Lecture 01: Introduction

Introduction to Machine Learning

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Contents

References

Except explicitly cited, the reference for the material in slides is:

- Murphy, K. P. (2022). *Probabilistic machine learning: an introduction.* MIT press.

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Note Block

Example Block

Remember Block

Section 1

Course Introduction

Subsection 1

State of Machine Learning

State of Machine Learning

Andrew Ng

Electricity transforms countless industries: transportation, manufacturing, healthcare, communications and more. AI (machine learning) will bring about an equally big transformation

What is Machine Learning

Machine Learning [1]

Consider the following three items:

- Experience E
- Class of tasks T
- Performance measure P

Machine learning is to improve the performance measured by P of a computer program on T using E

Machine Learning

Based on *Machine Learning*, definition we have the main following major types of machine learning:

- Supervised Learning
- Unsupervised Learning
- Reinforcement Learning

Section 2

Supervised Learning

Supervised Learning

Supervised Learning is:

- Task T: Finding mapping $f : \boldsymbol{x} \mapsto \boldsymbol{y}$ ($\boldsymbol{x} \in \mathcal{X} = \mathbb{R}^D$ and $\boldsymbol{y} \in \mathcal{Y}$)
  - $\boldsymbol{x}$: Features, Covariates or Predictors
  - $\boldsymbol{y}$: Label, Target or Response
- Experience E: Set of N input-output pairs $\mathcal{D} = \{(\boldsymbol{x}_n, \boldsymbol{y}_n)\}_{n=1}^{N}$
  - $\mathcal{D}$: Dataset
  - N: Sample size
- Performance measure P: Dependent on the task

Subsection 1

Classification

Classification

General Features:

- Task T: Finding mapping $f : \boldsymbol{x} \mapsto y$ ($\boldsymbol{x} \in \mathcal{X} = \mathbb{R}^D$ and $y \in \mathcal{Y}$)
- Experience E: Set of N input-output pairs $\mathcal{D} = \{(\boldsymbol{x}_n, y_n)\}_{n=1}^{N}$

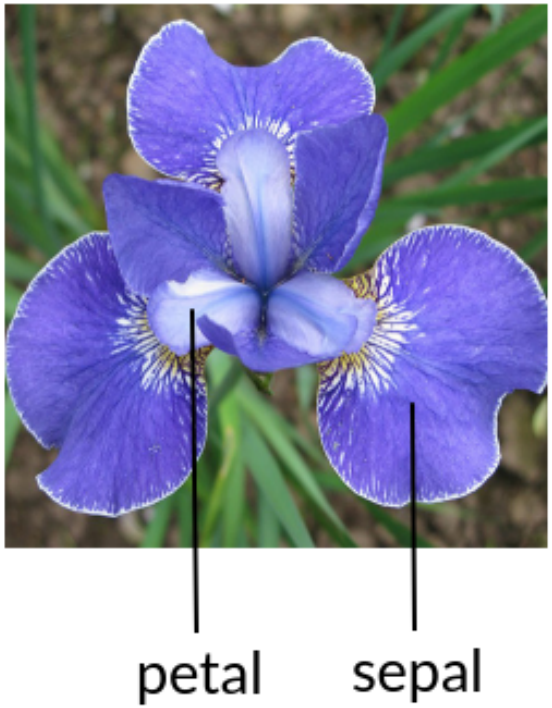
Specific Features:

- $\mathcal{Y} = \{1, 2, \ldots, C\}$ (Unordered and mutually exclusive labels)
- $P = \frac{1}{N} \sum_{n=1}^{N} \mathbb{I}(y_n \neq f(\boldsymbol{x}_n))$ where:

$$\mathbb{I}(e) = \begin{cases} 1 & \text{if } e \text{ is true} \\ 0 & \text{if } e \text{ is false} \end{cases}$$

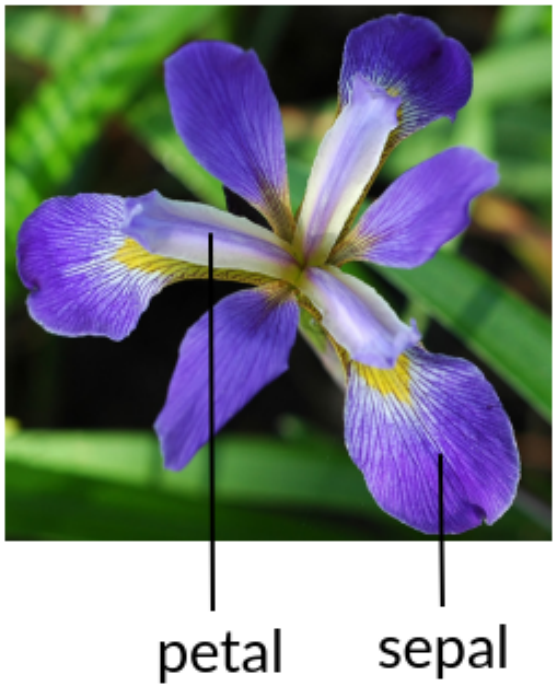
  - P is known as *Misclassification Error*

Example - Iris Flower Classification



(a) Setosa ($y = 1$)

(b) Versicolor ($y = 2$)



(c) Virginica ($y = 3$)

Figure: Different types of Iris flower

Example - Iris Flower Classification

$$f_1\left(\ \ \right) = \begin{cases} 1 \text{ (Setosa)} \\ 2 \text{ (Versicolor)} \\ 3 \text{ (Virginica)} \end{cases}$$

(a) Approach 1

$$f_2\Big(g\Big(\ \ \Big)\Big) = \begin{cases} 1 \text{ (Setosa)} \\ 2 \text{ (Versicolor)} \\ 3 \text{ (Virginica)} \end{cases}$$

$$g: \begin{bmatrix} \text{Sepal length} \\ \text{Sepal width} \\ \text{Petal length} \\ \text{Petal width} \end{bmatrix}$$

(b) Approach 2

Figure: Different types of Iris flower

Example - Iris Flower Classification

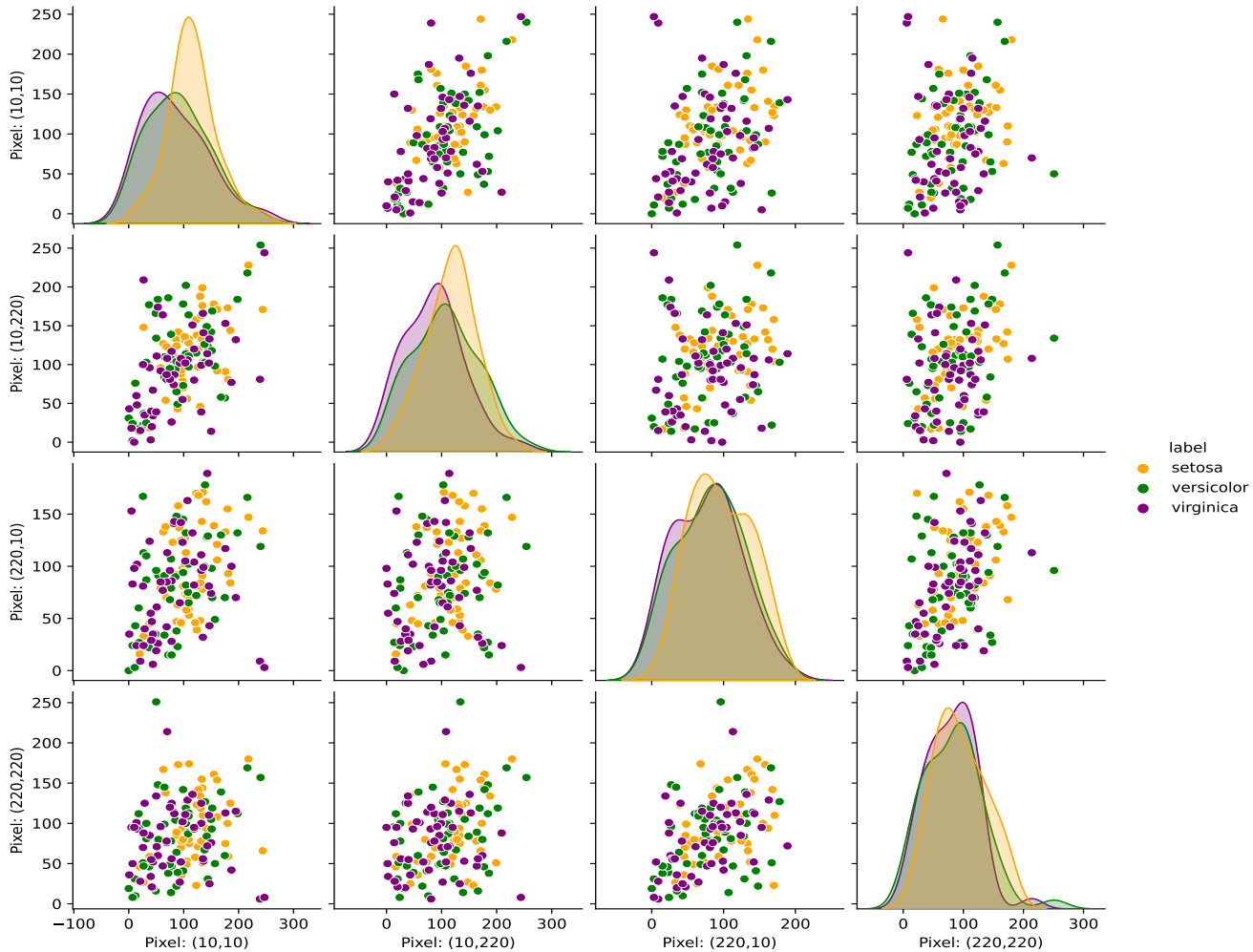


Figure: Exploratory data analysis - Approach 1

Example - Iris Flower Classification

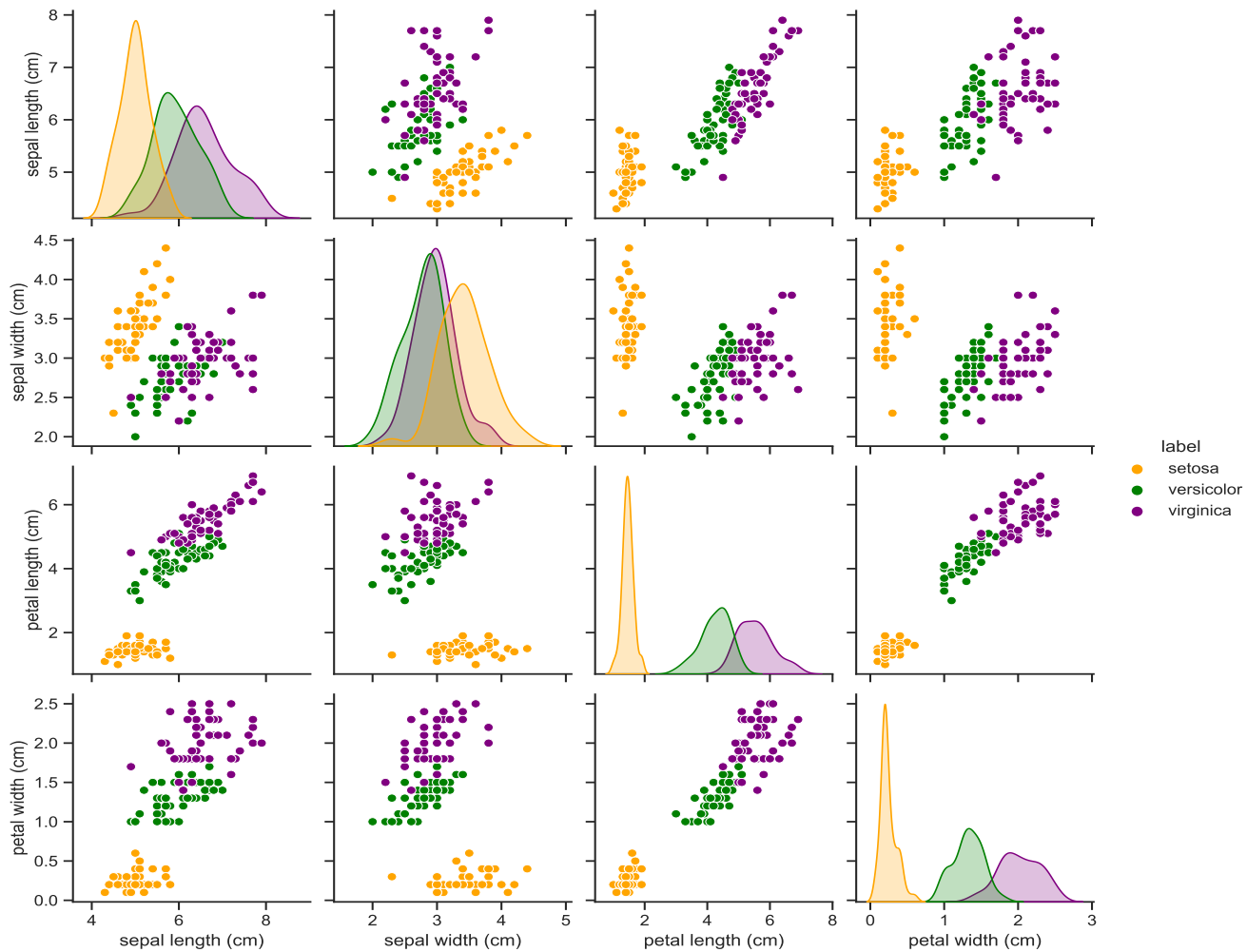
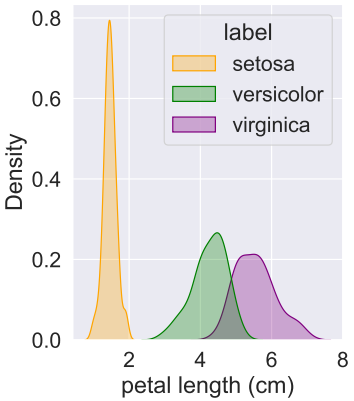
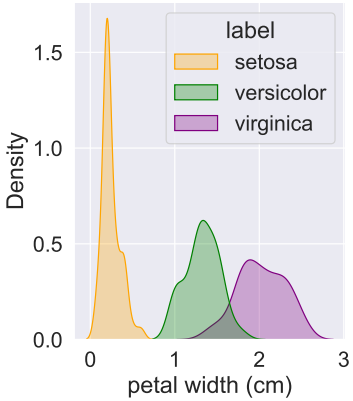


Figure: Exploratory data analysis - Approach 2

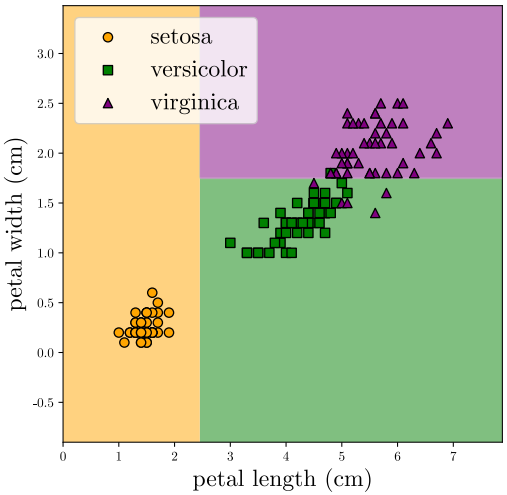
More on Approach 2



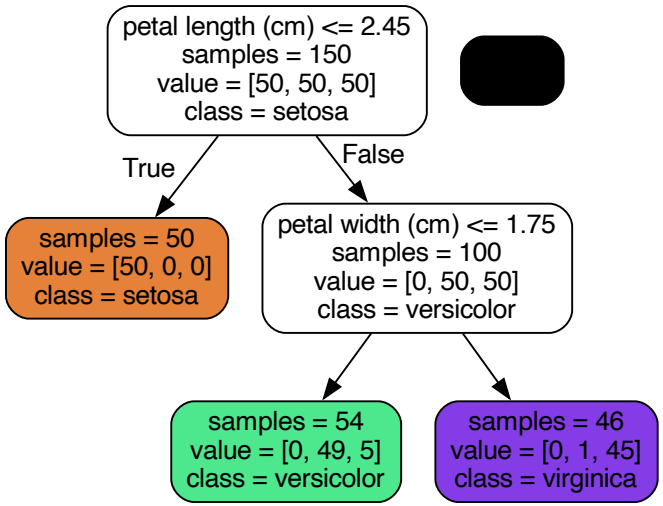
(a) Petal length



(b) Petal width



(c) Decision tree surface



(d) Decision tree

Automate Classification

Steps to Automate Classification

- Parameterizing mapping: $f(\cdot) \Rightarrow f(\cdot; \boldsymbol{\theta})$
- Finding suitable $\boldsymbol{\theta}$ $(\widehat{\boldsymbol{\theta}})$ using Experiment E (Model Fitting)
  - Enhancing performance measure $P \Rightarrow$ decreasing misclassification error

Note: Limitation with Misclassification Error

Inability to distinguish different errors

		$f(\boldsymbol{x}; \boldsymbol{\theta})$		
		Setosa	Versicolor	Virginica (Poisonous)
y	Setosa	0 (0)	1 (1)	1 (1)
	Versicolor	1 (1)	0 (0)	1 (1)
	Virginica (Poisonous)	1 (10)	1 (10)	0 (0)

Empirical Risk

Empirical Risk, the generalization of misclassification error is:

$$\mathcal{L} = \frac{1}{N} \sum_{n=1}^{N} l(y_n \neq f(\boldsymbol{x}_n; \boldsymbol{\theta}))$$

Using above definition, model fitting can be done via *Empirical Risk Minimization* (ERM) as:

$$\widehat{\boldsymbol{\theta}} = \underset{\boldsymbol{\theta}}{\operatorname{argmin}} \frac{1}{N} \sum_{n=1}^{N} l(y_n \neq f(\boldsymbol{x}_n; \boldsymbol{\theta}))$$

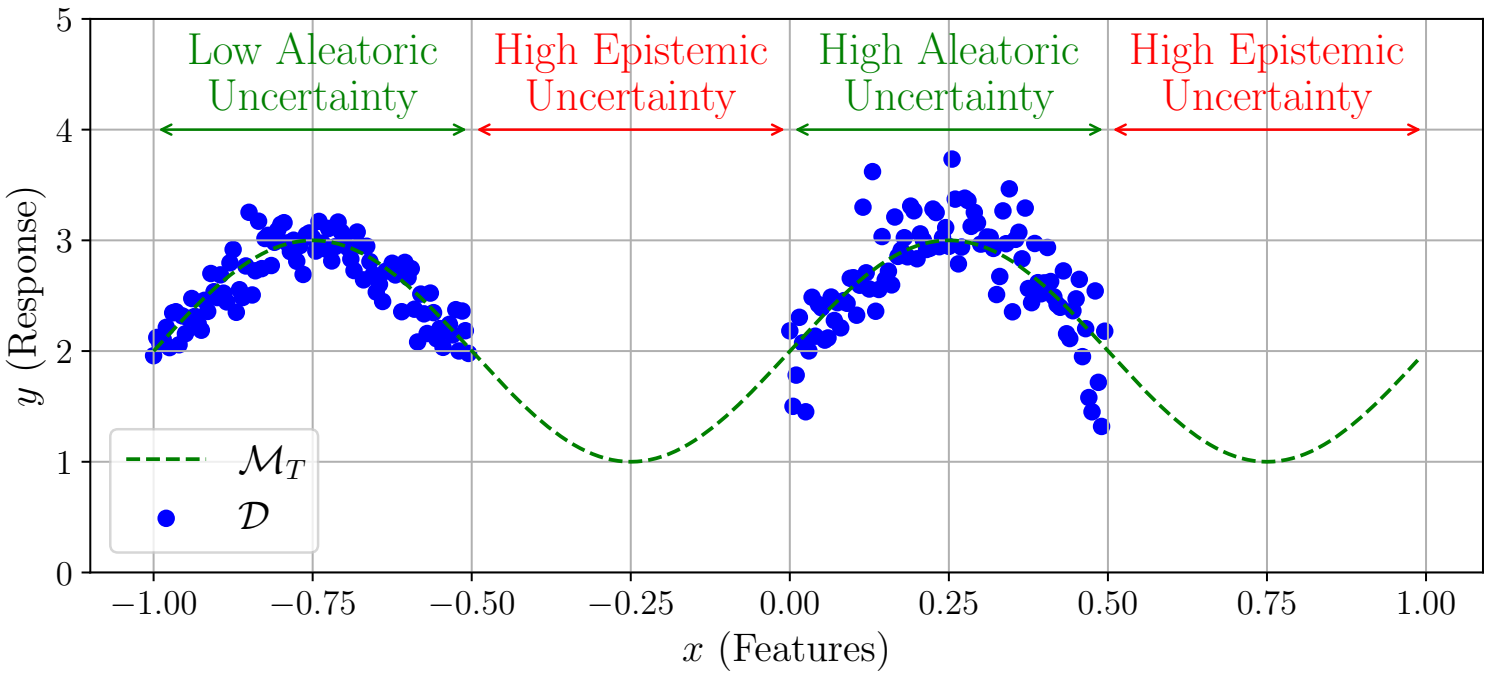
Uncertainty [2]

Epistemic Uncertainty (Model Uncertainty)

Uncertainty originated from lack of knowledge about true input-output mapping

Aleatoric Uncertainty (Data Uncertainty)

Uncertainty originated from inherent randomness in experiment E



Uncertainty in Classification

Capturing Uncertainty

To capture uncertainty, we can define *Conditional Probability Density* (CPD) as:

$$p(y = c|\boldsymbol{x}; \boldsymbol{\theta}) = f_c(\boldsymbol{x}; \boldsymbol{\theta}), \ \begin{cases} 0 \leq f_c \leq 1 \\ \sum_{c=1}^{C} f_c = 1 \end{cases}$$

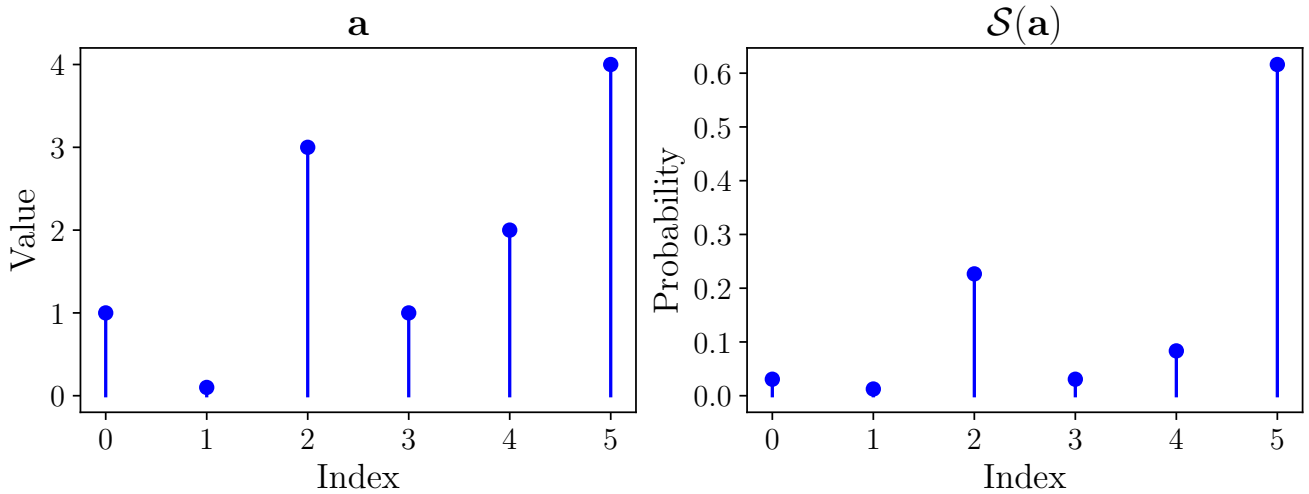
Softmax Function

Consider the *logits* vector defined as:

$$\boldsymbol{a} \triangleq [a_1, \ldots, a_C] = [f_1(\boldsymbol{x}; \boldsymbol{\theta}), \ldots, f_C(\boldsymbol{x}; \boldsymbol{\theta})] = \boldsymbol{f}(\boldsymbol{x}; \boldsymbol{\theta})$$

The softmax function for this vector is defined as:

$$\boldsymbol{\mathcal{S}} \triangleq \left[\frac{e^{a_1}}{\sum_{c'=1}^{C} e^{a_{c'}}}, \ldots, \frac{e^{a_C}}{\sum_{c'=1}^{C} e^{a_{c'}}} \right]$$



Application of Softmax Function in Classification

Capturing Uncertainty Using Softmax Function

Previously we define:

$$p(y = c|\boldsymbol{x}; \boldsymbol{\theta}) = f_c(\boldsymbol{x}; \boldsymbol{\theta}), \ \begin{cases} 0 \leq f_c \leq 1 \\ \sum_{c=1}^{C} f_c = 1 \end{cases}$$

Now using softmax we have:

$$p(y = c|\boldsymbol{x}; \boldsymbol{\theta}) = \boldsymbol{\mathcal{S}}_c(\boldsymbol{f}(\boldsymbol{x}; \boldsymbol{\theta}))$$

where the following constraints are met:

$$0 \leq \boldsymbol{\mathcal{S}}_c(\boldsymbol{f}(\boldsymbol{x}; \boldsymbol{\theta})) \leq 1, \ c = 1, 2, \ldots, C$$

$$\sum_{c=1}^{C} \boldsymbol{\mathcal{S}}_c(\boldsymbol{f}(\boldsymbol{x}; \boldsymbol{\theta})) = 1$$

Fitting Probabilistic Model

Maximum Likelihood Estimation

One approach to fit probabilistic models is *Maximum Likelihood Estimation* (MLE). We can equivalently define loss function as:

$$l(y, f(\boldsymbol{x}; \boldsymbol{\theta})) = -\log p(y|f(\boldsymbol{x}; \boldsymbol{\theta}))$$

Using above loss, the *Negative Log Likelihood* (NLL) over training set is:

$$\text{NLL}(\boldsymbol{\theta}) = -\frac{1}{N} \sum_{n=1}^{N} \log p(y_n|f(\boldsymbol{x}_n; \boldsymbol{\theta}))$$

Then the MLE for model parameters is:

$$\widehat{\boldsymbol{\theta}}_{mle} = \underset{\boldsymbol{\theta}}{\text{argmin}} \ \text{NLL}(\boldsymbol{\theta})$$

Subsection 2

Regression

Supervised Learning - Regression

Regression

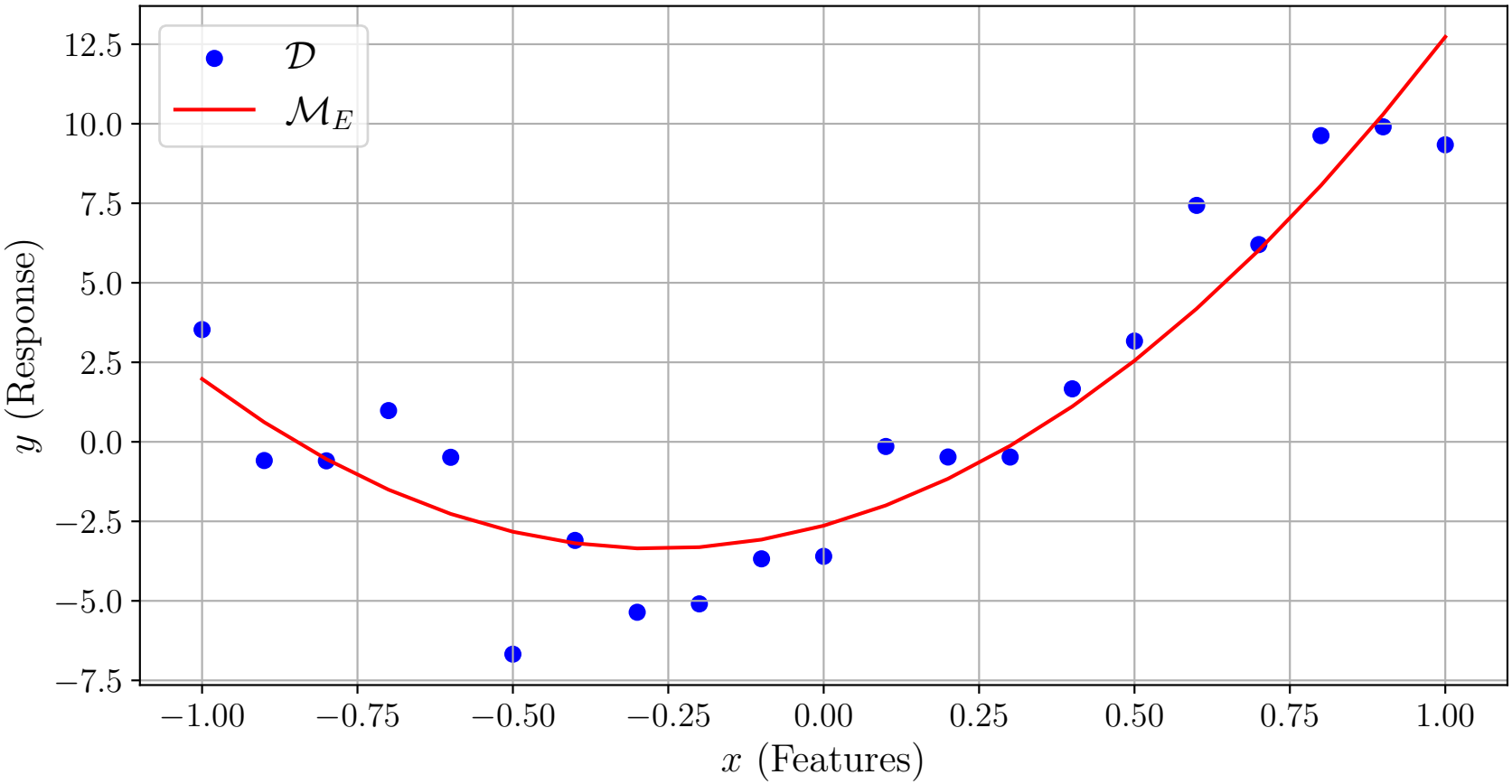
General Features:

- Task T: Finding mapping $f : \boldsymbol{x} \mapsto \boldsymbol{y}$ ($\boldsymbol{x} \in \mathcal{X} = \mathbb{R}^D$ and $y \in \mathcal{Y}$)
- Experience E: Set of N input-output pairs $\mathcal{D} = \{(\boldsymbol{x}_n, \boldsymbol{y}_n)\}_{n=1}^N$

Specific Features:

- $\mathcal{Y} = \mathbb{R}$
- $P = \frac{1}{N} \sum_{n=1}^N (y_n - f(\boldsymbol{x}_n; \boldsymbol{\theta}))^2$
  - P is known as *Mean Square Error* (MSE)

Example - One Dimensional Curve Fitting



Model Fitting in Regression

Model Fitting via ERM

Similar to classification, model parameters for regression problem can be found via ERM as:

$$\widehat{\boldsymbol{\theta}} = \underset{\boldsymbol{\theta}}{\operatorname{argmin}} \overbrace{\frac{1}{N}\sum_{n=1}^{N}(y_n - f(\boldsymbol{x}_n;\boldsymbol{\theta}))^2}^{\text{MSE}(\boldsymbol{\theta})}$$

Capturing Uncertainty in Regression

To capture uncertainty, we assume the output distribution to be Gaussian (Normal) as:

$$\mathcal{N}(y|\mu,\sigma^2) \triangleq \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2\sigma^2}(y-\mu)^2}$$

We make the mean depend on the inputs by defining $\mu \triangleq f(\boldsymbol{x}_n, \boldsymbol{\theta})$. Then we have the following CPD:

$$p(y|\boldsymbol{x};\boldsymbol{\theta}) = \mathcal{N}(y|f(\boldsymbol{x};\boldsymbol{\theta}),\sigma^2)$$

Subsection 3

Generalization

Overfitting and Generalization

Population Risk

Consider $p^\star(\boldsymbol{x}, y)$ to be the true generating distribution of training set. Then population risk is defined as:

$$\mathcal{L}(\boldsymbol{\theta}; p^\star) \triangleq \mathbb{E}_{p^\star(\boldsymbol{x},y)}[l(y, f(\boldsymbol{x}; \boldsymbol{\theta}))]$$

Generalization Gap

The difference $\mathcal{L}(\boldsymbol{\theta}; p^\star) - \mathcal{L}(\boldsymbol{\theta}; \mathcal{D}_{train})$ is called generalization gap where $\mathcal{L}(\boldsymbol{\theta}; \mathcal{D}_{train})$ is ERM defiend as:

$$\mathcal{L}(\boldsymbol{\theta}; \mathcal{D}_{train}) = \frac{1}{|\mathcal{D}_{train}|} \sum_{(\boldsymbol{x}_n, y_n) \in \mathcal{D}_{train}} l(y_n, f(\boldsymbol{x}_n; \boldsymbol{\theta}))$$

Overfitting

Overfitting occure when the generalization gap is large.

Population Risk

Population Risk Estimation

- In practice, we don't know $p^\star(\boldsymbol{x}, y)$.
- We partition the data into two subsets, known as the training set and test set.
- We use test set to estimate population risk as:

$$\mathcal{L}(\boldsymbol{\theta}; \mathcal{D}_{test}) = \frac{1}{|\mathcal{D}_{test}|} \sum_{(\boldsymbol{x}_n, y_n) \in \mathcal{D}_{test}} l(y_n, f(\boldsymbol{x}_n; \boldsymbol{\theta}))$$

Subsection 4

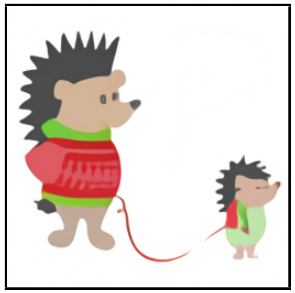
Real World Applications

Real World Classification: Super resolution [3]

Real World Classification: Image Generation [4]




(a) a tapir made of accordion. a tapir with the texture of an accordion.

(b) an illustration of a baby hedgehog in a christmas sweater walking a dog



(c) a neon sign that reads “backprop”. a neon sign that reads “backprop”. backprop neon sign

Real World Classification: Image Captioning [5]

A person riding a motorcycle on a dirt road.

Two dogs play in the grass.

A skateboarder does a trick on a ramp.

A dog is jumping to catch a frisbee.

A group of young people playing a game of frisbee.

Two hockey players are fighting over the puck.

A little girl in a pink hat is blowing bubbles.

A refrigerator filled with lots of food and drinks.

A herd of elephants walking across a dry grass field.

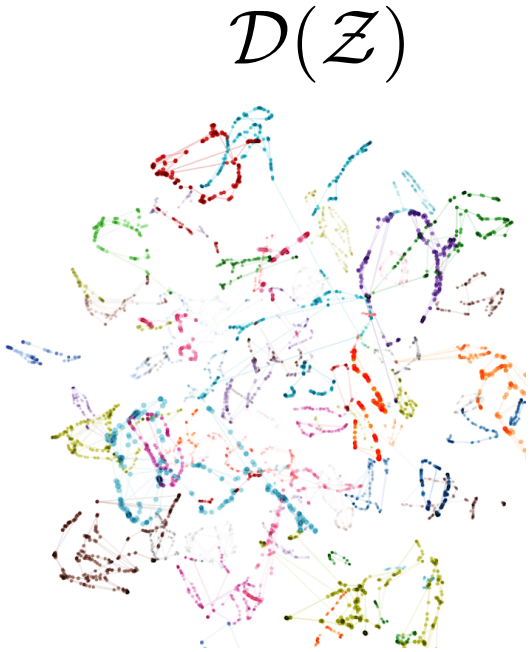
A close up of a cat laying on a couch.

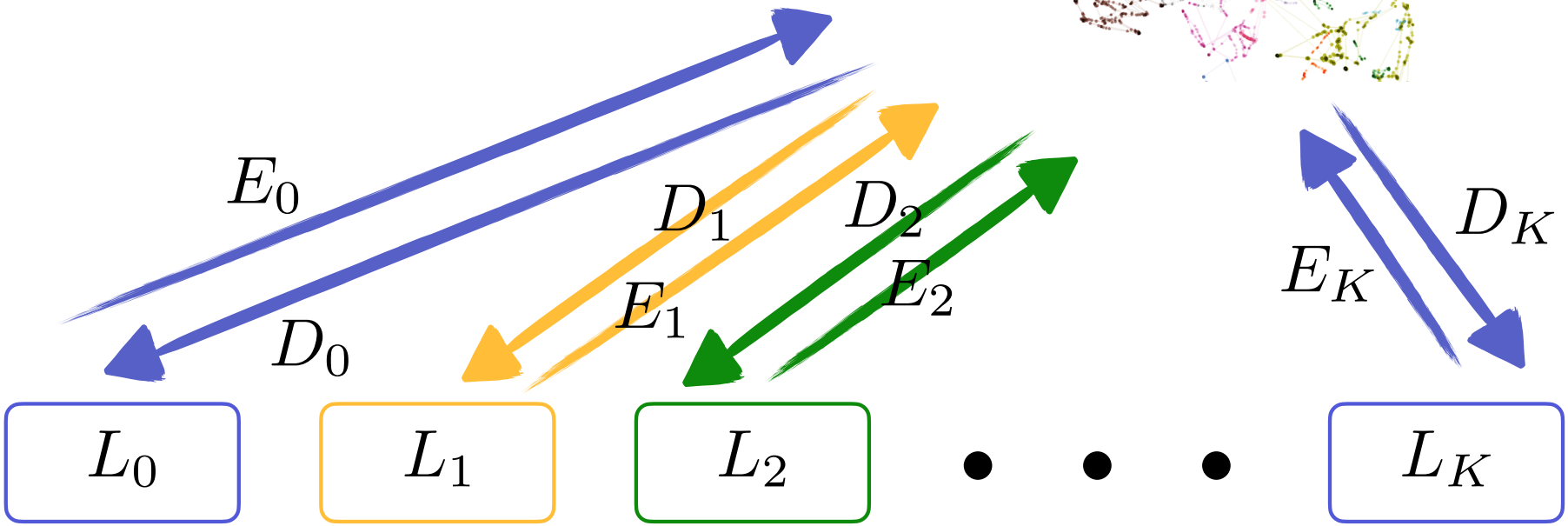
A red motorcycle parked on the side of the road.

A yellow school bus parked in a parking lot.

Real World Classification: Machine Translation [6]

Representation Space $\mathcal{Z} =$





Section 3

Unsupervised Learning

Unsupervised Learning

Unsupervised Learning is:

- Task T: Dependent on the task
- Experience E: Set of N samples $\mathcal{D} = \{\boldsymbol{x}_n\}_{n=1}^{N}$
- Performance measure P: Dependent on the task

Subsection 1

Clustering

Unsupervised Learning - Clustering

Clustering

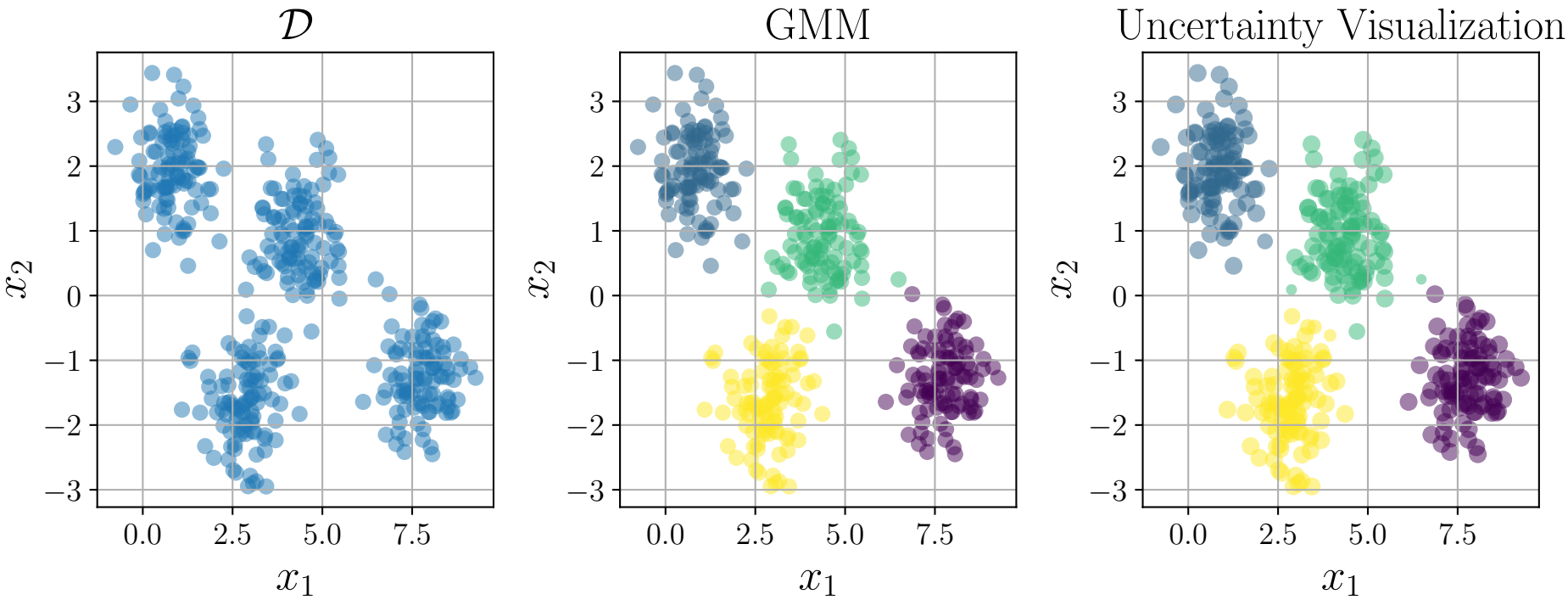
General Features:

- Experience E: Set of N samples $\mathcal{D} = \{\boldsymbol{x}_n\}_{n=1}^{N}$

Specific Features:

- Task T: Partition the input into regions that contains *similar* points.
- Performance measure in *Compression*: Compression loss

Clustering: Gaussian Mixture Model [7]



Subsection 2

Factors of Variation

Unsupervised Learning - Factors of Variation

Factors of Variation

General Features:

- Experience E: Set of N samples $\mathcal{D} = \{\boldsymbol{x}_n\}_{n=1}^{N}$

Specific Features:

- Task T: Projecting data into low dimensional subspace which captures its main aspects
- Performance measure: Performance of low dimensional data in various downstream tasks

Principle Component Analysis [8]

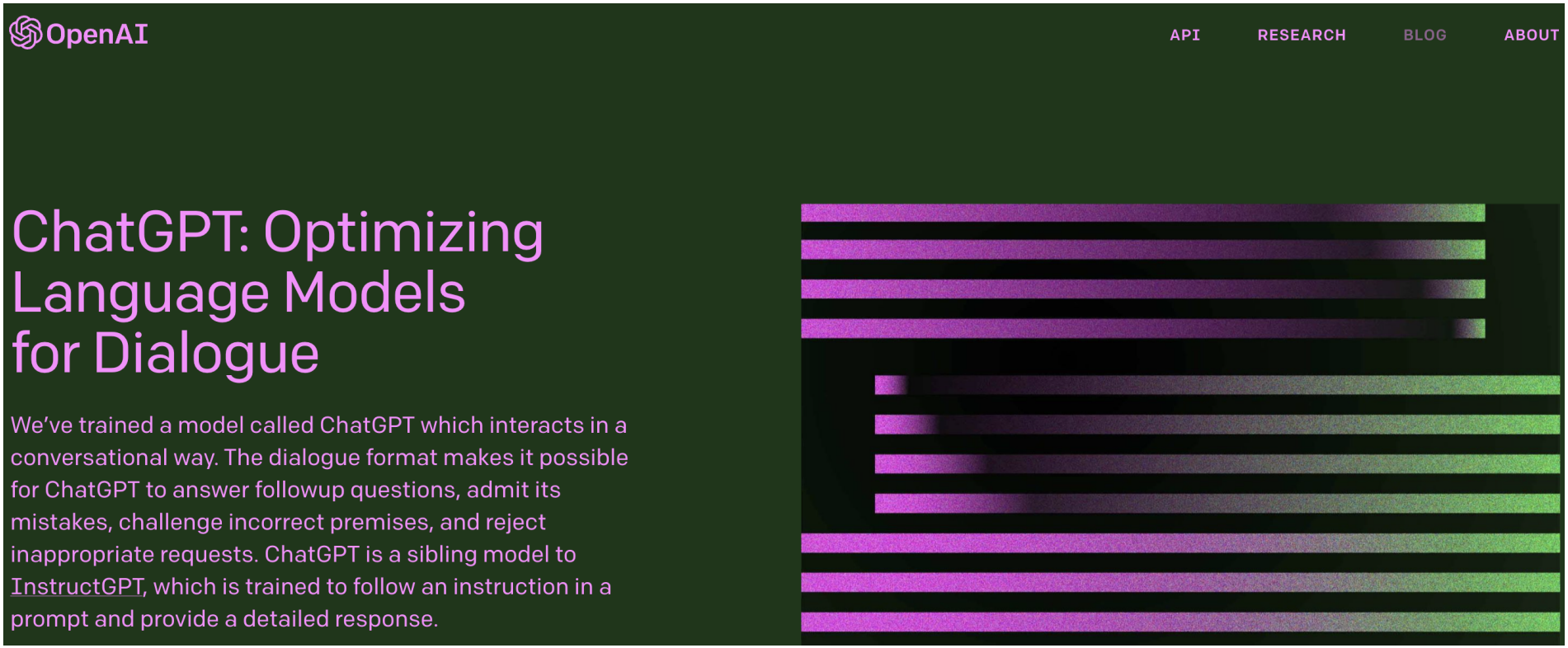
(a) Original 64×64 pixels

(b) Reconstructed from 8×8 pixels

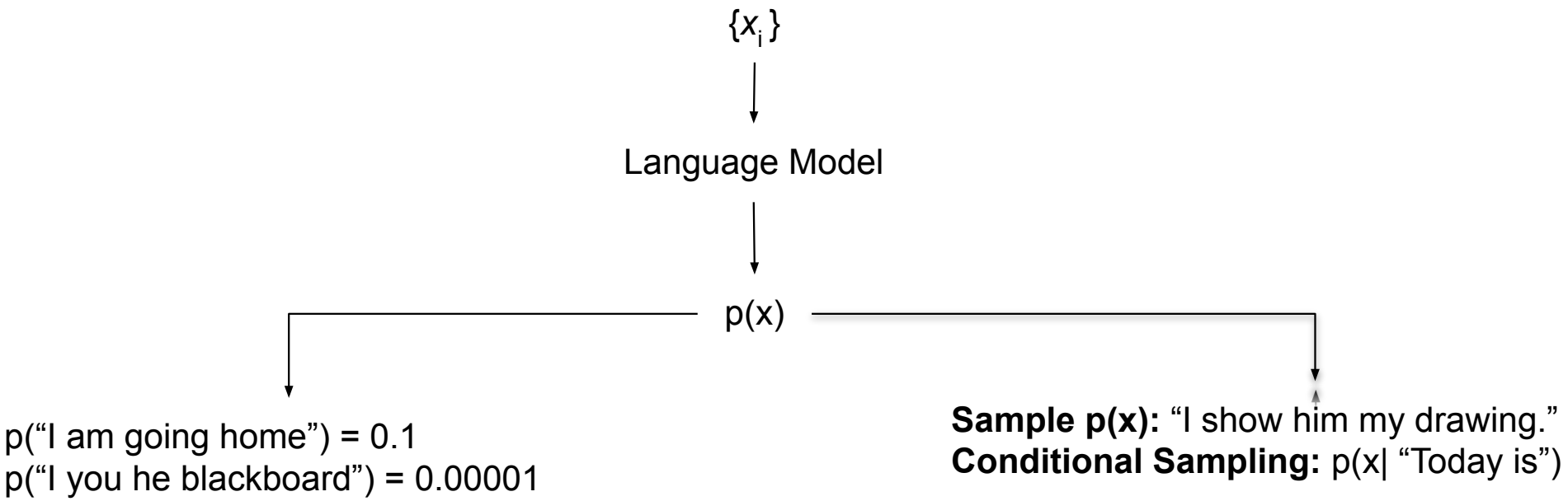
Subsection 3

Real World Applications

ChatGPT [9]


OpenAI
API
RESEARCH
BLOG
ABOUT
ChatGPT: Optimizing Language Models for Dialogue
We've trained a model called ChatGPT which interacts in a conversational way. The dialogue format makes it possible for ChatGPT to answer followup questions, admit its mistakes, challenge incorrect premises, and reject inappropriate requests. ChatGPT is a sibling model to InstructGPT, which is trained to follow an instruction in a prompt and provide a detailed response.

Language Model



Section 4

Reinforcement Learning

Reinforcement Learning

Reinforcement Learning is:

- Task T: Learning an agent to take action in different environmental conditions.
- Experience E: Set of N condition-action-reward triplet
- Performance measure P: Average reward

Reinforcement Learning

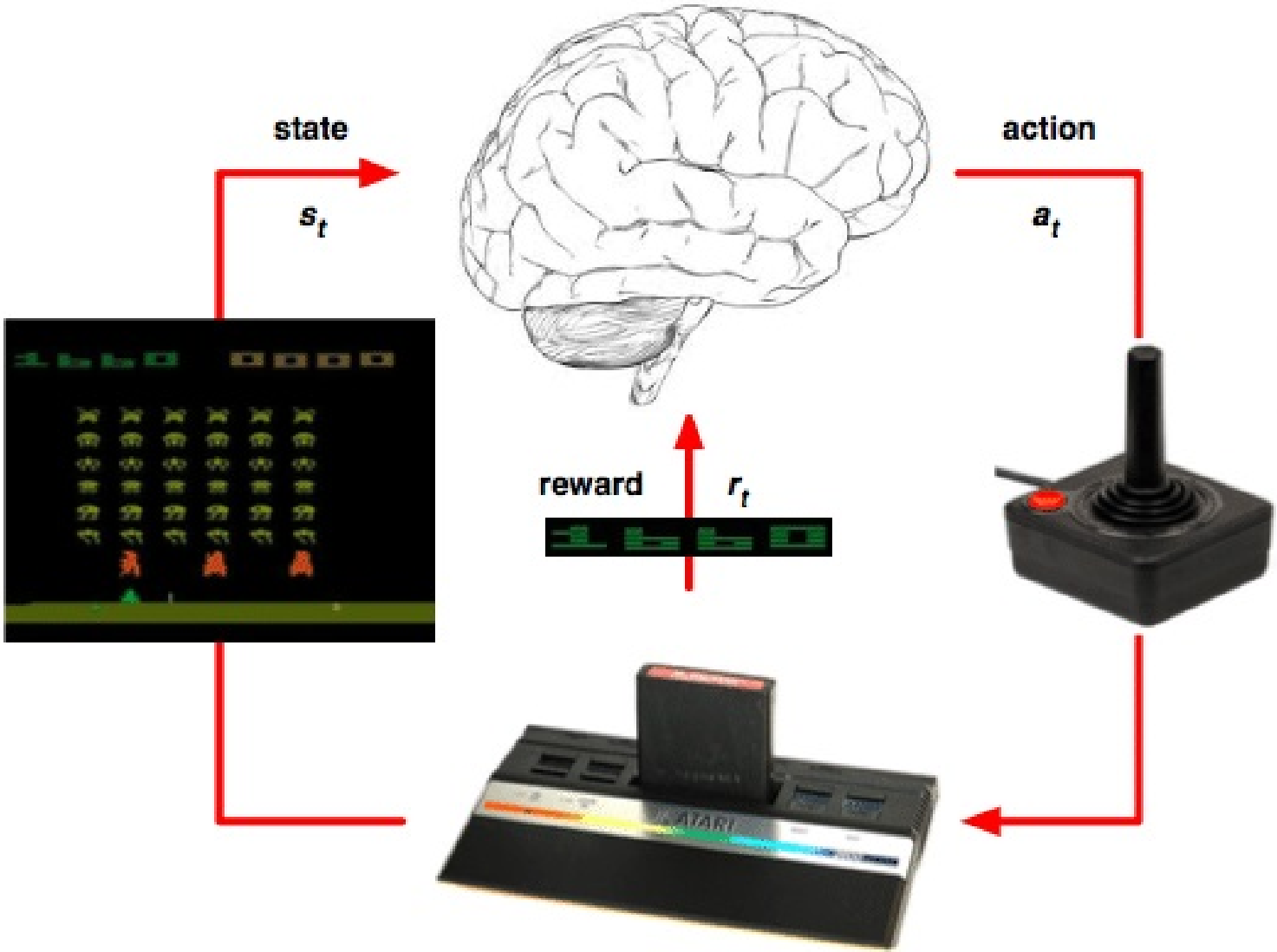
Playing an Atari game

- Task T: learning policy mapping $\boldsymbol{a} = \pi(\boldsymbol{x})$ where:
  - $\boldsymbol{a}$: Action
  - $\boldsymbol{x}$: Environmental conditions
- Experience E: Set of N triplet $\{(\boldsymbol{x}_n, \boldsymbol{a}_n, r_n)\}_{n=1}^{N}$
- Performance measure P: Maximizing the reward

Subsection 1

Real World Applications

Reinforcement Learning



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