# Machine Learning with Python

## MTH786U/P 2023/24

## Week 1: Introduction and maths preliminaries

Nicola Perra, Queen Mary University of London (QMUL)

n.perra@qmul.ac.uk

# Organisation

- Lecturer: Dr Nicola Perra
- Email: n.perra@qmul.ac.uk
- Office: Maths: MB-G26
- Office hours: Tuesdays 15:00-16:00 by request

Timetable

- Lectures: Tuesday 13:00-15:00
- Laboratory sessions: Friday 10:00-11:00

All relevant information also available on QMPlus page!

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There will be

- non-examinable weekly coursework (theory first, practice from week 4 on)
- a mid-term exam (theory questions)
- a final coding project

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- Submission of well-documented Jupyter notebook script
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$$\text{Final Grade} = 0.6 \times \text{Project Grade} + 0.4 \times \text{Exam Grade}$$

# Learning outcomes

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- formulate representative problems for supervised machine learning and derive mathematical models to solve them

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- write scientific reports

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- One to discuss previous week’s coursework, one to work on this week’s coursework

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To the best of your abilities; coursework is teamwork, so please engage with your peers

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Post your questions in the student forum

# WHAT IS MACHINE LEARNING?

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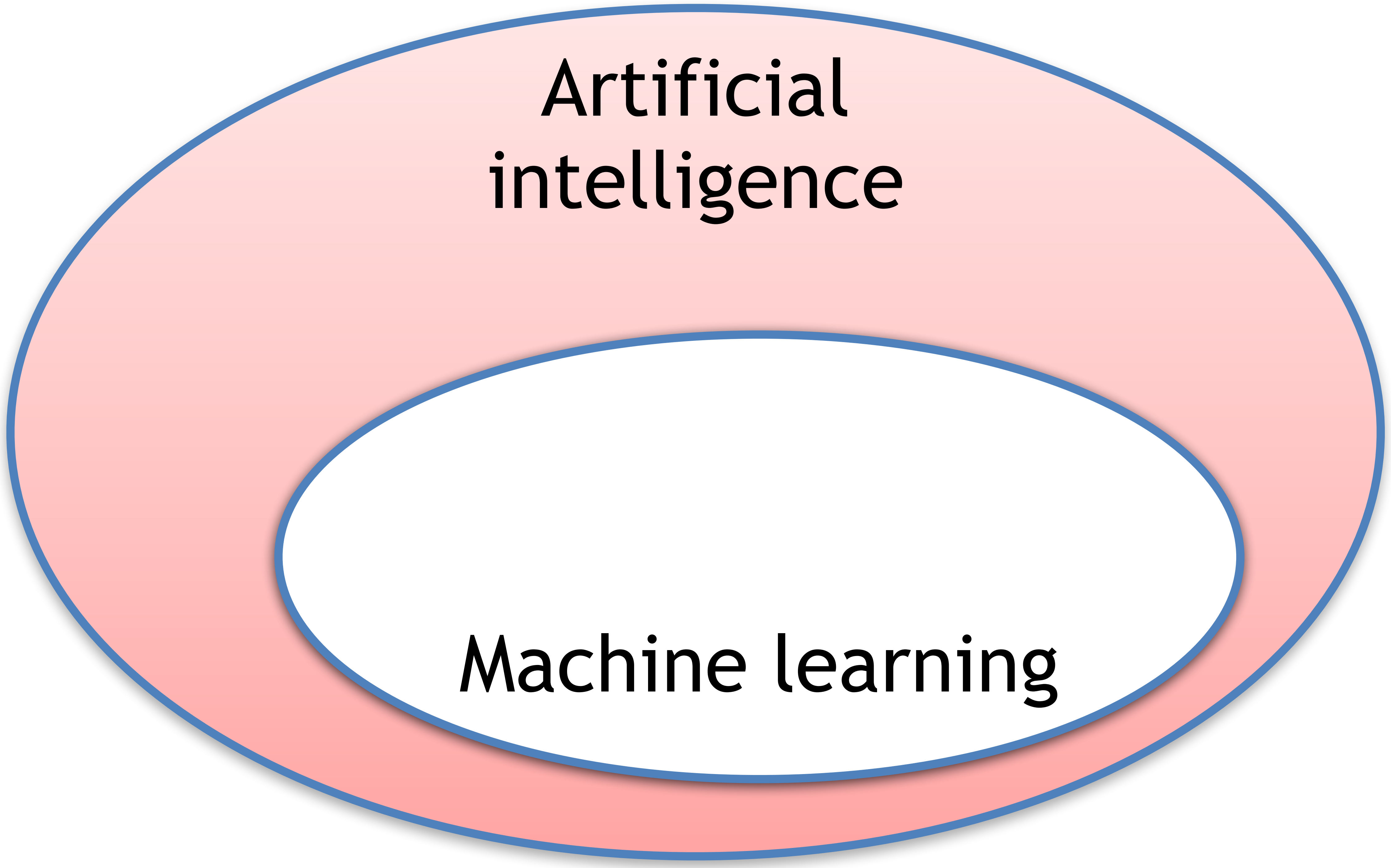
Is it the same as artificial intelligence?

Machine learning $\neq$ artificial intelligence...

Machine learning $\neq$ artificial intelligence...

...but machine learning $\subsetneq$ artificial intelligence



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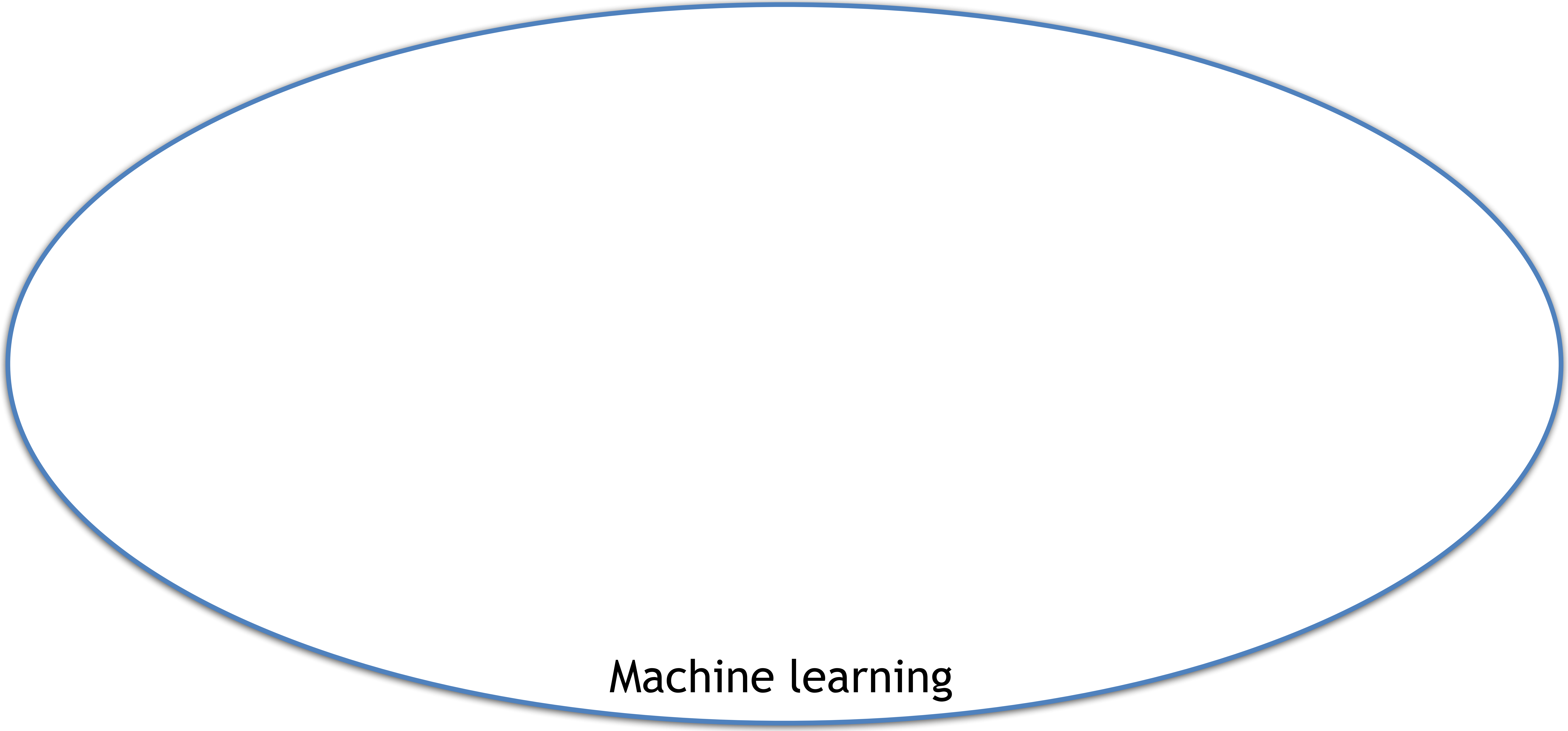

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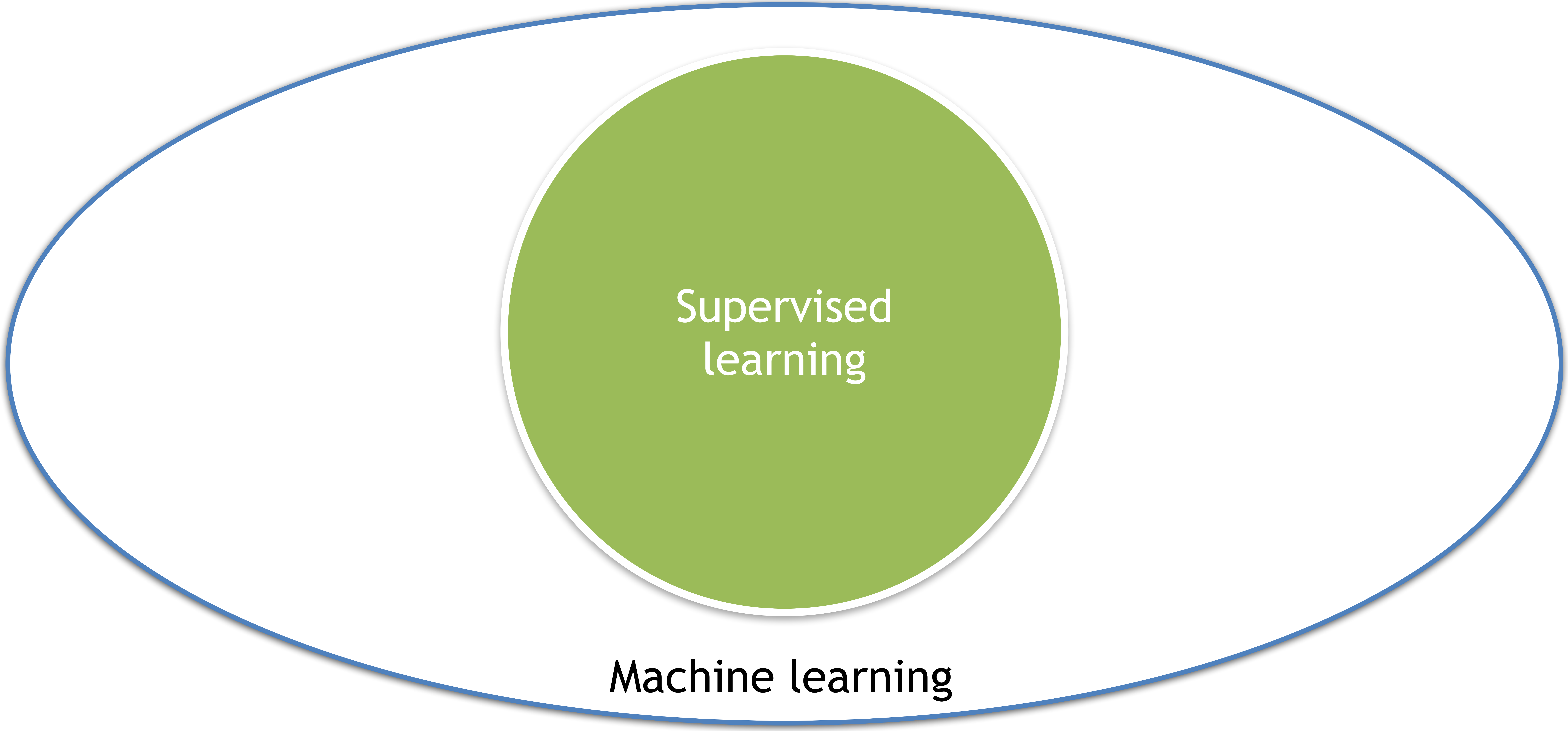

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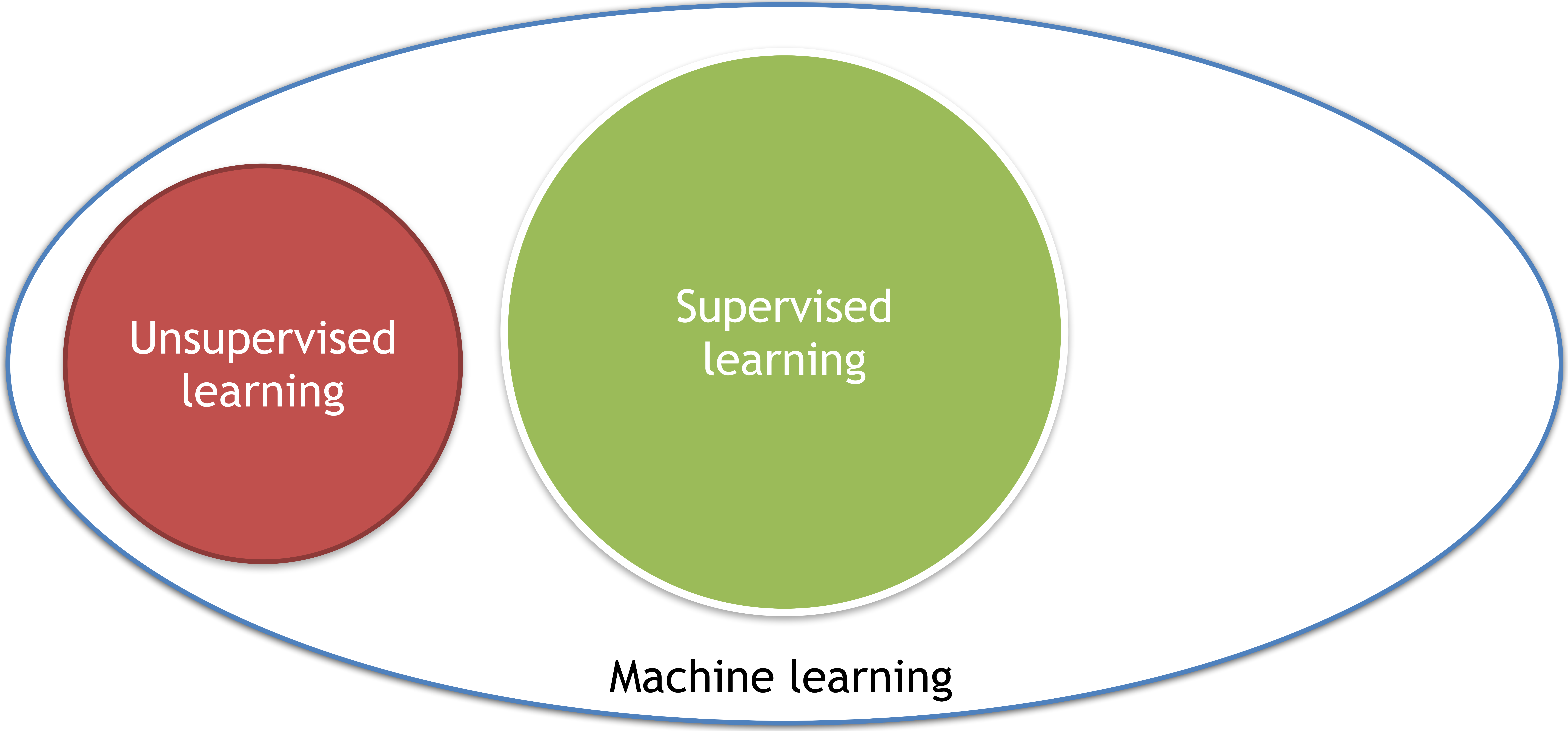

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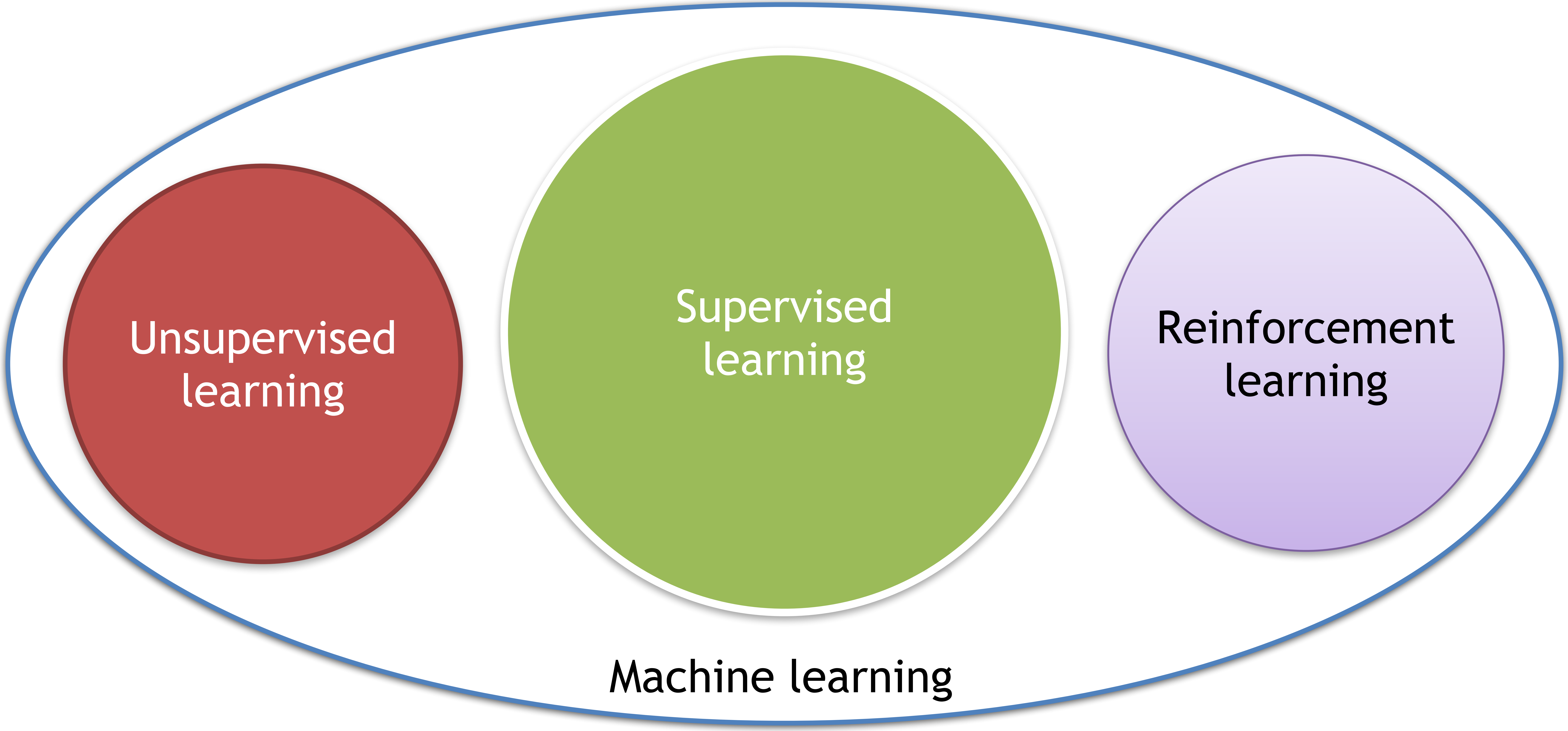

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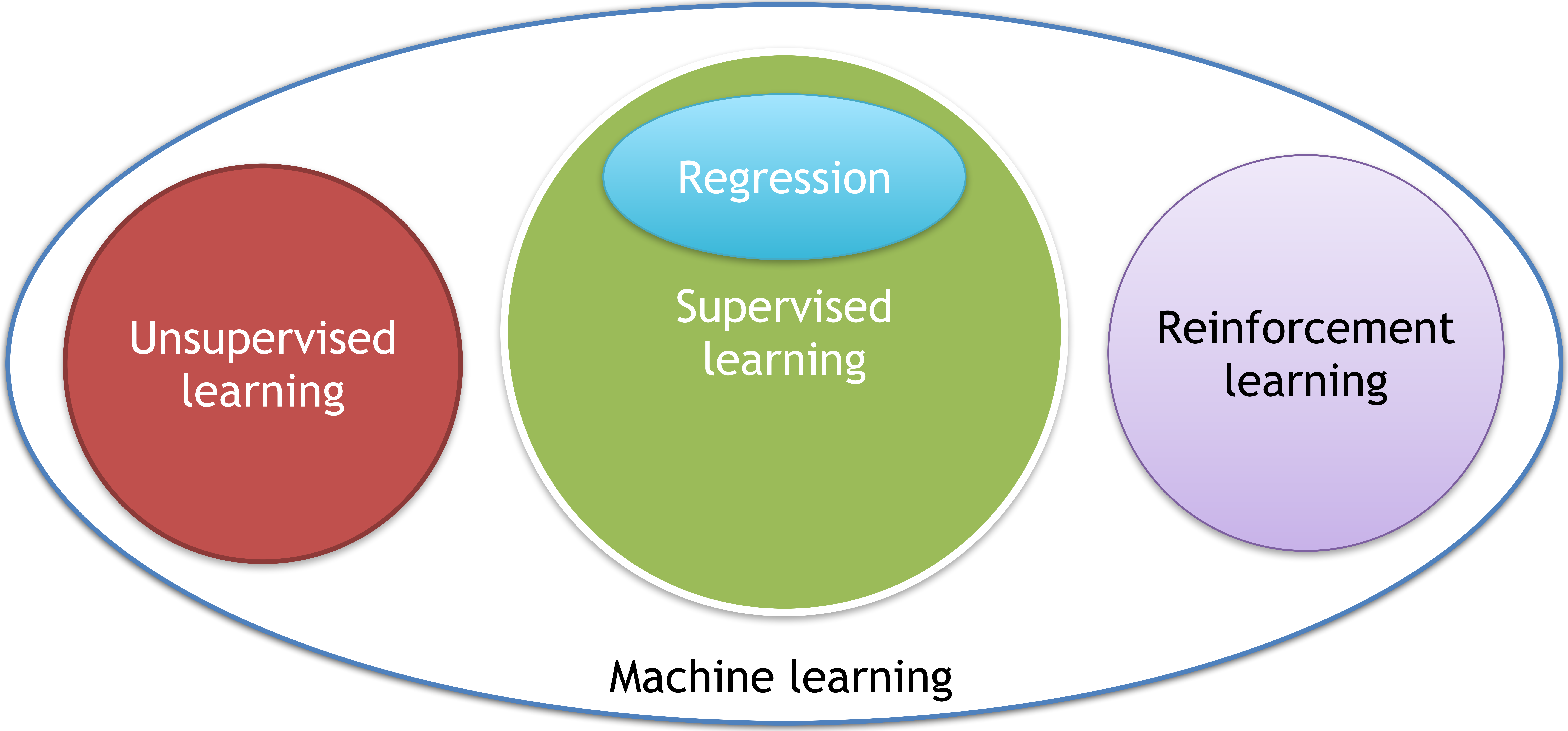

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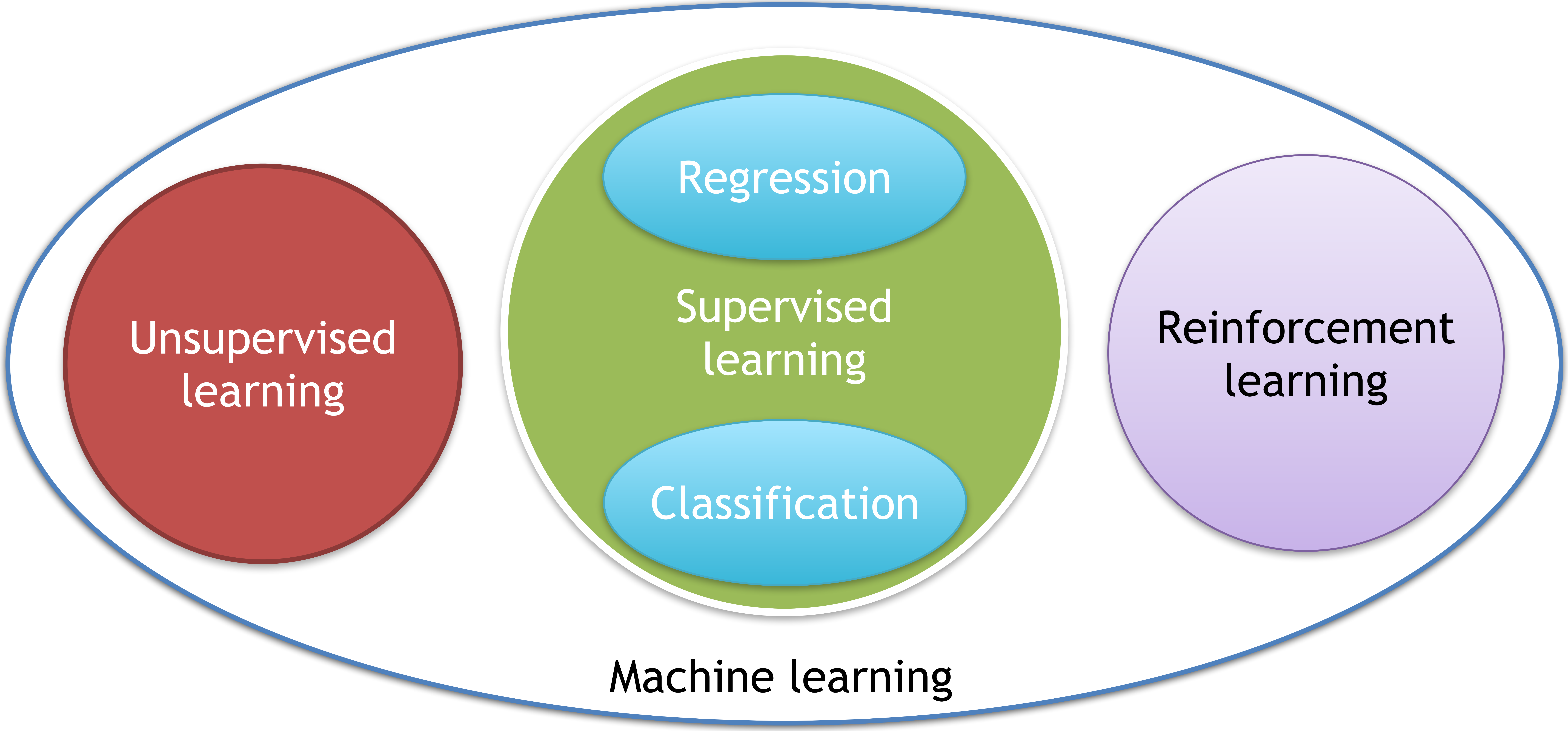

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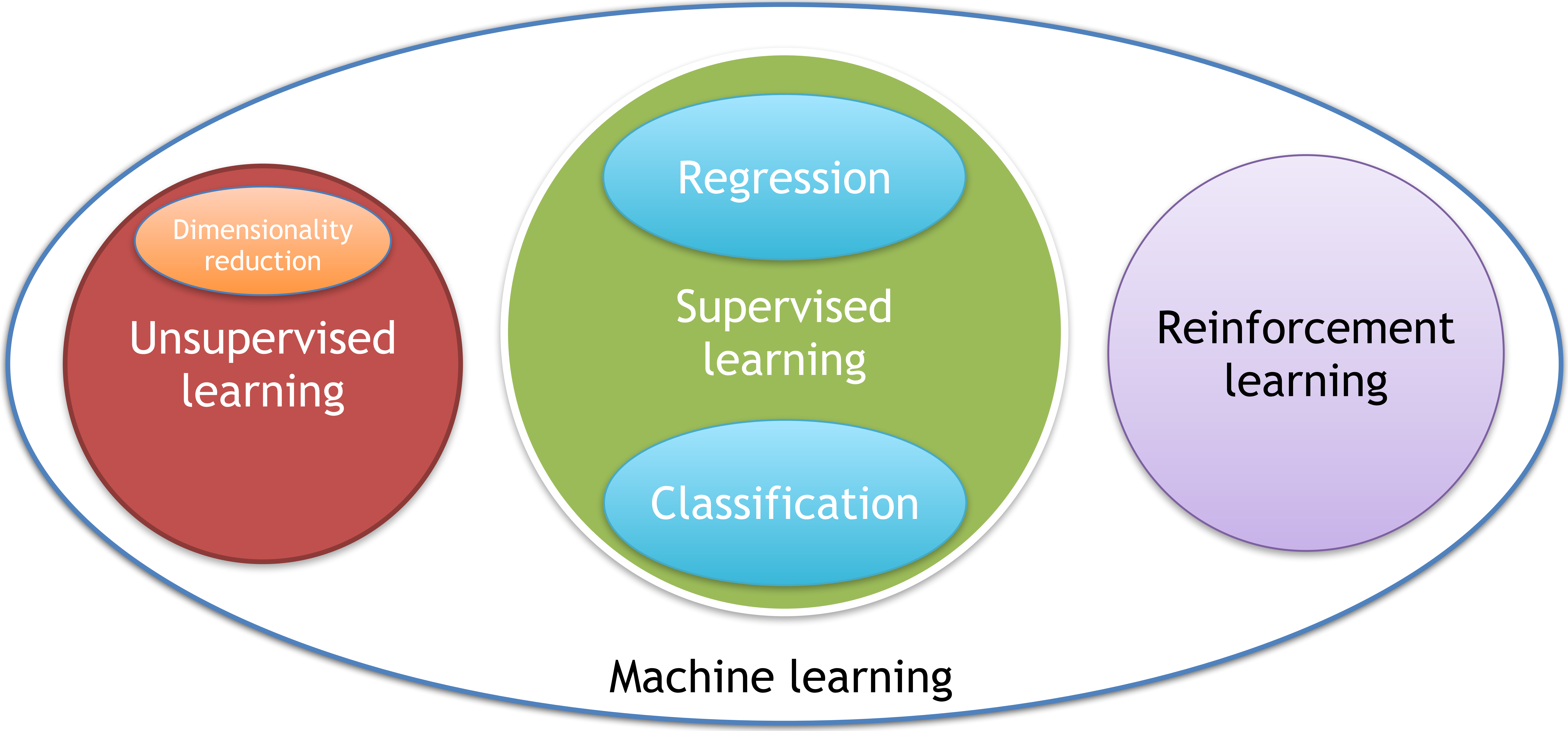

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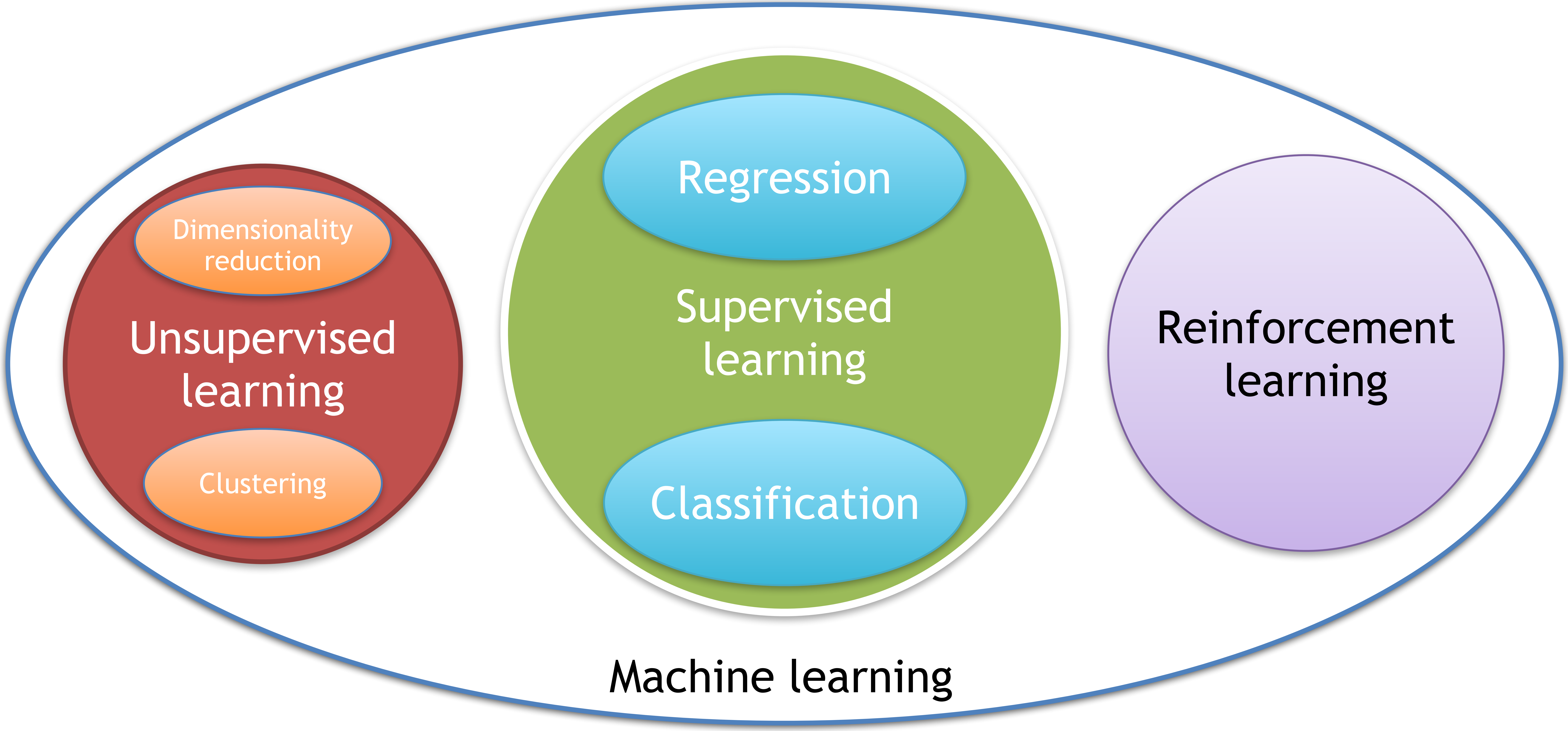

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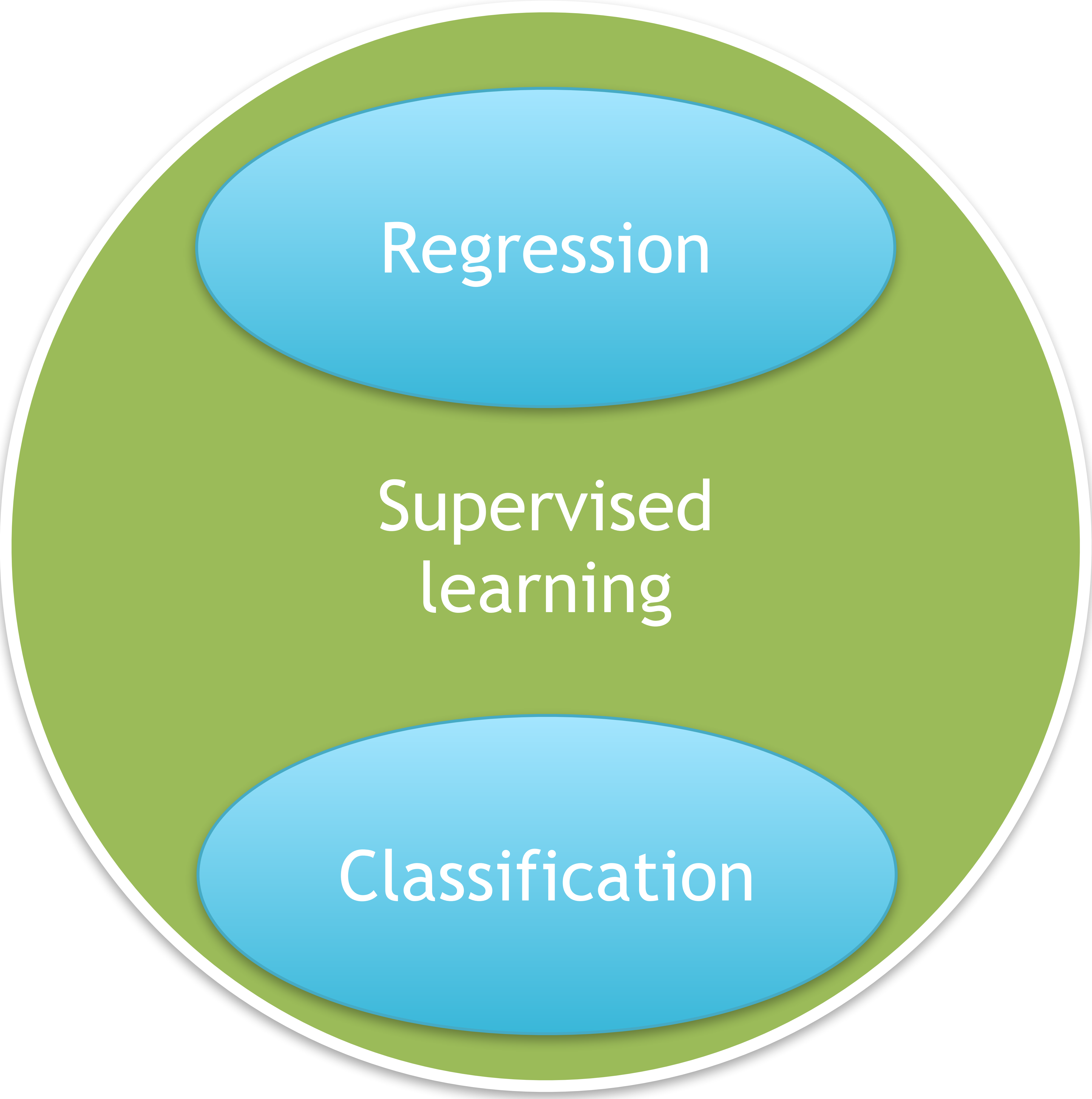
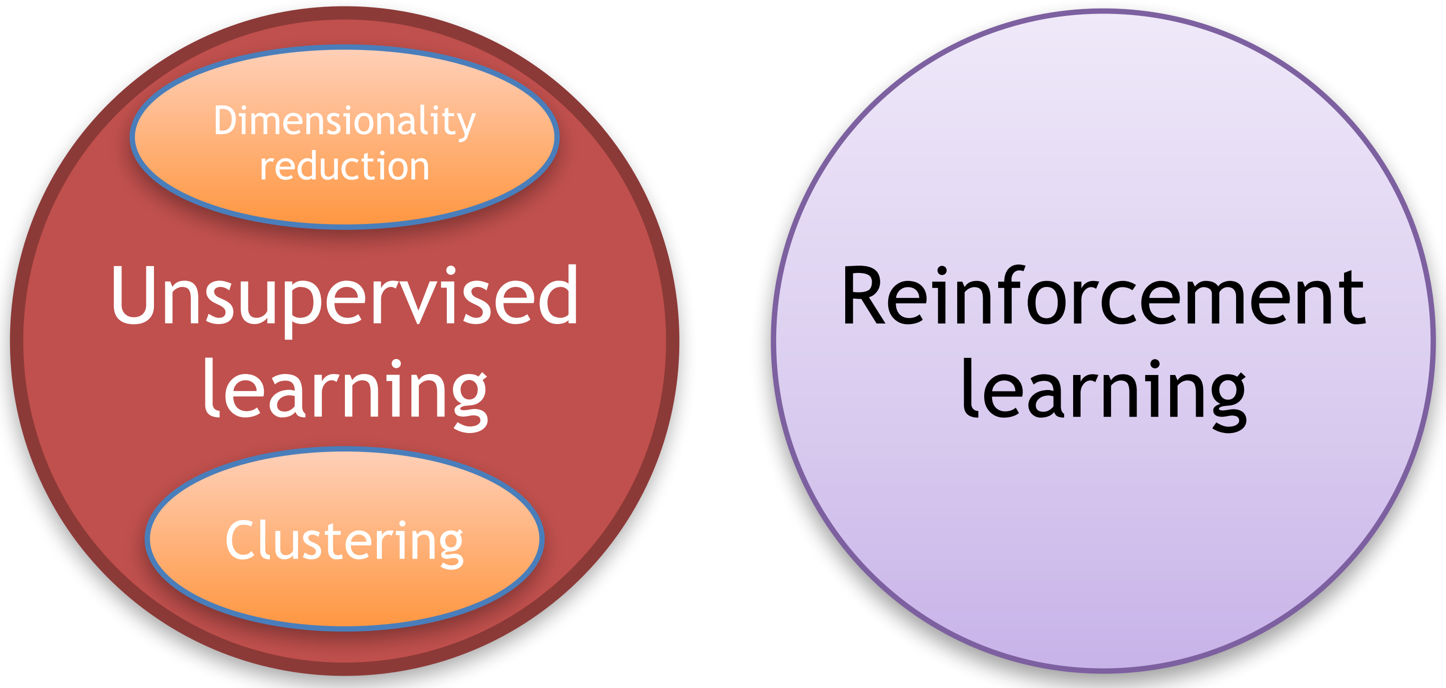



In this module, we solely focus on supervised machine learning &




will be covered in MTH793P

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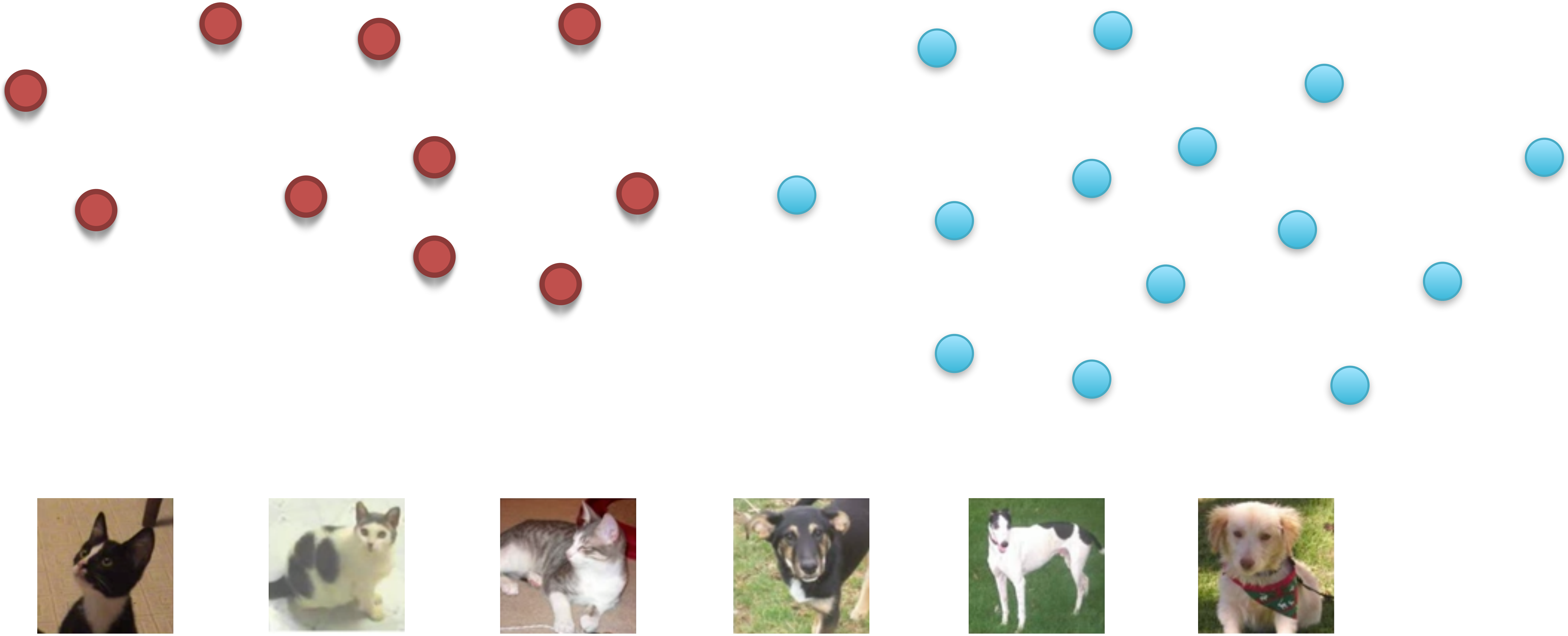
# What is supervised machine learning?

Classification

Example:

# What is supervised machine learning?



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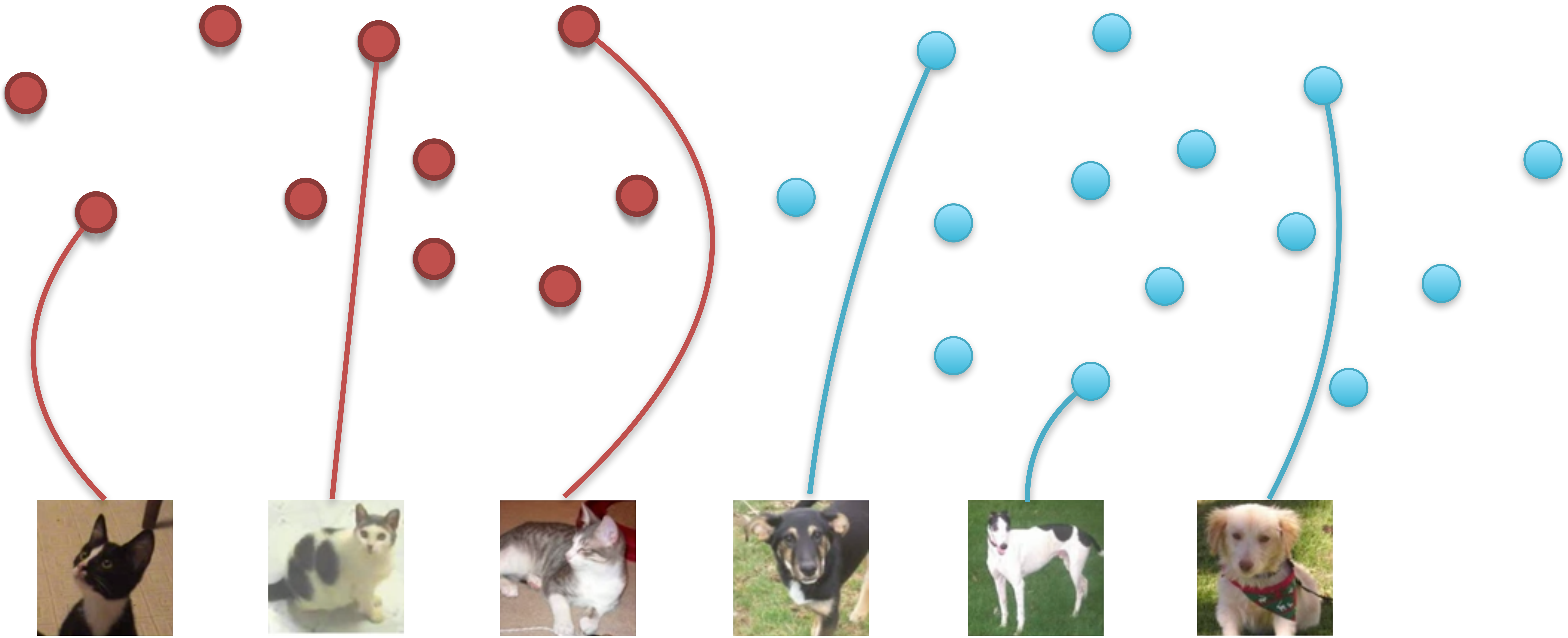

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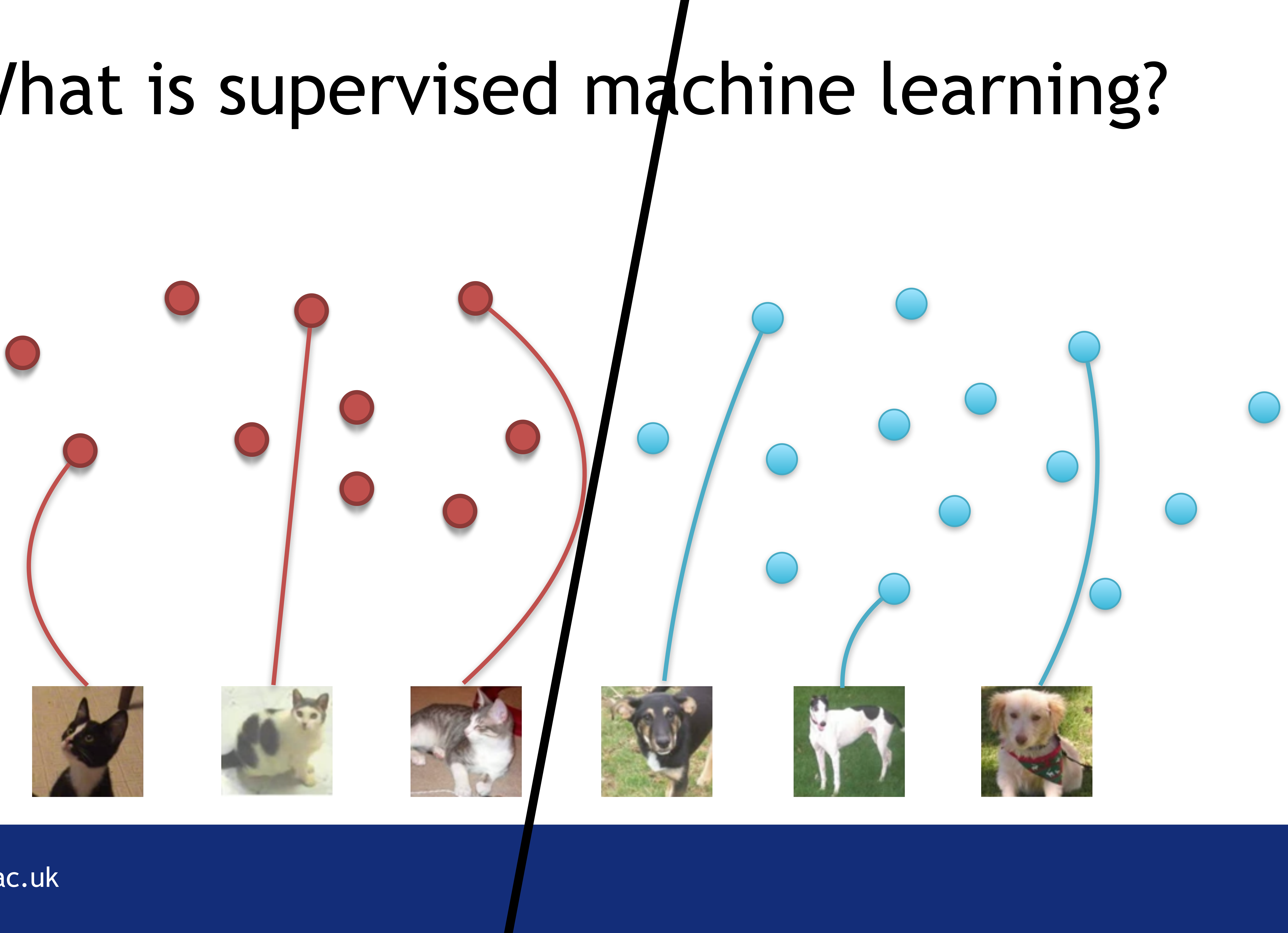

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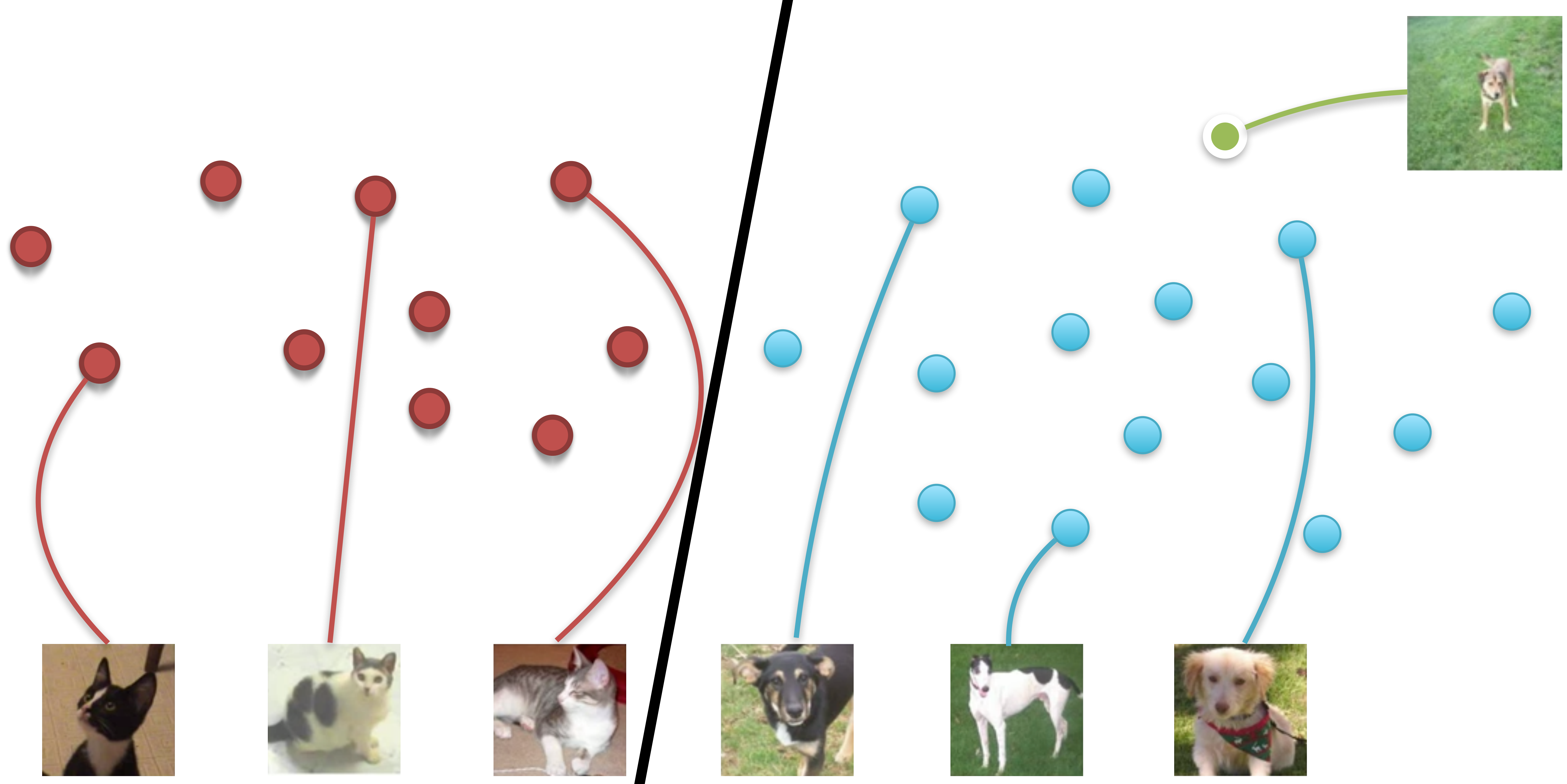

# What is supervised machine learning?

Mathematical model

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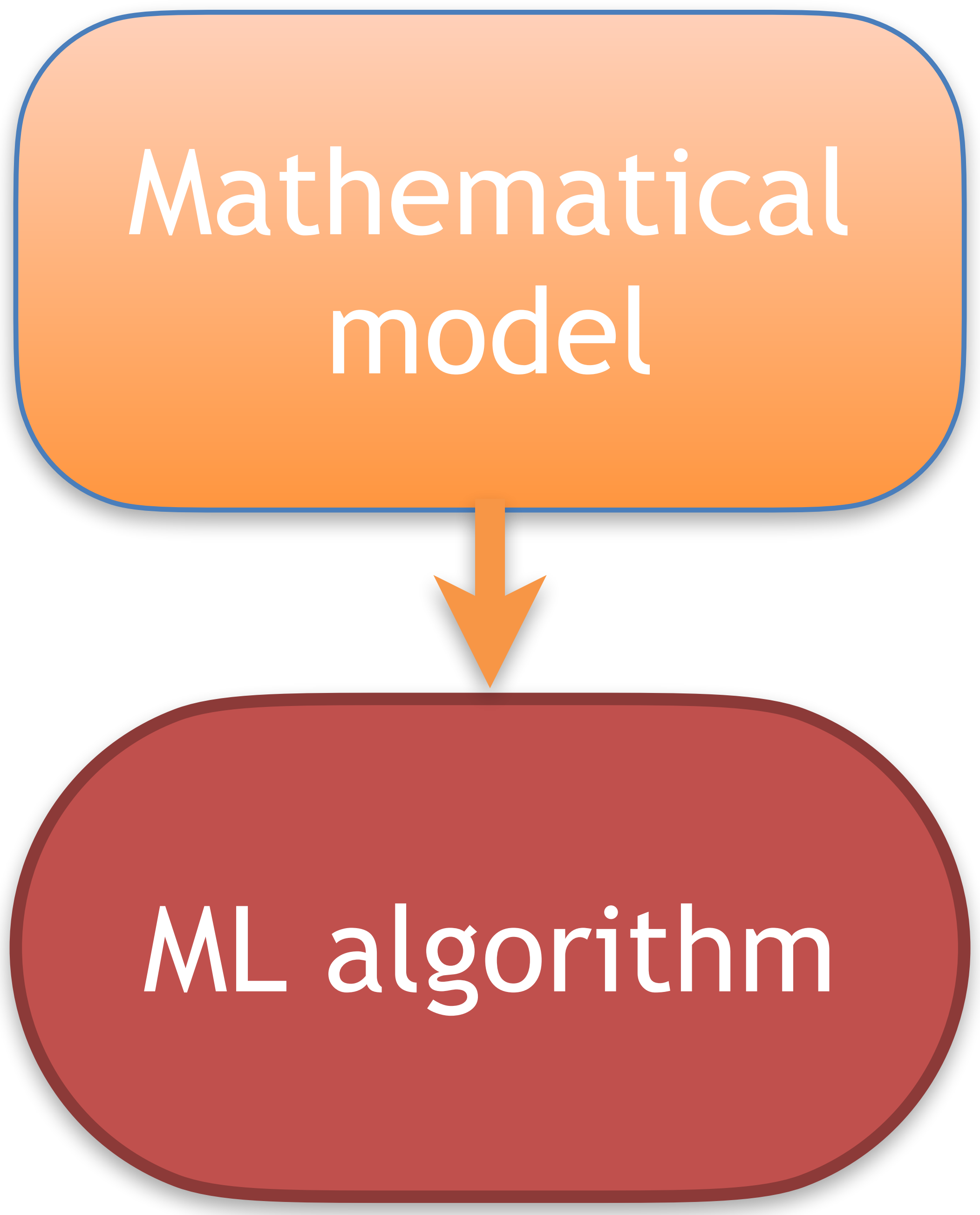

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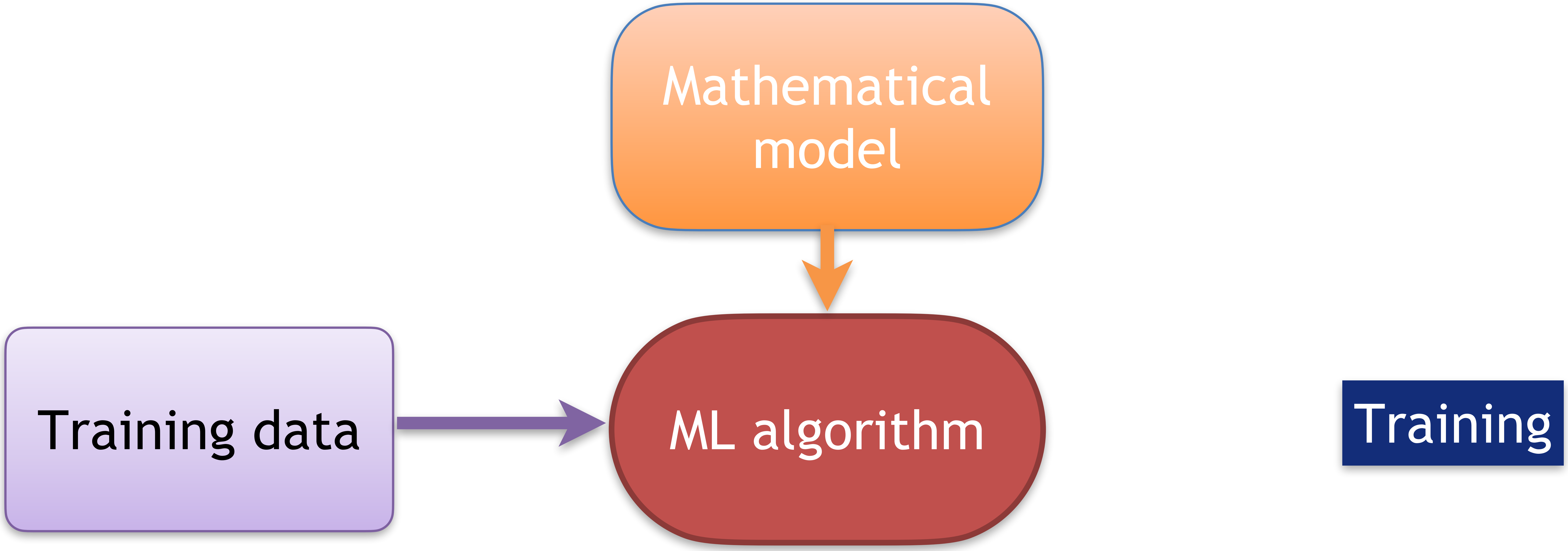

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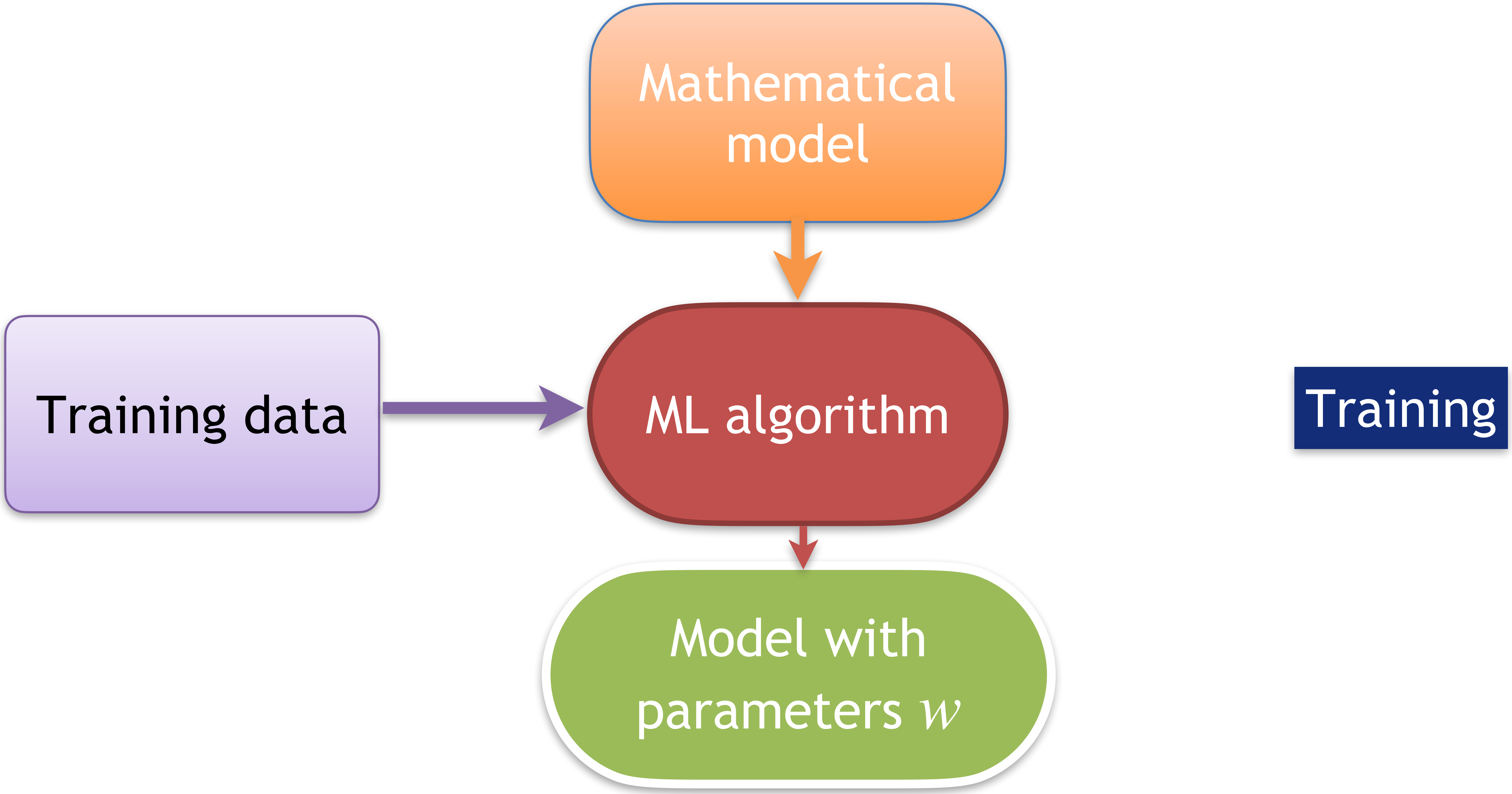

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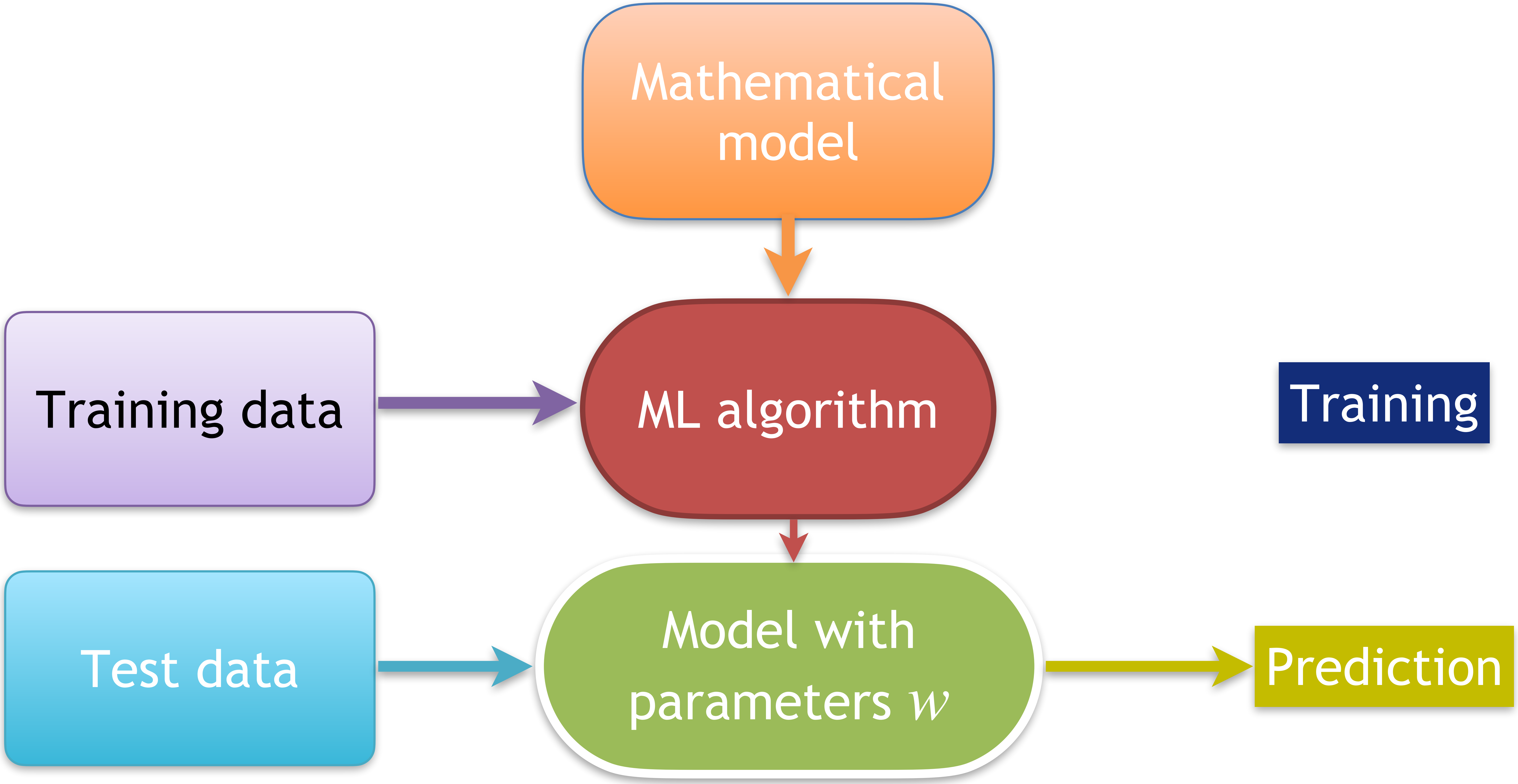

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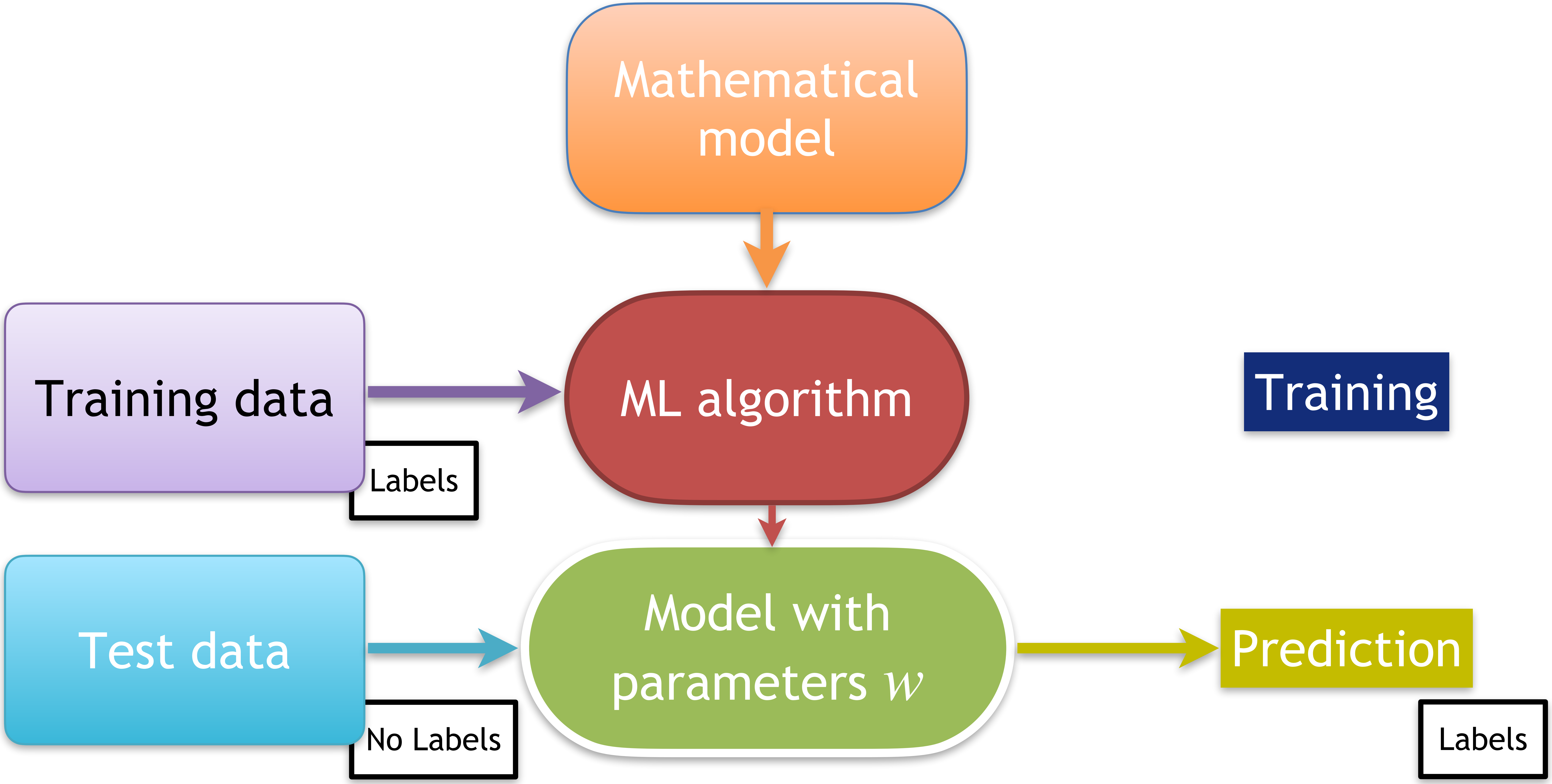
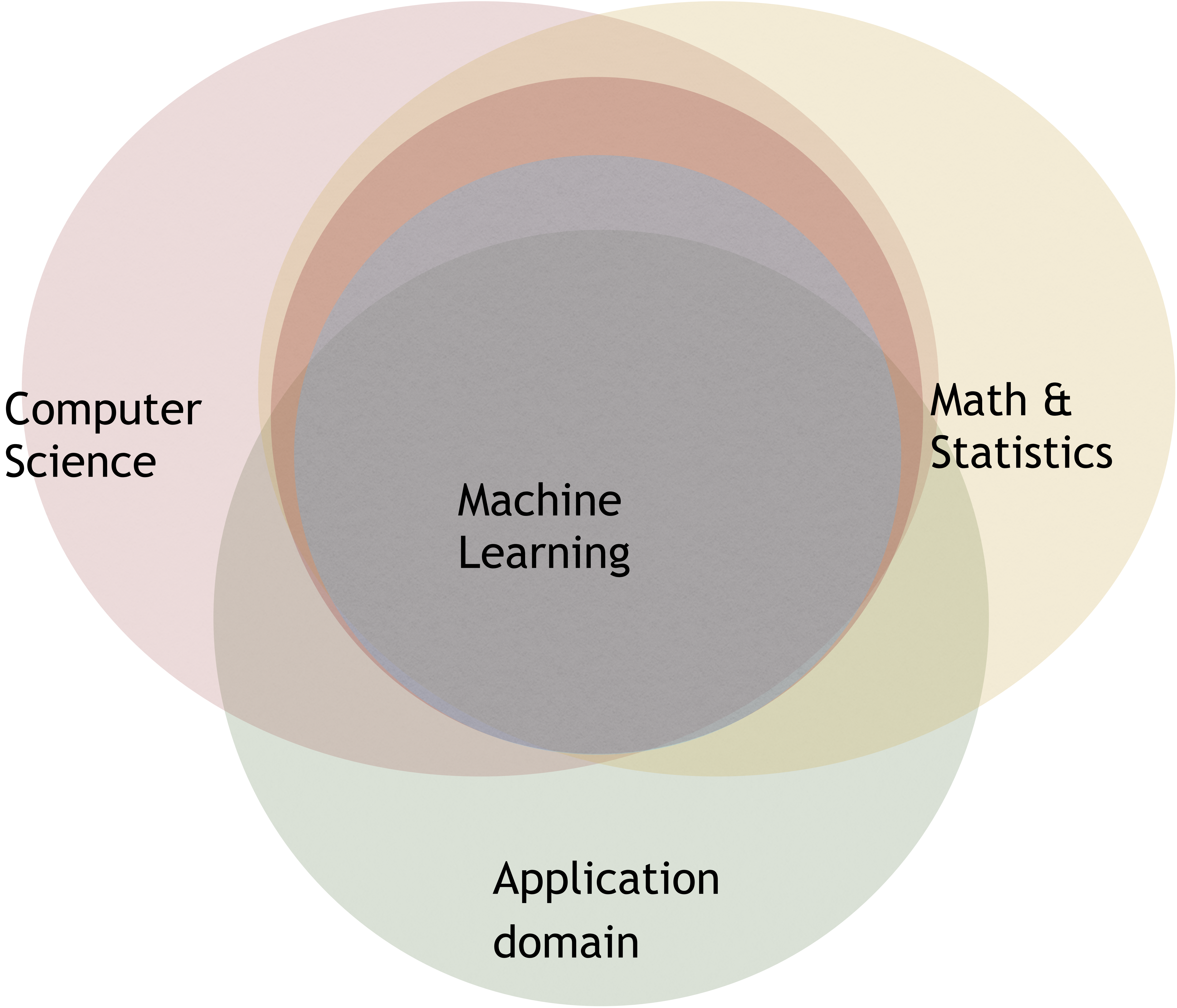
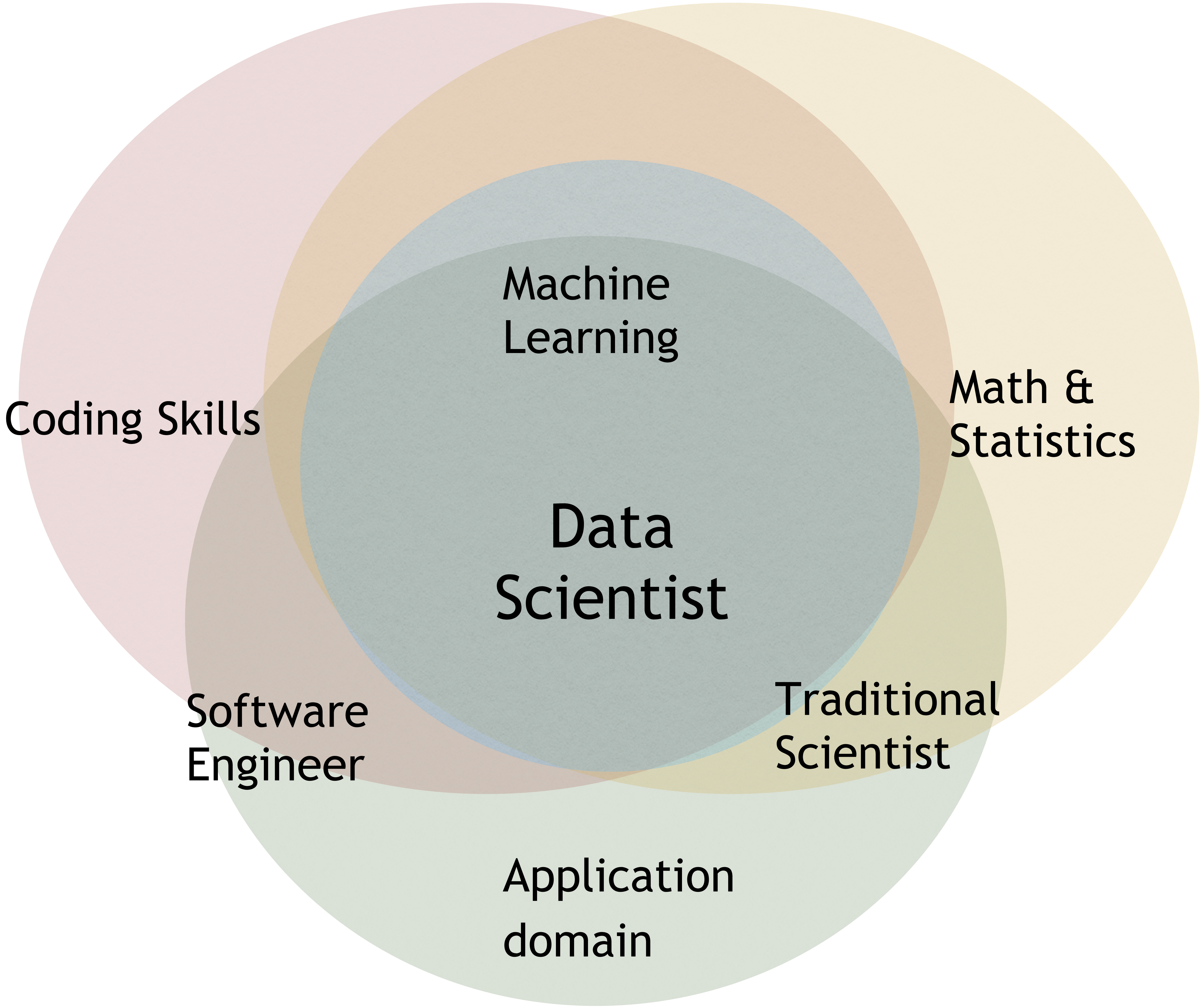


# ML and its broader context



# ML and jobs


Machine Learning
Coding Skills
Math & Statistics
Data Scientist
Software Engineer
Traditional Scientist
Application domain

# ML and jobs

Harvard Business Review

Coronavirus Magazine Popular Topics Podcasts Video Store The Big Idea Visual Library

Artwork: Tamar Cohen, Andrew J Buboltz, 2011, silk screen on a page from a high school yearbook, 8.5" x 12"

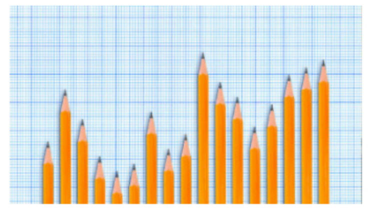
DATA

## Data Scientist: The Sexiest Job of the 21st Century

by Thomas H. Davenport and D.J. Patil

From the October 2012 Issue

WHAT TO READ NEXT

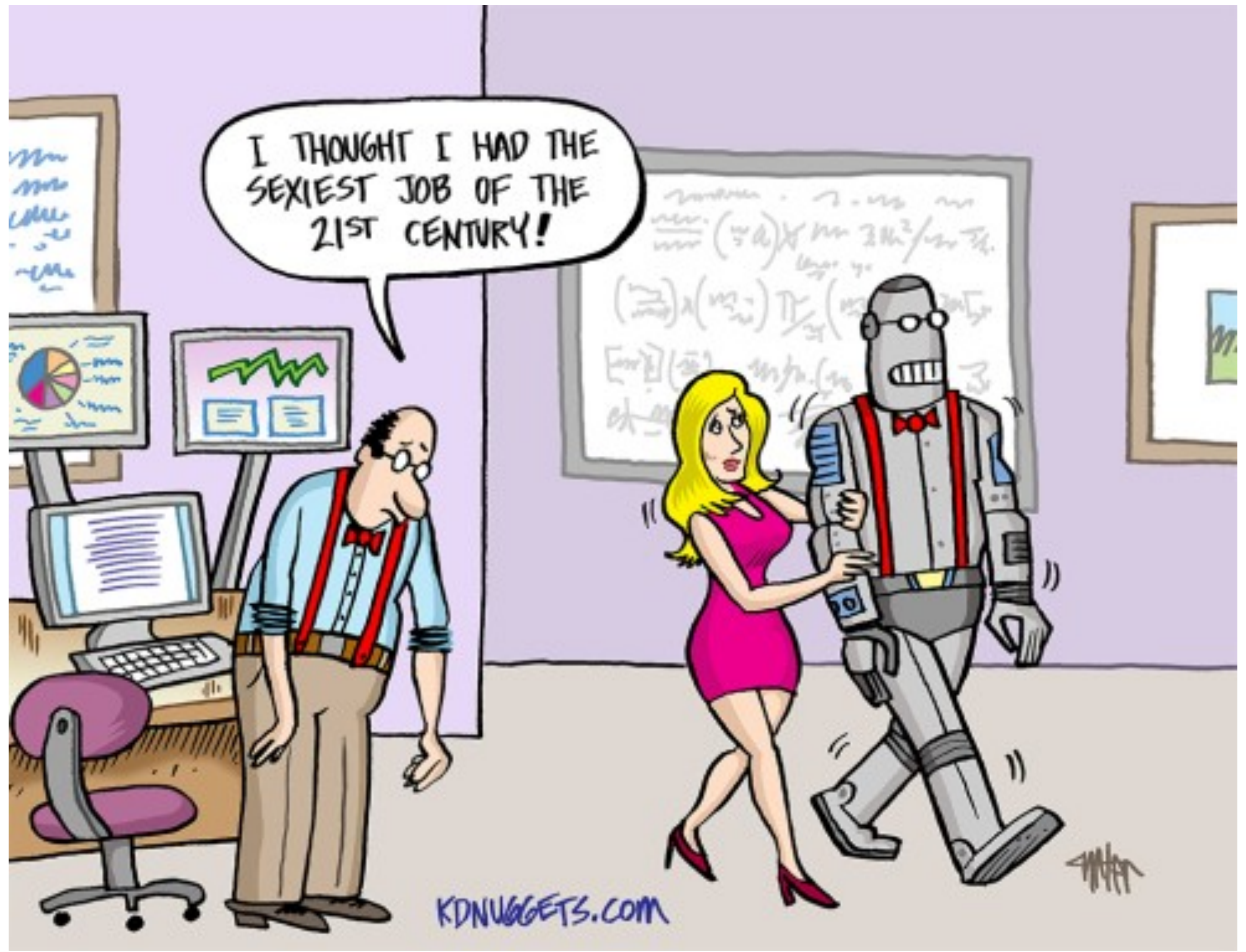


**What Data Scientists Really Do, According to 35 Data Scientists**

DATA SCIENTISTS

## Is 'Data Scientist' the 'Sexiest Job of the 21st Century'? And How Do You Get One of Your Own?

*Even if you're not versed in advanced analytics and data science, you can understand the thought process data scientists go through.*



# ML and jobs

## Royal Society: Dynamics of Data Science

Ensuring a Healthy Data Science Skills Landscape Across All Sectors in the UK

Britain is facing "explosive demand" for data science skills and its education system needs to change to keep up, according to a Burning Glass Technologies analysis commissioned by the Royal Society.

Demand for data scientists and data engineers tripled over the past five years, rising 231%. That's much faster than job postings overall in the UK, which rose 36%, according to the report, "Dynamics of data science skills."

Different regions saw different growth rates, from 79% in Wales to 269% in the North West and 563% in Northern Ireland. On average, salaries for these roles is £64,376, up 22% over the same period.

Job of the 21st Century

by Thomas H. Davenport and D.J. Patil

From the October 2012 Issue

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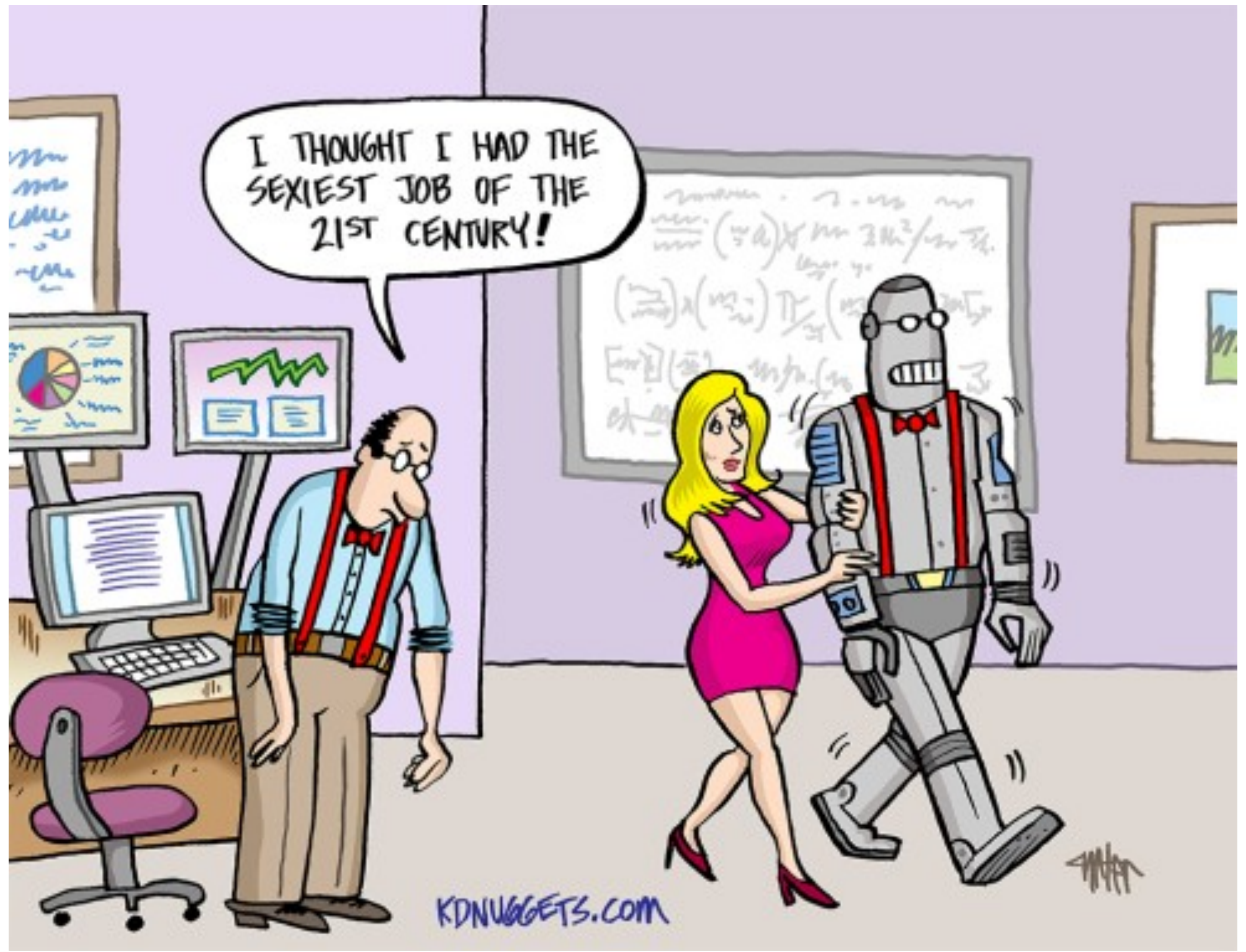
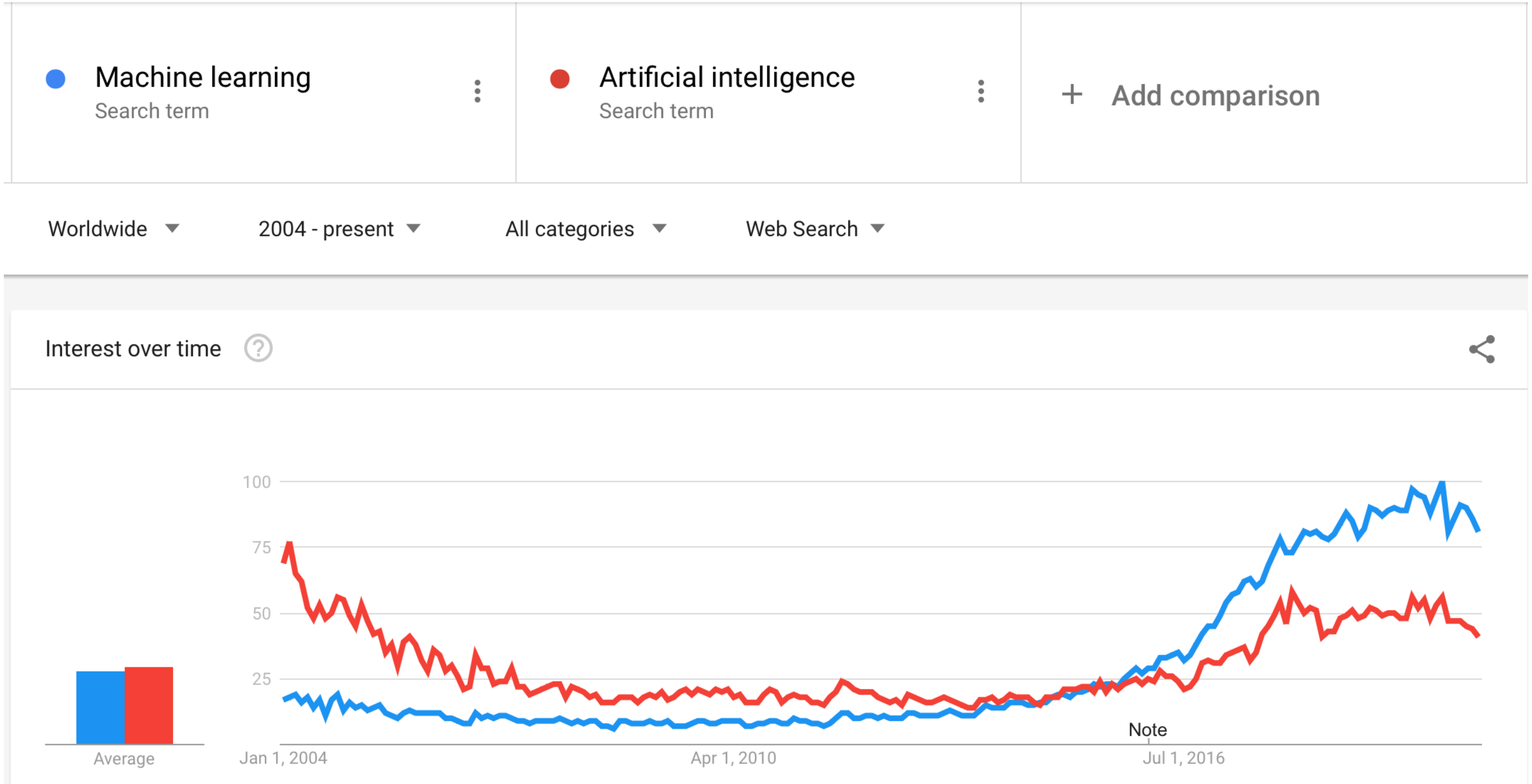


# ML popularity



# ML and jobs

The usual suspects

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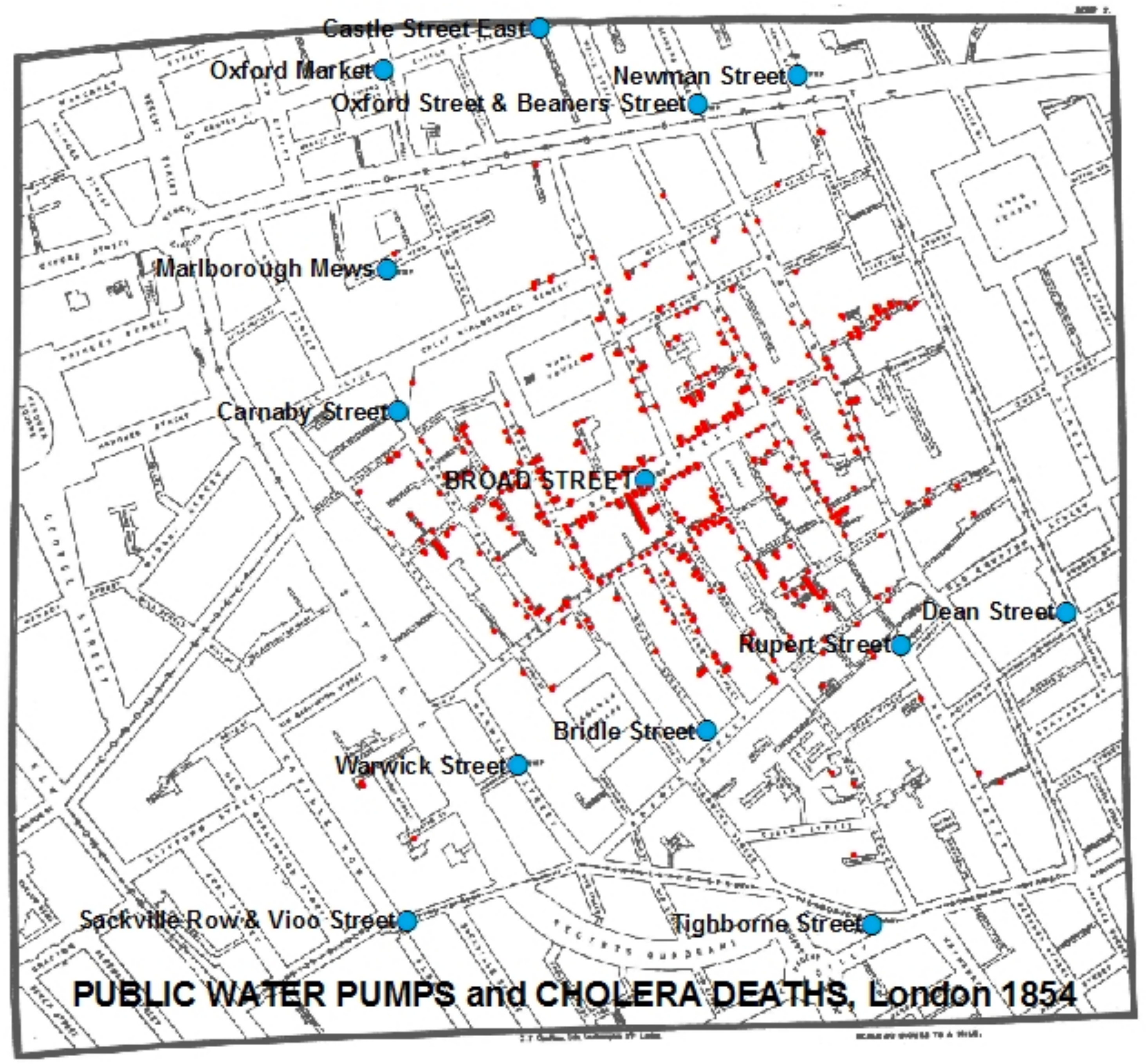
The usual suspects

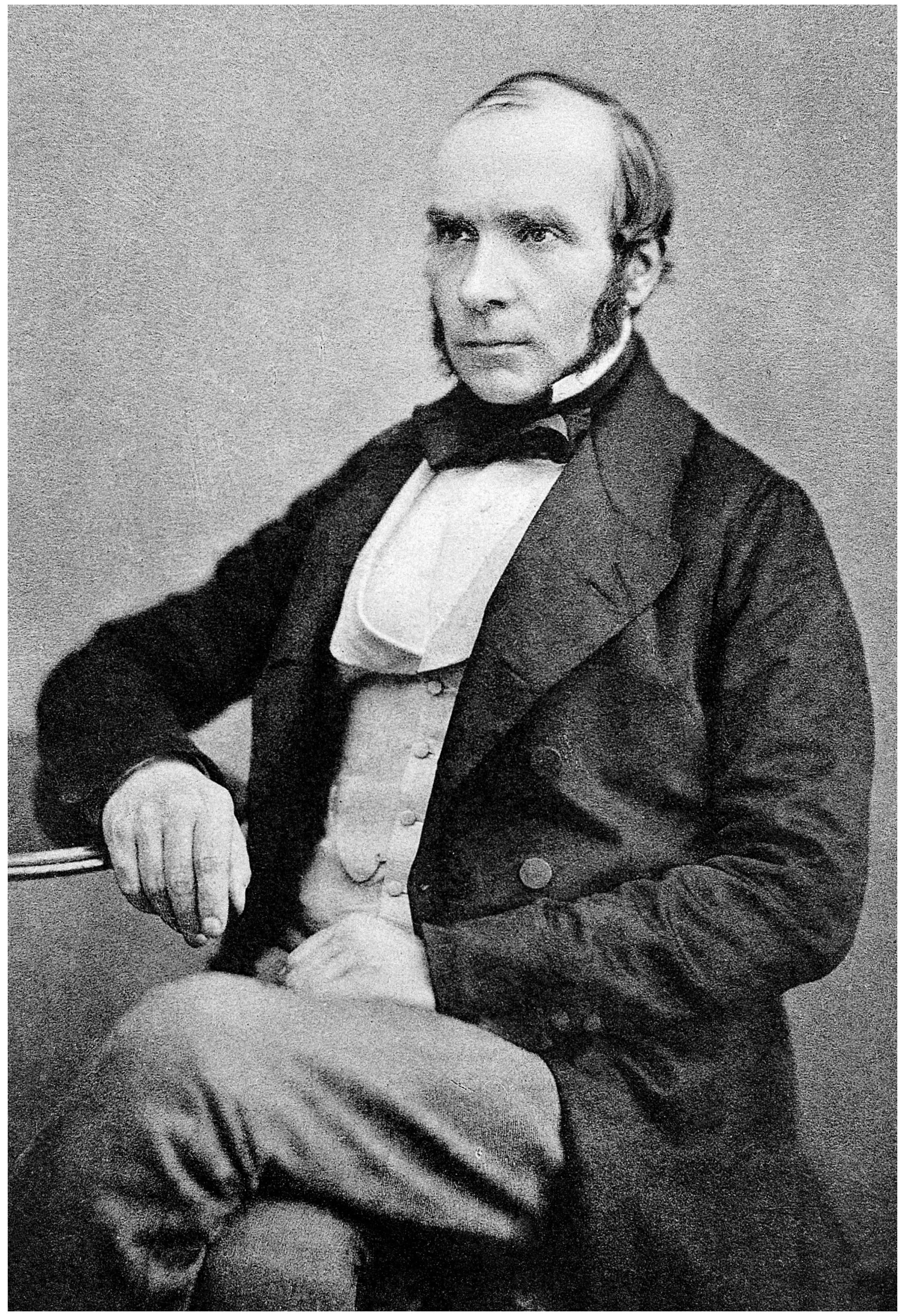
No longer just them

Majority of industries hiring data scientists

# Machine learning is not new




1854 Broad Street cholera outbreak



John Snow. ©Wikimedia commons

©Wikimedia commons

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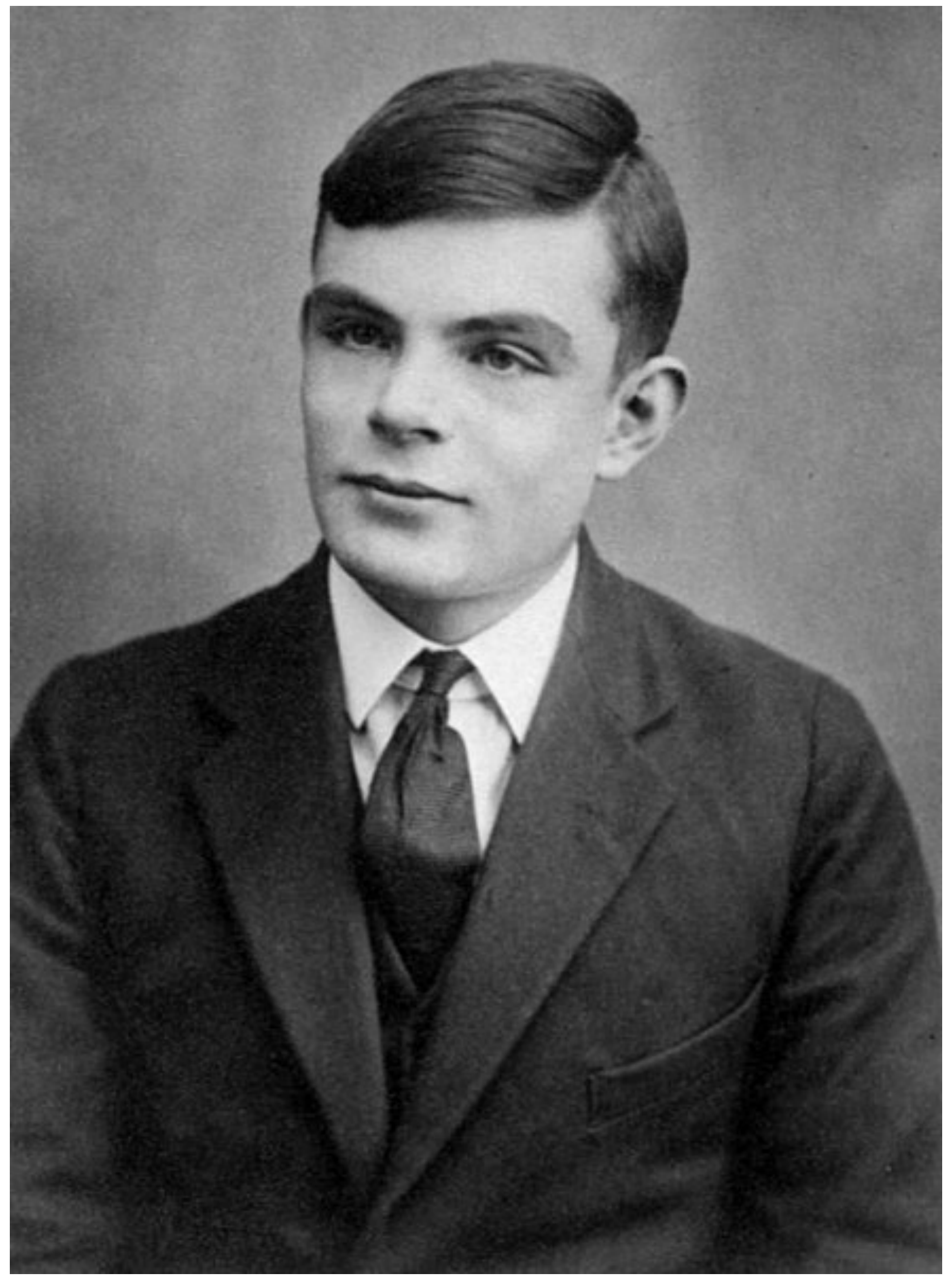

Turing

Rosenblatt

# What has changed?

*1950s:* $10^3$ FLOPS

*2020:* $10^{18}$ FLOPS

FLOPS -> floating point operations per second

# Challenges

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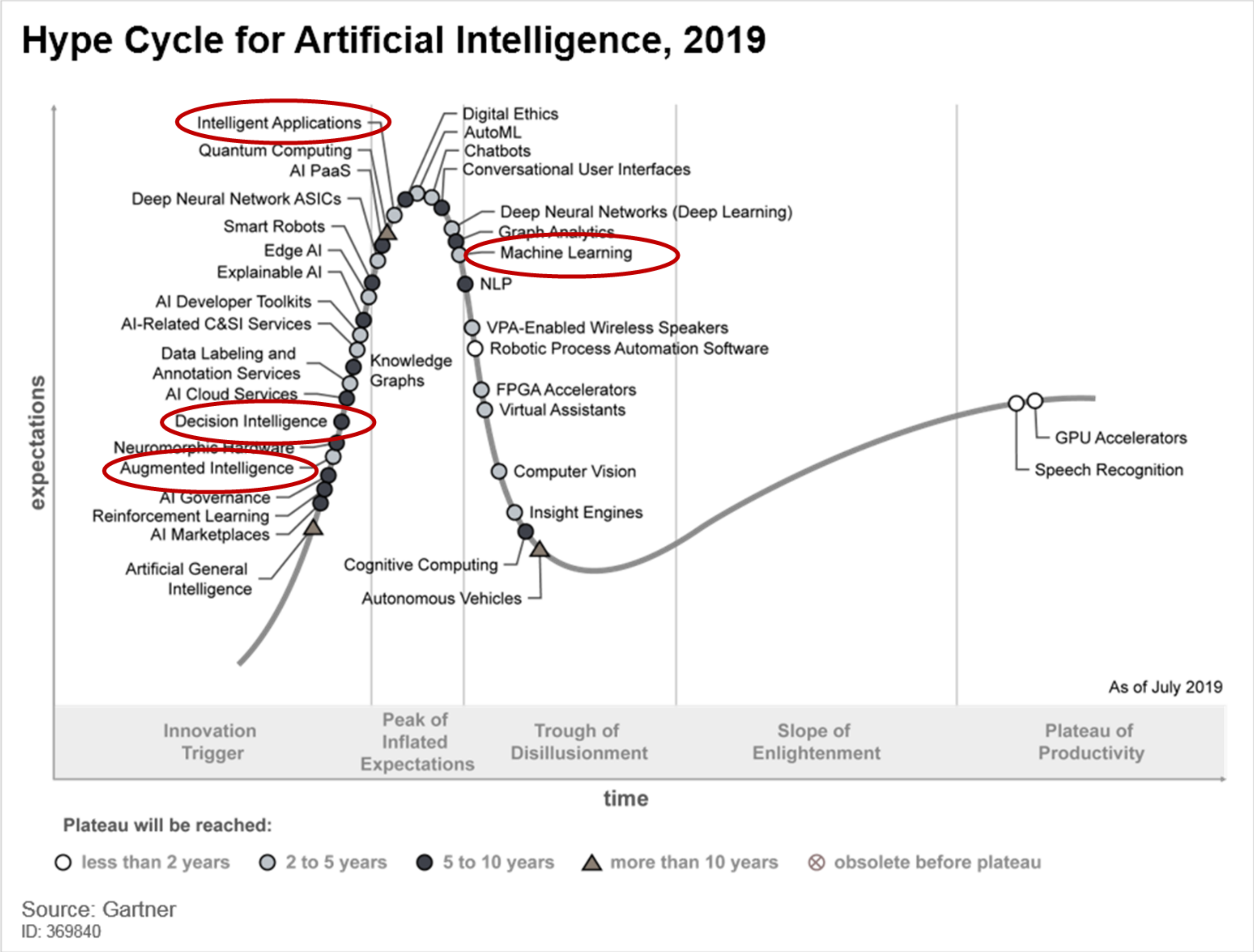
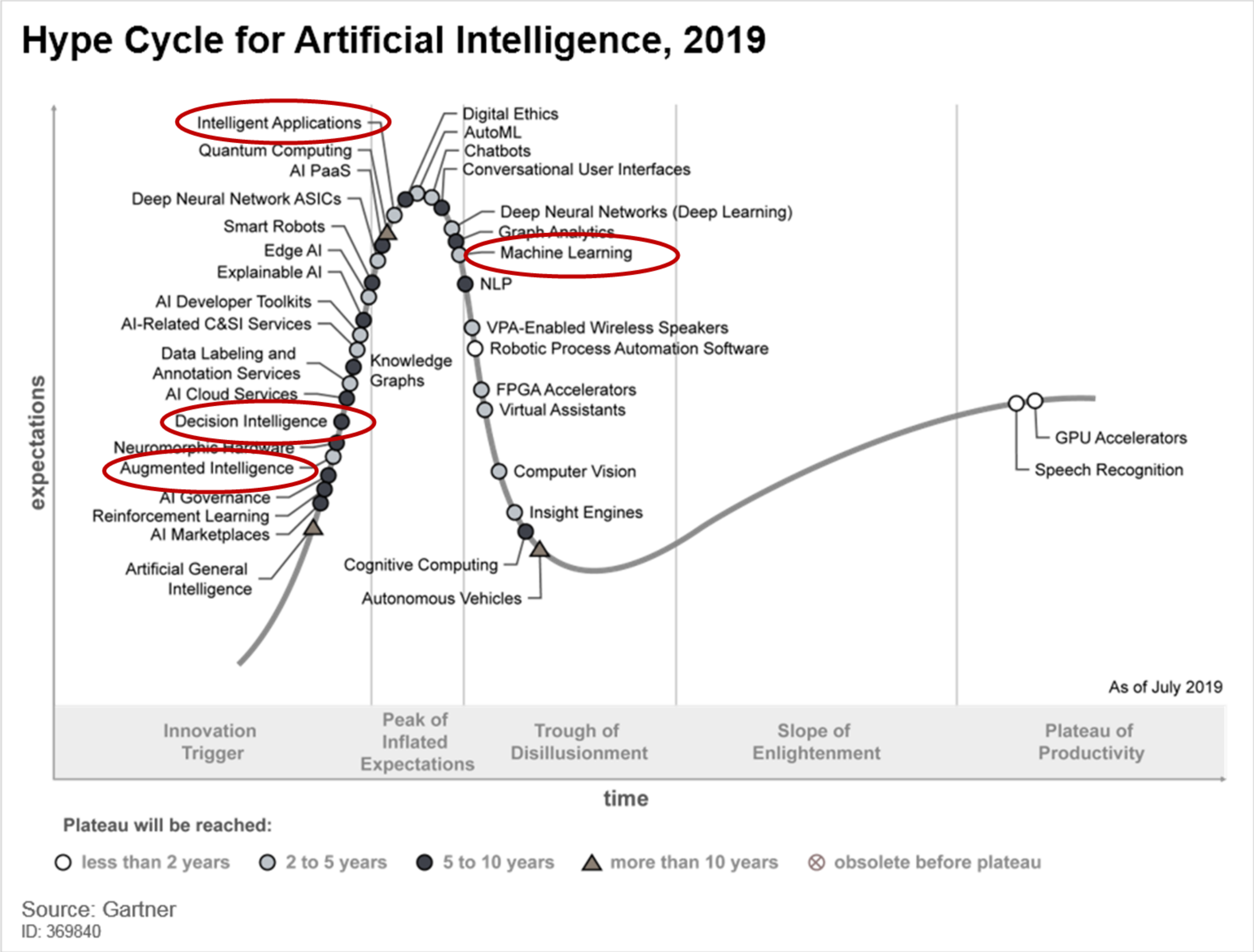
- Hype, i.e. cycles of AI and ML popularity



# Challenges

- Hype, i.e. cycles of AI and ML popularity
- Data Ethics, Privacy, Fairness

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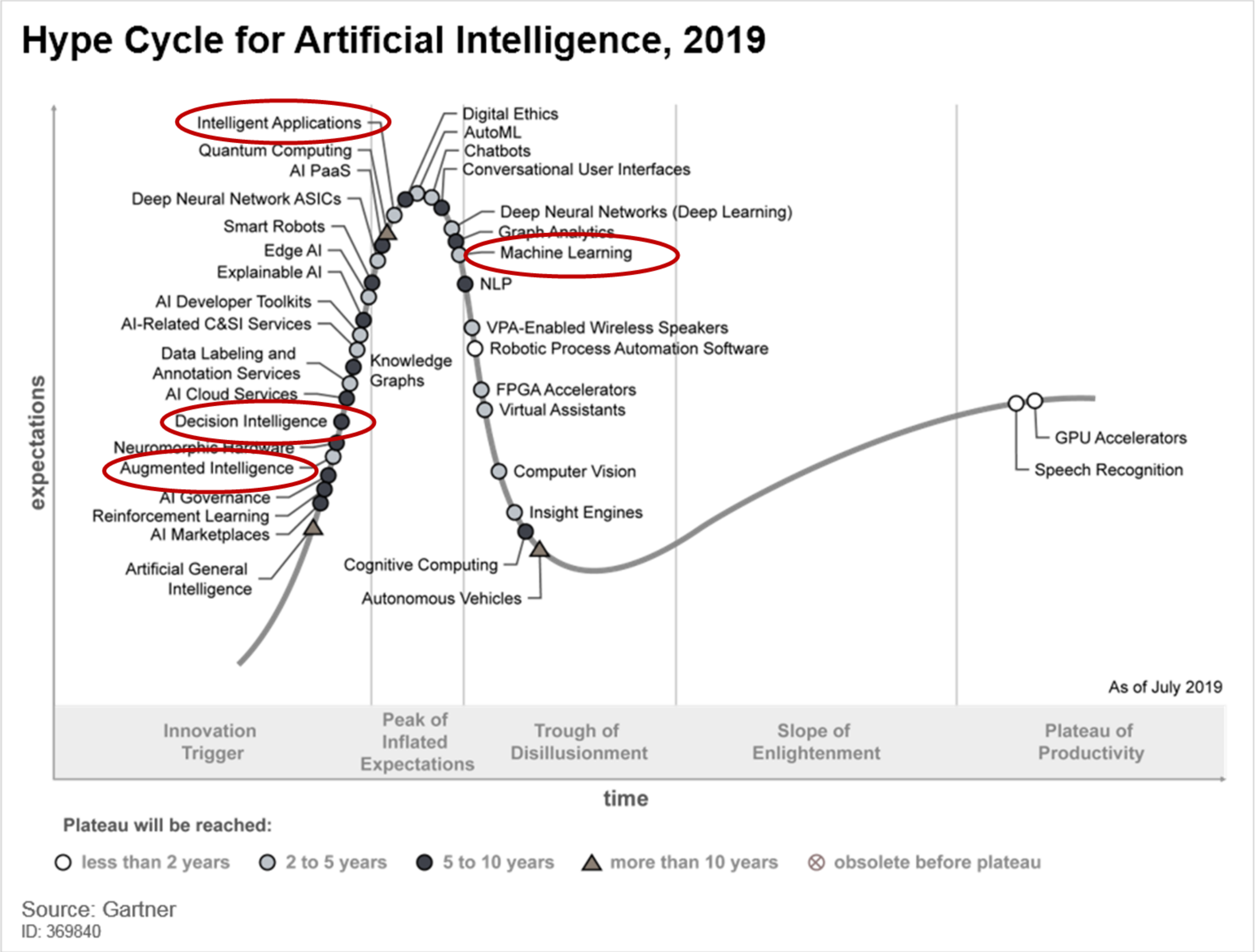

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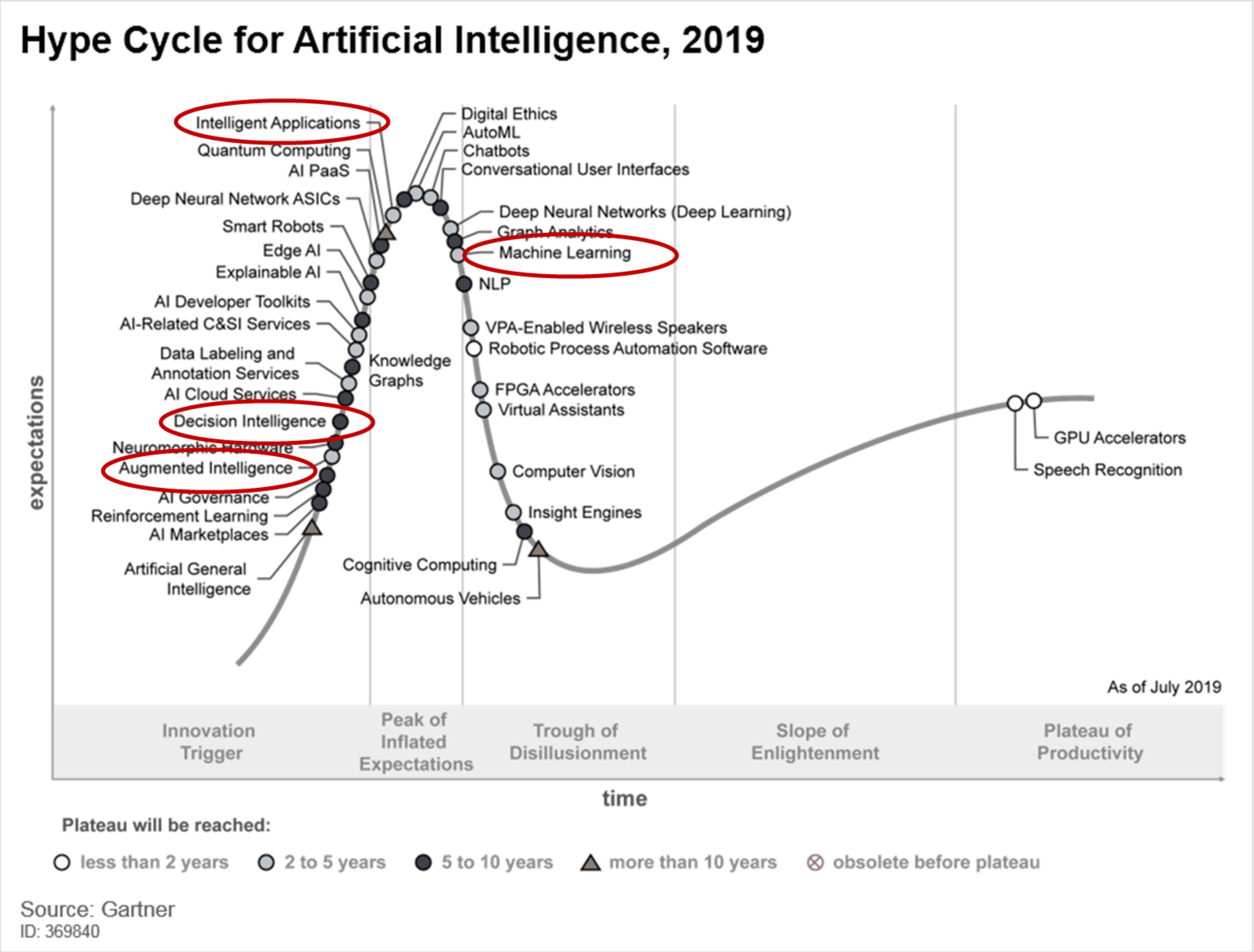
- Social Implications: threats from super-human AI? Job losses?



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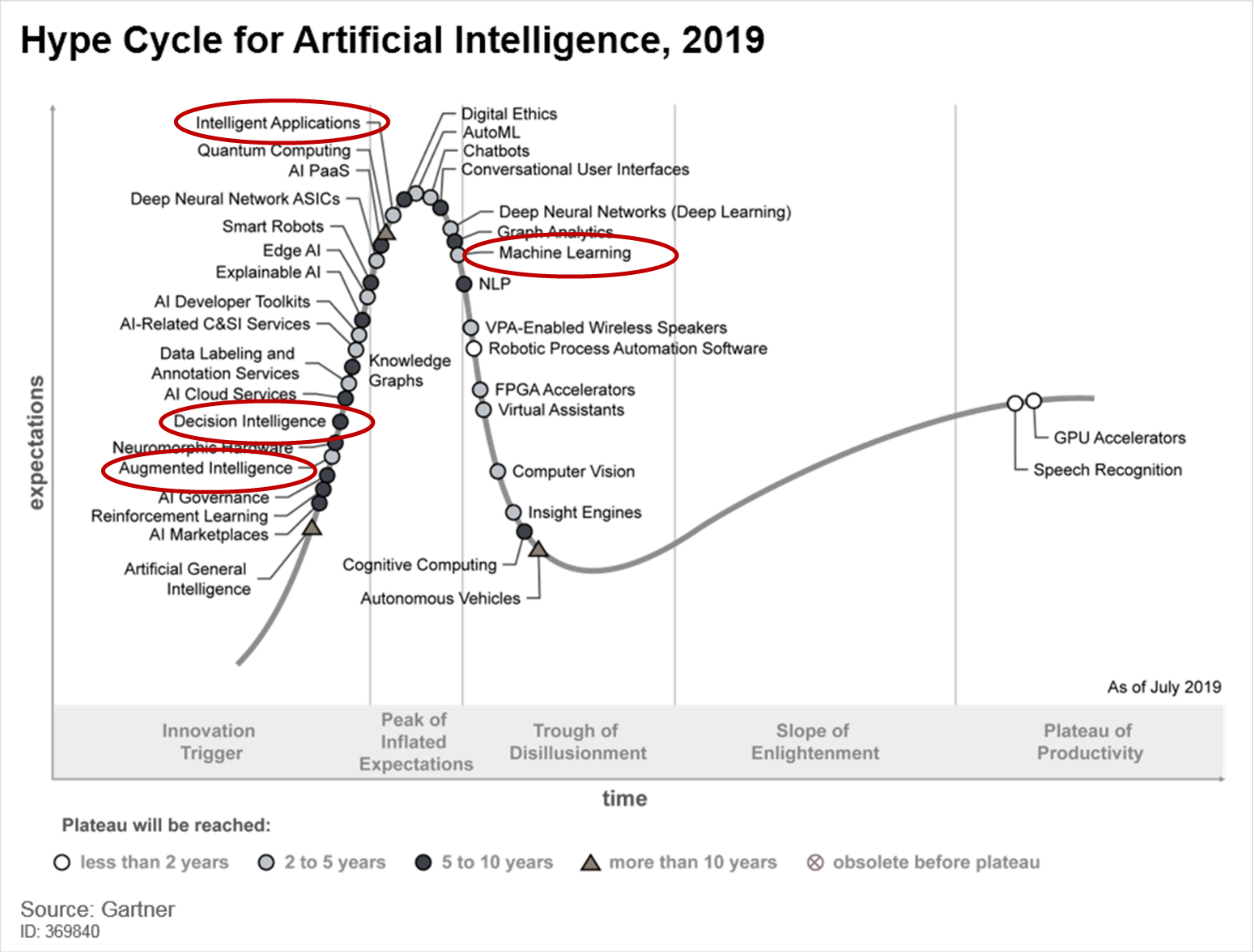
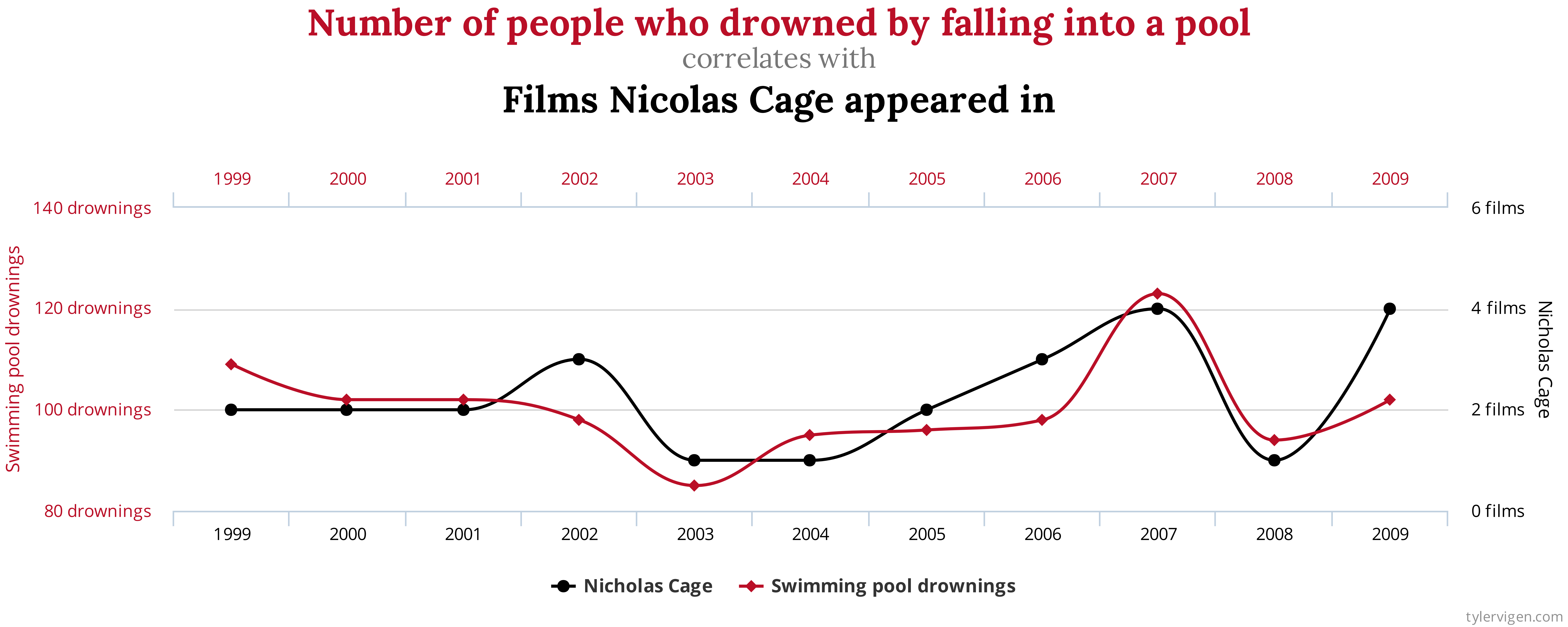



We need: scientific method, reproducible research, open source and open data

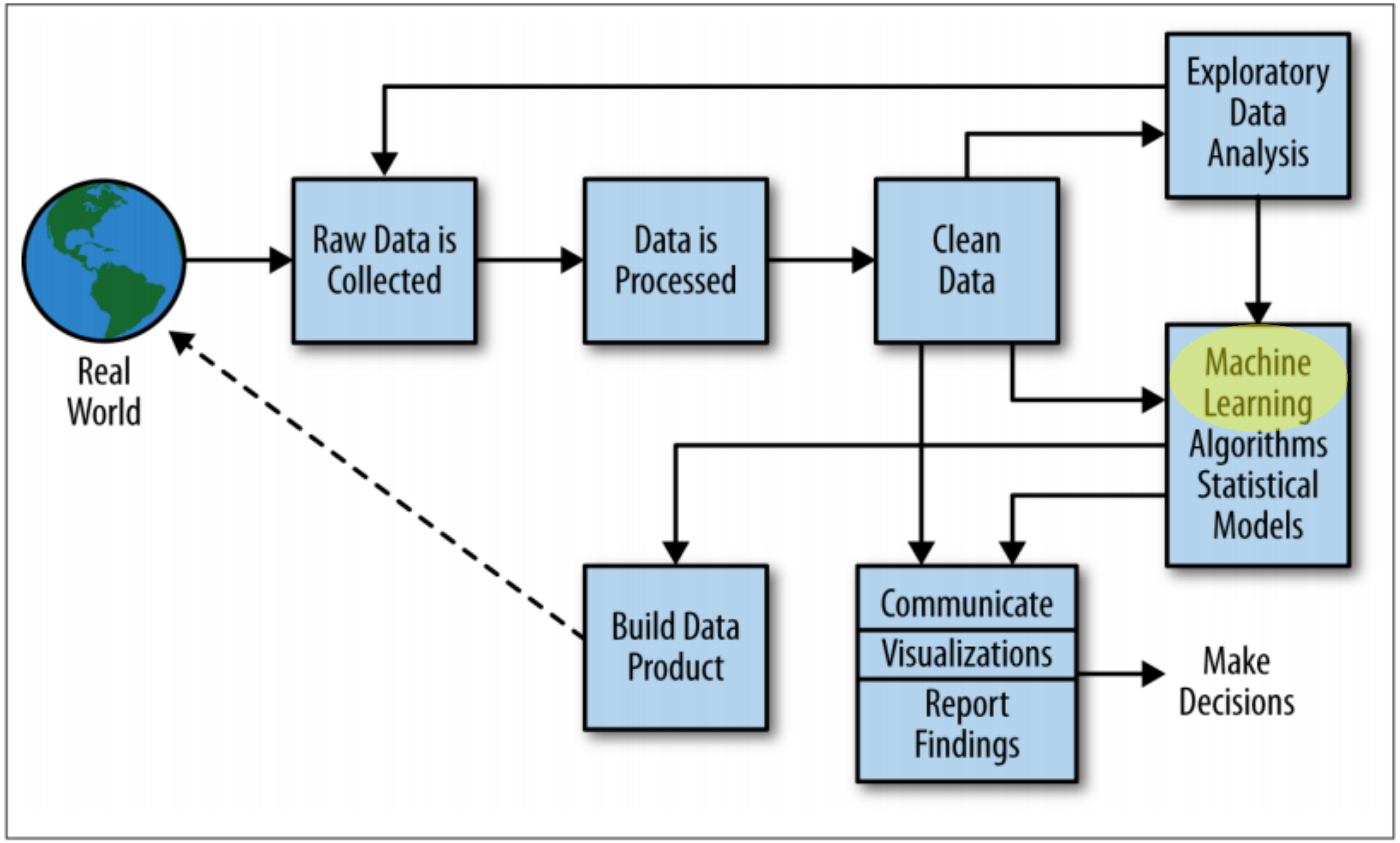
# Correlation ≠ causation*

What we not cover in this module: causal inference**




*in general, and without additional prior assumptions
**Pearl, Judea, Madelyn Glymour, and Nicholas P. Jewell. *Causal inference in statistics: A primer*. John Wiley & Sons, 2016.

# Machine learning is only a small part




From Schutt and O'Neil "Doing Data Science"

# LINEAR ALGEBRA

# Matrices and Vectors

Matrix: $$\mathbf{X} = \begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1d} \\ x_{21} & x_{22} & \cdots & x_{2d} \\ \vdots & & \ddots & \vdots \\ x_{s1} & x_{s2} & \cdots & x_{sd} \end{pmatrix} \in \mathbb{R}^{s\times d}$$

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You need to pay attention to the dimensions!

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# Matrices and Vectors

Example

$$\begin{pmatrix} 1 & 2 & 3 \\ 0 & 1 & 2 \\ 1 & -1 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 4 \\ 0 \end{pmatrix}$$

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General rule: rows times columns

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$$\begin{pmatrix} 1 & 2 & 3 \\ 0 & 1 & 2 \\ 1 & -1 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 4 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \times 1 + 2 \times 4 + 3 \times 0 \\ \\ \end{pmatrix}$$

# Matrices and Vectors

How do we compute the result of the multiplication?

General rule: rows times columns

$$\begin{pmatrix} 1 & 2 & 3 \\ 0 & 1 & 2 \\ 1 & -1 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 4 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \times 1 + 2 \times 4 + 3 \times 0 \\ \\ \end{pmatrix}$$

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The row times column rule can be written as

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Matrix: $$\mathbf{X} = \begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1d} \\ x_{21} & x_{22} & \cdots & x_{2d} \\ \vdots & & \ddots & \vdots \\ x_{s1} & x_{s2} & \cdots & x_{sd} \end{pmatrix} \in \mathbb{R}^{s \times d}$$

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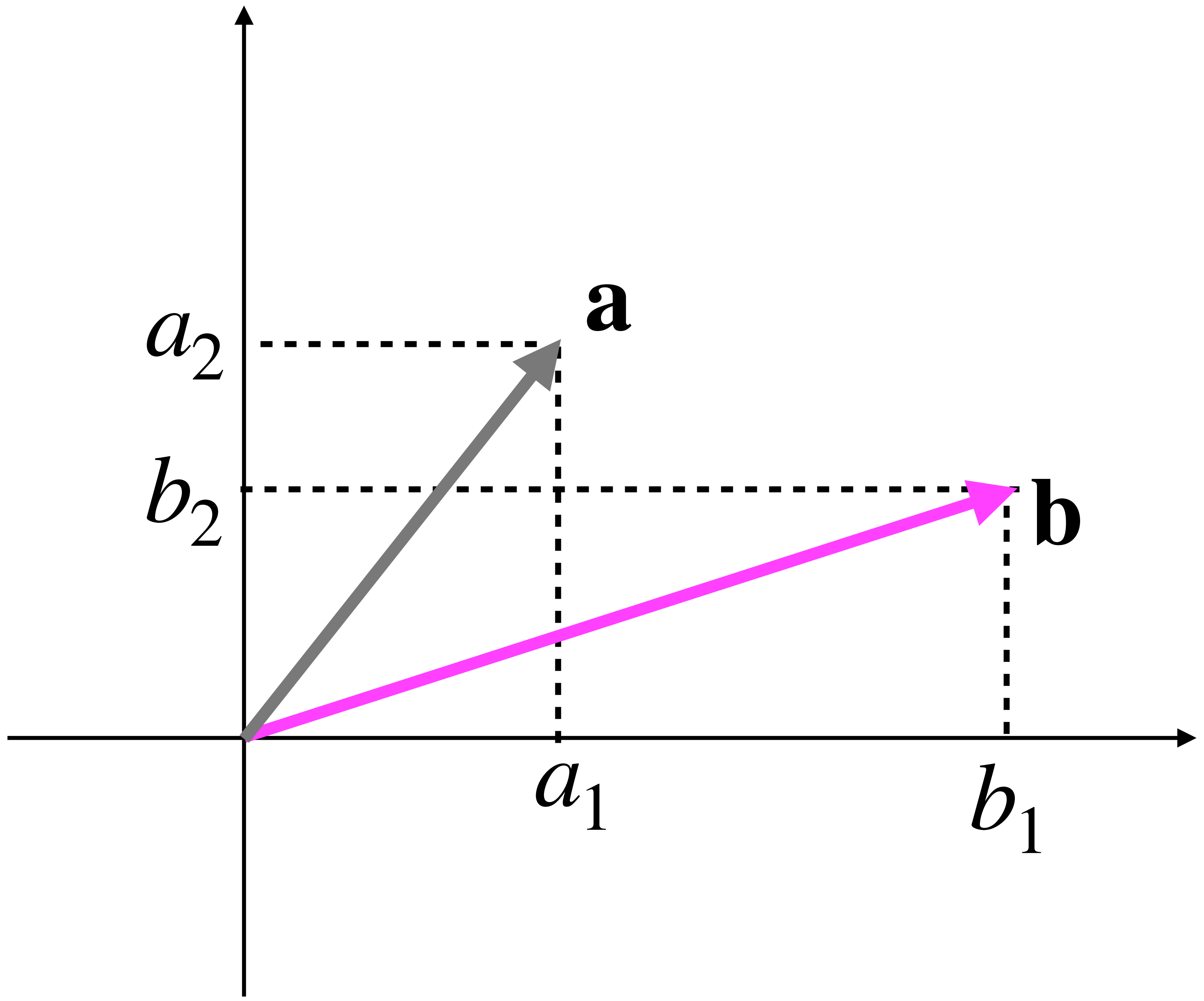
The transpose $X^\top$ of a matrix $X$ is defined as $$X^\top = \begin{pmatrix} x_{11} & x_{21} & \dots & x_{s1} \\ x_{12} & x_{22} & \dots & x_{s2} \\ \vdots & & \ddots & \vdots \\ x_{1d} & x_{2d} & \dots & x_{sd} \end{pmatrix} \in \mathbb{R}^{d \times s}$$

# Inner/dot/scalar product




$$\mathbf{a} = \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} \quad \mathbf{b} = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix} \quad \mathbf{a}, \mathbf{b} \in \mathbb{R}^{2\times1}$$

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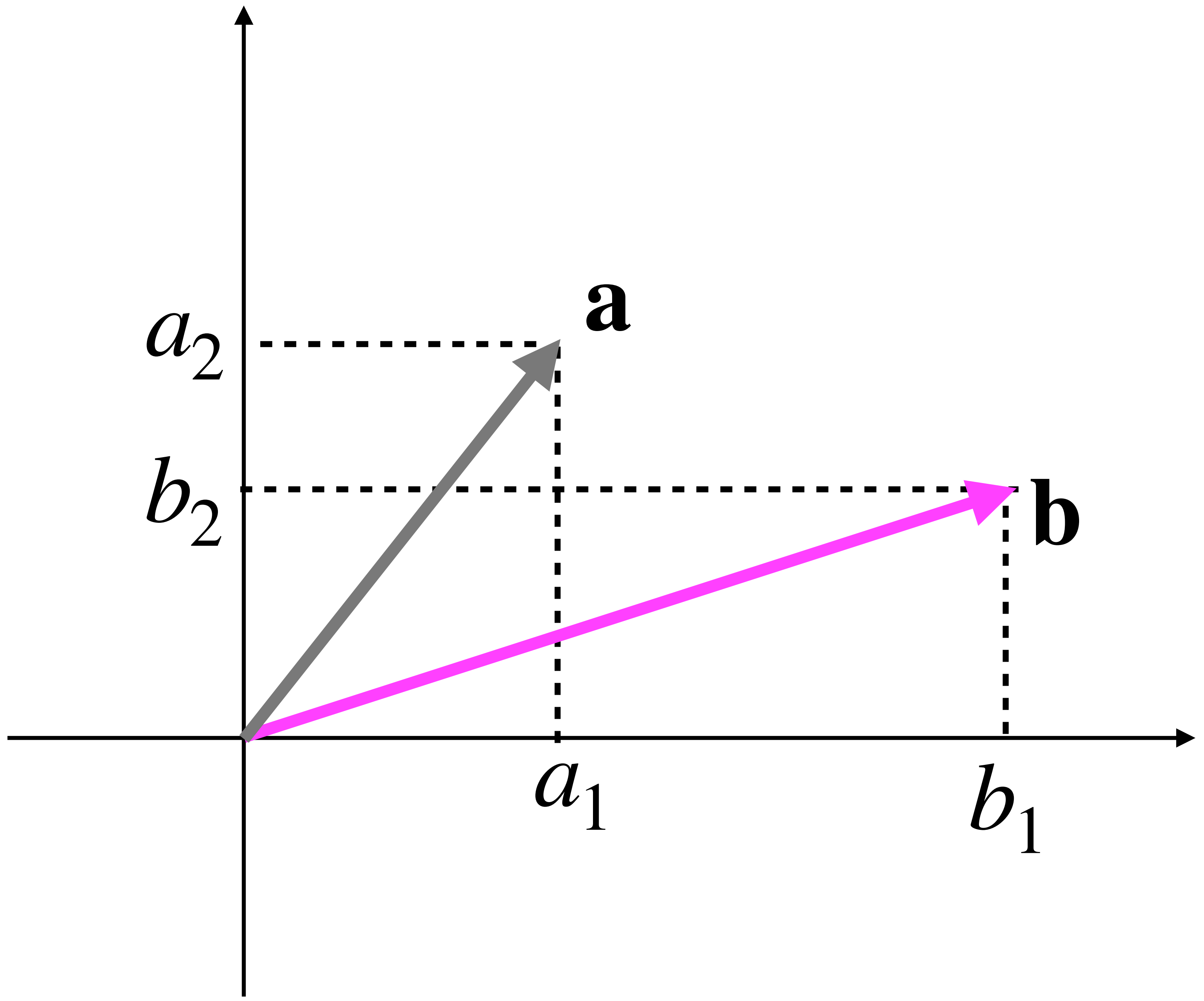


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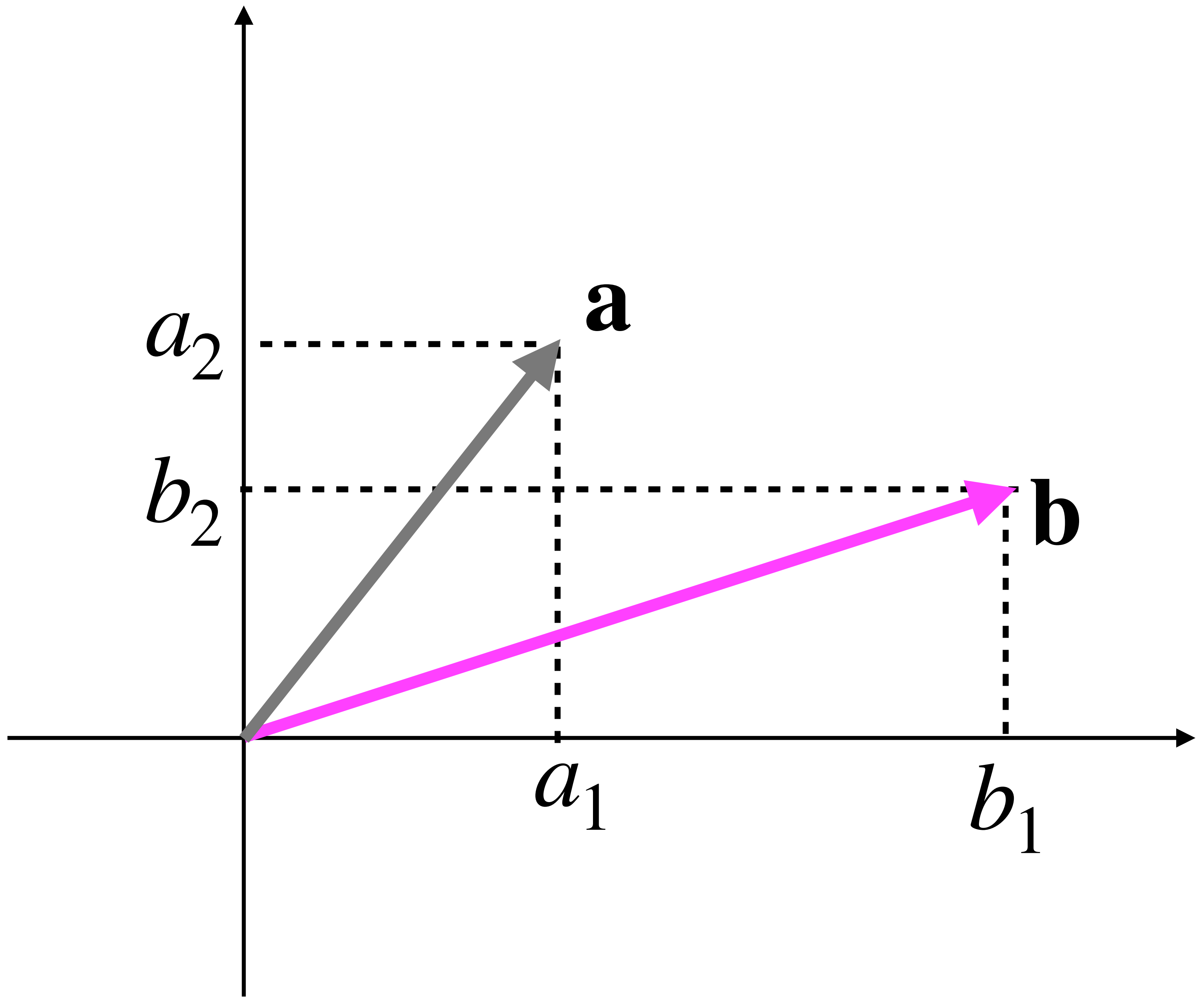


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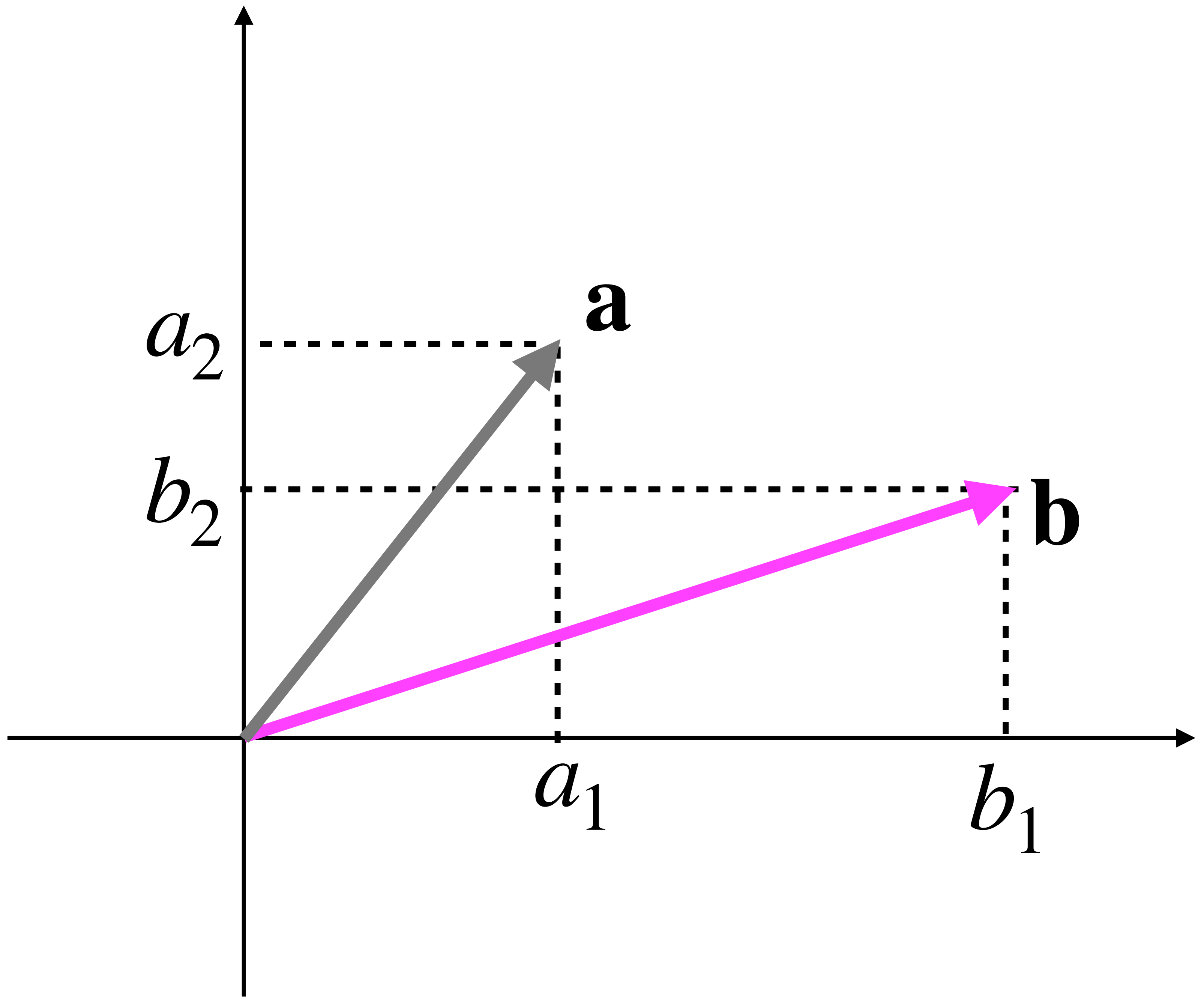


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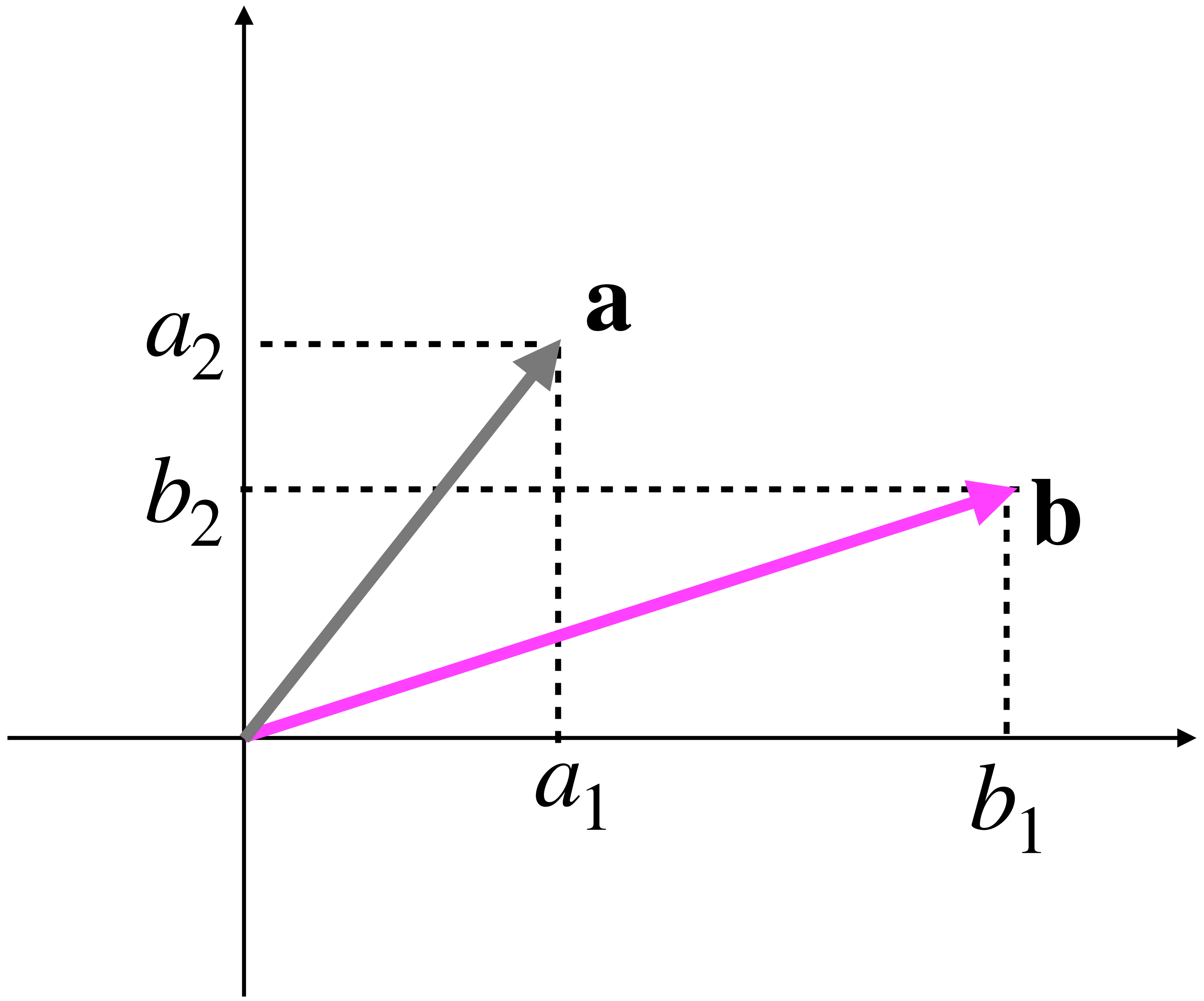


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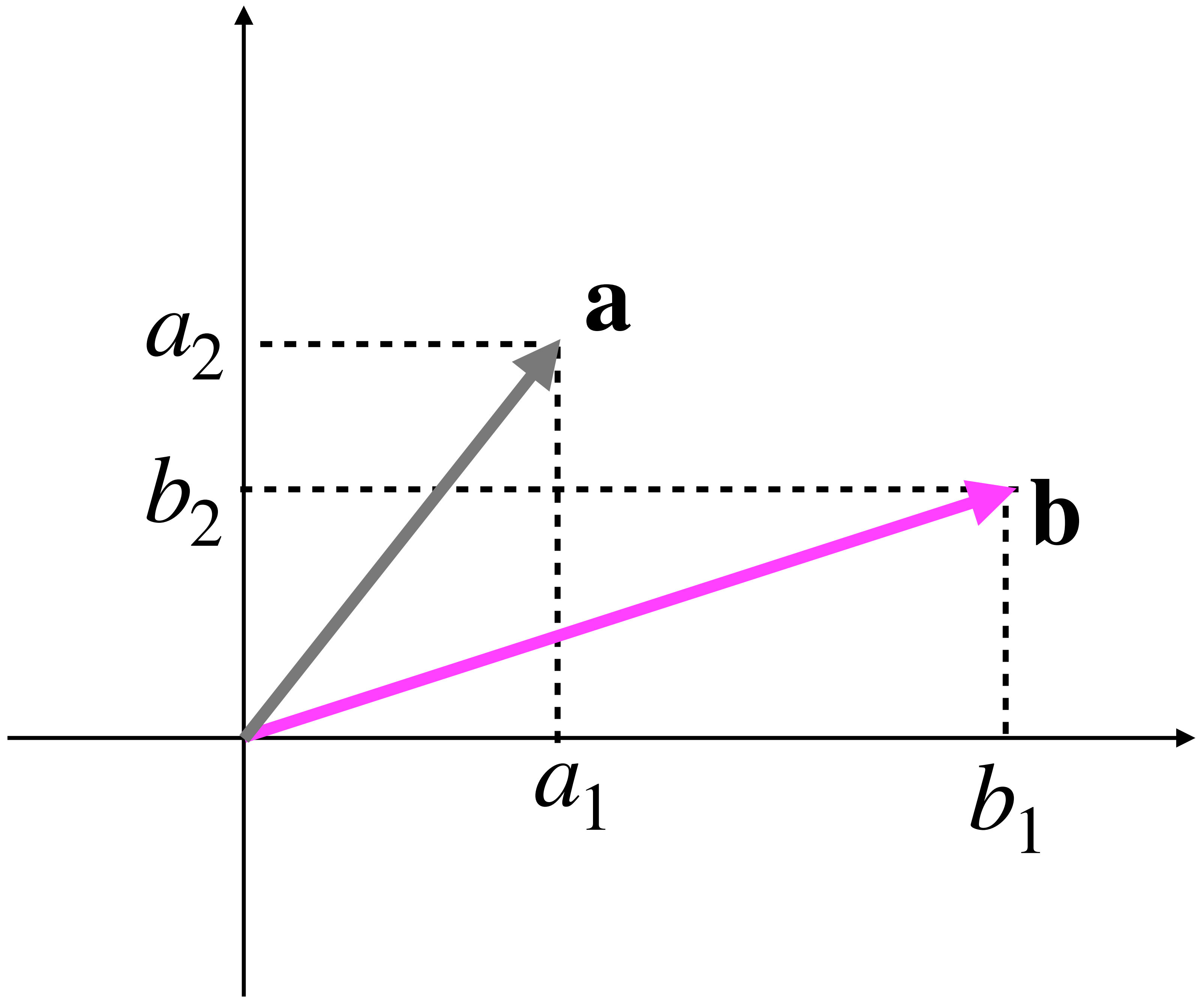


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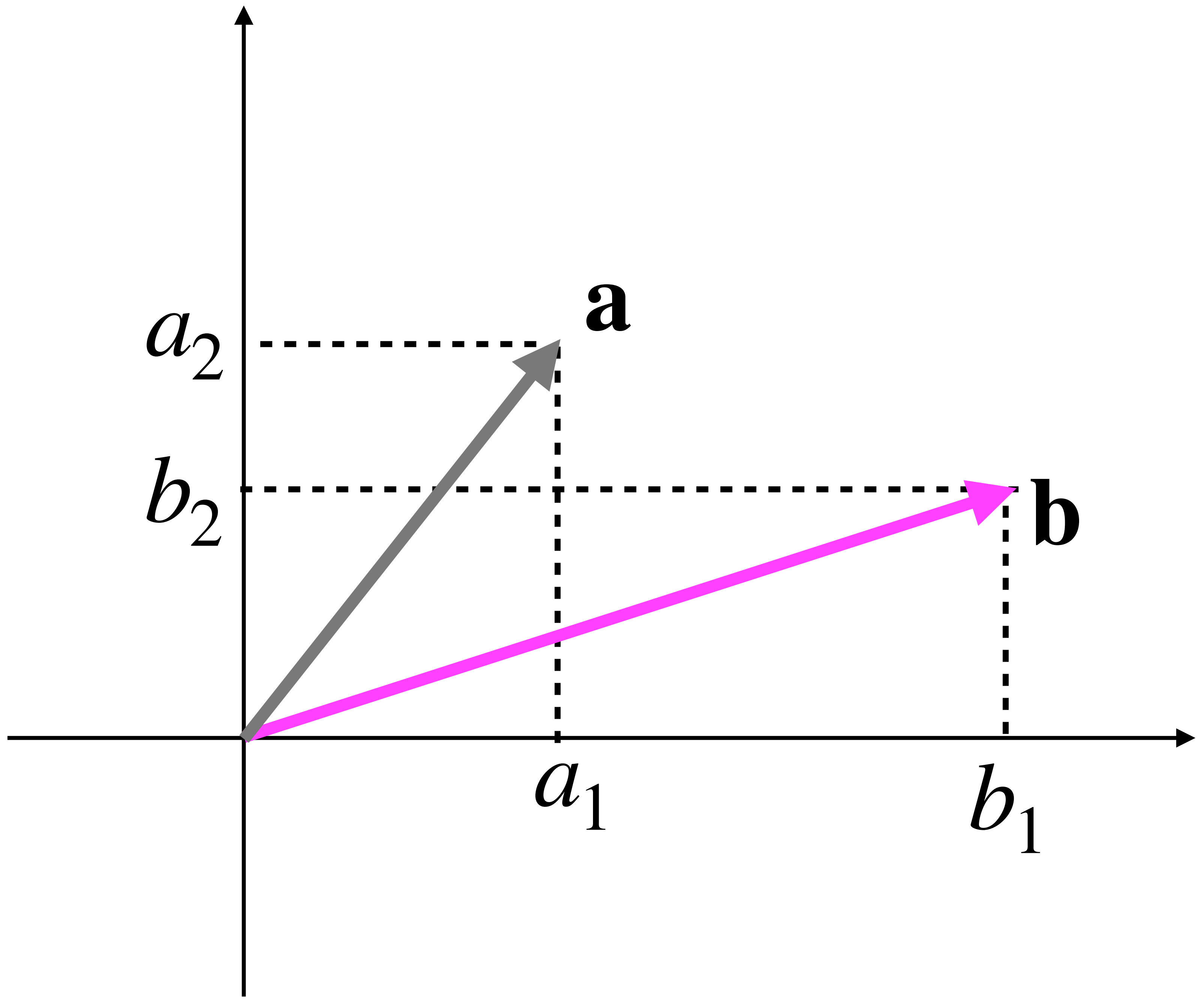


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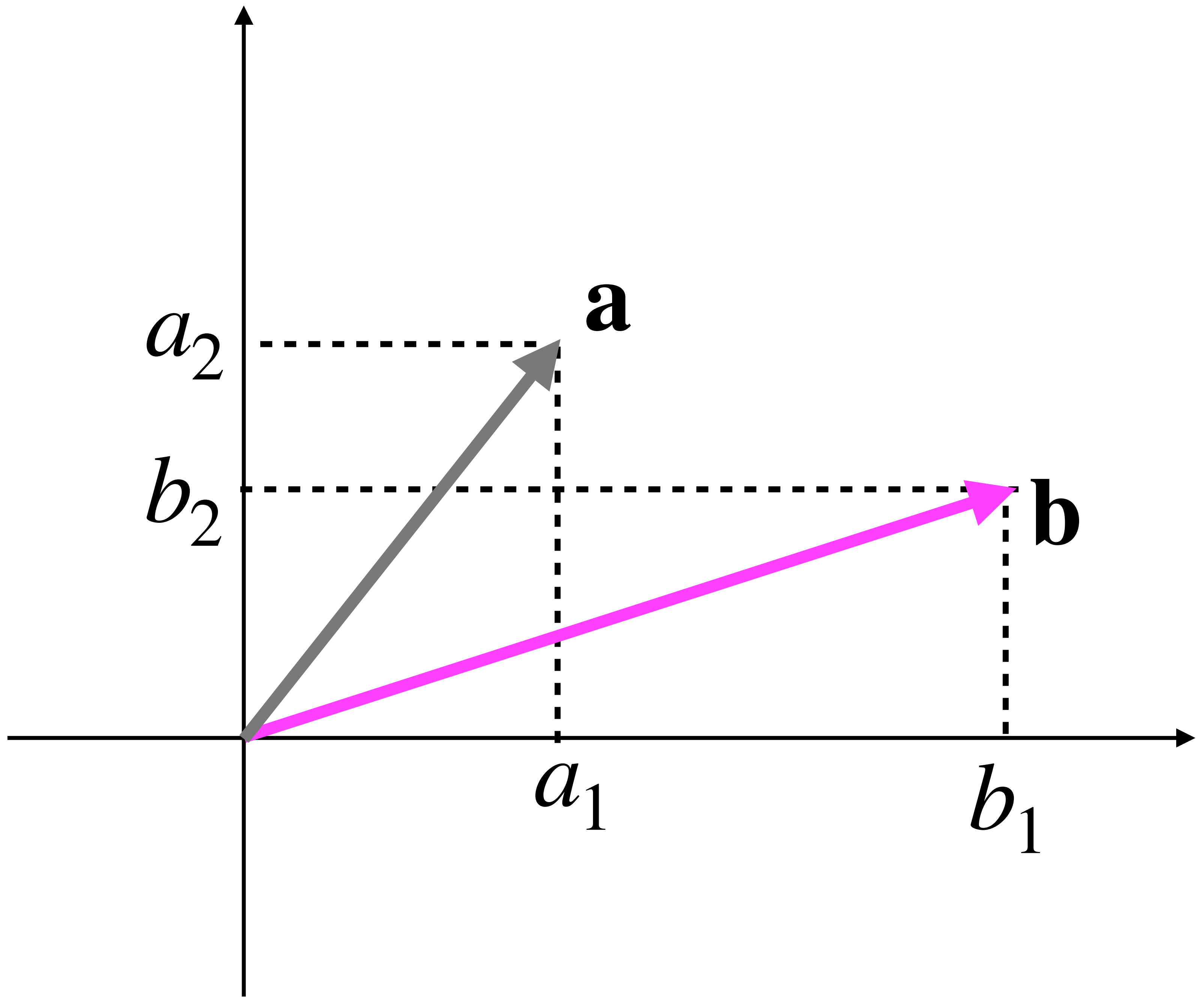


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$$\mathbf{a}^\top \mathbf{b} = (a_1 \quad a_2) \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}$$

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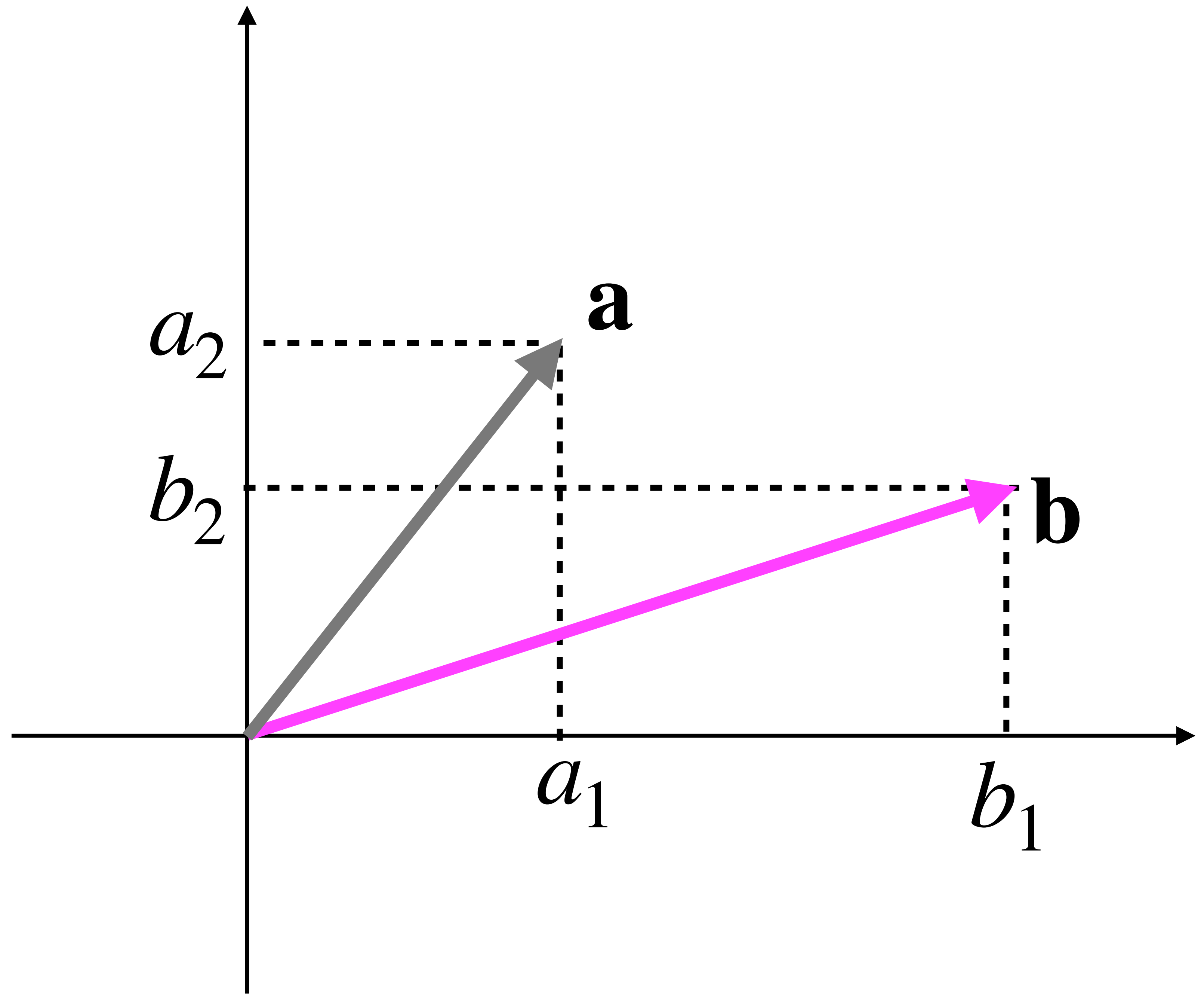


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$$\mathbf{a}^\top \mathbf{b} = \begin{pmatrix} a_1 & a_2 \end{pmatrix} \begin{pmatrix} b_1 \\ b_2 \end{pmatrix} = \mathbf{b}^\top \mathbf{a} = \begin{pmatrix} b_1 & b_2 \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}$$

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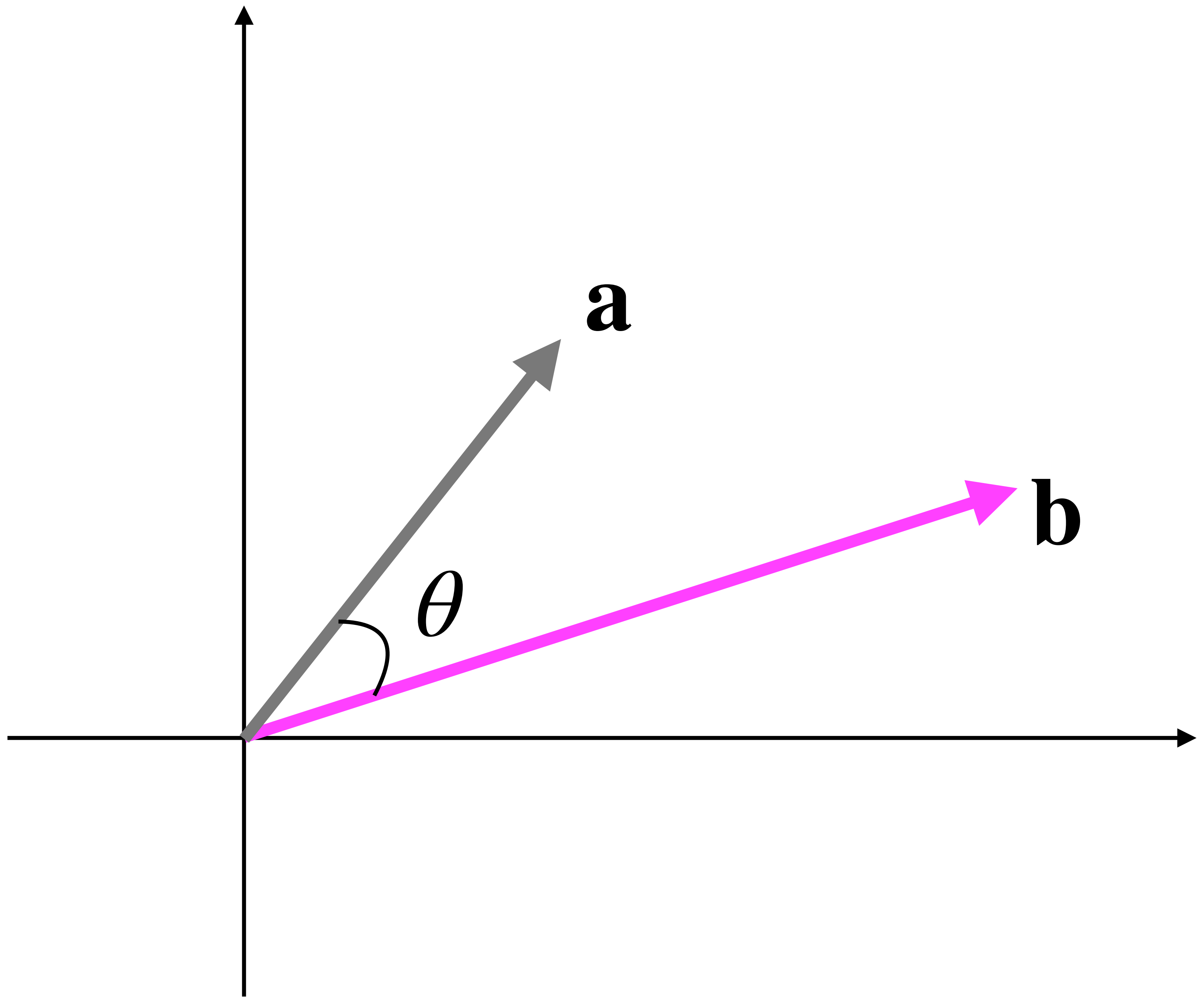


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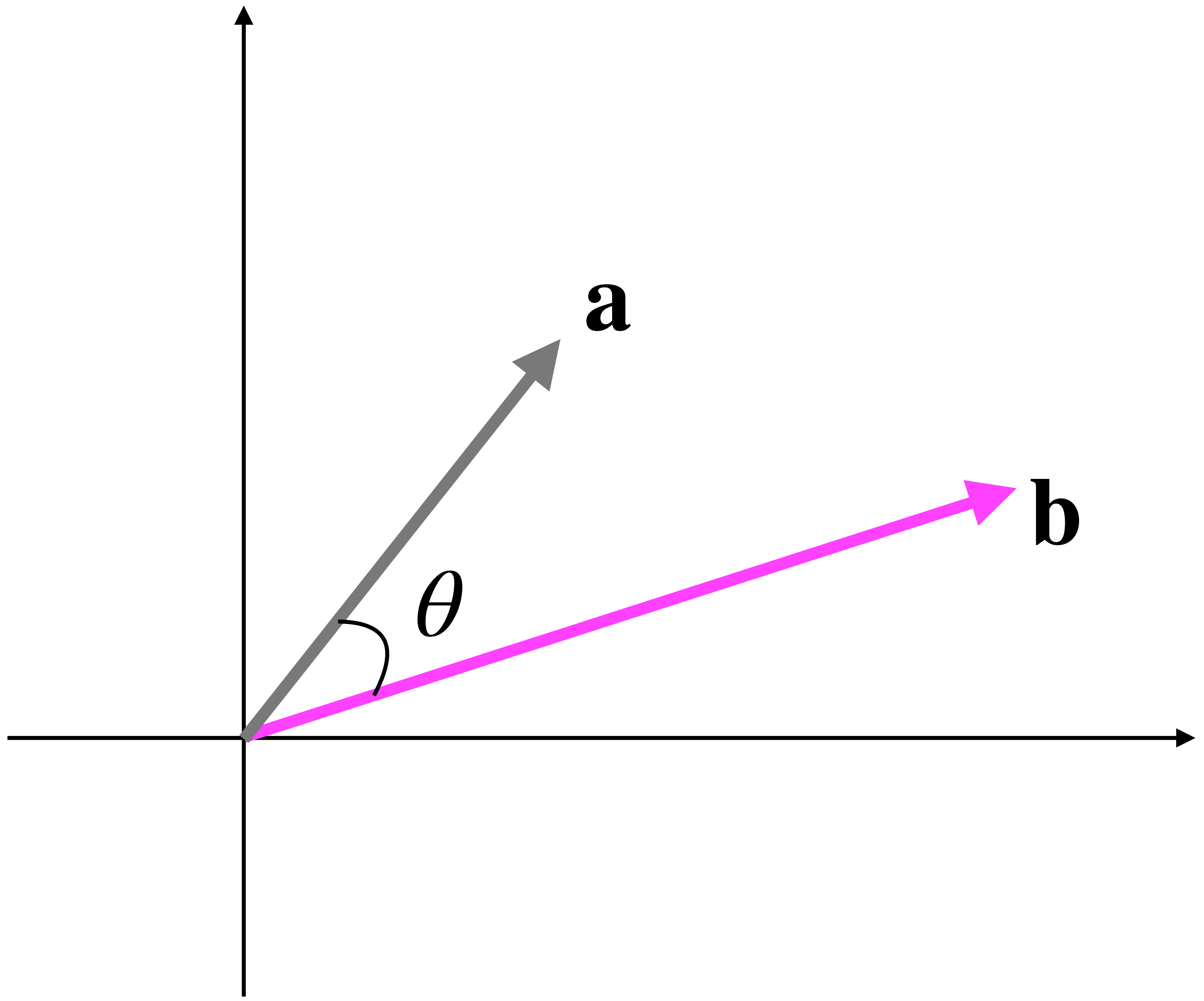


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$$\mathbf{a} \cdot \mathbf{b} = \|\mathbf{a}\| \|\mathbf{b}\| \cos\theta$$

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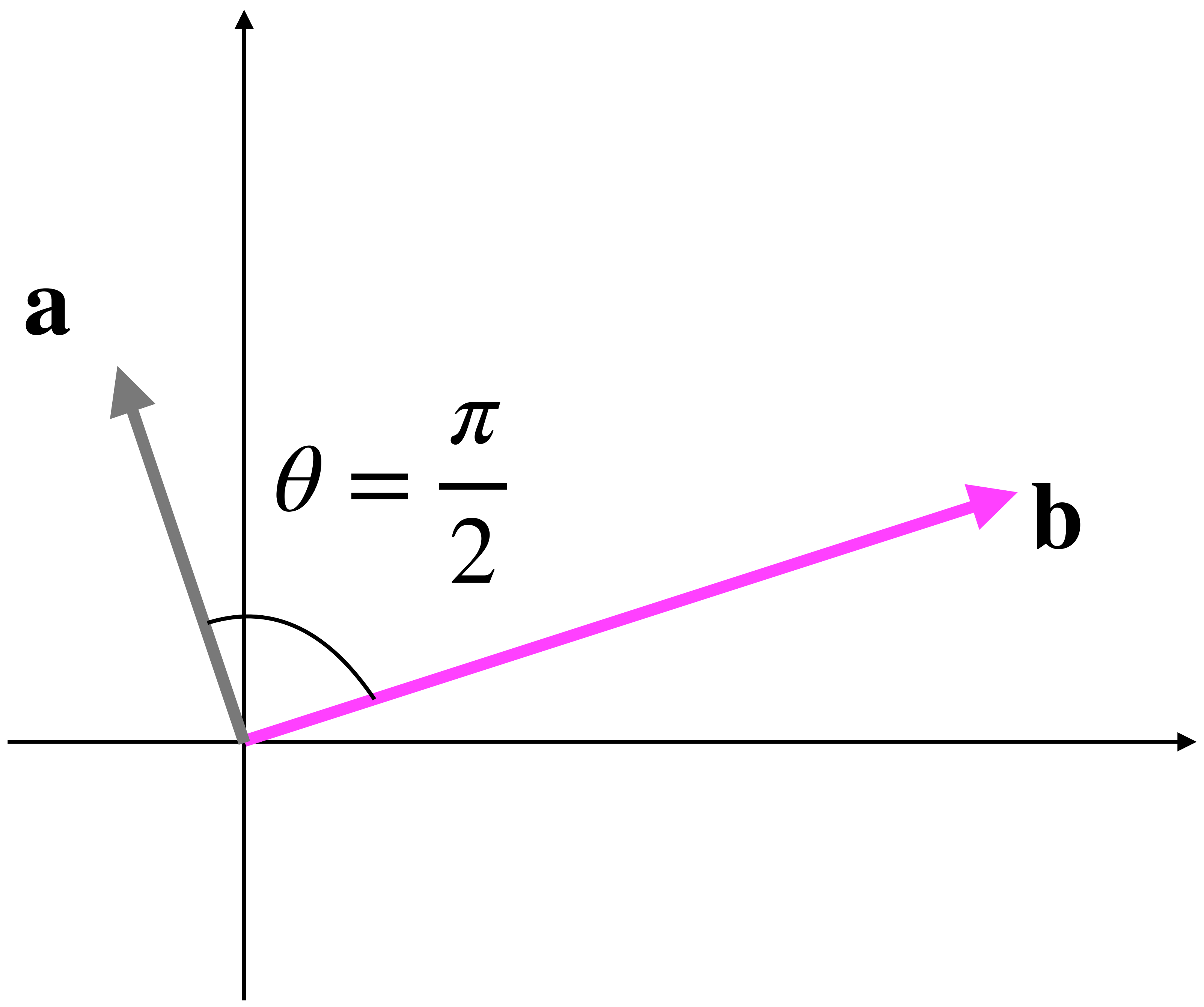
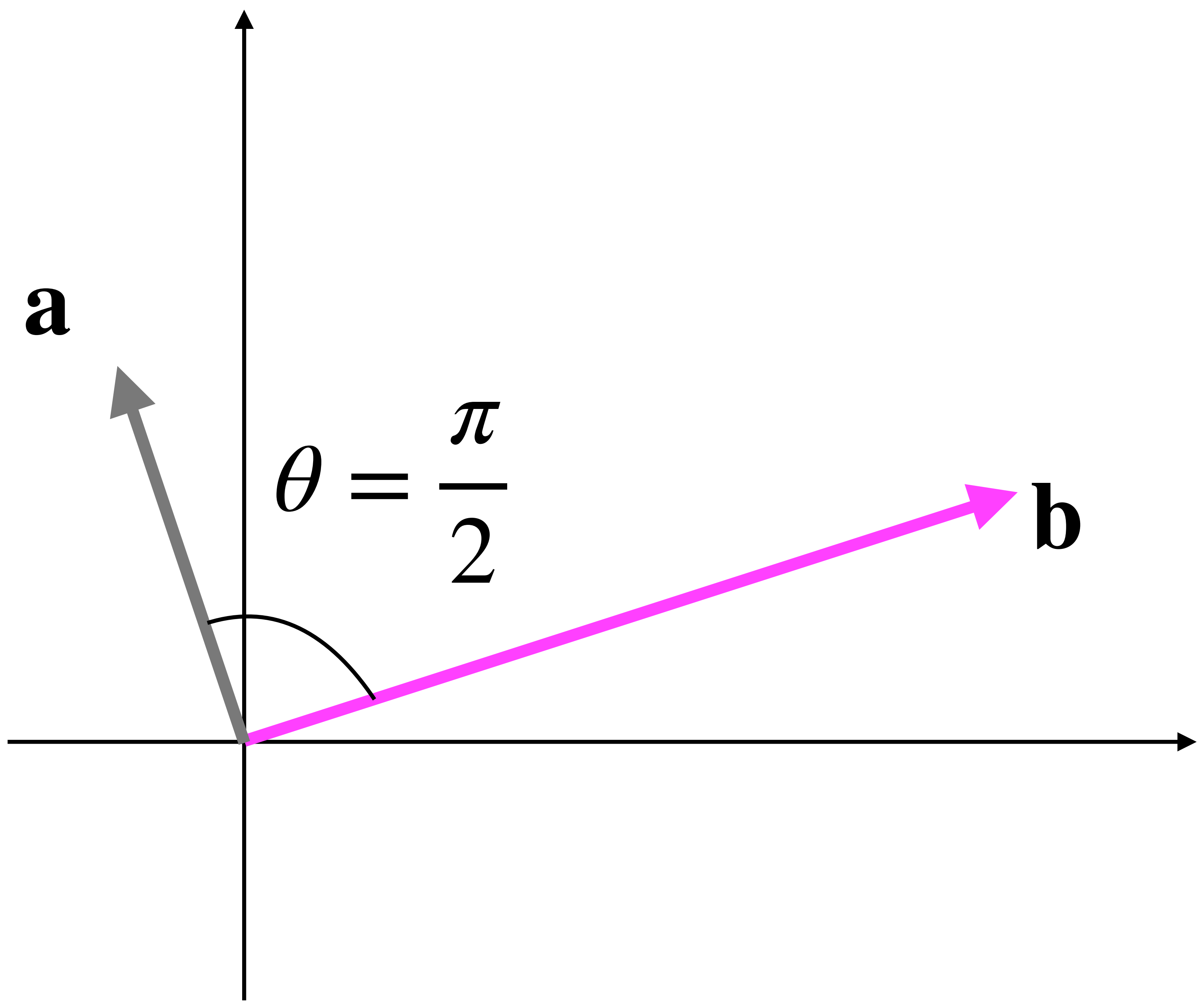


# Inner/dot/scalar product

What happens if the two vectors are orthogonal?



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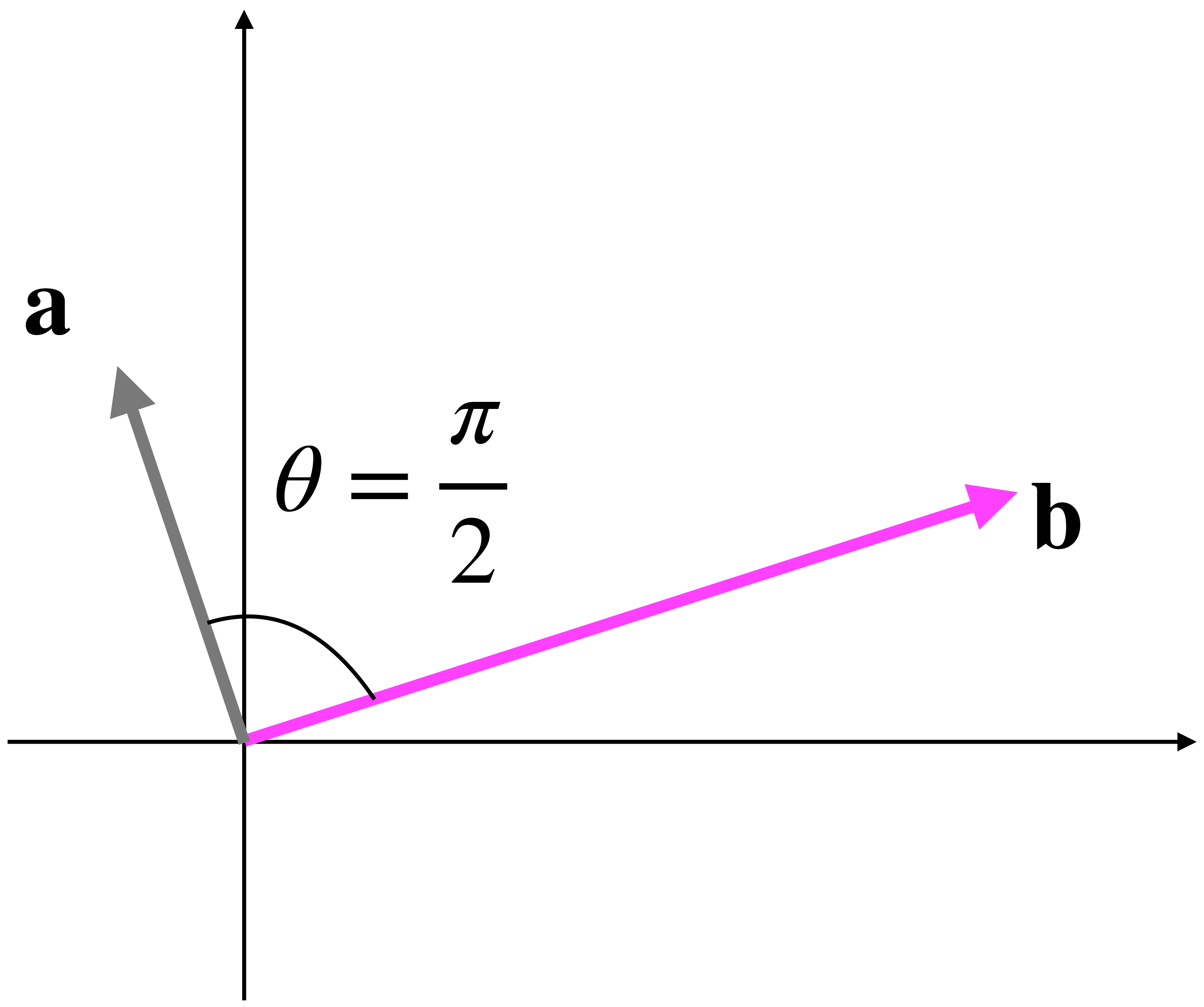


$$\mathbf{a} \cdot \mathbf{b} = \|\mathbf{a}\| \, \|\mathbf{b}\| \cos \frac{\pi}{2} = 0$$

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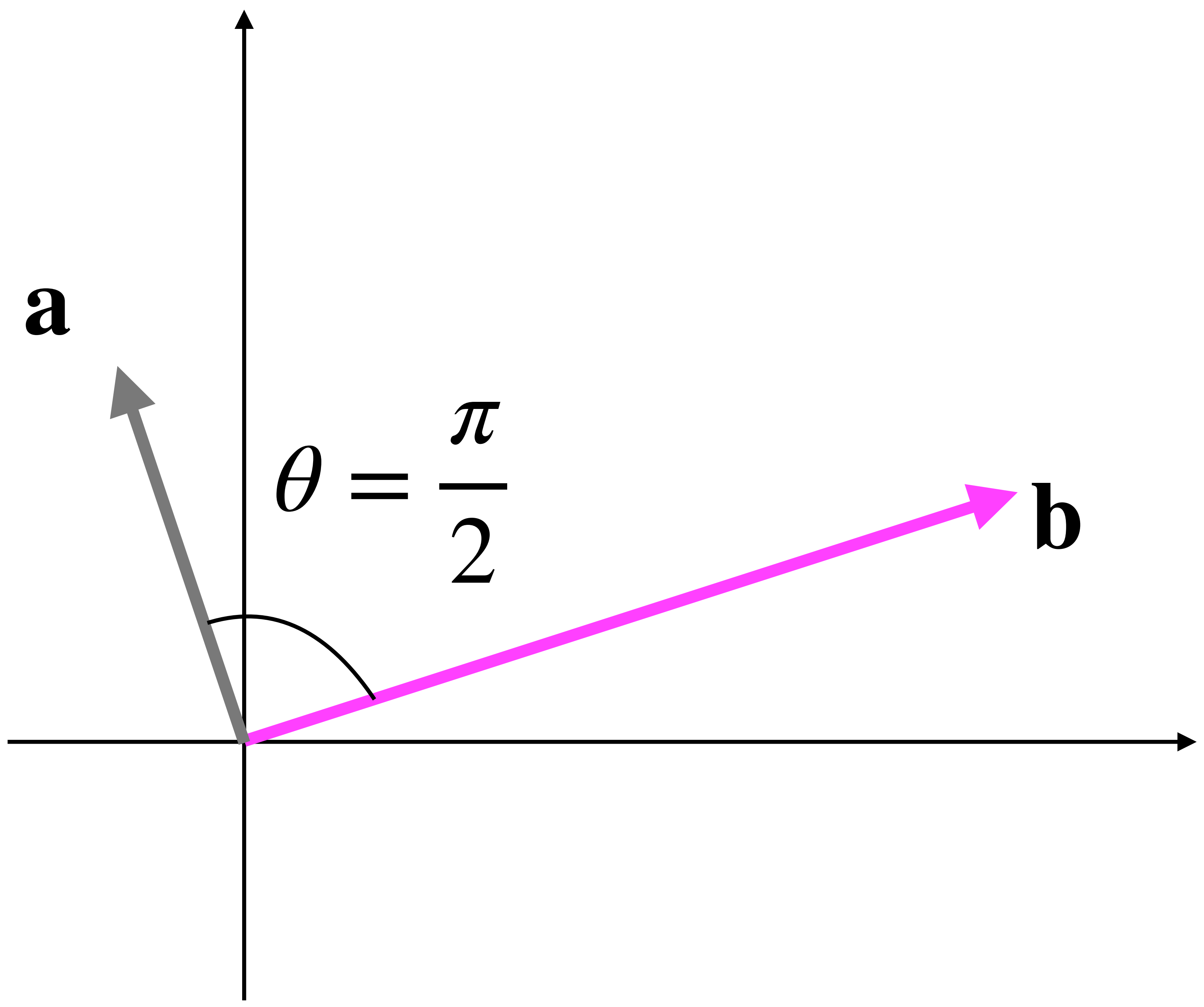


$$\mathbf{a} \cdot \mathbf{b} = \|\mathbf{a}\| \, \|\mathbf{b}\| \cos\frac{\pi}{2} = 0$$

The inner/dot/scalar product of two orthogonal vectors is zero!

# Inner/dot/scalar product

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Norm:

$$\|\mathbf{a}\| := \sqrt{\langle \mathbf{a}, \mathbf{a} \rangle} := \sqrt{\sum_{j=1}^{d} a_j^2}$$

# Eigenvalues and Eigenvectors

Given a squared matrix $\mathbf{X} \in \mathbb{R}^{d \times d}$ a vector $\mathbf{w_i} \in \mathbb{R}^{d \times 1}$ that satisfies this equation

$$\mathbf{X}\mathbf{w_i} = \lambda_{\mathbf{i}}\mathbf{w_i}$$

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It is called eigenvector of the matrix and lambda is the correspondent eigenvalue

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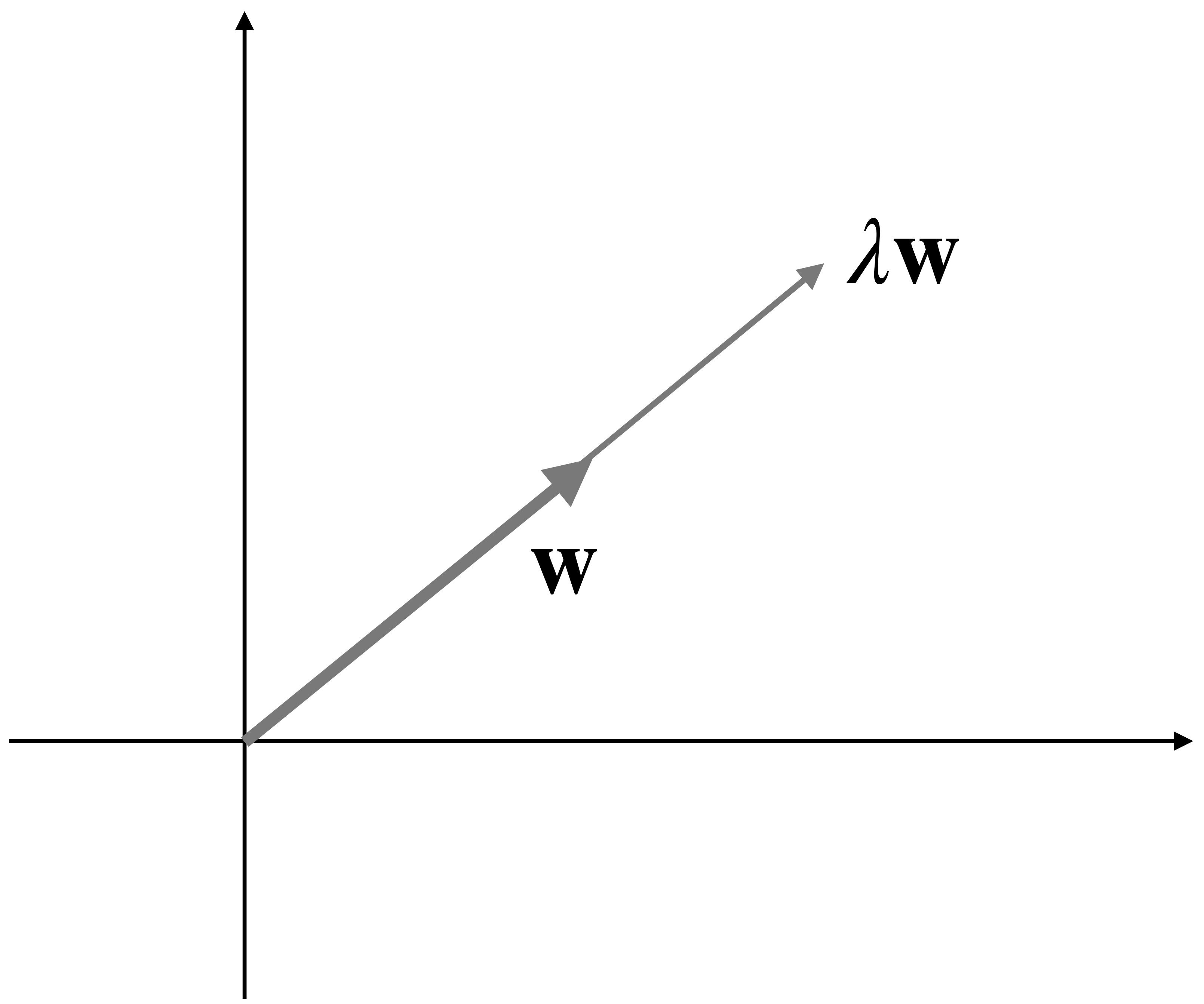


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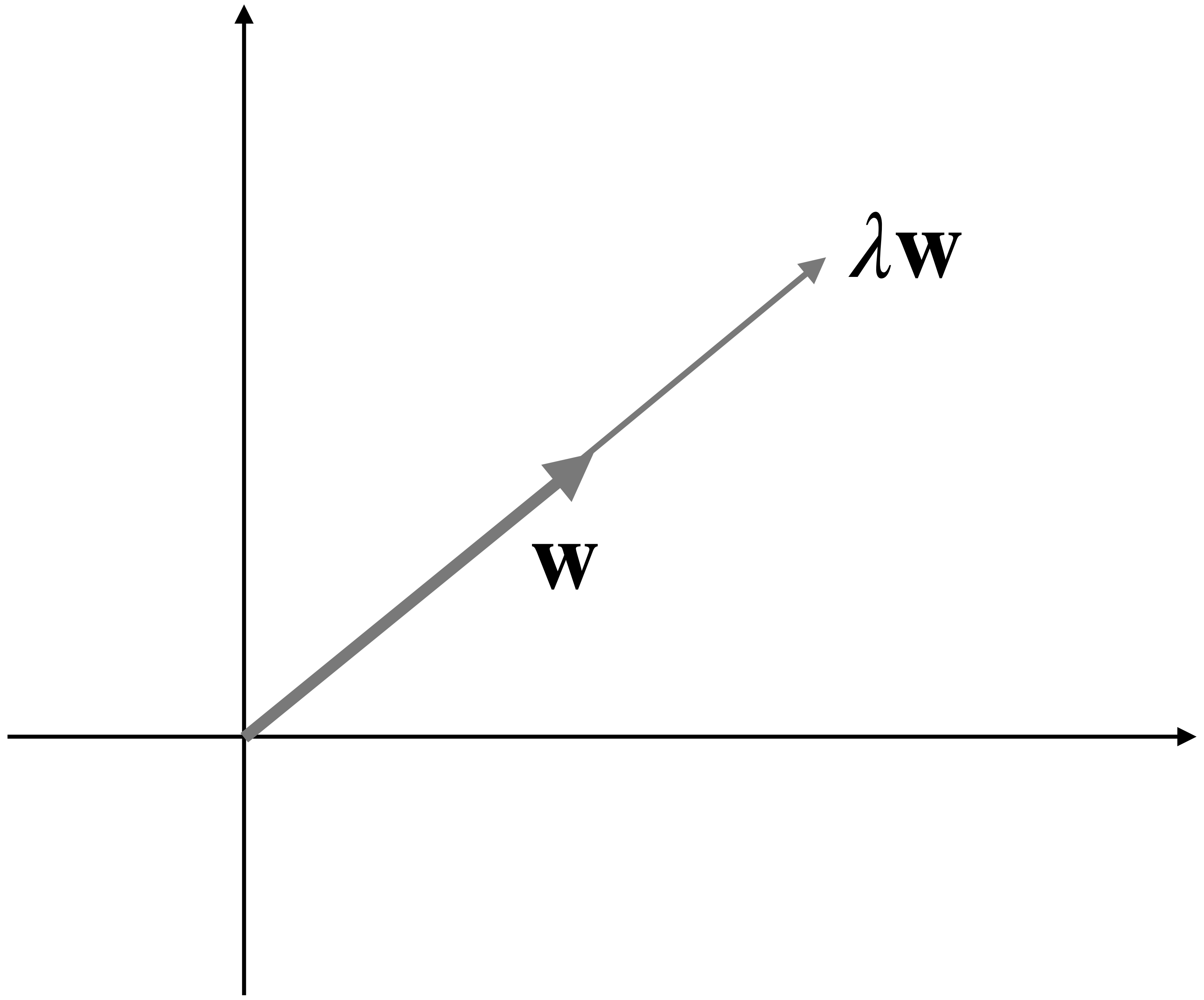


$$\mathbf{X}\mathbf{w_i} = \lambda_\mathbf{i}\mathbf{w_i}$$

The matrix is a linear transformation that acts on w squeezing or stretching it

# Eigenvalues and Eigenvectors

The equation

$$\mathbf{X}\mathbf{w_i} = \lambda_i \mathbf{w_i}$$

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$$\mathbf{X}\mathbf{w}_\mathbf{i} = \lambda_\mathbf{i}\mathbf{w}_\mathbf{i}$$

Can be written as

$$(\mathbf{X} - \lambda_\mathbf{i}\mathbf{I})\mathbf{w}_\mathbf{i} = 0$$

This has non zero solutions if and only if

$$\det(\mathbf{X} - \lambda_\mathbf{i}\mathbf{I}) = 0$$

Hence the goal is find solutions of this so-called characteristic equation

# Eigenvalues and Eigenvectors

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Symmetric matrices lead to $d$ real solutions and orthogonal eigenvectors!

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$$\mathbf{X}\mathbf{W} = \mathbf{W}\boldsymbol{\Lambda}$$

Where the matrix $\mathbf{W}$ contains, in the columns, the eigenvectors and $\boldsymbol{\Lambda}$ is a diagonal matrix whose entries are the eigenvalues

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This is the eigendecomposition of the matrix

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In the basis formed by the eigenvector the transformation is diagonal

# Singular value decomposition (SVD)

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As we will see soon, in most cases we will work with data matrices that are rarely squared. So how can we decompose such matrices?

Given a $\mathbf{X} \in \mathbb{R}^{s \times d}$ the transpose is $\mathbf{X}^\top \in \mathbb{R}^{d \times s}$ hence $\mathbf{X}^\top \mathbf{X} \in \mathbb{R}^{d \times d}$

# Singular value decomposition (SVD)

We then define $\mathbf{V} \in \mathbb{R}^{d\times d}$ such that of $\mathbf{X}^\top \mathbf{X}\mathbf{V_i} = \sigma_\mathbf{i}^\mathbf{2}\mathbf{V_i}$

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$\sigma_i$ are called singular values

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Furthermore

$$\mathbf{X}\mathbf{X}^\top\mathbf{U_i} = \sigma_\mathbf{i}\mathbf{X}\mathbf{V_i} = \sigma_\mathbf{i}^2\mathbf{U_i}$$

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$\mathbf{U_i}$ are the eigenvectors of $\mathbf{X}\mathbf{X}^\top$

# Singular value decomposition (SVD)

Summarizing

$$\mathbf{X}^\top \mathbf{X}\mathbf{V} = \sigma^2 \mathbf{V}$$

$$\mathbf{X}\mathbf{X}^\top \mathbf{U} = \sigma^2 \mathbf{U}$$

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$$\mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^{\top} = \mathbf{X}$$

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$$\mathbf{U}\boldsymbol{\Sigma} = \mathbf{X}\mathbf{V}$$

$$\mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^{\top} = \mathbf{X}$$ SVD of $\mathbf{X}$

# CALCULUS

# Calculus

Assume we have a function $f(\mathbf{x}) = f(x_1, x_2, \ldots, x_d)$

Where $\mathbf{x} = (x_1, x_2, \ldots, x_d)$

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The gradient is defined as

$$\nabla f(\mathbf{x}) = \begin{pmatrix} \frac{\partial}{\partial x_1} f(\mathbf{x}) \\ \frac{\partial}{\partial x_2} f(\mathbf{x}) \\ \vdots \\ \frac{\partial}{\partial x_d} f(\mathbf{x}) \end{pmatrix}$$

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It is a vector that indicates the direction of fastest increase of the function

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$$\Rightarrow \quad \nabla f(x) = 2 \begin{pmatrix} x_1 x_2^2 - y x_2 \\ x_1^2 x_2 - x_1 y \end{pmatrix}$$

# Calculus

Example: $f(x_1, \ldots, x_d) = \|\mathbf{x}\|^2$

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Let's see the details

$$\sum_{i=1}^{d} \frac{\partial}{\partial x_1} x_i^2 = \frac{\partial}{\partial x_1} x_1^2 + \frac{\partial}{\partial x_1} x_2^2 + \ldots + \frac{\partial}{\partial x_1} x_d^2$$

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$$\nabla f(\mathbf{x}) = 2\mathbf{x}$$

# Calculus

We can extend this to functions $f : \mathbb{R}^d \to \mathbb{R}^s$ with multiple outputs via the Jacobian matrix $J_f : \mathbb{R}^d \to \mathbb{R}^{s \times d}$ defined as

$$J_f(x) := \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_d} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_s}{\partial x_1} & \cdots & \frac{\partial f_s}{\partial x_d} \end{pmatrix}$$

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And we can even define a second-order derivative matrix (known as Hessian) via

$$H_f(x) := J_{\nabla f}(x)$$

# PROBABILITY & STATISTICS

# Probability & statistics

Assume we have a random variable $X$ with a finite no. of outcomes $x_1, x_2, \ldots, x_s$ and probabilities $\rho_1 = P(X = x_1), \rho_2 = P(X = x_2), \ldots, \rho_s = P(X = x_s)$. The expectation of $X$ is defined as

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It is simply a weighted average!

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Example: $s = 3$, $x_1 = 1$ ($\rho_1 = 1/2$), $x_2 = 11/10$ ($\rho_2 = 1/3$), $x_3 = 1/2$ ($\rho_3 = 1/6$)

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$$\implies \qquad \mathbb{E}_x[x_i] = \sum_{i=1}^{3} x_i \rho_i = \frac{1}{2} + \frac{11}{30} + \frac{1}{12} = \frac{19}{20} = 0.95$$

# Probability & statistics

Assume we have an absolutely continuous random variable $X$ with probability density function $\rho$. The expectation of $X$ is defined as

$$\mathbb{E}_x[x] := \int_{\mathbb{R}} x\,\rho(x)\,dx$$

# Probability & statistics

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Example: uniform random variable $X$ in $[a, b]$ with $\rho(x) = \begin{cases} \frac{1}{b-a} & x \in [a, b] \\ 0 & \text{otherwise} \end{cases}$

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If x is a constant?

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$$\mathbb{E}_x[x_i] := \sum_{i=1}^{s} x_i \rho_i$$

If x is a constant?

$$\mathbb{E}_x[c] := \sum_{i=1}^{s} c \rho_i$$

$$\mathbb{E}_x[c] := c \sum_{i=1}^{s} \rho_i = c$$

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The variance of a random variable $X$ is defined as

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$$\text{Var}_x[x] = \mathbb{E}_x\left[x^2 - 2x\mathbb{E}_x[x] + \mathbb{E}_x[x]^2\right]$$

$$= \mathbb{E}_x[x^2] - 2\mathbb{E}_x[x]\mathbb{E}_x[x] + \mathbb{E}_x\left[\mathbb{E}_x[x]^2\right]$$

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$$\mathbb{E}_x[x_i] := \sum_{i=1}^{s} x_i \rho_i$$

If x is a constant?

$$\mathbb{E}_x[c] := \sum_{i=1}^{s} c \rho_i$$

$$\mathbb{E}_x[c] := c \sum_{i=1}^{s} \rho_i = c$$

# Probability & statistics

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Its square-root

$$\sigma_x := \sqrt{\text{Var}_x[x]}$$

is known as standard deviation

# Probability & statistics

Two random variables $X$ and $Y$ are independent if their joint PDF factors, i.e.

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The collection of random variables is independent and identically distributed (i.i.d.) if in addition we have

$$\rho_{X_1} = \rho_{X_2} = \cdots = \rho_{X_n}$$

# TUTORIAL ON FRIDAY

We will discuss the solutions of Coursework 0

To make the most of these tutorials, attempt completing the coursework before!