Chapter 1 : Introduction

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Contents

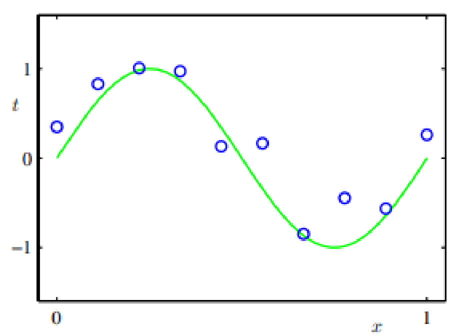
1. Introduction

- Training set: $\{\mathbf{x_1}, ..., \mathbf{x_N}\}$, to tune the parameters of an adaptive model
- Target vector: $\mathbf{t}$, the identity of the corresponding training set digit.
- Training phase / Learning phase / Generalization
- Preprocessing: to transform the original input variables into some new space of variables $\rightarrow$ easy to recognition pattern
  - purpose: (dimensinolality reduction $\rightarrow$) (1) feature extraction, (2) to speed up computation

- Application
  - supervised learning: classification, regression
  - unsupervised learning: clustering, density estimation
  - reinforcement learning: finding suitable actions to take in a given situation in order to maximize a reward.

1.1 Example: Polynomial Curve Fitting

Goal: to exploit the training set in order to make predictions of the value $\hat{t}$ of the target variable for some new value $\hat{x}$ of the input variable.



- trying to discover the underlying function $\sin(2\pi)$

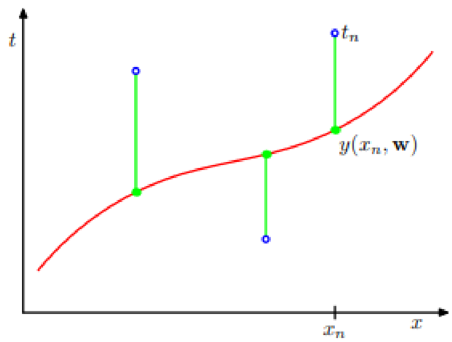
$$y(x, \mathbf{w}) = w_0 + w_1 x + w_2 x^2 + ... + w_M x^M = \sum_{j=0}^{M} w_j x^j \tag{1.1}$$

- M is order of the polynomial
- $y(x, \mathbf{w})$is a nonlininear function of x and a linear function of the coefficients $\mathbf{w}$.

Step 1: choosing the value of $\mathbf{w}$ to minimize error function, $E(\mathbf{w})$.

- error function

$$E(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\{y(x_n, \mathbf{w}) - t_n\}^2 \tag{1.2}$$



- by the sum of the squareds of the errors between the predictions $y(x_n, \mathbf{w})$ for each data point x_n and the corresponding target value t_n
- 1/2: for convenience
- result is positive quantity and that would be zero, iff the function $y(x_n, \mathbf{w})$ were to pass exactly through each training data point.

(ex.1.1)

$$\frac{\partial E}{\partial w_i} = \sum_{n=1}^{N}\{y(x_n, \mathbf{w}) - t_n\}x_n^i = 0$$

$$\sum_{n=1}^{N} y(x_n, \mathbf{w})x_n^i = \sum_{n=1}^{N} t_n x_n^i$$

$$\sum_{n=1}^{N}(\sum_{j=0}^{M} w_j x_n^j)x_n^i = \sum_{n=1}^{N} t_n x_n^i$$

$$\sum_{n=1}^{N}\sum_{j=0}^{M} w_j x_n^{(j+i)} = \sum_{n=1}^{N} t_n x_n^i$$

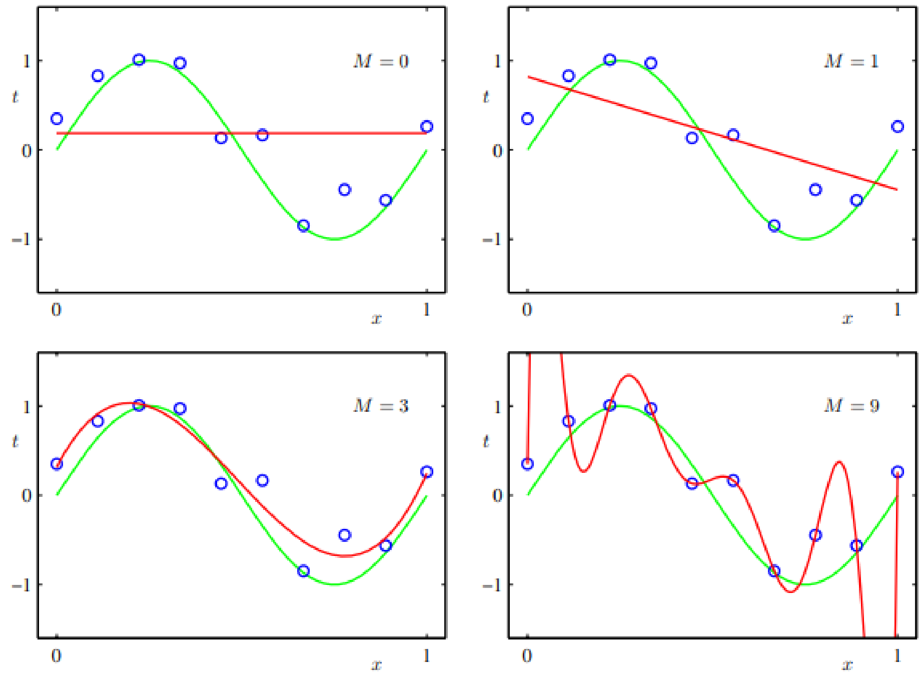
$$\sum_{j=1}^{M}\sum_{n=0}^{N} x_n^{(j+i)} w_j = \sum_{n=1}^{N} t_n x_n^i$$

$$\sum_{j=1}^{M} A_{ij} w_j = T_i$$

$\therefore$ the jcoefficients $\mathbf{w}$ that minimize the error function are given by the solution to above set of linear equations.

Step 2: choosing the order M of polynomial (*model comparison* or *model seleiction*)

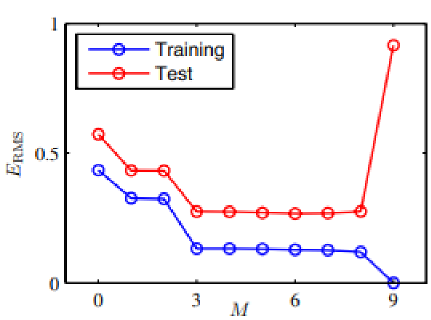
- over-fitting: eventhough, when polynomial passes exactly through each data point ($M = 9$), error function is 0, $E(\mathbf{w}^*) = 0$, the fitted curve oscillates widly and gives a very poor representation of the function $\sin(2\pi x)$.



- **root mean squre error, RMS error**

$$E_{RMS} = \sqrt{2E(\mathbf{w}^*)/N} \tag{1.3}$$

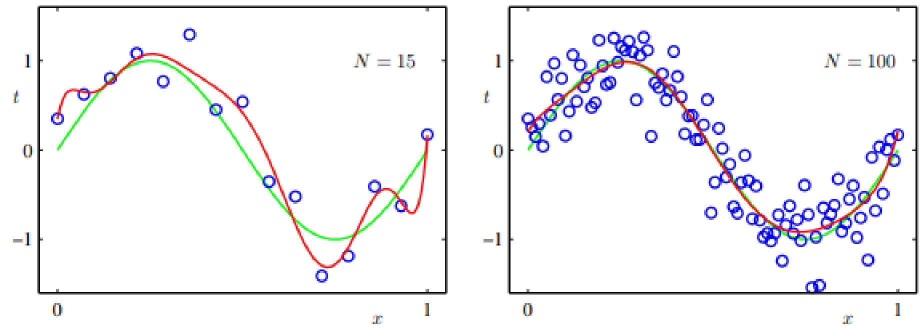
- the division by N: it could be to compare different sizes of data sets on an equal footing
- square root: measured on the same scale as the target variable t.



	$M = 0$	$M = 1$	$M = 6$	$M = 9$
$w_0^\star$	0.19	0.82	0.31	0.35
$w_1^\star$		-1.27	7.99	232.37
$w_2^\star$			-25.43	-5321.83
$w_3^\star$			17.37	48568.31
$w_4^\star$				-231639.30
$w_5^\star$				640042.26
$w_6^\star$				-1061800.52
$w_7^\star$				1042400.18
$w_8^\star$				-557682.99
$w_9^\star$				125201.43

- (*over-fitting problem*) larger values of M $\rightarrow$ the more flexible, increasing the coefficients $\mathbf{w}^*$ $\rightarrow$ increasingly tuned to the random noise on the target values

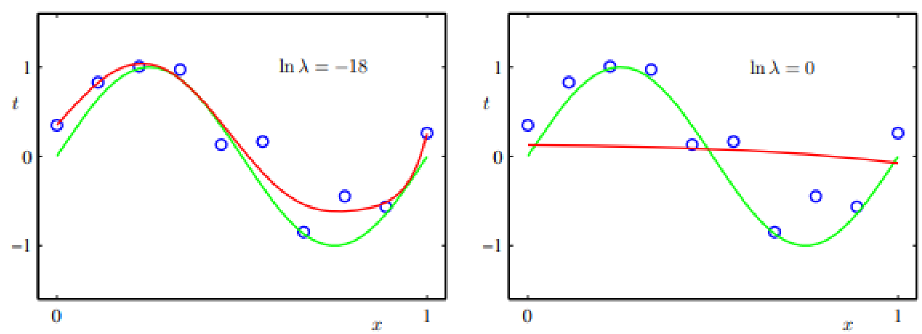
- **over come the over-fitting problem**
  - increaing the size of data set
  - Bayesian method
  - (for limit size) Regularization: adding the penalty term to the error function (1.2)



- **Regularization**

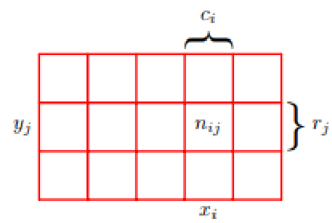
$$\tilde{E}(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\{y(x_n, \mathbf{w}) - t_n\}^2 + \frac{\lambda}{2} \parallel \mathbf{w} \parallel^2 \tag{1.4}$$

- λ: reactive importance of the regularization term compared with the sum-of-squres error term.
  - zero: overfitting $\rightarrow$ desired: good for fitting $\rightarrow$ too large: poor fit
- w_0: normally omitted from the regularizer ($\because$ it depend on theh choice of orgin for the garget variable)
- shrinkage method (e.g. ridge regression, weight decay,...)



	$\ln \lambda = -\infty$	$\ln \lambda = -18$	$\ln \lambda = 0$
$w_0^\star$	0.35	0.35	0.13
$w_1^\star$	232.37	4.74	-0.05
$w_2^\star$	-5321.83	-0.77	-0.06
$w_3^\star$	48568.31	-31.97	-0.05
$w_4^\star$	-231639.30	-3.89	-0.03
$w_5^\star$	640042.26	55.28	-0.02
$w_6^\star$	-1061800.52	41.32	-0.01
$w_7^\star$	1042400.18	-45.95	-0.00
$w_8^\star$	-557682.99	-91.53	0.00
$w_9^\star$	125201.43	72.68	0.01

1.2 Probabililty Theory



- joint probability:

$$p(X = x_i, Y = y_i) = \frac{n_{ij}}{N} \tag{1.5}$$

- sum rule (marginal probability):

$$p(X = x_i) = \frac{c_i}{N} = \frac{\sum_j n_{ij}}{N} = \sum_{j=1}^{L} p(X = x_i, Y = y_j) \tag{1.7}$$

- condition probability:

$$p(Y = y_i|X = x_i) = \frac{n_{ij}}{c_i} \tag{1.8}$$

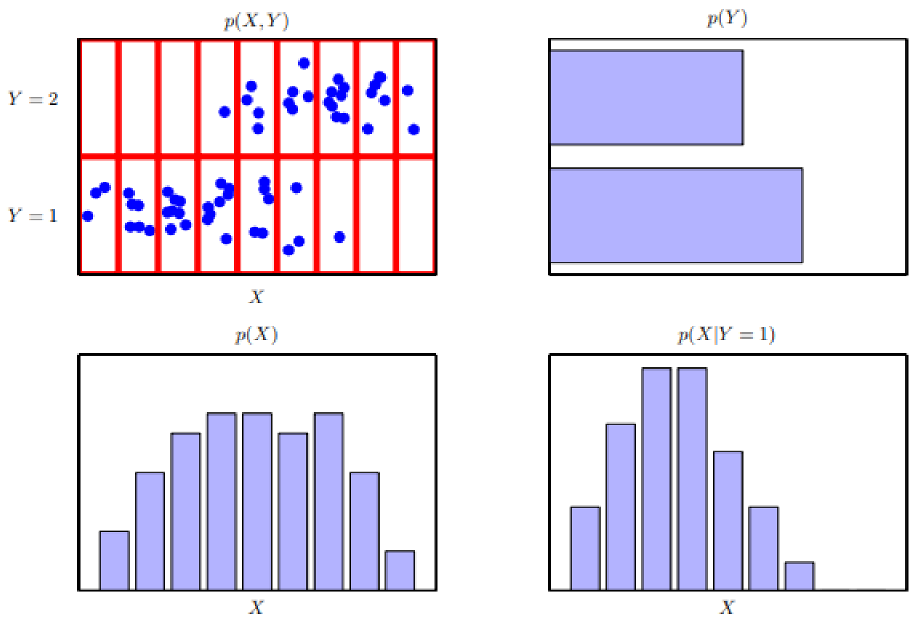
- product rule:

$$p(X = x_i, Y = y_i) = \frac{n_{ij}}{N} = \frac{n_{ij}}{c_{ij}} \cdot \frac{c_{ij}}{N} = p(Y = y_i|X = x_i)p(X = x_{ij}) \tag{1.9}$$

- Bayes' theorem

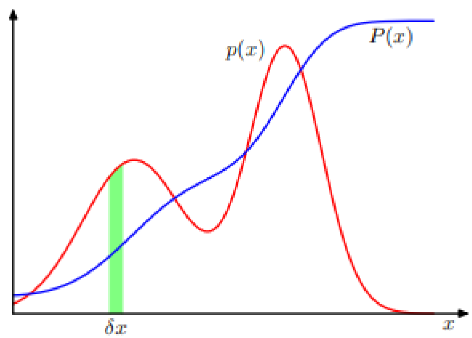
$$p(Y|X) = \frac{p(X|Y)p(Y)}{p(X)} = \frac{p(X|Y)p(Y)}{\sum_Y p(X|Y)p(Y)} \tag{1.13}$$

- independent: $p(X, Y) = p(X)p(Y)$



1.2.1 Probability densities

- **probability density**: If the probability of a real-valued variable x falling in the interval $(x, x+\delta x)$ is given by $p(x)\delta x$for $\delta x \to 0$, then $p(x)$ is probability density.



$$p(x \in (a,b)) = \int_a^b p(x)dx \tag{1.24}$$

s.t

$$p(x) \geqslant 0 \tag{1.25}$$

$$\int_{-\infty}^{\infty} p(x)dx = 1 \tag{1.26}$$

- probability density transforms (due to Jacobian factor)
  - Jacobian factor: $J_{ki} \equiv \frac{\partial y_k}{\partial x_i}$
  - if $x = g(y)$, $f(x) = \tilde{f}(y) = f(g(y)) \to p_y(y) \neq p_x(x)$
  - *(ex.1.4)* the concept of the maximum of a probability density is dependent on the choice of variable.

$$p_y(y) = p_x(x)\left|\frac{d_x}{d_y}\right| = \frac{d(p_x(g(y))|g'(y)|)}{dy} \tag{1.27}$$

maximum value is calculated by $dp_y(y)/dy|_{\hat{y}} = 0$

$$\begin{aligned}
\frac{dp_y(y)}{dy} &= \frac{d(p_x(g(y))|g'(y)|)}{dy} && (1)\\
&= \frac{d(p_x(g(y)))}{dy}|g'(y)| + p_x(g(y))\frac{d|g'(y)|}{dy} && (2)\\
&= \frac{dp_x(g(y))}{dg(y)}\frac{dg(y)}{dy}|g'(y)| + p_x(g(y))\frac{d|g'(y)|}{dy} && (3)\\
&= \frac{dp_x(x)}{dx}\frac{dg(y)}{dy}|g'(y)| + p_x(g(y))\frac{d|g'(y)|}{dy} = p_x(g(y))\frac{d|g'(y)|}{dy} && (4)
\end{aligned}$$

If $p_x(x) = 2x, x \in [0,1]$, the maximum value of variable $\hat{x}$ is 1. And given that $x = sin(y)$, it transform to the $p_y(y) = 2sin(y)|cos(y)|(= sin(2y)), y \in [0, \pi/2]$, and the $\hat{y}$ is $\pi/4$. $\therefore \hat{x} \neq sin(\hat{y})$

- **cumulative discribution function**: the probability that x lies in the interval $(-\infty, z)$
- **probability mass function** : $p(x)$ when x is a discrete variable.

$$P(z) = \int_{-\infty}^{z} p(x)dx \tag{1.28}$$

- The sum and product ruels, Bayes' therom of probability densities

$$p(x) = \int p(x, y)dy \tag{1.31}$$

$$p(x, y) = p(y|x)p(x) \tag{1.32}$$

1.2.2 Expectations and covariabces

- **expectation of** $f(x)$: weighted by the relative probabilities of the different values of x.

$$\mathbb{E}[f] = \sum_x p(x)f(x) \; or \int p(x)f(x)dx \tag{1.33}$$

- if there is N of points, the expectation can be approximated as

$$\mathbb{E}[f] \simeq \frac{1}{N}\sum_{n=1}^{N} f(x_n) \tag{1.35}$$

- **conditional expectiation**

$$\mathbb{E}_x[f|y] = \sum_x p(x|y)f(x) \tag{1.37}$$

- **variance**: measurment of how much variability there is in $f(x)$ around its mean value $\mathbb{E}[f(x)]$.

$$\begin{aligned} var[f] &= \mathbb{E}[(f(x) - \mathbb{E}[f(x)])^2] \\ &= \mathbb{E}[f(x)^2 - 2f(x)\mathbb{E}[f(x)]] + \mathbb{E}[f(x)]^2 \\ &= \mathbb{E}[f(x)^2 - 2\mathbb{E}[f(x)\mathbb{E}[f(x)]]] + \mathbb{E}[f(x)]^2 \\ &= \mathbb{E}[f(x)^2] - 2\mathbb{E}[f(x)]^2 + \mathbb{E}[f(x)]^2 \end{aligned} \tag{1.38}$$

$$var[f] = \mathbb{E}[(f(x)]^2 - \mathbb{E}[f(x)]^2 \tag{1.39}$$

- **covariance**: expresses the extent to which x and y vary together. (if x and y is independent, cov=0)

$$\begin{aligned} cov[x, y] &= \mathbb{E}_{x,y}[\{x - \mathbb{E}[x]\}\{y - \mathbb{E}[y]\}] \\ &= \mathbb{E}_{x,y}[xy - x\mathbb{E}[y] - y\mathbb{E}[x] + \mathbb{E}[x]\mathbb{E}[y]] \\ &= \mathbb{E}_{x,y}[xy] - \mathbb{E}_{x,y}[x\mathbb{E}[y]] - \mathbb{E}_{x,y}[y\mathbb{E}[x]] + \mathbb{E}[x]\mathbb{E}[y] \\ &= \mathbb{E}_{x,y}[xy] - \mathbb{E}[x]\mathbb{E}[y] - \mathbb{E}[y]\mathbb{E}[x] + \mathbb{E}[x]\mathbb{E}[y] \\ &= \mathbb{E}_{x,y}[xy] - \mathbb{E}[x]\mathbb{E}[y]] \end{aligned} \tag{1.41}$$

(vector)

$$\begin{aligned} cov[\mathbf{x}, \mathbf{y}] &= \mathbb{E}_{\mathbf{x},\mathbf{y}}[\{\mathbf{x} - \mathbb{E}[\mathbf{x}]\}\{\mathbf{y}^{\mathbf{T}} - \mathbb{E}[\mathbf{y}^{\mathbf{T}}]\}] \\ &= \mathbb{E}_{\mathbf{x},\mathbf{y}}[\mathbf{x}\mathbf{y}^{\mathbf{T}}] - \mathbb{E}[\mathbf{x}]\mathbb{E}[\mathbf{y}^{\mathbf{T}}]] \end{aligned} \tag{1.42}$$

1.2.3 Bayesian probabilities

- **Purpose**: to address and quantify the uncertainty that surrounds the appropriate choice for the model parameters $\mathbf{w}$
- **Bayes' theorem**: at the uncertain event,
  - (1) (prior probability) Suppose some opinion based on exist knowldge
  - (2) obtain fresh evidence
  - (3) (posterior probability) revise the uncertainty about (1)opinion
  - that is, to convert a prior probability into a posterior probability by incorporating the evidence provided by the observed data

$$p(\mathbf{w}|\mathcal{D}) = \frac{p(\mathcal{D}|\mathbf{w})p(\mathbf{w})}{p(\mathcal{D})} = \frac{p(\mathcal{D}|\mathbf{w})p(\mathbf{w})}{\int p(\mathcal{D}|\mathbf{w})p(\mathbf{w})} \tag{1.43}$$

- $p(\mathbf{w})$: prior probability, assumptions about $\mathbf{w}$, before observing the data
- $p(\mathcal{D}|\mathbf{w}), \mathcal{D} = \{t_1, t_2, ..., t_n\}$: likelihood function, how probable the observed data set is for different settings of the parameter vector $\mathbf{w}$
- $p(\mathbf{w}|\mathcal{D})$: posterior probability, to evaluate the uncertainty in w after observing D.
- $p(\mathcal{D})$: normalization constant
- **Frequentist paradigms**
  - frequentist estimator $\rightarrow$ maximum likelihood (maximize $p(\mathbf{w}|\mathcal{D})$)
  - or minimize the *error* by the *error function*
- **Bayesian view**: provide a quantification of uncertainty using probabilities.
  - Advantage: the inclusion of prior knowledge arises naturally
  - Criticism: at the prior distribution is often selected on the basis of mathematical convenience rather than as a reflection of any prior beliefs
  - To reduce the dependence on the prior $\rightarrow$ noninformative priors
  - Limitation: for using Bayeesian, need to marginalize over the whole of parameter space (it is difficult!)

1.2.4 The Gaussian distribution

$$\mathcal{N}(x|\mu,\sigma^2) = \frac{1}{(2\pi\sigma^2)^{1/2}} exp\{-\frac{1}{2\sigma^2}(x-\mu)^2\} \tag{1.46}$$

- precision: $\frac{1}{\sigma^2}$

- **vector form**

$$\mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu},\boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{D/2}}\frac{1}{|\boldsymbol{\Sigma}|^{1/2}} exp\{-\frac{1}{2}(\mathbf{x}-\mu)^T\Sigma(\mathbf{x}-\mu)\} \tag{1.52}$$

It is probability density

(1) $\mathcal{N}(x|\mu,\sigma^2) > 0$

(2)

$$\int_{-\infty}^{\infty}\mathcal{N}(x|\mu,\sigma^2) = 1 \tag{1.48}$$

(ex.1.7)

$$\int_{-\infty}^{\infty} exp\{-\frac{1}{2\sigma^2}(x-\mu)^2\}dx = \sqrt{2\pi\sigma^2}$$

$$\int_{-\infty}^{\infty} exp\{-\left(\frac{x-\mu}{\sqrt{2\sigma^2}}\right)^2\}dx = \sqrt{2\pi\sigma^2}$$

$$\int_{-\infty}^{\infty} e^{-z^2}dz = \sqrt{\pi} \text{ ,where } z = \left(\frac{x-\mu}{\sqrt{2\sigma^2}}\right), dx = \sqrt{2\sigma^2 dz}$$

transform the spherical coordinate system

$$\int_{-\infty}^{\infty} e^{-x^2}dx\int_{-\infty}^{\infty} e^{-y^2}dy = \int\int_{-\infty}^{\infty} e^{-(x^2+y^2)}dxdy = \pi$$

$$= \int_0^{2\pi}\int_0^{\infty} e^{-r^2}rdrd\theta = \int_0^{2\pi}\int_0^{\infty}(-1/2)e^u dud\theta = \pi$$

- **expectation**

$$\mathbb{E}[x] = \int_{-\infty}^{\infty} \mathcal{N}(x|\mu, \sigma^2) x dx = \mu \tag{1.49}$$

(ex.1.8)

$$\begin{aligned}
\int_{-\infty}^{\infty} \mathcal{N}(x|\mu, \sigma^2) x dx &= \int_{-\infty}^{\infty} \frac{1}{(2\pi\sigma^2)^{1/2}} exp\{-\frac{1}{2\sigma^2}(x-\mu)^2\} x dx \\
&= \int_{-\infty}^{\infty} \frac{1}{(2\pi\sigma^2)^{1/2}} exp\{-\frac{1}{2\sigma^2}y^2\}(y+\mu) dy \ (y = x-\mu) \\
&= \mu \int_{-\infty}^{\infty} \frac{1}{(2\pi\sigma^2)^{1/2}} exp\{-\frac{1}{2\sigma^2}y^2\} dy + \int_{-\infty}^{\infty} \frac{1}{(2\pi\sigma^2)^{1/2}} exp\{-\frac{1}{2\sigma^2}y^2\} y dy \\
&= \mu + 0 = \mu
\end{aligned}$$

- **variance**

$$\mathbb{E}[x^2] = \int_{-\infty}^{\infty} \mathcal{N}(x|\mu, \sigma^2) x^2 dx = \mu^2 + \sigma^2 \tag{1.50}$$

$$var[x] = \mathbb{E}[x^2] - \mathbb{E}[x]^2 = \sigma^2 \tag{1.51}$$

- The maximum of a distribution is known as its mode. For a Gaussian, the mode = mean

(ex.1.8)

$$\begin{aligned}
Var[x] &= \int_{-\infty}^{\infty} (x-\mu)^2 \mathcal{N}(x|\mu, \sigma^2) x dx, f(x) = \mathcal{N}(x|\mu, \sigma^2) \\
&= \int_{-\infty}^{\infty} x^2 f(x) - 2\mu x f(x) + \mu^2 f(x) dx \\
&= \int_{-\infty}^{\infty} x^2 f(x) dx - 2\mu \int_{-\infty}^{\infty} x f(x) dx + \mu^2 \int_{-\infty}^{\infty} f(x) dx \\
&= \int_{-\infty}^{\infty} x^2 f(x) dx - 2\mu \cdot \mu + \mu^2 \cdot 1 \\
&= \int_{-\infty}^{\infty} x^2 f(x) dx - \mu^2 = \mathbb{E}[x^2] - \mathbb{E}[x]^2
\end{aligned}$$

$\therefore \mathbb{E}[x^2] = Var[x] + \mu^2 = \sigma^2 + \mu$

Goal: determine μ, σ parameters from the data set

- **maximize the (log) likelihood function**

$$\ln p(\mathbf{x}|\mu, \sigma^2) = -\frac{1}{2\sigma^2}\sum_{n=1}^{N}(x_n - \mu)^2 - \frac{1}{2}\ln\sigma^2 - \frac{N}{2}\ln(2\pi) \tag{1.54}$$

- why log?
  - (1) simplifies the subsequent mathematical analysis (2) good for underflow the numerical precision of the computer
- **sample mean**: maximizint (1.54) whith respect to μ

$$\mu_{ML} = \frac{1}{N}\sum_{n=1}^{N} x_n \tag{1.55}$$

(ex.1.11)

$$\begin{aligned}
\frac{\partial}{\partial\mu}(\sum_{n=1}^{N}(x_n - \mu)^2) &= 0 \\
\frac{\partial}{\partial\mu}(\sum_{n=1}^{N}(x_n^2 - 2x_n\mu + \mu^2)) &= 0 \\
\sum_{n=1}^{N}(-2x_n + 2\mu) &= 0 \\
\sum_{n=1}^{N} 2x_n &= 2N\mu \\
\therefore \mu_{ML} &= \frac{1}{N}\sum_{n=1}^{N} x_n
\end{aligned}$$

- **sample variance**: maximizint (1.54) whith respect to σ^2
  - the solution (μ_{ML}) and $\sigma^2_{ML}$is decopled. → calculation order does not matter

$$\sigma^2_{ML} = \frac{1}{N}\sum_{n=1}^{N}(x_n - \mu_{ML})^2 \tag{1.55}$$

(ex.1.11)

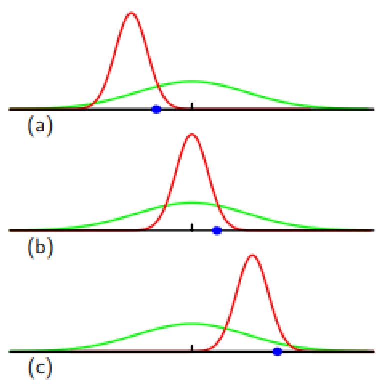
$$\begin{aligned}
\frac{\partial}{\partial\sigma^2}(-\frac{1}{2\sigma^2}\sum_{n=1}^{N}(x_n - \mu)^2 - \frac{N}{2}\ln\sigma^2) &= 0 \\
\frac{1}{2}\sum_{n=1}^{N}(x_n - \mu)^2 - \frac{N}{2}\sigma^2 &= 0 \\
\therefore \sigma^2_{ML} &= \frac{1}{N}\sum_{n=1}^{N}(x_n - \mu_{ML})^2
\end{aligned}$$

- **Limit: bias problem**
  - μ_{ML} is unbias, σ^2_{ML} is bias
  - at the variance, bias (underestimat) $\rightarrow$ over fitting
  - more complex models with many parameters $\rightarrow$ more bias $\rightarrow$ over fitting

$$\mathbb{E}[\mu_{ML}] = \mu \tag{1.57}$$

$$\mathbb{E}[\sigma^2_{ML}] = \frac{N-1}{N}\sigma^2 \tag{1.58}$$

$$\therefore \text{unbias variable : } \tilde{\sigma}^2 = \frac{N}{N-1}\sigma^2 = \frac{1}{N-1}\sum_{n=1}^{N}(x_n - \mu_{ML})^2 \tag{1.59}$$



1.2.5 Curve fitting re-visited

Goal: to predictions for the target variable t given some new value of the input variable x on the basis of a set of training data comprising N input values $x = (x_1, ..., x_N)^T$ and their corresponding target values $t = (t_1, ..., t_N)^T$ (from a probabilistic perspective)

assume that it is a Gaussian distribution

$$p(t|x, \mathbf{w}, \beta) = \mathcal{N}(t|y(x, \mathbf{w}), \beta^{-1}) \tag{1.60}$$

Step 1: usingthe training set $\{\mathbf{x}, \mathbf{t}\} \rightarrow$ finding an unknown $\mathbf{w}$ & β by maximum likelihood

$$p(\mathbf{t}|\mathbf{x}, \mathbf{w}, \beta) = \prod_{n=1}^{N} \mathcal{N}(t_n|y(x_n, \mathbf{w}), \beta^{-1}) \tag{1.61}$$

$$\ln p(\mathbf{t}|\mathbf{x}, \mathbf{w}, \beta) = -\frac{\beta}{2} \sum_{n=1}^{N} \{y(x_n, \mathbf{w}) - t\}^2 + \frac{N}{2} \ln \beta - \frac{N}{2} \ln(2\pi) \tag{1.62}$$

- $\mathbf{w}_{ML}$: minimize $\frac{\beta}{2} \sum_{n=1}^{N} \{y(x_n, \mathbf{w}) - t\}^2$ (=1.2)
- β_{ML}:

$$\frac{1}{\beta} = \frac{1}{N} \sum_{n=1}^{N} \{y(x_n, \mathbf{w}_{ML}) - t_n\}^2 \tag{1.62}$$

- Having determined the parameters $\mathbf{w}$ and $\beta \rightarrow$ predictive distribution that gives the probability distribution over t

$$p(t|x, \mathbf{w}_{ML}, \beta_{ML}) = \mathcal{N}(t|y(x, \mathbf{w}_{ML}), \beta_{ML}^{-1}) \tag{1.63}$$

Step 2: introduce a prior distribution for Bayesian approach

- **prior**

$$p(\mathbf{w}, \alpha) = \mathcal{N}(\mathbf{w}|\mathbf{0}, \alpha^{-1}\mathbf{I}) = (\frac{\alpha}{2\pi})^{(M+1)/2} \exp\{-\frac{\alpha}{2} \mathbf{w}^T \mathbf{w}\} \tag{1.65}$$

- α: precision (hyperparameter), $M + 1$:the total number of elements in the vector $\mathbf{w}$ for an M_{th} order polynomial
- **posterior**

$$p(\mathbf{w}|\mathbf{x}, \mathbf{t}, \alpha, beta) = p(\mathbf{t}|\mathbf{x}, \mathbf{w}, \beta) p(\mathbf{w}, \alpha) \tag{1.66}$$

- **MAP**: maximizing the posterior distribution, determine w by finding the most probable value of w given the data (a point estimate)

$$\text{minimize } \frac{\beta}{2} \sum_{n=1}^{N} \{y(x_n, \mathbf{w}_{ML}) - t_n\}^2 + \frac{\alpha}{2} \mathbf{w}^T \mathbf{w} \tag{1.67}$$

- It is same as (1.4) with a regularization parameter given by $\lambda = \alpha/\beta$.

1.2.6 Bayesian curve fitting

- Marginalizations of $\mathbf{w} \rightarrow$ predict $\mathbf{w}$ as a distribution

$$p(t|x, \mathbf{x}, \mathbf{t}) = \int p(t|x, \mathbf{w}) p(\mathbf{w}|\mathbf{x}, \mathbf{t}) d\mathbf{w} \tag{1.68}$$

- $p(t|x, \mathbf{w})$: (1.60), $p(\mathbf{w}|\mathbf{x}, \mathbf{t})$: posterior, normalizing the right-hand side of (1.66)

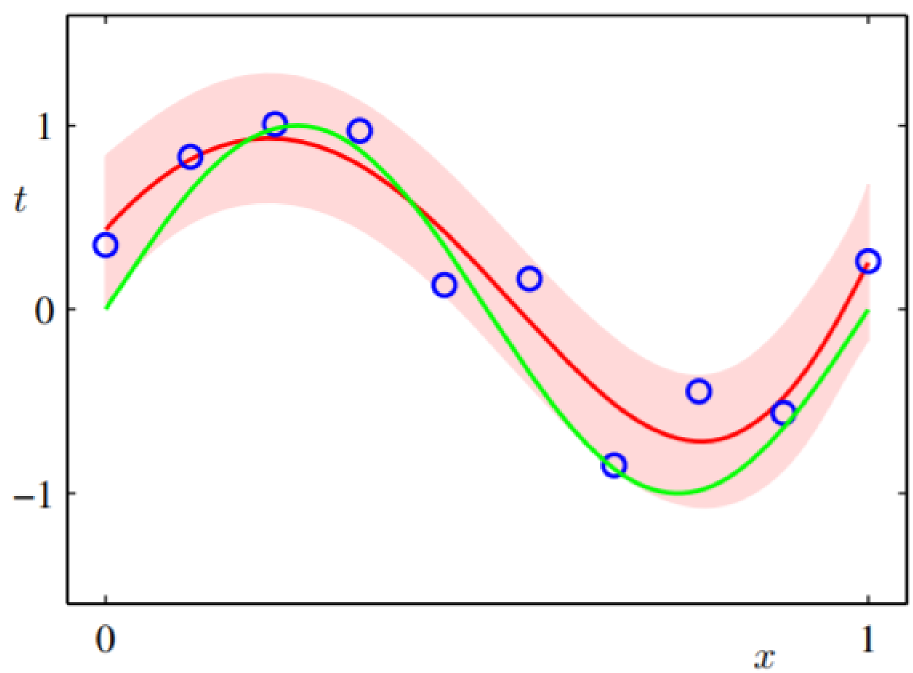
$$p(t|x, \mathbf{x}, \mathbf{t}) = \mathcal{N}(t|m(x), s^2(x)) \tag{1.69}$$

$$m(x) = \beta \phi(x)^T \mathbf{S} \sum_{n=1}^{N} \phi(x_n) t_n \tag{1.70}$$

$$s^2(x) = \beta^{-1} + \phi(x)^T \mathbf{S} \phi(x) \tag{1.70}$$

$$\mathbf{S}^{-1} = \alpha \mathbf{I} + \beta \sum_{n=1}^{N} \phi(x_n) \phi(x_n)^T \tag{1.72}$$

- β^{-1}: the uncertainty in the predicted value of t, $\phi(x)^T \mathbf{S} \phi(x)$: the uncertainty of $\mathbf{w}$ (a consequence of the Bayesian treatment)



1.3 Model Selection

- Select the number of free parameters (order)
- In the maximum likelihood approach, the performance on the training set is not a good indicator of predictive performance on unseen data ($\because$ over-fitting)
- $\therefore$ setting a validation set $\rightarrow$ select the one having the best predictive performance
- However, the supply of data for training and testing will be limited $\rightarrow$ **cross validation**
- **cross validation drawback**:
  - larger the number of factor of S, more the training runs
- **Information criteria**
  - akaike information criterion, AIC: add panalty term which is number of adjustable parameters at the log likelihood
  - Bayesian information criterion, BIC (Section 4.4.1)
- **Information criteria limits**:
  - not take account of the uncertainty in the model parameters
  - tend to favour overly simple model

1.4 The Curse of Dimensionality

- **The Curse of Dimensionality**: when the dimensionality increases, the volume of the space increases so fast that the available data become sparse

(example)

$$y(\mathbf{x}, \mathbf{w}) = w_0 + \sum_{i=1}^{D} w_i x_i + \sum_{i=1}^{D}\sum_{j=1}^{D} w_{ij} x_i x_j + \sum_{i=1}^{D}\sum_{j=1}^{D}\sum_{k=1}^{D} w_{ijk} x_i x_j x_k \tag{1.74}$$

- As the number of input variables D increases, so the number of independent coefficients $\propto D^3$
- For a polynomial of order M, the number of coefficients $\propto D^M$

1.5 Decision Theory

- When combined with probability theory, allows us to make optimal decisions in situations involving uncertainty
- **Inference**: Determination of $p(x, t)$ from a set of training data
  - $p(x, t)$: complete summary of the uncertainty associated with these variables
  - any of the quantities appearing in Bayes' theorem can be obtained from the joint distribution $p(x, t)$ by either marginalizing or conditioning with respect to the appropriate variables

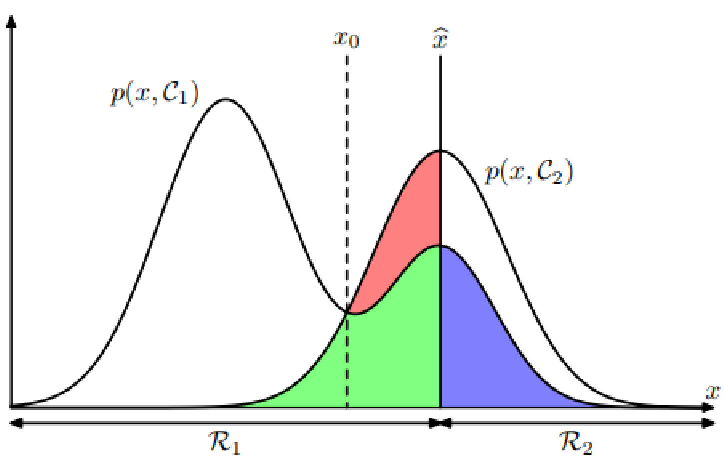
$$p(\mathcal{C}_k|\mathbf{x}) = \frac{p(\mathbf{x}|\mathcal{C}_k)p(\mathcal{C}_k)}{p(\mathbf{x})} \tag{1.77}$$

1.5.1 Minimizaing the misclassification rate

Goal: to make as few misclassifications as possible

- Decision region: a rule - *assigns each value of x to one of the available classes*- will divide the input space into regions $\mathcal{R}_k$ for each class, such that all points in $\mathcal{R}_k$ are assigned to class $\mathcal{C}_k$
- Decision boundary or decision surface: the boundaries between decision regions

$$\begin{aligned} \text{maximize } p(correct) &= \sum_{k=1}^{K} p(\mathbf{x} \in \mathcal{R}_k, \mathcal{C}_k) \\ &= \sum_{k=1}^{K} \int_{\mathcal{R}_k} p(\mathbf{x}, \mathcal{C}_k) d\mathbf{x} \end{aligned} \tag{1.79}$$



- The optimal choice for $\hat{x}$ is where the curves for $p(x, C_1)$ and $p(x, C_2)$ cross, corresponding to $\hat{x} = x_0$, because in this case the red region disappears.

1.5.2 Minimizing the expected loss

- **cost function** or **loss function** : overall measure of loss incurred in taking any of the available decisions or actions, $L_{kj}p(\mathbf{x}, \mathcal{C}_k)$

Goal: to minimize the total loss incurred

(loss matrix)

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

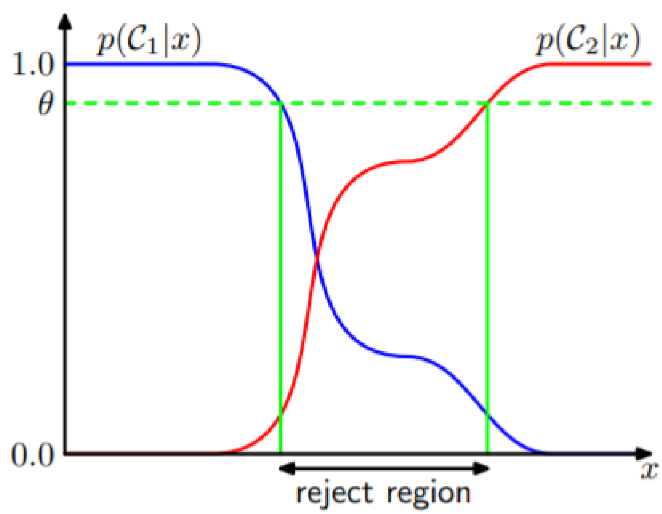
- The loss function depends on the true class, which is unknown.

$$\begin{aligned} \text{minimize } \mathbb{E}[L] &= \sum_k \sum_j \int_{\mathcal{R}_j} L_{kj} p(\mathbf{x}, \mathcal{C}_k) d\mathbf{x} \qquad (1.80) \\ &= \sum_k \sum_j \int_{\mathcal{R}_j} L_{kj} p(\mathcal{C}_k|\mathbf{x}) p(\mathbf{x}) d\mathbf{x} \end{aligned}$$

$$\text{minimize } \sum_k L_{kj} p(\mathcal{C}_k|\mathbf{x}) \qquad (1.81)$$

1.5.3 The reject option

- somtimes $p(\mathcal{C}_k|\mathbf{x})$ is too small (= joint distributions $p(x, C_k)$s are similar value)
- In areas where it is difficult to make a decision, the reject option could be better



1.5.4 Inference and decision

- Decision problem process: inference stage (train the posterior) $\rightarrow$ decision stage *or* using discriminant function
- **(a) generative model**
  - (1) solve theh inference problem, Determining the class-conditional densities $p(x|\mathcal{C}_k)$ for each class $\mathcal{C}_k$ individually
  - (2) separately infer the prior class probabilities $p(C_k)$
  - or model the joint distribution $p(x, C_k)$ directly and then normalize
  - (3) obtain the posterior probabilities
  - Advantage: using $p(x) \rightarrow$ outlier detection or novelty detection
  - Limit: excessively demanding of data, to find the joint distribution
- **(b) discriminative model**
  - obtain a posterior probability directly
  - (1) solve the inference problem
  - (2) using the decision theory
  - (3) to assign each new $\mathbf{x}$ to one of the classes
- **(c) using discriminant function**
  - discriminant function $\rightarrow$ directly assigning
  - In this case, probabilities play no role
- The reasons for the posterior probabilities
  - Minimizing risk
  - Reject option
  - Compensating for class priors
  - Combining models

1.5.5 Loss functions for regression

Goal: to choose $y(x)$ so as to minimize the average, or expected, loss $\mathbb{E}[L]$.

$$\text{minimize } \mathbb{E}[L] = \int\int L(t, y(\mathbf{x})p(\mathbf{x}, t)d\mathbf{x}dt \tag{1.86}$$

- A common loss function in regression problems: $L(t, y(\mathbf{x})) = \{y(\mathbf{x}) - t\}^2$
- **Regression function**: the conditional average of t conditioned on $\mathbf{x}$
  - The regression function $y(x)$, which minimizes the expected squared loss,is given by the mean of the conditional distribution $p(t|x)$.

$$\text{minimize } \mathbb{E}[L] = \int\int \{y(\mathbf{x} - t)\}^2 p(\mathbf{x}, t)d\mathbf{x}dt \tag{1.87}$$

$$\frac{\delta\mathbb{E}[L]}{\delta y(\mathbf{x})} = 2\int \{y(\mathbf{x}) - t\}p(\mathbf{x}, t)dt \tag{1.88}$$

(appendix D)

$$\begin{aligned}
\int y(\mathbf{x})p(\mathbf{x}, t)dt - \int tp(\mathbf{x}, t)dt = 0 \\
y(\mathbf{x})p(\mathbf{x}) = \int tp(\mathbf{x}, t)dt \\
y(x) = \frac{\int tp(\mathbf{x}, t)dt}{p(x)} = \frac{\int tp(t|\mathbf{x})p(x)dt}{p(x)}
\end{aligned}$$

$$y(x) = \frac{\int tp(\mathbf{x}, t)dt}{p(x)} = \int tp(t|\mathbf{x})dt = \mathbb{E}_t[t|\mathbf{x}] \tag{1.89}$$

- slightly different way,

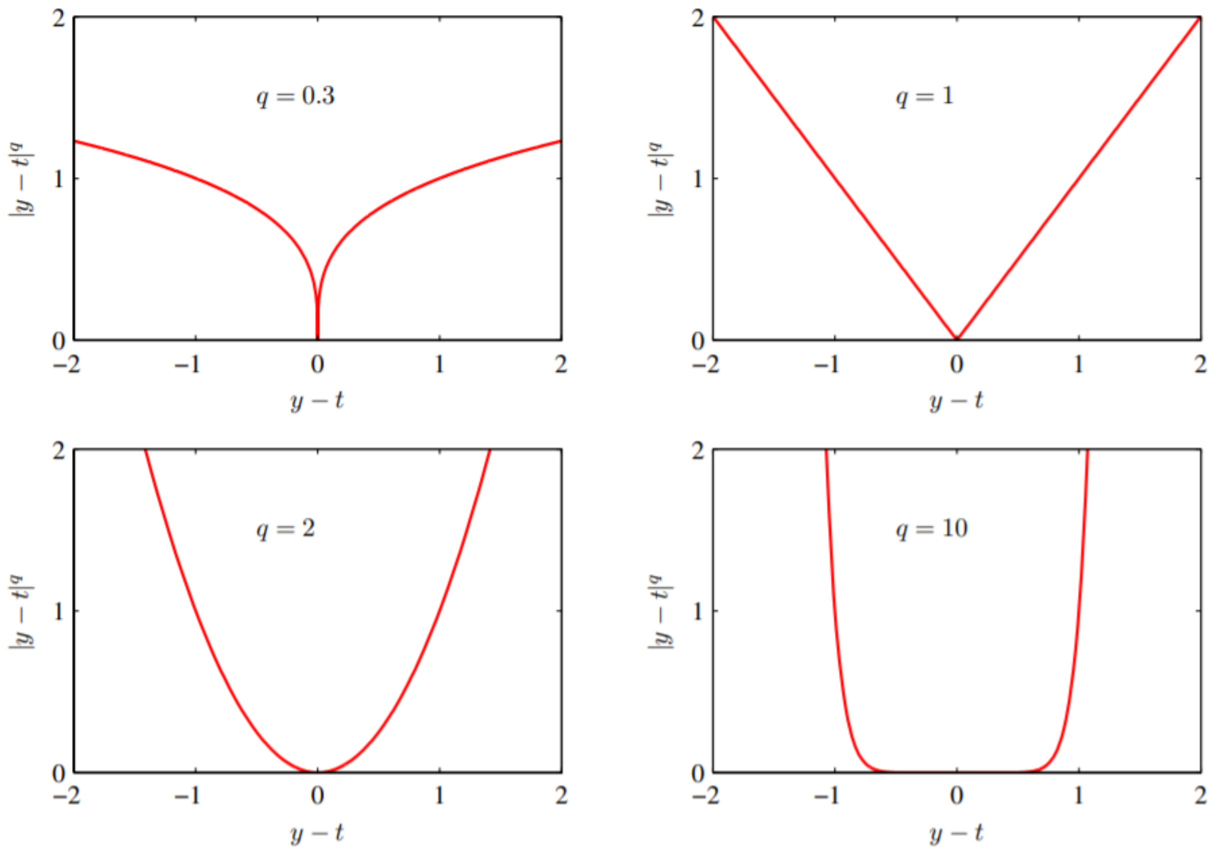
$$\begin{aligned}
\{y(\mathbf{x}) - t\}^2 &= \{y(\mathbf{x}) - \mathbb{E}[t|\mathbf{x}] + \mathbb{E}[t|\mathbf{x}] - t\}^2 \\
&= \{y(\mathbf{x}) - \mathbb{E}[t|\mathbf{x}]\}^2 + 2\{y(\mathbf{x}) - \mathbb{E}[t|\mathbf{x}]\}\{\mathbb{E}[t|\mathbf{x}] - t\} + \{\mathbb{E}[t|\mathbf{x}] - t\}^2
\end{aligned}$$

$$\begin{aligned}
\mathbb{E}[L] &= \int \{y(\mathbf{x}) - \mathbb{E}[t|\mathbf{x}]\}^2 + 2\{y(\mathbf{x}) - \mathbb{E}[t|\mathbf{x}]\}\{\mathbb{E}[t|\mathbf{x}] - t\} + \{\mathbb{E}[t|\mathbf{x}] - t\}^2 p(\mathbf{x}, t)dt \\
&= \int \{y(\mathbf{x}) - \mathbb{E}[t|\mathbf{x}]\}^2 p(\mathbf{x})d\mathbf{x} + \int \{\mathbb{E}[t|\mathbf{x}] - t\}^2 p(\mathbf{x})d\mathbf{x} = var[t|\mathbf{x}]p(\mathbf{x})
\end{aligned} \tag{1.90}$$

- second term
  - the variance of the distribution of t, averaged over $\mathbf{x}$
  - the irreducible minimum value of the loss function, noise

- another loss function: Minkowski loss

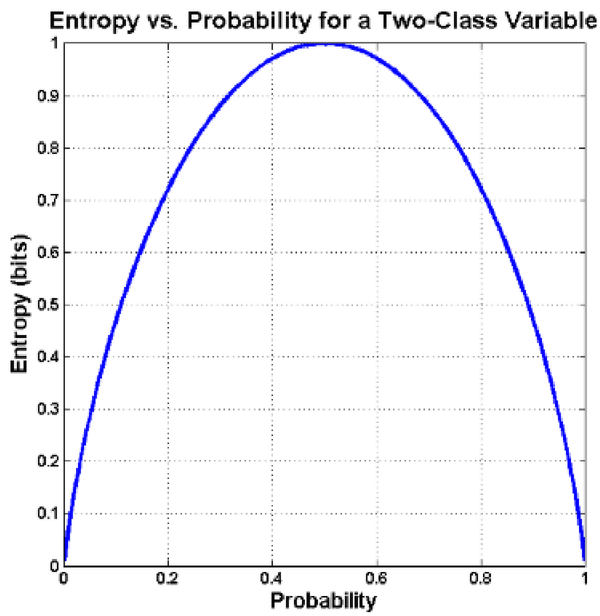
$$\mathbb{E}[L_q] = \int\int |y(\mathbf{x}) - t|^q p(\mathbf{x}, t) d\mathbf{x} dt \tag{1.91}$$



1.6 Information Theory

- **Entropy**: the average amount of information needed to specify the state of a random variable
  - low probability events → high information content → low entropy
  - nonuniform distribution's entropy < uniform (that is, uniform distribution has lower information than nonuniform one.)
  - Entropy is pasitive value ($\because$ p is probability, $0 \leqslant p_i \leqslant 1$)
  - *(ex. 1.29)* If all of the $p(x_i)$ are equal and given by $p(x_i) = 1/M$ where M is the total number of states x_i, the Entropy is maximized.

$$\mathrm{H}[x] = -\sum_x p(x) \log_2 p(x) \tag{1.93}$$



(ex. 1.29)

Jensen's Inequality

$$f(\sum_{i=1}^{N} p_i x_i) \leq \sum_{i=1}^{N} p_i f(x_i)$$

(proof) if $f(x)$ is convex,

$$\begin{aligned} f(\sum_{i=1}^{N} p_i x_i) &= f(p_1 x_1 + (1-p_1)\sum_{i=2}^{N} \frac{p_i}{1-p_1} x_i) \\ &\leq p_1 f(x_1) + (1-p_1)\sum_{i=2}^{N} \frac{p_i}{1-p_1} f(x_i) = p_1 f(x_1) + \sum_{i=2}^{N} p_i f(x_i) = \sum_{i=1}^{N} p_i f(x_i) \end{aligned}$$

Show that the entropy of distribution $p(x)$ satisfies $\mathbf{H}[\mathbf{x}] \leq \ln M$

$$\mathrm{H}[x] = -\sum_{i=1}^{M} p(x_i) \log p(x_i) = \sum_{i=1}^{M} p(x_i) \log \frac{1}{p(x_i)}$$

$\log \mu$ is concave, so, it is satisfied that $\sum_{i=1}^{N} p_i f(x) \leq f(\sum_{i=1}^{N} p_i x_i)$.

$f(x)$ is log function,

$$\therefore \sum_{i=1}^{M} p(x_i) \log \frac{1}{p(x_i)} \leq \log(\sum_{i=1}^{M} p_i(x_i) \cdot \frac{1}{p(x_i)}) = \log M$$

At the gaussian distribution, ...

1.6.1 Relative entropy and mutual information

- **Kullback-Leibler divergence, KL divergence, relative entropy**
  - Consider unknown distribution $p(\mathbf{x}) \rightarrow$ *modeling* $\rightarrow$ approximating distribution $q(\mathbf{x})$
  - the average *additional* amount of information required to specify the value of $\mathbf{x}$ as a result of using $q(\mathbf{x})$ instead of the true distribution $p(\mathbf{x})$
  - not a symmetrical quantity ($\mathrm{KL}(p||q) \neq \mathrm{KL}(q||p)$)
  - *(ex. 1.33)* KL satifies KL≥ 0 with equality iff, $p(\mathbf{x}) = q(\mathbf{x})$

$$\begin{aligned}
\mathrm{KL}[p||q] &= -\int xp(\mathbf{x}) \ln q(\mathbf{x}) d\mathbf{x} - (-\int p(\mathbf{x}) \ln p(\mathbf{x}) d\mathbf{x}) \\
&= -\int p(\mathbf{x}) \ln \frac{q(\mathbf{x})}{p(\mathbf{x})} d\mathbf{x}
\end{aligned} \tag{1.113}$$

(ex. 1.33)

i) $\mathrm{KL}[p||q] = 0$ iff, $p = q$

$$\begin{aligned}
\mathrm{KL}[p||q] &= \sum_i p_i \log \frac{p_i}{q_i} \\
&\geq -\log[\sum_i p_i \frac{q_i}{p_i}] = -\log[\sum_i q_i] = 0
\end{aligned}$$

ii) minimize $\mathrm{KL}[p||q] = 0$, s.t. $\sum_i p_i = 1$

$$\begin{aligned}
\epsilon &= \mathrm{KL}[p||q] + \lambda(1 - \sum_i p_i) = \sum_i p_i \log \frac{p_i}{q_i} + \lambda(1 - \sum_i p_i) \\
&= [\sum_i p_i (\log \frac{p_i}{q_i} - \lambda)] + \lambda \\
&= \sum p_i (\log p_i - \log q_i - \lambda) + \lambda \\
\frac{\partial \epsilon}{\partial p_k} &= (\log p_k - \log q_k - \lambda) + p_k \frac{1}{p_k} = 0 \\
&= \log p_k - \log q_k + 1 - \lambda = 0 \\
\log p_k &= \log q_k + (\lambda - 1) \\
p_k &= q_k \exp(\lambda - 1) \\
&\Leftrightarrow \sum_i q_i \exp(\lambda - 1) = 1, \therefore \lambda = 1 \\
\therefore p_i = q_i &
\end{aligned}$$

Further more,

$$\frac{\partial^2 \epsilon}{\partial p_i^2} = \frac{1}{p_i}, \frac{\partial^2 \epsilon}{\partial p_i \partial p_j} = 0$$

, That is Hessian >0 (p.d). $\therefore p_i = q_i$ is genuine minimal.

- **Mutual information**
  - How close to be independent by considering the KL divergence
  - *(ex.1.41)*$I(\mathbf{x},\mathbf{y}) \geq 0$ with equality iff, $\mathbf{x}$ and $\mathbf{y}$ are independent.

$$
\begin{aligned}
\mathrm{I}[\mathbf{x},\mathbf{y}] &\equiv \mathrm{KL}[p(x,y)||p(x)p(y)] \\
&= -\int\int p(\mathbf{x},\mathbf{y}) \ln(\frac{p(\mathbf{x}p(\mathbf{y}))}{p(\mathbf{x},\mathbf{y})}) d\mathbf{x}d\mathbf{y}
\end{aligned}
\tag{1.120}
$$

$$
\mathrm{I}[\mathbf{x},\mathbf{y}] = -\mathrm{H}(\mathbf{y}|\mathbf{x}) + \mathrm{H}(\mathbf{y}) = -\mathrm{H}(\mathbf{x}|\mathbf{y}) + \mathrm{H}(\mathbf{x}) \tag{1.121}
$$

(ex.1.41)

$$
\begin{aligned}
\mathrm{I}[\mathbf{x},\mathbf{y}] &= \mathrm{KL}[p(\mathbf{x},\mathbf{y})||p(\mathbf{x})p(\mathbf{y})] = \sum p(\mathbf{x},\mathbf{y}) \log \frac{p(\mathbf{x},\mathbf{y})}{p(\mathbf{x})p(\mathbf{y})} \\
&= \sum\sum p(\mathbf{x},\mathbf{y}) \log \frac{p(\mathbf{x},\mathbf{y})}{p(\mathbf{y})} - \sum\sum p(\mathbf{x},\mathbf{y}) \log p(\mathbf{x}) \\
(p(\mathbf{x},\mathbf{y}) &= p(\mathbf{x})p(\mathbf{y}|\mathbf{x}) = p(\mathbf{y})p(\mathbf{x}|\mathbf{y})) \\
&= \sum\sum p(\mathbf{y})p(\mathbf{x}|\mathbf{y}) \log p(\mathbf{x}|\mathbf{y}) - \sum\sum p(\mathbf{x},\mathbf{y}) \log p(\mathbf{x}) \\
&= \sum_y p(\mathbf{y}) \sum_x p(\mathbf{x}|\mathbf{y}) \log p(\mathbf{x}|\mathbf{y}) - \sum_x (\sum_y p(\mathbf{x},\mathbf{y}) \log p(\mathbf{x})) \\
&= -\mathrm{H}(\mathbf{x}|\mathbf{y}) + \mathrm{H}(\mathbf{x})
\end{aligned}
$$