Introduction to Machine Learning

WSS ML Workshop

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WSS 2024

Outline

- Introduction and Motivation
- ML Problems
  - Supervised Learning
  - Unsupervised Learning
  - Reinforcement Learning
- Loss Function and Optimization
- Generalization and Overfitting

Machine Learning: Motivation

Extensive influence of Machine Learning across multitude of applications and everyday life:

- Computer Vision
- Signal Processing
- Audio and Speech Recognition
- Natural Language Processing
- Computational Social Science
- Control

Machine Learning: Motivation

Extensive influence of Machine Learning across multitude of applications and everyday life:

- Computational Biology and Bioinformatics
- Medicine, Diagnosis and Health Care
- Computational Neuroscience
- Brain-Computer Interface
- Financial Forecasting
- Recommender Systems

Machine Learning: Motivation

Why ML applications are growing?

- Improved machine learning algorithms
- Availability of data

  (Increased data capture, networking, …)
- Algorithms too complex to write by hand
  - Demand for complex systems

    (high-dimensional, multi-modal, …)
  - Demand for self-customization to user or environment

Machine Learning: Concept

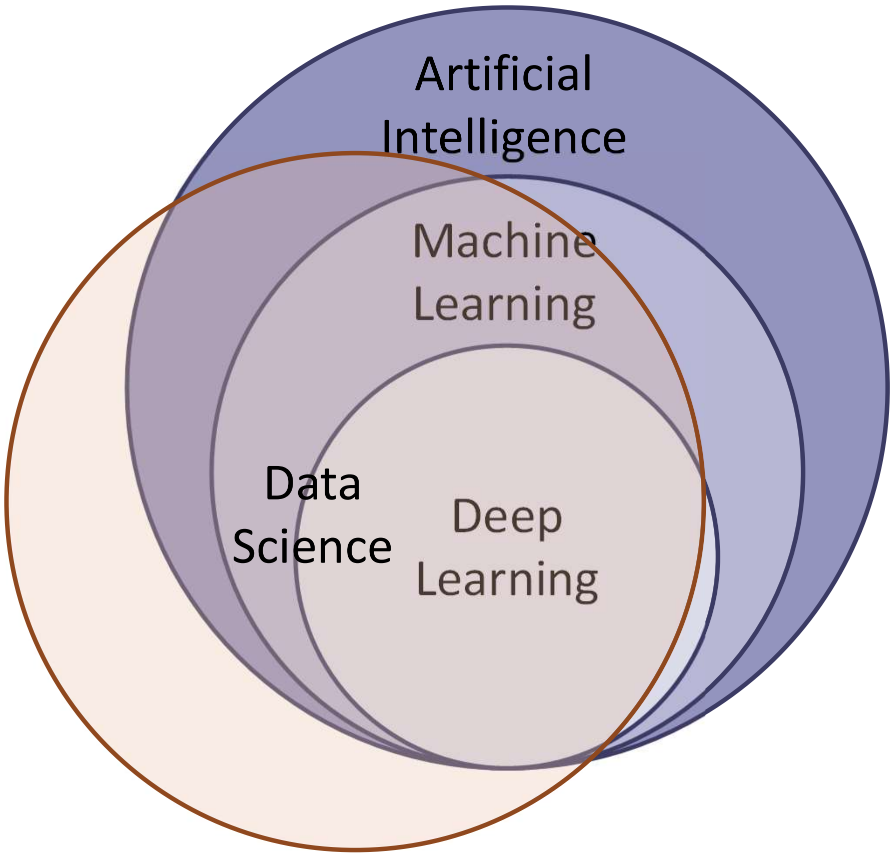
- Making machines learn!
- Using statistical models and algorithms to perform a specific task by learning data patterns, without being explicitly programmed
- **Generalization** to new unseen examples.

Machine Learning: Main Recipe

- A pattern exist …
- We do not know it mathematically!
- We have data on it :)

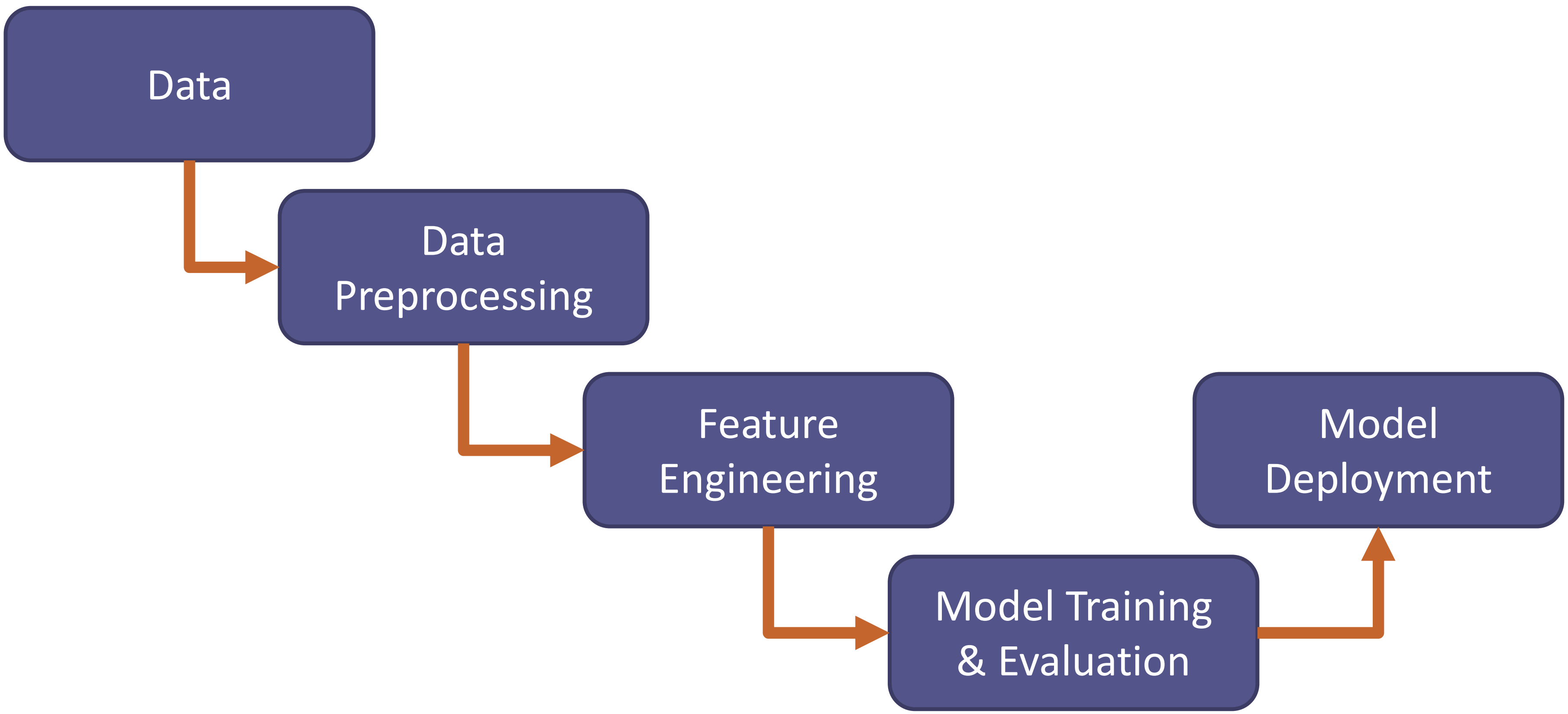
Machine Learning: Role of Data

What’s the scope?



Machine Learning: Main Steps

- Typical steps:



Main ML Problems

- Supervised Learning
  - Classification
  - Regression
- Unsupervised Learning
  - Density Estimation
  - Generative Modeling
  - Clustering
  - Dimensionality Reduction
- Reinforcement Learning
  - Multi-armed Bandit

Supervised Learning vs. Unsupervised Learning

- Supervised learning

  Given: Training set

  Labeled set of N input-output pairs $D = \{(x^{(i)}, y^{(i)})\}_{i=1}^{N}$

  Goal: Learning a mapping from x to y

Supervised Learning vs. Unsupervised Learning

- Supervised learning

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- Unsupervised learning

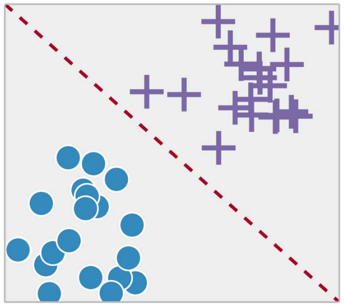
  Given: Training set

  $$D = \{(x^{(i)})\}_{i=1}^{N}$$

  Goal: Revealing structure in the observed data and finding groups or intrinsic structures in the data

Supervised Learning: Classification vs. Regression

- Classification: predict a discrete target variable e.g. $y \in \{1, 2, \dots, C\}$



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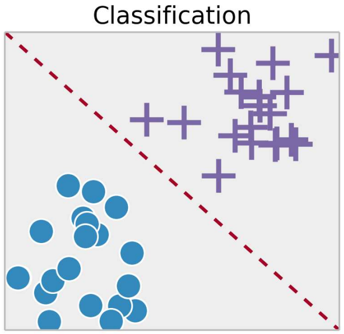
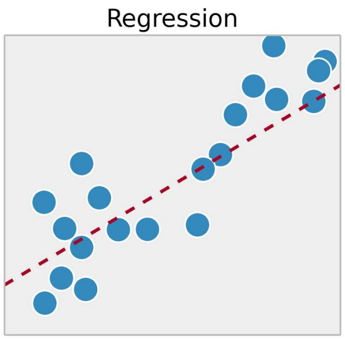


- Regression: predict a continuous target variable e.g. $y \in [0, 1]$



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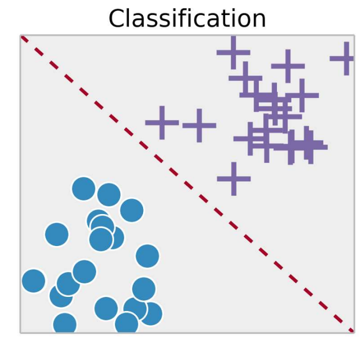

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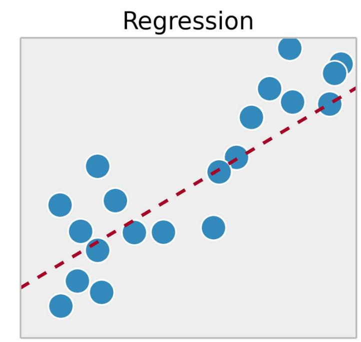

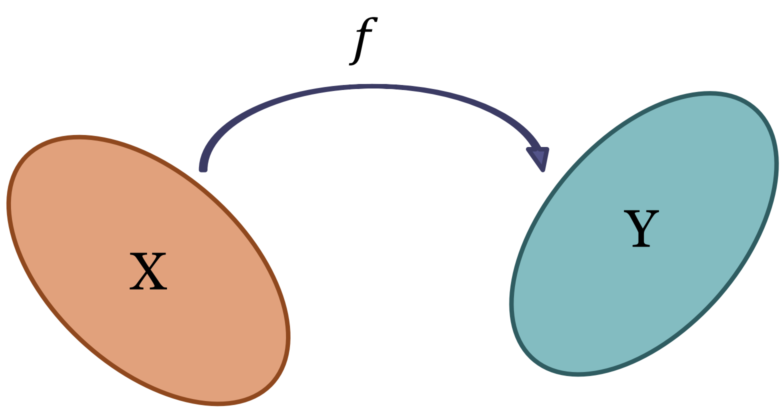

Classification

- A function $f : R^n \to \{1, \ldots, k\}$ specifies which of k categories an input vector x belongs to.

Classification

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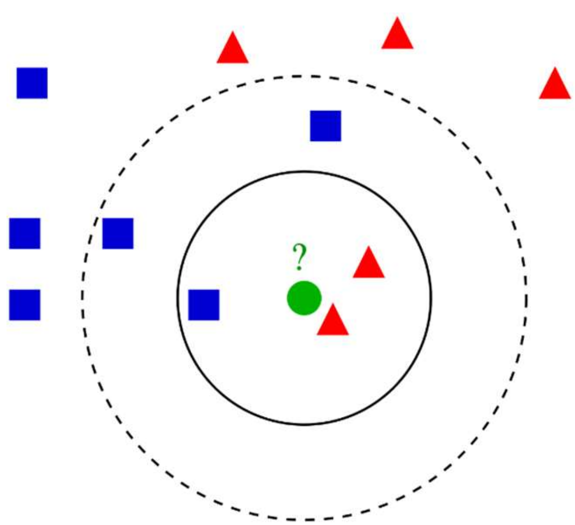
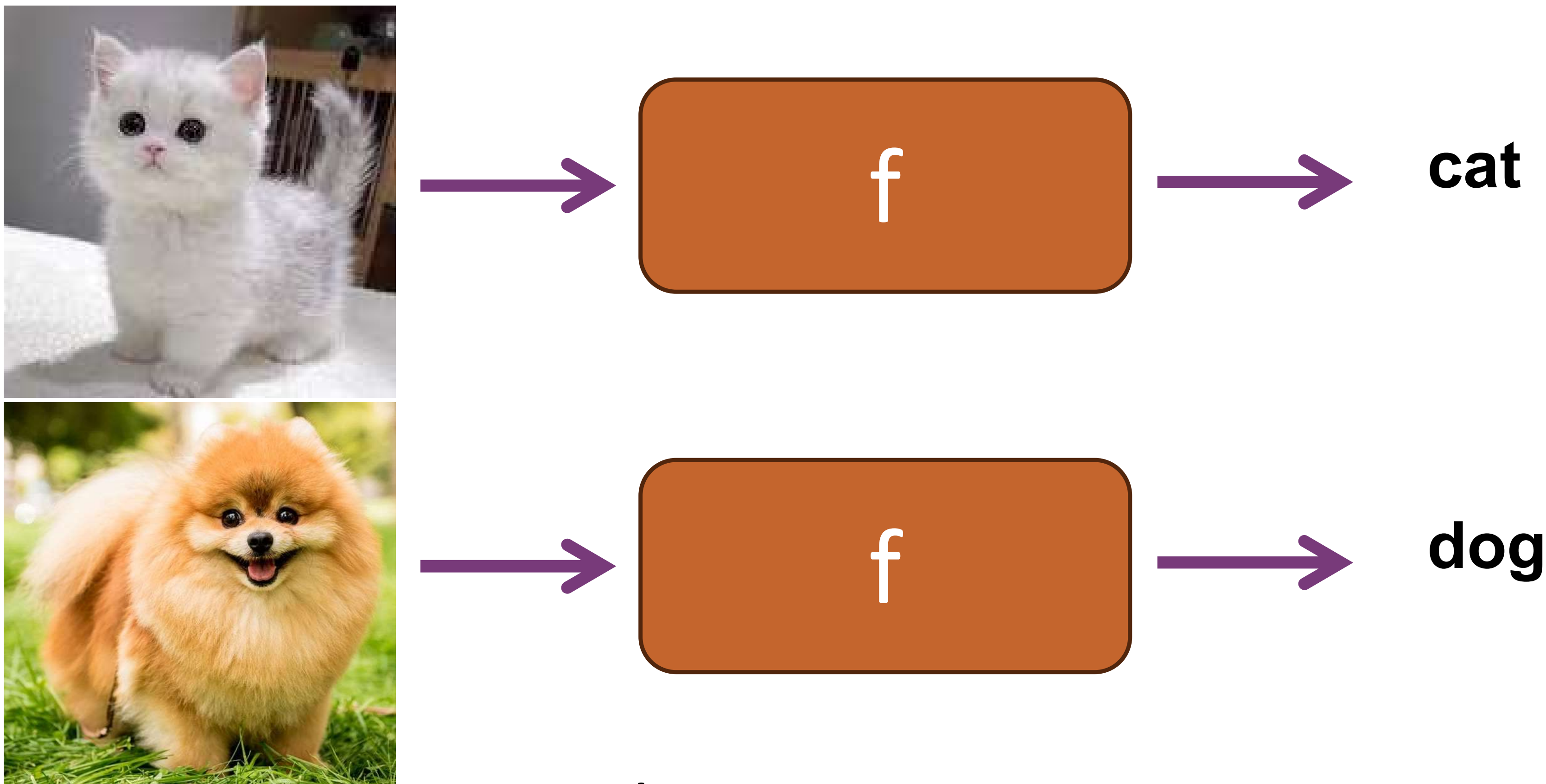
- Case Study: KNN (K Nearest Neighbors)
  - Stores all training cases and classify new cases based on similarity measure (like Euclidean distance)



Classification

More advanced applications:



Object Recognition

Regression

- A function $f\ :R^n \rightarrow R$ that maps an input vector x to a continues value y.

Regression

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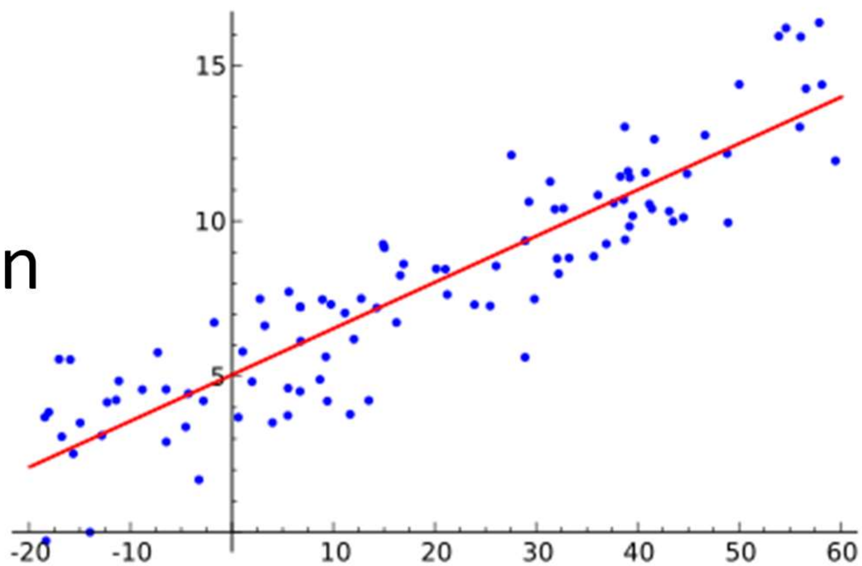
- Case study: Linear Regression

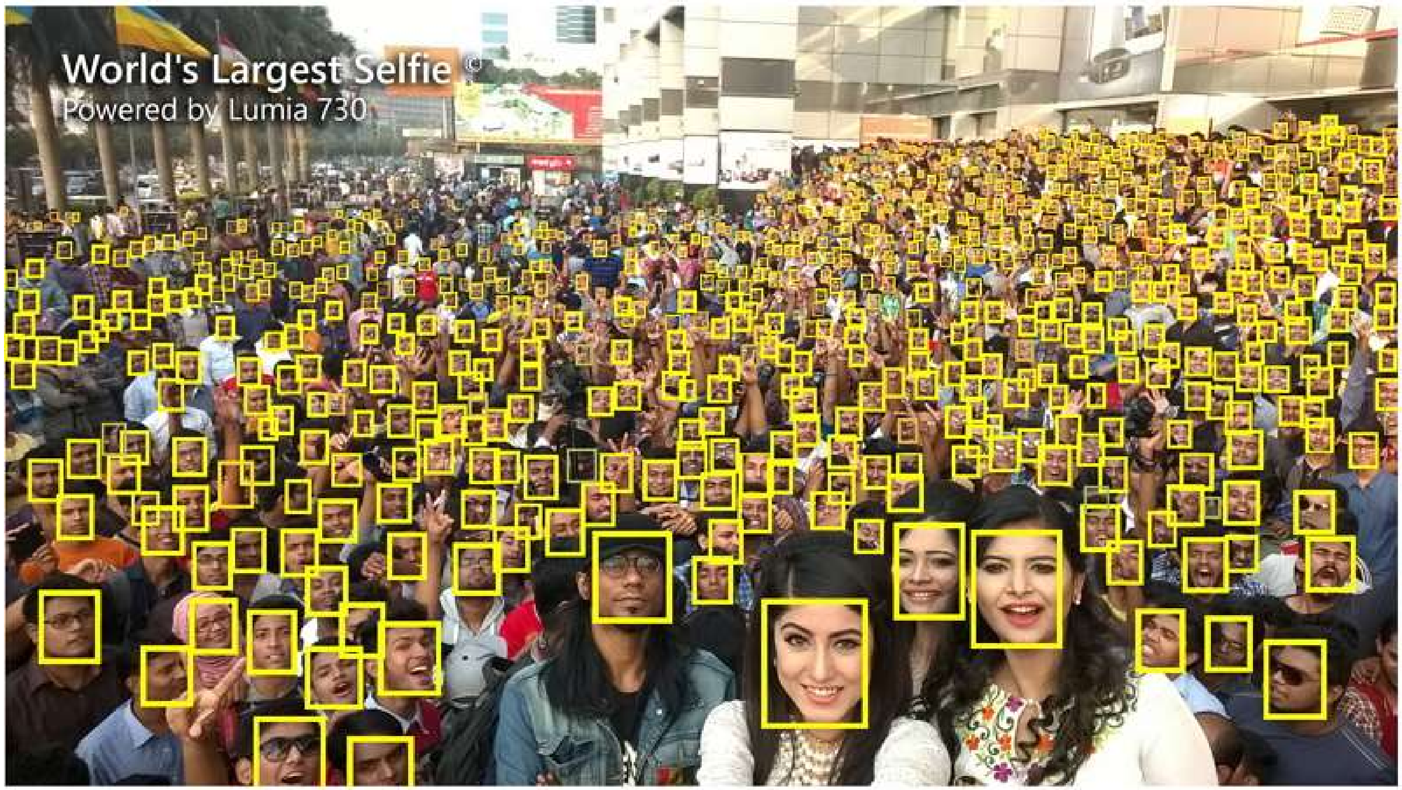
$$f(x; w) = \mathrm{w}_0 + \mathrm{w}_1\mathrm{x}$$



$w = [w_0, w_1]$: Parameters that be estimated during optimization

Regression

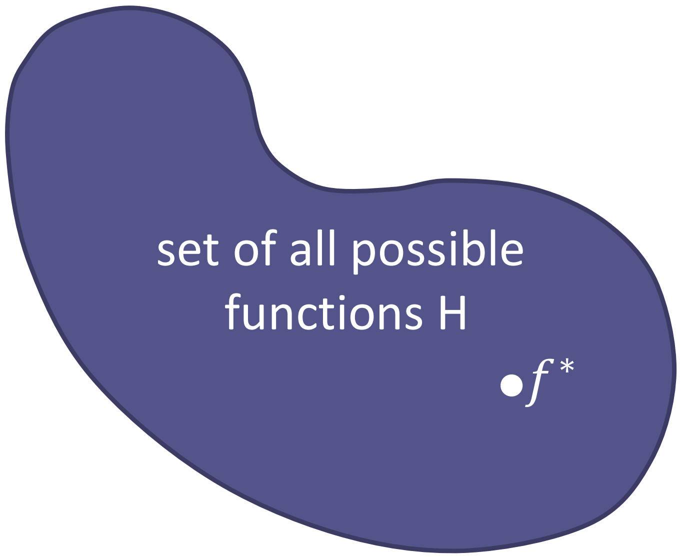
- More advanced applications:



Object Detection

Hypothesis Class and Inductive Bias

- The aim of supervised learning is to find f^* (best solution) from **hypothesis space** (e. g. the set of all possible functions)

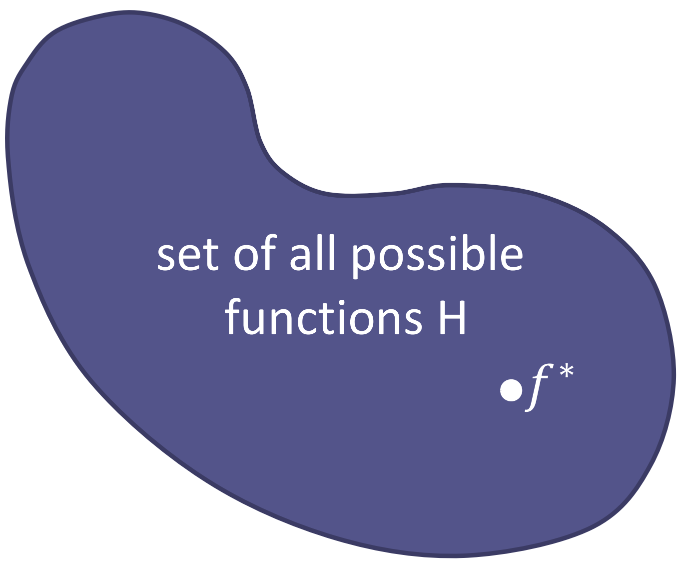


Hypothesis Class and Inductive Bias

- The aim of supervised learning is to find f^* (best solution) from **hypothesis space** (e. g. the set of all possible functions)
- Example:

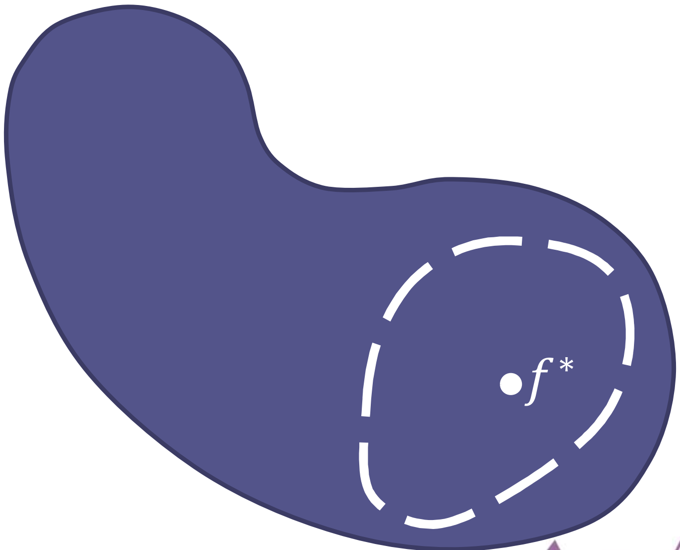
In linear regression the hypothesis space include all possible functions with the form of

$$f(x; w_0, w_1) = w_0 + w_1 x$$



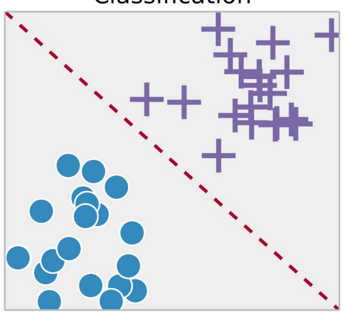
Hypothesis Class and Inductive Bias

- **Inductive bias** is the set of assumptions that a learner uses to predict outputs of given inputs.
- Some times we use our knowledge about the nature of data to **restrict** the hypothesis space.

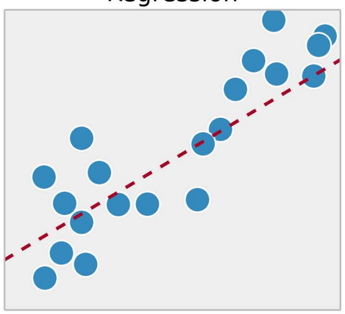


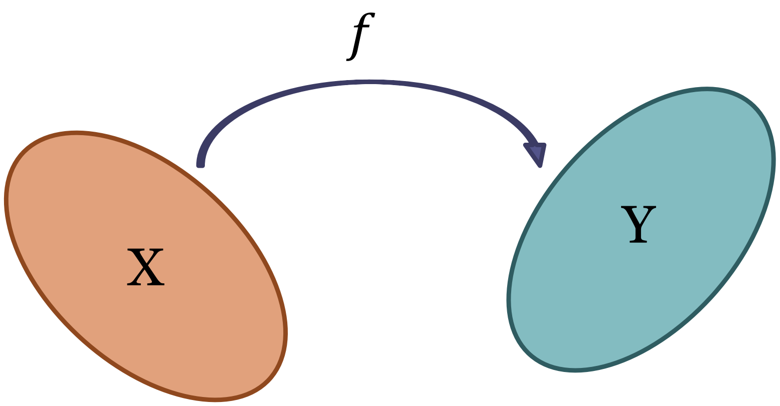
Supervised Learning (Recap)

- Classification: predict a discrete target variable e.g. $y \in \{1, 2, \dots, C\}$



- Regression: predict a continuous target variable e.g. $y \in [0, 1]$





Unsupervised Learning

Unsupervised learning

Given: Training set

$$D = \{(x^{(i)})\}_{i=1}^{N}$$

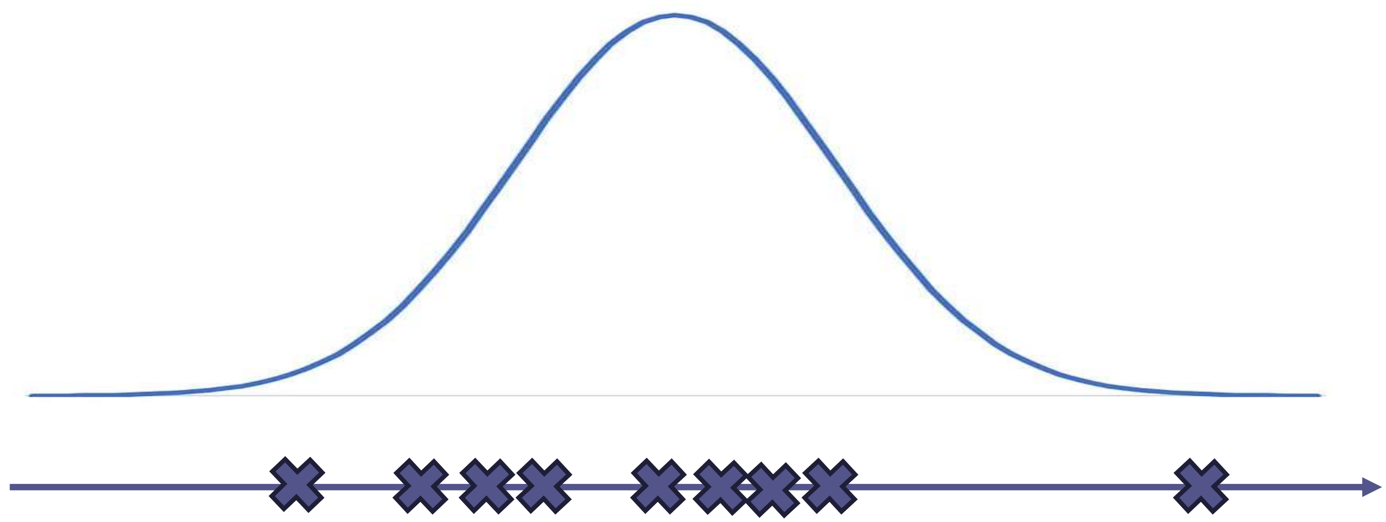
Goal: Revealing structure in the observed data and finding groups or intrinsic structures in the data

Main Approaches:

- Density Estimation
- Generative Modelling
- Clustering
- Dimensionality Reduction

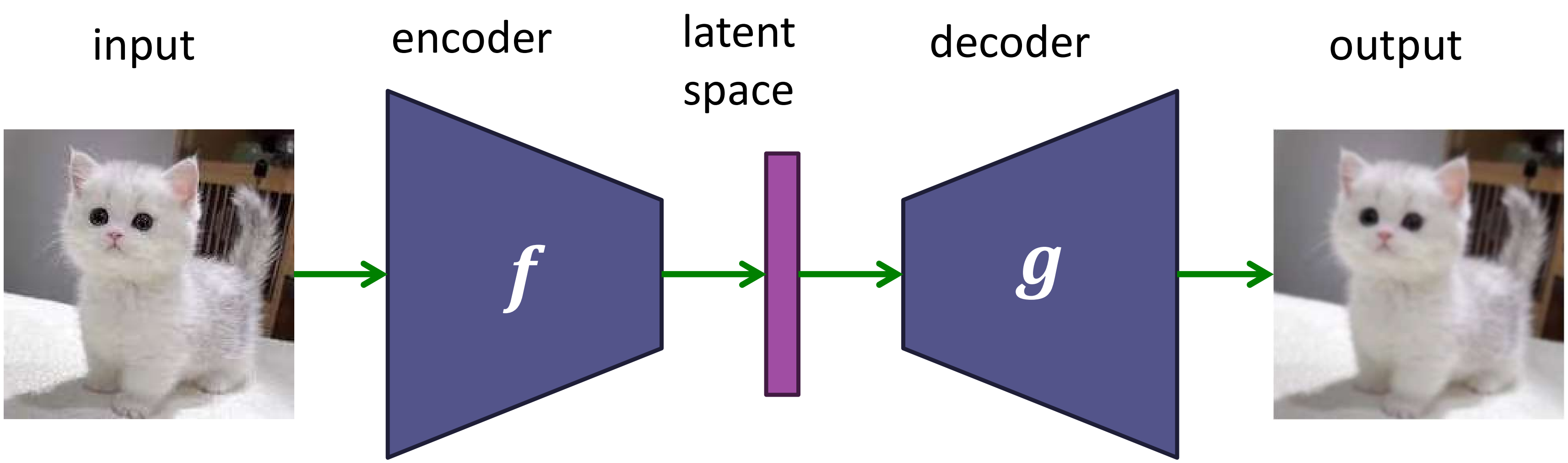
Density Estimation

- Estimating the probability density function $p(\boldsymbol{x})$, given a set of data points $\{\boldsymbol{x}^{(i)}\}_{i=1}^{N}$ drawn from it.



Density Estimation

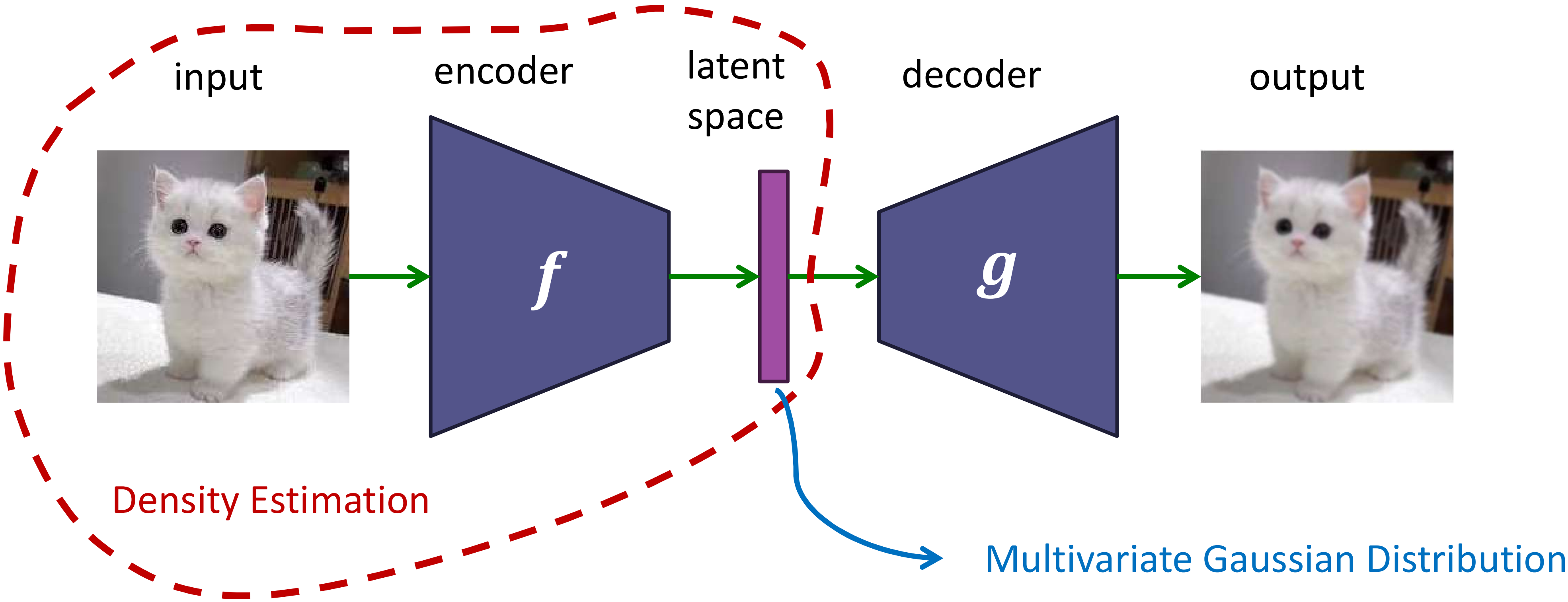
More sophisticated applications:



Variational Autoencoder (VAE)

Density Estimation

More sophisticated applications:

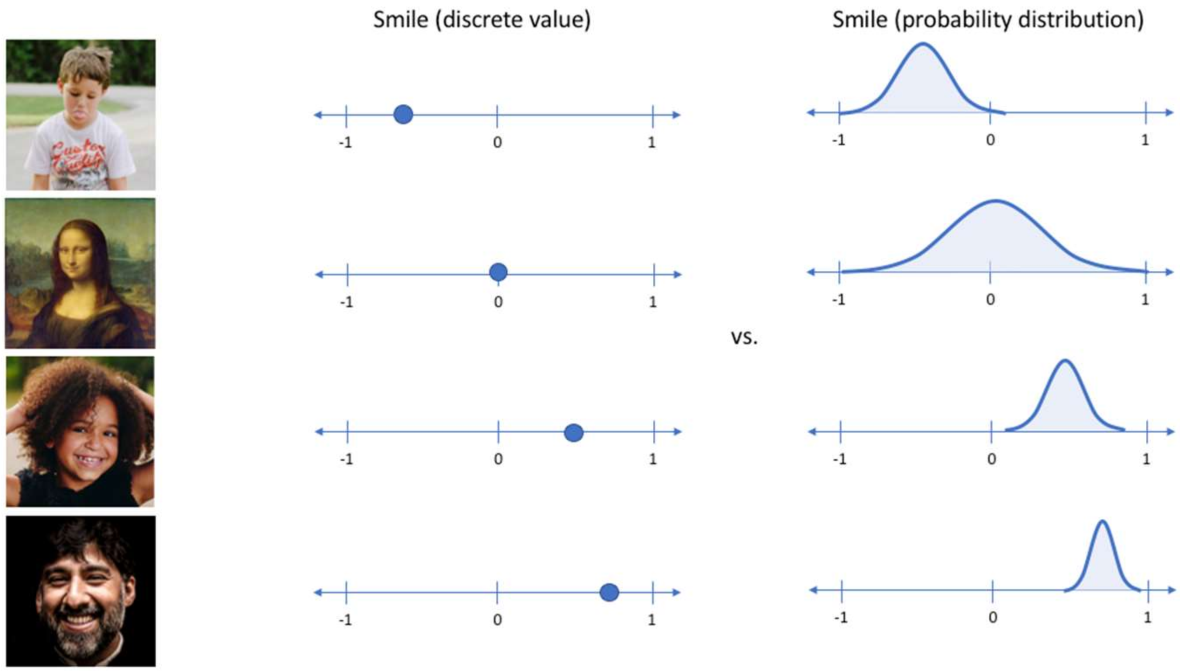


Variational Autoencoder (VAE)

Density Estimation

More sophisticated applications:

latent variable value



Variational Autoencoder (VAE)

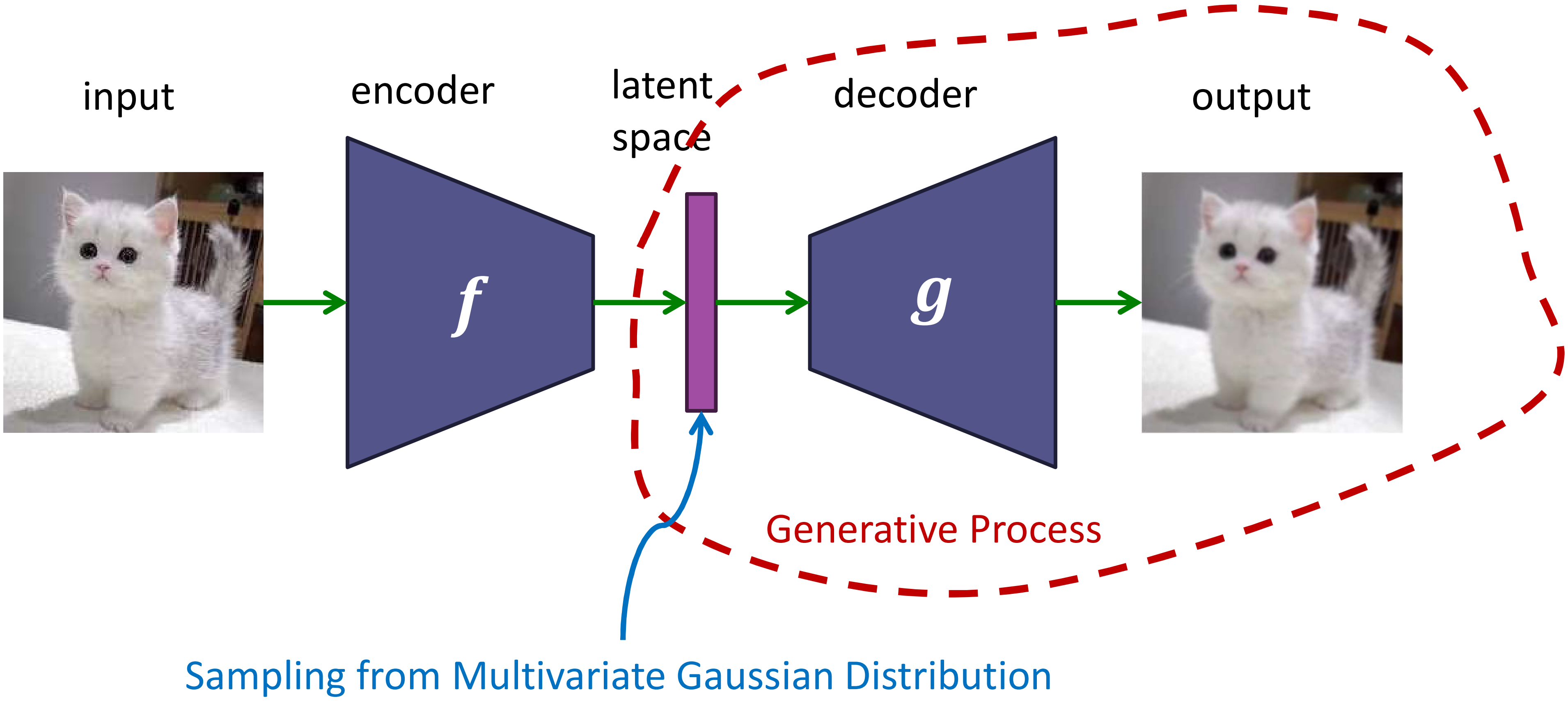
Generative Modeling

- Sampling new data points based on observed data distribution.

- This can be achieved with / without explicitly learning density function $p(\boldsymbol{x})$.

Generative Modeling:

More sophisticated applications (explicit density estimation)



Variational Autoencoder (VAE)

Generative Modeling:

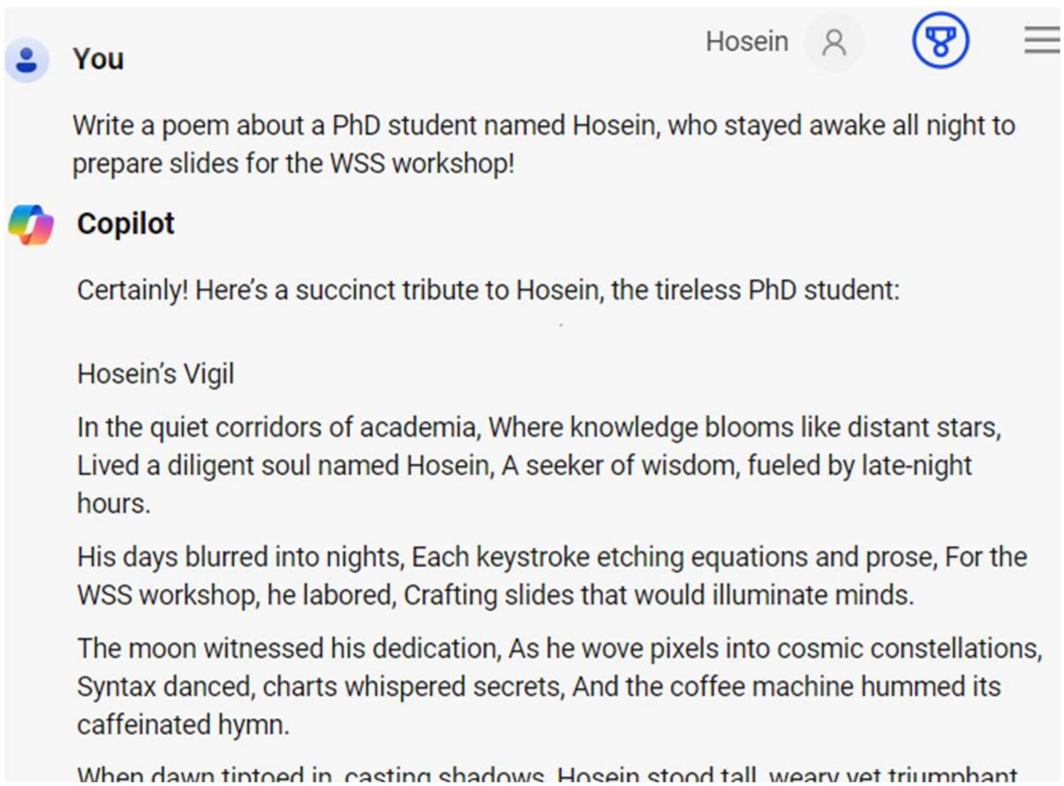
More sophisticated applications (implicit density estimation)

- Generative Adversarial Networks (GANs)
- Diffusion Models

Generative Modeling:

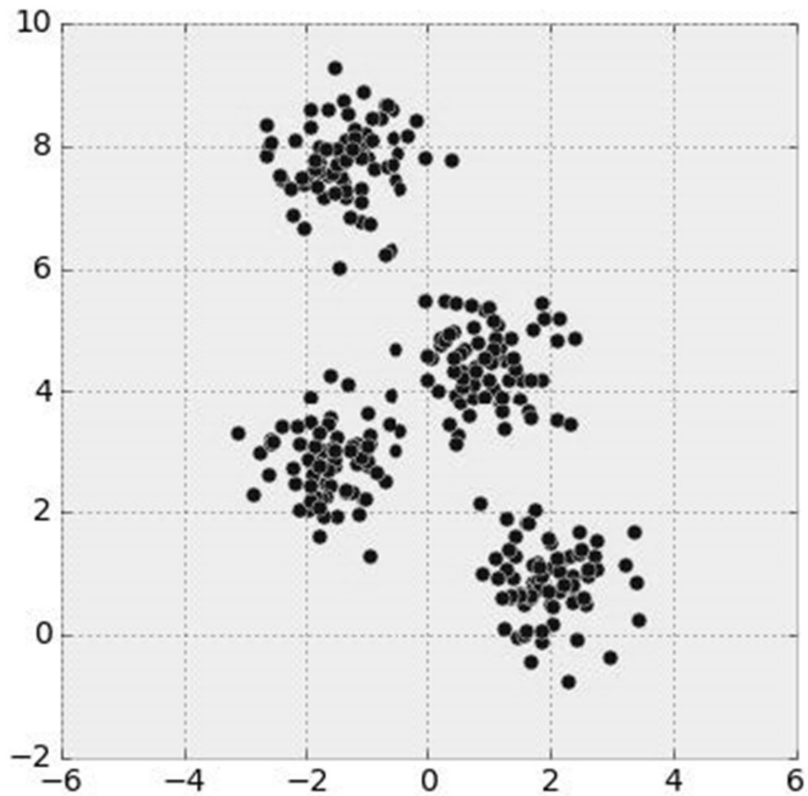
More sophisticated applications (implicit density estimation)

- Large Language Models (LLMs)
- Generative pre-trained transformers (GPT)



Clustering

- A technique to assign each point into a specific group.



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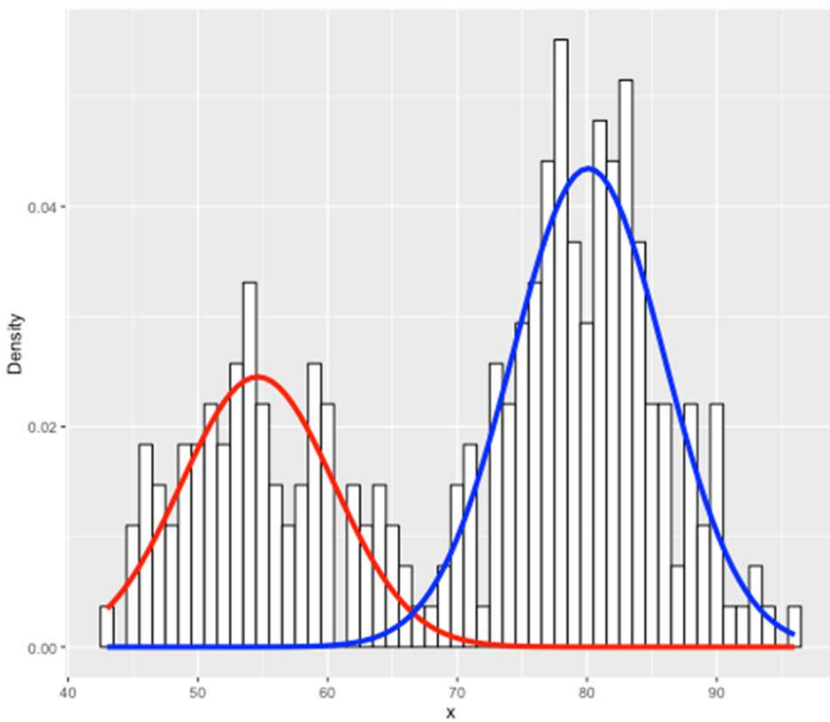

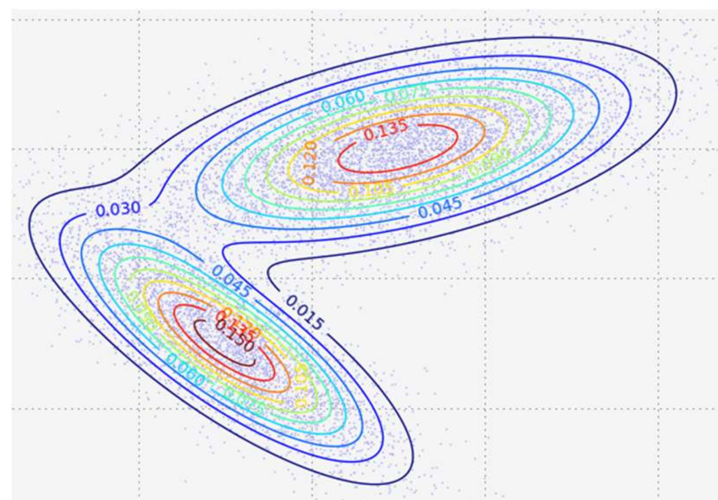

Gaussian Mixture Model

Clustering: Case Study

K-means Algorithm:

1. Choose number of clusters K.
2. Pick K random points as cluster centers (centroid)
3. Compute the distance between data points and all centroids
4. Assign each data point to the closest centroid
5. Compute the centroids for the clusters (by averaging)
6. Iterate steps 3-5 until convergence (no centroid change)

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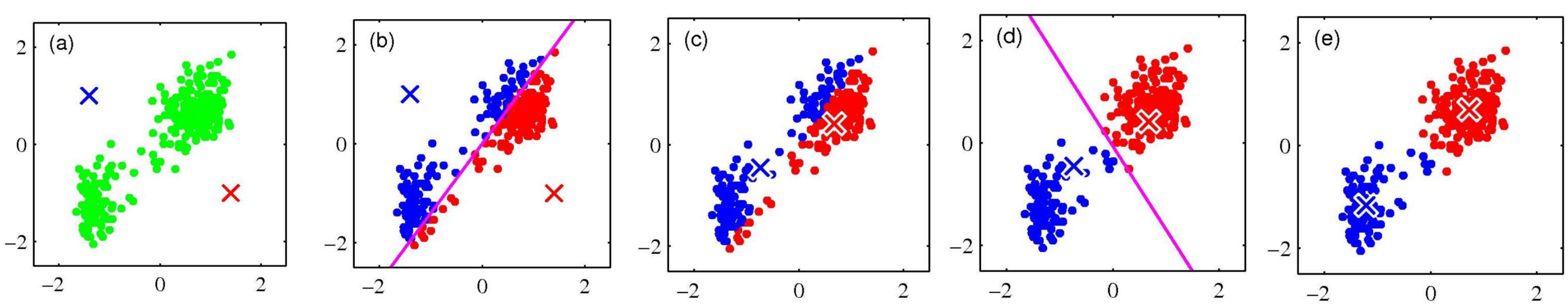
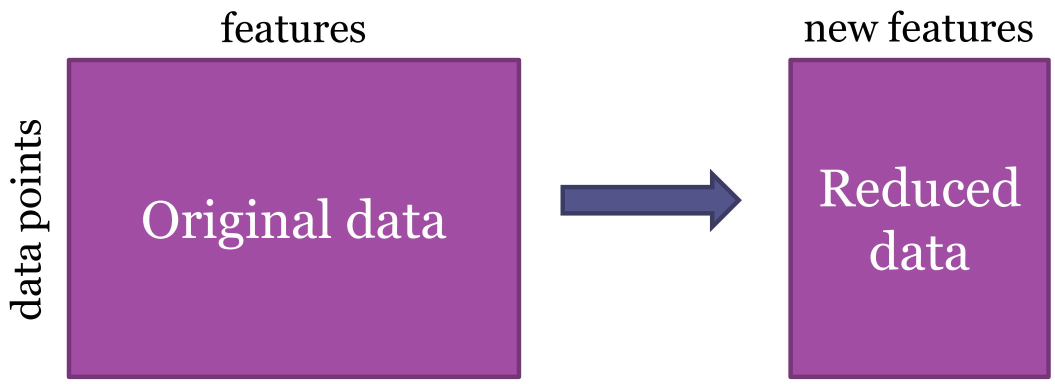


(2) (3-4) (5) (3-4) (6)

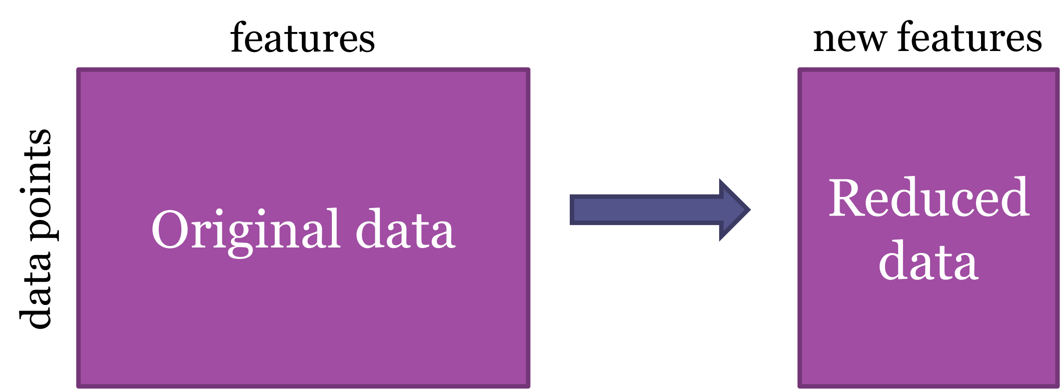
Dimensionality Reduction

- A technique to find a lower-dimensional representation of data features that preserves some of its properties.



Dimensionality Reduction

- A technique to find a lower-dimensional representation of data features that preserves some of its properties.
- Motivations:
  - Computation
  - Visualization
  - Feature extraction



Dimensionality Reduction

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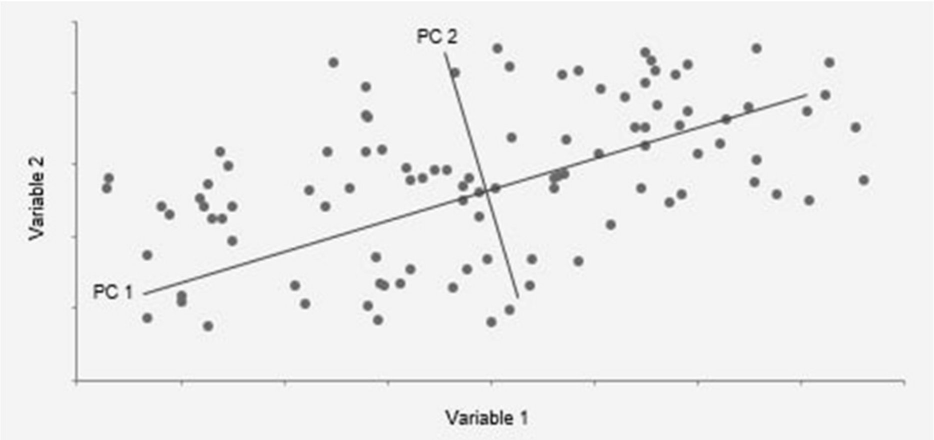
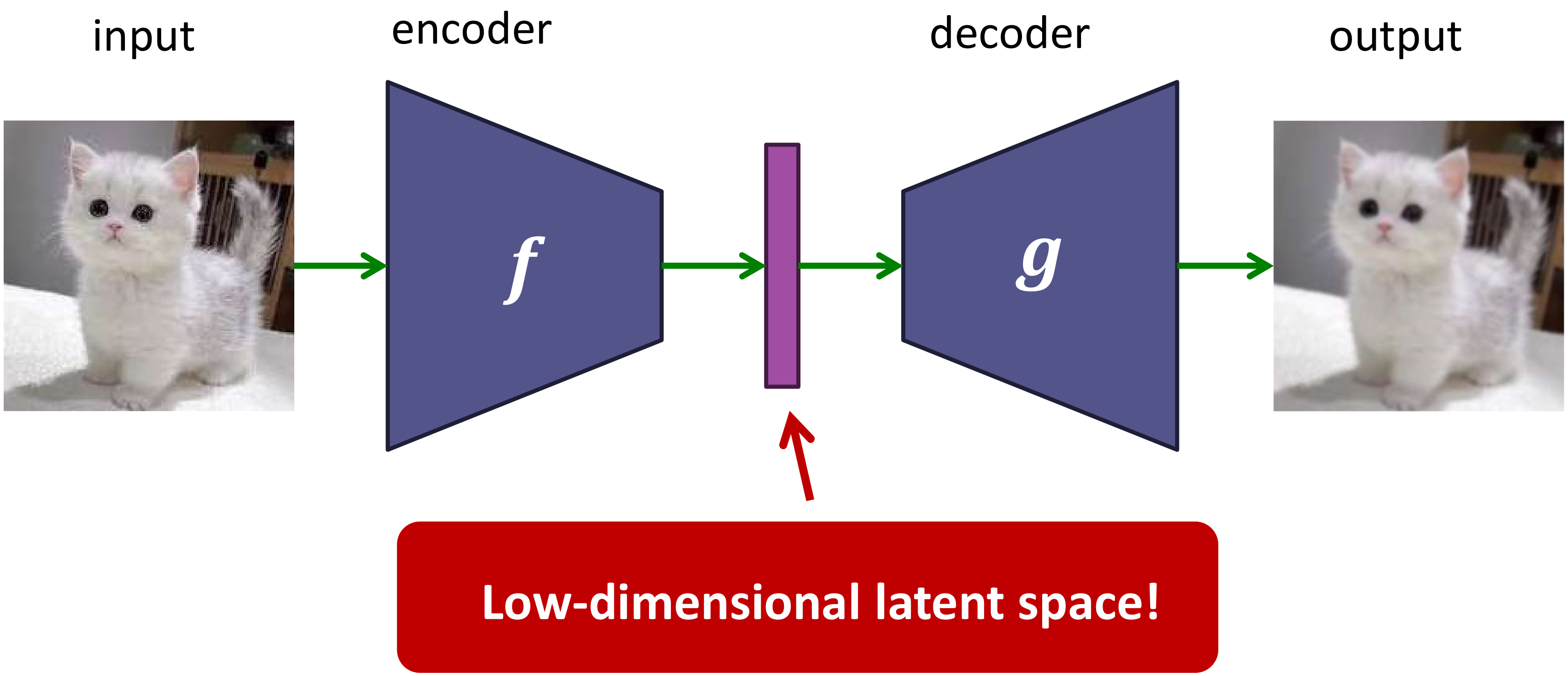
- Case Study:
  Principal Component Analysis (PCA)



Dimensionality Reduction

More sophisticated methods:



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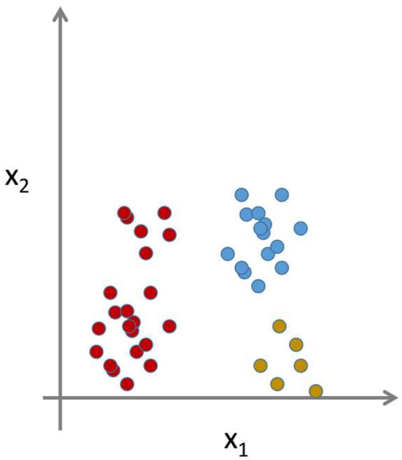
Supervised Learning vs. Unsupervised Learning



	discrete	Continues
supervised	**classification**	**regression**
unsupervised	**clustering**	**dimensionality reduction**