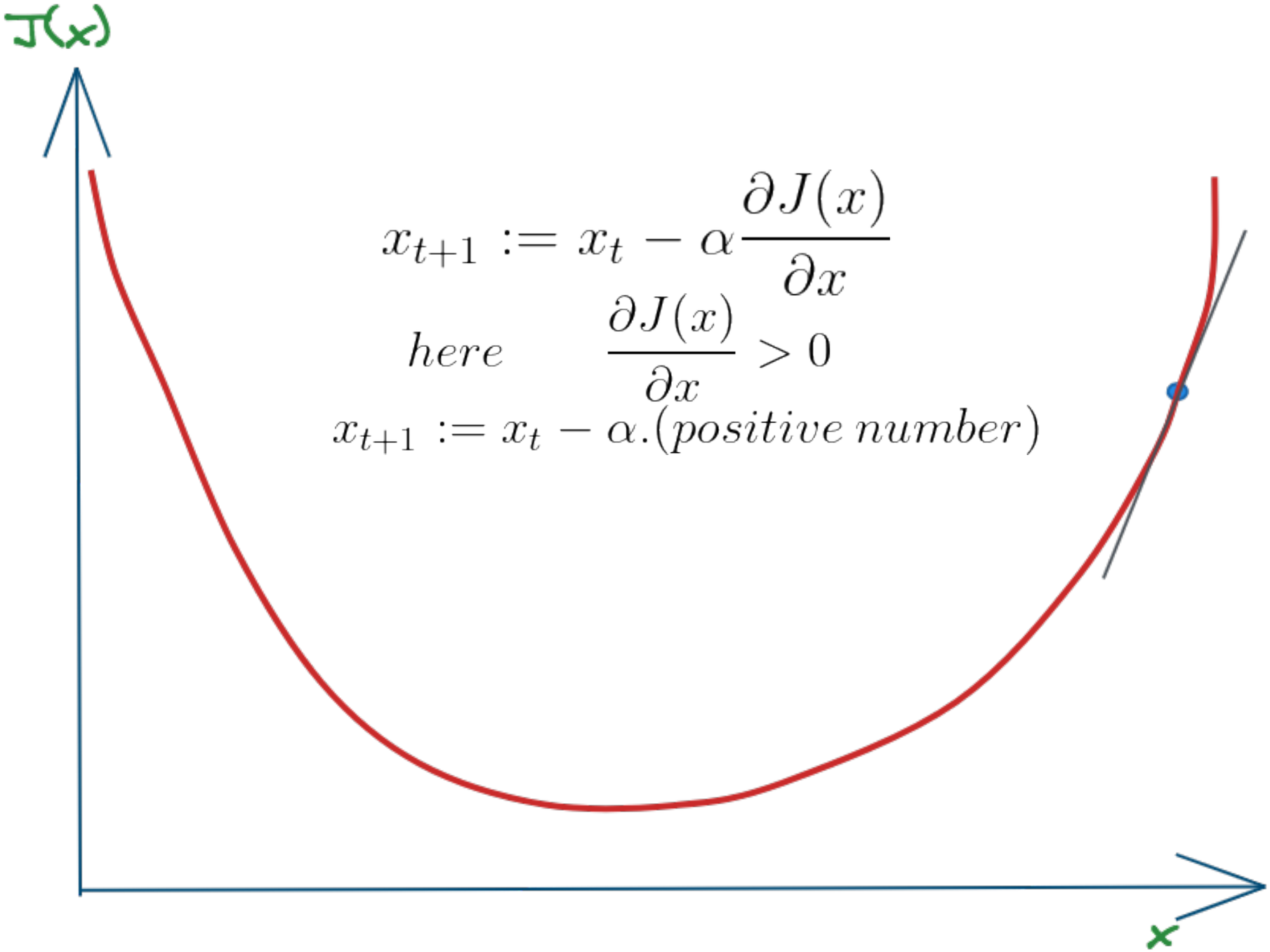
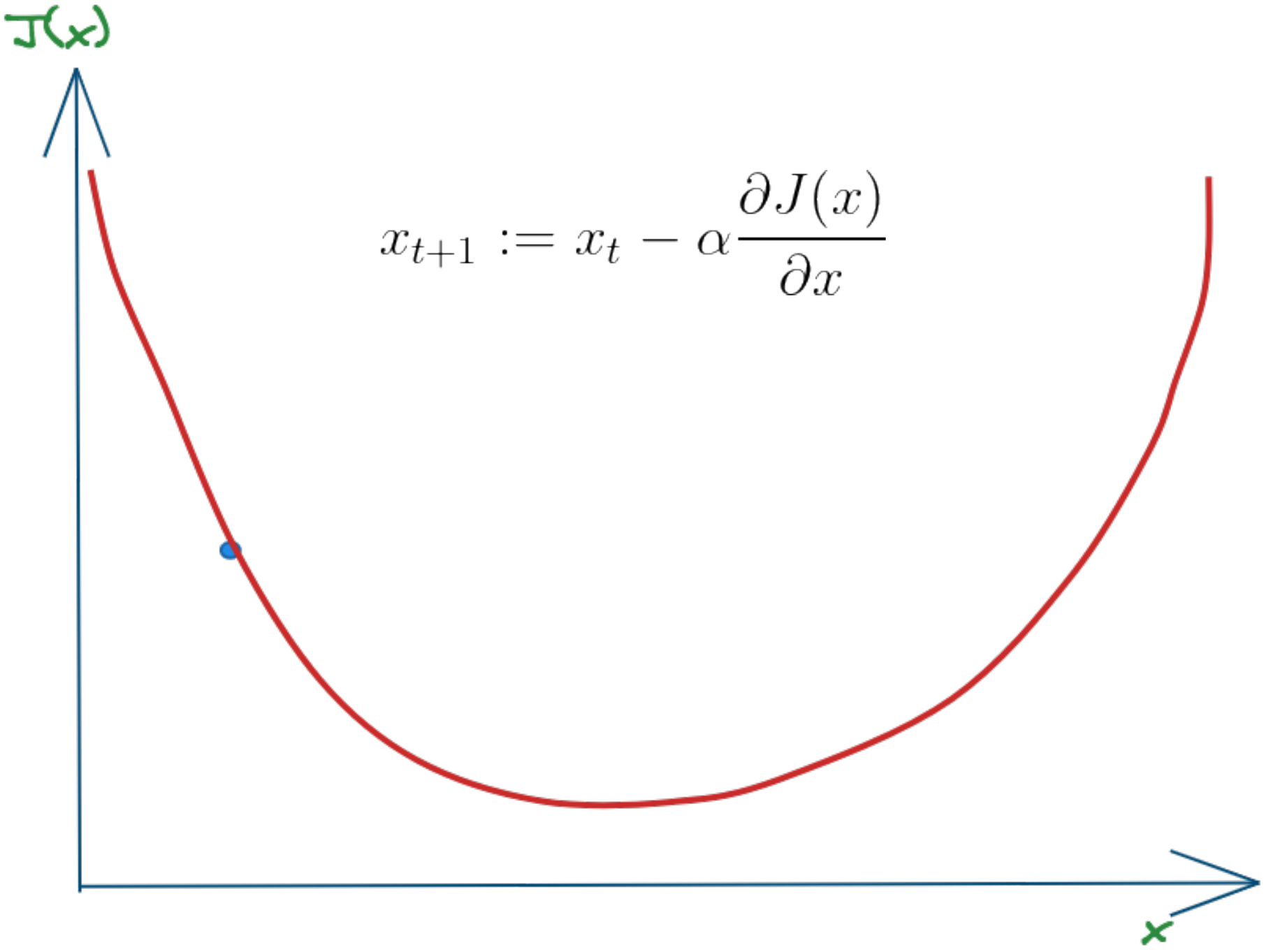


$$x_{t+1} := x_t - \alpha \frac{\partial J(x)}{\partial x}$$

$$here \quad \frac{\partial J(x)}{\partial x} > 0$$

$$x_{t+1} := x_t - \alpha.(positive\ number)$$

Gradient Descent intuition



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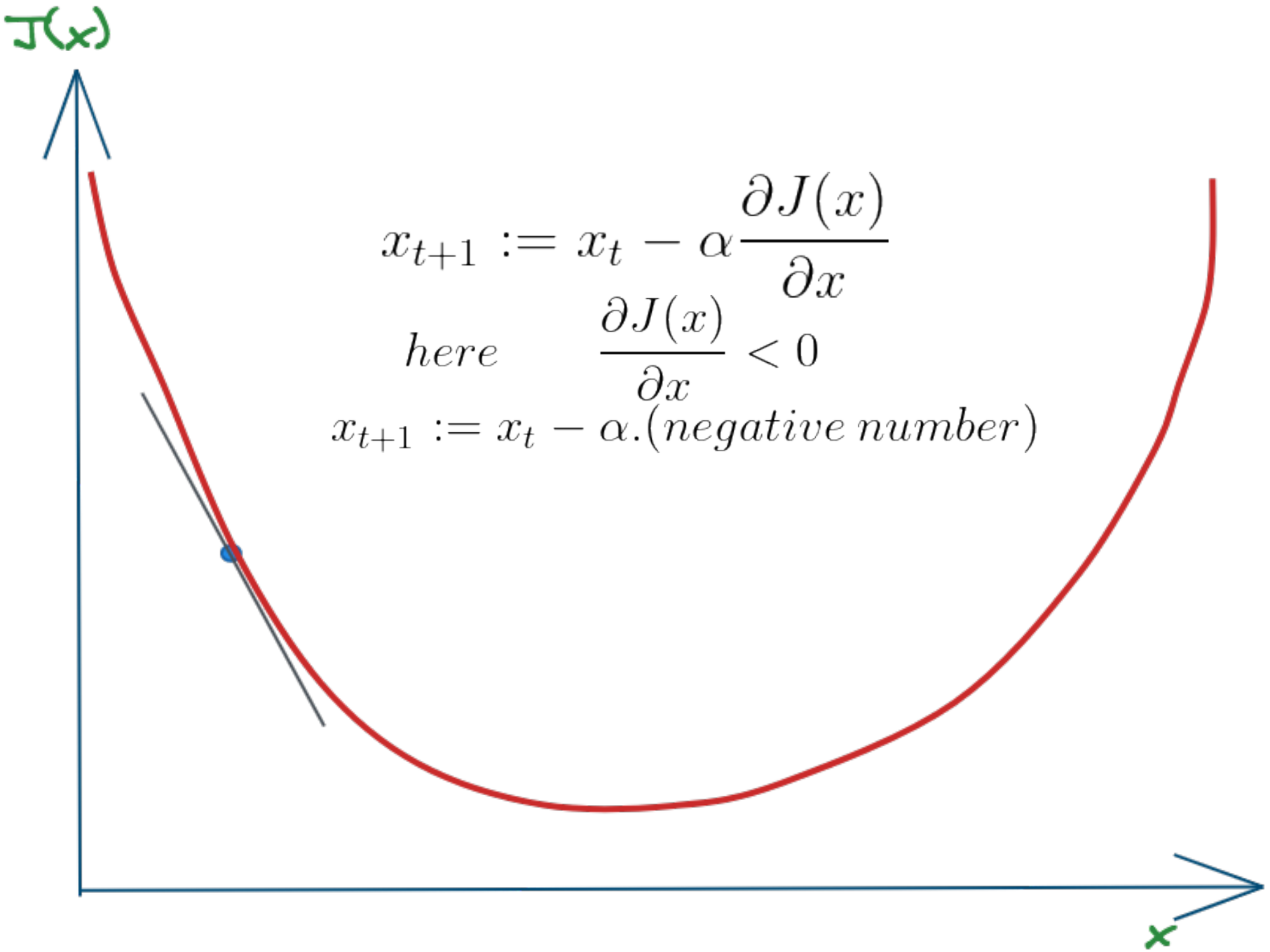

$$x_{t+1} := x_t - \alpha \frac{\partial J(x)}{\partial x}$$

$$here \qquad \frac{\partial J(x)}{\partial x} < 0$$

$$x_{t+1} := x_t - \alpha.(negative\ number)$$

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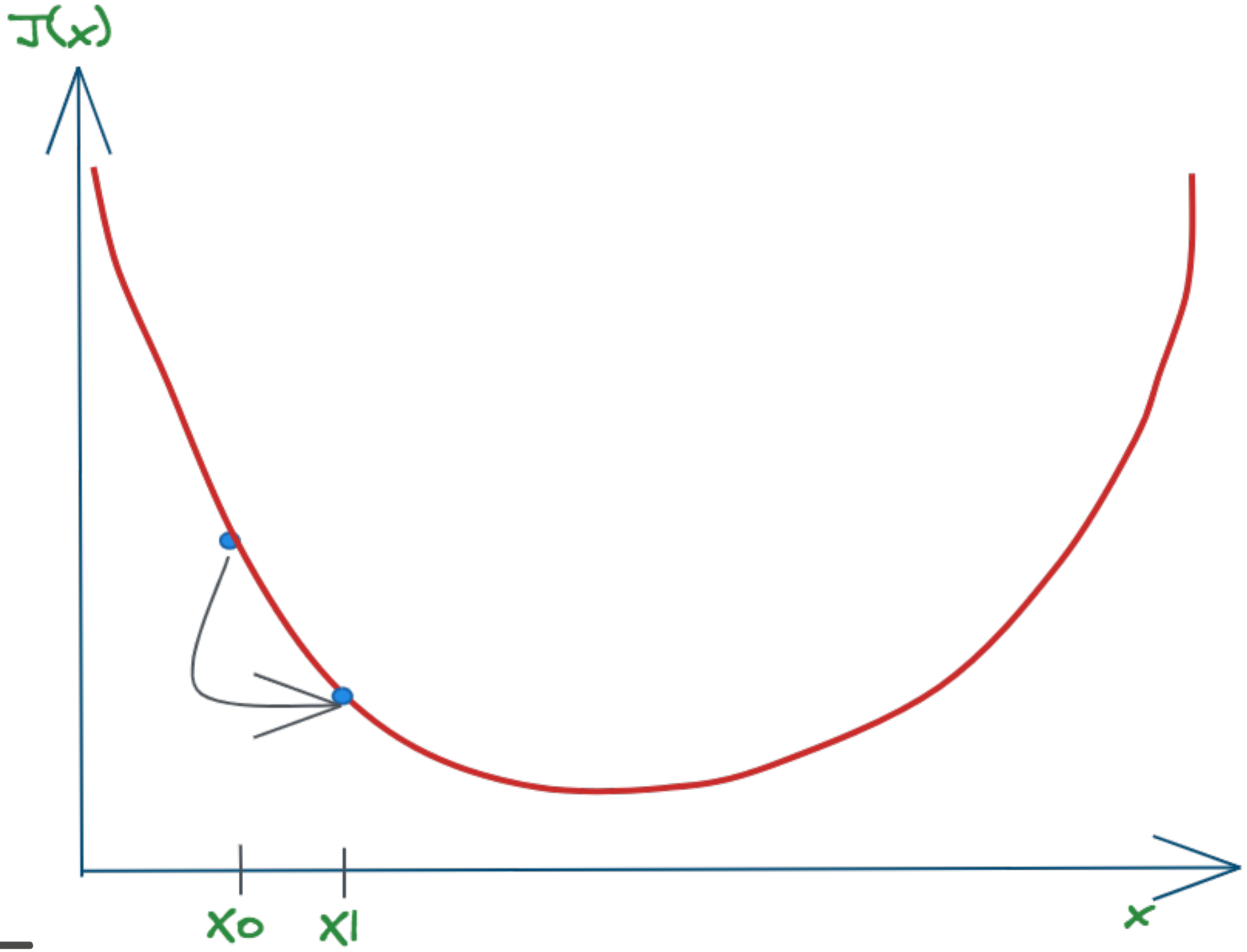

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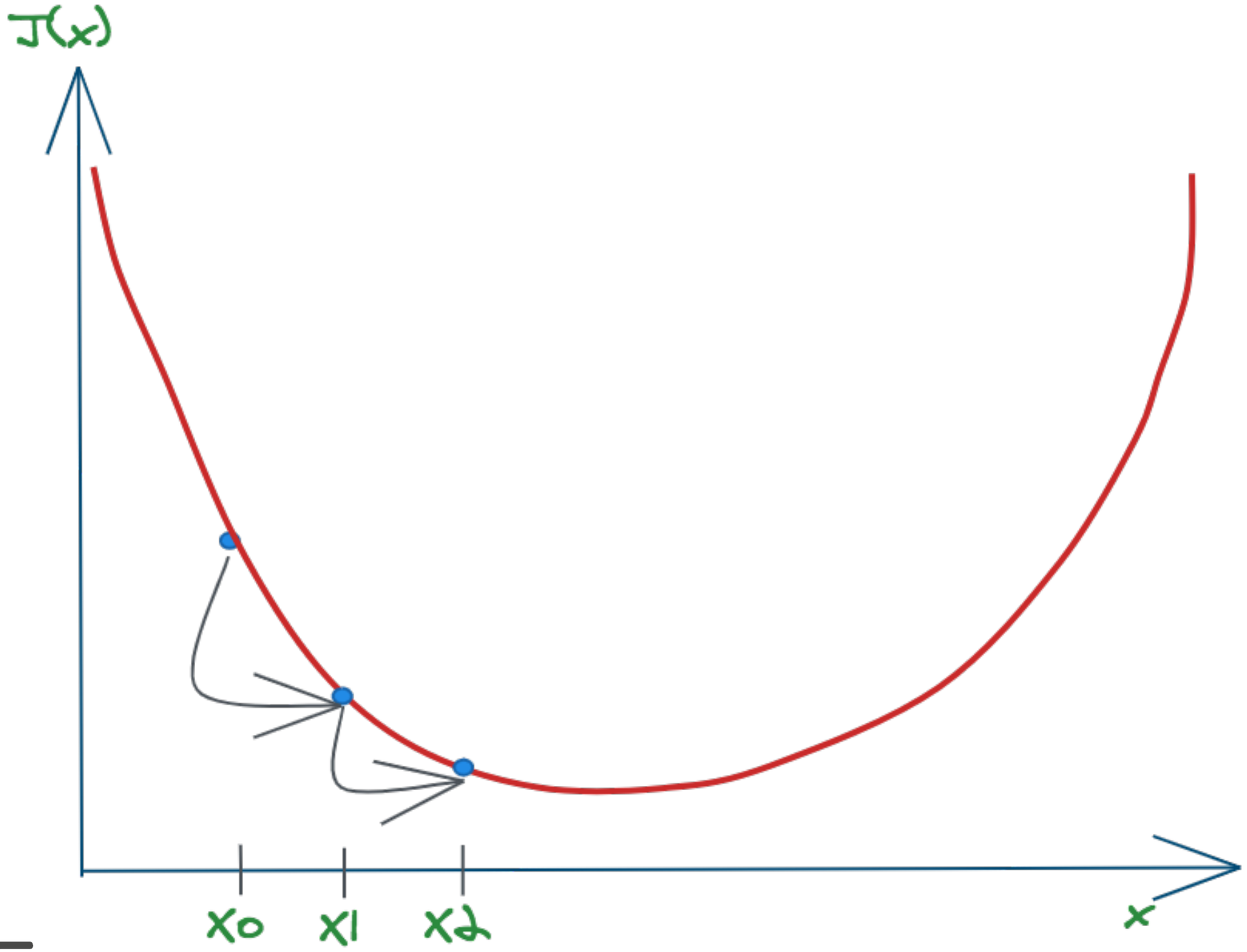

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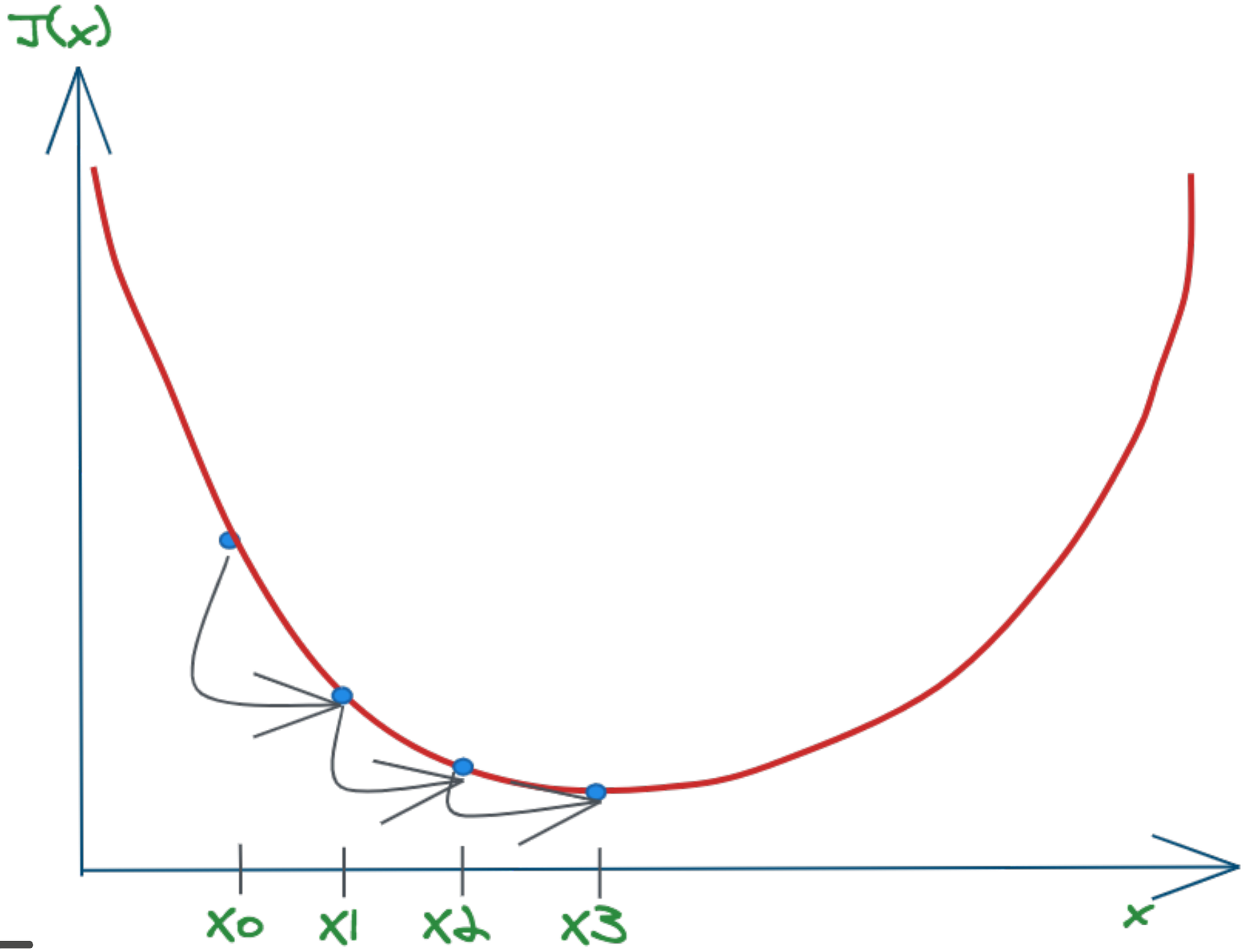

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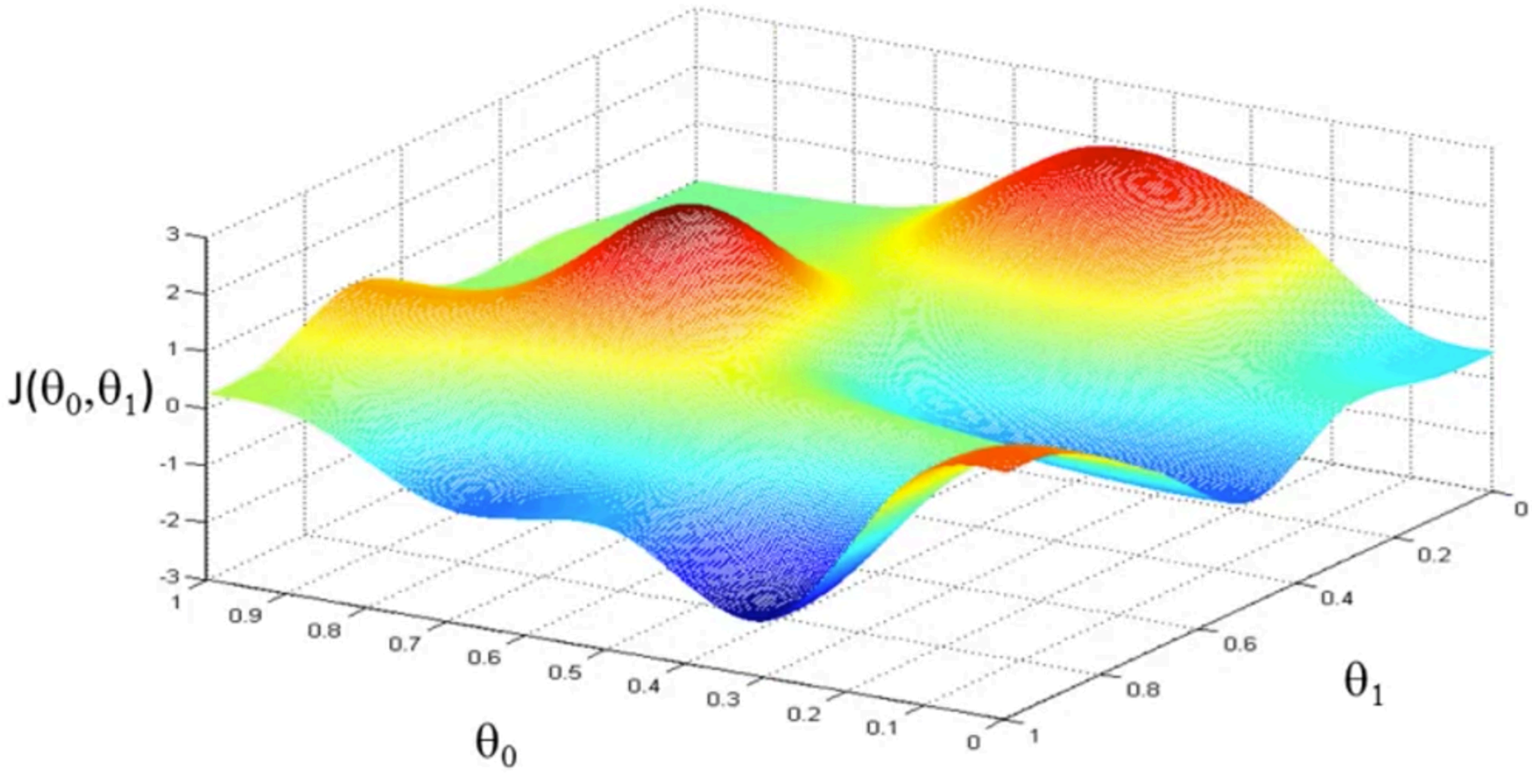
- What we've seen on a 1-dimension can be **generalized** to any number of dimensions



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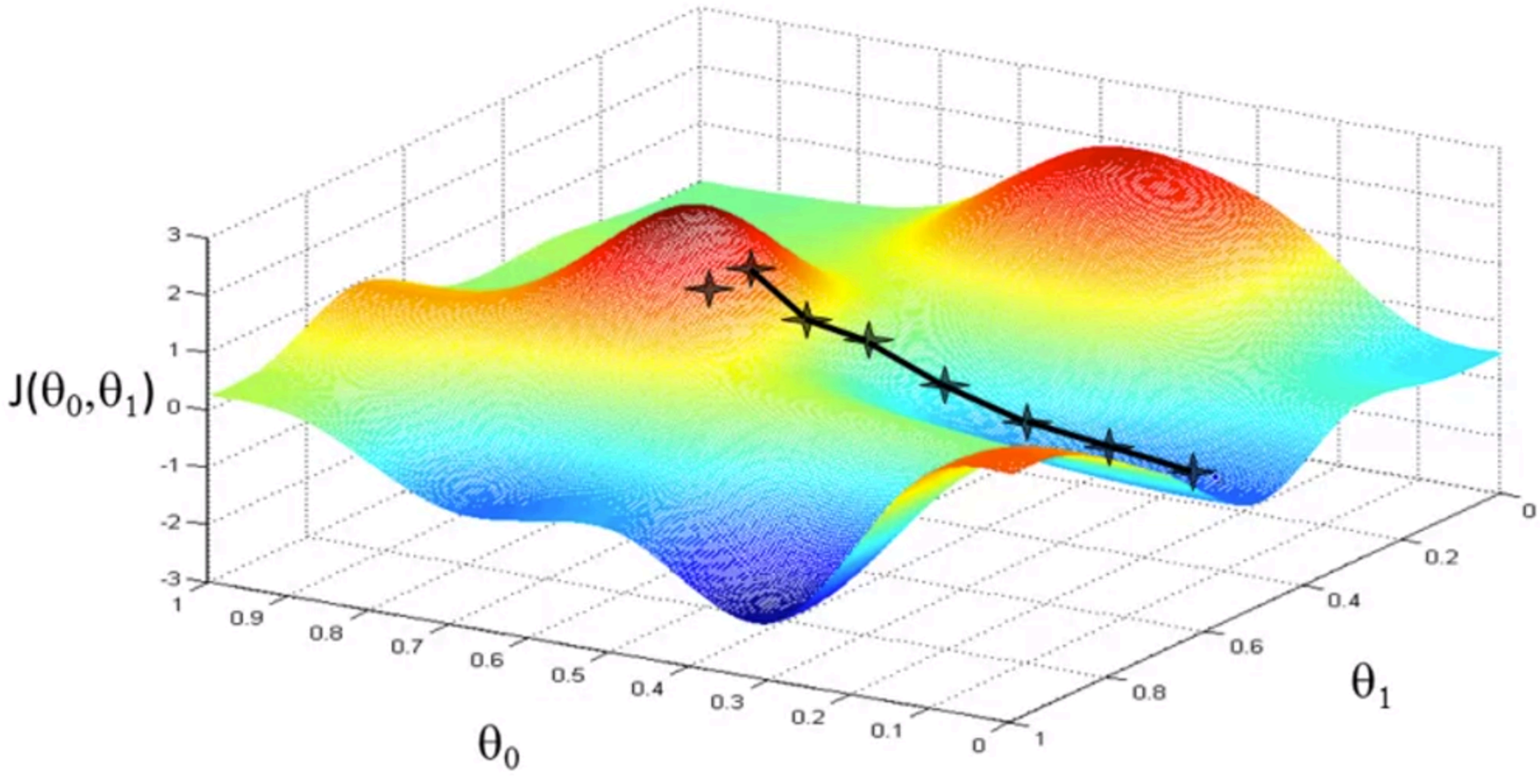

Gradient Descent algorithm

- The general algorithm can be described as the following:

$$Repeat\ until\ convergence:$$
$$\left\{ For\ each\ j \in [1, N]: \quad \theta_j := \theta_j - \alpha \frac{\partial J(\theta_1, \theta_2, ..., \theta_N)}{\partial \theta_j} \right\}$$

Step size

Partial derivative

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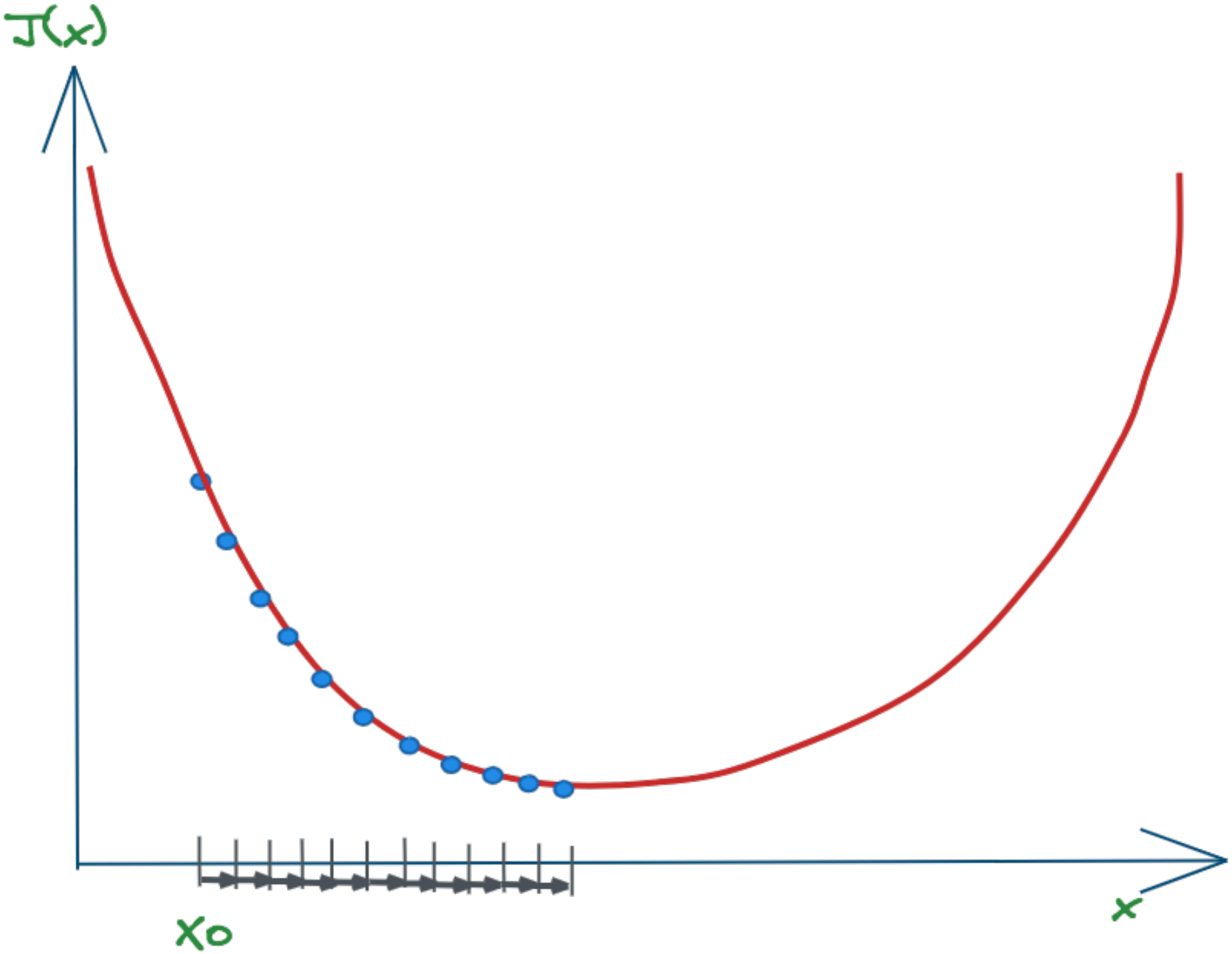
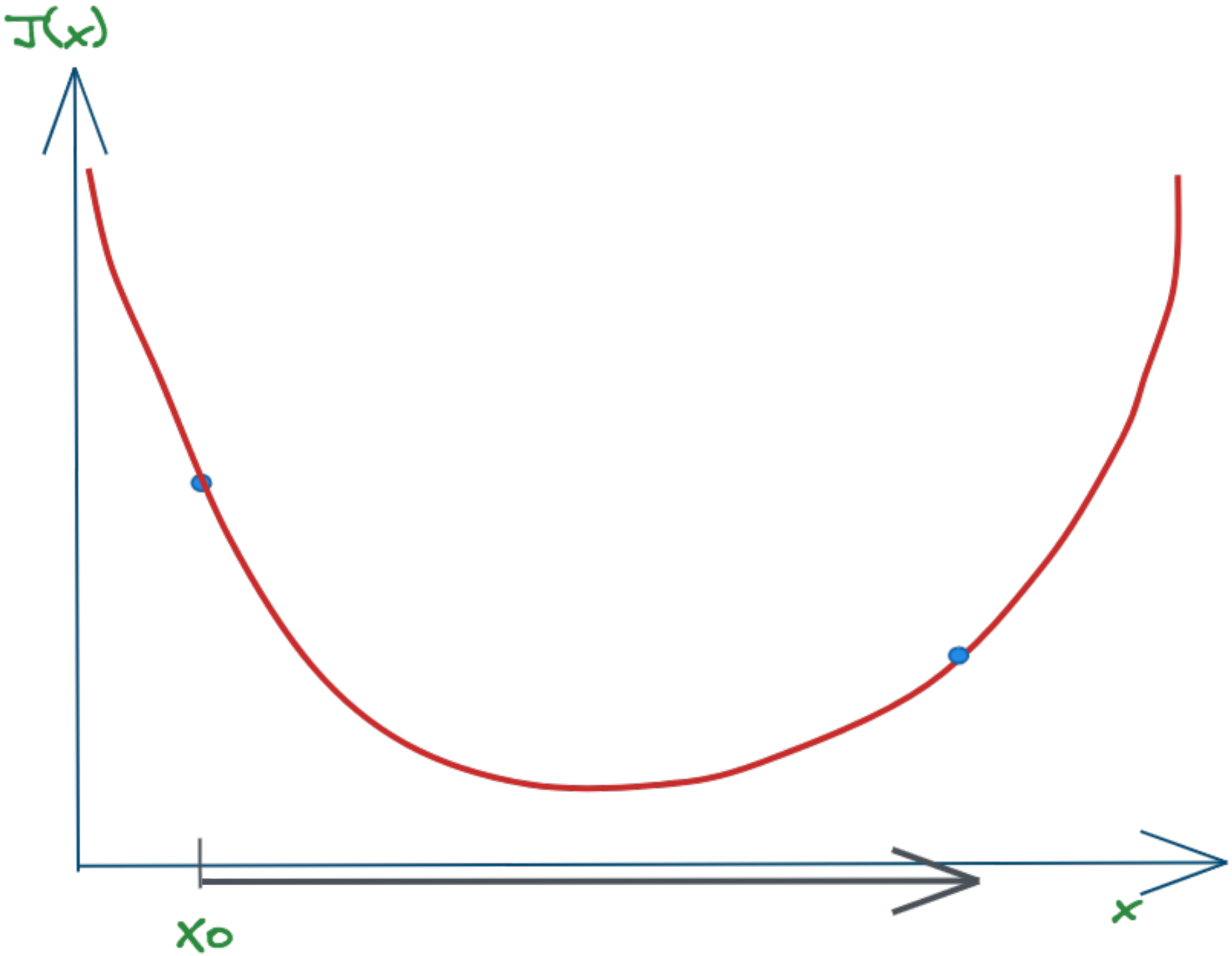
Gradient Descent algorithm

- If the step size is too small, the convergence will be **slow**



Gradient Descent algorithm

- If the step size is too big, we may **overshoot** the minimum



Gradient Descent for Linear Regression

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- The **gradient descent** iterations are then defined for **each parameter:**

$$\theta_0 := \theta_0 - \frac{\alpha}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_0^{(i)}$$

$$\theta_1 := \theta_1 - \frac{\alpha}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_1^{(i)}$$

$$\dots$$

$$\theta_N := \theta_N - \frac{\alpha}{m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_N^{(i)}$$

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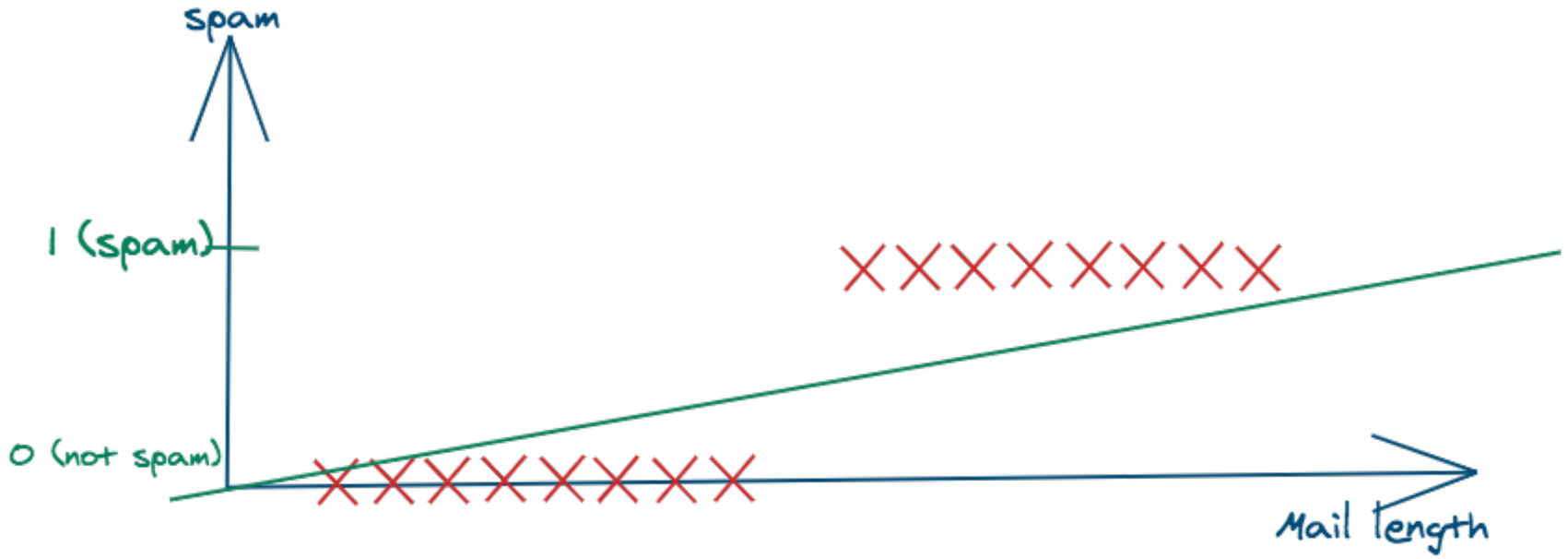
- In the linear regression case, we have the **guarantee** that we will reach a **local minimum**

Classification

- In **classification**, the output takes values in a **finite unordered** set (spam/not spam, fraudulent/not fraudulent …)

- Let's try fitting a **linear model** to a **classification** task



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- The linear model is defined as $h_\theta(x) = \theta^T x$
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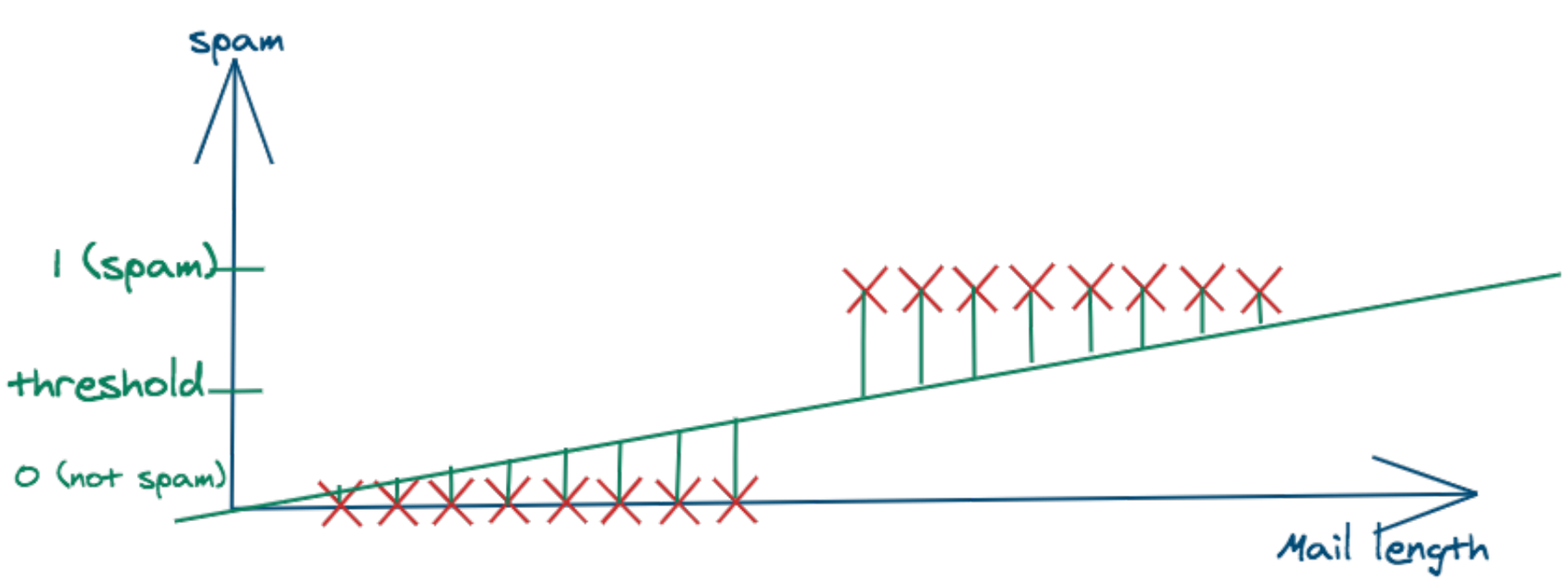

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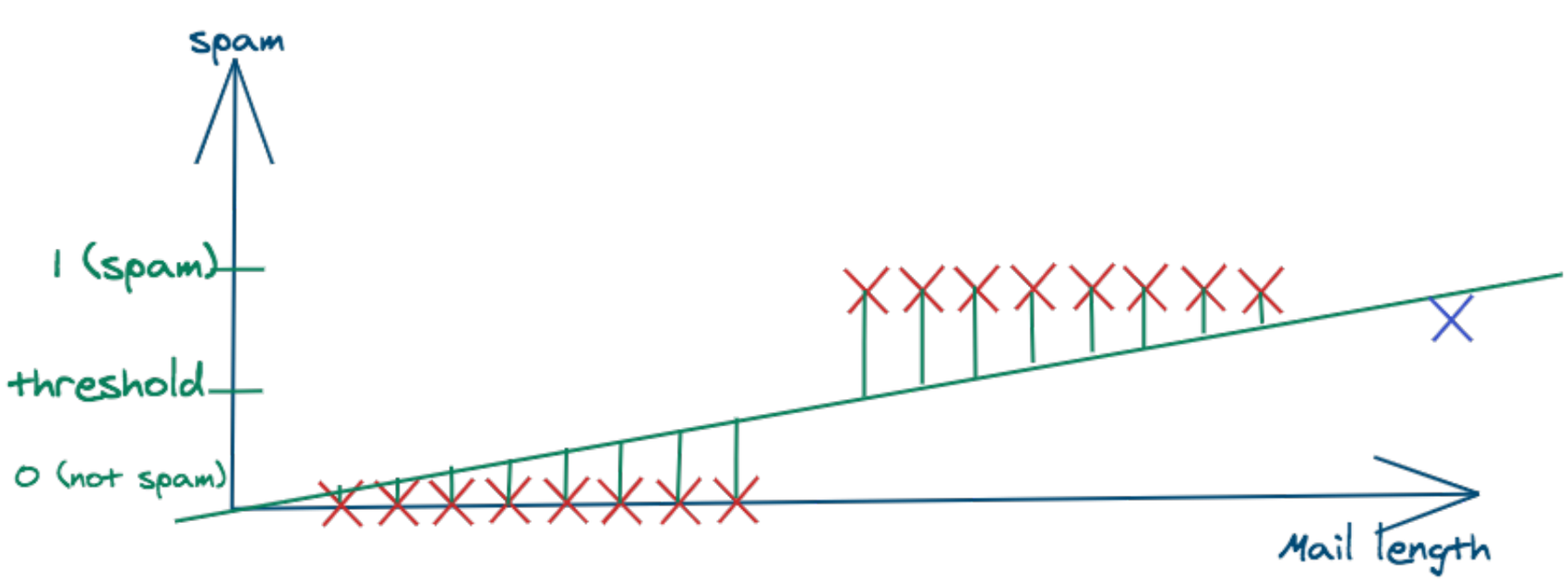

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  - It takes values in R, not in [0,1]
- We want the values of our **classifier** to be in the [0,1] range to be interpreted as **probabilities**

Logistic Regression

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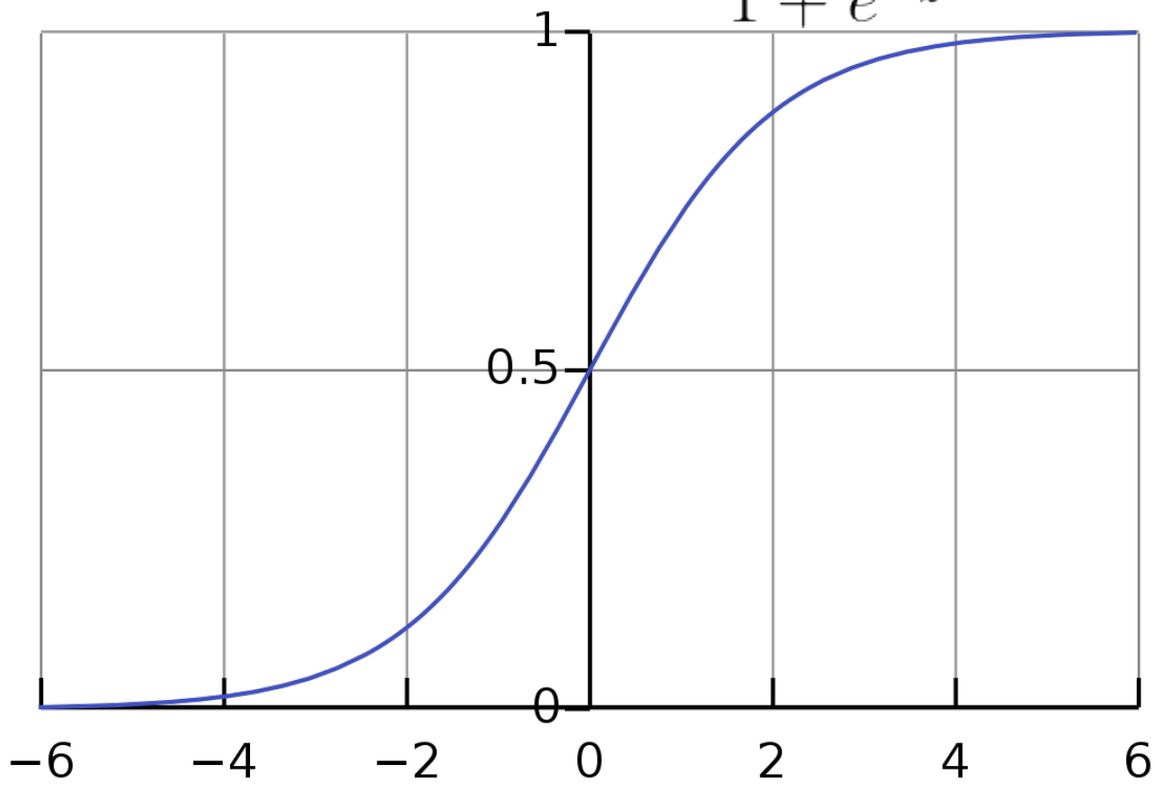
- In **logistic regression**, we add a **sigmoid** function

$$h_\theta(x) = \sigma(\theta^T x)$$

$$where \quad \sigma(z) = \frac{1}{1 + e^{-z}}$$



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- Now to find the **best set of parameters**, we need to define a **cost function**, just like we did for linear regression

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- For **Linear Regression**, we defined our cost function as:

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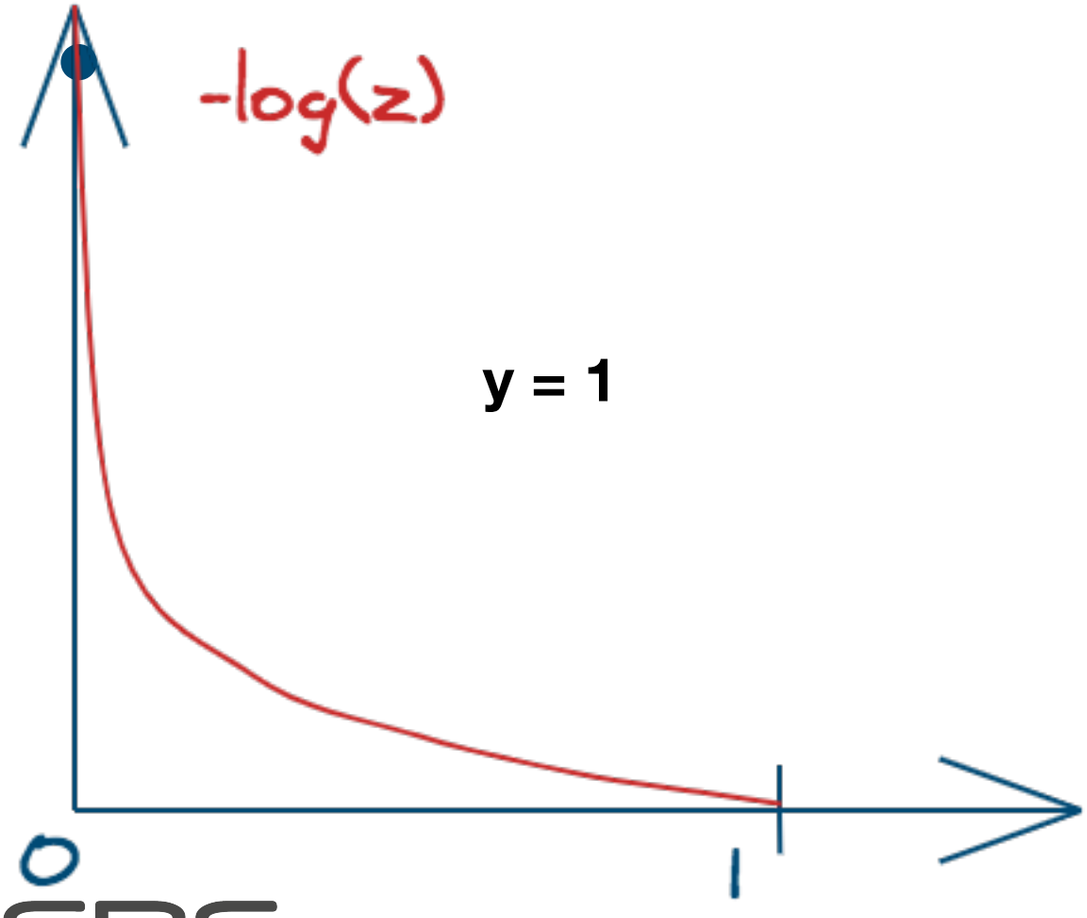
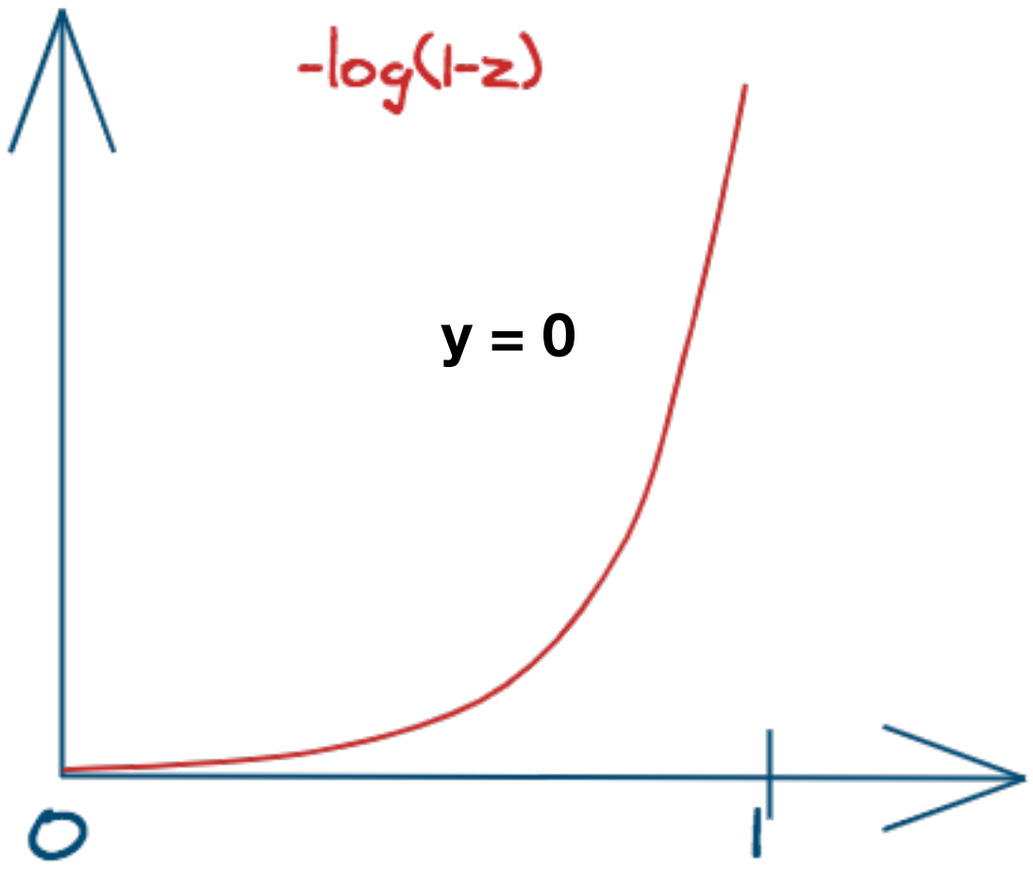
- We need to define a **convex cost function**

Logistic Regression

- We define the following **cost function** for logistic regression

$$Cost(h_\theta(x), y) = \begin{cases} -log(h_\theta(x)), & \text{if } y = 1 \\ -log(1 - h_\theta(x)), & \text{if } y = 0 \end{cases}$$





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- We can **rewrite** $Cost(h_\theta(x), y) = \begin{cases} -log(h_\theta(x)), & \text{if } y = 1 \\ -log(1 - h_\theta(x)), & \text{if } y = 0 \end{cases}$

as $Cost(h_\theta(x), y) = -y * log(h_\theta(x)) - (1 - y) * log(1 - h_\theta(x))$

Logistic Regression

- We can **rewrite** our cost function for a given **dataset**

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- Once we have defined our **cost function**, we just need to use the **gradient descent** to find the **best set of parameters**, identically to the linear regression model

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- But what if our target is **not linear**, or if the decision space is **not linearly separable**?

Non-Linear Models: Randomized Trees & Forests

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- We then model $$f(X) = \sum_{m=1}^{M} \beta_m h_m(X)$$

Non-linear models

- Examples of transformations

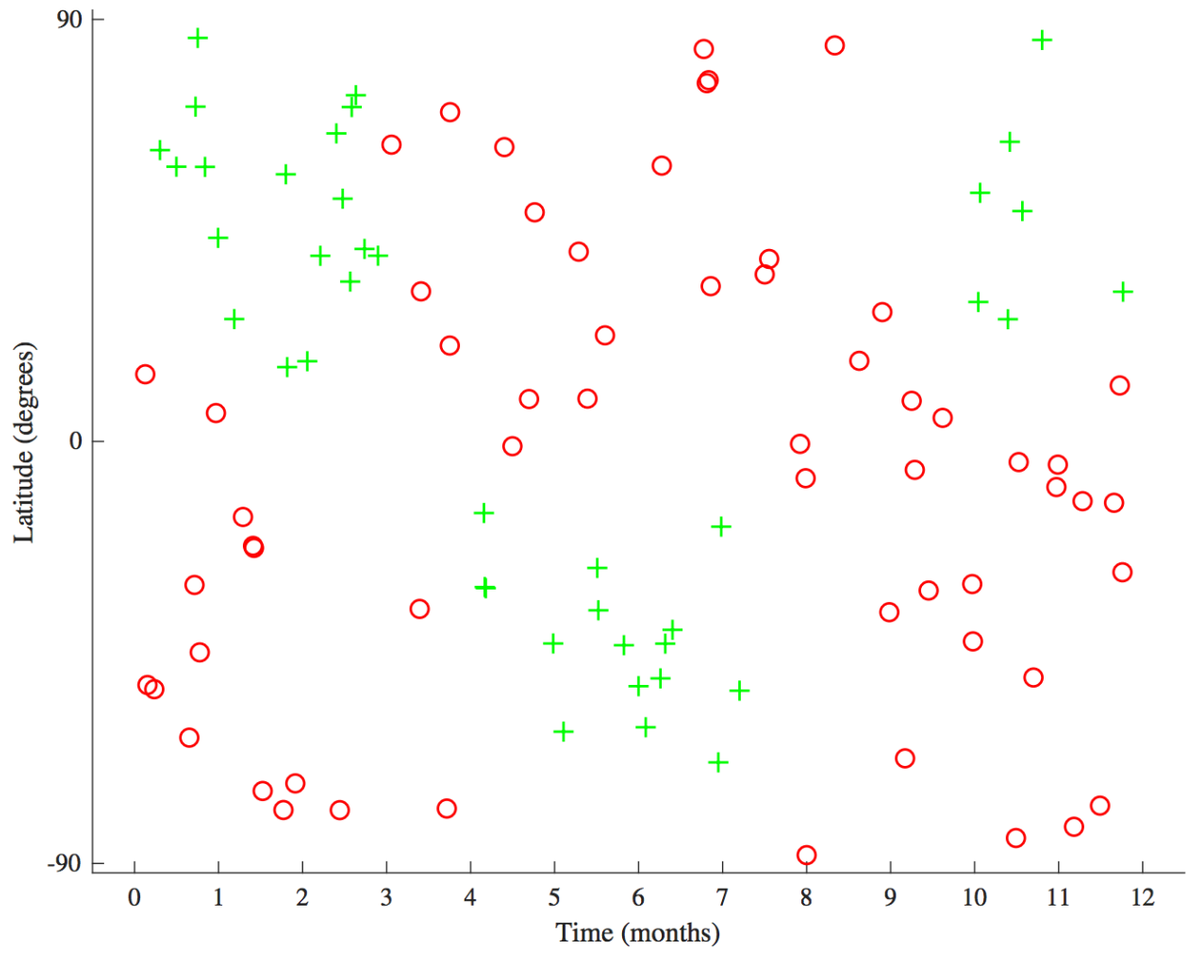
Polynomial transformations: $h_m(X) = X_j^2 \text{ or } X_j X_k$

Non-linear transformations: $h_m(X) = log(X_j) \text{ or } \sqrt{X_j}$

An indicator for a region of X_k $h_m(X) = \mathbb{I}(L_m \leq X_k < U_m)$

Non-linear models

- Example of a non-linearly separable decision space: a very simplistic snow prediction model (based on latitude and month)



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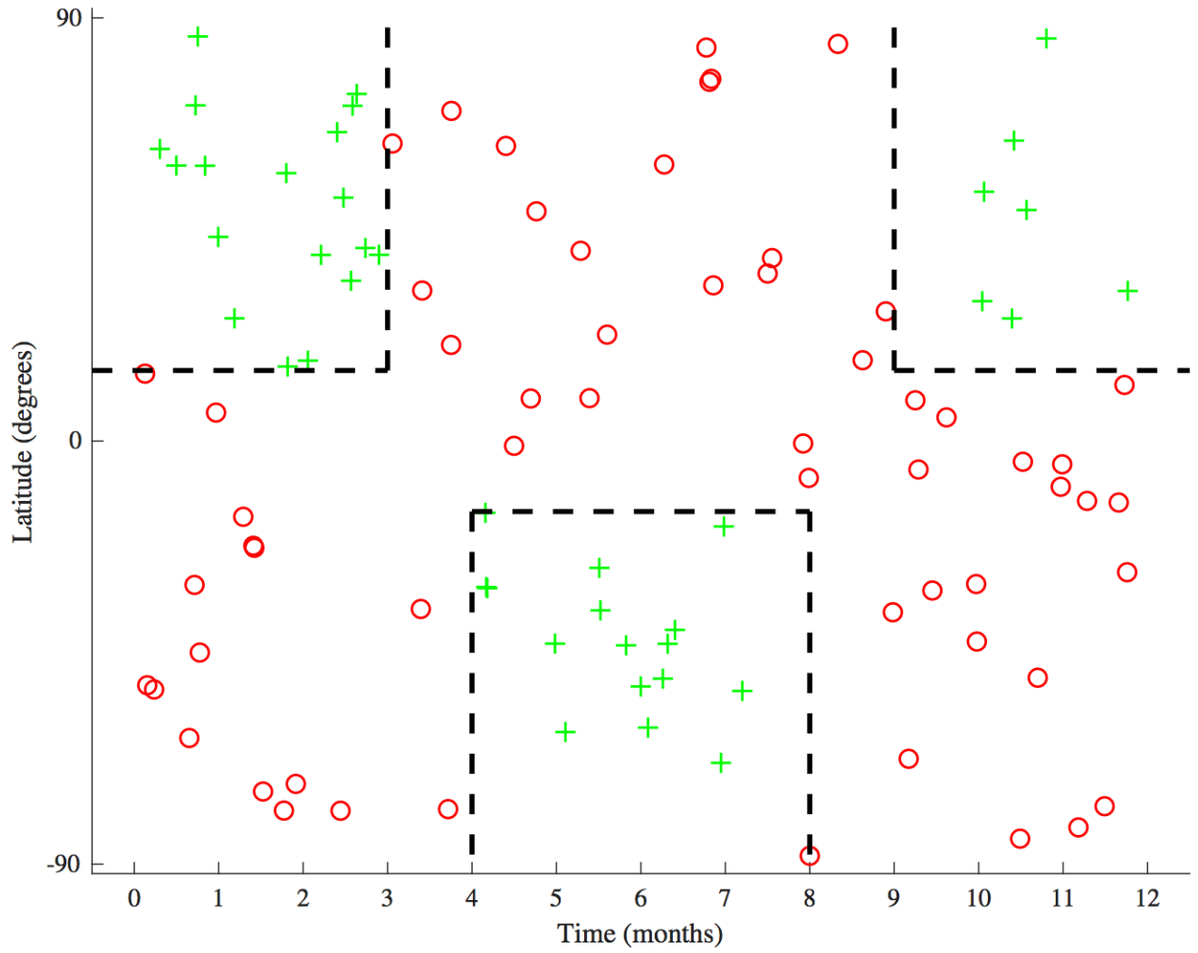


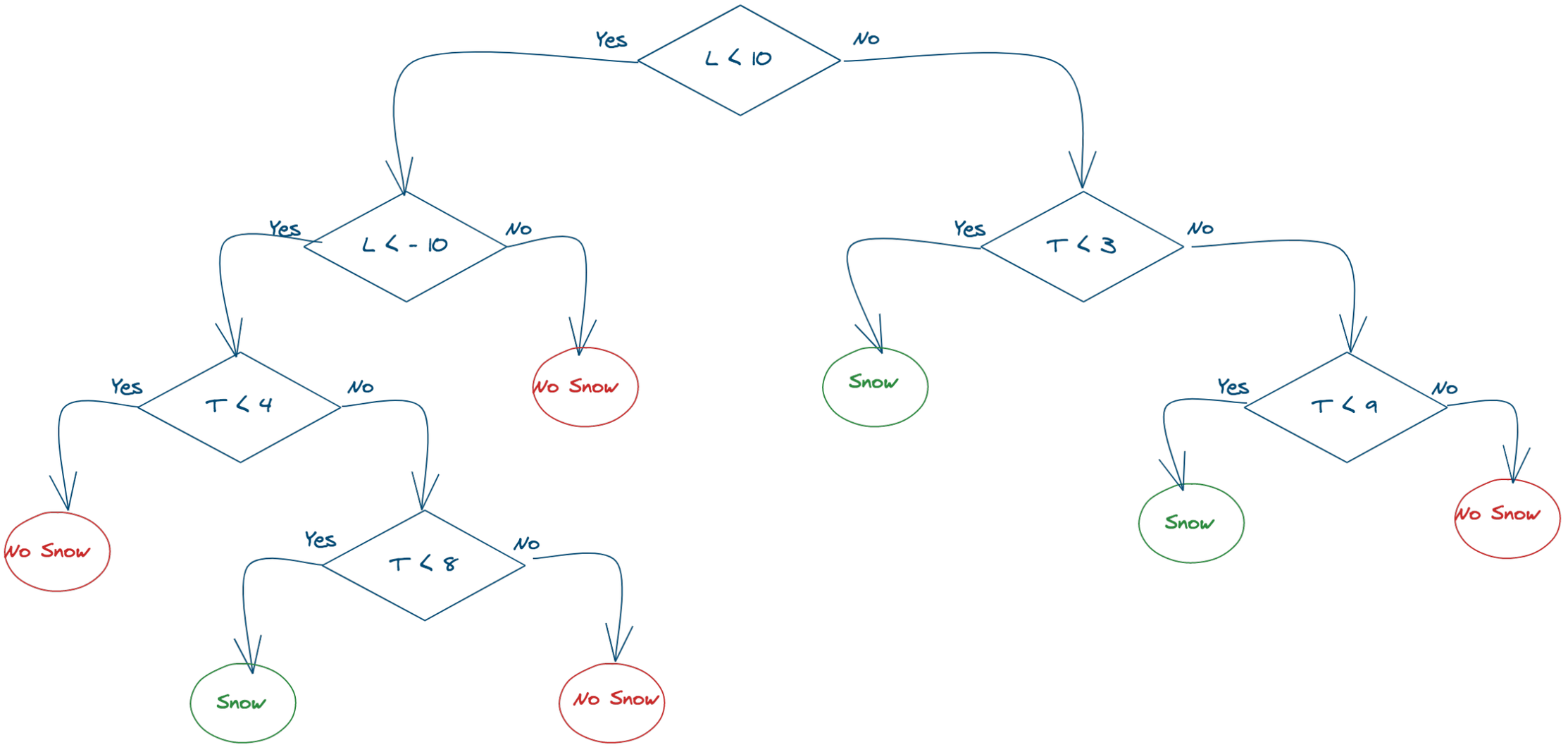
Non-linear models

- Snow prediction model: let's try to model what we see:

$$\begin{aligned}
&\text{If Latitude} \geq 10 \text{ and Month} < 3 \text{ then Snow} \\
&\text{If Latitude} \leq -10 \text{ and } 4 \leq \text{Month} < 8 \text{ then Snow} \\
&\text{If Latitude} \geq 10 \text{ and Month} \geq 9 \text{ then Snow} \\
&\text{Else No Snow}
\end{aligned}$$

Non-linear models

- Snow prediction model: this is what we call a **decision tree**



Classification And Regression Trees (CART)

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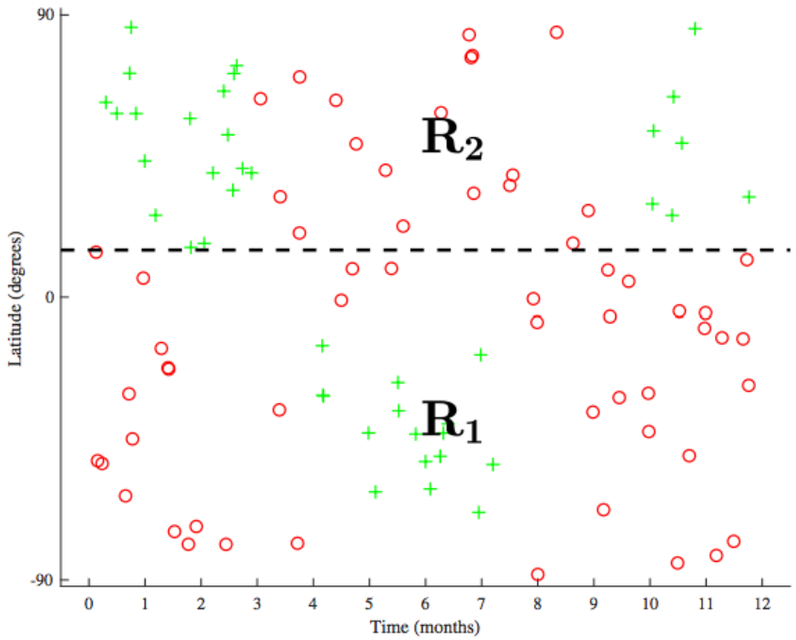
- Formally, given a parent region R_p , a feature index j and a threshold t, we obtain two child regions R_1 and R_2 as follows:

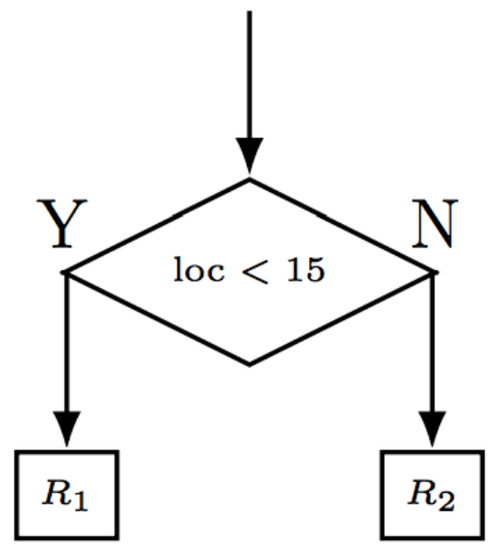
$$R_1 = \{X | X_j < t, X \in R_p\}$$
$$R_2 = \{X | X_j \geq t, X \in R_p\}$$

Classification And Regression Trees (CART)

- Let's see it in action for the snow example



(a)



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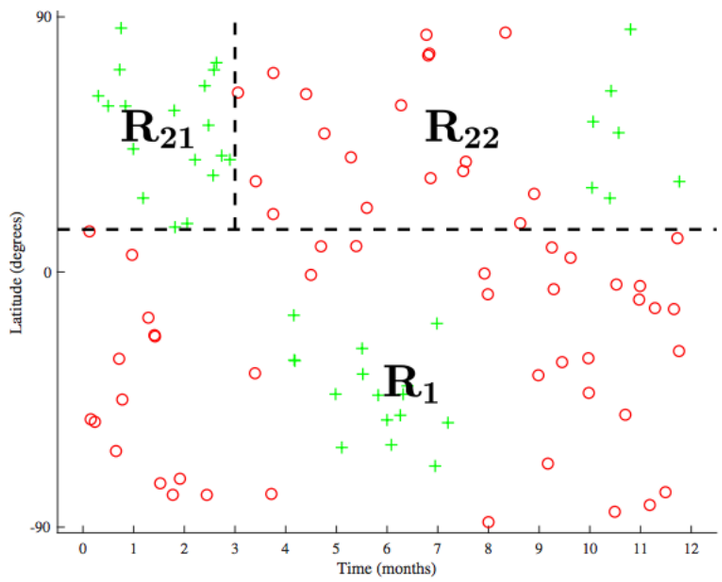
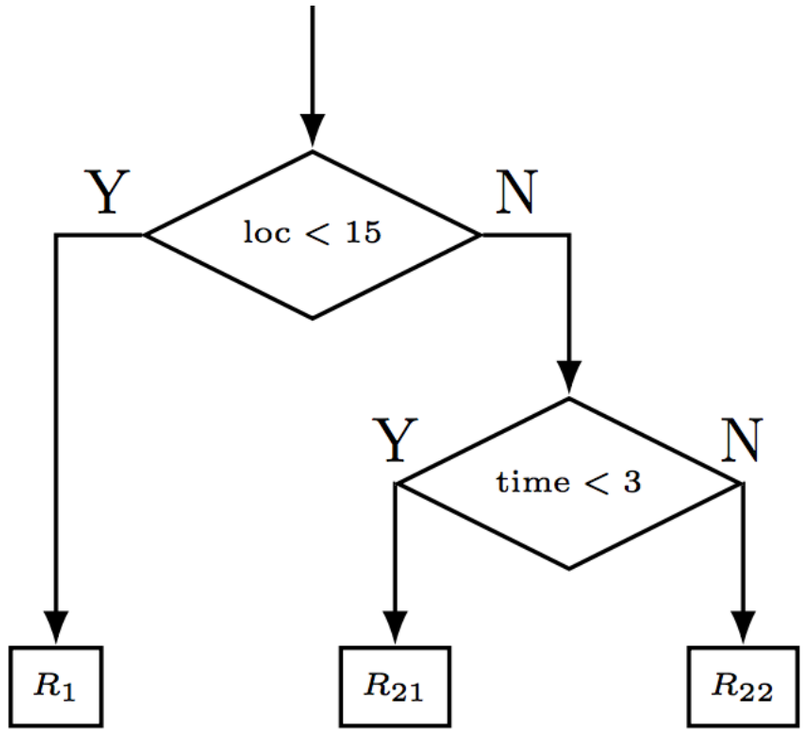


(b)



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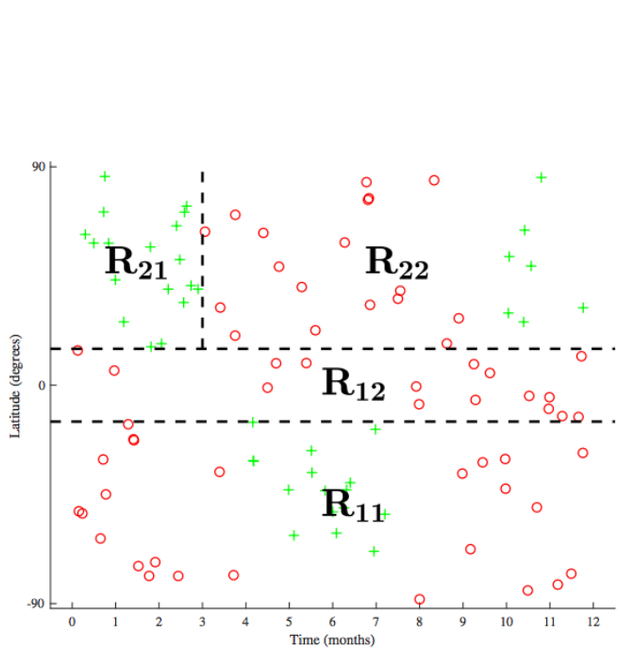
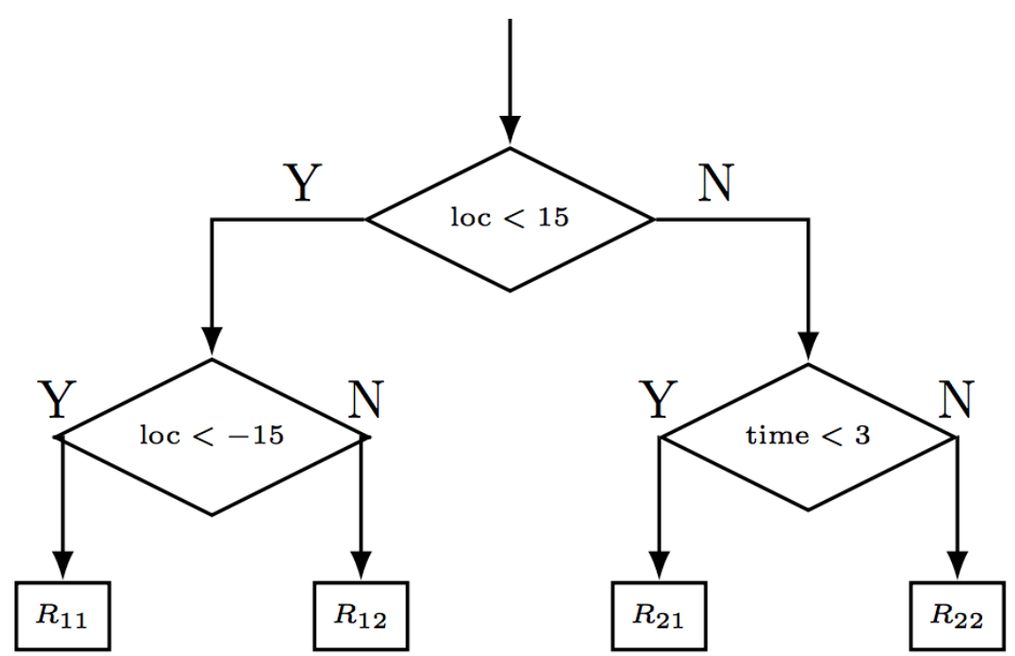


(c)



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- We select the leaf region, feature, and threshold that will **maximize** our **decrease** in loss

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- We continue until we meet a **stopping criterion**

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$$L_{misclass}(R) = 1 - max_c(\hat{p}_c)$$

where $\hat{p}_c$ is the proportion of examples in R that are of class c

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- From an **information-theoretic** perspective, **cross-entropy** measure the number of bits needed to specify the outcome (or class) given that the distribution is known. The decrease of loss from parent to child is known as **information gain**

Classification And Regression Trees (CART)

- We need to define a specific loss L for each task
  - For **regression**, for each data point x_i we have an associated value y_i
  - The final **prediction** for a region R is the mean of all the values in the region

$$\hat{y} = \frac{\sum_{i \in R} y_i}{|R|}$$

- We define the **squared loss** as

$$L_{squared}(R) = \frac{\sum_{i \in R} (y_i - \hat{y})^2}{|R|}$$

Classification And Regression Trees (CART)

- Let's talk about some **stopping criteria**

- The simplest criteria would be to fully grow the tree: continue until each leaf region contains exactly one training data point

- But this would be **expensive** and the model would **overfit**

- We need other stopping **heuristics**

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  - **Maximum Number of Nodes**: Stop if a tree has more leaf nodes than a fixed threshold

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- A better approach is called **pruning**: we first fully grow the tree, and then prune away nodes that minimally decrease the loss

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- A **Random Forest** is an **ensemble** of **Decision Trees**, trained with the **bagging** method: these trees are **merged** together to get a more **accurate** and **stable** prediction

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3. Each tree is grown to the largest extent possible (**no pruning**)

Random Forest

- Once all the trees are grown, to make a prediction we can either:
  - Do a **majority vote** for **classification** tasks
  - **Average** all the trees' **estimates** for **regression** tasks

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