



### Supervised Learning:

Find a mapping  $f$  from input features  $x$  to target outputs  $t$  using **labelled** training data (input-output pairs).

### Unsupervised Learning:

Find interesting patterns in the data, e.g., find clusters, where **no target labels are given** (only inputs are given).

**Reinforcement Learning:** Find a sequence of actions that produce a high reward signal in an environment.

**Training Set:** Used to learn the (*parameters* of) the mapping  $f$  from input features to the predicted output

**Validation Set:** Used to choose *hyperparameters* or model settings that are not provided by the learning algorithm

**Test Set:** Used to estimate how well the model will *generalize* to new data and how well the model will perform when deployed

Training:

**k-Nearest Neighbours:** No training necessary; just store the data

**Decision Trees:** Greedy method: find the optimum split at each node, where "optimum" is determined by a loss, e.g., information gain

**Linear Regression and Classification:** Find weights  $w$  that minimize a cost function, e.g., mean square error or average cross entropy loss across the training set

$x_j^{(i)}$  represents the  $j$ -th feature of the  $i$ -th training example

**Hypothesis** (model, predictor) is a function  $f$  that maps input  $x$  to output prediction  $y$

**Voronoi diagram** partitions space into regions closest to each data

**kNN:**  $k$  too small may overfit (sensitive to noise),  $k$  too large would underfit (fail to capture regularities)

$k < \sqrt{n}$ , choose  $k$  with highest validation accu-

racy

We use test data to estimate generalization error 60% training, 20% validation and test

We normalize each dimension to zero mean and unit variance

**Curse of dimensionality:** data not dense in high dimensions, and hard to calculate distances. Most points are approximately equally distanced, squared Euclidean distance becomes dominated by the average behavior, making distances converge

**Overfitting:** High training accuracy, poor test accuracy; model too complex, small data set, noise in data; regularization, better hyperparameters, better model

**Underfitting:** Low training and test accuracy; model too simple, bad hyperparameters, bad model; adjust hyperparameters, regularization, normalization

### Decision Tree Output:

Most common value for discrete classification, or mean value for regression. Use greedy heuristic to construct decision tree based on (highest) information gain

More certain outcome has lower entropy, i.e. not uniformly distributed

**Entropy** characterizes uncertainty of random variable

**Conditional Entropy** characterizes uncertainty of random variable given another random variable

**Information Gain** measures informativeness of variable

Process: Pick a feature, compare all possible splits, choose the one with highest IG, repeat recursively

We may minimize squared error instead:  $SE = \sum_{i=1}^N (f(x^{(i)}) - t^{(i)})^2$

A model is a set of assumptions (restrictions) about the structure of  $f$ . The model or architecture restricts the

hypothesis  $f$  space

**Goal of Linear Regression:** find  $w$  (weights) and  $b$  (bias) minimizing  $\mathcal{E}(w, b) = \mathcal{E}(w)$

Let  $X$  be matrix with  $N \times (D + 1)$  shape with each  $x^{(i)}$ , then  $y = Xw$ . **Gradient Descent** is more general than matrix inversion for finding  $w$ . Each GD update costs  $O(ND)$ ,  $w \leftarrow w - \alpha \nabla_w \mathcal{E}(w) = w - \frac{\alpha}{N} X^T (Xw - t)$ , or  $w_i \leftarrow w_i - \alpha \frac{\partial \mathcal{E}}{\partial w_i}$ , where initially  $\alpha = 0.002$ ,  $w_i = b = 0$

If  $\alpha$  too small, training is slow, if  $\alpha$  large, diverges

We may generalize linear regression by mapping input feature to another space, by feature mapping (or basis expansion):  $\psi(x) : \mathbb{R}^D \rightarrow \mathbb{R}^d$ , and treat  $\mathbb{R}^d$  as input space, e.g. polynomial  $\psi(x) = (1, x, \dots, x^M)^T$ , then  $y = \psi(x)^T w$ . Adjust the degree of polynomial to avoid underfitting or overfitting

**regularizer** or **penalty** is function that qualifies how much we prefer one hypothesis (penalize large weights). Both polynomial degree  $M$  and  $\lambda$  are hyperparameters

$\lambda$  large cause underfit,  $\lambda$  small cause overfit

We want each feature's values to be indicators or orderable

**ML Algorithm Design:** 1. Choose model; 2. Define loss function; 3. Choose regularizer; 4. Fit model by minimizing regularized cost, using **optimization algorithm**.

$t = 1$  for positive example,  $t = 0$  or  $-1$  for negative example

For **Linear Binary Classification Model**, let  $z = w^T x$ , then  $y = 1$  if  $z \geq 0$ , else  $y = 0$ , decision boundary being hyperplane  $z = 0$

Given small training set, go over each data point to find restrictions of  $w_i$ , if region in weight space satisfying all constraints is non-empty, then this **feasible region** makes

the problem (in-)feasible and the training set **linearly separable**

Use square error loss function would cause correctly classified points with high loss; use indicator loss function would cause gradient be zero e.w.; use sigmoid plus square loss won't update much for very wrongly classified example, i.e. poor gradient signal

We use sigmoid to smooth the output of each choice of  $w$  between 0 and 1, then use cross entropy loss function to penalize the model for being wrong

$w \leftarrow w - \frac{\alpha}{N} \sum_{i=1}^N (y^{(i)} - t^{(i)}) x^{(i)}$ , same as linear regression

**hypothesis space  $\mathcal{H}$**  set of all possible  $h$  a model can represent, i.e. all linear functions for linear regression

Members of  $\mathcal{H}$  with algorithm's preference determine **inductive bias**

Algorithm is **parametric** if  $\mathcal{H}$  is defined by a set of parameters (linear and logistic regression, neural network; counter-example kNN)

Previously we used **full batch gradient descent** of  $\frac{\partial \mathcal{E}}{\partial w}$ , we may estimate  $\frac{\partial \mathcal{E}}{\partial w}$  using subset of data if  $N$  too large, via **stochastic gradient descent**: computing average of a small number of examples called **mini-batch** with a **batch size**.

inner loop is **iteration** (each mini-batch), outer is **epoch** (one update)

num\_iter = num\_epoch \*  $N / \text{batch\_size}$

**Accuracy:**

$$\frac{1}{N} \sum_{i=1}^N \mathbb{I}[t^{(i)} = y^{(i)}]$$

**Error:**  $1 - \text{Accuracy}$

**Euclidean:**

$$\|x^{(a)} - x^{(b)}\|_2 = \sqrt{\sum_{j=1}^d (x_j^{(a)} - x_j^{(b)})^2}$$

**Cosine Similarity:**

$$\text{cosine}(x^{(a)}, x^{(b)}) = \frac{x^{(a)} \cdot x^{(b)}}{\|x^{(a)}\|_2 \|x^{(b)}\|_2}$$

**Mean:**

$$\bar{x} = \frac{1}{N} \sum_{i=1}^N x^{(i)} = \mu$$

**Variance:**

$$\sigma^2 = \frac{1}{N} \sum_{i=1}^N (x^{(i)} - \bar{x})^2$$

**Standard Deviation:**

$$\sigma = \sqrt{\sigma^2}$$

**Normalization:**

$$\tilde{x}_j^{(i)} = \frac{x_j^{(i)} - \mu_j}{\sigma_j}$$

**Entropy:**

$$H(X) = -\mathbb{E}_{X \sim p}[\log_2 p(X)]$$

$$= -\sum_{x \in X} p(x) \log_2 p(x)$$

$$H(X, Y) = -\sum_{x \in X} \sum_{y \in Y} p(x, y) \log_2 p(x, y)$$

$$H(Y|X) = -\sum_{y \in Y} p(y|x) \log_2 p(y|x)$$

$$H(Y|X) = \sum_{x \in X} p(x) H(Y|x)$$

$$= -\sum_{x \in X} \sum_{y \in Y} p(x, y) \log_2 p(y|x)$$

$$H(X, Y) = H(Y, X) = H(X|Y) + H(Y|X)$$

$$H \geq 0, H(Y|Y) = 0, H(Y|X) \leq H(Y)$$

$$H(Y|X) = H(Y) \text{ if } X \text{ and } Y \text{ ind.}$$

$$\text{Information Gain: } IG(Y|X) = H(Y) - H(Y|X)$$

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$$\nabla_{\mathbf{w}} \mathcal{E}(\mathbf{w}) = 0: \quad \mathbf{w} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{t}$$

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**$L^2$  Regularizer:**

$$\mathcal{R}(\mathbf{w}) = \frac{1}{2} \|\mathbf{w}\|_2^2 = \frac{1}{2} \sum_{j=1}^D w_j^2$$

**Regularized cost function:**

$$\mathcal{E}_{\text{reg}}(\mathbf{w}) = \mathcal{E}(\mathbf{w}) + \lambda \mathcal{R}(\mathbf{w})$$

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**Logistic / Sigmoid function:**

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

Both sigmoid and square loss:

$$\frac{\partial \mathcal{L}}{\partial w_j} = (y - t)y(1 - y)x_j$$

**Cross Entropy Loss:**

$$\mathcal{L}_{\text{CE}}(y, t)$$

$$= \begin{cases} -\log(y) & \text{if } t = 1 \\ -\log(1 - y) & \text{if } t = 0 \end{cases}$$

$$= -t \log(y) - (1 - t) \log(1 - y)$$

$$\frac{\partial \mathcal{L}_{\text{CE}}}{\partial w_j} = (y - t)x_j$$

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**3rd column cont.,**

batch size too large =  
expensive, too small =  
noisy

center and normalize to  
avoid ravines

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**Graph of kNN:** Draw  
tangent line at each mid-  
point, connect regions  
with same class

**Graph of Decision  
Tree:** Draw axis-aligned  
lines to split regions

**IG of Decision Tree:**

First calculate the en-  
tropy  $H(Y)$  with prob-  
ability (percentages) of  
each class, similarly for  
 $H(Y|\text{right})$ ,  $H(Y|\text{left})$ ,  
then  $IG = H(Y) -$   
 $p(\text{right})H(Y|\text{right}) -$   
 $p(\text{left})H(Y|\text{left})$

**Shape:** # of rows  $\times$  #  
of columns

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Linear Regression:  
Square error loss func-  
tion, with average loss  
cost function

Logistic Regression: Sig-  
moid function, with cross  
entropy loss function

Decision Tree: Greedy  
method, with informa-  
tion gain loss function

kNN: No training, with  
Euclidean distance for  
lower dimension  $D$