Machine Learning: Overview

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What is machine learning?

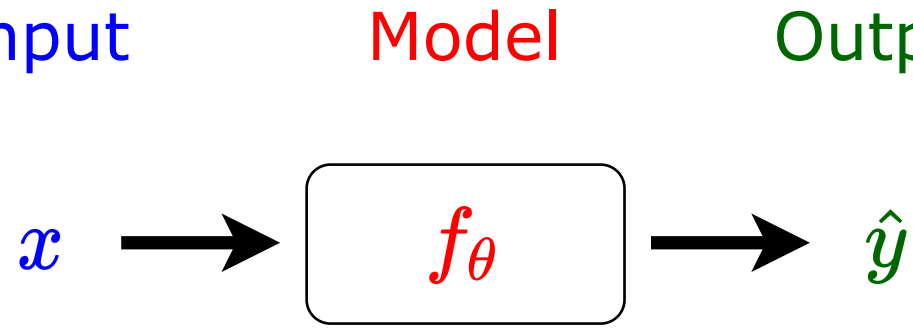
> *A computer program is said to learn from experience E with respect to some class of tasks T, and performance measure P, if its performance at tasks in T, as measured by P, improves with experience E.*
>
> — Tom Mitchell

There are many different kinds of ML, depending on

- the task T we wish the system to learn
- the performance measure P we use to evaluate the system
- the training signal or experience E we give it.

What is machine learning?

- Supervised learning. We get observed inputs $\mathcal{D} = \{\boldsymbol{x}_n : n = 1 : N\}$ and corresponding outputs y_n. We learn a mapping f from inputs to outputs.



- Unsupervised learning. We just get observed inputs $\mathcal{D}$ without any corresponding outputs. We try to make sense of data.
- Reinforcement learning. An **agent** has to learn how to interact with its environment. This can be encoded by a **policy** $a = \pi(\boldsymbol{s})$, which specifies which action a to perform in response to each possible input $\boldsymbol{s}$ (environmental state).

What is machine learning?

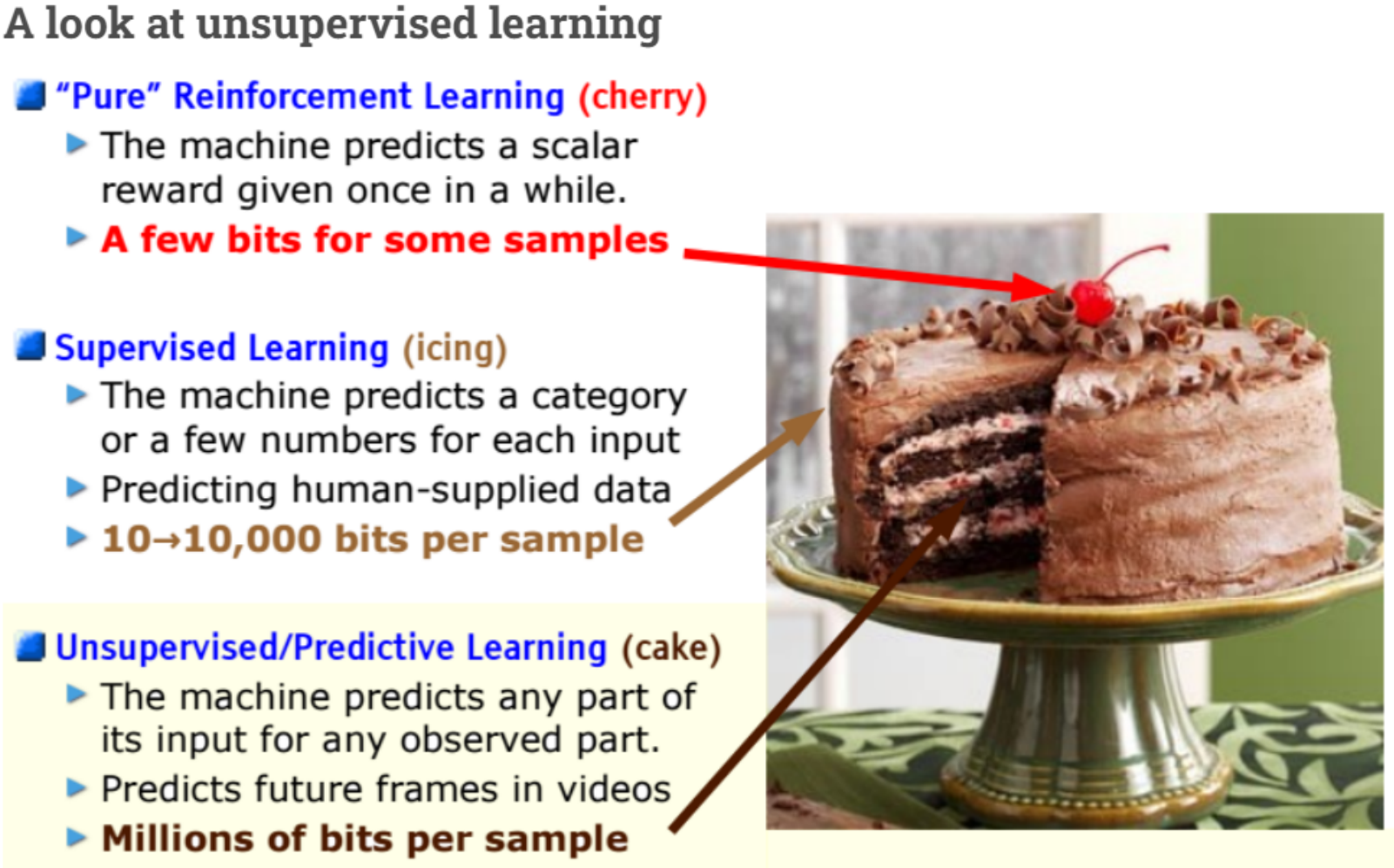


Figure: Yann LeCun's talk on Predictive Learning. *NIPS 2016*.

Supervised Learning - Classification

Learning a mapping $f_{\boldsymbol{\theta}} : \mathbb{R}^{W \times H} \to \{\text{"cat"}, \text{"non-cat"}\}$.

Input Model Output

f_θ

"cat"

Supervised Learning - Regression

Learning a mapping $f_{\boldsymbol{\theta}} : \mathbb{R}^N \to \mathbb{R}$.

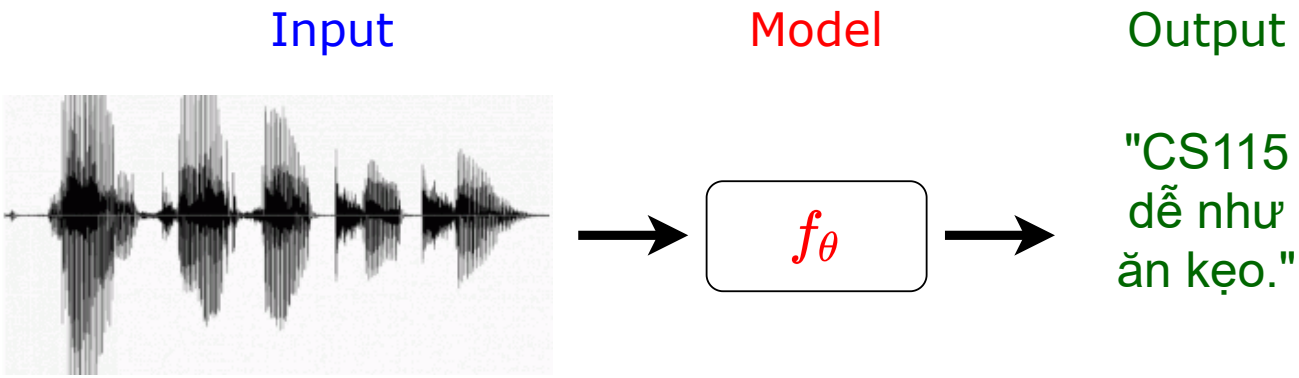
Input Model Output

f_θ

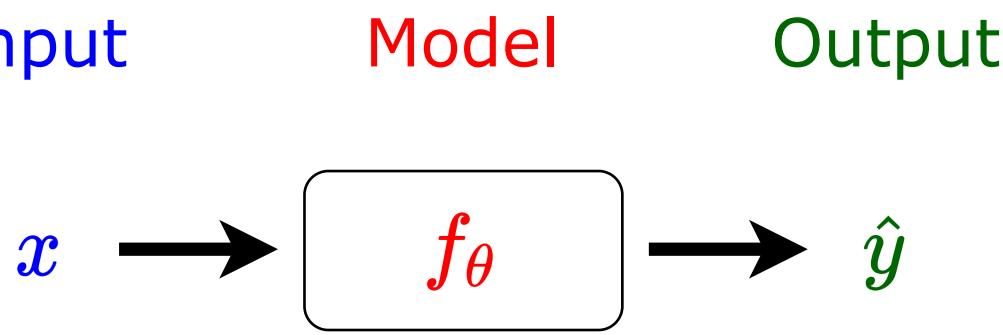
$50,312

Supervised Learning - Structured Prediction

Learning a mapping $f_{\boldsymbol{\theta}} : \mathbb{R}^N \to \{1, 2, \ldots, L\}^M$.



Supervised learning



The most common form of ML is **supervised learning**.

- The task T is to learn a mapping f from inputs $\boldsymbol{x} \in \mathcal{X}$ to outputs $y \in \mathcal{Y}$: Estimate **parameters $\boldsymbol{\theta}$** from training data $\{(\boldsymbol{x}_n, y_n)\}_{n=1}^N$.
- The inputs $\boldsymbol{x}$ are also called the **features**, or **predictors**.
- The output y is also known as the **label**, **target**, or **response**.
- The experience E is a set of N input-output pairs $\mathcal{D} = \{(\boldsymbol{x}_n, y_n)\}_{n=1}^N$, known as the **training set**. N is called the **sample size**.
- The performance measure P depends on the type of output we are predicting.

Classification

In **classification** problems, the output space is

- a set of C unordered and mutually exclusive labels known as **classes** $\mathcal{Y} = \{1, 2, \ldots, C\}$.
- If there are just two classes, $y \in \{0, 1\}$ or $y \in \{+1, -1\}$, it is called **binary classification**.

(a) (b) (c)

Figure: Classifying Iris flowers into 3 subspecies: setosa, versicolor and virginica.

Classification

In **image classification**,

- The $\mathcal{X}$ is the set of images, which is very high-dimensional.
- For a color image with $C = 3$ channels (RGB) and $D_1 \times D_2$ pixels, we have $\mathcal{X} = \mathbb{R}^D$, where $D = C \times D_1 \times D_2$.
- Learning a mapping $f : \mathcal{X} \to \mathcal{Y}$ from images to labels is challenging.

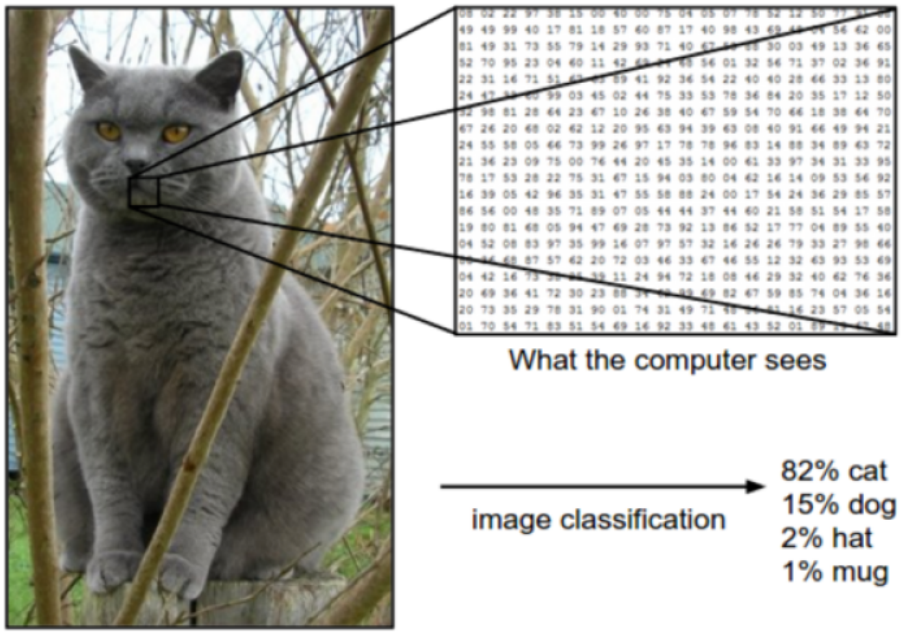


Figure: Illustration of the image classification problem.

Classification

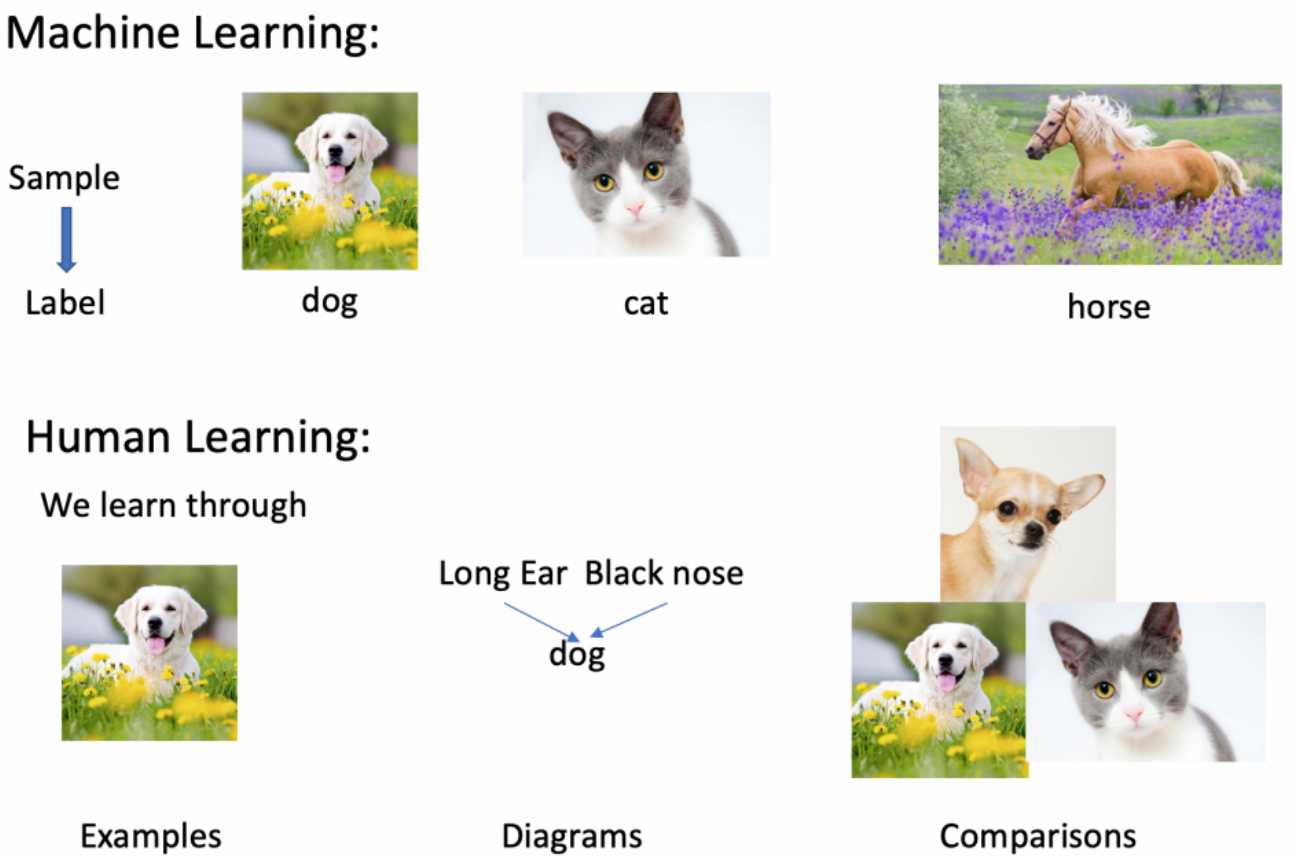


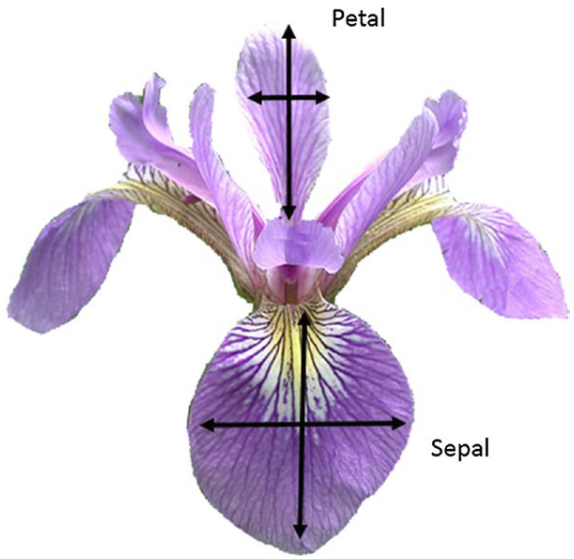
Figure: Machine learning vs. Human learning[1]

[1] https://blog.ml.cmu.edu/2019/03/29/building-machine-learning-models-via-comparisons/

Classification

The **Iris dataset** is a collection of 150 labeled examples of Iris flowers, 50 of each type, described by 4 features

- sepal length, sepal width, petal length, petal width.
- The input space is much lower-dimensional $\mathcal{X} = \mathbb{R}^4$.
- These numeric features are highly informative.

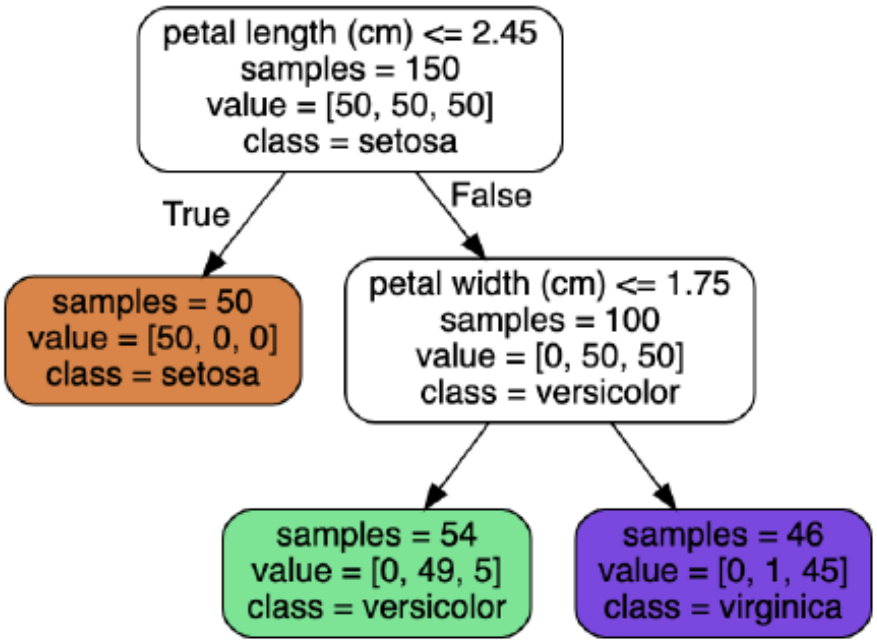


index	sl	sw	pl	pw	label
0	5.1	3.5	1.4	0.2	setosa
1	4.9	3.0	1.4	0.2	setosa
	...				
50	7.0	3.2	4.7	1.4	Versicolor
	...				
149	5.9	3.0	5.1	1.8	Virginica

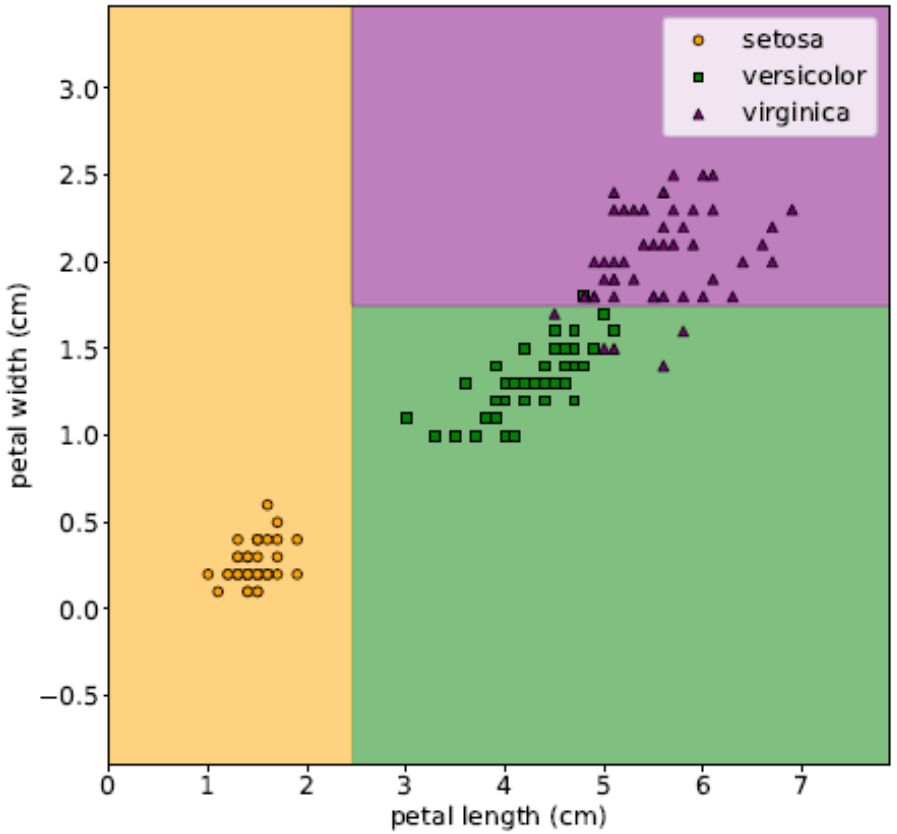
Figure: A subset of the Iris design matrix.

- A small dataset of features can be stored as an $N \times D$ **design matrix**.

Learning a classifier



(a)



(b)

Figure: A decision tree on Iris dataset, using just petal length and width features.

Learning a classifier

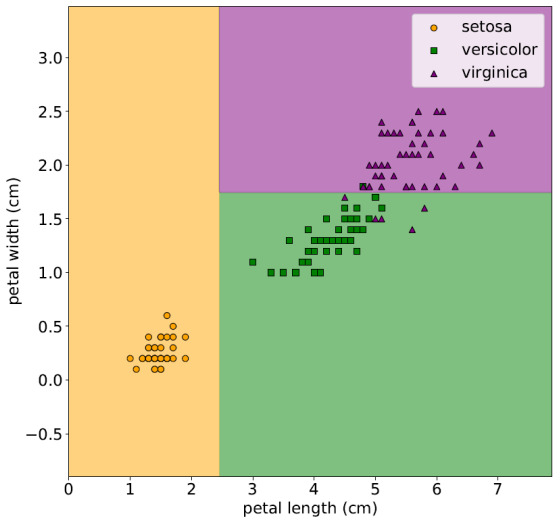


Figure: Decision surface

- We apply a **decision rule** to the Iris dataset

$$f_1(\boldsymbol{x};\boldsymbol{\theta}) = \begin{cases} \text{Setosa if petal length} < 2.45 \\ \text{Versicolor or Virginica otherwise} \end{cases}$$

- This rule defines a 1d **decision boundary** at $x_{\text{petal length}} = 2.45$, partitioning the input space into 2 regions.
- We add another **decision rule** to inputs that fail the first rule.

$$f_2(\boldsymbol{x};\boldsymbol{\theta}) = \begin{cases} \text{Versicolor if petal width} < 1.75 \\ \text{Virginica otherwise} \end{cases}$$

- Both rules induces a 2d **decision surface**.

Learning a classifier

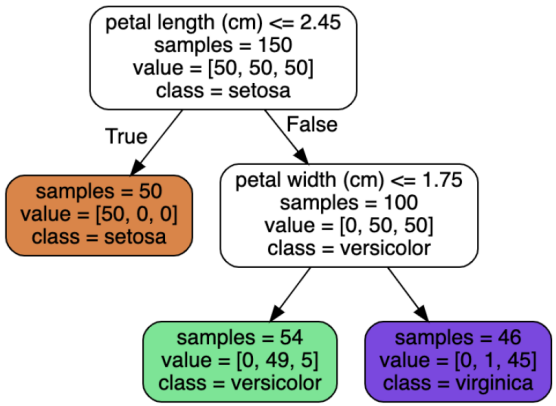


Figure: Decision tree

- We can arrange the rules f_1, f_2 into a tree structure, called a **decision tree**.
- We can represent the tree by storing, for each internal node:
  - the feature index that is used.
  - the corresponding threshold value.
- We denote all these **parameters** by $\boldsymbol{\theta}$.

Empirical risk minimization

The goal of supervised learning is

- to automatically come up with classification models.
- to reliably predict the labels for any given input.

The **misclassification rate** on the training set can be used to measure performance on this task:

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

where $\mathbb{I}(e)$ is the binary **indicator function**:

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

This assumes all errors are equal.

Empirical risk minimization

- It may happen that some erros are more costly than others.
- Suppose that setosa & Versicolor are tasty but Virginica is poisonous.
- We might use the asymmetric **loss function** $\ell(y, \hat{y})$ as below.

		Estimate		
		Setosa	Versicolor	Virginica
Truth	Setosa	0	1	1
	Versicolor	1	0	1
	Virginica	10	10	0

The **empirical risk** is the average loss of the predictor on the training set:

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

The misclassification rate is equal to the empirical risk when we use **zero-one loss**:

$$\ell_{01}(y, \hat{y}) = \mathbb{I}(y \neq \hat{y})$$

Empirical risk minimization

The problem of **model fitting** or **training** can be defined as finding a setting of parameters that minimizes the empirical risk on the training set:

$$\hat{\boldsymbol{\theta}} = \operatorname*{argmin}_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{\theta}) = \operatorname*{argmin}_{\boldsymbol{\theta}} \frac{1}{N} \sum_{n=1}^{N} \ell(y_n, f(\boldsymbol{x}_n; \boldsymbol{\theta}))$$

This is called **empirical risk minimization**.

However, our true goal is:

- to minimize the expected loss on **future data** that we have not seen,
- to **generalize**, rather than just do well on the training set.

Uncertainty

We can't perfectly predict the exact output given the input, due to

- lack of knowledge of the input-output mapping (**model uncertainty**)
- and/or intrinsic (irreducible) stochasticity in the mapping (**data uncertainty**).

We capture our uncertainty using **conditional probability distribution**:

$$p(y = c|\boldsymbol{x}; \boldsymbol{\theta}) = f_c(\boldsymbol{x}; \boldsymbol{\theta})$$

where $f : \mathcal{X} \to [0, 1]^C$ maps inputs to a probability distribution over the C possible output labels.

Uncertainty

Since $f_c(\boldsymbol{x}; \boldsymbol{\theta})$ returns the probability of class label c, we require

$$0 \leq f_c \leq 1 \text{ for each } c, \text{ and } \sum_{c=1}^{C} f_c = 1$$

To avoid this restriction, it is common to require the model to return unnormalized log-probabilities. We can then use the **softmax function** to convert these to probabilities

$$\mathcal{S}(\boldsymbol{a}) = \left[\frac{e^{a_1}}{\sum_{c=1}^{C} e^{a_c}}, \ldots, \frac{e^{a_C}}{\sum_{c=1}^{C} e^{a_c}} \right]$$

$\mathcal{S} : \mathbb{R}^C \to [0,1]^C$, and satisfied $0 \leq \mathcal{S}(\boldsymbol{a})_c \leq 1$ and $\sum_{c=1}^{C} \mathcal{S}(\boldsymbol{a})_c = 1$.

The inputs to the softmax, $\boldsymbol{a} = f(\boldsymbol{x}; \boldsymbol{\theta})$, are called **logits**.

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

Uncertainty

The overall model is defined as

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

A special case is when f is an **affine function**

$$f(\boldsymbol{x}; \boldsymbol{\theta}) = b + \boldsymbol{w}^T \boldsymbol{x} = b + w_1 x_1 + w_2 x_2 + \ldots + w_D x_D$$

where $\boldsymbol{\theta} = (b, \boldsymbol{w})$ are the parameters of the model. $\boldsymbol{w}$ are called the **weights** and b is called the **bias**. This model is called **logistic regression**. We can define $\tilde{\boldsymbol{w}} = [b, w_1, \ldots, w_D]$ and $\tilde{\boldsymbol{x}} = [1, x_1, \ldots, x_D]$ so that

$$\tilde{\boldsymbol{w}}^T \tilde{\boldsymbol{x}} = b + \boldsymbol{w}^T \boldsymbol{x}$$

This converts the affine function into a **linear function**. For simplicity, we can just write the prediction function as

$$f(\boldsymbol{x}; \boldsymbol{\theta}) = \boldsymbol{w}^T \boldsymbol{x}$$

Maximum likelihood estimation

- When fitting probabilistic models, we can use the **negative log probability** as our loss function:

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

- A good model is one that assigns a high probability to the true output y for each corresponding input $\boldsymbol{x}$
- The average negative log probability of the training set is given by

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

- This is called the **negative log likelihood**.
- If we minimize this, we can compute the **maximum likelihood estimate** (MLE):

$$\hat{\boldsymbol{\theta}}_{\text{MLE}} = \underset{\boldsymbol{\theta}}{\operatorname{argmin}}\, \text{NLL}(\boldsymbol{\theta})$$

Regression

- Suppose we want to predict a real-valued quantity $y \in \mathbb{R}$ instead of a class label $y \in \{1, \ldots, C\}$.
- E.g., in the case of Iris flowers, y might be the average height of the plant, or the degree of toxicity.

This type of problem is known as **regression**.

Regression

- Regression is very similar to classification, but since the output $\hat{y} = f(\boldsymbol{x}; \boldsymbol{\theta})$ is real-valued, we need to use a different loss function.
- Why don't we use the misclassification rate with the zero-one loss?

$$\mathcal{L}(\boldsymbol{\theta}) = \frac{1}{N} \sum_{n=1}^{N} \ell_{01}(y, \hat{y}) = \frac{1}{N} \sum_{n=1}^{N} \mathbb{I}(y_n \neq f(\boldsymbol{x}_n; \boldsymbol{\theta}))$$

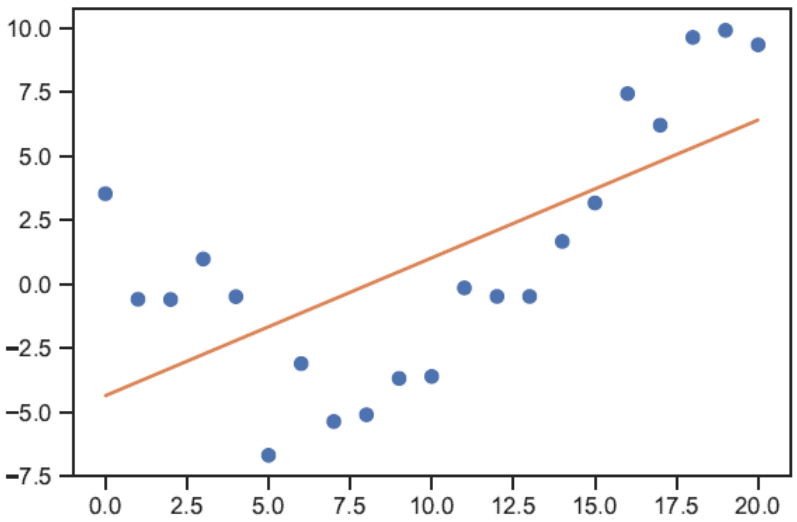
- The most common choice is **quadratic loss**, or ℓ_2 loss.

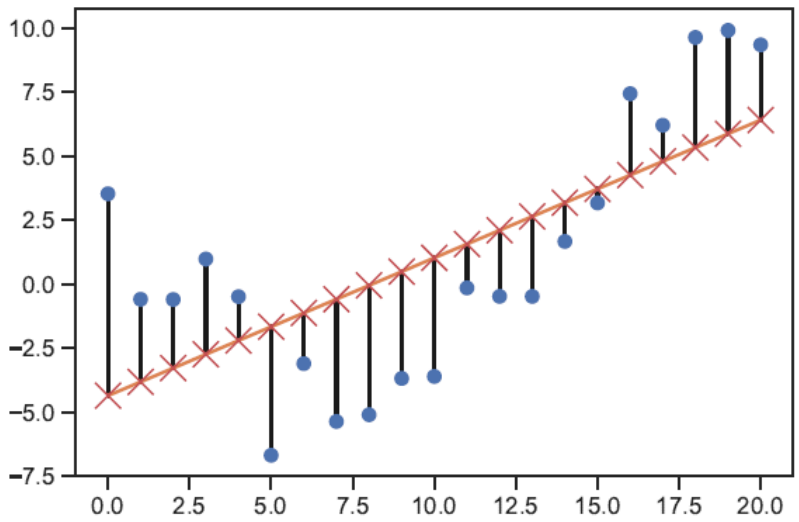
$$\ell_2(y, \hat{y}) = (y - \hat{y})^2$$

- This penalizes large **residuals** $y - \hat{y}$ more than small ones.
- The empirical risk when using quadratic loss is equal to the **mean squared error** (MSE):

$$\mathcal{L}(\boldsymbol{\theta}) = \text{MSE}(\boldsymbol{\theta}) = \frac{1}{N} \sum_{n=1}^{N} (y_n - f(\boldsymbol{x}_n; \boldsymbol{\theta}))^2$$

Linear Regression





We can fit the 1d data above using a **simple linear regression** model:

$$f(x; \boldsymbol{\theta}) = b + wx$$

where w is the **slope**, and b is the **offset**. $\boldsymbol{\theta} = (w, b)$ are the parameters of the model. By adjusting $\boldsymbol{\theta}$, we can minimize the sum of squared errors until we find the **least squares solution**:

$$\hat{\boldsymbol{\theta}} = \underset{\boldsymbol{\theta}}{\operatorname{argmin}} \, \mathrm{MSE}(\boldsymbol{\theta})$$

Linear Regression

If we have multiple input features, we can write

$$f(\boldsymbol{x};\boldsymbol{\theta}) = b + w_1 x_1 \ldots + w_D x_D = b + \boldsymbol{w}^T \boldsymbol{x}$$

where $\boldsymbol{\theta} = (\boldsymbol{w}, b)$. This is called **multiple linear regression**.

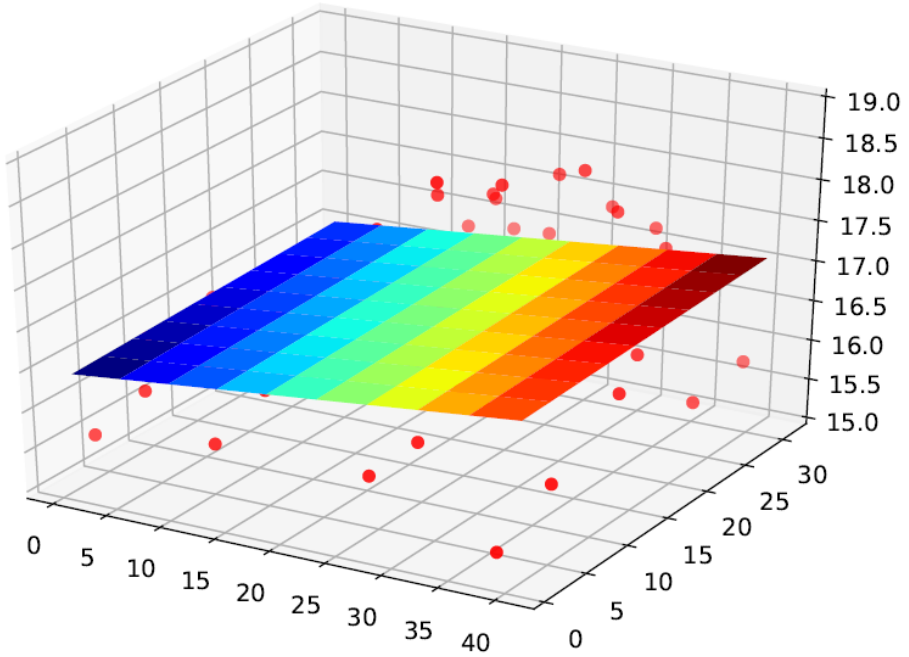
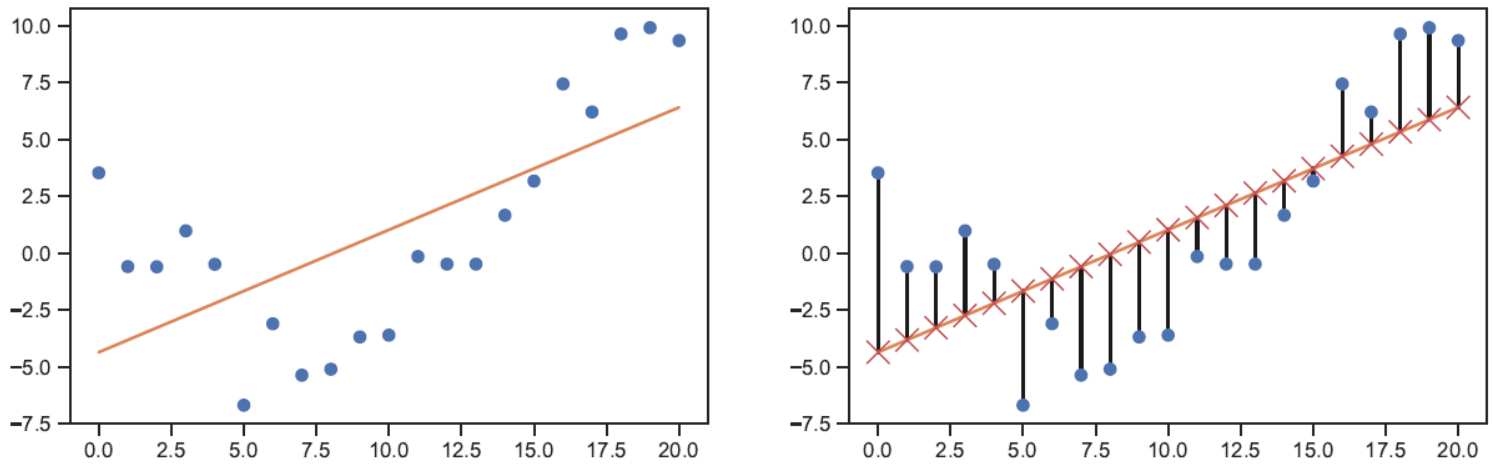


Figure: We predict the temperature as a function of 2d location in a room. Linear model: $f(\boldsymbol{x};\boldsymbol{\theta}) = b + w_1 x_1 + w_2 x_2$

Polynomial regression



We can improve the fit by a **polynomial regression** model of degree D:

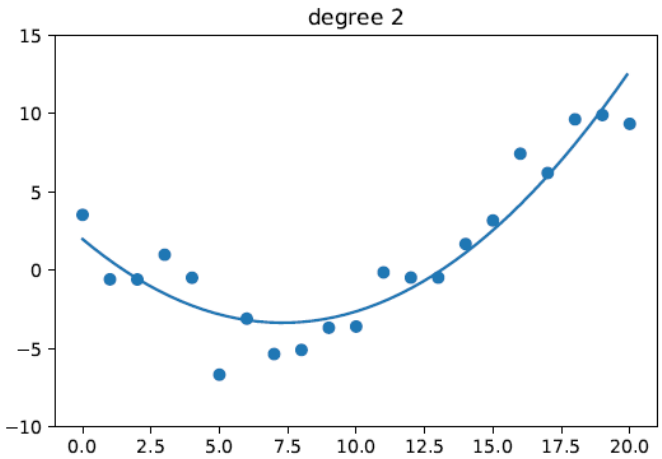
$$f(x; \boldsymbol{w}) = \boldsymbol{w}^T \phi(x)$$

where $\phi(x)$ is a feature vector derived from the input:

$$\phi(x) = [1, x, x^2, \ldots, x^D]$$

This is an example of **feature engineering**.

Polynomial regression



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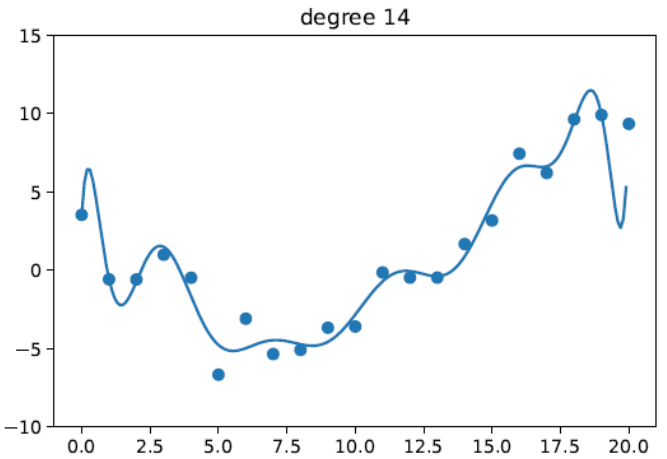

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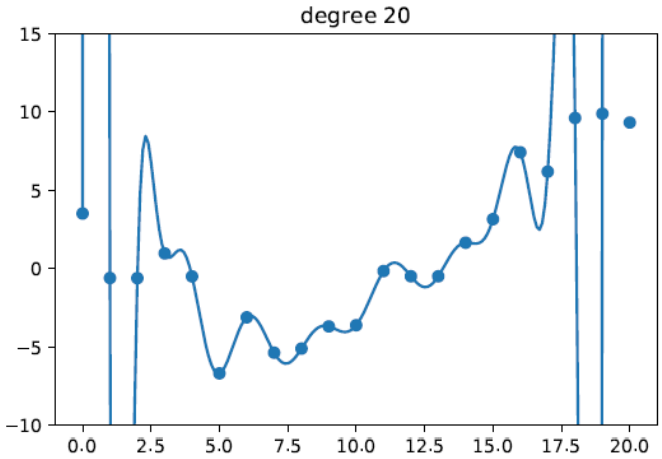

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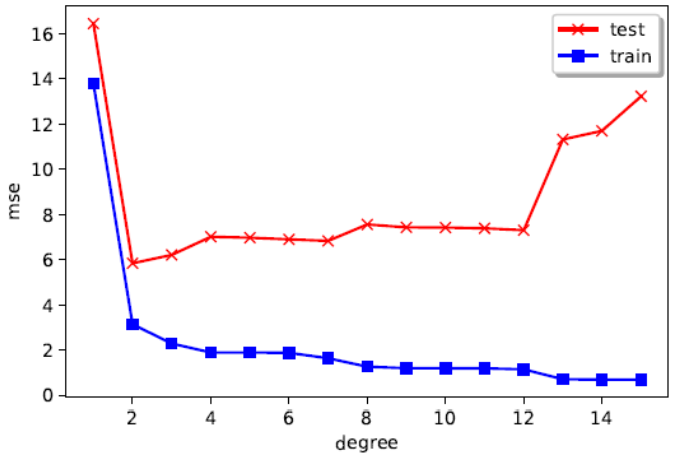
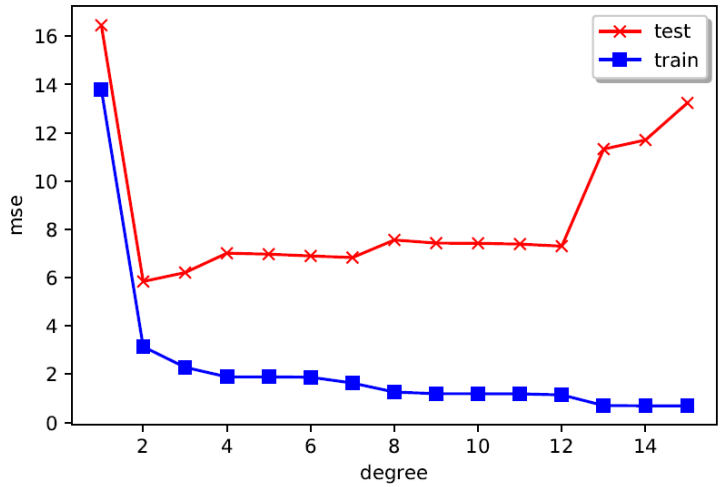


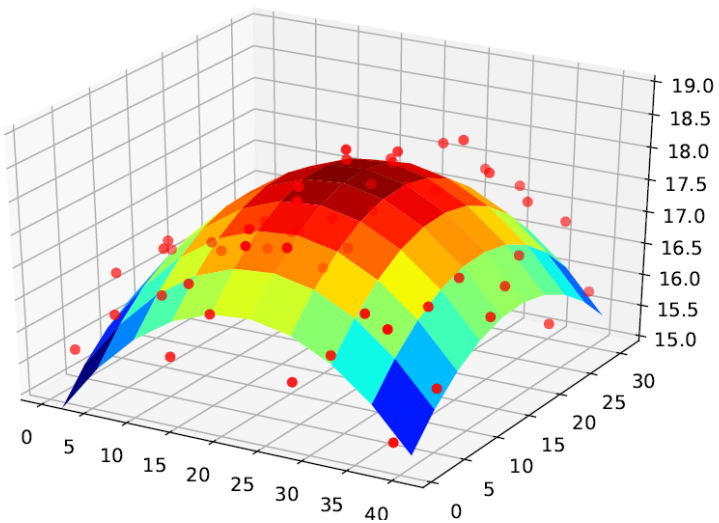
(d)

Polynomial regression



- Using $D = 2$ results in a much better fit.
- We can keep increasing D, and hence the number of parameters in the model, until $D = N - 1$.
- In this case, we have one parameter per data point, so we can perfectly **interpolate** the data. The resulting model will have 0 MSE.
- However, the resulting function will not be a good predictor.
- A model that perfectly fits the training data, but which is too complex, is said to suffer from **overfitting**.

Polynomial regression



- We can apply polynomial regression to multi-dimensional inputs.
- For example, we use a quadratic expansion of the inputs as the prediction function for the temperature model

$$f(\boldsymbol{x}; \boldsymbol{w}) = w_0 + w_1 x_1 + w_2 x_2 + w_3 x_1^2 + w_4 x_2^2$$

- The prediction function is still a linear function of the parameters $\boldsymbol{w}$, even though it is a nonlinear function of the original input $\boldsymbol{x}$.

Deep neural networks

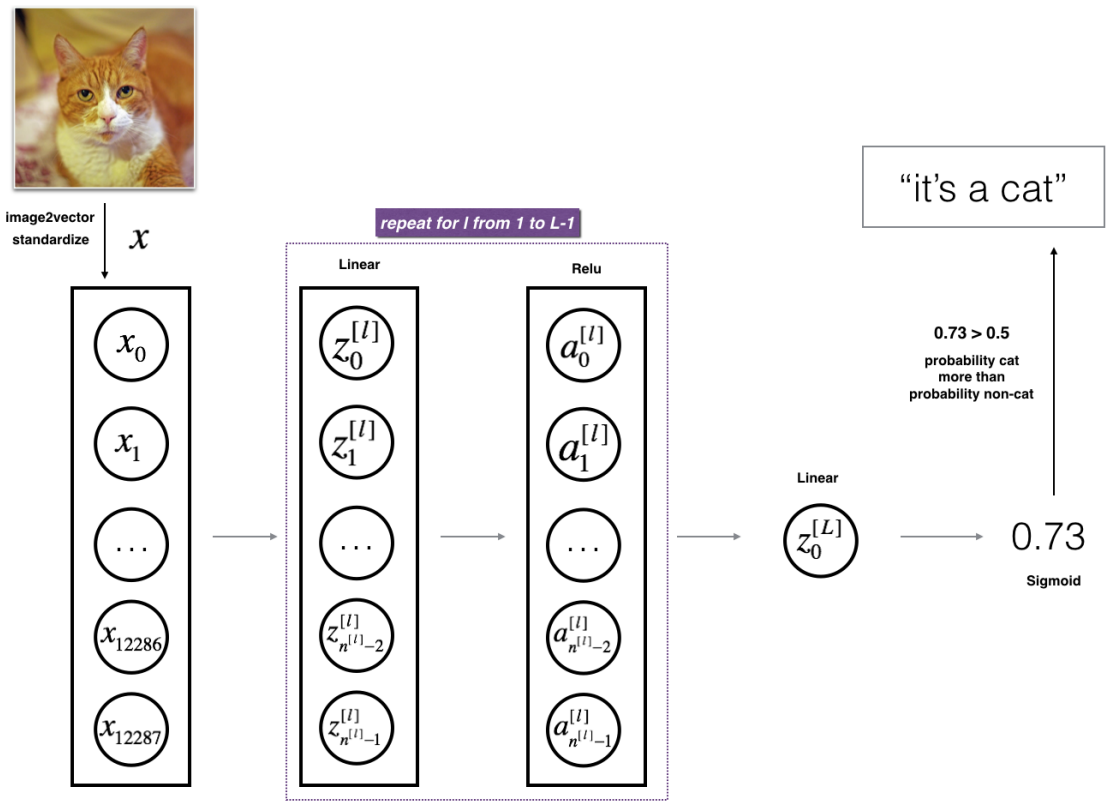
- Previously, we manually specify the transformation of the input features (feature engineering). For example, in polynomial regression

$$\phi(\boldsymbol{x}) = [1, x_1, x_2, x_1^2, x_2^2, \ldots]$$

- We can create more powerful models by learning to do such *nonlinear* **feature extraction** automatically.
- We let $\phi(\boldsymbol{x})$ have its own set of parameters $\boldsymbol{V}$:

$$f(\boldsymbol{x}; \boldsymbol{w}, \boldsymbol{V}) = \boldsymbol{w}^T \phi(\boldsymbol{x}; \boldsymbol{V})$$

Deep neural networks

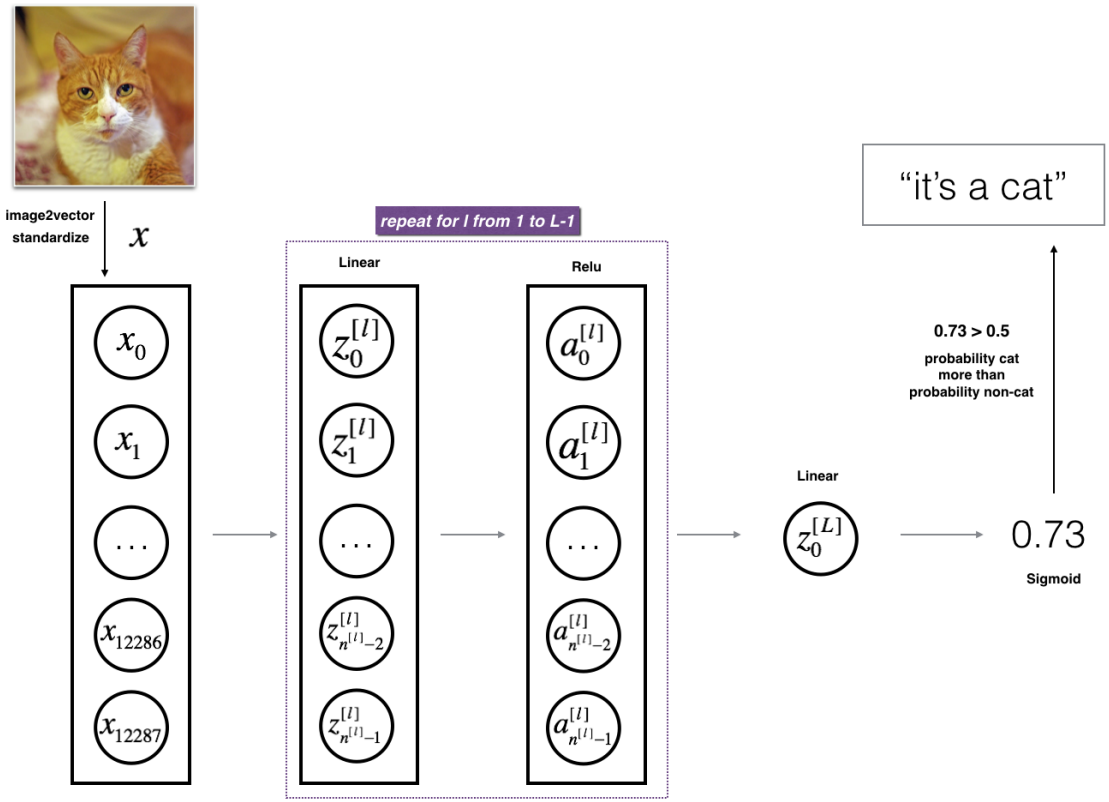


The **feature extractor** $\phi(\boldsymbol{x}; \boldsymbol{V})$ is a composition of simpler functions. The resulting model is a stack of L nested functions:

$$f(\boldsymbol{x}; \boldsymbol{\theta}) = f(\boldsymbol{x}; \boldsymbol{w}, \boldsymbol{V}) = f_L(f_{L-1}(\ldots(f_1(\boldsymbol{x}))\ldots))$$

where $f_\ell(\boldsymbol{x}) = f(\boldsymbol{x}; \boldsymbol{\theta}_\ell)$ is the function at layer ℓ.

Deep neural networks



$$f(\boldsymbol{x}; \boldsymbol{w}, \boldsymbol{V}) = \boldsymbol{w}^T \phi(\boldsymbol{x}; \boldsymbol{V})$$

Typically, the final layer L is *linear* and has the form

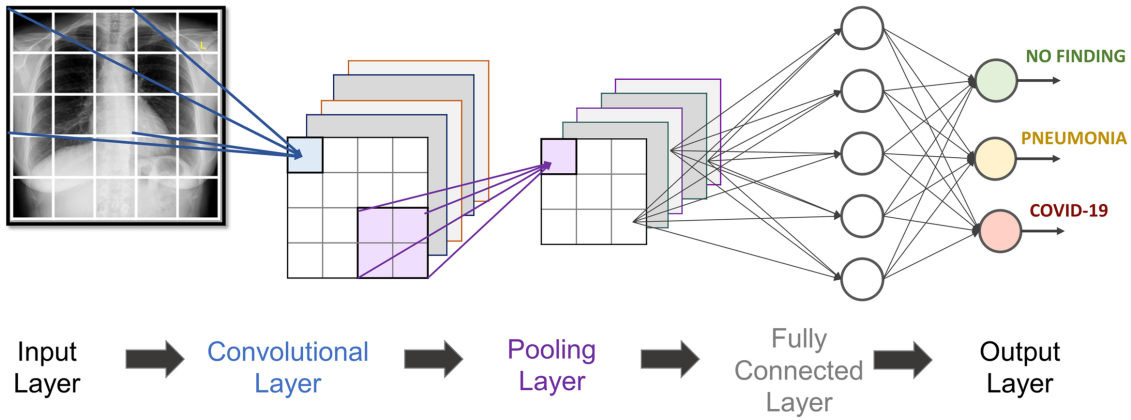
$$f_L(\boldsymbol{x}) = \boldsymbol{w}^T f_{1:L-1}(\boldsymbol{x})$$

where $f_{1:L-1}(\boldsymbol{x})$ is the **learned** feature extractor $\phi(\boldsymbol{x}; \boldsymbol{V})$.

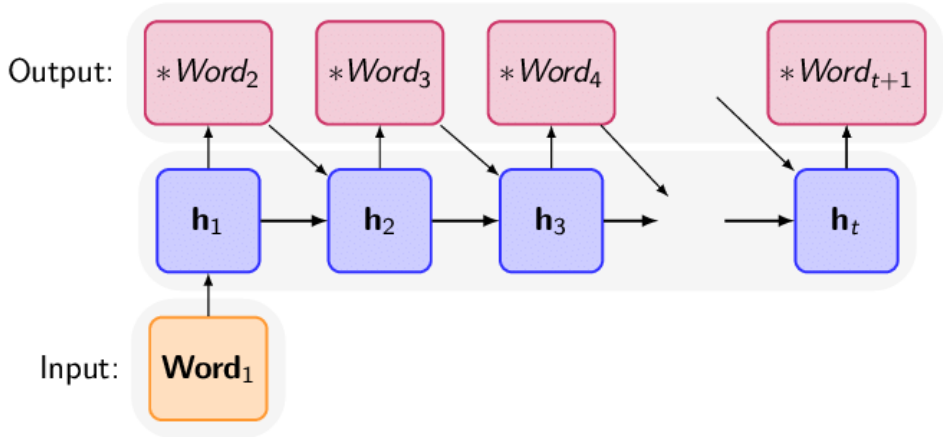
Deep neural networks

Common DNN variants are:

- Convolutional neural networks (CNNs) for images.



- Recurrent neural networks (RNNs) for sequences.



Overfitting and Generalization

- We can rewrite the empirical risk equation as

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

$$\mathcal{L}(\boldsymbol{\theta}; \mathcal{D}_{\text{train}}) = \frac{1}{|\mathcal{D}_{\text{train}}|} \sum_{(\boldsymbol{x}, y) \in \mathcal{D}_{\text{train}}} \ell(y, f(\boldsymbol{x}; \boldsymbol{\theta}))$$

  where $\mathcal{D}_{\text{train}}$ is the size of the training set $\mathcal{D}_{\text{train}}$.
- This makes explicit which dataset the loss is being evaluated on.
- With a complex enough model (or simply by memorizing all training data), we can achieve **zero** training loss.
- But we care about prediction accuracy on new data, that are not in the training set.
- A model that perfectly fits the training data, but which is too complex, is said to suffer from **overfitting**.

Overfitting and Generalization

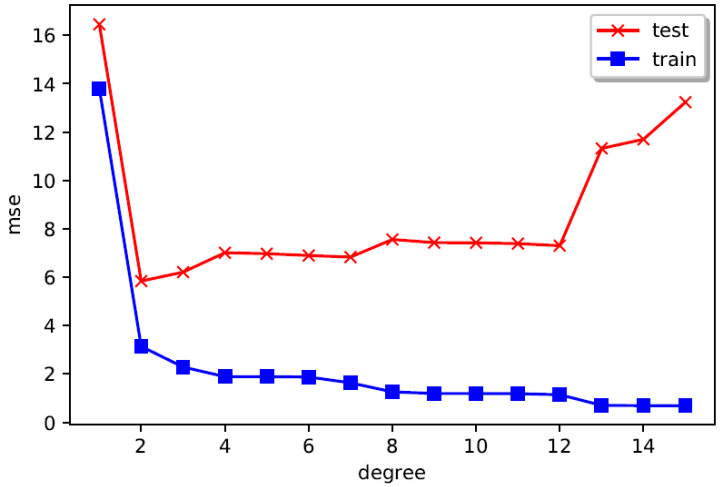
- Let $p^*(\boldsymbol{x}, y)$ denote the true (and unknown) distribution of the training data. Instead of the empirical risk, we have the **population risk** (or the theoretical expected loss):

$$\mathcal{L}(\boldsymbol{\theta}; p^*) = \mathbb{E}_{p^*(\boldsymbol{x},y)}[\ell(y, f((x); \boldsymbol{\theta}))]$$

- The difference $\mathcal{L}(\boldsymbol{\theta}; p^*) - \mathcal{L}(\boldsymbol{\theta}; \mathcal{D}_{\text{train}})$ is the **generalization gap**.
- If a model has a large generalization gap (i.e., low empirical risk but high population risk), it is a sign of overfitting.
- However, in practice, we don't know p^*.
- We partition the data we have into two subsets: the training set and the **test set**. We approximate the population risk using the **test risk**:

$$\mathcal{L}(\boldsymbol{\theta}; \mathcal{D}_{\text{test}}) = \frac{1}{|\mathcal{D}_{\text{test}}|} \sum_{(\boldsymbol{x},y)\in\mathcal{D}_{\text{test}}} \ell(y, f(\boldsymbol{x}; \boldsymbol{\theta}))$$

Overfitting and Generalization



- The training error goes to 0 as the model becomes more complex.
- The test error has a **U-shaped curve**:
  - On the left, where $D = 1$, the model is **underfitting**.
  - On the right, where $D >> 1$, the model is **overfitting**.
  - When $D = 2$, the model complexity is "just right".
- The most complex model has the most **degrees of freedom** $\rightarrow$ minimum training loss.
- We should pick the model with the minimum test loss.

Overfitting and Generalization

- In practice, we partition the data into 3 sets: a training set, a test set, and a **validation set**.
- The training set is used for model fitting.
- The validation set is used for model selection.
- The test set is used to estimate future performance (i.e., the population risk).
- The test set is NOT used for model fitting or model selection.

No free lunch theorem

All models are wrong, but some models are useful.

— George Box

- There is no single best model that works optimally for all kinds of problems.
- A set of assumptions (**inductive bias**) that works well in one domain may work poorly in another.
- We pick a suitable model based on domain knowledge, and/or trial and error (using model selection techniques).
- It is important to have many models and algorithmic techniques to choose from.