PRML Chapter I : Introduction

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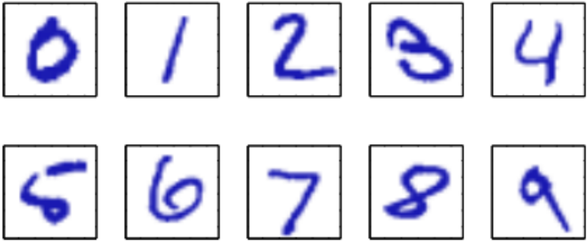
Introduction



- Training Set & Test Set & validation set
- Supervised learning & Unsupervised learning & Weakly-supervised learning &Semi-supervised learning
- Pre-process
- Classfication & Regression
- reinforcement learning

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  - Supervised learning:Applications in which the training data comprises examples of the input vectors along with their corresponding target vectors.$\{ X_{data}, Y_{label}\}$ is known in advance.
  - Unsupervised learning :The goal in such unsupervised learning problems may be to discover groups of similar examples within the data.

- **Weakly-supervised learning**:
  - incomplete supervision:One (usually very small) subset of the training set is labeled, while the other data is not labeled.
  - inexact supervision: Image has only coarse-grained labels.
  - inaccurate supervision:The labels given by the model are not always true values.

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- **Semi-supervised learning**:
  - Semi-supervised learning is to enable learners to use unlabeled samples to improve learning performance without relying on external interaction.

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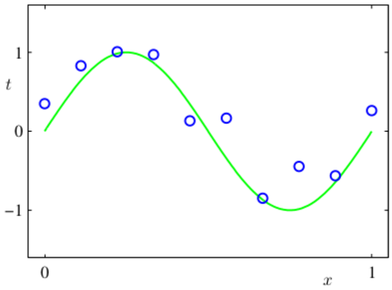
  The technique of reinforcement learning is concerned with the problem of finding suitable actions to take in a given situation in order to maximize a reward.

Section 1.1 Example:Polynomial Curve Fitting

Example:Polynomial Curve Fitting



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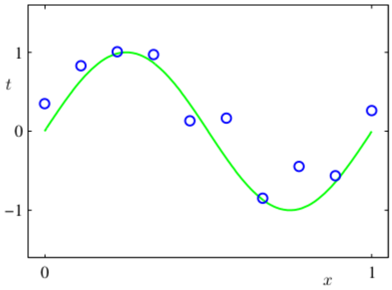

Our goal is to train a function $y(x)$ which takes a vector X as input and produce the prediction of Y.
$y(x, w) = w_0 + w_1 x + w_2 x^2 + \ldots w_M x^M = \sum_{j=0}^{M} w_j x^j$

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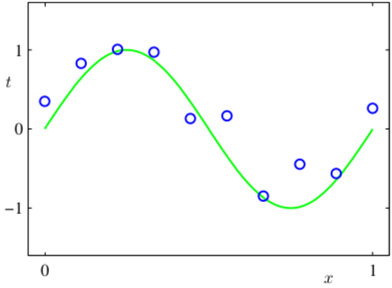

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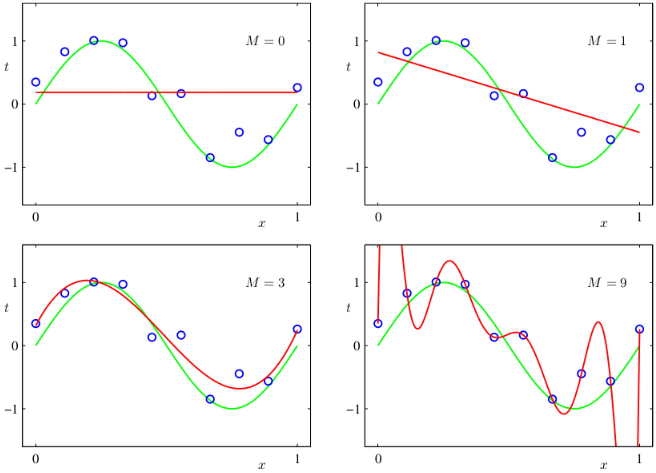
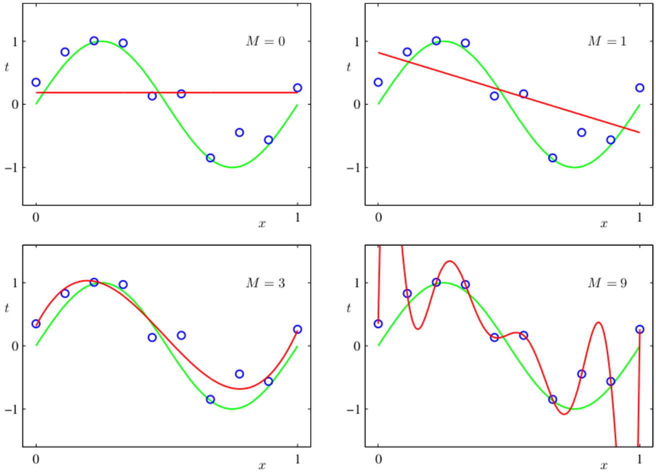
$y(x, w) = w_0 + w_1 x + w_2 x^2 + \ldots w_M x^M = \sum_{j=0}^{M} w_j x^j$

$E(w) = \frac{1}{2} \sum_{n=1}^{N} \{y(x_n, w) - t_n\}^2$


M = 0
M = 1
M = 3
M = 9
t
x
1
0
−1
0
1



Model comparsion(Model Selection), **Over-fitting**, **Regularization**, a **Penalty Term** to the error function

	$M=0$	$M=1$	$M=3$	$M=9$
w_0^*	0.19	0.82	0.31	0.35
w_1^*		-1.27	7.99	232.37
w_2^*			-25.43	-5321.83
w_3^*			17.37	48568.31
w_4^*				-231639.30
w_5^*				640042.26
w_6^*				-1061800.52
w_7^*				1042400.18
w_8^*				-557682.99
w_9^*				125201.43

Error Function: $E(w) = \frac{1}{2}\sum_{n=1}^{N}\{y(x_n, w) - t_n\}^2 + \frac{\lambda}{2}\|w\|^2$

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	$M=0$	$M=1$	$M=3$	$M=9$
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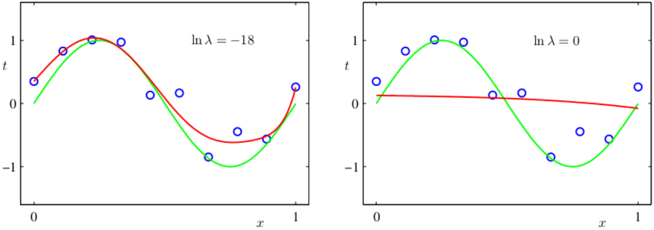

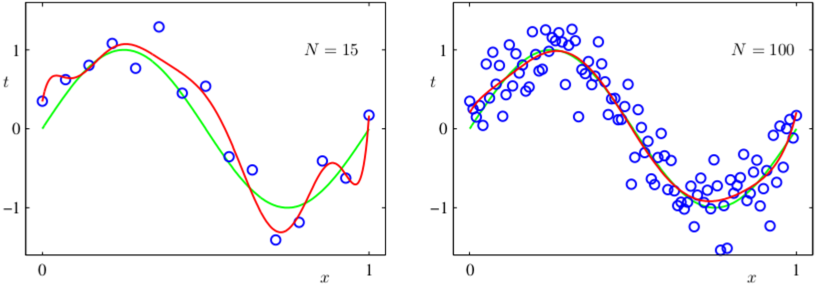

- We see that increasing the size of the data set reduces the over-fitting problem.

Section 1.2 Probability Theory

Probability densities & Expectations and covariances

- joint probability : $P(X = x_i, Y = y_j)$
- marginal probability: $P(X = x_i) = \sum_{j=1}^{L} P(X = x_i, Y = y_j)$
- conditional probability : $P(Y = y_j | X = x_i)$
- **sum rule**: $P(X) = \sum_Y P(X, Y)$
- **product rule**: $P(X, Y) = P(Y|X)P(X)$
- probability densities : $p(x \in (a, b)) = \int_a^b p(x)dx$
- expections: $\mathbb{E}[f] = \sum_x p(x)f(x)$ & $\mathbb{E}[f] = \int p(x)f(x)dx$
- variances: $var[f] = \mathbb{E}[f(x)^2] - \mathbb{E}[f(x)]^2$
- covariance: $cov[x, y] = [\mathbb{E}_{x,y}\{x - \mathbb{E}[x]\}\mathbb{E}\{y - \mathbb{E}[y]\}]$

Bayesian probabilities

So far in this chapter, we have viewed probabilities in terms of the frequencies of random, repeatable events. We shall refer to this as the **classical** or **frequentist** interpretation of probability.

Bayesian probabilities

- **Prior probability**： cause −> effect
- **Posterior probability**： effect −> cause

Bayesian probabilities

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定义

$p(Y|X) = \frac{p(X|Y)p(Y)}{p(X)}$,$p(X) = \sum_Y p(X|Y)p(Y)$

Bayesian probabilities

- Teacher : Student = 1:1
  The probability of a teacher coming to the office on weekends is 0.2
  The probability of a student coming to the office on weekends is 0.6
- There's a man in the office on weekends, so what's the probability that he's a student?
- W–> T/S, X–> coming to office
- $p(W_1) = 0.5$ $p(W_2) = 0.5$

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- $p(X|W_1) = 0.2, p(X|W_2) = 0.6$
- $p(X) = p(X|W_1)p(W_1) + p(X|W_2)p(W_2) = 0.4$

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- $p(W_1|X) = \frac{p(X|W_1)P(W_1)}{p(X)} = 0.25$

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- $p(W_1|X) = \frac{p(X|W_1)P(W_1)}{p(X)} = 0.25$
- $p(W_2|X) = \frac{p(X|W_2)P(W_2)}{p(X)} = 0.75$

The Gaussian distribution

The most important probability distributions for continuous variables, called the normal or Gaussian distribution.

定义

$$N(x|\mu,\sigma^2) = \frac{1}{(2\pi\sigma^2)^{\frac{1}{2}}} exp\{-\frac{1}{2\sigma^2}(x-\mu)^2\}$$

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$$x = \{x_1, x_2 ... x_N\}$$

Independent and Identically Distributed

$$p(x_1, ...x_N|\mu,\sigma^2) = \prod_{n=1}^{N} N(x_n|\mu,\sigma^2)$$

The Gaussian distribution

The log likelihood function can be written in the form

$$\ln p(\mathbf{x}|\mu, \sigma^2) = -\frac{1}{2\sigma^2}\sum_{n=1}^{N}(x_n - \mu)^2 - \frac{N}{2}\ln\sigma^2 - \frac{N}{2}\ln(2\pi)$$

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Maximizing with respect to σ^2:

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Var:

$$E(\sigma_{ML}^2) = \frac{N-1}{N}\sigma^2$$

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The Gaussian distribution

- So that on average the maximum likelihood estimate will obtain the correct mean but will underestimate the true variance by a factor $\frac{N-1}{N}$.
- Note that the bias of the maximum likelihood solution becomes less significant as the number N of data points increases, and in the limit $N \to \infty$ the maximum likelihood solution for the variance equals the true variance of the distribution that generated the data.

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- it is assumed that t is Gaussian: $p(t|x, w, \beta) = N(t|y(x, w), \beta^{-1})$
- **precision parameter** β corresponding to the inverse variance of the distribution.

Curve fitting re-visited

$$p(\mathbf{t} \mid \mathbf{x}, \boldsymbol{w}, \beta) = \prod_{n=1}^{N} \mathcal{N}(t_n \mid y(x_n, \boldsymbol{w}), \beta^{-1})$$

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$$\frac{1}{\beta_{ML}} = \frac{1}{N} \sum_{n=1}^{N} \{y(x_n, \boldsymbol{w}_{ML}) - t_n\}^2$$

$$p(t \mid x, \boldsymbol{w}_{ML}, \beta_{ML}) = \mathcal{N}(t \mid y(x, \boldsymbol{w}_{ML}), \beta_{ML}^{-1})$$

Curve fitting re-visited

- The polynomial coefficients are treated as random variables with a Gaussian distribution taken over a vector of dimension M+1:

$$p(\boldsymbol{w} \mid \alpha) = \mathcal{N}(\boldsymbol{w} \mid \mathbf{0}, \alpha^{-1}\boldsymbol{I}) = \left(\frac{\alpha}{2\pi}\right)^{\frac{M+1}{2}} \exp\left\{-\frac{\alpha}{2}\boldsymbol{w}^T\boldsymbol{w}\right\}$$

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- **maximum posterior** or **MAP**.We take the negative logarithm,we throw out constant terms and we get:

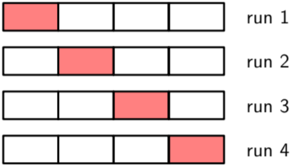
$$\frac{\beta}{2}\sum_{n=1}^{N}\{t_n - y(x_n,\boldsymbol{w})\}^2 + \frac{\alpha}{2}\boldsymbol{w}^\top\boldsymbol{w}$$

Section 1.3 Model Selection

Model Selection : Cross validation

- With regularized least squares, the regularization coefficient λ also controls the effective complexity of the model.
- For more complex models, such as mixture distributions or neural networks there may be multiple parameters governing complexity.
- we need to determine the values of such parameters, and the principal objective in doing so is usually to achieve the best predictive performance on new data.
- Furthermore, as well as finding the appropriate values for complexity parameters within a given model, we may wish to consider a range of different types of model in order to find the best one for our particular application.
- It may be necessary to keep aside a third test set on which the performance of the selected model is finally evaluated.

Cross Validation



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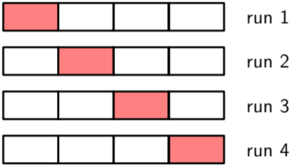
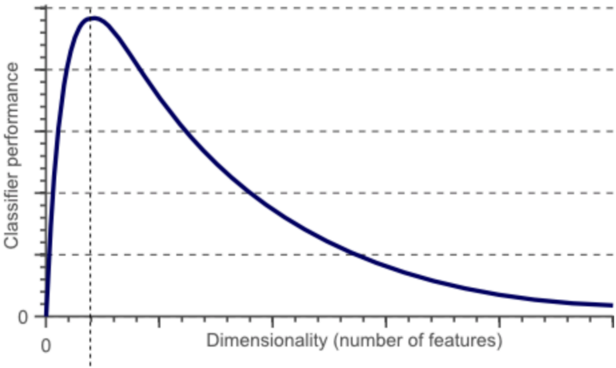


- When data is particularly scarce, it may be appropriate to consider the case $S = N$, where N is the total number of data points, which gives the **leave-one-out** technique.
- One major drawback of cross-validation is that the number of training runs that must be performed is increased by a factor of S.

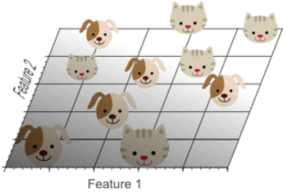
Section 1.4 The Curse of Dimensionality

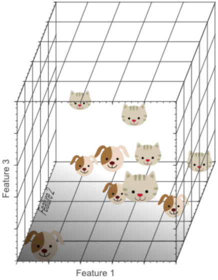
The Curse of Dimensionality

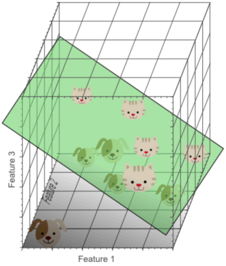
When reading machine learning papers, we often see that some writers refer to "curse of dimensionality", What kind of "disaster" is it? what is its importance in classification.

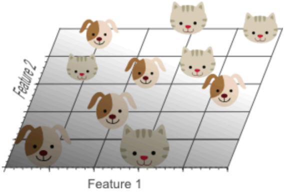


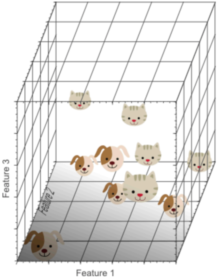
the Curse of Dimensionality

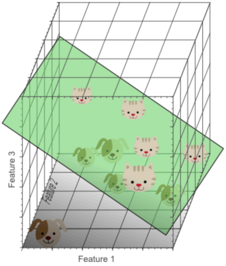












- **Sample density**
- **Feature space**

Section 1.5 Decision Theory

Decision Theory

- The decision problem:
  - **classification problem**
  - given x,predict t according to a probablistic model $p(x, t)$

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- Two basic requirements:
  - The probability distribution of the population of each category is known.
  - The number of categories to be classified is certain.
- Important quantity:$p(C_k|x)$

$$p(C_k|x) = \frac{p(x,C_k)}{p(x)} = \frac{p(x,C_k)}{\sum_{k=1}^{2} p(x,C_k)}$$

- Intution:choose k that maximizes $p(C_k|x)$

Decision Theory-Minimizing the misclassification rate

- **Decision region:** $R_i = \{\ x : \mathit{pred}(x) = C_i\ \}$
- **Decision Boundaries or Decision Surfaces**： The boundaries between decision regions

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- $p(correct) = p(x \in R_x, C_x)$

Decision Theory-Minimizing the expected loss

- Suppose that, for a new value of x, the true class is C_k and that we assign x to class C_j (where j may or may not be equal to k).
- In so doing, we incur some level of loss that we denote by L_{kj} , which we can view as the k, j element of a loss matrix.
- **Cost**/**Loss** of a decision:L_{kj} = predict C_j while truth is C_k

$$\begin{array}{cc} & \begin{array}{cc} \text{cancer} & \text{normal} \end{array} \\ \begin{array}{c} \text{cancer} \\ \text{normal} \end{array} & \begin{pmatrix} 0 & 1000 \\ 1 & 0 \end{pmatrix} \end{array}$$

$$\mathbb{E}(L) = \sum_k \sum_j \int_{R_j} L_{kj} p(\mathbf{x}, C_k) dx$$

$$\mathbb{E}[L] = \int_{R2} L_{1,2} p(x, C_1) + \int_{R1} L_{2,1} p(x, C_2)$$

$$\sum L_{kj} p(C_k|x)$$

The reject option

- For the 0/1 loss,pred(x) $=$ $argmax_k p(C_k|x)$
  - Note: K classes–> $1/K \leq maxp(C_k|x) \leq 1$
- When max $p(C_k|x)$ –>1/K the confidence in the prediction decreases

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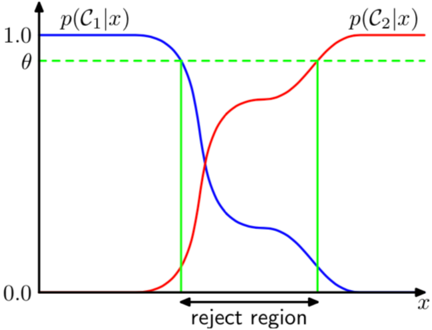

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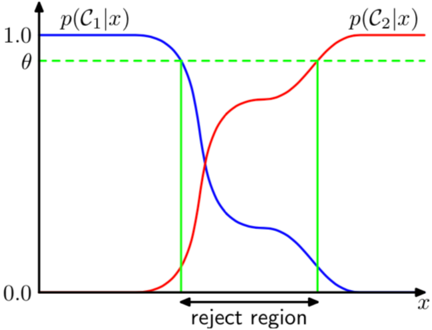

- Motivation:switch between automatic/human decision

Inference and decision

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   1. generative
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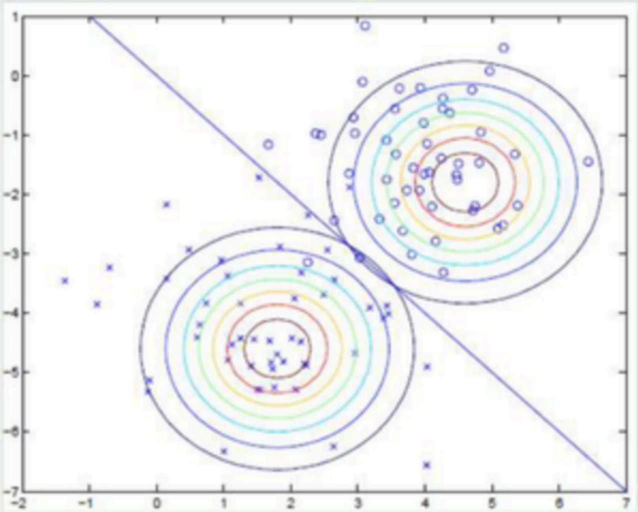
2. learn a discriminant funtion $f(x)$
   - directly map input to class labels
   - for binary classification, $f(x)$ is typically defined as the sign $(+1/\text{-}1)$ of an auxiliary funtion


1
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7

Inference and decision

- probabilistic generative models:
  - pros:access to $p(x)$ $->$ easy detection of outliers
  - cons:estimation the joint probability $p(x, C_k)$ can be computational and data demanding.
- probabilistic discrimative models:
  - pros:less demanding than the generative approach
- discriminant functions:
  - pros:a single learning problem
  - cons:no access to $p(C_k|x)$

Loss functions for regression

- The regression setting:quantitative target t $\in R$
- Typical regression loss-function : $L(t, y(x)) = (y(x) - t)^2$
  - the **squared loss**
- The decision problem = minimize the expected loss:

$$\mathbb{E}[L] = \int_X \int_{\mathcal{R}} L(t, y(x)) p(x, t) dx dt$$

- Note: general class of loss functions $L(x, y(x)) = |y(x) - t|^2$

Section 1.6 Information Theory

Information Theory-Entropy

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(Convention: $p\log p = 0$ if p=0, $\log$–>$\ln$(in nats))

Information Theory-Entropy

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- $\{a, b, c, d, e, f, g, h\}$: $\{\frac{1}{2}, \frac{1}{4}, \frac{1}{8}, \frac{1}{16}, \frac{1}{64}, \frac{1}{64}, \frac{1}{64}, \frac{1}{64}\}$

$$H[x] = -\frac{1}{2}\log_2\frac{1}{2} - \frac{1}{4}\log_2\frac{1}{4} - \frac{1}{8}\log_2\frac{1}{8} - \frac{1}{16}log_2\frac{1}{16} - \frac{4}{64}\log_2\frac{1}{64} = 2 \text{ bits}$$

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- Consider how we would transmit the identity of the variable' s state to a receiver:
    - 0, 10, 110, 1110, 111100, 111101, 111110, 111111
    - average code length: $\frac{1}{2}x1 + \frac{1}{4}x2 + \frac{1}{8}x3 + \frac{1}{16}x4 + 4x\frac{1}{64}x6$ =2 bits

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- The **noiseless coding theorementropy** is a lower bound on the number of bits needed to transmit the state of a random variable.

Information Theory-Entropy

- Differential entropy:

$$H[X] = -\int p(x) \ln p(x) dx$$

Relative entropy and mutual information

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$$\begin{aligned} \mathrm{KL}(p\|q) &= -\int p(\mathbf{x}) \ln q(\mathbf{x})\, \mathrm{d}\mathbf{x} - \left(-\int p(\mathbf{x}) \ln p(\mathbf{x})\, \mathrm{d}\mathbf{x}\right) \\ &= -\int p(\mathbf{x}) \ln \left\{\frac{q(\mathbf{x})}{p(\mathbf{x})}\right\} \mathrm{d}\mathbf{x}. \end{aligned}$$

- **relative entropy | Kullback-Leibler divergence**

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- **relative entropy | Kullback-Leibler divergence**
- $KL(p\|q) \not\equiv KL(q\|p)$

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- Kullback-Leibler divergence satisfies $KL(\mathrm{p}\|\mathrm{q}) \geq 0$ with equality if, and only if, $p(x) = q(x)$.

Relative entropy and mutual information

- Kullback-Leibler divergence satisfies $KL(\mathrm{p}\|\mathrm{q}) \geq 0$ with equality if, and only if, $p(x) = q(x)$.
- A function os convex iff every cord lies above the function
- Any value of x in the interval from $x = a$ to $x = b$ can be written in the form $\lambda a + (1 - \lambda)b$ where $0 \leq \lambda \leq 1$.

$$f(\lambda a + (1 - \lambda)b) \leq \lambda f(a) + (1 - \lambda)f(b)$$

- strictly convex function:if the equality is satisfied only for $\lambda = 0$ and $\lambda = 1$.
- Jensen's inequality for convex functions:

$$E[f(x)] \geq f(E[x])$$

$$f\left(\int \boldsymbol{x}p(\boldsymbol{x})\ \mathrm{d}\boldsymbol{x}\right) \leq \int f(\boldsymbol{x})p(\boldsymbol{x})\ \mathrm{d}\boldsymbol{x}$$

- When applied to $KL(p\|q)$:

$$
\begin{aligned}
KL(p\|q) &= -\int p(x)\ln\frac{q(x)}{p(x)}dx \\
&> -\ln\int p(x)\times\frac{q(x)}{p(x)}dx \quad \text{(because } -\ln \text{ is stricly convex)} \\
&= -\ln\int q(x)dx = -\ln 1 = 0
\end{aligned}
$$

Moreover,straightforward to see that $KL(p\|p)$ =0

Mutual information

- Consider the joint distribution between two sets of variables x and y given by p(x, y).
- If the sets of variables are independent, p(x, y) = p(x)p(y).
- If the variables are not independent, we can gain some idea of whether they are ‘close’ to being independent by considering the Kullback-Leibler divergence between the joint distribution and the product of the marginals

$$\begin{aligned} \mathrm{I}[\mathbf{x}, \mathbf{y}] &\equiv \mathrm{KL}(p(\mathbf{x}, \mathbf{y}) \| p(\mathbf{x}) p(\mathbf{y})) \\ &= -\iint p(\mathbf{x}, \mathbf{y}) \ln \left(\frac{p(\mathbf{x}) p(\mathbf{y})}{p(\mathbf{x}, \mathbf{y})} \right) \mathrm{d}\mathbf{x}\, \mathrm{d}\mathbf{y} \end{aligned}$$

Mutual information

- From the properties of the Kullback-Leibler divergence, we see that I(x,y) $\geq$ 0 with equality if, and only if, x and y are independent.
- Using the sum and product rules of probability, we see that the mutual information is related to the conditional entropy through

$$I[\boldsymbol{x}, \boldsymbol{y}] = H[\boldsymbol{x}] - H[\boldsymbol{x} \mid \boldsymbol{y}] = H[\boldsymbol{y}] - H[\boldsymbol{y} \mid \boldsymbol{x}]$$

- Thus we can view the mutual information as the reduction in the uncertainty about x by virtue of being told the value of y (or vice versa). From a Bayesian perspective, we can view p(x) as the prior distribution for x and p(x|y) as the posterior distribution after we have observed new data y. The mutual information therefore represents the reduction in uncertainty about x as a consequence of the new observation y.