Mathematic Foundation and Basic Concept

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Recap: Prerequisites

- Basic knowledge of probabilities
 - Bayes rule, chain rule, probability distribution ...
- Basic knowledge of information theory
 - Self-information, Shannon entropy, differential entropy ...
 - Kullback-Leibler (KL) divergence
- Basic knowledge of machine learning/deep learning
 - "Machine Learning", "Pattern Recognition and Machine Learning"
 - "Computer Vision", "Natural Language Processing" ...
- Basic programming language
 - Python

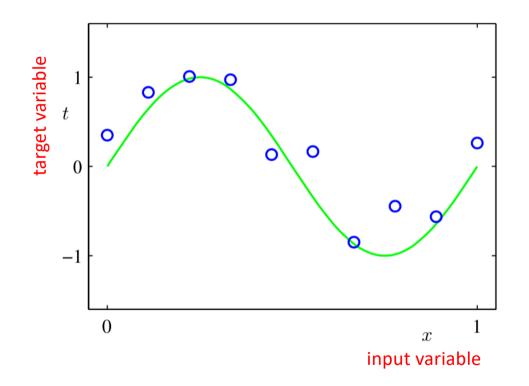
Mathematic Foundation and Basic Concept

- Example: Regression Polynomial Curve Fitting
- Probability Theory
- Decision Theory
- Information Theory

• Example: Regression - Polynomial Curve Fitting

- Probability Theory
- Decision Theory
- Information Theory

• Problem Definition



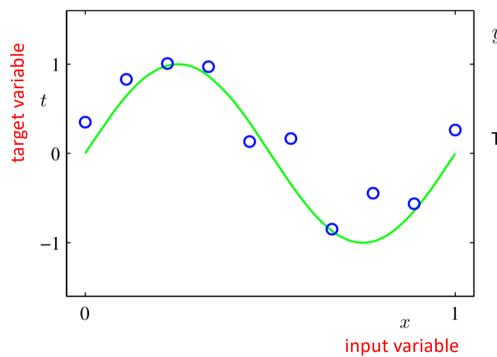
• A training dataset of N = 10 points

1

Predict the target value *t* given the input *x* ٠

$$\mathbf{x} \equiv (x_1, \dots, x_N)^{\mathrm{T}}$$
 A row vector with N elements $\mathbf{t} \equiv (t_1, \dots, t_N)^{\mathrm{T}}$

• Simple Model: Polynomial Function



M order polynomial:

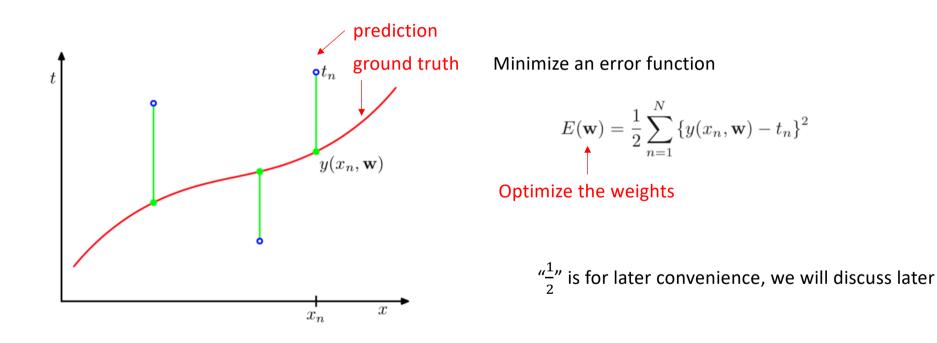
$$y(x, \mathbf{w}) = w_0 + w_1 x + w_2 x^2 + \ldots + w_M x^M = \sum_{j=0}^M w_j x^j$$

 $\mathbf{w} = (w_1, \ldots, w_M)^{\mathrm{T}}$ Weights: a row vector with M elements

The appropriate value \hat{t} :

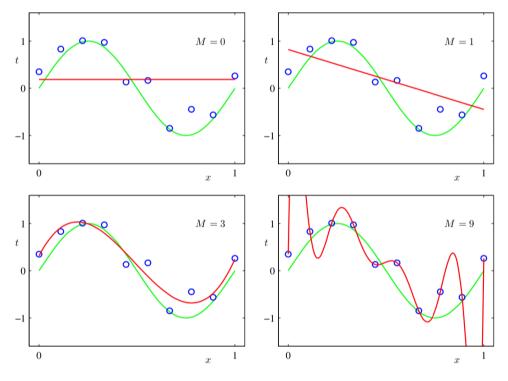
 $\hat{t} = \mathbf{x}^{\mathrm{T}} \mathbf{w}$

• Error Function





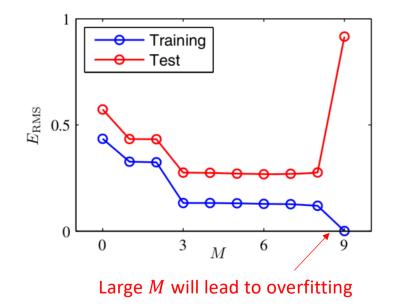
• Model Capacity and Overfitting



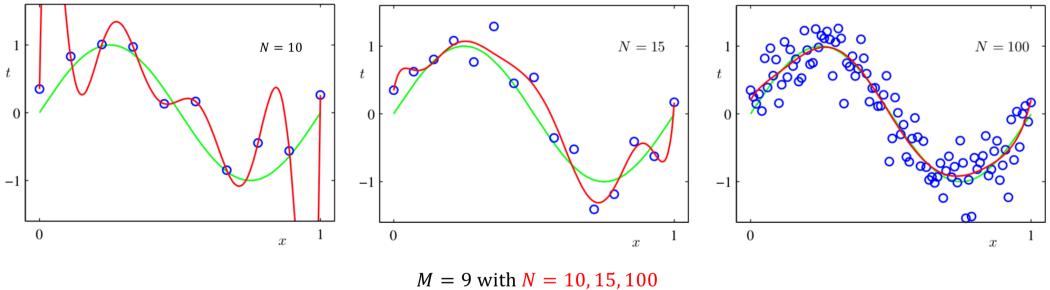
M order polynomial

Root mean square error:

$$E_{
m RMS} = \sqrt{2E(\mathbf{w}^{\star})/N}$$
 Averaged/mean error $E(\mathbf{w}^{\star}) = 0$ Optimized weights

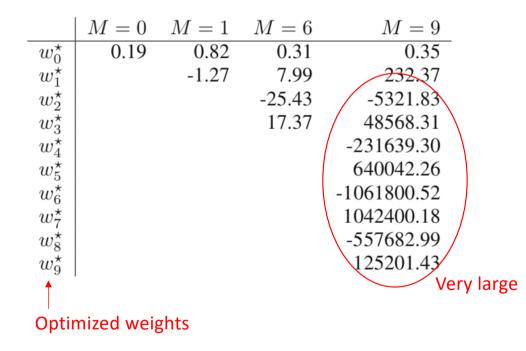


• Solution1 : More Training Data Point



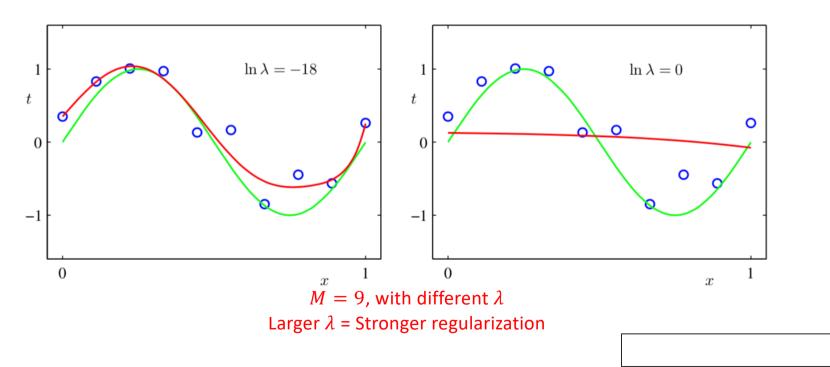
M = 9 with N = 10, 15, 100More data points = Better generalization

• Solution2 : Weight Regularization

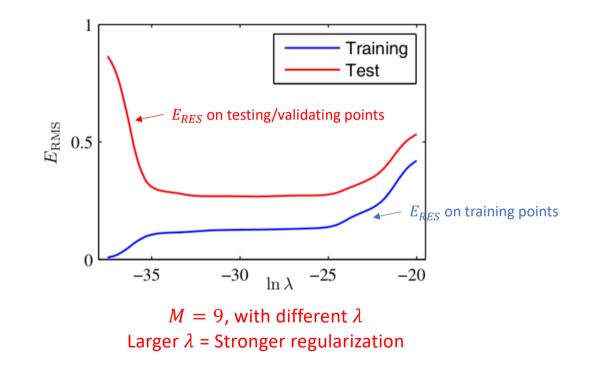


• Solution2 : Weight Regularization

$$\widetilde{E}(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^{N} \{y(x_n, \mathbf{w}) - t_n\}^2 + \frac{\lambda}{2} \|\mathbf{w}\|^2$$
$$\|\mathbf{w}\|^2 \equiv \mathbf{w}^{\mathrm{T}} \mathbf{w} = w_0^2 + w_1^2 + \ldots + w_M^2$$



• Solution2 : Weight Regularization



- Example: Regression Polynomial Curve Fitting
- Probability Theory
- Decision Theory
- Information Theory

- The probability of an event is the fraction of times that event occurs out of the total number of trials
- The probability must lie in the interval [0, 1]
- A box contains red and blue balls, we randomly pick 100 balls from a box, and 90 balls are red

$$p(ball = red) = \frac{90}{100} = 0.9$$

Joint probability: $X = x_i$ and $Y = y_i$ happen together

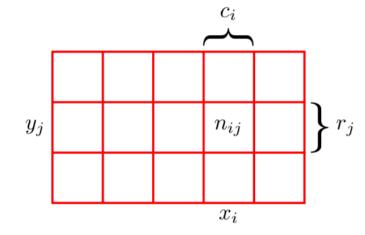
$$p(X = x_i, Y = y_j) = \frac{n_{ij}}{N}$$

Given ..

$$p(X = x_i) = \frac{c_i}{N}$$

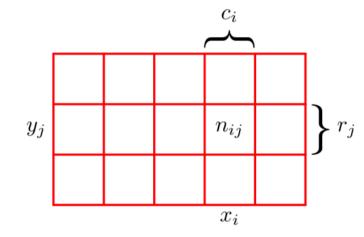
So.. We have the **sum rule of probability**

$$p(X = x_i) = \sum_{j=1}^{L} p(X = x_i, Y = y_j)$$





Conditional probability: $Y = y_i$ given $X = x_i$



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

As we know:

$$p(X = x_i, Y = y_j) = \frac{n_{ij}}{N} \qquad p(X = x_i) = \frac{c_i}{N}$$

We can have the **product rule of probability**

$$p(X = x_i, Y = y_j) = \frac{n_{ij}}{N} = \frac{n_{ij}}{c_i} \cdot \frac{c_i}{N}$$
$$= p(Y = y_j | X = x_i) p(X = x_i)$$

Variable Value

• The Rules of Probability

$$\label{eq:posterior} \begin{array}{ll} \mbox{sum rule} & p(X) = \sum_Y p(X,Y) \\ \mbox{product rule} & p(X,Y) = p(Y|X)p(X) \end{array}$$

• Bayes' theorem

Given the **product rule**:

$$p(X,Y) = p(Y|X)p(X)$$

 $p(Y,X) = p(X|Y)p(Y)$
symmetry property $p(X,Y) = p(Y,X)$

We can have the **Bayes' theorem**:

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

Using the sum rule ($p(X) = \sum_{Y} p(X, Y)$), we can have:

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

• Bayes' theorem

posterior \propto likelihood \times prior

• The Rules of Probability

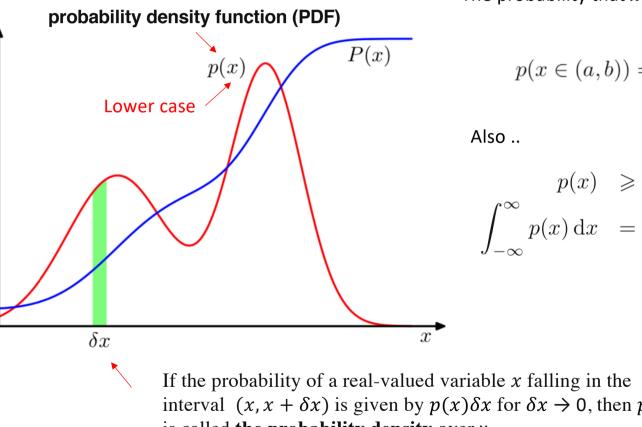
sum rule
$$p(X) = \sum_{Y} p(X, Y)$$

product rule $p(X, Y) = p(Y|X)p(X)$
Bayes' theorem $p(Y|X) = \frac{p(X|Y)p(Y)}{p(X)}$
where $p(X) = \sum_{Y} p(X|Y)p(Y)$

- Independent Events
 - If X and Y are independent

Bayes' theorem
$$p(Y|X) = \frac{p(X|Y)p(Y)}{p(X)}$$
 $p(Y|X) = p(Y)$
product rule $p(X,Y) = p(Y|X)p(X)$ $p(X,Y) = p(X)p(Y)$

Probability Densities ٠



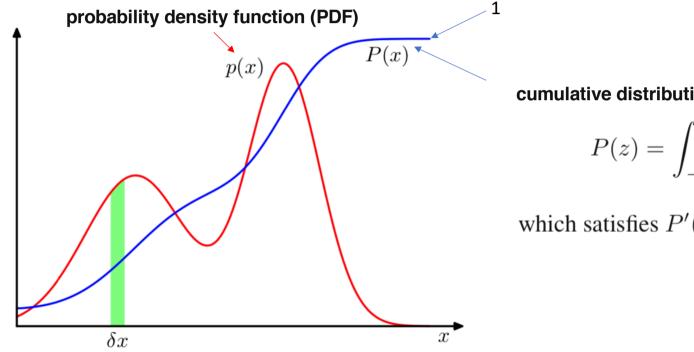
The probability that x will lie in an interval (a, b) is given by:

$$p(x \in (a, b)) = \int_{a}^{b} p(x) \, \mathrm{d}x$$

$$p(x) \ge 0$$
$$\int_{-\infty}^{\infty} p(x) \, \mathrm{d}x = 1$$

interval $(x, x + \delta x)$ is given by $p(x)\delta x$ for $\delta x \to 0$, then p(x)is called **the probability density** over x.

• Probability Densities



cumulative distribution function

$$P(z) = \int_{-\infty}^{z} p(x) \, \mathrm{d}x$$

which satisfies P'(x) = p(x)

• Expectations and Covariances

The average value of some function f(x) under a probability distribution p(x) is called the **expectation** of f(x) and will be denoted by E[f]:

For a continuous distribution:

$$\mathbb{E}[f] = \int p(x)f(x) \,\mathrm{d}x$$

For a discrete distribution:

$$\mathbb{E}[f] = \sum_{x} p(x)f(x)$$

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

It becomes exact in the limit $N \to \infty$

• Expectations and Covariances

In the case of **continuous variables**, expectations are expressed in terms of an integration with respect to the corresponding probability density

$$\mathbb{E}[f] = \int p(x)f(x) \, \mathrm{d}x$$

The conditional expectation with respect to a conditional distribution

$$\mathbb{E}_{x}[f|y] = \sum_{x} p(x|y)f(x)$$

• Expectations and Covariances

The variance of f(x):

$$\operatorname{var}[f] = \mathbb{E}\left[\left(f(x) - \mathbb{E}[f(x)]\right)^2\right]$$
$$= \mathbb{E}[f(x)^2] - \mathbb{E}[f(x)]^2$$

For two random variables x and y, the **covariance** is:

$$cov[x, y] = \mathbb{E}_{x, y} \left[\left\{ x - \mathbb{E}[x] \right\} \left\{ y - \mathbb{E}[y] \right\} \right] \\ = \mathbb{E}_{x, y} [xy] - \mathbb{E}[x] \mathbb{E}[y]$$

For two vectors of random variables **x** and **y**, the **covariance matrix**:

The **variance** of the variable *x*:

$$\operatorname{var}[x] = \mathbb{E}[x^2] - \mathbb{E}[x]^2$$

$$\begin{aligned} \operatorname{cov}[\mathbf{x}, \mathbf{y}] &= \mathbb{E}_{\mathbf{x}, \mathbf{y}} \left[\{ \mathbf{x} - \mathbb{E}[\mathbf{x}] \} \{ \mathbf{y}^{\mathrm{T}} - \mathbb{E}[\mathbf{y}^{\mathrm{T}}] \} \right] \\ &= \mathbb{E}_{\mathbf{x}, \mathbf{y}}[\mathbf{x} \mathbf{y}^{\mathrm{T}}] - \mathbb{E}[\mathbf{x}] \mathbb{E}[\mathbf{y}^{\mathrm{T}}]. \end{aligned}$$

The covariance of the components of a vector **x** with each other:

$$\operatorname{cov}[\mathbf{x}] \equiv \operatorname{cov}[\mathbf{x}, \mathbf{x}]$$

- Bayesian Probabilities
 - Frequentist: Probability in terms of frequencies of random, repeatable events.
 - Do not work if the event is not repeatable, e.g., the probability of the Arctic ice cap disappear.
 - **Bayesian**: Degree of belief.

- Frequentist Probability
 - Maximum Likelihood

A widely used frequentist estimator is maximum likelihood, in which θ is set to the value that maximizes the likelihood function $p(X | \theta)$.

• Given $x \sim iid \sim p(x|\theta)$, $p(X|\theta) = \prod_{i=1}^{N} p(x_i|\theta)$

•
$$\theta_{\text{MLE}} = \arg \max_{\theta} \log p(X|\theta) = \arg \max_{\theta} \sum_{i=1}^{N} \log p(x_i|\theta)$$

- Bayesian Probabilities
 - θ : random variables, $\theta \sim p(\theta) \leftarrow$ prior
 - MAP: Maximum A Posterior

 $p(\theta|X) = \frac{p(X|\theta)p(\theta)}{p(X)} \propto p(X|\theta)p(\theta)$ posterior
normalization constant

•
$$\theta_{MAP} = \arg \max_{\theta} p(\theta|X) = \arg \max_{\theta} p(X|\theta)p(\theta)$$

Bayes can evaluate the **uncertainty** in θ after we have observed X in the form of the posterior probability $p(\theta|X)$.

- Bayesian Probabilities
 - θ : random variables, $\theta \sim p(\theta) \leftarrow$ prior
 - Bayesian Estimation

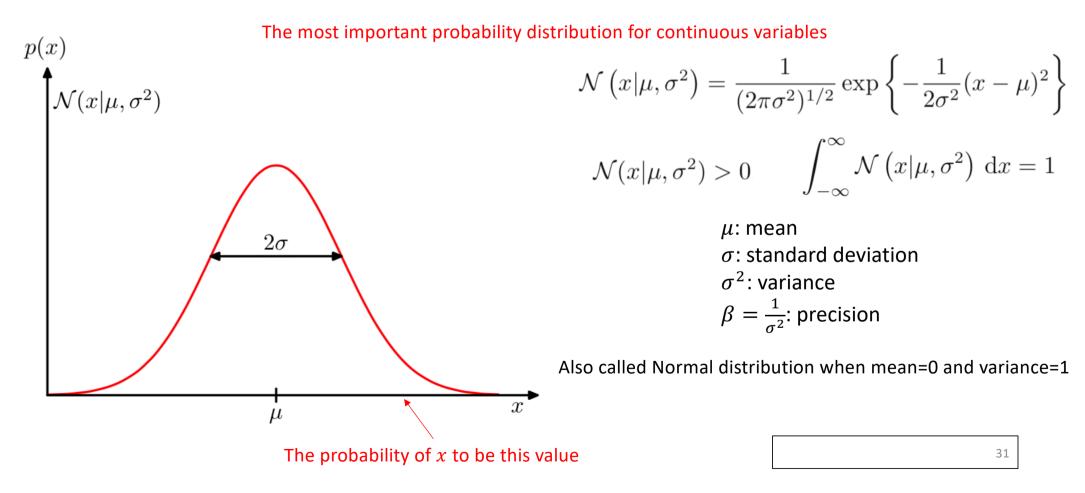
$$p(\theta|X) = \frac{p(X|\theta)p(\theta)}{p(X)} = \frac{p(X|\theta)p(\theta)}{\int_{\theta} p(X|\theta)p(\theta)d\theta}$$

- Bayesian Prediction
 - Given dataset X and a sample \tilde{x} find $p(\tilde{x}|X)$ via θ

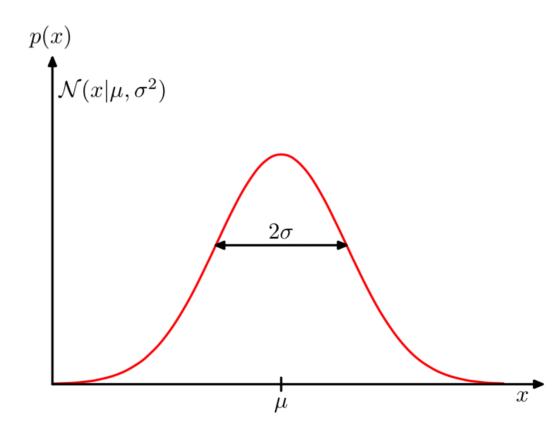
$$p(\tilde{x}|X) = \int_{\theta} p(\tilde{x}, \theta|X) d\theta = \int_{\theta} p(\tilde{x}|\theta) p(\theta|X) d\theta = \int_{\theta} p(\tilde{x}|\theta) p(\theta|X) d\theta$$



• The Gaussian Distribution



• The Gaussian Distribution



$$\mathbb{E}[x] = \int_{-\infty}^{\infty} \mathcal{N}\left(x|\mu, \sigma^2\right) x \, \mathrm{d}x = \mu$$

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

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

• The Gaussian Distribution

D-dimensional vector x of continuous variables

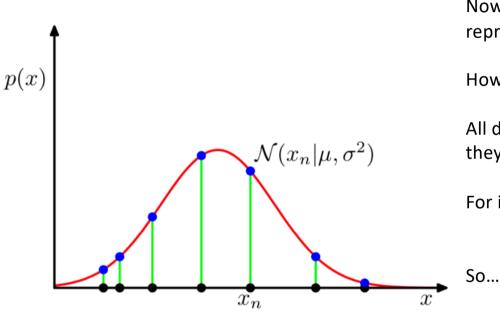
$$\mathcal{N}(\mathbf{x}|\boldsymbol{\mu},\boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{D/2}} \frac{1}{|\boldsymbol{\Sigma}|^{1/2}} \exp\left\{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{\mathrm{T}}\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right\}$$

 μ is called the mean, the D × D matrix

 Σ is called the covariance

 $|\Sigma|$ denotes the determinant of Σ

The Gaussian Distribution



Now suppose that we have a dataset of observations $\mathbf{x} = (x_1, ..., x_N)^T$, representing N observations of the scalar variable x.

How to determine the mean and variance according to the dataset??

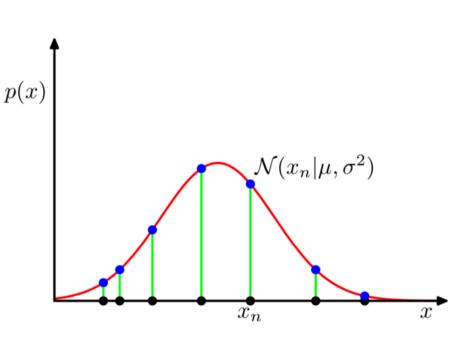
All data points are sampled independently from the same distribution, they are **independent and identically distributed (i.i.d)**.

For i.i.d variables, we can have the joint probability as follow

$$p(\mathbf{x}) = p(x_1) p(x_1) p(x_1) \dots p(x_N)$$

$$p(\mathbf{x}|\boldsymbol{\mu}, \sigma^2) = \prod_{n=1}^N \mathcal{N}\left(x_n | \boldsymbol{\mu}, \sigma^2\right)$$

The Gaussian Distribution



Maximum Likelihood

To find the "best" mean and variance, we can maximize the probability of the parameters given the data

$$p(\mathbf{x}|\mu,\sigma^2) = \prod_{n=1}^{N} \mathcal{N}\left(x_n|\mu,\sigma^2\right)$$

In practice, it is more convenient to maximize the log of the likelihood function. The logarithm is a monotonically increasing function, maximization of the log of a function is equivalent to maximization of the function itself

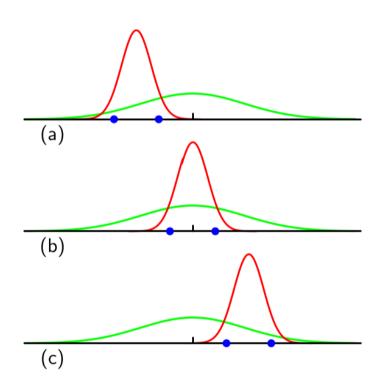
$$\ln p\left(\mathbf{x}|\mu,\sigma^{2}\right) = -\frac{1}{2\sigma^{2}}\sum_{n=1}^{N}(x_{n}-\mu)^{2} - \frac{N}{2}\ln\sigma^{2} - \frac{N}{2}\ln(2\pi)$$

So.. the maximum likelihood solution:

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

$$\sigma_{\rm ML}^2 = \frac{1}{N} \sum_{n=1}^{N} (x_n - \mu_{\rm ML})^2$$

• The Gaussian Distribution



$$\begin{split} \mathbb{E}[\mu_{\mathrm{ML}}] &= \mu \\ \mathbb{E}[\sigma_{\mathrm{ML}}^2] &= \left(\frac{N-1}{N}\right)\sigma^2 \end{split}$$

On average the maximum likelihood estimate will obtain the correct mean but will underestimate the true variance by a factor (N - 1)/N.

The following estimate for the variance parameter is unbiased.

$$\tilde{\sigma}^2 = \frac{N}{N-1} \sigma_{\rm ML}^2 = \frac{1}{N-1} \sum_{n=1}^{N} (x_n - \mu_{\rm ML})^2$$

- Example: Regression Polynomial Curve Fitting
- Probability Theory
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- An example
- Basic intuition
- Minimizing the misclassification rate
- Minimizing the expected loss
- The reject option
- Loss functions for regression

• A example

A medical diagnosis problem in which we have taken an X-ray image of a patient, and we wish to determine whether the patient has cancer or not.

We are interested in **the probabilities of the two classes** given the **image**, which are given by p(Ck|x). Using Bayes' theorem, these probabilities can be expressed in the form :

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

Note that any of the quantities appearing in Bayes' theorem can be obtained from the joint distribution p(x, Ck) by either marginalizing or conditioning with respect to the appropriate variables.

We can now interpret p(Ck) as the prior probability for the class Ck, and p(Ck|x) as the corresponding posterior probability. Thus p(C1) represents the probability that a person has cancer, before we take the X-ray measurement.

Similarly, p(C1|x) is the corresponding probability, revised using Bayes' theorem in light of the information contained in the X-ray.

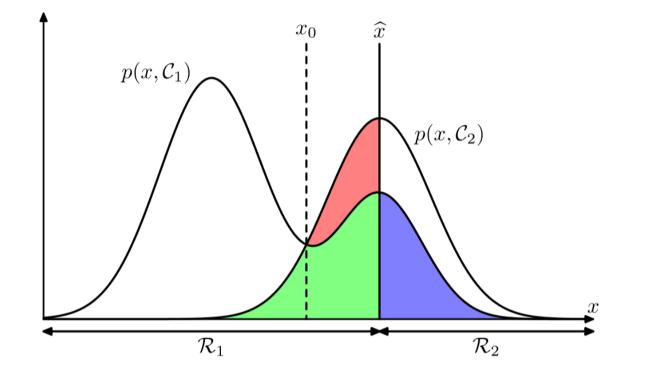
• Basic intuition

If our aim is to minimize the chance of assigning x to the wrong class, then intuitively we would choose the class having the higher posterior probability. We now show that this intuition is correct, and we also discuss more general criteria for making decisions.

• Minimizing the misclassification rate

A mistake occurs when an input vector belonging to class C1 is assigned to class C2 or vice versa. The probability of this occurring is given by

$$p(\text{mistake}) = p(\mathbf{x} \in \mathcal{R}_1, \mathcal{C}_2) + p(\mathbf{x} \in \mathcal{R}_2, \mathcal{C}_1)$$
$$= \int_{\mathcal{R}_1} p(\mathbf{x}, \mathcal{C}_2) \, \mathrm{d}\mathbf{x} + \int_{\mathcal{R}_2} p(\mathbf{x}, \mathcal{C}_1) \, \mathrm{d}\mathbf{x}.$$



• Minimizing the expected loss

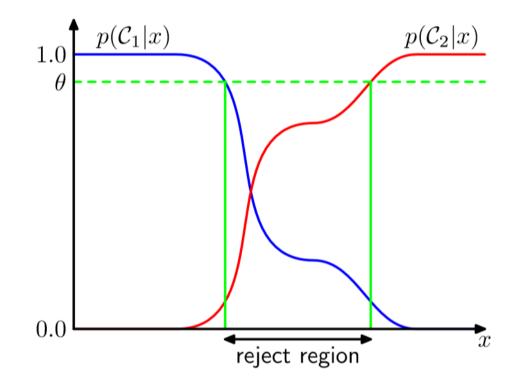
Loss function, also called a cost function, which is a single, overall measure of loss incurred in taking any of the available decisions or actions.

Our goal is then to minimize the total loss incurred.

We seek to minimize the average loss, where the average is computed with respect to this distribution, which is given by

$$\mathbb{E}[L] = \sum_{k} \sum_{j} \int_{\mathcal{R}_{j}} L_{kj} p(\mathbf{x}, \mathcal{C}_{k}) \, \mathrm{d}\mathbf{x}$$

• The reject option



• Loss functions for regression

For regression problems, loss is given by

$$\mathbb{E}[L] = \iint L(t, y(\mathbf{x})) p(\mathbf{x}, t) \, \mathrm{d}\mathbf{x} \, \mathrm{d}t.$$

A common choice of loss function in regression problems is the squared loss. In this case, the expected loss can be written:

$$\mathbb{E}[L] = \iint \{y(\mathbf{x}) - t\}^2 p(\mathbf{x}, t) \,\mathrm{d}\mathbf{x} \,\mathrm{d}t.$$

We can expand the square term as follows:

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

$$= \{y(\mathbf{x}) - \mathbb{E}[t|\mathbf{x}]\}^{2} + 2\{y(\mathbf{x}) - \mathbb{E}[t|\mathbf{x}]\}\{\mathbb{E}[t|\mathbf{x}] - t\} + \{\mathbb{E}[t|\mathbf{x}] - t\}^{2}$$
Expectation = 0
We obtain an expression for the loss function in the form:
$$\mathbb{E}[L] = \int \{y(\mathbf{x}) - \mathbb{E}[t|\mathbf{x}]\}^{2}p(\mathbf{x}) d\mathbf{x} + \int \operatorname{var}[t|\mathbf{x}]p(\mathbf{x}) d\mathbf{x}$$

- Example: Regression Polynomial Curve Fitting
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Basic intuition

- Learning that an unlikely event has occurred is more informative than learning that a likely event has occurred.
 - E.g.
 - "the sun rose this morning" : uninformative
 - "there was a solar eclipse this morning": informative.

Basic intuition

- We would like to quantify information in a way that formalizes this intuition. Specifically:
 - Likely events should have low information content, and in the extreme case, events that are guaranteed to happen should have no information content whatsoever.
 - Less likely events should have higher information content.
 - Independent events should have additive information.
 - E.g. Finding out that a tossed coin has come up as heads twice should convey twice as much information as finding out that a tossed coin has come up as heads once.

Self-information

• In order to satisfy all three of these properties, we define the self information of an event x to be

$$I(x) = -\log P(x).$$

(use log to mean the natural logarithm, with base e. I(x) is therefore written in units of nats)

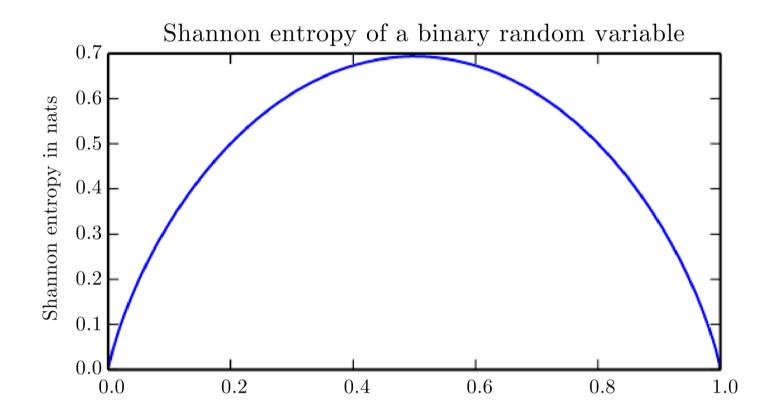
Shannon entropy

• Self-information deals only with a single outcome. We can quantify the amount of uncertainty in an entire probability distribution using the Shannon entropy:

$$H(\mathbf{x}) = \mathbb{E}_{\mathbf{x} \sim P}[I(x)] = -\mathbb{E}_{\mathbf{x} \sim P}[\log P(x)].$$

• The Shannon entropy of a distribution is the expected amount of information in an event drawn from that distribution. It gives a lower bound on the number of bits (if the logarithm is base 2, otherwise the units are different) needed on average to encode symbols drawn from a distribution P.

Example for Shannon entropy



KL divergence

• If we have two separate probability distributions P(x) and Q(x) over the same random variable x, we can measure how different these two distributions are using the Kullback-Leibler (KL) divergence:

$$D_{\mathrm{KL}}(P||Q) = \mathbb{E}_{\mathbf{x}\sim P}\left[\log\frac{P(x)}{Q(x)}\right] = \mathbb{E}_{\mathbf{x}\sim P}\left[\log P(x) - \log Q(x)\right].$$

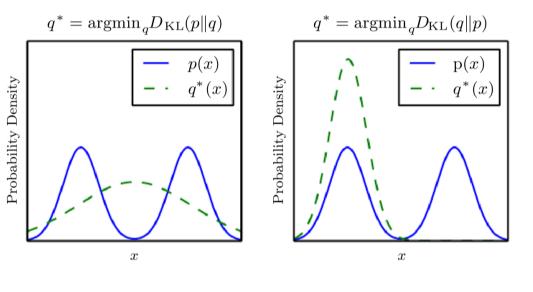
 In the case of discrete variables, it is the extra amount of information needed to send a message containing symbols drawn from probability distribution P, when we use a code that was designed to minimize the length of messages drawn from probability distribution.



KL divergence

- Because the KL divergence is non-negative and measures the difference between two distributions, it is often conceptualized as measuring some sort of distance between these distributions.
 - Not a true distance measure because it is not symmetric.
 - It is nonnegative.

KL divergence



- Which direction of the KL divergence to use?
 - Some applications require an approximation that usually places high probability anywhere that the true distribution places high probability: left one
 - Other applications require an approximation that rarely places high probability anywhere that the true distribution places low probability: right one

$$D_{\mathrm{KL}}(P \| Q) = \mathbb{E}_{\mathbf{x} \sim P} \left[\log \frac{P(x)}{Q(x)} \right] = \mathbb{E}_{\mathbf{x} \sim P} \left[\log P(x) - \log Q(x) \right].$$

Cross-entropy

 A quantity that is closely related to the KL divergence is the crossentropy H(P,Q) = H(P) + D_{KL}(P||Q), which is similar to the KL divergence but lacking the term on the left:

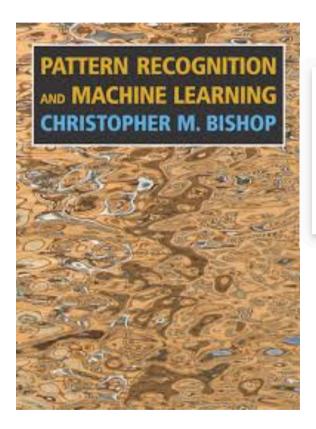
$$H(P,Q) = -\mathbb{E}_{\mathbf{x}\sim P} \log Q(x).$$

• Minimizing the cross-entropy with respect to Q is equivalent to minimizing the KL divergence, because does not participate in the omitted term.

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Reference





Free Download

https://github.com/zsdonghao/deep-learningbook/blob/master/All-in-one-pdf 《Deep Learning》 all-in-one.pdf

Thanks