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JOHNS HOPKINS
WHITING SCHOOL
of ENGINEERING

Artificial Intelligence in Predictive Health and Laboratory Research

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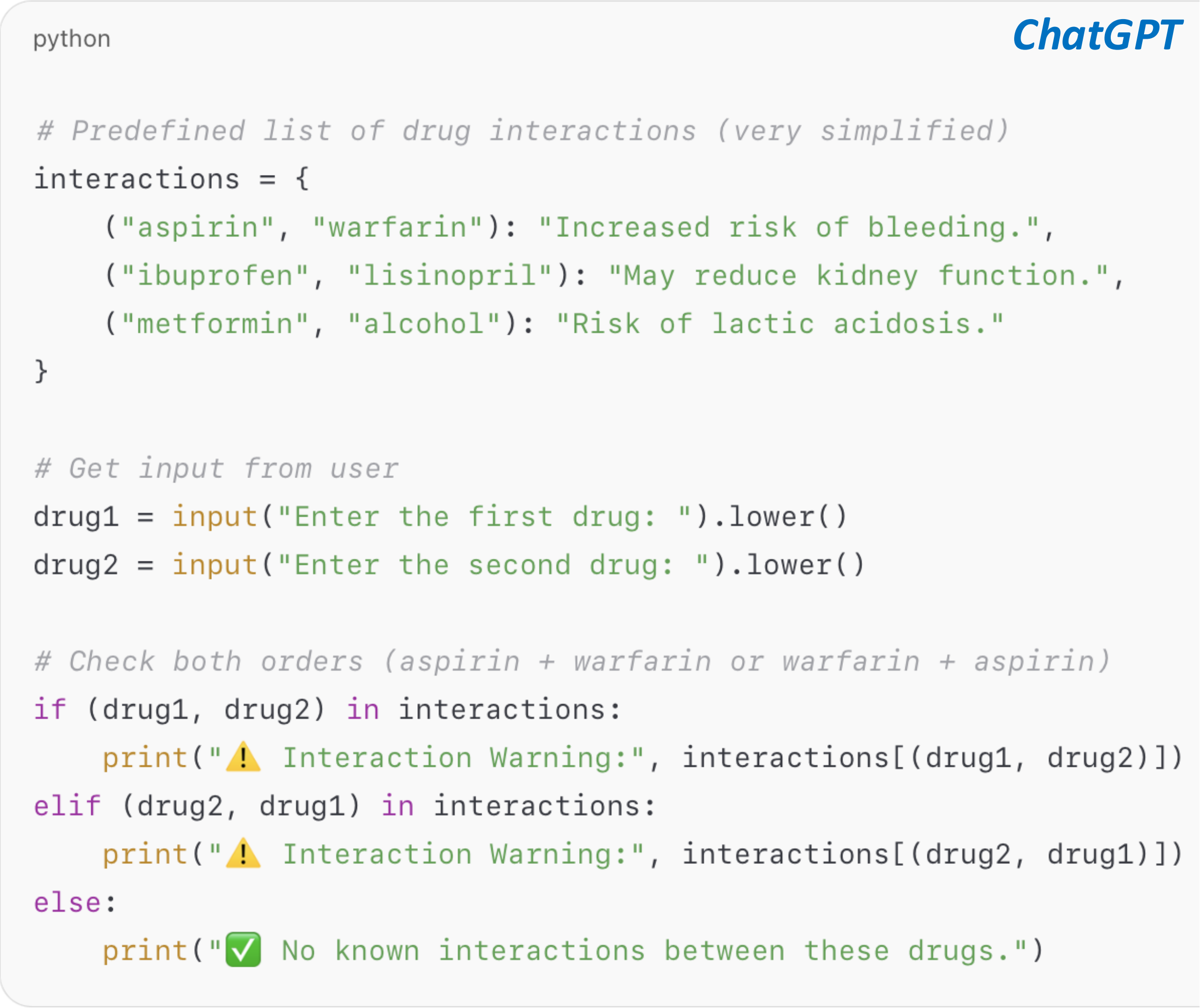
Exciting Recent Developments!

Cute owl professor writing drug names on a computer, photorealistic style.

DALL.E 2

Write a Drug Interaction Checker code to check if two drugs interact with each other using a small predefined list of known interactions.

ChatGPT



```python
# Predefined list of drug interactions (very simplified)
interactions = {
    ("aspirin", "warfarin"): "Increased risk of bleeding.",
    ("ibuprofen", "lisinopril"): "May reduce kidney function.",
    ("metformin", "alcohol"): "Risk of lactic acidosis."
}

# Get input from user
drug1 = input("Enter the first drug: ").lower()
drug2 = input("Enter the second drug: ").lower()

# Check both orders (aspirin + warfarin or warfarin + aspirin)
if (drug1, drug2) in interactions:
    print("⚠️ Interaction Warning:", interactions[(drug1, drug2)])
elif (drug2, drug1) in interactions:
    print("⚠️ Interaction Warning:", interactions[(drug2, drug1)])
else:
    print("✅ No known interactions between these drugs.")
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Exciting Recent Developments!

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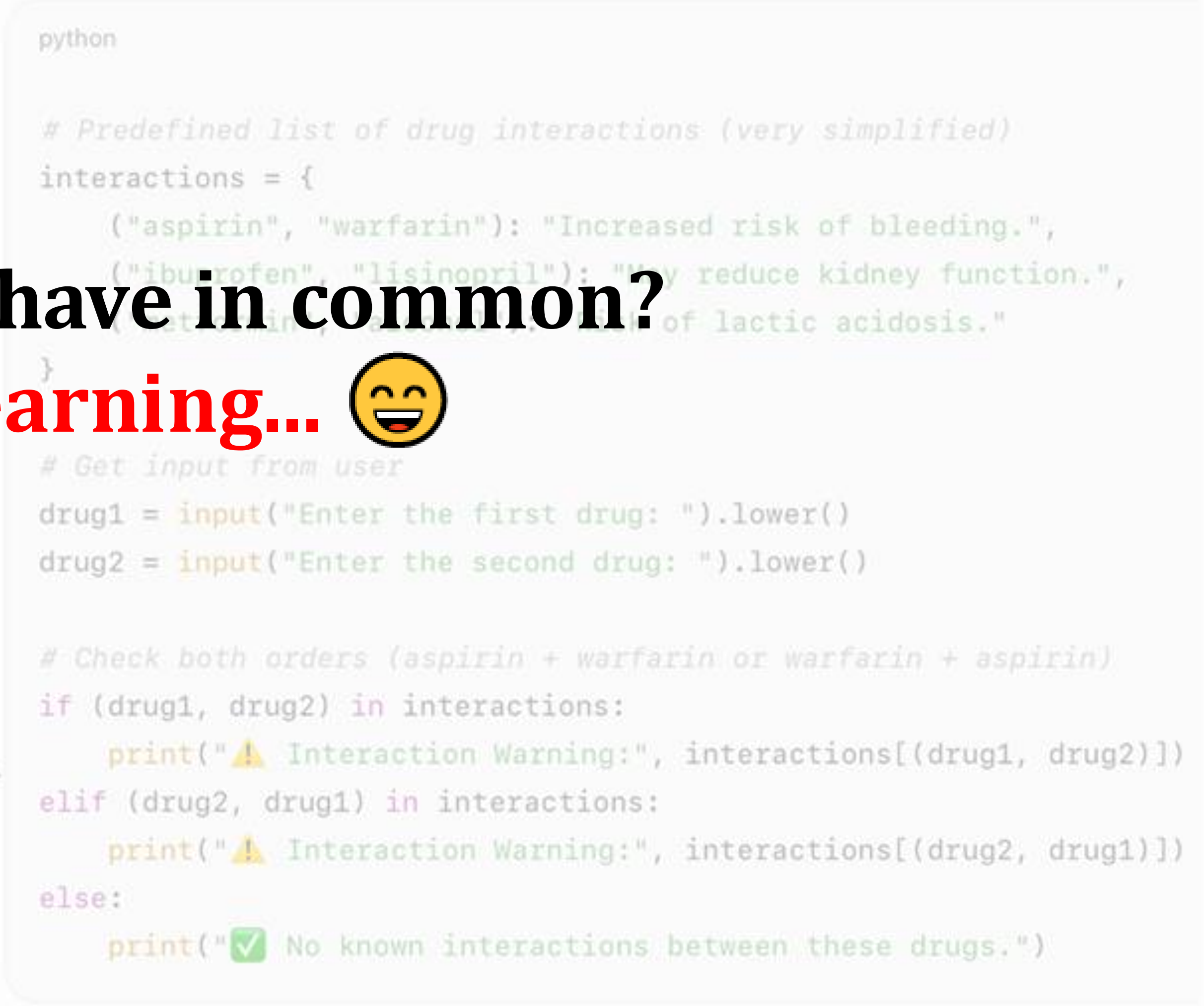
DALL.E 2

What do these all have in common?

Machine Learning... 😄

ChatGPT coding: Write a Drug Interaction Checker code to check if two drugs interact with each other using a small predefined list of known interactions.



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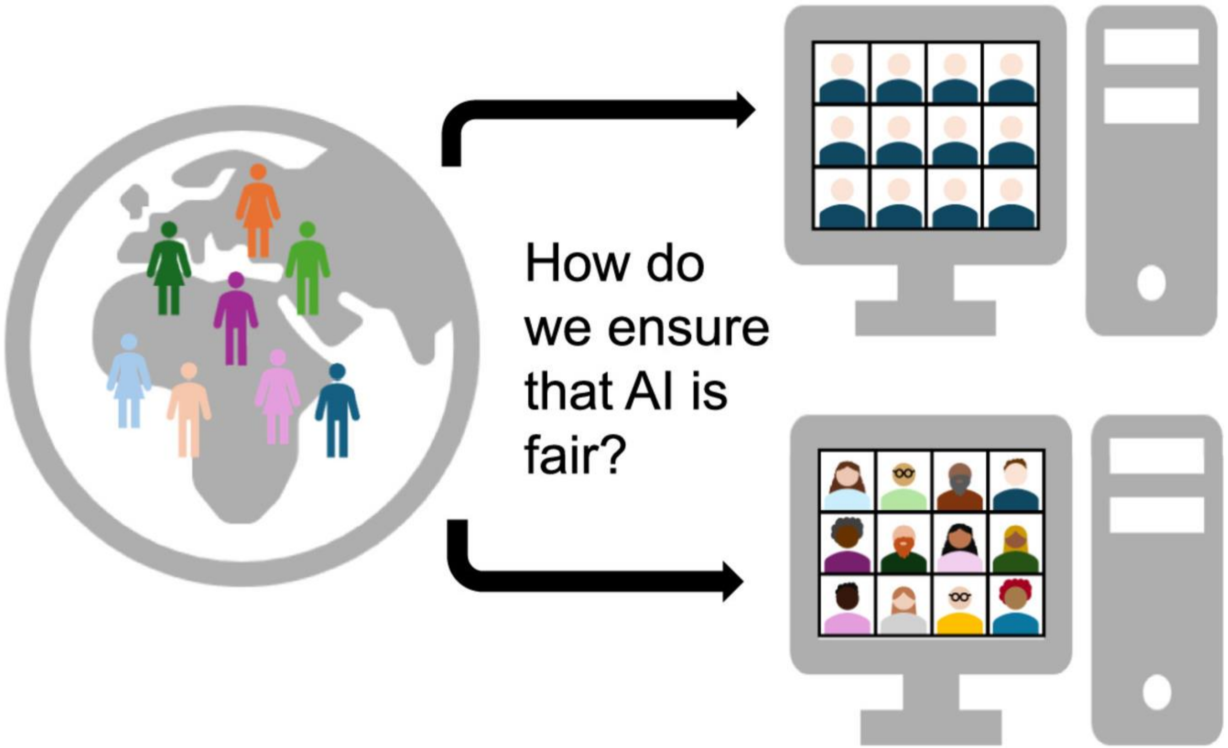
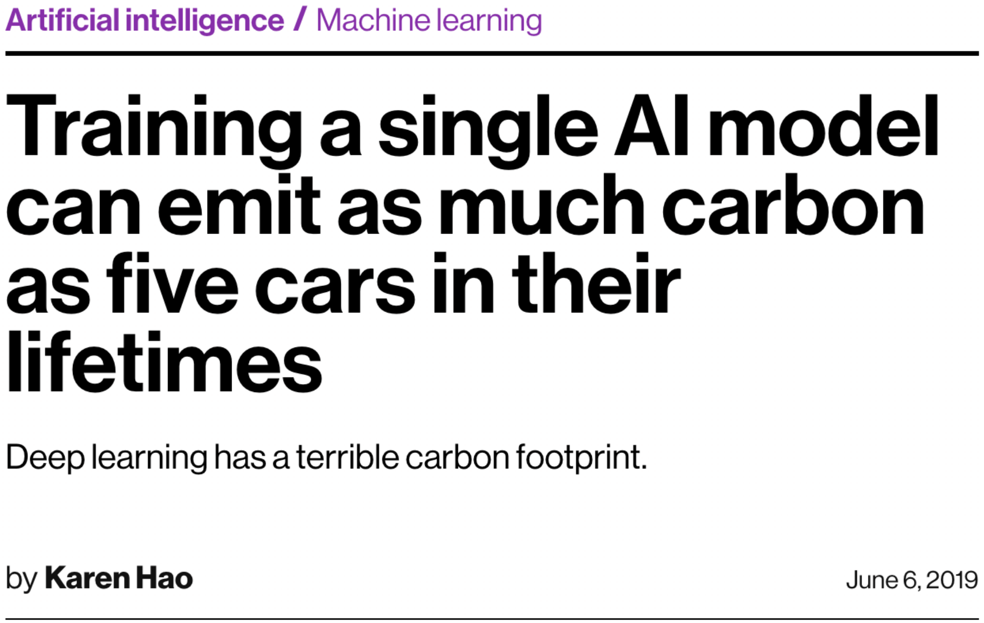
Worrisome Recent Development



Fairness in AI for healthcare



Artificial intelligence / Machine learning

Training a single AI model can emit as much carbon as five cars in their lifetimes

Deep learning has a terrible carbon footprint.

by **Karen Hao**

June 6, 2019

Need for Efficient AI Models

What do these all have in common?

Machine Learning... 😔

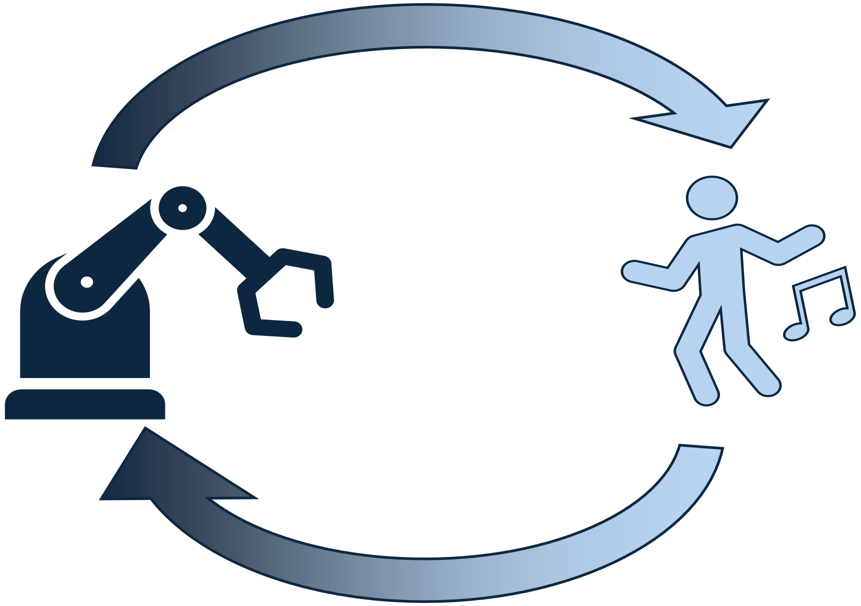
Our Goals in this Course

- Understand the core high-level ideas that lead to the success of machine learning-based methods.

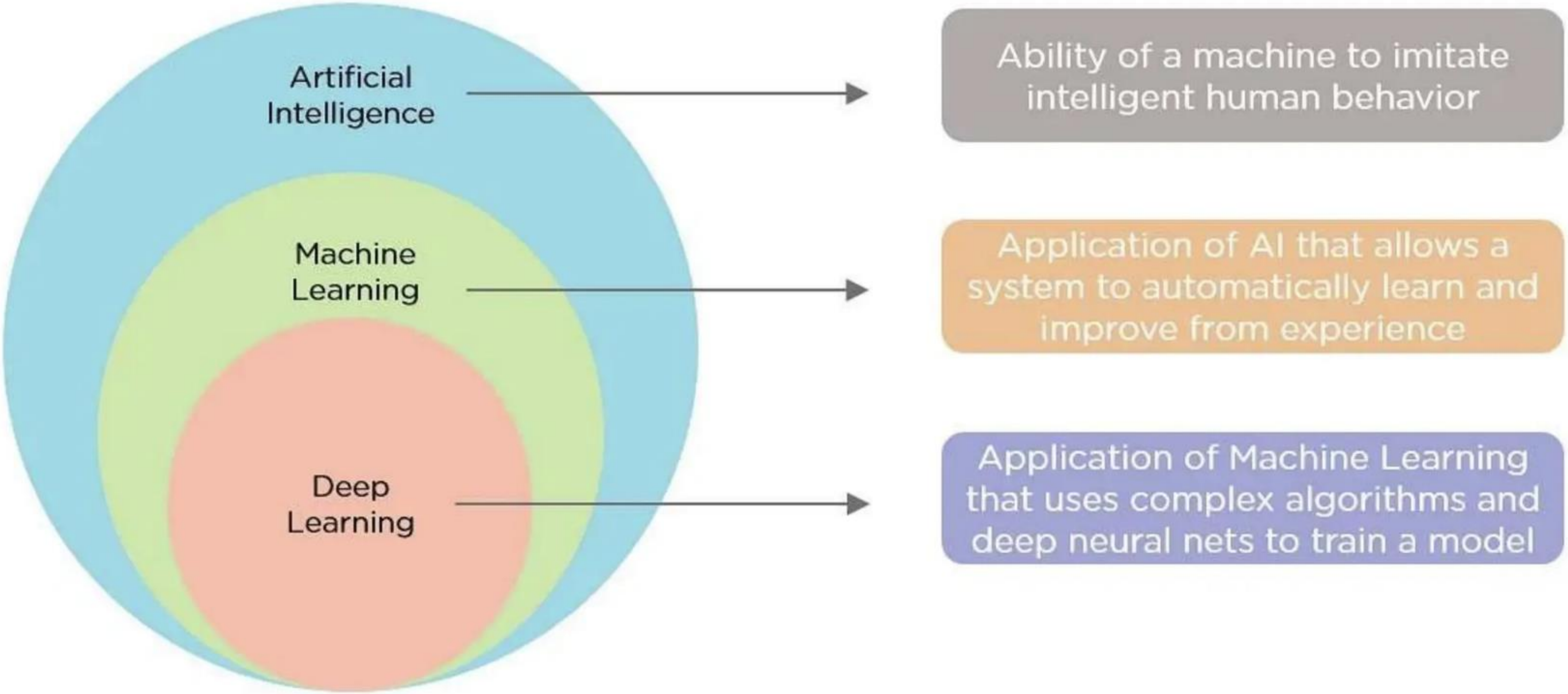
- Gain hands-on experience implementing deep learning models for solving problems in pharmacy/healthcare.

Human Vs Machine Learning

Relaxed Alertness



Human	Machine
Rest and Digest	Training
Fight-or-flight	Prediction



Ability of a machine to imitate intelligent human behavior

Application of AI that allows a system to automatically learn and improve from experience

Application of Machine Learning that uses complex algorithms and deep neural nets to train a model

Beginning of Artificial Intelligence

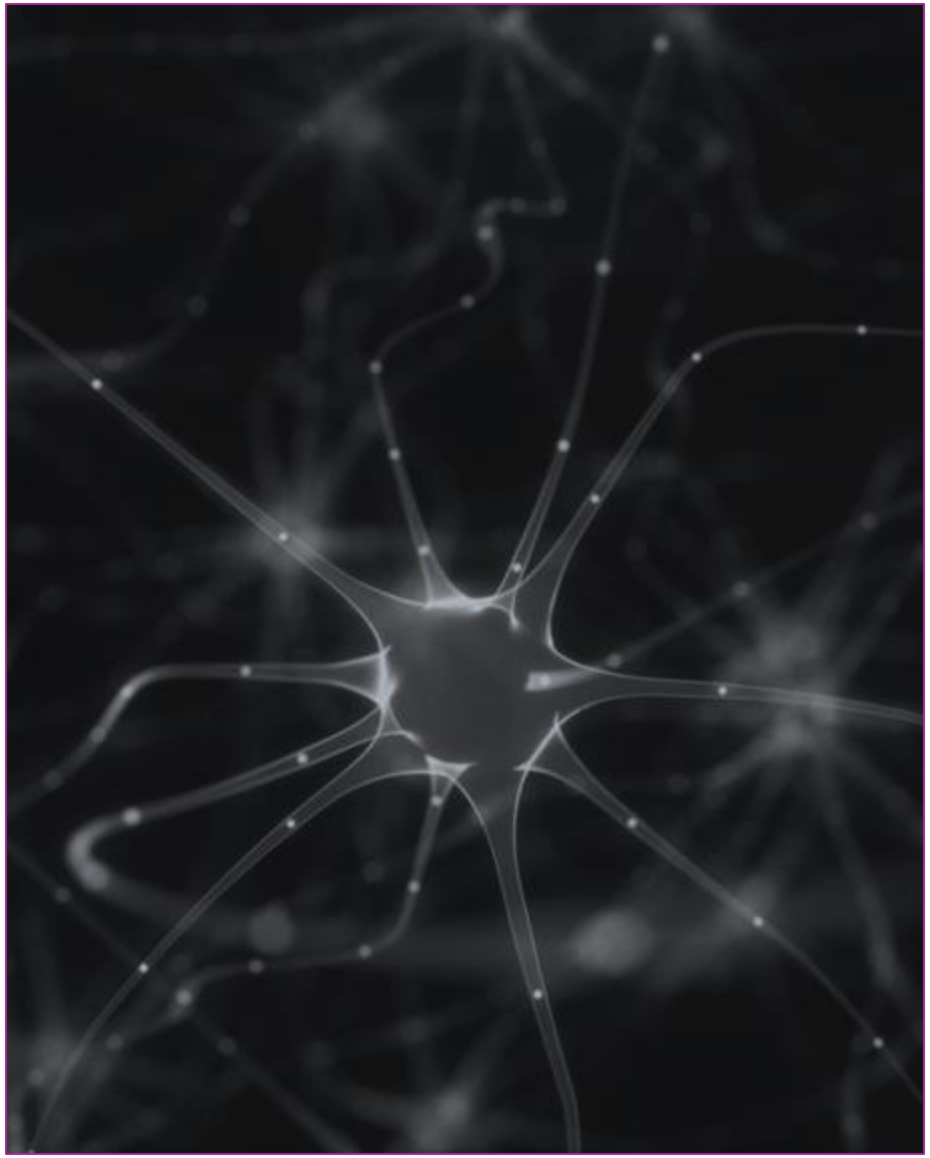
Computers are made in part to complete human tasks

Early on, generalized intelligence looked possible

Turned out to be harder than expected

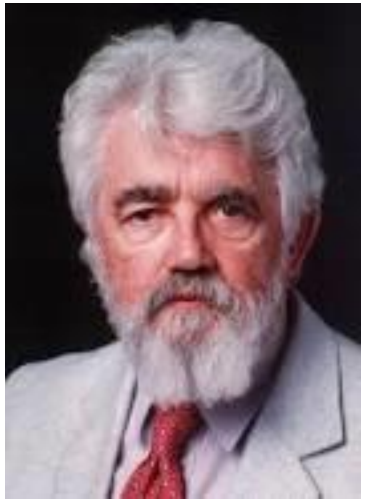
Early Neural Networks

- Inspired by biology
- Created in the 1950’s
- Outclassed by Von Neumann Architecture

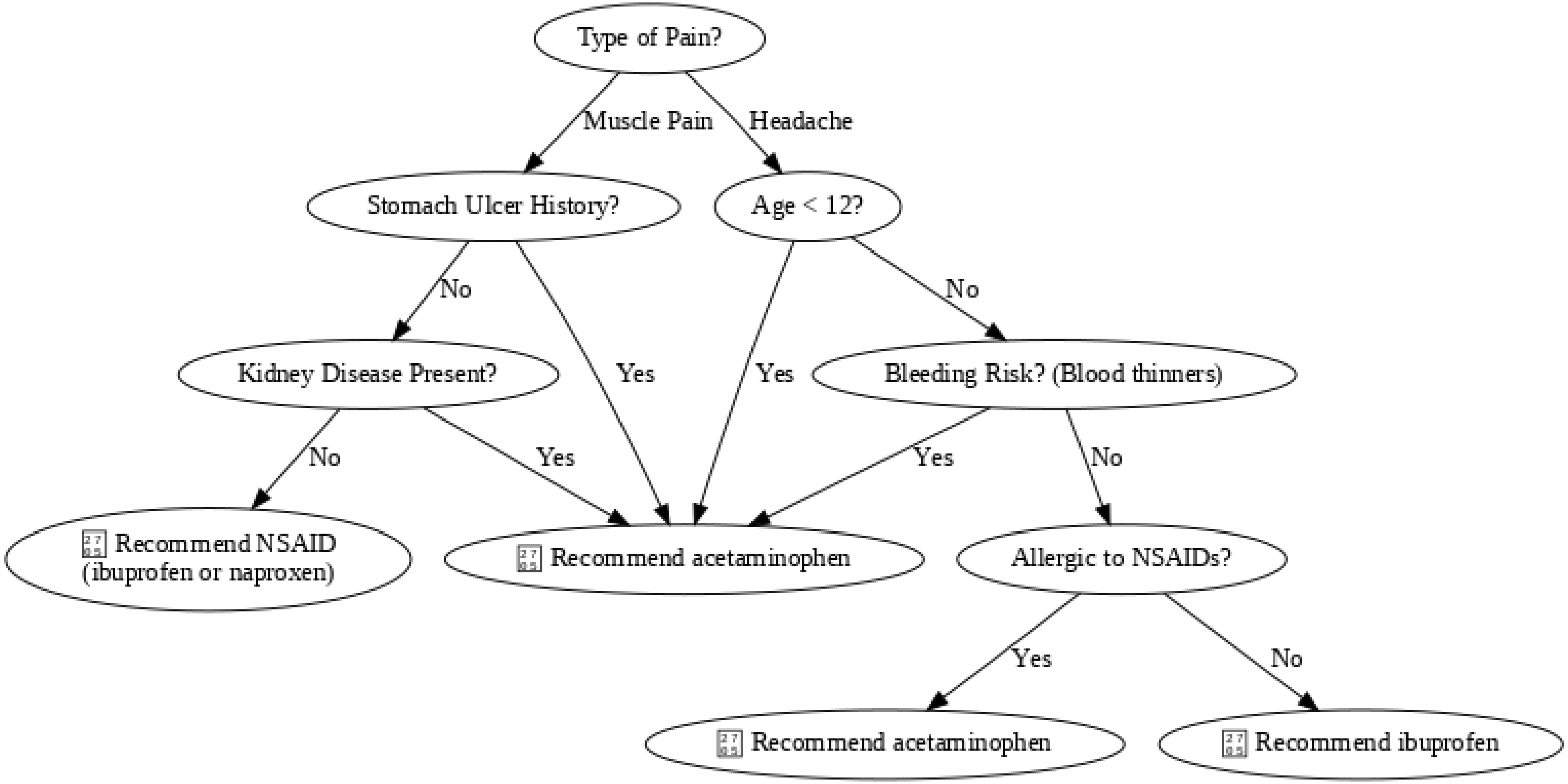


Artificial Intelligence

"AI is ... the science and engineering of making intelligent machines." - John McCarthy



Symbolic Artificial Intelligence

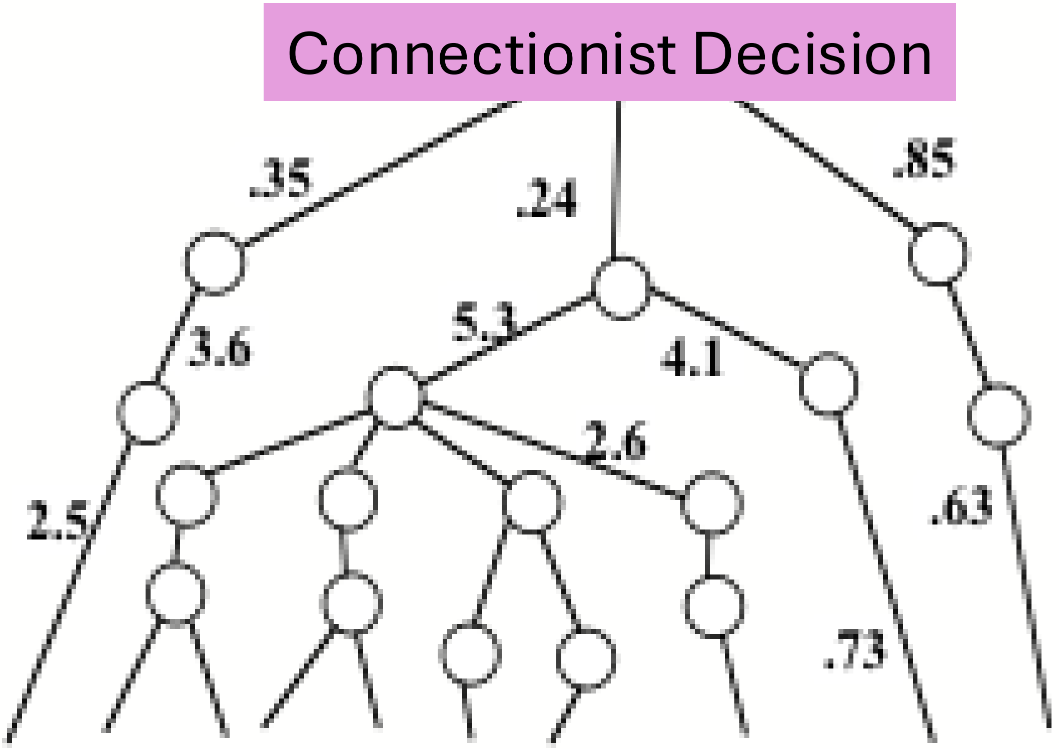


Symbolic AI: Based on high-level representations of problem, logic, and search.

Symbolic AI

- Highly complex
- Programmed by hundreds of engineers
- Rigorous programming of many rules

Connectionist Artificial Intelligence



Using Artificial Neural Networks to build intelligent machines.

How Do Children Learn?

- Expose them to lots of data
- Give them the “correct answer”
- They will pick up the important patterns on their own

the
DEEP
LEARNING
Revolution

Data

- Networks need a lot of information to learn from.
- The digital era and the internet has supplied that data.

Computing Power

Need a way for our artificial "brain" to observe lots of data within a practical amount of time.

What is deep learning?

> “Deep learning flips traditional programming on its head”

Traditional Programming for Building a Classifier

1. Define a set of rules for classification
2. Program those rules into the computer
3. Feed it examples, and the program uses the rules to classify

Machine Learning for Building a Classifier

1. Show model the examples with the answer of how to classify
2. Model takes guesses, we tell it if it’s right or not
3. Model learns to correctly categorize as it’s training. The system learns the rules on its own

This is a Fundamental Shift

When to choose deep learning?

Classic Programming

If rules are clear and straightforward, often better to program it

Deep Learning

If rules are nuanced, complex, difficult to discern, use deep learning

Problem Statement

Problem: Is this patient at risk for diabetes?

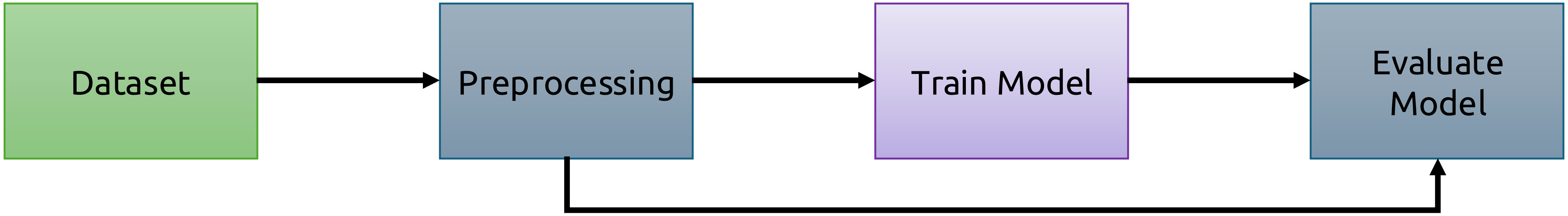
You have data on 1000 patients with just two pieces of information:

- Age
- BMI (Body Mass Index)

And you know which ones developed diabetes within 5 years.

The Classification Task: When a new patient walks in (age 45, BMI 28), predict: Will they develop diabetes? YES, or NO?

Machine Learning Pipeline

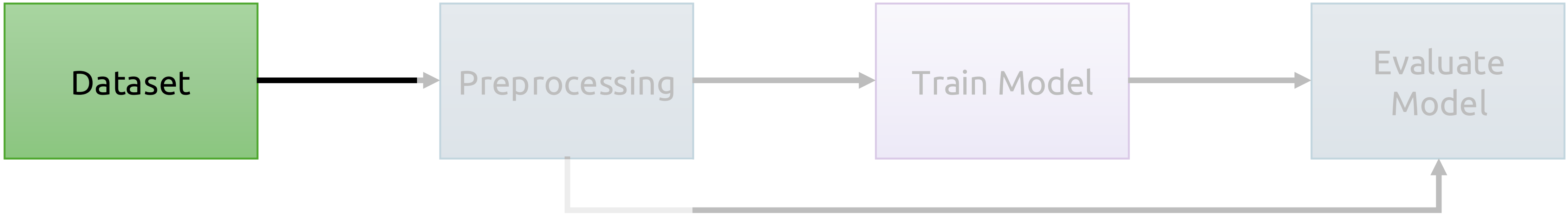

Dataset

Preprocessing

Train Model

Evaluate Model

Machine Learning Pipeline


Dataset

Preprocessing

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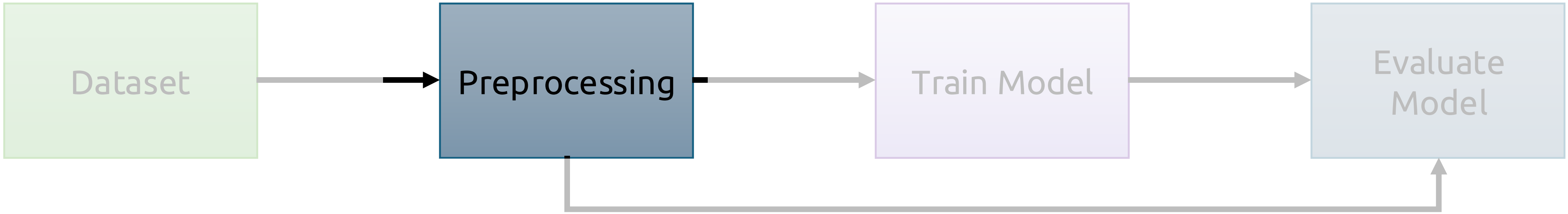
Evaluate Model

Data

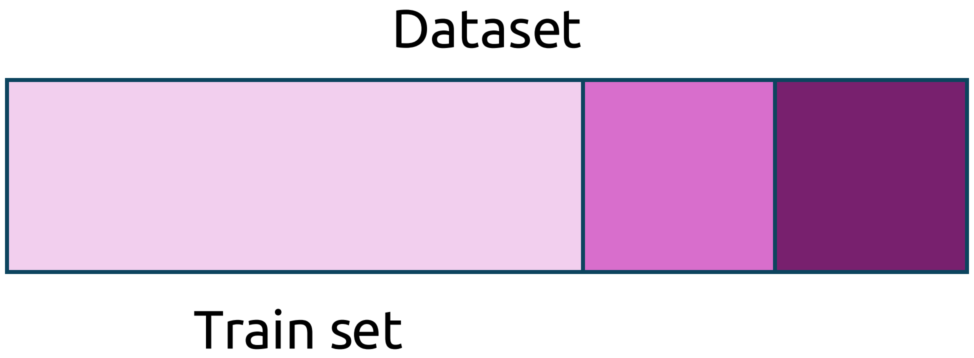
#	Age	BMI	Developed Diabetes?
0001	23	22.1	No
0002	34	24.8	No
0003	45	29.3	**Yes**
0004	28	21.5	No
0005	52	31.2	**Yes**
0006	38	26.7	No
0007	61	33.8	**Yes**
…	…	…	…
…	…	…	…
1000	29	23.4	No

Machine Learning Pipeline



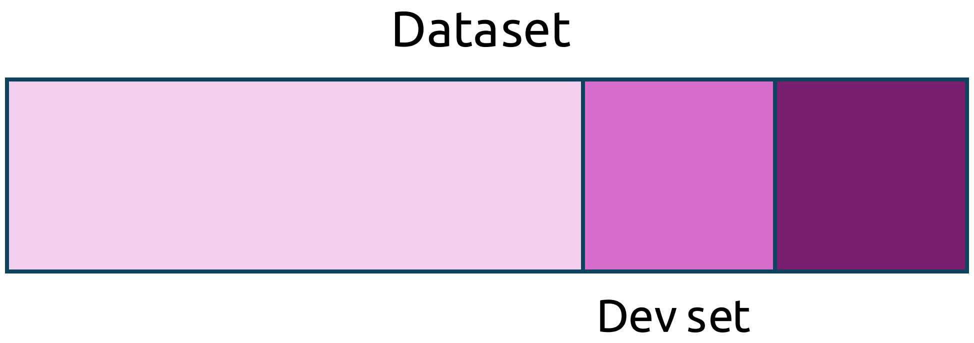
Train, validation, and test sets

- ***Train set*** — used to adjust the parameters of the model



Train, validation, and test sets

- ***Train set*** — used to adjust the parameters of the model
- ***Validation set*** — used to test how well we're doing as we develop
  - Prevents ***overfitting***, something you will learn later!
  - Also known as the ***development set***



Train, validation, and test sets

- ***Train set*** — used to adjust the parameters of the model
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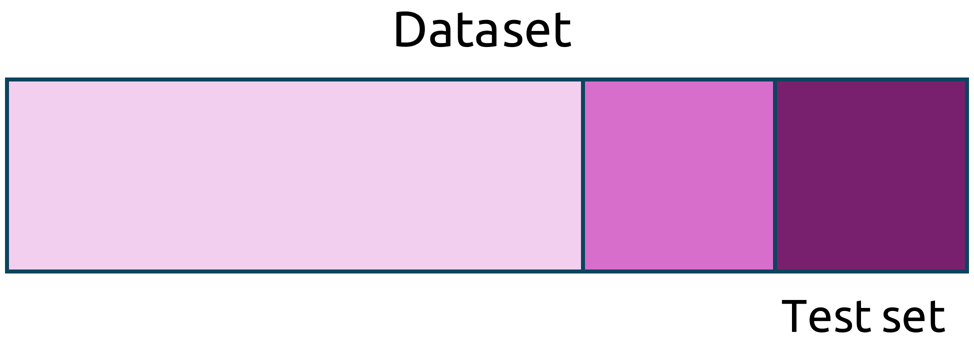
- ***Test set*** — used to evaluate the model once the model is done



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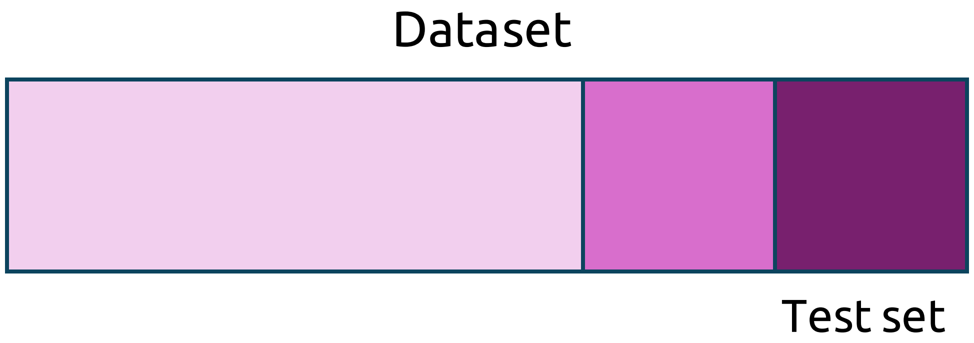


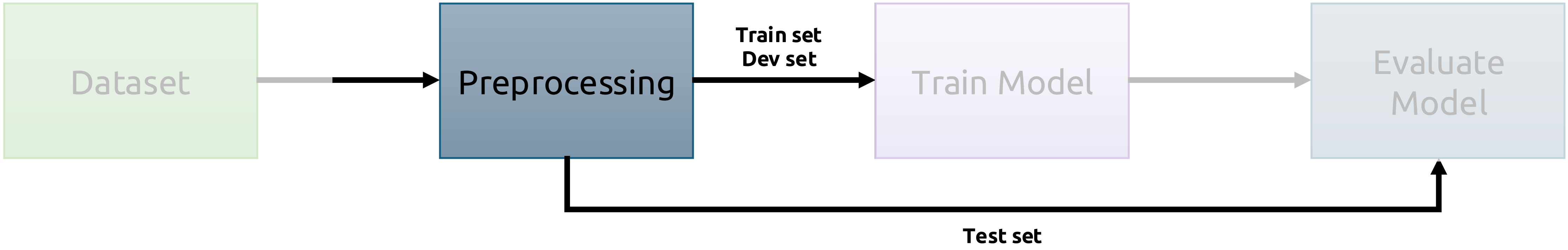
Question: Why do we need a separate test set?

Train, validation, and test sets

For the patient records

- 800 train records
- 100 validation records
- 100 test records

Machine Learning Pipeline



Dataset

Preprocessing

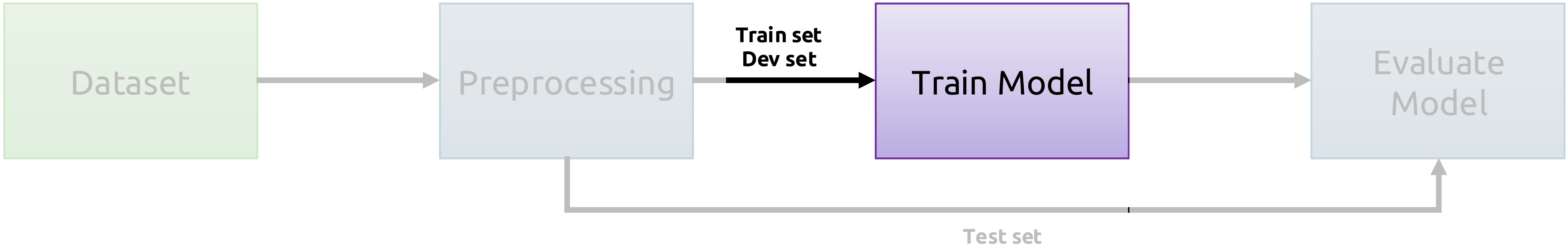
Train set
Dev set

Train Model

Evaluate Model

Test set

Machine Learning Pipeline



Dataset

Preprocessing

Train set
Dev set

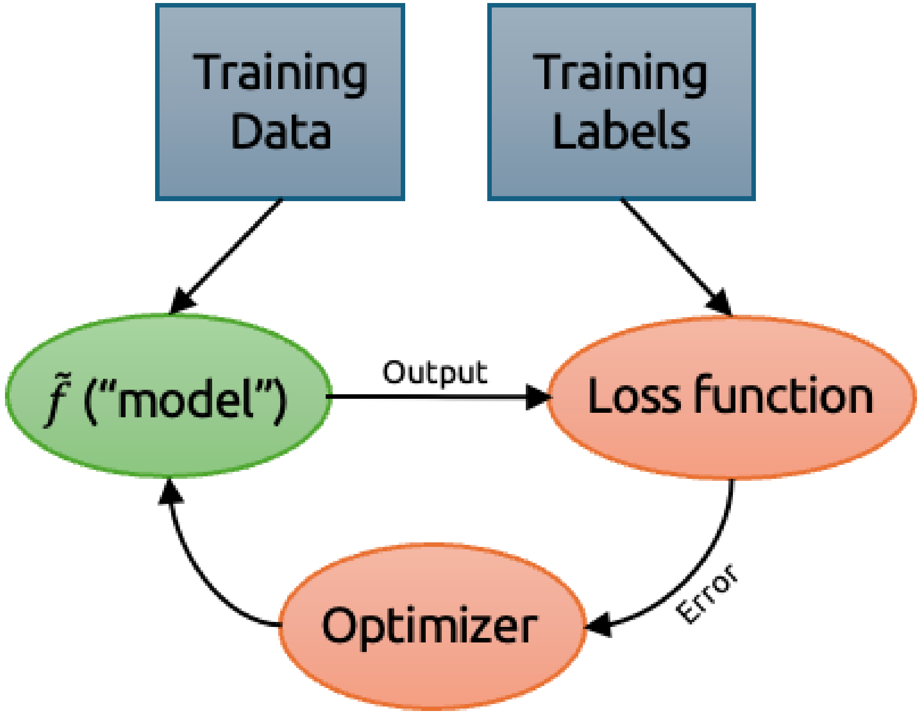
Train Model

Evaluate Model

Test set

Classification: Problem Setup

- Each x in our dataset is called an ***input***
  - x is represented by 2 features: [a1, a2]. a1 = age, a2 is BMI
- Each y in our dataset is called a ***label***
  - y is the corresponding answer/classification, one of two possibilities
- We refer to each (x, y) as an ***example***
- This is a ***supervised learning*** task



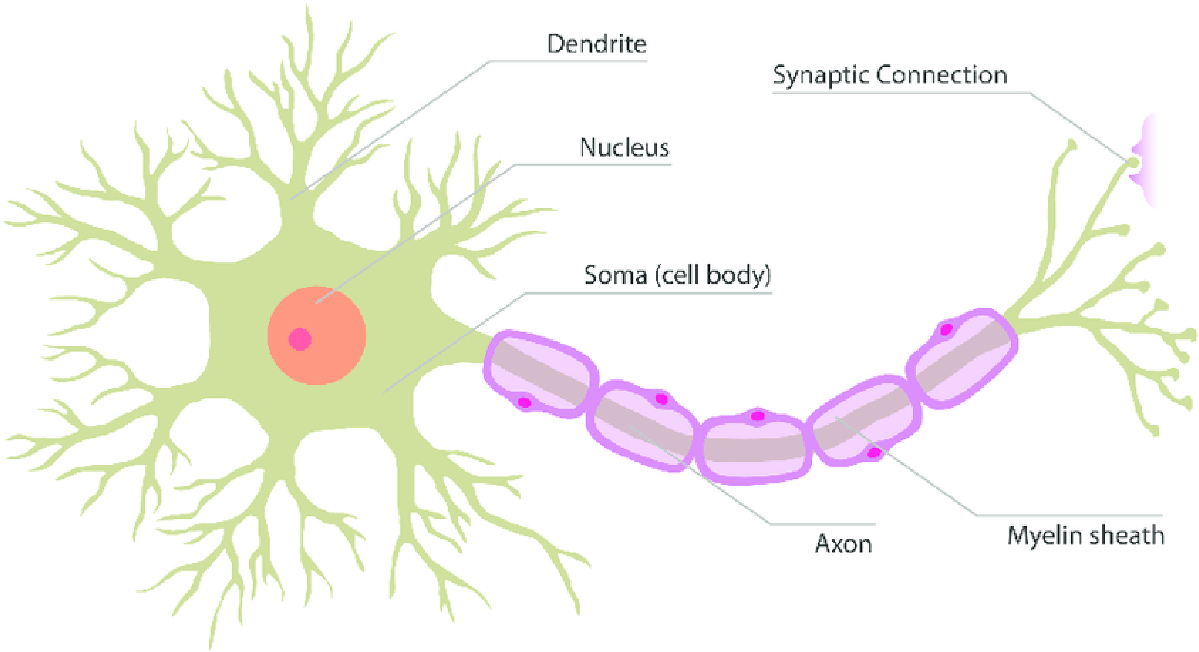
Perceptron: Our first neural network!

- "An electronic device which was constructed in accordance with biological principles and showed an ability to **learn**"
- Proposed by Frank Rosenblatt in 1958 (Cornell Aeronautical Laboratory)
- Initially simulated on an IBM 704 computer

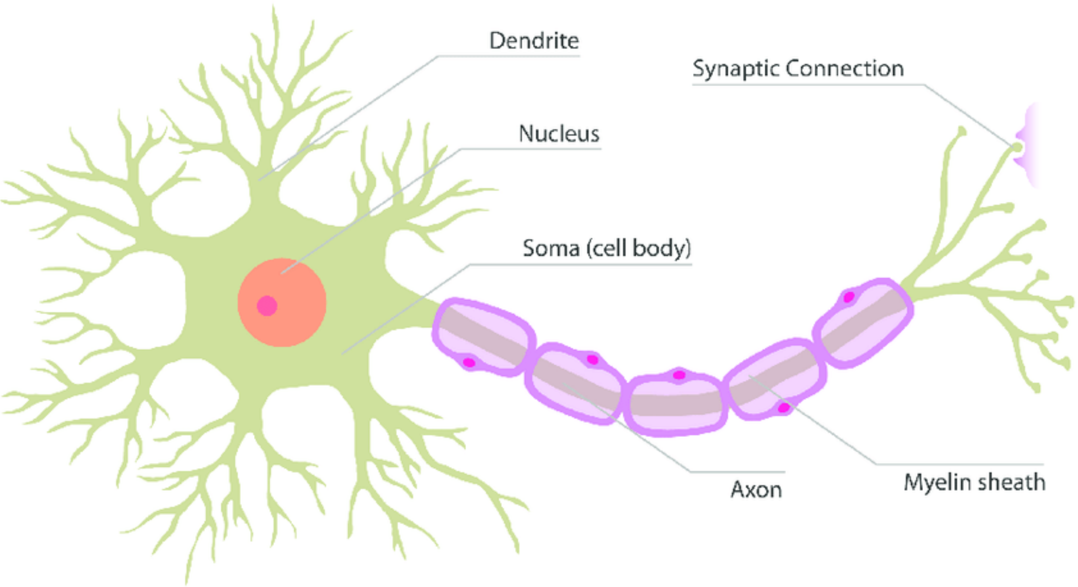
Images from Wikipedia

Biological motivation

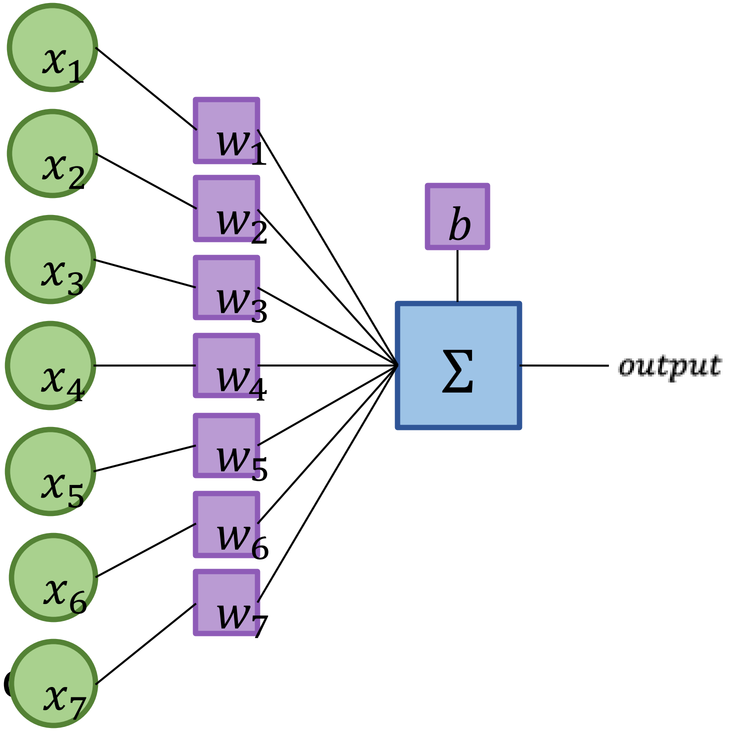
- Loosely inspired by neurons, basic working unit of the brain
- Serve to transmit information between cells



The Perceptron



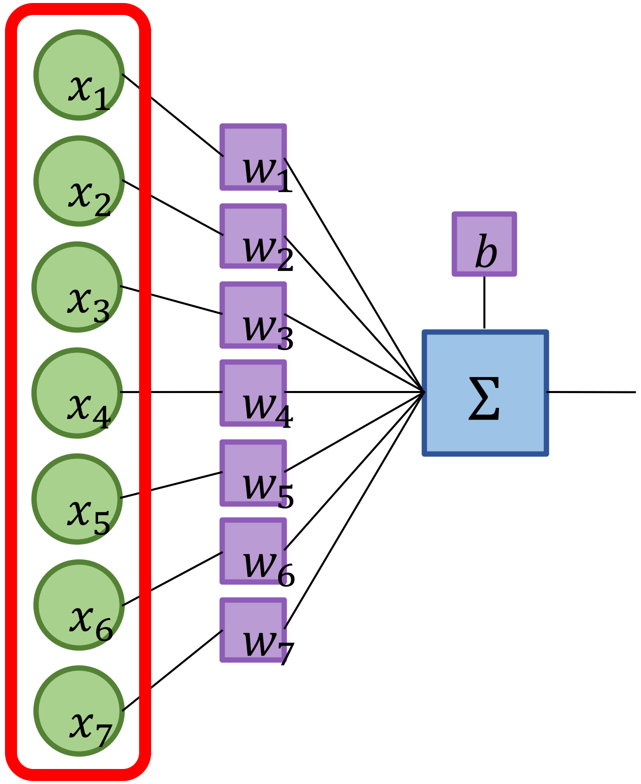
Biological Neur



Artificial Neuron (Perceptron)

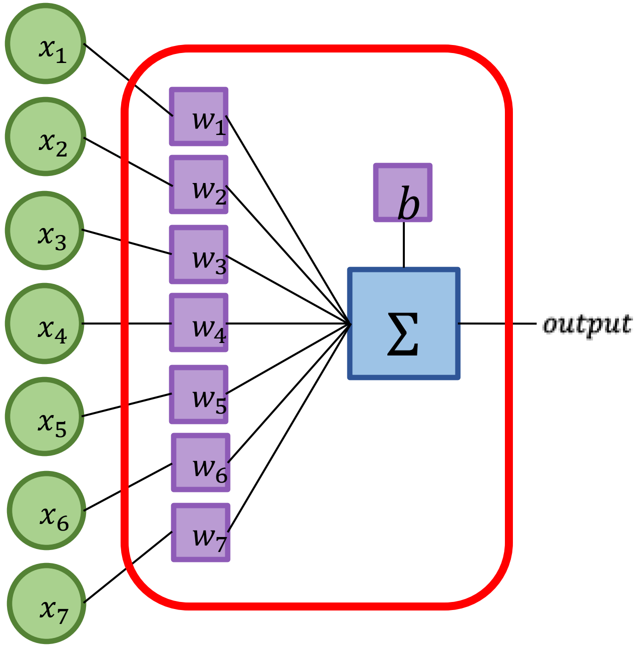
Input

- Input: a vector of numbers $\mathbf{x} = [x_1, x_2, \dots x_n]$



Predicting with a Perceptron

1. Multiply each input x_i by its corresponding weight w_i, sum them up.
2. Add the bias b



Predicting with a Perceptron

1. Multiply each input x_i by its corresponding weight w_i, sum them up.
2. Add the bias b
3. If the result value is greater than 0, return 1, otherwise return 0

$$f_{\Phi}(x) = \begin{cases} 1, & if\ b + \sum_{i=0}^{n} w_i\, x_i > 0 \\ 0, & otherwise \end{cases}$$

4. As a binary classifier, 1 indicates that x is a member of the class and 0, not a member

Linear Neurons

These are simple but computationally limited.

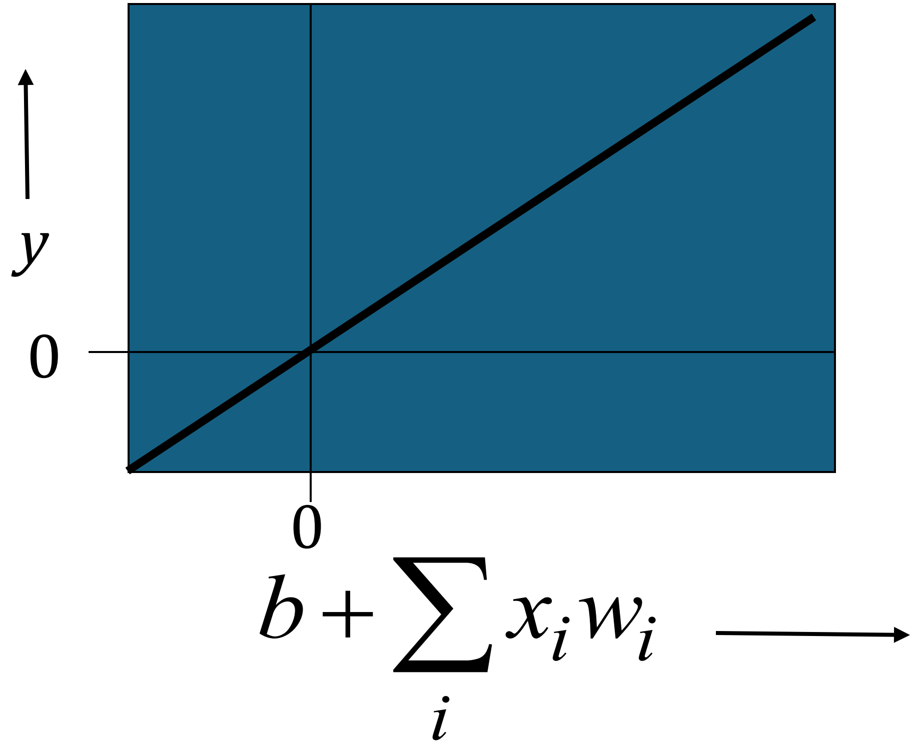
i-th Input

$$y = \sum_i x_i w_i$$

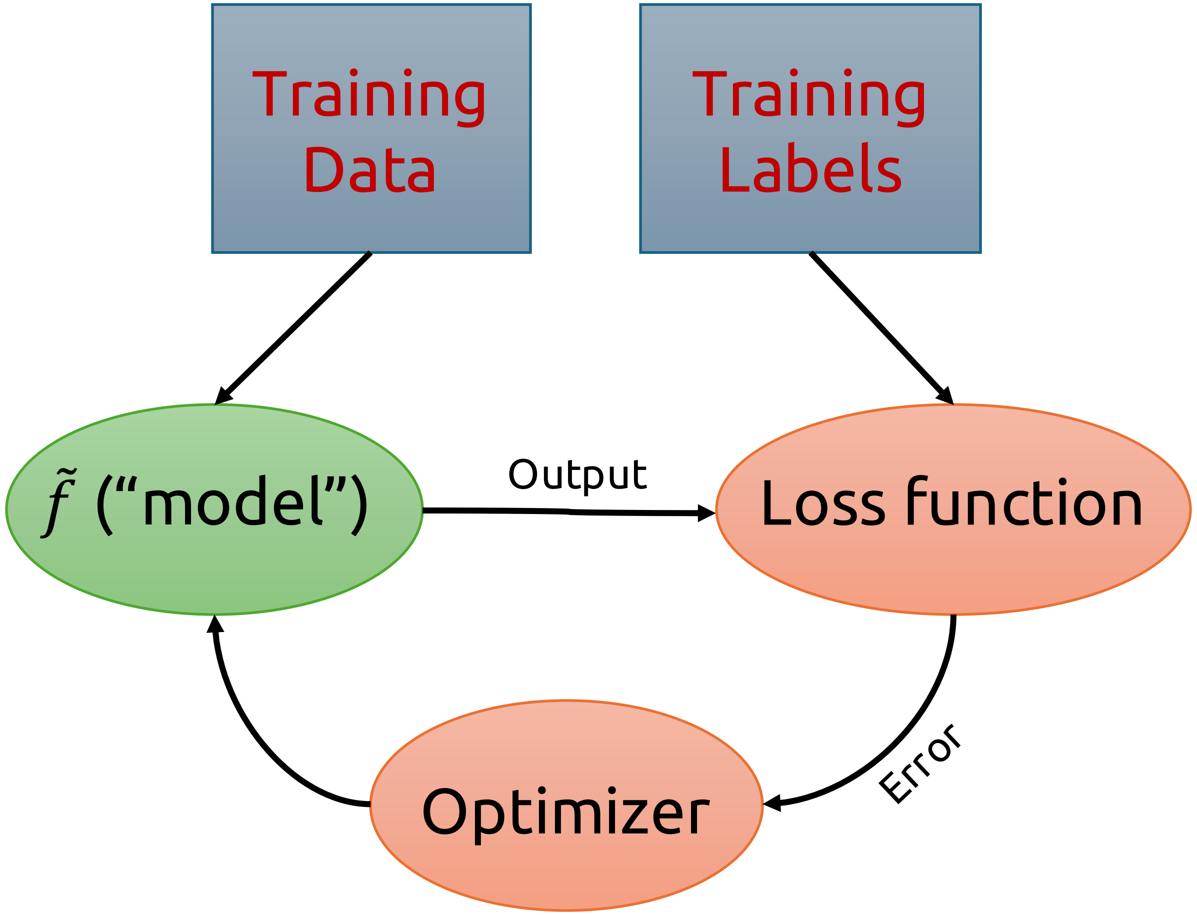
output

Index over input connections

Weights on i-th neuron

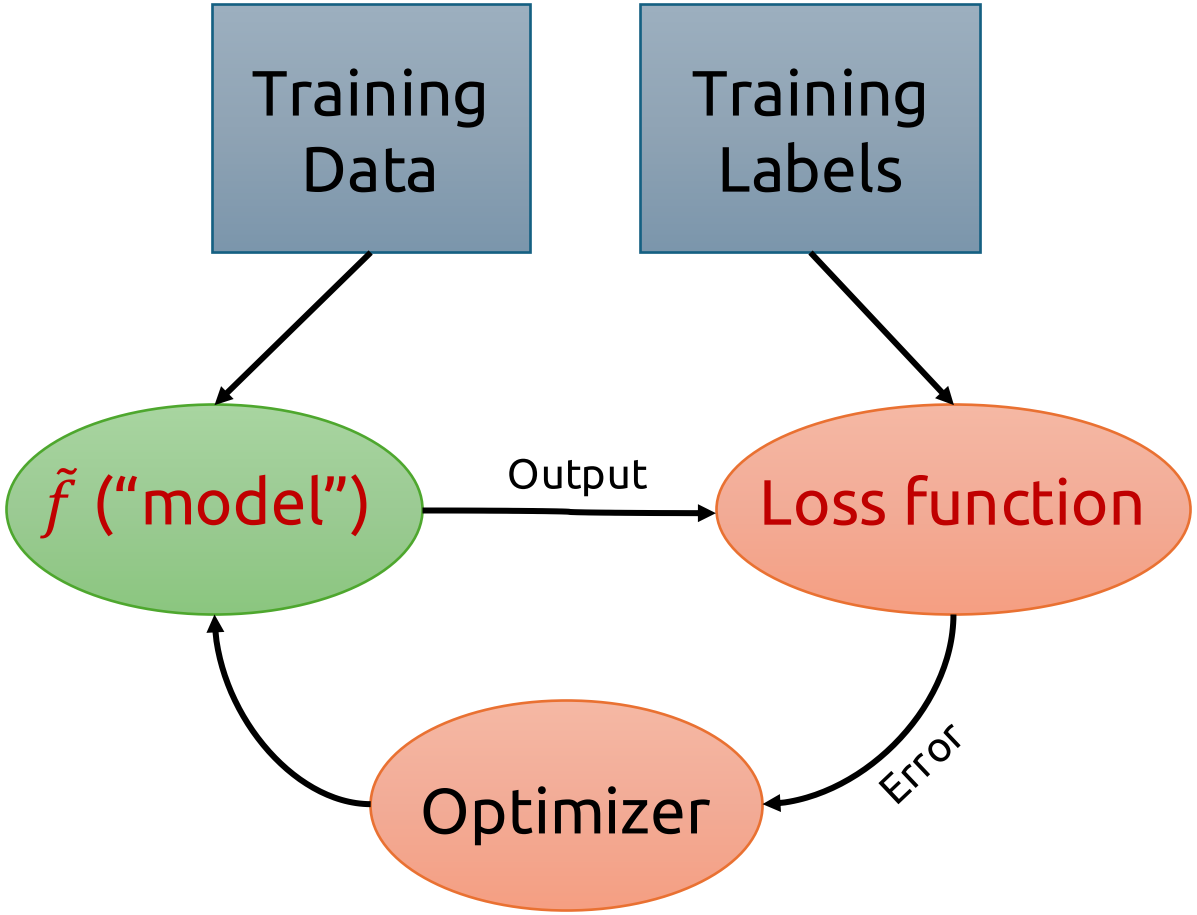


Supervised Learning



Collect training data and labels

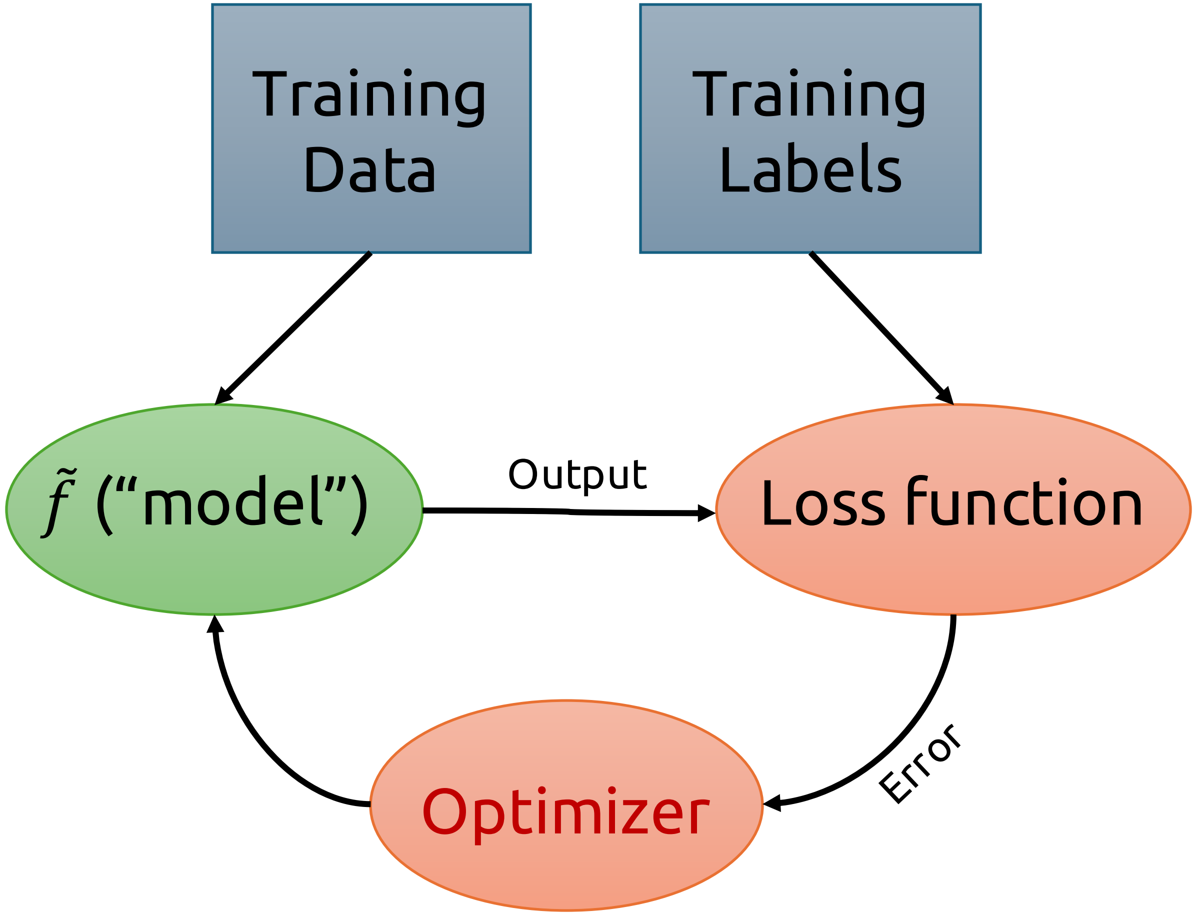
Supervised Learning



Collect training data and labels

Specify hypothesis class $\mathcal{H}$ and loss function

Supervised Learning



Collect training data and labels

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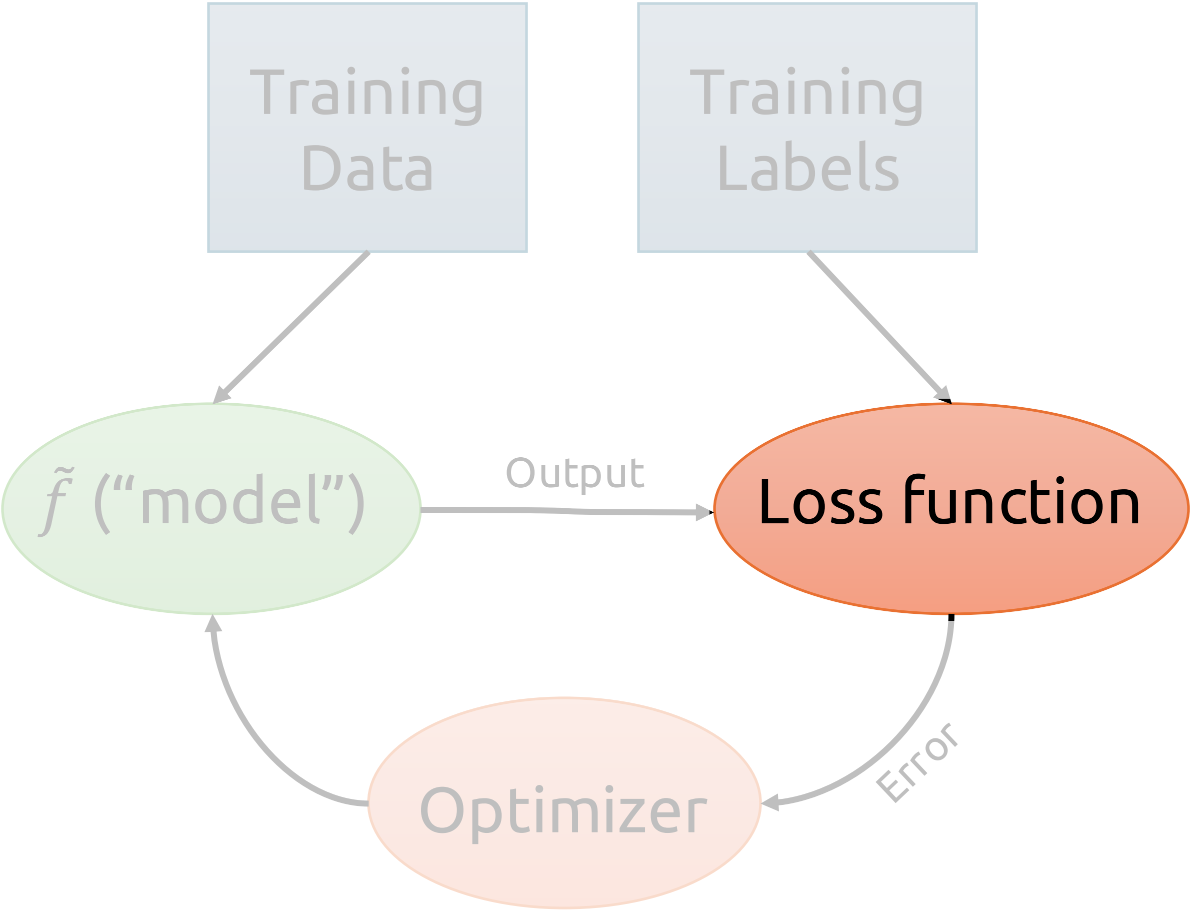
Learning: Find $f \in \mathcal{H}$ that minimizes the *empirical loss* on *training* data

A Critical Ingredient: Loss function



Loss function: How far $f(x)$ is from y

We want to minimize the loss.

Loss function – Measure of How Wrong Are We?

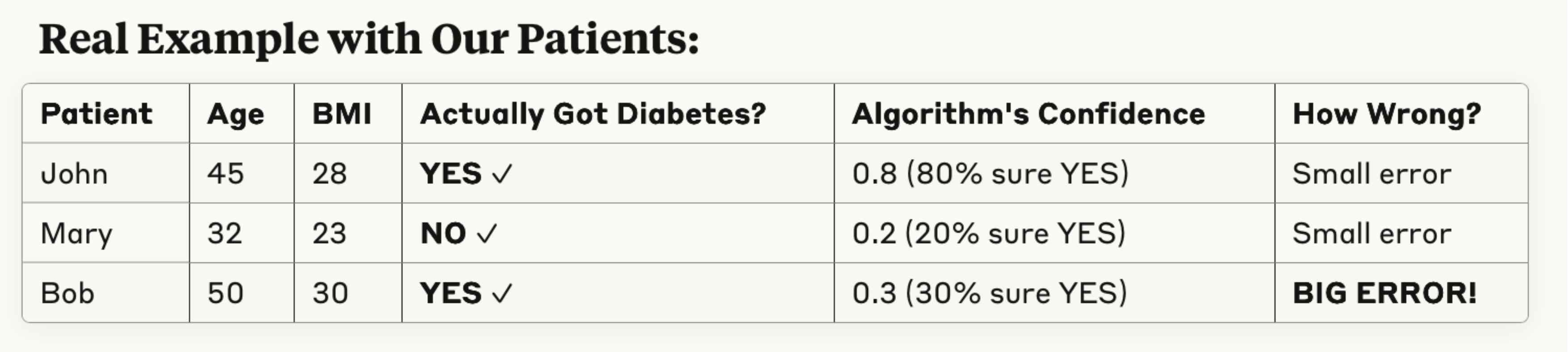
Imagine you're a pharmacy student doing clinical rotations. Every time you predict whether a patient will develop diabetes, you're either **right** or **wrong**. But how do we measure "how wrong" the computer is so it can improve?

Simple Scoring System

Let's say our algorithm doesn't just say "YES" or "NO" - it gives a **confidence score** between 0 and 1:

- 0.1 = "Very unlikely to get diabetes"
- 0.9 = "Very likely to get diabetes"
- 0.5 = "50-50 chance"

Loss function – Measure of How Wrong Are We?



Real Example with Our Patients:

Patient	Age	BMI	Actually Got Diabetes?	Algorithm's Confidence	How Wrong?
John	45	28	**YES** ✓	0.8 (80% sure YES)	Small error
Mary	32	23	**NO** ✓	0.2 (20% sure YES)	Small error
Bob	50	30	**YES** ✓	0.3 (30% sure YES)	**BIG ERROR!**

The Loss Function is Like a Penalty System

Think of it like losing points in a video game:

When the algorithm is confident AND correct:

- Patient has diabetes, algorithm says 90% chance → **Small penalty** (like -1 point)

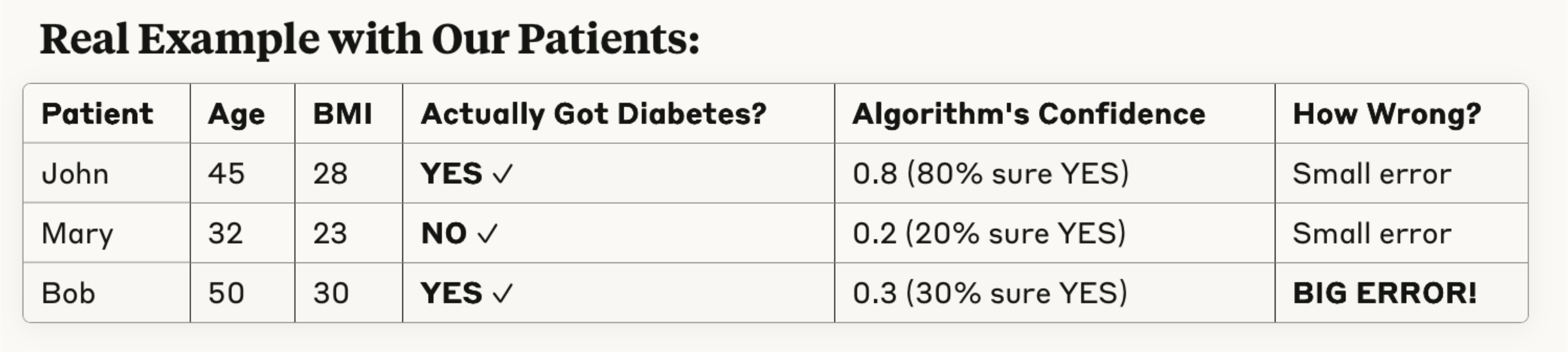
When the algorithm is confident BUT wrong:

- Patient has diabetes, algorithm says 10% chance → **HUGE penalty** (like -100 points)

When the algorithm is uncertain:

- Patient has diabetes, algorithm says 50% chance → **Medium penalty** (like -20 points)

Loss function – Measure of How Wrong Are We?



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The **binary loss function** calculates these penalties mathematically. The algorithm's goal is to **minimize total penalties** across all patients.

Key insight: The algorithm doesn't just want to be right - it wants to be **confidently right** and **uncertainly wrong** (rather than confidently wrong).

This is exactly like studying for an exam - you don't just want to know the right answer, you want to be confident when you know it and admit uncertainty when you don't!

Loss Function in Classification

$$\hat{L}(f) = -\frac{1}{N}\sum_{i=1}^{N} y_i \cdot log(p(y_i)) + (1 - y_i) \cdot log(1 - p(y_i))$$

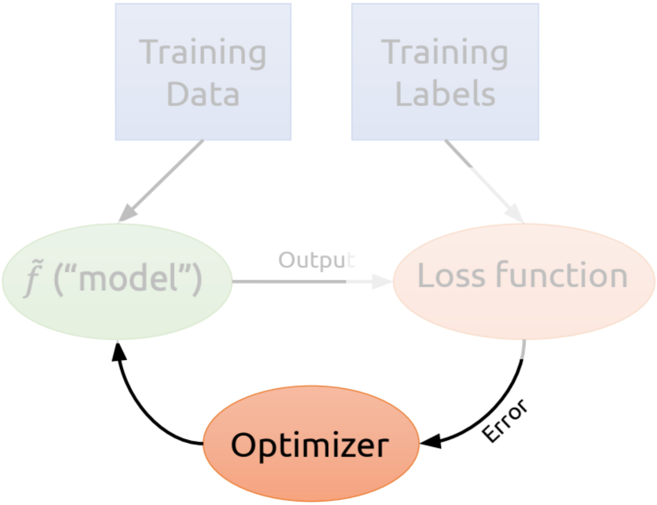
y_i is the **label** (**1 for** yes to diabetes and **0 for no to diabetes**) and
$\boldsymbol{p}(\boldsymbol{y_i})$ is the predicted **probability of the cases being yes** for all **N** points.

Linear Regression: Optimization

- We want to minimize

$$\hat{L}(f) = -\frac{1}{N}\sum_{i=1}^{N} y_i \cdot log(p(y_i)) + (1 - y_i) \cdot log(1 - p(y_i))$$

- The algorithm to minimize the loss function is called an **optimizer**.



Thank you