Northeastern University
Khoury College of
Computer Sciences

Final Review

DS 4400 | Machine Learning and Data Mining I

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Spring 2026

Wednesday | April 15th, 2026

Models Seen So Far

Supervised

- Linear Regression
- Naive Bayes
- Logistic Regression
- Decision Trees
- k-NN
- Neural Networks
- LDA
- CNNs

Unsupervised

- PCA
- k-Means Clustering
- Hierarchical Clustering
- Autoencoders & VAE

Models Seen So Far

Supervised		Unsupervised
Linear Regression	Naive Bayes	PCA
Logistic Regression	Decision Trees	k-Means Clustering
k-NN	Neural Networks	Hierarchical Clustering
LDA	CNNs	Autoencoders & VAE

Naive Bayes Classifier

- Like LDA, Naive Bayes is a generative classifier using Bayes' theorem

$$\mathbb{P}(Y = k \,|\, X = x) = \frac{\mathbb{P}(X = x \,|\, Y = k) \cdot \mathbb{P}(Y = k)}{\mathbb{P}(X = x)}$$

- The challenge:
  - Estimating $\mathbb{P}(X \,|\, Y = k)$ for high-dimensional X is difficult.

Naive Bayes Classifier

Naive Bayes assumes features are conditionally independent given the class

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- The challenge:
  - Estimating $\mathbb{P}(X \,|\, Y = k)$ for high-dimensional X is difficult.
  - With d features, each taking v possible values, we'd need to estimate v^d parameters per class - **exponential in dimensionality**.

Naive Bayes Classifier

- Example:
  - For spam classification with words “free” and “money”
    - Reality: $\mathbb{P}$("free", "money" | spam) $\neq \mathbb{P}$("free"|spam) $\cdot \mathbb{P}$(“money" | spam)
    - These words are correlated in spam emails
    - Naive Bayes pretends they're **independent**

Naive Bayes Classifier

Want to predict:

$$\mathbb{P}(Y = k \,|\, X = x) = \frac{\mathbb{P}(X = x \,|\, Y = k) \cdot \mathbb{P}(Y = k)}{\mathbb{P}(X = x)}$$

Naive Assumption:

$$\mathbb{P}(X = x \,|\, Y = k) = \mathbb{P}(x_1, x_2, x_3, \ldots, x_d \,|\, Y = k) = \Pi_{j=1}^{d} \mathbb{P}(x_j \,|\, Y = k)$$

Naive Bayes Classifier

How do you find $\mathbb{P}(x_j \mid Y = k)$?

Naive Bayes Classifier

$$\mu_{kj} = \frac{1}{N_k} \sum_{i:y_i=k} x_{ij}$$

$$\sigma_{kj}^2 = \frac{1}{N_k} \sum_{i:y_i=k} (x_{ij} - \mu_{kj})^2$$

Gaussian Naive Bayes

For continuous features, assume each feature follows a Gaussian Distribution

$$\mathbb{P}(x_j \mid Y = k) = \frac{1}{\sqrt{2\pi\sigma_{kj}^2}} \cdot e^{-\frac{(x_j - \mu_{kj})^2}{2\sigma_{kj}^2}}$$

Each class-feature combination has its own mean μ_{kj} and variance σ_{kj}^2

Naive Bayes Classifier

Multinomial Naive Bayes

For discrete features/count data like word frequencies

$$\mathbb{P}(x_j \mid Y = k) = \theta_{kj}^{x_j}$$

Where θ_{kj} is the probability of feature j in class k and x_j is the count of feature j

$$\theta_{kj} = \frac{\text{count of feature } j \text{ in class } k}{\text{total count of all features in class } k}$$

Naive Bayes Classifier

Bernoulli Naive Bayes

For binary data like word frequencies

$$\mathbb{P}(x_j \mid Y = k) = \theta_{kj}^{x_j} \cdot (1 - \theta_{kj})^{1 - x_j}$$

Where θ_{kj} is the probability of feature j in class k and x_j is the count of feature j

$$\theta_{kj} = \frac{\text{count of feature } j \text{ in class } k}{\text{total samples in class } k}$$

Naive Bayes Classifier

Example

Task

Classify emails as spam or not spam

Training Data

Document	x_1 = “free”	x_2 = “money”	x_3 = “meeting”	x_4 = “lunch”	Class
1	3	2	0	0	spam
2	2	1	0	0	spam
3	0	0	2	1	not spam
4	0	0	1	2	not spam

Naive Bayes Classifier

Example

$$\theta_{kj} = \frac{\text{count of feature } j \text{ in class } k}{\text{total count of all features in class } k}$$

Task

Classify emails as spam or not spam

$$\mathbb{P}(\textbf{spam}) = \frac{2}{4} = 0.5$$

$$\mathbb{P}(\textbf{not spam}) = \frac{2}{4} = 0.5$$

Training Data

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$$\mathbb{P}(\textbf{spam}) = \frac{2}{4} = 0.5$$

$$\mathbb{P}(\textbf{not spam}) = \frac{2}{4} = 0.5$$

For **spam** class:

Laplace Smoothing

- $\mathbb{P}(\text{"free"}|\text{spam}) = \frac{(5+1)}{(8)} = \frac{6}{8} = 0.75$

Naive Bayes Classifier

Example

$$\theta_{kj} = \frac{\text{count of feature } j \text{ in class } k}{\text{total count of all features in class } k}$$

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For **spam** class:

- $\mathbb{P}(\text{"free"}|\text{spam}) = \frac{(5+1)}{(8)} = \frac{6}{8} = 0.75$
- $\mathbb{P}(\text{"money"}|\text{spam}) = \frac{(3+1)}{(8)} = \frac{4}{8} = 0.5$
- $\mathbb{P}(\text{"meeting"}|\text{spam}) = \frac{(0+1)}{(8)} = \frac{1}{8} = 0.125$
- $\mathbb{P}(\text{"lunch"}|\text{spam}) = \frac{(0+1)}{(8)} = \frac{1}{8} = 0.125$

Naive Bayes Classifier

Example

$$\theta_{kj} = \frac{\text{count of feature } j \text{ in class } k}{\text{total count of all features in class } k}$$

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$$\mathbb{P}(\textbf{spam}) = \frac{2}{4} = 0.5$$

$$\mathbb{P}(\textbf{not spam}) = \frac{2}{4} = 0.5$$

For **not spam** class:

- $\mathbb{P}(\text{"free"}|\text{not spam}) = \frac{(0+1)}{(6)} = \frac{1}{6} = 0.166$
- $\mathbb{P}(\text{"money"}|\text{not spam}) = \frac{(0+1)}{(6)} = \frac{1}{6} = 0.166$
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Naive Bayes Classifier

Example

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New Email: $x =$ “free money”

Naive Bayes Classifier

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New Email: $x =$ “free money”

$$\mathbb{P}(spam \mid x) = \mathbb{P}(Y = spam) \cdot \Pi_{j=1}^{d} \mathbb{P}(x_j \mid Y = spam)$$

Naive Bayes Classifier

Example

$$\theta_{kj} = \frac{\text{count of feature } j \text{ in class } k}{\text{total count of all features in class } k}$$

$$\mathbb{P}(x_j \mid Y = k) = \theta_{kj}^{x_j}$$

For **spam** class:

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New Email: $x =$ “free money”

$$\mathbb{P}(spam \mid x) = \mathbb{P}(Y = spam) \cdot \Pi_{j=1}^{d} \mathbb{P}(x_j \mid Y = spam)$$

$$\mathbb{P}(spam \mid x) = 0.5 \cdot (0.75)^1 \cdot (0.5)^1 = 0.1875$$

Naive Bayes Classifier

Example

$$\theta_{kj} = \frac{\text{count of feature } j \text{ in class } k}{\text{total count of all features in class } k}$$

$$\mathbb{P}(x_j \mid Y = k) = \theta_{kj}^{x_j}$$

For **spam** class:

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New Email: $x =$ “free money”

$$\mathbb{P}(spam \mid x) = \mathbb{P}(Y = spam) \cdot \Pi_{j=1}^{d} \mathbb{P}(x_j \mid Y = spam)$$

$$\mathbb{P}(spam \mid x) = 0.5 \cdot (0.75)^1 \cdot (0.5)^1 = 0.1875$$

$$\mathbb{P}(not\ spam \mid x) = \mathbb{P}(Y = not\ spam) \cdot \Pi_{j=1}^{d} \mathbb{P}(x_j \mid Y = not\ spam)$$

$$\mathbb{P}(not\ spam \mid x) = 0.5 \cdot (0.166)^1 \cdot (0.166)^1 = 0.013$$

Naive Bayes Classifier

Pros

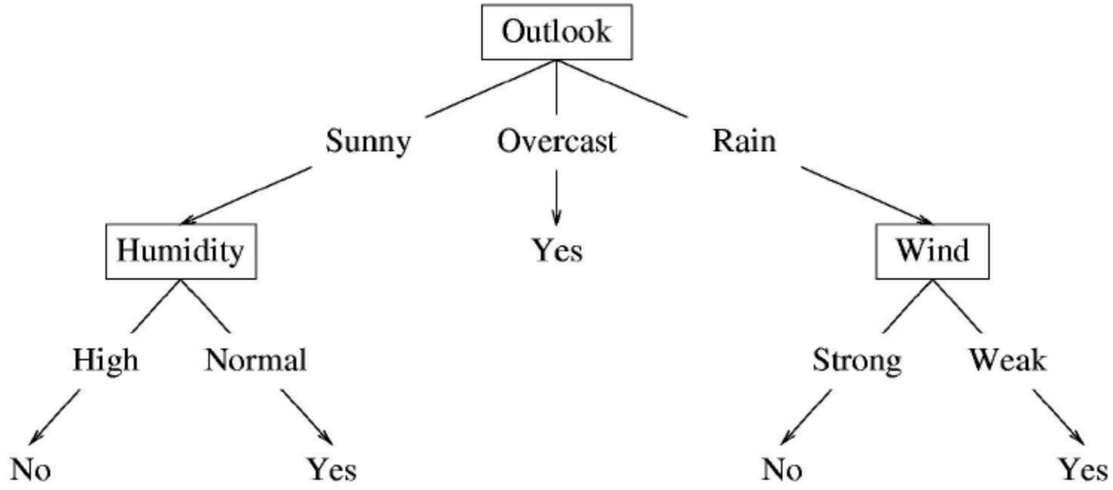
- Extremely fast training (just counting)
- Fast prediction
- Handles high-dimensional data well
- Works with **small training** sets
- Handles missing features naturally
- Easy to implement and interpret
- Often surprisingly accurate

Cons

- Independence assumption is usually wrong
- Probability estimates are unreliable
- Cannot learn feature interactions
- Continuous features require distributional assumptions
- Correlated features are “double-counted”

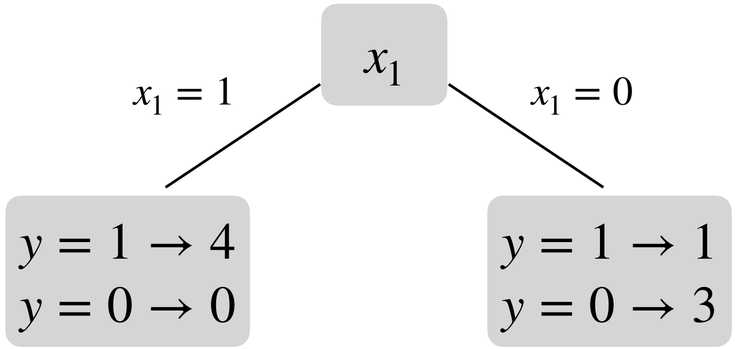
Decision Trees

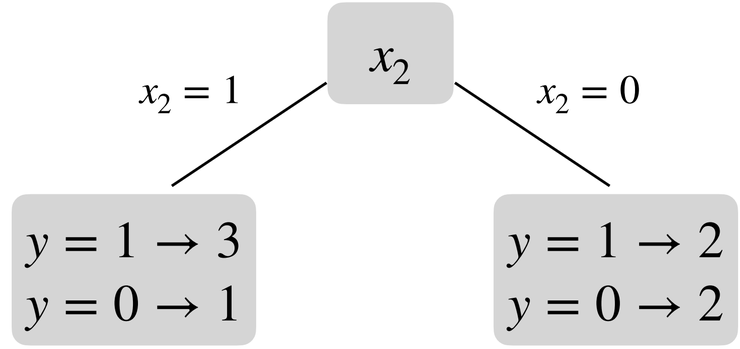
Play Outside? (y)	Humidity (X1)	Wind (X2)	Outlook (X3)
Yes	Normal	Strong	Sunny
Yes	Low	Weak	Overcast
No	High	Weak	Rain



Decision Trees

y	x_1	x_2
1	1	1
1	1	0
1	1	1
1	1	0
1	0	1
0	0	0
0	0	1
0	0	0





How do we decide which is better?

Entropy Measures - Information Gain

Use counts at leaf nodes to define probabilities, so we can measure uncertainty

Entropy

- Entropy measures **uncertainty** or **surprise**.
- The **more uncertain** you are about an outcome, the **higher the entropy**.
- **Entropy is maximized when all outcomes are equally likely.**
- For outcomes with probabilities $p_1, p_2, \ldots, p_n$:

$$H = -\sum_i p_i log_2(p_i)$$

Entropy

- Why Entropy Matters in Decision Trees
  - We want splits that **reduce uncertainty** about the class label.
  - A split that creates pure nodes (all one class) reduces entropy to zero.
    - **Before split:** Mixed classes, high entropy
    - **After good split**: Purer nodes, lower entropy
    - Information gain = entropy reduction

Entropy

- Node 1 has 75% class A, 25% class B:

$$H = -0.75log_2(0.75) - 0.25log_2(0.25) = 0.811 \text{ bits}$$

- Node 2 has 50% class A and 50% class B:

$$H = -0.5log_2(0.5) - 0.5log_2(0.5) = 1 \text{ bit}$$

- Node 1 has **lower entropy** (less uncertainty) than node 2.

Measuring Split Quality: Impurity Functions

- A good split separates classes.
- We measure node **impurity** - how mixed the classes are - and choose splits that maximize impurity reduction.

Measuring Split Quality: Impurity Functions

Gini Impurity

- Let p_k be the proportion of class k samples in a node

$$Gini(D) = 1 - \sum_{k=1}^{K} p_k^2 = \sum_{k=1}^{K} p_k(1 - p_k)$$

- **Interpretation**: Probability of misclassifying a randomly chosen sample if labeled according to the class distribution.
- **Properties**:
  - Minimum = 0 when node is pure (all one class)
  - Maximum = $1 - \frac{1}{K}$ when classes are equally distributed
  - For binary: max = 0.5 at p = 0.5
- **Example (binary classification):**
  - Node with 100% class A: Gini = 1 - 1^2 = **0 (pure)**
  - Node with 50% each: Gini = 1 - 0.5^2 - 0.5^2 = 0.5 (maximum impurity)
  - Node with 90% class A: Gini = 1 - 0.9^2 - 0.1^2 = 0.18

Measuring Split Quality: Impurity Functions

Information Gain

- We want splits that reduce **impurity** (i.e., Gini, Entropy).
- Information gain measures this reduction:

$$Gain(D, split) = Impurity(D) - \sum_{k \in \text{classes}} \frac{|D_k|}{|D|} \cdot Impurity(D_k)$$

Measuring Split Quality: Impurity Functions

Information Gain

- We want splits that reduce **impurity** (i.e., Gini, Entropy).
- Information gain measures this reduction:

weighted average impurity of child nodes

$$Gain(D, split) = Impurity(D) - \sum_{k \in \text{classes}} \frac{|D_k|}{|D|} \cdot Impurity(D_k)$$

Measuring Split Quality: Impurity Functions

Information Gain

- Information gain measures this reduction:

$$Gain(D, split) = Impurity(D) - \sum_{k \in \text{outcomes}} \frac{|D_k|}{|D|} \cdot Impurity(D_k)$$

100 Days
60 Play, 40 Don’t Play

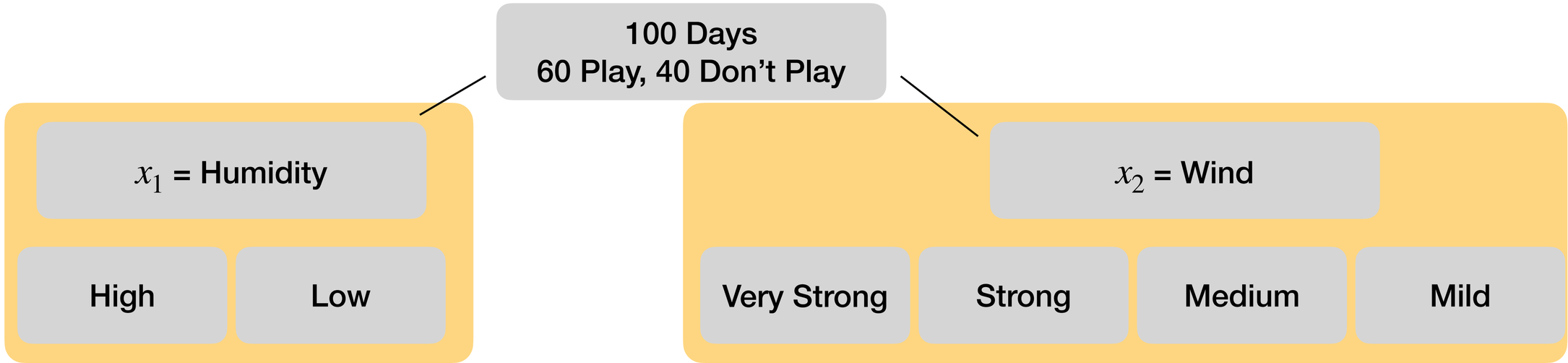
Measuring Split Quality: Impurity Functions

Information Gain

Step 1: Decide between Wind and Humidity

- Information gain measures this reduction:

$$Gain(D, split) = Impurity(D) - \sum_{k \in \text{outcomes}} \frac{|D_k|}{|D|} \cdot Impurity(D_k)$$



Measuring Split Quality: Impurity Functions

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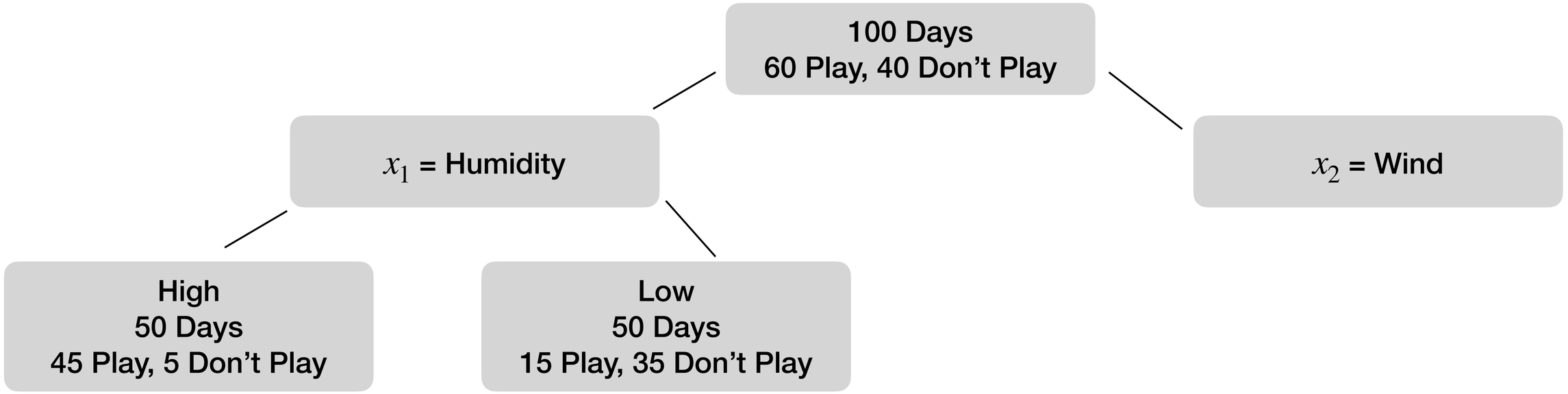

$H = -0.9log_2(0.9) - 0.1log_2(0.1) = 0.469\ bits$

$H = -0.3log_2(0.3) - 0.7log_2(0.7) = 0.881\ bits$

Measuring Split Quality: Impurity Functions

Information Gain

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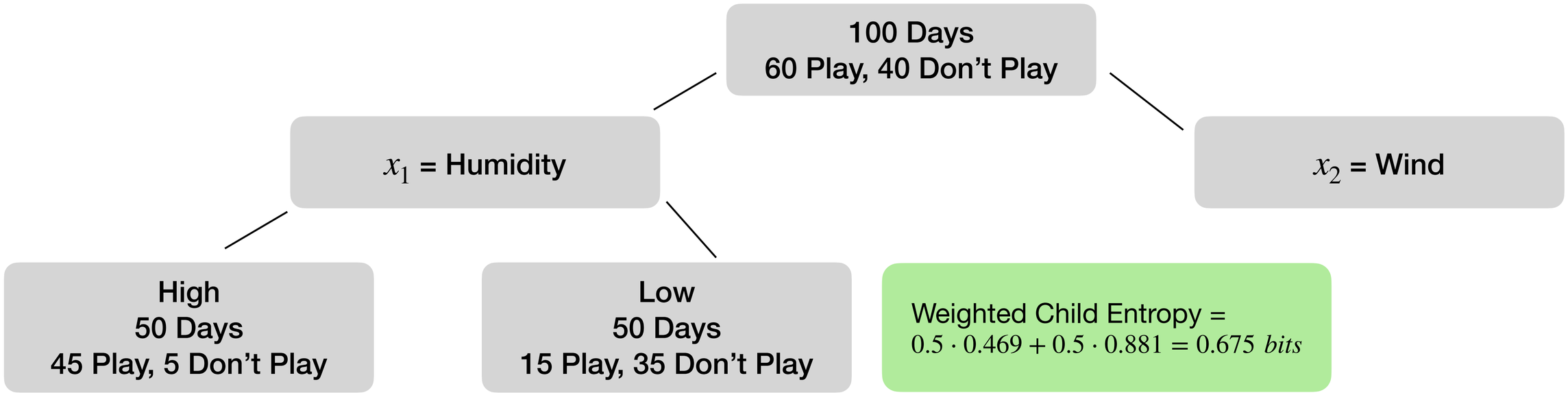

$H = -0.9log_2(0.9) - 0.1log_2(0.1) = 0.469$ *bits*

$H = -0.3log_2(0.3) - 0.7log_2(0.7) = 0.881$ *bits*

Measuring Split Quality: Impurity Functions

Information Gain

- Information gain measures this reduction:

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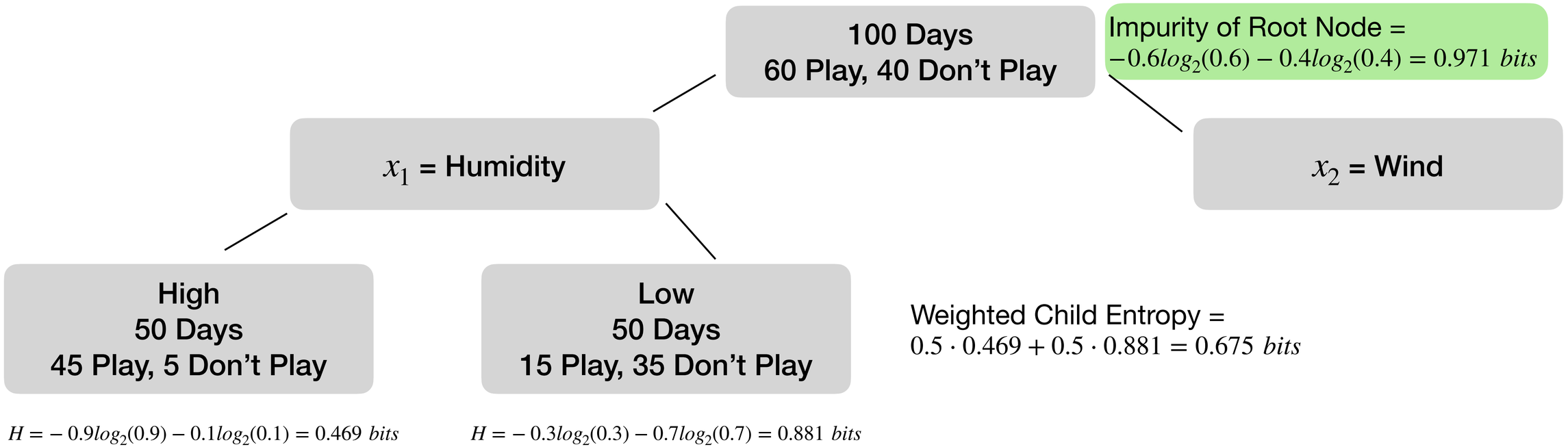

Measuring Split Quality: Impurity Functions

Information Gain

Information Gain = 0.971 - 0.675 = **0.296 bits**

- Information gain measures this reduction:

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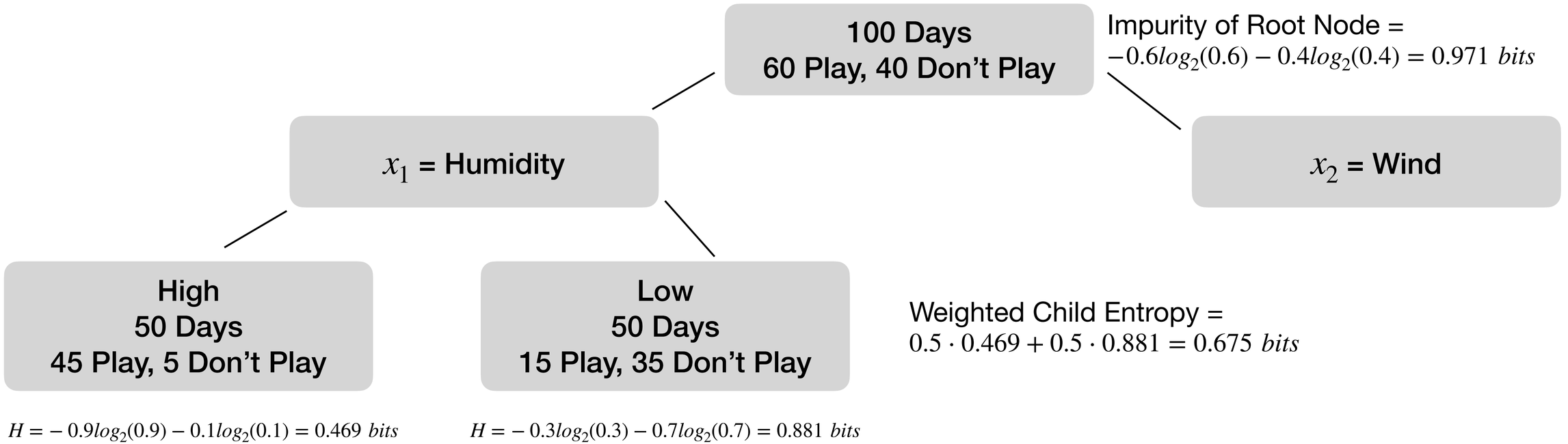


Stopping Criteria

When to stop splitting and create a leaf

Hyperparameters

- **Maximum depth reached**: depth $\geq$ **max_depth**
- **Minimum samples:** node has fewer than **min_samples_split** samples
- **Minimum samples per leaf:** split would create child with < **min_samples_leaf**
- **Pure node:** all samples belong to same class
- **No information gain:** best split doesn't improve impurity
- **Maximum leaf nodes:** tree already has **max_leaf_nodes** leaves

Stopping Criteria

Overfitting & Pruning

- Deep trees overfit - they memorize training data, **creating leaves with very few samples**.
- Signs of overfitting:
  - Training accuracy ≈ 100%
  - Test accuracy much lower
  - **Very deep tree with many leaves**

Decision Trees

Pros and Cons

Pros

- Highly interpretable (visualize as flowchart)
- No feature scaling required
- Handles numerical and categorical features
- Handles missing values
- Captures non-linear relationships
- Automatic feature selection
- Fast prediction: O(depth)

Cons

- High variance (unstable)
- Prone to overfitting
- Greedy algorithm (no global optimum)
- Axis-aligned splits only (can't capture diagonal boundaries efficiently)
- Biased toward high-cardinality features

Ensemble Methods

The Fundamental Idea

- A single decision tree is unstable and prone to overfitting.
- Ensemble methods combine multiple trees to create a more robust model.
- **Key Insight:**
  - Combining many “weak” learners can create a “strong” learner.
- **Analogy:**
  Asking 100 people to estimate something and averaging their answers is often more accurate than asking one expert.

Ensemble Methods

The Fundamental Idea

Method	Strategy	Trees Trained	Key Idea
Bagging	Parallel	Independently	Reduce variance via averaging
Random Forest	Parallel	Independently + High Depth	Bagging + random feature subsets
Boosting	Sequential	Each corrects previous	Reduce bias via focusing on errors

Bagging
Bootstrap Aggregating

- Bootstrap sampling:
  - Sample **N** points with replacement from a dataset of **N** points.
- **Bagging Algorithm**
  - Create **B** bootstrap samples from the training data
  - Train one decision tree on each bootstrap sample
  - Combine predictions:
    - Classification: Majority vote
    - Regression: Average

Bagging
Evaluation - Out-of-Bag (OOB)

- For each sample x_i, find all trees that **did not** include it in their bootstrap sample
- Get predictions from **only those trees**
- Aggregate these predictions
- Compute error across all samples
- OOB error approximates test error without needing a separate validation set.

Random Forests

Pros and Cons

Pros

- Excellent accuracy out-of-the-box
- Robust to overfitting
- Handles high-dimensional data
- Provides feature importance
- Built-in OOB validation
- Parallelizable (trees are independent)
- Minimal tuning required

Cons

- Less interpretable than single tree
- Can be slow for very large datasets
- Not optimal for sparse, high-dimensional data (like text)

Boosting

- Unlike bagging (parallel, independent trees), boosting trains trees **sequentially**
  - Each subsequent tree trying to **correct the errors of the previous trees**.
- **Intuition**: Each tree focuses on the samples that **previous trees got wrong**.

AdaBoost - Adaptive Boosting

- **Key idea**:
  - Maintain weights on samples.
  - Increase weights on misclassified samples so the next tree focuses on them.

AdaBoost - Adaptive Boosting

Algorithm

- Initialize weights: $w_i = \frac{1}{N}$ for all samples
- For $t = 1 \rightarrow T$:
    1. Train weak learner h_t on weighted data
    2. Compute weighted error: $\epsilon_t = \frac{\sum w_i \cdot I(y_i \neq h_t(x_i))}{\sum w_i}$
    3. Compute tree weight: $\alpha_t = \frac{0.5 \cdot ln(1 - \epsilon_t)}{\epsilon_t}$
    4. Update sample weights: $w_i \leftarrow w_i \cdot exp(-\alpha_t \cdot y_i \cdot h_t(x_i))$ (Normalize so weights sum to 1)
- Final prediction: $H(x) = sign(\sum \alpha_t \cdot h_t(x))$

AdaBoost - Adaptive Boosting

- Intuition Behind the Updates
  - Tree weight α_t :
    - If error ϵ_t = 0.5 (random):
      - α_t = 0 (ignore this tree)
    - If error $\epsilon_t \to 0$ (perfect):
      - $\alpha_t \to \infty$ (trust this tree completely)
    - If error $\epsilon_t \to 1$ (anti-correlated)
      - $\alpha_t \to -\infty$ (flip its predictions)

$$\epsilon_t = \frac{\sum w_i \cdot I(y_i \neq h_t(x_i))}{\sum w_i}$$

$$\alpha_t = \frac{0.5 \cdot ln(1 - \epsilon_t)}{\epsilon_t}$$

When to use what?

Random Forest

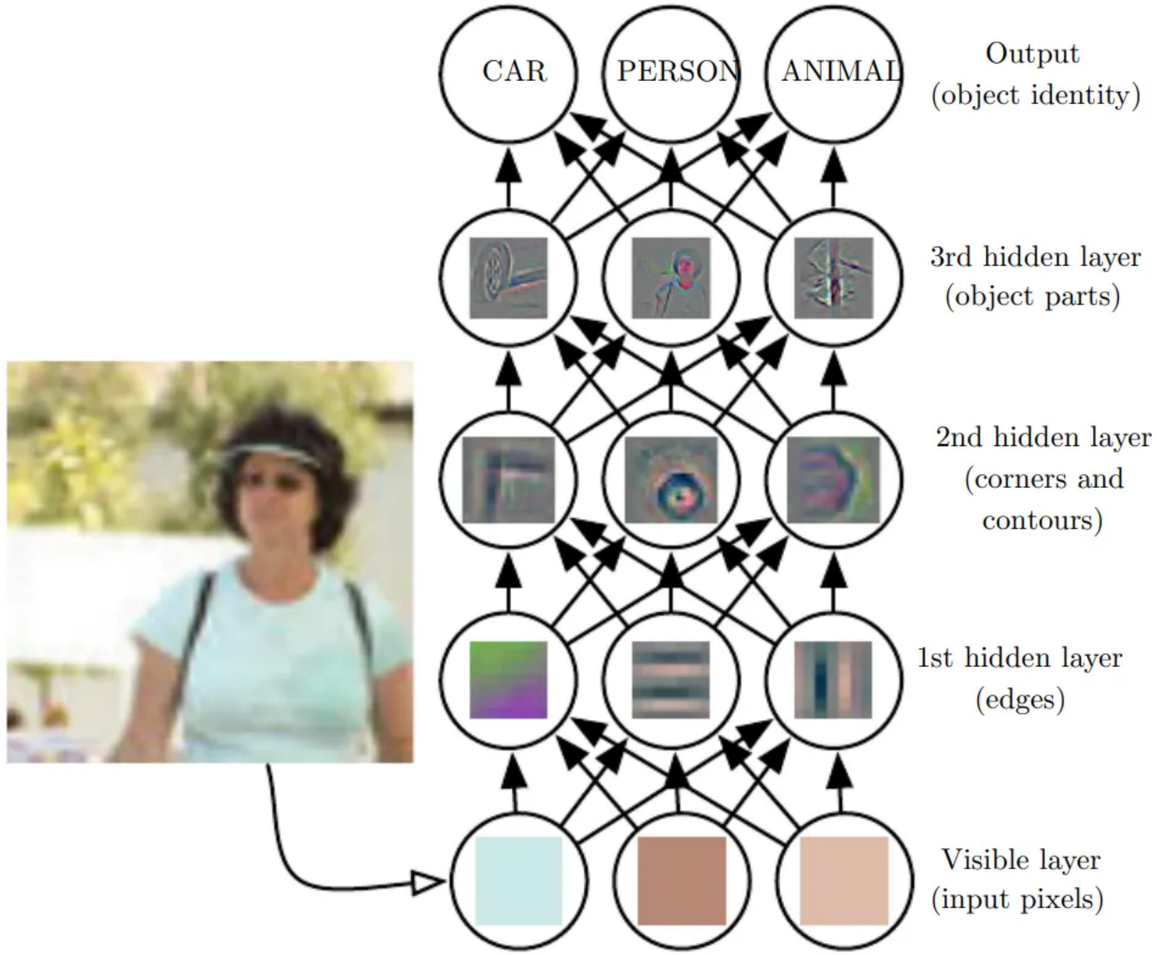
- Good default choice
- When interpretability (feature importance) matters
- When you want robustness without tuning
- When you have noisy labels

Gradient Boosting
(XGBoost / LightGBM / CatBoost)

- When you need maximum accuracy
- Structured/tabular data competitions
- When you have time to tune hyperparameters
- When training data is clean

Deep Learning

- Why is deep learning needed?
  - Learnable transformations of data
- Limitations of Linear Models - can only learn **linear** decision boundaries



Deep Learning

Composing Functions

Solution: Add **non-linearity** between compositions

$$h = \sigma(W_1 x + b_1)$$

$$\hat{y} = W_2 h + b_2$$

Deep Learning

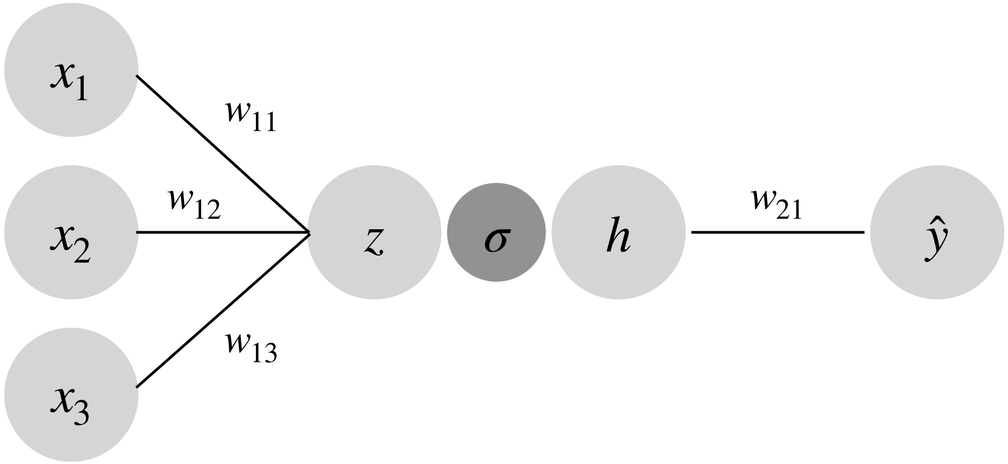
Composing Functions

$$x = [x_1 \quad x_2 \quad x_3]$$

$$h = \sigma(W_1 x + b_1)$$

$$W_1 = \begin{bmatrix} w_{11} \\ w_{12} \\ w_{13} \end{bmatrix} \quad W_2 = [w_{21}]$$

$$\hat{y} = W_2 h + b_2$$



Deep Learning

Composing Functions

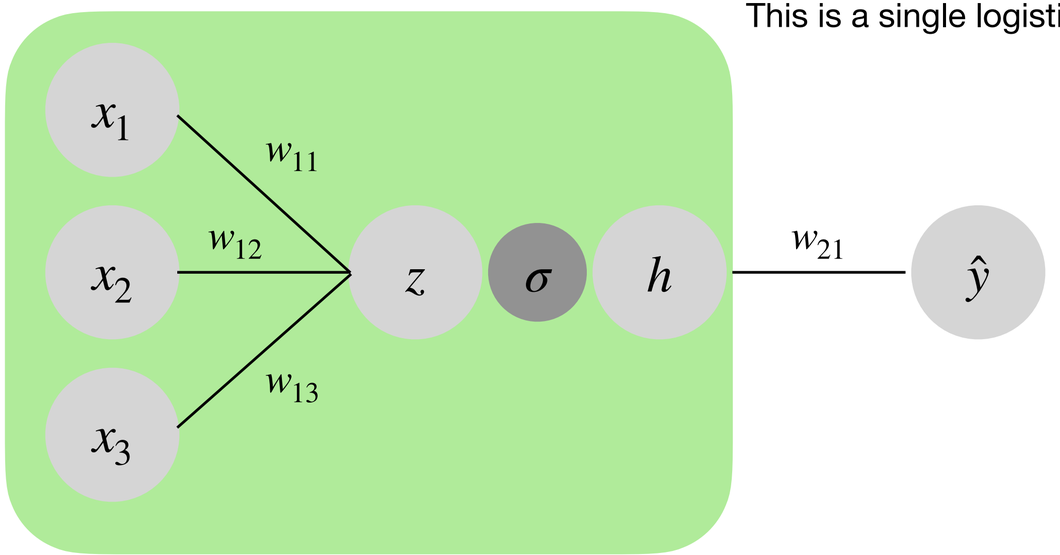
$$x = [x_1 \quad x_2 \quad x_3]$$

$$h = \sigma(W_1 x + b_1)$$

$$W_1 = \begin{bmatrix} w_{11} \\ w_{12} \\ w_{13} \end{bmatrix} \quad W_2 = [w_{21}]$$

$$\hat{y} = W_2 h + b_2$$

This is a single logistic regression unit



Deep Learning

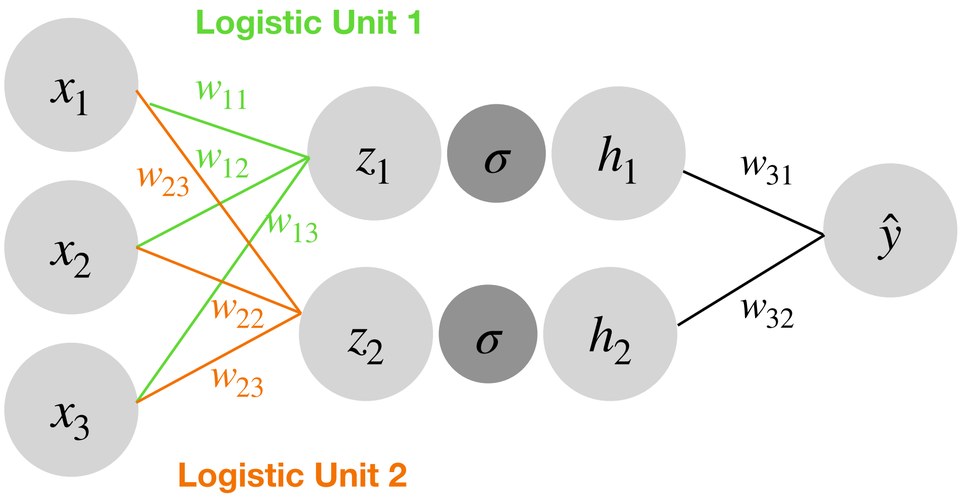
Composing Functions

$$x = [x_1 \quad x_2 \quad x_3]$$

$$h = \sigma(W_1 x + b_1)$$

$$W_1 = \begin{bmatrix} w_{11} & w_{21} \\ w_{12} & w_{22} \\ w_{13} & w_{23} \end{bmatrix} \qquad W_2 = \begin{bmatrix} w_{31} \\ w_{32} \end{bmatrix}$$

$$\hat{y} = W_2 h + b_2$$



Deep Learning

Composing Functions

$$x = [x_1 \quad x_2 \quad x_3]$$

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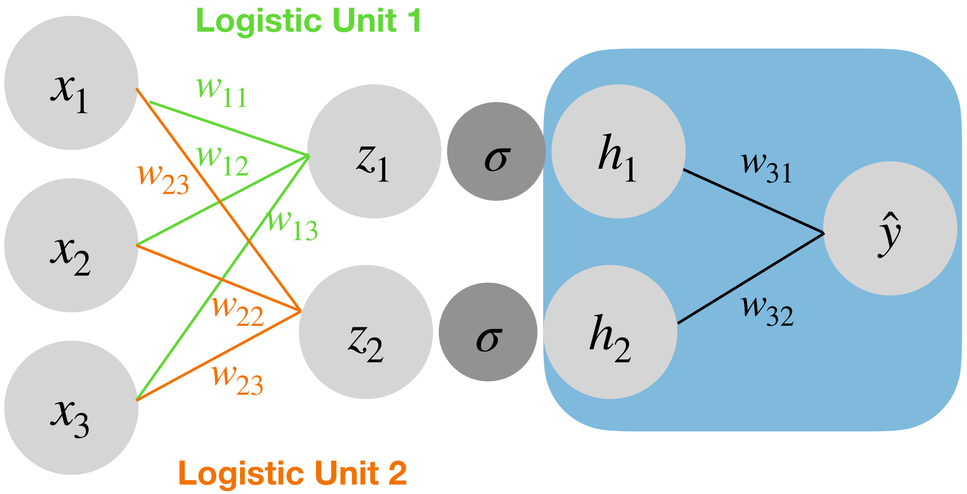
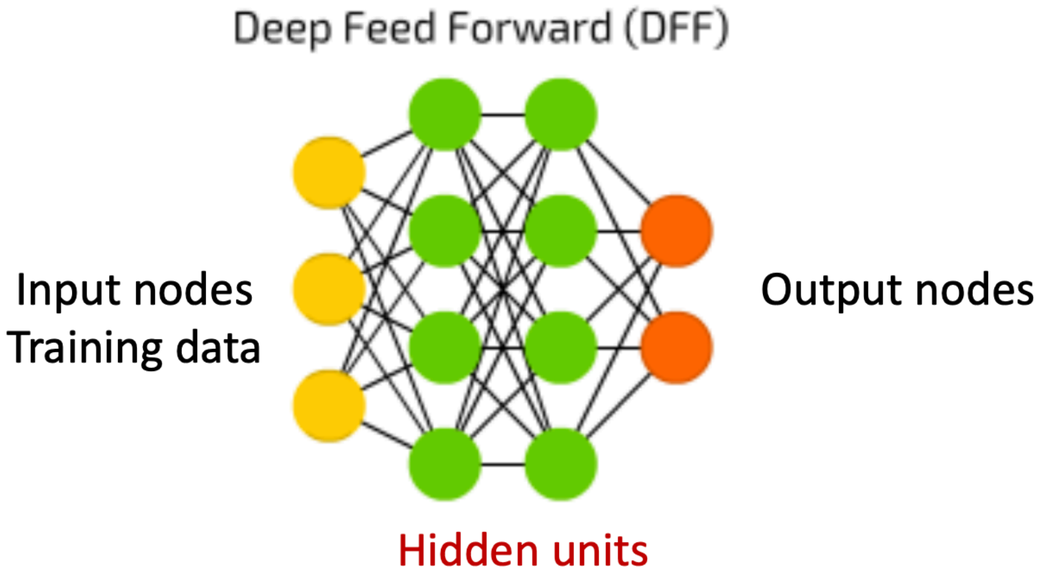


This is also a Logistic Unit!
It takes as **input** the outputs of the previous layer

Deep Learning

Neural Networks



- Each link has a weight
- Each hidden unit has an activation function
- Training data is input in the left, output is generated on the right

Deep Learning

Multi Layer Perceptron (MLP)

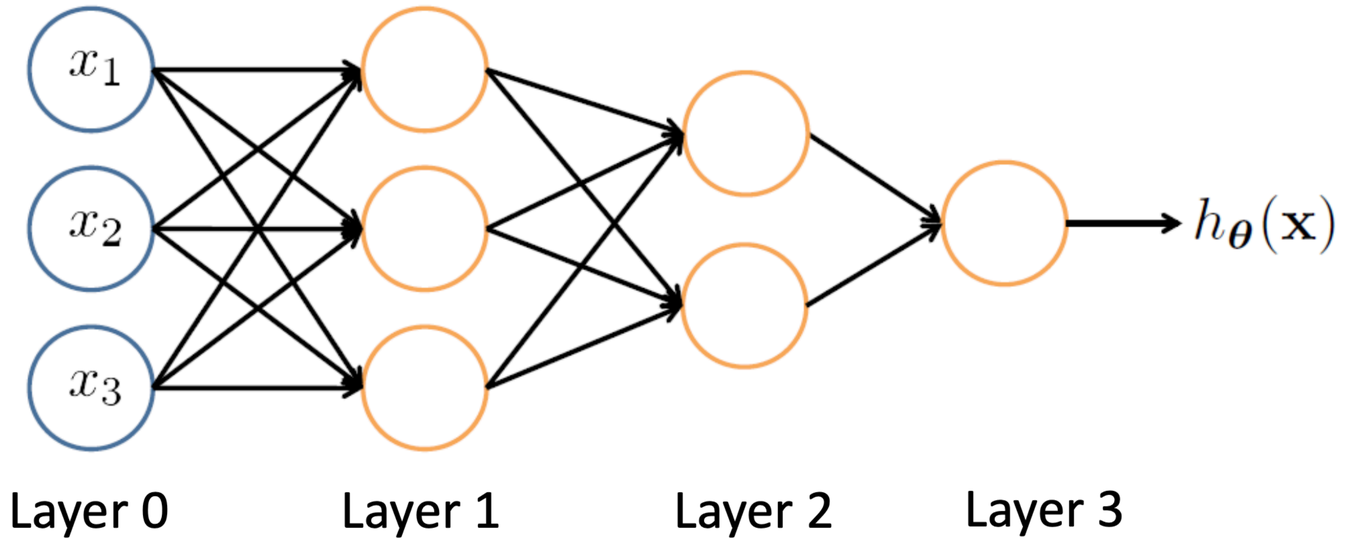
Number of layers L = 3

Computation:

$a^{[0]} = x$ (input)
For each layer $l = 1,2,...L$:

$z^{[l]} = W^{[l]}a^{[l-1]} + b^{[l]}$ (linear transform)
$a^{[l]} = \sigma^{[l]}(z^{[l]})$ (activation)

Final Output: $h_\theta(x) = \hat{y} = a^{[L]}$



Deep Learning

Activation Functions

- Why Activation Functions Matter
  - Introduce non-linearity (**essential for learning complex patterns**)
  - Control the range of outputs
  - Affect gradient flow during training

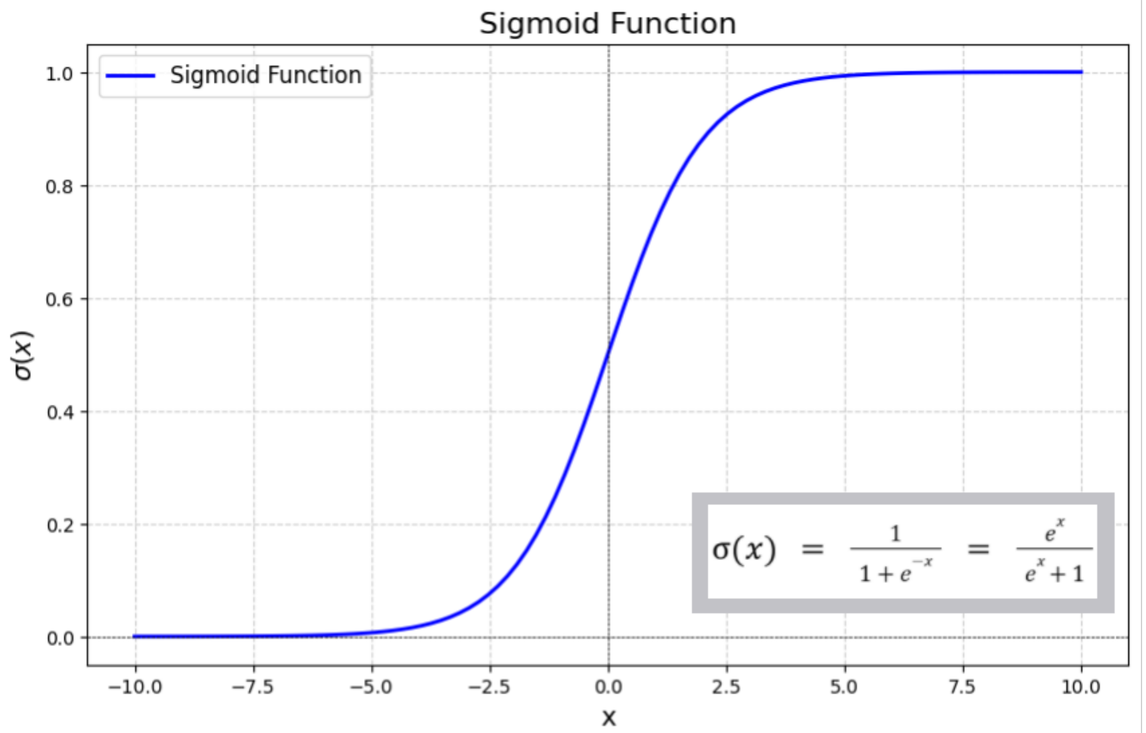
Deep Learning

Activation Functions

- Sigmoid Function

$$\sigma(x) = \frac{1}{1 + e^{-x}}$$

Range: [0, 1]



Pros: Smooth, bounded, interpretable as probability

Cons: Vanishing gradients (saturates at extremes), not zero-centered, expensive exponential operation. Slow due to exponentiation operation.

Use: Output layer for binary classification

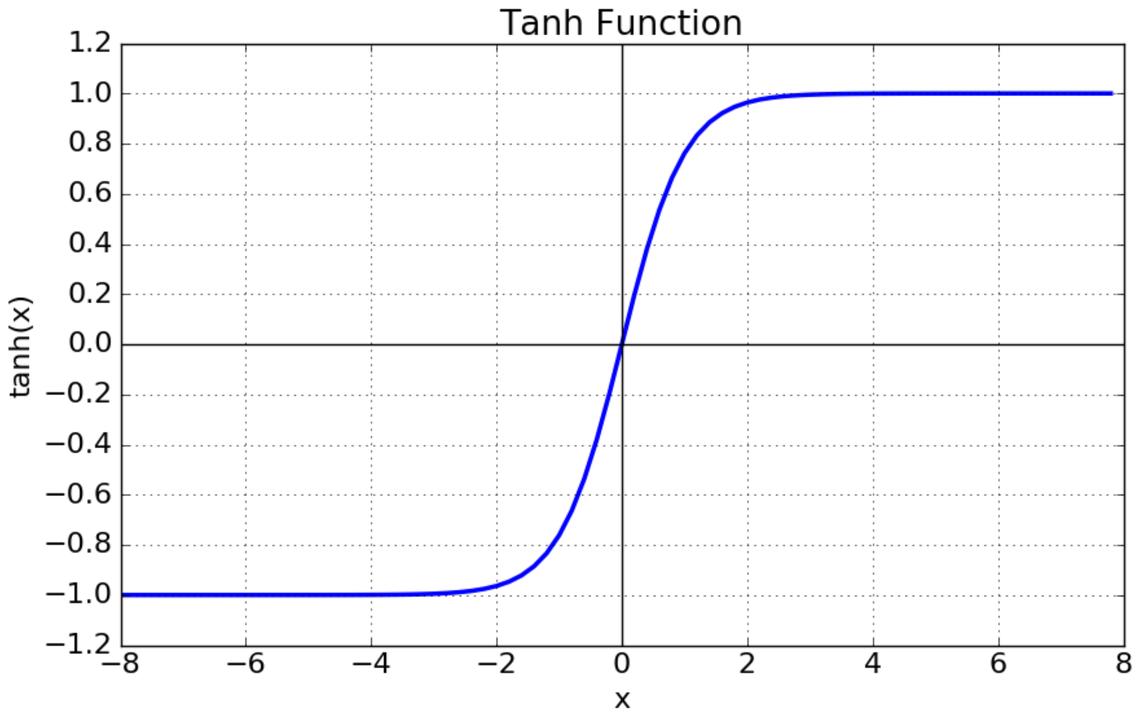
Deep Learning

Activation Functions

- Tanh Function

$$\tanh(x) = \frac{e^{x} - e^{-x}}{e^{x} + e^{-x}}$$

Range: [-1, 1]



Pros: Zero-centered (better than sigmoid), stronger gradients

Cons: Still has vanishing gradient problem. Slow due to exponentiation operation.

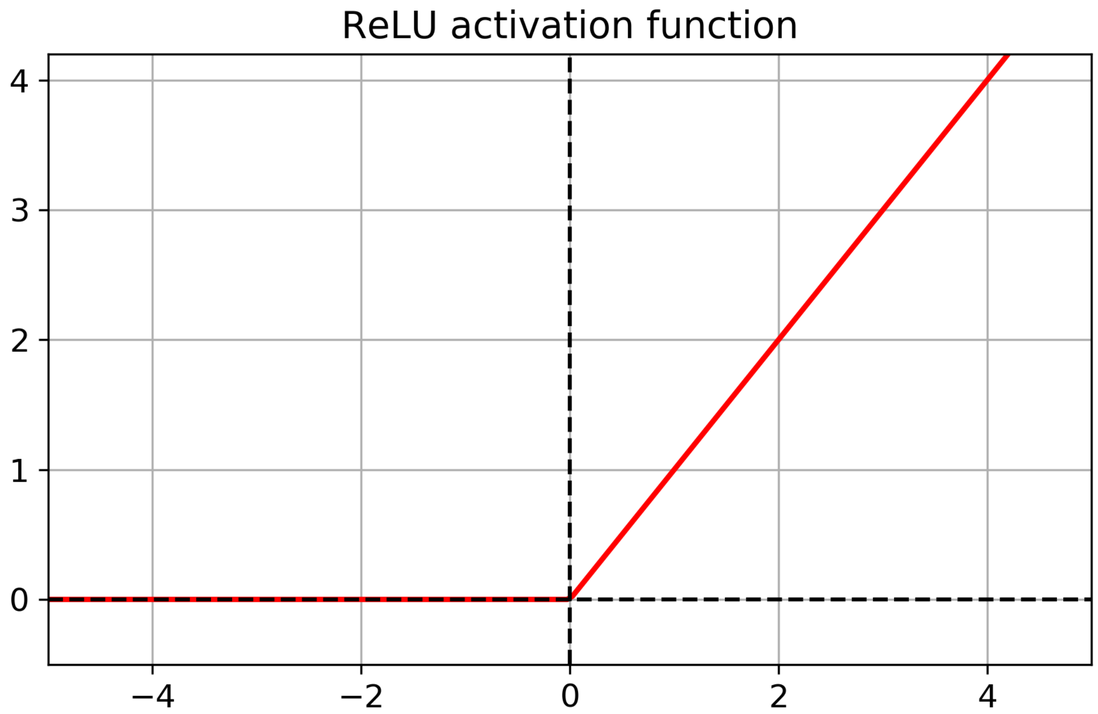
Use: Hidden layers (historically), RNNs

Deep Learning

Activation Functions

- ReLU Function (Rectified Linear Unit)

$$ReLU(x) = max(0,\ x) = \begin{cases} x & x > 0 \\ 0 & x \leq 0 \end{cases}$$



Range: [0, ∞)

Pros: No vanishing gradient (for x > 0), computationally efficient, sparse activation

Cons: “Dying ReLU” problem (neurons stuck at 0), not zero-centered

Use: Default for hidden layers in most networks

Deep Learning

Activation Functions

- Leaky ReLU Function

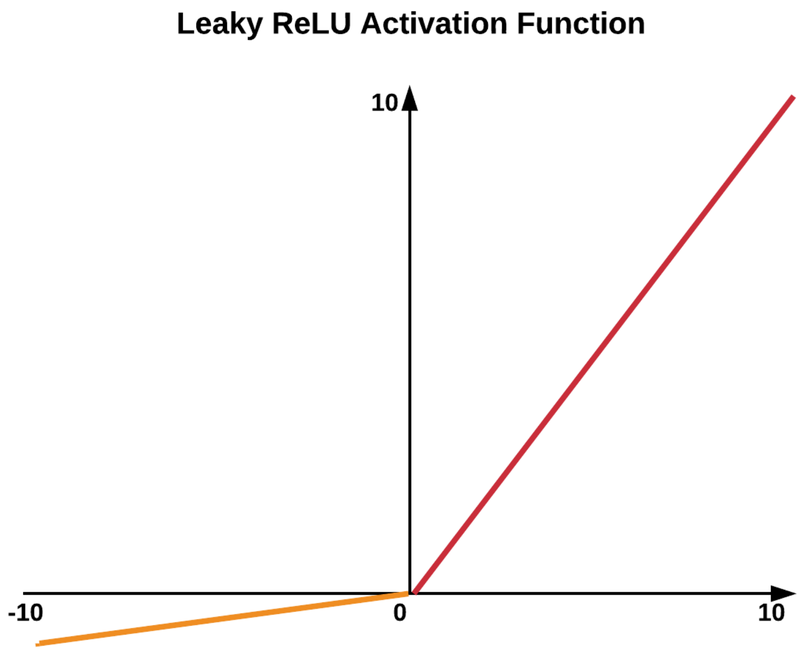
$$ReLU(x) = \begin{cases} x & x > 0 \\ \alpha x & x \leq 0 \end{cases}$$

Range: $(-\infty, \infty)$

Pros: Prevents dying ReLU

Cons: Extra hyperparameter $(\alpha = 0.01)$

Use: Default for hidden layers in most networks



Deep Learning

Activation Functions

- Softmax (**Output** Layer)

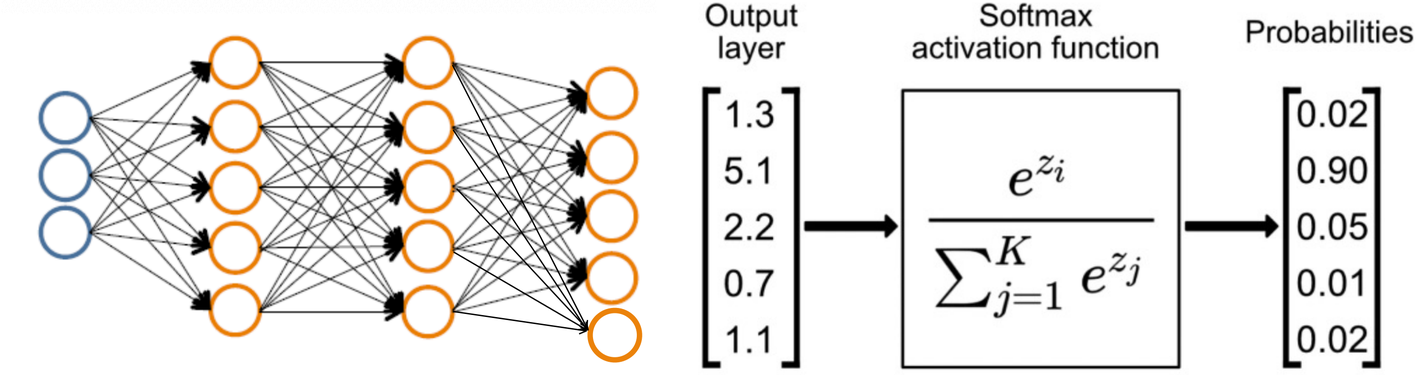
$$softmax(x)_k = \frac{e^{x_k}}{\sum_{j=1}^{K} e^{x_j}}$$

If we have multi-class probability, what loss function can we use?

Categorical Cross Entropy Loss:

$$\ell_\theta(x) = -\frac{1}{N}\sum_{i=1}^{N}\sum_{k=1}^{K} y_{ik} log(\hat{y}_{ik})$$

Output: Probability distribution over K classes (sums to 1)



Deep Learning
Activation Functions

If we have multi-class probability, what loss function can we use?

Categorical Cross Entropy Loss:

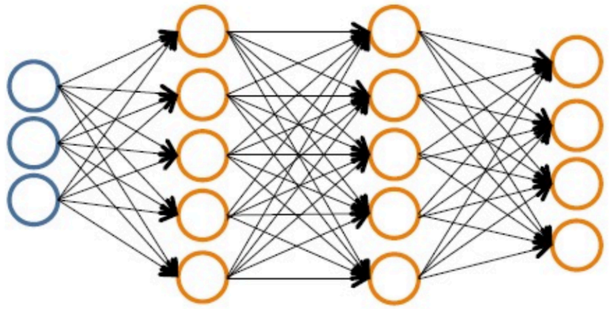
$$\ell_\theta(x) = -\frac{1}{N}\sum_{i=1}^{N}\sum_{k=1}^{K} y_{ik} log(\hat{y}_{ik})$$


Pedestrian


Car


Motorcycle


Truck



$$h_\Theta(\mathbf{x}) \in \mathbb{R}^K$$

We want:

$$h_\Theta(\mathbf{x}) \approx \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$
when pedestrian

$$h_\Theta(\mathbf{x}) \approx \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$$
when car

$$h_\Theta(\mathbf{x}) \approx \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}$$
when motorcycle

$$h_\Theta(\mathbf{x}) \approx \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$
when truck

Deep Learning
Weight Initialization

- Poor initialization causes:
  - **Vanishing signals**: Activations shrink to zero through layers
  - **Exploding signals**: Activations grow unboundedly
  - **Symmetry**: If all weights are equal, all neurons compute the same thing
    - **All Zeros**
      - Problem: All neurons compute the same thing. Gradients are identical. Symmetry is never broken. Network cannot learn.
    - **All Same Value**
      - Same problem as zeros - symmetry is not broken.

Deep Learning

Regularization

- Deep networks have **millions** of parameters - they can **memorize** training data.
- We need regularization to improve generalization.

Deep Learning

Regularization

- L_2 Regularization
  - Add penalty on weight magnitude to loss

$$L_\theta(x) = L_\theta(x) + \lambda \sum_l \|W^{[l]}\|_F^2$$

  - **Effect**: Pushes weights toward zero, preferring simpler models.

Deep Learning

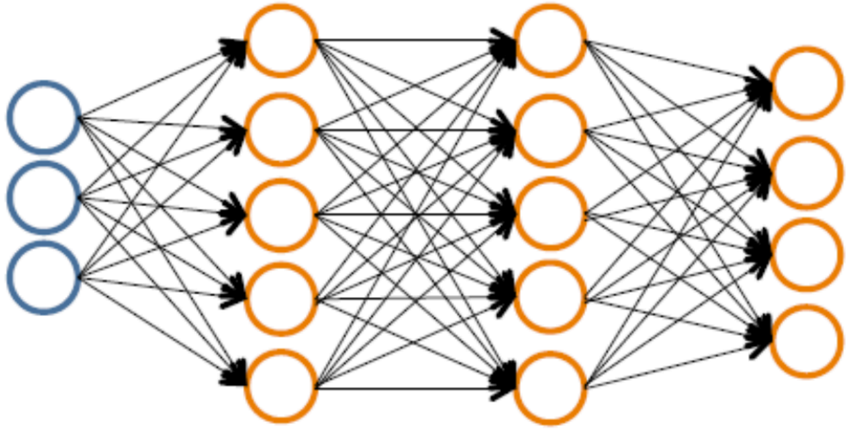
Regularization

- L_1 Regularization
  - Add penalty on weight magnitude to loss

$$L_\theta(x) = L_\theta(x) + \lambda \sum_l \|W^{[l]}\|_1$$

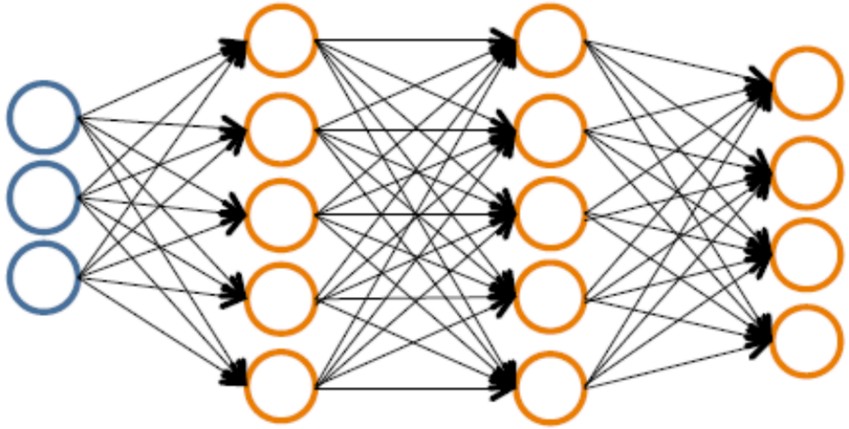
  - **Effect**: Encourages **sparsity** (many weights become exactly zero)

Deep Learning
Regularization



- Dropout Regularization
  - During training: randomly set activations to zero with probability p
  - During inference: Use all neurons, no dropout
  - **Intuition:**
    - Forces network to not rely on any single neuron
    - Approximately trains an ensemble of 2^n sub-networks
    - Prevents **co-adaptation** of neurons

Deep Learning
Regularization



- Batch Normalization
  - Normalize **activations** within each mini-batch

$$\hat{z} = \frac{z - \mu_B}{\sqrt{\sigma_B^2}}$$

$$\tilde{z} = \gamma \cdot \hat{z} + \beta$$

  - **Benefits**:
    - Reduces internal covariate shift
    - Allows higher learning rates
    - Acts as regularization (noise from batch statistics)
    - Reduces sensitivity to initialization

Deep Learning

Backpropagation

Layer 1 (Hidden Layer):

$$z^{[1]} = W^{[1]}x + b^{[1]}$$
$$a^{[1]} = \text{ReLU}(z^{[1]})$$

Layer 2 (Output Layer):

$$z^{[2]} = W^{[2]}a^{[1]} + b^{[2]}$$
$$\hat{y} = \sigma(z^{[2]})$$

Loss Function: $L = -\left[y \log \hat{y} + (1-y)\log(1-\hat{y})\right]$

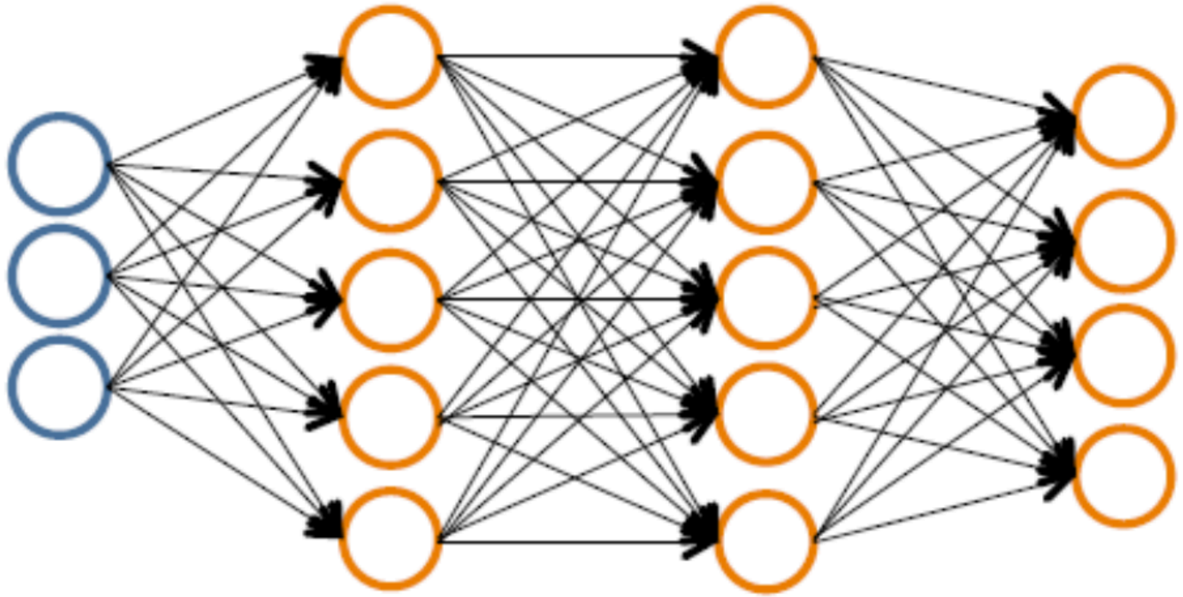
Forward Pass: Compute and store all intermediate values:

$$x \xrightarrow{W^{[1]},b^{[1]}} z^{[1]} \xrightarrow{\text{ReLU}} a^{[1]} \xrightarrow{W^{[2]},b^{[2]}} z^{[2]} \xrightarrow{\sigma} \hat{y} \to L$$

Deep Learning

Backpropagation

1. Forward Propagation



2. Backward Propagation

3. ?

Equations –

$$z^{[1]} = w^{[1]} a^{[0]} + b^{[1]}$$

$(2 \times 4) \times (4 \times m)$

$$a^{[1]} = \sigma(z^{[1]})$$

$(2 \times m)$

$$z^{[2]} = w^{[2]} a^{[1]} + b^{[2]}$$

$(1 \times 2) \times (2 \times m)$

$$a^{[2]} = \sigma(z^{[2]})$$

$(1 \times m)$

$$\mathcal{L} = \frac{1}{2}(y - \hat{y})^2$$

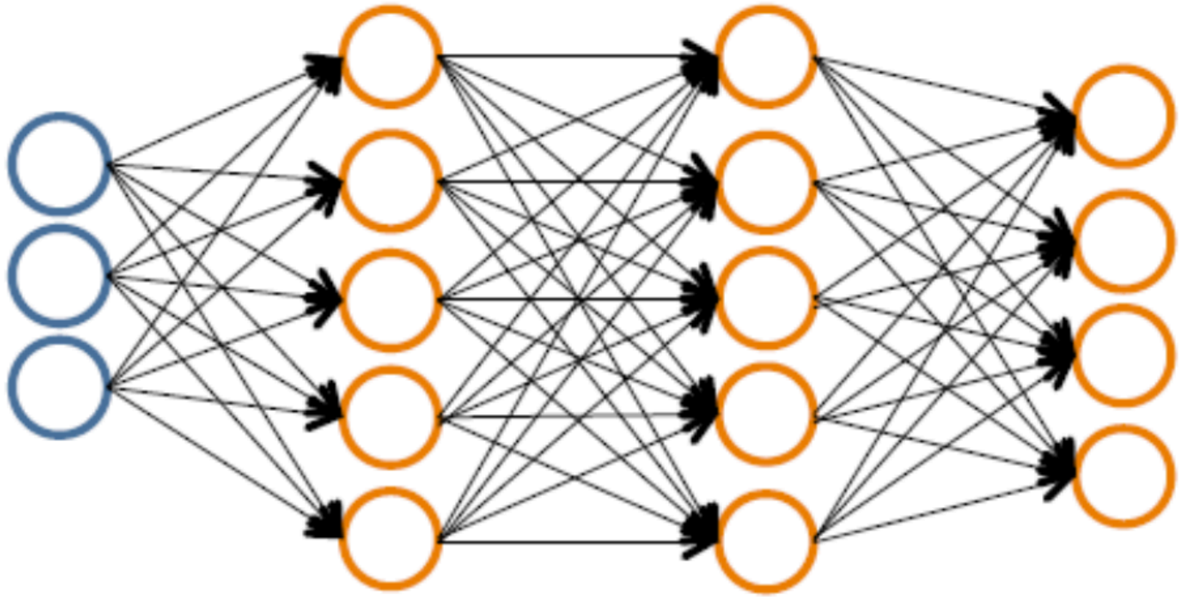
Final Equations –

$$da^{[2]} = a^{[2]} - y$$
$$dz^{[2]} = da^{[2]} \, g'(z^{[2]})$$
$$dw^{[2]} = dz^{[2]} \, a^{[1]}$$
$$da^{[1]} = dz^{[2]} \, w^{[2]}$$
$$dz^{[1]} = da^{[1]} \, g'(z^{[1]})$$
$$dw^{[1]} = dz^{[1]} \, a^{[0]}$$

Deep Learning

Backpropagation

1. Forward Propagation



2. Backward Propagation

3. Update Weights - Gradient Descent

Equations -

$$z^{[1]} = w^{[1]} a^{[0]} + b^{[1]}$$

$(2 \times 4) \times (4 \times m)$

$$a^{[1]} = \sigma(z^{[1]})$$

$(2 \times m)$

$$z^{[2]} = w^{[2]} a^{[1]} + b^{[2]}$$

$(1 \times 2) \times (2 \times m)$

$$a^{[2]} = \sigma(z^{[2]})$$

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$$\mathcal{L} = \frac{1}{2}(y - \hat{y})^2$$

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Convolutional Neural Networks

- An image is represented as a grid of pixel values
- Lets say this image os 224x224 RGB image
  - ~ 150 million parameters in the first layer alone
  - Why is this a problem?
    - **Too many parameters**: Overfitting, memory issues
    - **No spatial structure**: Flattening destroys 2D relationships
    - **No translation invariance**: A cat in the corner vs. center looks completely different to an MLP

Convolutional Neural Networks

- CNNs exploit these insights through:
  - **Local receptive fields**: Each neuron sees only a small region
  - **Weight sharing:** Same detector (filter) applied across entire image
  - **Pooling:** Reduces spatial dimensions, adds invariance

Convolutional Neural Networks

- 2D filters “slide” over the entire dataset
- Each filter learns something about the data

Convolutional Neural Networks

$$\begin{bmatrix} -1 & 0 & 1 \\ -1 & 0 & 1 \\ -1 & 0 & 1 \end{bmatrix}$$ — Vertical Edge Filter

$$\begin{bmatrix} 10 & 10 & 10 & 0 & 0 & 0 \\ 10 & 10 & 10 & 0 & 0 & 0 \\ 10 & 10 & 10 & 0 & 0 & 0 \\ 10 & 10 & 10 & 0 & 0 & 0 \\ 10 & 10 & 10 & 0 & 0 & 0 \\ 10 & 10 & 10 & 0 & 0 & 0 \end{bmatrix} * \begin{bmatrix} -1 & 0 & 1 \\ -1 & 0 & 1 \\ -1 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 0 & -30 & -30 & 0 \\ 0 & -30 & -30 & 0 \\ 0 & -30 & -30 & 0 \end{bmatrix}$$

Convolutional Neural Networks

$$\begin{bmatrix} -1 & 0 & 1 \\ -1 & 0 & 1 \\ -1 & 0 & 1 \end{bmatrix}$$ — Vertical Edge Filter

$$\frac{1}{9}\begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}$$ — Blur (Averaging)

$$\begin{bmatrix} -1 & -1 & -1 \\ 0 & 0 & 0 \\ 1 & 1 & 1 \end{bmatrix}$$ — Horizontal Edge Filter

$$\begin{bmatrix} 0 & -1 & 0 \\ -1 & 5 & -1 \\ 0 & -1 & 0 \end{bmatrix}$$ — Sharpen

Convolutional Neural Networks

- Key idea of CNNs - **learn filter values** rather than hand designing them
- A convolutional layer has **multiple filters**, each producing one output channel (feature map).
- Instead of having a fixed vertical edge filter like

$$\begin{bmatrix} -1 & 0 & 1 \\ -1 & 0 & 1 \\ -1 & 0 & 1 \end{bmatrix}$$

- You learn filters like

$$\begin{bmatrix} \theta_{10} & \theta_{11} & \theta_{12} \\ \theta_{13} & \theta_{14} & \theta_{15} \\ \theta_{16} & \theta_{17} & \theta_{18} \end{bmatrix}$$

Convolutional Neural Networks

- Key idea of CNNs - **learn filter values** rather than hand designing them
- A convolutional layer has **multiple filters**, each producing one output channel (feature map).
- Instead of having a fixed vertical edge filter like

$$\begin{bmatrix} -1 & 0 & 1 \\ -1 & 0 & 1 \\ -1 & 0 & 1 \end{bmatrix}$$

- You learn filters like

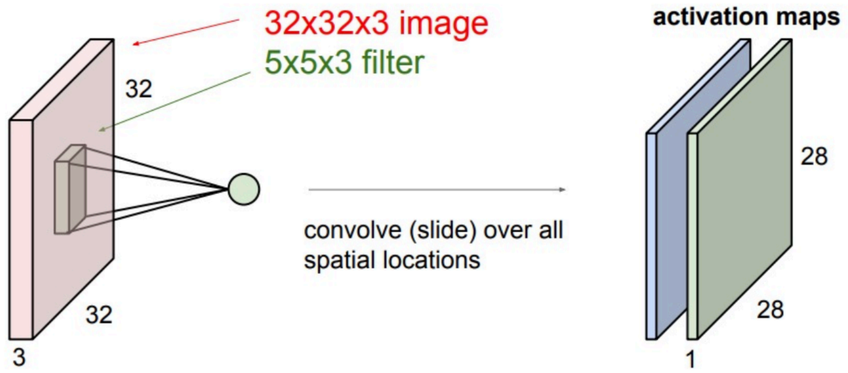
$$\text{Filter 1: } \begin{bmatrix} \theta_{10} & \theta_{11} & \theta_{12} \\ \theta_{13} & \theta_{14} & \theta_{15} \\ \theta_{16} & \theta_{17} & \theta_{18} \end{bmatrix} \quad \text{Filter 2: } \begin{bmatrix} \theta_{20} & \theta_{21} & \theta_{22} \\ \theta_{23} & \theta_{24} & \theta_{25} \\ \theta_{26} & \theta_{27} & \theta_{28} \end{bmatrix}$$

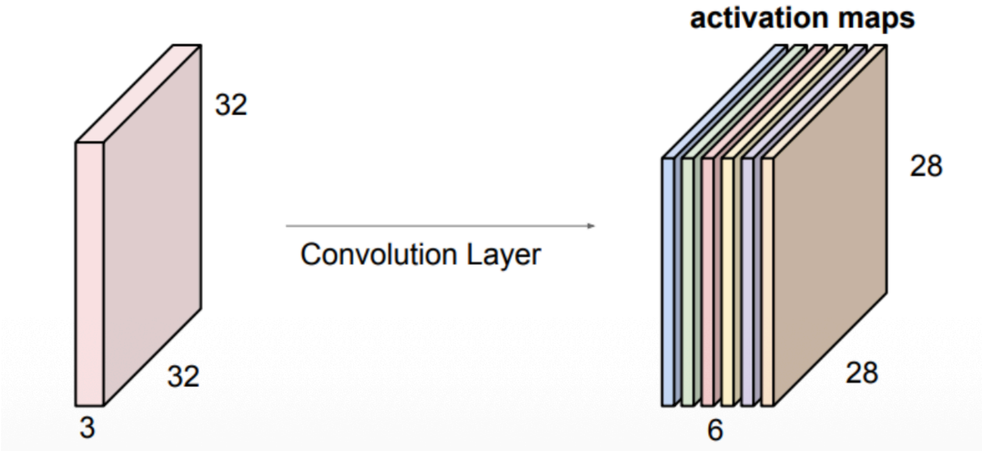
Convolutional Neural Networks

- Key idea of CNNs - **learn filter values** rather than hand designing them
- A convolutional layer has **multiple filters**, each producing one output channel (feature map).
- Input: $H_{in} \times W_{in} \times C_{in}$ (height x width x channels)
- Output: $H_{out} \times W_{out} \times C_{out}$ (one channel per filter)
- Each filter has shape $k \times k \times C_{in}$

Convolutional Neural Networks

- Input: $H_{in} \times W_{in} \times C_{in}$ (height x width x channels)
- Output: $H_{out} \times W_{out} \times C_{out}$ (one channel per filter)
- Each filter has shape $k \times k \times C_{in}$
- **Example**
  - Input Image: $32 \times 32 \times 3$ (RGB Image), 6 filters
  - Each filter: $5 \times 5 \times 3 = 75$ parameters
  - Output Shape: $28 \times 28 \times 6$ (why 28?)
  - Total parameters = 75 x 6 = 450, compared to 32 x 32 x 3 x 1000 = 3M parameters for MLP





Convolutional Neural Networks

Stride and Padding

- Output Shape: $28 \times 28 \times 16$ (why 28?)
- Stride captures how many pixels the filter moves each step

Stride = 2

$$\begin{bmatrix} 10 & 10 & 10 & 0 & 0 & 0 \\ 10 & 10 & 10 & 0 & 0 & 0 \\ 10 & 10 & 10 & 0 & 0 & 0 \\ 10 & 10 & 10 & 0 & 0 & 0 \\ 10 & 10 & 10 & 0 & 0 & 0 \\ 10 & 10 & 10 & 0 & 0 & 0 \end{bmatrix} * \begin{bmatrix} -1 & 0 & 1 \\ -1 & 0 & 1 \\ -1 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 0 & 30 & -30 & 0 \\ 0 & 30 & -30 & 0 \\ 0 & 30 & -30 & 0 \end{bmatrix}$$

Convolutional Neural Networks

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Convolutional Neural Networks

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Stride = 2

Next Stride?

Convolutional Neural Networks

Stride and Padding

- Output Shape: $28 \times 28 \times 16$ (why 28?)
- Stride captures how many pixels the filter moves each step

$$\begin{bmatrix} 0 & 10 & 10 & 10 & 0 & 0 & 0 & 0 \\ 0 & 10 & 10 & 10 & 0 & 0 & 0 & 0 \\ 0 & 10 & 10 & 10 & 0 & 0 & 0 & 0 \\ 0 & 10 & 10 & 10 & 0 & 0 & 0 & 0 \\ 0 & 10 & 10 & 10 & 0 & 0 & 0 & 0 \\ 0 & 10 & 10 & 10 & 0 & 0 & 0 & 0 \end{bmatrix} * \begin{bmatrix} -1 & 0 & 1 \\ -1 & 0 & 1 \\ -1 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 0 & 30 & -30 & 0 \\ 0 & 30 & -30 & 0 \\ 0 & 30 & -30 & 0 \end{bmatrix}$$

Stride = 2

Padding

Convolutional Neural Networks

Stride and Padding

- Output Shape: $28 \times 28 \times 16$ (why 28?)
- Stride captures how many pixels the filter moves each step
- Stride and padding change the shape of the output matrix
- With no padding, input size n, filter size k and stride s :
  - Output Size = $\lfloor \frac{n-k}{s} \rfloor + 1$
- With padding p:
  - Output Size = $\lfloor \frac{n+2p-k}{s} \rfloor + 1$

Convolutional Neural Networks

Pooling

- Pooling reduces spatial dimensions, providing:
  - Translation invariance
  - Reduced computation
  - Larger receptive field
- Example - **Max** Pool = (3x3) with stride = 3

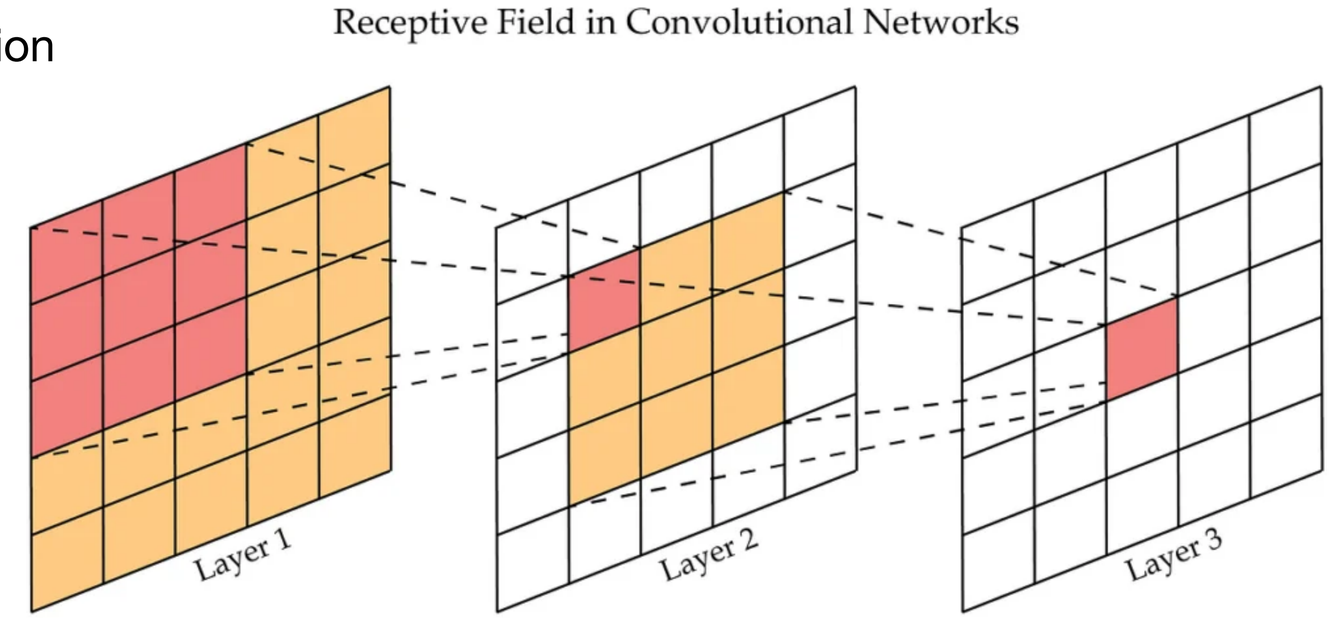
$$\begin{bmatrix} 10 & 10 & 10 & 0 & 0 & 0 \\ 10 & 10 & 10 & 0 & 0 & 0 \\ 10 & 10 & 10 & 0 & 0 & 0 \\ 10 & 10 & 10 & 0 & 0 & 0 \\ 10 & 10 & 10 & 0 & 0 & 0 \\ 10 & 10 & 10 & 0 & 0 & 0 \end{bmatrix} \rightarrow \begin{bmatrix} 10 & 0 \\ 10 & 0 \end{bmatrix}$$

Convolutional Neural Networks

Pooling

- The receptive field is the **region of the input** that influences a particular output neuron.
- With stacking, receptive fields grow:
  - Layer 1 (3×3 filter): Each filter sees 3×3 input region
  - Layer 2 (3×3 filter): Each filter sees 5×5 input region
  - Layer 3 (3×3 filter): Each filter sees 7×7 input region

$$\begin{bmatrix} 1 & 10 & 1 & 0 & 1 & 0 \\ 1 & 10 & 1 & 0 & 1 & 0 \\ 1 & 10 & 1 & 0 & 1 & 0 \\ 10 & 0 & 0 & 1 & 0 & 0 \\ 10 & 0 & 0 & 1 & 0 & 0 \\ 10 & 0 & 0 & 1 & 0 & 0 \end{bmatrix} \rightarrow \begin{bmatrix} 4 & 0.3 \\ 3.3 & 0.3 \end{bmatrix}$$



Dimensionality Reduction

Metric	PCA	t-SNE	UMAP
Type	Linear	Non-Linear	Non-Linear
Preserves	Global Variance	Local Neighborhoods	Local + Global
Speed	Very Fast	Slow	Fast
Deterministic	Yes	No	Consistent but not deterministic
Interpretable	Somewhat	No	No
New Data	Yes	No	Yes
Use Cases	Preprocessing, quick visualization	Visualization	Visualization

Principal Component Analysis (PCA)

Motivation

- PCA finds new axes (principal components) such that:
  - PC1: Direction of maximum variance
  - PC2: Direction of maximum remaining variance, **orthogonal** to PC1
  - PC3: Direction of maximum remaining variance, **orthogonal to PC1 and PC2**

Principal Component Analysis (PCA)

Formulation

- **Goal:** Find a linear transformation that projects data onto directions of maximum variance.
- Given data matrix $X \in \mathbb{R}^{n \times d}$ (n samples, d features)
  - Compute covariance matrix

$$C = \frac{1}{n-1} X^T X$$

  - Compute Eigen-decomposition of C

$$Cv_i = \lambda_i v_i$$

Principal Component Analysis (PCA)

Formulation

- Given data matrix $X \in \mathbb{R}^{n \times d}$ (n samples, d features)
  - Compute covariance matrix

$$C = \frac{1}{n-1} X^T X$$

  - Compute Eigen-decomposition of C

$$Cv_i = \lambda_i v_i$$

  - Sort Eigenvalues $\lambda_1 \geq \lambda_2 \ldots \geq \lambda_n$
  - Project into generated dimensions

$$Z = XW_k \text{ where } W_k = [v_1, v_2, \ldots v_k]$$

Principal Component Analysis (PCA)

Features, Pros and Cons

- Always make sure to normalize input features (say mean-variance normalization)
  - Without normalization: Features with larger variance dominate
  - With normalization: All features contribute equally

- Pros:
  - Multicollinearity Handling: Creates new, uncorrelated variables to address issues when **original features are highly correlated**.
  - Noise Reduction: Eliminates components with low variance
  - Data Compression: Represents data with fewer components reduce storage needs and speeding up processing.
  - Outlier Detection: Identifies unusual data points by showing which ones deviate significantly in the reduced space.

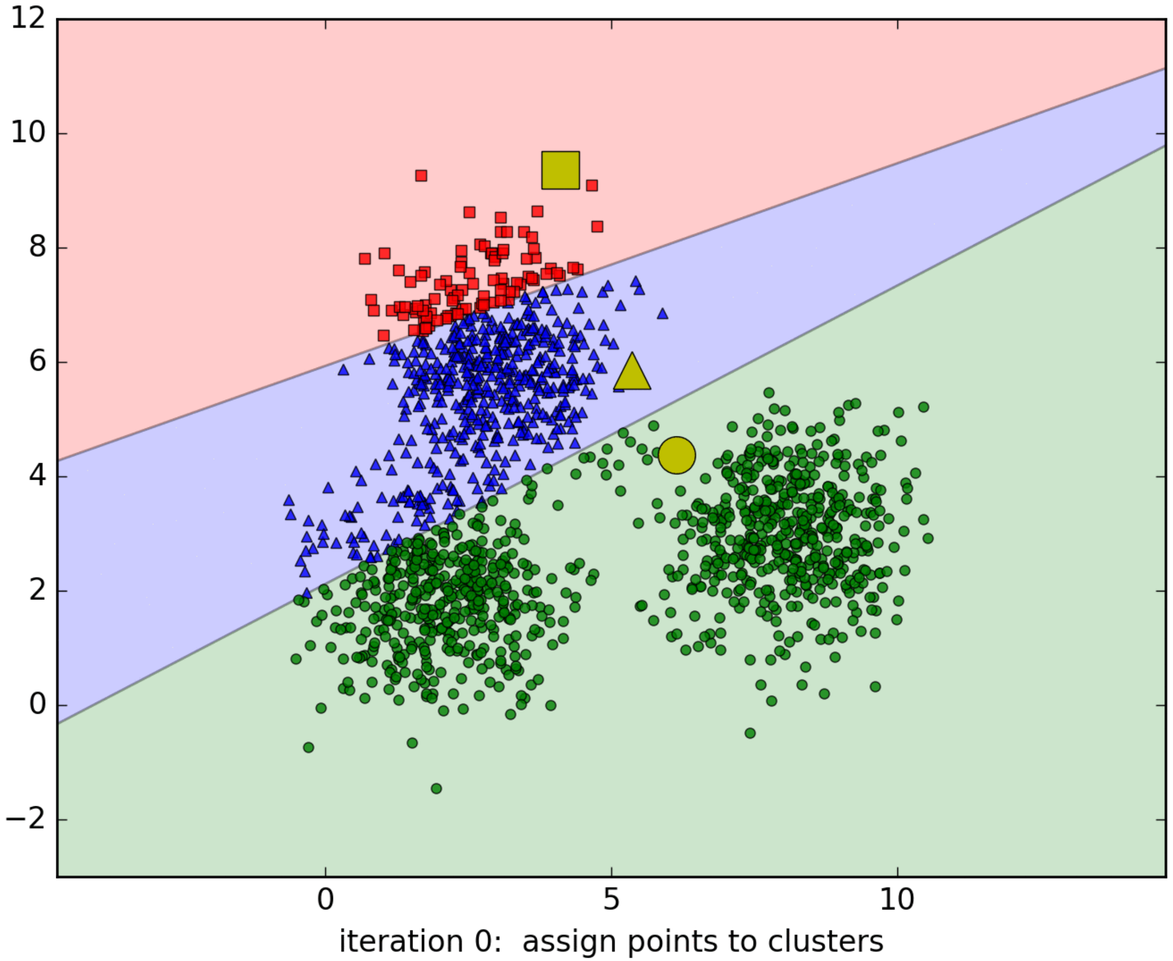
- Cons:
  - Assumes linear relationships, can't capture non-linear structure
  - Maximum variance direction may not be most informative - variance $\neq$ importance
  - Outliers can dominate variance
  - Lack of interpretability - PCs are mixtures of original features

Clustering

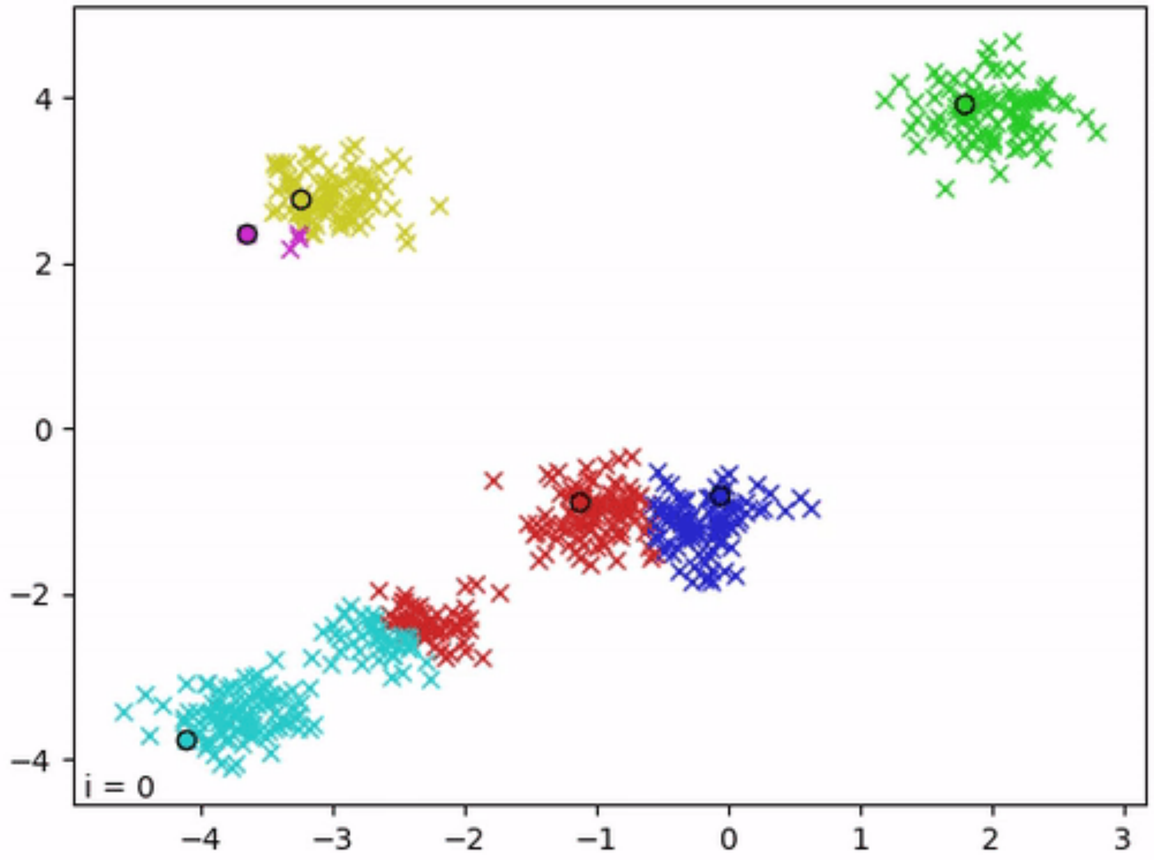
- **Goal:** Partition data into groups (clusters) such that:
  - Points within a cluster are similar
  - Points in different clusters are dissimilar
  - Unlike classification, **clusters are discovered**, not predefined.

Clustering

K-Means Clustering



iteration 0: assign points to clusters



Clustering

K-Mean Clustering

- **Input:** Data X, number of clusters k
- Randomly initialize k cluster centroids $\mu_1, \mu_2, \ldots, \mu_k$
- Repeat until convergence:
  - **ASSIGN:** For each point x_i, assign to nearest centroid μ

$$c_i = arg\min_j \|x_i - \mu_j\|^2$$

  - **UPDATE**: Recompute centroids as cluster means

$$\mu_j = \frac{1}{|C_j|}\sum_{i \in C_j} x_i$$

- **Return** cluster assignments and centroids

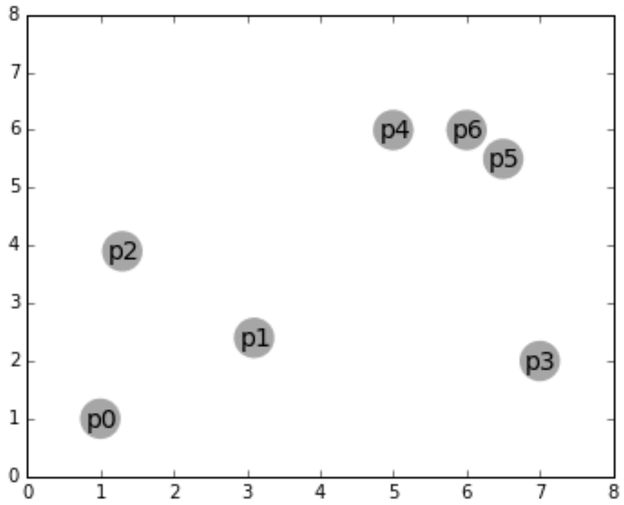
Clustering

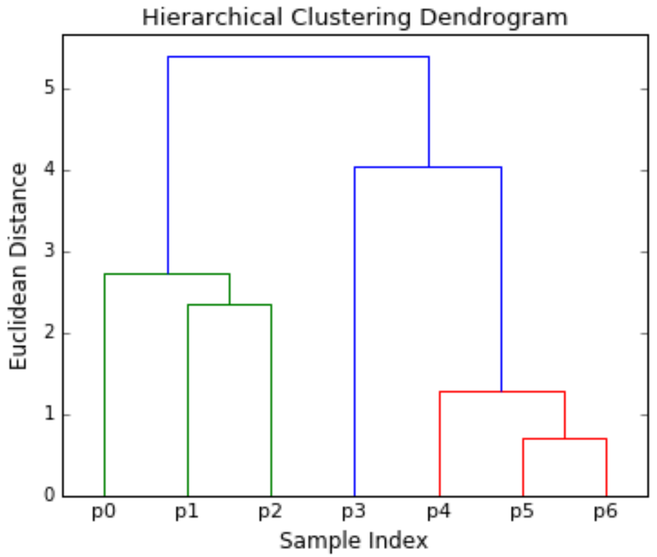
K-Mean Clustering - When to use?

- Good for:
  - Large datasets (scales well: $O(nkd)$ per iteration)
  - Roughly spherical, similar-sized clusters
  - When you know approximate number of clusters
- Not good for:
  - Non-convex cluster shapes
  - Clusters of very different sizes/densities
  - When number of clusters is unknown

Clustering

Hierarchical Clustering





- Agglomerative Algorithm

1. Start: Each point is its own cluster (n clusters)
2. Compute distance between all pairs of clusters
3. Merge the two closest clusters
4. Repeat steps 2-3 until only one cluster remains
5. Record the merge history (dendrogram)

Clustering

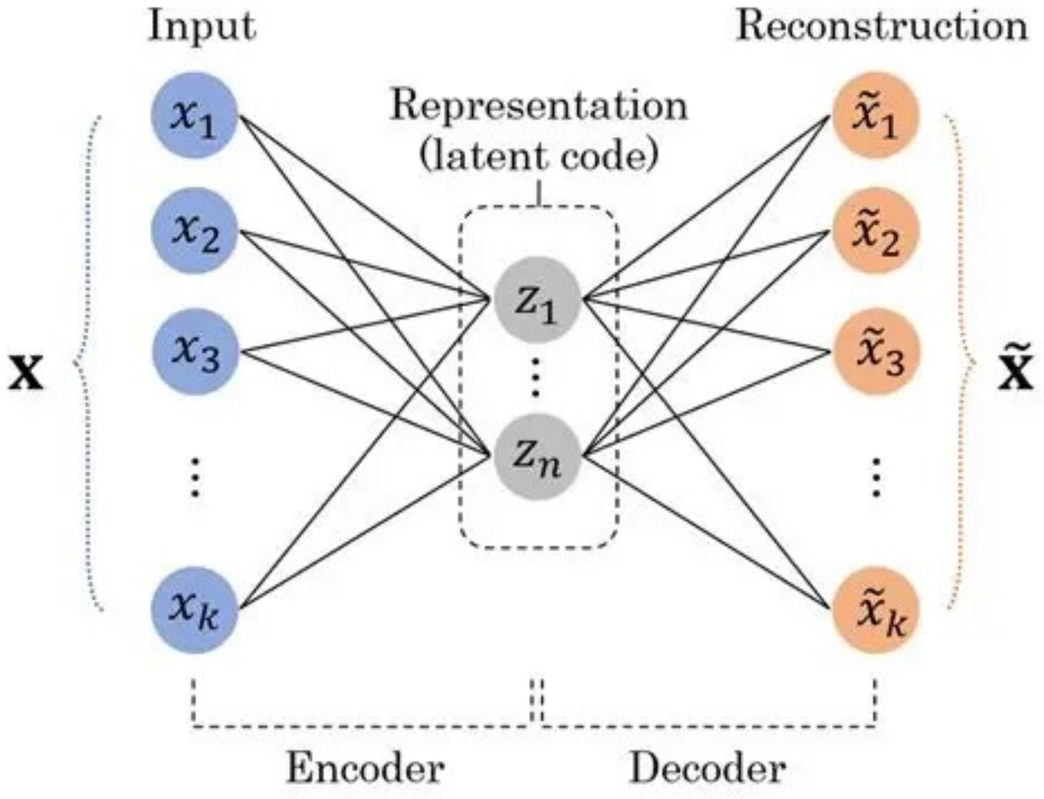
Hierarchical Clustering - Pros and Cons

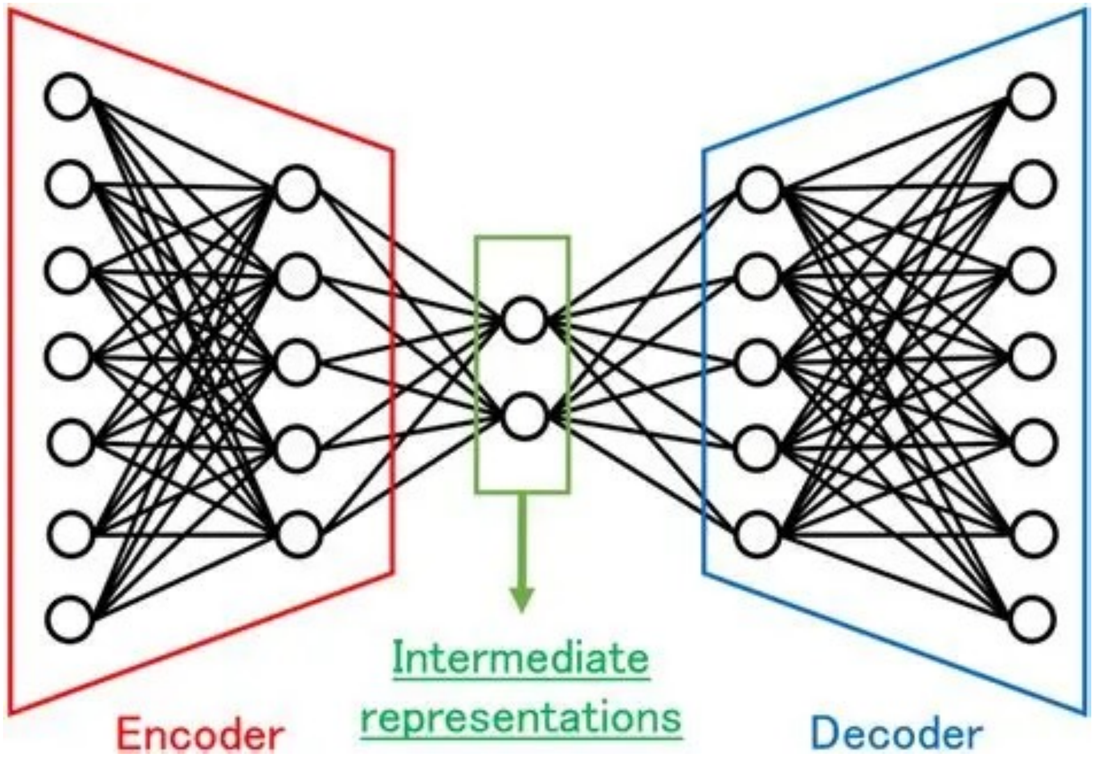
- Advantages:
  - No need to specify k in advance
  - Produces hierarchy (useful for taxonomy)
  - Dendrogram is informative
  - Any distance metric can be used
  - Deterministic (unlike K-Means)
- Disadvantages:
  - Slow: $O(n^3)$ time, $O(n^2)$space
  - Cannot “undo” a merge (greedy)
  - Sensitive to noise and outliers
  - Not suitable for large datasets

Autoencoders

Dimensionality Reduction using Deep Learning

- An autoencoder is a neural network trained to **reconstruct** its input.





Autoencoders

Dimensionality Reduction using Deep Learning

- An autoencoder is a neural network trained to **reconstruct** its input.
- **Encoder:** Compresses input to lower-dimensional latent representation
- **Latent space:** Compressed representation (bottleneck)
- **Decoder:** Reconstructs input from latent code
- **Training objective:** Minimize reconstruction error

$$L = ||x - \hat{x}||^2$$

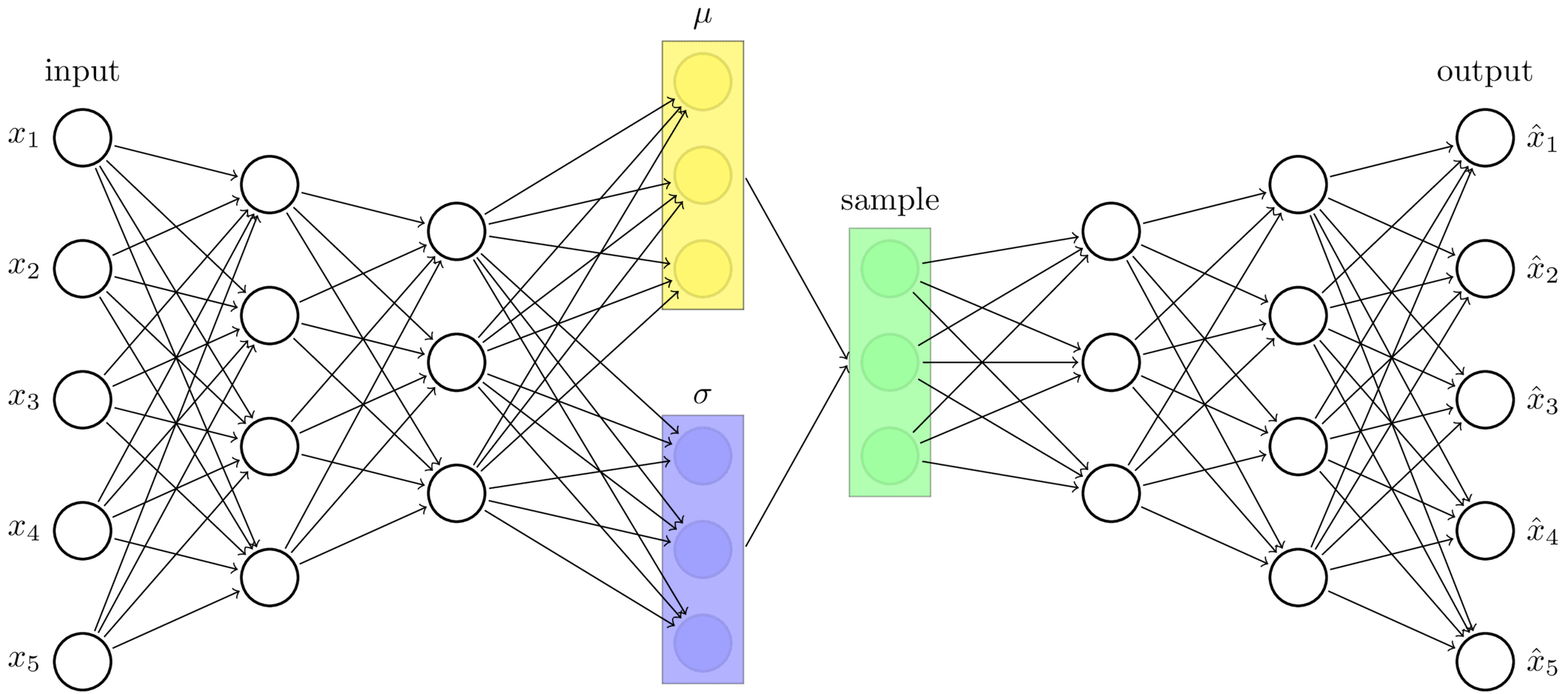
Variational Autoencoders

Dimensionality Reduction using Deep Learning

- Standard autoencoders learn a **deterministic** mapping to latent space (this is true for all neural networks in general)
- The latent space may have “holes”, i.e., regions that don't correspond to valid data.
- You can't sample from it to generate new data.
- **VAE Key Idea**
  - Instead of encoding to a point, encode to a **probability distribution.** The encoder outputs **parameters of a Gaussian distribution**, and we sample from it

Variational Autoencoders

Dimensionality Reduction using Deep Learning



Variational Autoencoders

Dimensionality Reduction using Deep Learning

- The Reparameterization Trick
  - **Problem**: Can't backpropagate through random sampling.
  - **Solution**: Reparameterize the sampling
    - $z = \mu + \sigma \cdot \epsilon, \quad \epsilon \sim \mathcal{N}(0,1)$
    - The randomness from sampling is now in ϵ and gradients can flow through μ and σ

Variational Autoencoders

Dimensionality Reduction using Deep Learning

- VAE Loss Function
  - Two Components
    - Reconstruction Loss - How well can the model reconstruct the input?

$$L_{recon} = ||x - \hat{x}||^2$$

    - KL Divergence - How close is the learned distribution to the original?

$$L_{KL} = KL(q(z|x) \ ||p(z))$$

  - Total Loss: $L = L_{recon} + L_{KL}$

The KL divergence **regularizes** the latent space:

- Encourages latent distributions to be close to $\mathcal{N}(0,1)$
- Creates a smooth, continuous latent space
- Enables **generation**: Sample$z \sim \mathcal{N}(0,1)$, decode to generate new data
- Without KL term, the encoder could **learn very narrow distributions** (essentially points), losing the generative property.