Report

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Discriminate Method Review

1. Logistic Regression
   Assume $y = 0$ or $y = 1$,and $h_w(x) = \frac{1}{1-e^{w^T x}}$
2. Perceptron Learning Algorithm
   $h_w(x)$ is a threshold function:

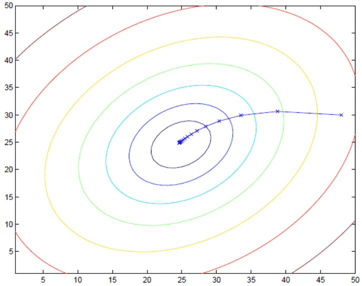
$$h_w(x) = g_w(w^T x) = \begin{cases} 1 & \text{if } w^T x \geq 0 \\ -1 & \text{otherwise} \end{cases}$$

Gradient descent Review

Batch Gradient descent

Repeat for each parameter :

$$w_i := w_i + \alpha \frac{\partial}{\partial w_i} Loss(h_w(x), y)$$



Gradient descent Review(2)

The normal equations:
For a function $f : \mathbb{R}^{m\times n} \to \mathbb{R}$ define the derivative of f with respect to A to be:

$$\nabla_A f(A) = \begin{pmatrix} \frac{\partial}{\partial A_{11}} & \cdots & \frac{\partial}{\partial A_{1n}} \\ \vdots & \ddots & \vdots \\ \frac{\partial}{\partial A_{m1}} & \cdots & \frac{\partial}{\partial A_{mn}} \end{pmatrix}$$

For examples, suppose $A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}$ is a 2-by-2 matrix,and:

$$f(A) = \frac{3}{2}A_{11} + 5A_{12}^2 + A_{21}A_{22}$$

Then we have:

$$\nabla_A f(A) = \begin{pmatrix} \frac{3}{2} & 10A_{12} \\ A_{22} & A_{21} \end{pmatrix}$$

Define of **trace** operator. For an n-by-n matrix A:

$$trA = \sum_{i=1}^{n} A_{ii}$$

Gradient descent Review(3)

For two matrices A and B,such that ABC is square,we have:

$$trAB = trBA$$

As corollaries:

$$trABC = trCAB = trBCA$$

Here A and B is square matrices and a is real number:

$$\begin{aligned} trA &= trA^T \\ tr(A+B) &= trA + trB \\ traA &= atrA \end{aligned}$$

Gradient descent Review(4)

Some facts without proof:

$$
\begin{aligned}
\nabla_A tr AB &= B^T \\
\nabla_{A^T} f(A) &= (\nabla_A f(A))^T \\
\nabla_A tr ABA^T C &= CAB + C^T AB^T
\end{aligned}
$$

Revisit Least Squares:
define **design matrix**X to be the m-by-n matrix:

$$X = \begin{pmatrix} x_1^{(1)} & \dots & x_n^{(1)} \\ \vdots & \ddots & \vdots \\ x_1^{(m)} & \dots & x_n^{(m)} \end{pmatrix}$$

Gradient descent Review(5)

define $\vec{y}$ be m-dimensional vector:

$$\vec{y} = \begin{pmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(m)} \end{pmatrix}$$

Since $h_w(x^{(i)}) = (x^{(i)})^T w$:

$$\begin{aligned} X w - \vec{y} &= \begin{pmatrix} (x^{(1)})^T w \\ \vdots \\ (x^{(m)})^T w \end{pmatrix} - \begin{pmatrix} y^{(1)} \\ \vdots \\ y^{(m)} \end{pmatrix} \\ &= \begin{pmatrix} h_w(x^{(1)}) - y^{(1)} \\ \vdots \\ h_w(x^{(m)}) - y^{(m)} \end{pmatrix} \end{aligned}$$

Gradient descent Review(5)

Using the face that for $\vec{z}$,we have $\vec{z}^T\vec{z} = \Sigma_i \vec{z}_i^2$:

$$\begin{aligned}
\frac{1}{2}(Xw - \vec{y})^T(Xw - \vec{y}) &= \frac{1}{2}\sum_{i=1}^{m}(h_w(x^{(i)}) - y^{(i)})^2 \\
&= J(w)
\end{aligned}$$

$$\begin{aligned}
\nabla_w J(w) &= \nabla_w \frac{1}{2}(Xw - \vec{y})^T(Xw - \vec{y}) \\
&= \frac{1}{2}\nabla_w tr(w^T X^T Xw - w^T X^T \vec{y} - \vec{y}^T Xw + \vec{y}^T\vec{y}) \\
&= \frac{1}{2}\nabla_w (trw^T X^T Xw - 2tr\vec{y}^T Xw) \\
&= \frac{1}{2}(X^T Xw + X^T Xw - 2X^T w) \\
&= X^T Xw - X^T\vec{y}
\end{aligned}$$

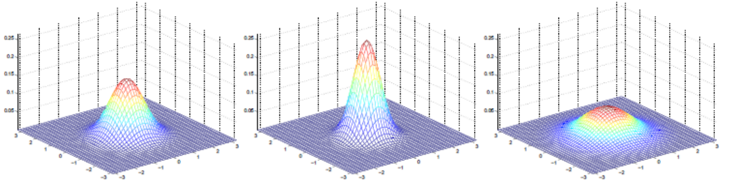
What are Generative Learning algorithms

- Consider a classification problem: distinguish between benign tumors and malignant tumors.
- Given a training set, an algorithm like logistic regression or the perceptron algorithm (basically) tries to find a straight line that is, a decision boundarythat separates the benign tumor and malignant tumor. Algorithms that try to learn $P(y|x)$ directly are called **discriminative learning algorithms**.
- Different approach: Fist we can build a model of what benign tumors look like. Then we build a seperate model of what malignant tumors look like. Finally, to classify a new sample,we can match the new sample with each model,to see whether one model matches better than one other model. Algorithms that try to learn $P(x|y)$(and $P(y)$) are called **generative learning algorithms**.

The multivariate normal distribution

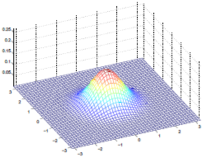
Suppose these is a multivariate normal distribution is parameterized by a **mean vector** $\mu \in \mathbb{R}^n$ and a **covariance matrix** $\Sigma \in \mathbb{R}^{n \times n}$,its density is given by:

$$p(x;\mu,\Sigma) = \frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu)\right)$$

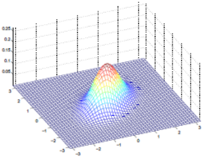


$\Sigma = I$ $\Sigma = 0.6I$; $\Sigma = 2I$.

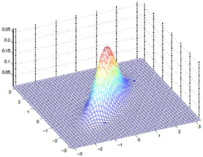
The multivariate normal distribution(2)



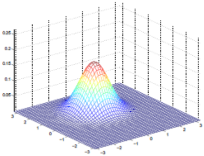
$$\Sigma = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$



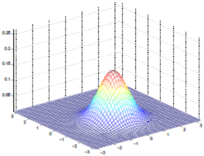
$$\Sigma = \begin{bmatrix} 1 & 0.5 \\ 0.5 & 1 \end{bmatrix}$$



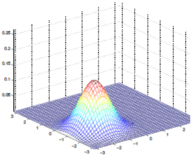
$$\Sigma = \begin{bmatrix} 1 & 0.8 \\ 0.8 & 1 \end{bmatrix}$$



$$\mu = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$



$$\mu = \begin{bmatrix} -0.5 \\ 0 \end{bmatrix}$$



$$\mu = \begin{bmatrix} -1 \\ -1.5 \end{bmatrix}$$

The Gaussian Discriminant Analysis model(1)

GDA Model is:

$$\begin{aligned} y &\sim Bernoulli(\phi) \\ x|y=0 &\sim \mathcal{N}(\mu_0, \Sigma) \\ x|y=1 &\sim \mathcal{N}(\mu_1, \Sigma) \end{aligned}$$

Writing out the distribution:

$$p(y) = \phi^y (1-\phi)^y$$

$$p(x|y=0) = \frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(x-\mu_0)^T\Sigma^{-1}(x-\mu_0)\right)$$

$$p(x|y=1) = \frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(x-\mu_1)^T\Sigma^{-1}(x-\mu_1)\right)$$

The Gaussian Discriminant Analysis model(2)

The log-likelihood is:

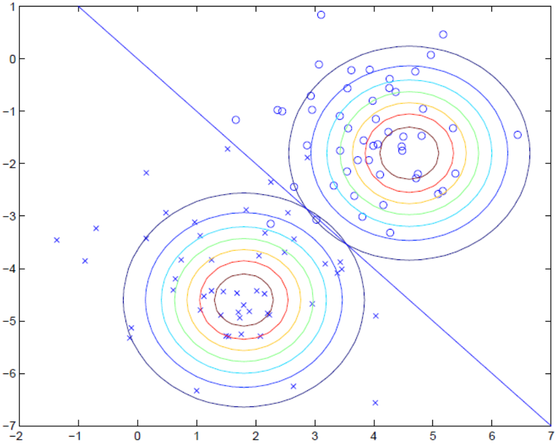
$$
\begin{aligned}
l(\phi, \mu_0, \mu_1, \Sigma) &= \log \prod_{i=1}^{m} p(x^{(i)}, y^{(i)}; \phi, \mu_0, \mu_1, \Sigma) \\
&= \log \prod_{i=1}^{m} p(x^{(i)} | y^{(i)}; \mu_0, \mu_1, \Sigma) p(y^{(i)}; \phi)
\end{aligned}
$$

By maximizing l with respect to the parameters,we find the maximum likelihood estimate of parameters to be:

$$
\begin{aligned}
\phi &= \frac{1}{m} \sum_{i:y^{(i)}=1}^{m} y^{(i)} \\
\mu_0 &= \frac{\sum_{i:y^{(i)}=0}^{m} x^{(i)}}{\sum_{i:y^{(i)}=0}^{m} y^{(i)}} \\
\mu_1 &= \frac{\sum_{i:y^{(i)}=1}^{m} x^{(i)}}{\sum_{i:y^{(i)}=1}^{m} y^{(i)}} \\
\Sigma &= \frac{1}{m} \sum_{i=1}^{m} (x^{(i)} - \mu_{y^{(i)}})(x^{(i)} - \mu_{y^{(i)}})^T
\end{aligned}
$$

The Gaussian Discriminant Analysis model(3)

Pictorially, what the algorithm is doing can be seen in as follows:



Discussion: GDA and logistic regression

If we view $p(y=1|x;\phi,\mu_0,\mu_1,\Sigma)$ as a function of x, there is a fact that:

$$p(y=1|x;\phi,\Sigma,\mu_0,\mu_1)=\frac{1}{1+\exp(-w^Tx)}$$

This is exactly the form that logistic regression used to model $p(y=1|x)$.
In fact in binary division problem:

$$p(x|y=1)\sim ExpFamily(x,\eta)\Rightarrow p(y=1|x)=Sigmoid$$

When would we prefer one model over another?

- GDA makes stronger modelling assumptions, and is more data efficient (i.e., requires less training data to learn well) when the modeling assumptions are correct or at least approximately correct.
- Logistic regression makes weaker assumptions, and is significantly more robust to deviations from modeling assumptions.

Bayes' formula

Suppose that we have the prior probability $P(\omega_j)$ and the conditional densities $p(x|\omega_j)$, the posterior probability can be written as:

$$P(\omega_j|x) = \frac{p(x|\omega_j)P(\omega_j)}{p(x)},$$

where

$$p(x) = \sum_{j=1}^{c} p(x|\omega_j)P(\omega_j).$$

Bayes' formula can be expressed informally in English:

$$posterior = \frac{likelihood \times prior}{evidence}.$$

Bayesian Decision Theory Continuous Features

Let $\omega_1, \ldots, \omega_c$ be the finite set of c states of nature ("categories") and $\alpha_1, \ldots, \alpha_a$ be the finite set of a possible action. The Loss function $\lambda(\alpha_i|\omega_j)$ describe the loss incurred for taking action α_i when the state of nature is ω_j. The posterior probability $P(\omega_j|x)$ can be compute from $P(\omega_j|x)$ by Bayes'formula:

$$P(\omega_j|x) = \frac{p(x|\omega_j)P(\omega_j)}{p(x)}$$

where the evidence is now

$$p(x) = \sum_{j=1}^{c} p(x|\omega_j)P(\omega_j)$$

Bayesian Decision Theory Continuous Features(2)

Suppose that we observe a particular x and that we contemplate taking action α_i.

$$R(\alpha_i|x) = \sum_{j=1}^{c} \lambda(\alpha_i|\omega_j)P(\omega_j|x)$$

In decision-theoretic terminology, an expected loss is called a risk, and $R(\alpha_i|x)$ is called the **conditional risk**. If we define loss function to be

$$\lambda(\alpha_i|\omega_j) = \begin{cases} 0 & i = j \\ 1 & i \neq j \end{cases} \quad i, j = 1, \ldots, c.$$

Condition risk will be

$$R(\alpha_i|x) = \sum_{j=1}^{c} \lambda(\alpha_i|\omega_j)P(\omega_j|x) = 1 - P(\omega_i|x)$$

Classifiers, Discriminant Functions and Decision Surfaces

For 0-1 Loss function case, we can simplely let the discriminant functions to be $g_i(x) = P(\omega_i|x)$. More generally, if we replace every $g_i(x)$ by $f(g_i(x))$, where $f(\cdot)$ is a monotonically increasing fuction, the resulting classification is unchanged.

$$g_i(x) = P(\omega_i|x) = \frac{p(x|\omega_i)P(\omega_i)}{\sum_{j=1}^{c} p(x|\omega_j)P(\omega_j)}$$

$$g_i(x) = p(x|\omega_i)P(\omega_i)$$

$$g_i(x) = \log p(x|\omega_i) + \log P(\omega_i)$$

Discriminant Functions for the Normal Density

if $p(x|\omega_i) \sim \mathcal{N}(\mu_i, \Sigma_i)$,

$$g_i(x) = -\frac{1}{2}(x-\mu_i)^T\Sigma_i^{-1}(x-\mu_i) - \frac{d}{2}\log 2\pi - \frac{1}{2}\log|\Sigma_i| + \log P(\omega_i)$$

Case: $\Sigma_i = \sigma^2 I$
Ignore terms which are independent of i, we obtain:

$$\begin{aligned} g_i(x) &= -\frac{\|x-\mu_i\|^2}{2\sigma^2} + \log P(\omega_i) \\ &= -\frac{1}{2\sigma^2}(x^Tx - 2\mu_i^Tx + \mu_i^T\mu_i) + \log P(\omega_i) \end{aligned}$$

Since x^Tx is the same for all i's, we obtain

$$g_i(x) = w_i^T x + w_{i0}$$

where

$$w_i = \frac{1}{\sigma^2}\mu_i, \quad w_{i0} = -\frac{1}{2\sigma^2}\mu_i^T\mu_i + \log P(\omega_i)$$

Discriminant Functions for the Normal Density(2)

For two class, we can set $g_i(x) = g_j(x)$:

$$w^T(x - x_0) = 0,$$

where,

$$w = \mu_i - \mu_j$$

and,

$$x_0 = \frac{1}{2}(\mu_i + \mu_j) - \frac{\sigma^2}{\|\mu_i - \mu_j\|} \log \frac{P(\omega_i)}{P(\omega_j)}(\mu_i - \mu_j)$$

Discriminant Functions for the Normal Density(3)

Case $\Sigma_i = \Sigma$:

$$g_i(x) = w^T x + w_0$$

where

$$w_i = \Sigma^{-1}\mu_i, \quad w_{i0} = -\frac{1}{2}\mu_i^T \Sigma^{-1}\mu_i + \log P(\omega_i)$$

Case $\Sigma_i =?$

$$g_i = x^T W_i x + w_i^T x + w_{i0}$$

where,

$$W_i = -\frac{1}{2}\Sigma_i^{-1}, \quad w_i = \Sigma_i^{-1}\mu_i$$

and,

$$w_{i0} = -\frac{1}{2}\mu_i^T \Sigma_i^{-1}\mu_i - \frac{1}{2}\log|\Sigma_i| + \log P(\omega_i)$$

Bayesian estimation

In Bayesian estimation, we consider parameter θ to be a random variable. Any information we might have about θ prior to observing the samples is assumed to be contained in a *known* prior density $p(\theta)$. Observation of the samples converts this to a posterior density $p(\theta|\mathcal{D})$
Knowing that our goal is to compute $p(x|\mathcal{D})$, we do this by:

$$p(x|\mathcal{D}) = \int p(x, \theta|\mathcal{D})d\theta$$

then:

$$p(x|\mathcal{D}) = \int p(x|\theta)p(\theta|\mathcal{D})d\theta$$

Bayesian estimation(2)

Suppose μ is the only unknown parameter, and

$$p(x|\mu) \sim \mathcal{N}(\mu, \sigma^2).$$

Our prior knowledge we might have about μ can be expressed by a known prior density $p(\mu)$.

$$p(\mu) \sim \mathcal{N}(\mu_0, \sigma_0^2)$$

To obtain the posterior probability:

$$\begin{aligned} p(\mu|\mathcal{D}) &= \frac{p(\mathcal{D}|\mu)p(\mu)}{\int p(\mathcal{D}|\mu)p(\mu)} \\ &= \alpha \prod_{k=1}^{n} p(x_k|\mu)p(\mu) \end{aligned}$$

Bayesian estimation(3)

Since $p(x_k|\mu) \sim \mathcal{N}(\mu, \sigma^2)$ and $p(\mu) \sim \mathcal{N}(\mu_0, \sigma_0^2)$:

$$
\begin{aligned}
p(\mu|\mathcal{D}) &= \alpha \prod_{k=1}^{n} \overbrace{\frac{1}{\sqrt{2\pi}\sigma} \exp\Big[-\frac{1}{2}\Big(\frac{x_k-\mu}{\sigma}\Big)^2\Big]}^{p(x_k|\mu)} \overbrace{\frac{1}{\sqrt{2\pi}\sigma_0} \exp\Big[-\frac{1}{2}\Big(\frac{\mu-\mu_0}{\sigma_0}\Big)^2\Big]}^{p(\mu)} \\
&= \alpha' \exp\left[-\frac{1}{2}\left(\sum_{k=1}^{n}\left(\frac{\mu-x_k}{\sigma}\right)^2 + \left(\frac{\mu-\mu_0}{\sigma_0}\right)^2\right)\right] \\
&= \alpha'' \exp\left[-\frac{1}{2}\left[\Big(\frac{n}{\sigma^2}+\frac{1}{\sigma_0^2}\Big)\mu^2 - 2\left(\frac{1}{\sigma^2}\sum_{k=1}^{n} x_k + \frac{\mu_0}{\sigma_0^2}\right)\mu\right]\right], \qquad (
\end{aligned}
$$

Now we know $p(\mu|\mathcal{D})$ is a Gaussian distribution, If we write $p(\mu|\mathcal{D} \sim \mathcal{N}(\mu_n \sigma_n^2))$,we obtain:

$$\mu_n = \left(\frac{n\sigma_0^2}{n\sigma_0^2+\sigma^2}\right)\bar{x_n} + \frac{\sigma^2}{n\sigma_0^2+\sigma^2}\mu_0$$

$$\sigma_n^2 = \frac{\sigma_0^2\sigma^2}{n\sigma_0^2+\sigma^2}$$

Now we need to compute the $p(x|\mathcal{D})$:

$$\begin{aligned}
p(x|\mathcal{D}) &= \int p(x|\mu)p(\mu|\mathcal{D})\ d\mu \\
&= \int \frac{1}{\sqrt{2\pi}\sigma} \exp\left[-\frac{1}{2}\Big(\frac{x-\mu}{\sigma}\Big)^2\right] \frac{1}{\sqrt{2\pi}\sigma_n}\exp\left[-\frac{1}{2}\Big(\frac{\mu-\mu_n}{\sigma_n}\Big)^2\right] d\mu \\
&= \frac{1}{2\pi\sigma\sigma_n} \exp\left[-\frac{1}{2}\frac{(x-\mu_n)^2}{\sigma^2+\sigma_n^2}\right] f(\sigma,\sigma_n),
\end{aligned}$$

Hence,

$$p(x|\mathcal{D}) \sim \mathcal{N}(\mu_n, \sigma^2 + \sigma_n^2)$$

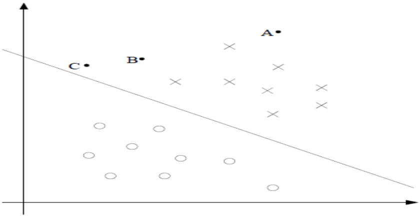
Margin(1)

Previous:
Consider logistic regression,we compute $w^T x$ then we:

- Predict "1" iff $w^T x \geq 0$.
- Predict "0" iff $w^T x < 0$.

The larger $w^T x$ is,the larger also is $h_w(x) = p(y|x; w)$:

- if $w^T x \gg 0$ then we are very "confident" predicting "1".
- if $w^T x \ll 0$ then we are very "confident" predicting "0".



Margin(2)

To make our discussion of SVMs easier,we need to change our notation:
we use $y \in 1, -1$ to denote class label, and change classifier as:

$$h_{w,b}(x) = g(w^T x + b)$$

Here g is a threshold function.
Given a training example $(x^{(i)}, y^{(i)})$,we define **functional margin** of (w, b) with respect to the training example.

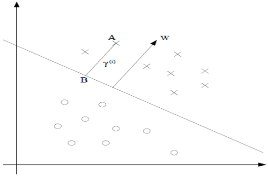
$$\hat{\gamma}^{(i)} = y^{(i)}(w^T x^{(i)} + b)$$

A large functional margin represents a confident and a correct prediction.But by exploiting our freedom to scale w and b, we can make the functional margin arbitrarily large without really changing anything meaningful.
Given a training set S,we also define the function margin of (w, b) with respect to S:

$$\hat{\gamma} = \min_{i=1,\dots,m} \hat{\gamma}^{(i)}$$

Margin(3)

Lets talk about **geometric margins**. Consider the picture below:



Suppose A is $x^{(i)}$,then B is $x^{(i)} - \gamma^{(i)} \cdot (w/\|w\|)$,B lies on the decision boundary,Hence:

$$w^T \left(x^{(i)} - \gamma^{(i)} \cdot \frac{w}{\|w\|} \right) + b = 0$$

Solving for $\gamma^{(i)}$ yields:

$$\gamma^{(i)} = \left(\frac{w}{\|w\|} \right)^T x^{(i)} + \frac{b}{\|w\|}$$

Margin(4)

More generally,define geometric margins of (w, b) with respect to a training example $(x^{(i)}, y^{(i)})$ to be

$$\gamma^{(i)} = y^{(i)} \left(\left(\frac{w}{\|w\|} \right)^T x^{(i)} + \frac{b}{\|w\|} \right)$$

Given a training set S, we also define the geometric margin of (w, b) with respect to S to be the smallest of the geometric margins on the individual training examples:

$$\gamma = \min_{i=1,\ldots,m} \gamma^{(i)}$$

The optimal margin classifier

Given a training set,We try to find a decision boundary that maximizes the margin. We can pose the following optimization problem

$$\begin{aligned} \max_{\gamma,w,b} \quad & \gamma \\ s.t. \quad & y^{(i)}(w^T x^{(i)} + b) \geq \gamma, i = 1, \dots, m \\ & \|w\| = 1. \end{aligned}$$

The "$\|w\|$" constraint is a nasty(non-convex) constraint. Transform to a nicer one:

$$\begin{aligned} \max_{\gamma,w,b} \quad & \frac{\hat{\gamma}}{\|w\|} \\ s.t. \quad & y^{(i)}(w^T x^{(i)} + b) \geq \hat{\gamma}, i = 1, \dots, m \end{aligned}$$

We get rid of "$\|w\| = 1$" which we don't like. But the downside is that we now have a nasty(non-convex) objective function.

The optimal margin classifier(2)

Since we can add an arbitrary scaling constraint on w and b without changing anything.We introduce a scaling constraint:

$$\hat{\gamma} = 1$$

Plugging this into our problem above,and noting that maximizing $\hat{\gamma}/\|w\| = 1/\|w\|$ is the same thing as minimizing$\|w\|^2$, we now have the following optimization problem:

$$\begin{aligned} \min_{\gamma,w,b} \quad & \frac{1}{2}\|w\|^2 \\ s.t. \quad & y^{(i)}(w^T x^{(i)} + b) \geq 1, i = 1, \ldots, m \end{aligned}$$

Now,we have an optimization problem with a convex quadratic objective and only linear constraints.This optimization problem can be solved using commercial quadratic programming (QP) code.

Lagrange duality

Consider problem of the following form:

$$\begin{aligned} \min_{w} \quad & f(w) \\ s.t. \quad & h_i(w) = 0, i = 1, \ldots, l. \end{aligned}$$

Define **Lagrangian** to be

$$\mathcal{L}(w, \beta) = f(w) + \sum_{i=1}^{l} \beta_i h_i(w)$$

Here,the β_i's are called the **Lagrange multipliers**. Set $\mathcal{L}$'s partial derivatives to zero:

$$\frac{\partial \mathcal{L}}{\partial w_i} = 0; \frac{\partial \mathcal{L}}{\partial \beta_i} = 0$$

We can solve for w and β

Lagrange duality(2)

Consider the following, which we call the **primal** optimization problem:

$$\begin{aligned} \min_{w} \quad & f(w) \\ s.t. \quad & g_i(w) \leq 0, i = 1, \ldots, k \\ & h_i(w) = 0, i = 1, \ldots, l \end{aligned}$$

Define **generalized Lagrangian**

$$\mathcal{L}(w, \alpha, \beta) = f(w) + \sum_{i=1}^{k} \alpha_i g_i(w) + \sum_{i=1}^{l} \beta_i h_i(w).$$

Here the α_i's and β_i's are the Lagrange multipliers.Consider the quantity:

$$\theta_{\mathcal{P}} = \max_{\alpha, \beta : \alpha_i \geq 0} f(w) + \sum_{i=1}^{k} \alpha_i g_i(w) + \sum_{i=1}^{l} \beta_i h_i(w)$$

Here,the "$\mathcal{P}$" subscript stands for "primal".

Lagrange duality(3)

Let some w be given. If w violates any of the primal constraints,then it's easy to verify that $\theta_{\mathcal{P}} = \infty$. Conversely, if the constraints are indeed satisfied for a particular value of w,then $\theta_{\mathcal{P}} = f(w)$.Hence,

$$\theta_{\mathcal{P}}(w) = \begin{cases} f(w) & \text{if } w \text{ satisfied primal conatraints} \\ \infty & \text{otherwise} \end{cases}$$

If we consider the minimization problem

$$\min_{w} \theta_{\mathcal{P}}(w) = \min_{w} \max_{\alpha,\beta,\alpha_i \geq 0} \mathcal{L}(w, \alpha, \beta)$$

It is the same problem of primal problem.Define optimal value of the objective to be $p^* = \min_w \theta_{\mathcal{P}}(w)$

Lagrange duality(4)

Define:

$$\theta_{\mathcal{D}}(\alpha, \beta) = \min_{w} \mathcal{L}(w, \alpha, \beta).$$

Here,the "$\mathcal{D}$" subscript stands for "dual".
Now the **dual** optimization problem:

$$\max_{\alpha,\beta:\alpha_i \geq 0} \theta_{\mathcal{D}}(\alpha, \beta) = \max_{\alpha,\beta:\alpha_i \geq 0} \min_{w} \mathcal{L}(w, \alpha, \beta)$$

define the optimal value of the dual problems objective to be $d^* = \max_{\alpha,\beta:\alpha_i \geq 0} \theta_{\mathcal{D}}(\alpha, \beta)$.
It can easily be shown that

$$d^* = \max_{\alpha,\beta:\alpha_i \geq 0} \min_{w} \mathcal{L}(w, \alpha, \beta) \leq \min_{w} \max_{\alpha,\beta:\alpha_i \geq 0} \mathcal{L}(w, \alpha, \beta) = p^*$$

However under certain conditions,we will have $d^* = p^*$

Lagrange duality(5)

Let's see what these conditions are:

- f and the g_i's are convex;
- h_i's are affine;
- g_i's are (strictly) feasible; this means that there exits some w so that $g_i(w) < 0$ for all i.

w^*,α^* and β^* satisfy the **Karush-Kuhn-Tucker** (**KKT**) **conditions**, which are as follows:

$$\begin{aligned}
\frac{\partial}{\partial w_i}\mathcal{L}(w^*, \alpha^*, \beta^*) &= 0, i = 1, \dots, n \\
\frac{\partial}{\partial \beta_i}\mathcal{L}(w^*, \alpha^*, \beta^*) &= 0, i = 1, \dots, l \\
\alpha_i^* g_i(w^*) &= 0, i = 1, \dots, k \\
g_i(w^*) &\leq 0, i = 1, \dots, k \\
\alpha^* &\geq 0, i = 1, \dots, k
\end{aligned}$$

The optimal margin classifier(3)

we posed the following (primal) optimization problem for finding the optimal margin classifier:

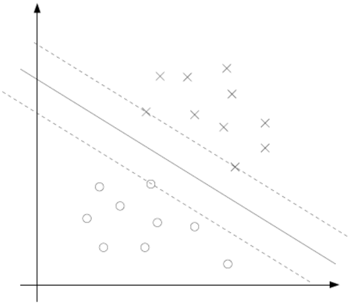
$$\begin{aligned} \min_{\gamma,w,\beta} \quad & \frac{1}{2}\|w\|^2 \\ s.t \quad & y^{(i)}(w^T x^{(i)} + b) \geq 1, i = 1, \ldots, m \end{aligned}$$

We can write the constraints as:

$$g_i(x) = 1 - y^{(i)}(w^T x^{(i)} + 1) \leq 0, i = 1, \ldots, m$$

Note that from the KKT condition,we will have $\alpha_i > 0$ only for that training example that have function margin exactly equal to one

The optimal margin classifier(4)



The points with the smallest margins are exactly the ones closest to the decision boundary;here, these are the three points which are called the **support vectors** in this problem.

The optimal margin classifier(5)

Construct Lagrangian for our problem:

$$\mathcal{L}(w,b,\alpha) = \frac{1}{2}\|w\|^2 - \sum_{i=1}^{m}[y^{(i)}(w^T x^{(i)} + b) - 1]$$

Note that there are only α_i but no β_i Lagrange multipliers. To minimize $\mathcal{L}(w,b,\alpha)$ for fix α:

$$\nabla_w \mathcal{L}(w,b,\alpha) = w - \sum_{i=1}^{m} \alpha_i y^{(i)} x^{(i)} \overset{\text{set}}{=} 0$$

This implies that:

$$w = \sum_{i=1}^{m} \alpha_i y^{(i)} x^{(i)} \tag{1}$$

The optimal margin classifier(6)

As for the derivation with respect to b,we obtain:

$$\frac{\partial}{\partial b}\mathcal{L}(w,b,\alpha)=\sum_{i=1}^{m}\alpha_i y^{(i)}=0 \tag{2}$$

Plugging w back into the Lagrangian:

$$\mathcal{L}(w,b,\alpha)=\sum_{i=1}^{m}\alpha_i-\frac{1}{2}\sum_{i,j=1}^{m}y^{(i)}y^{(j)}\alpha_i\alpha_j\langle x^{(i)},x^{(j)}\rangle$$

We obtain the following dual problem:

$$\begin{aligned}\max_{\alpha}\quad & W(\alpha)=\sum_{i=1}^{m}\alpha_i-\frac{1}{2}\sum_{i,j=1}^{m}y^{(i)}y^{(j)}\alpha_i\alpha_j\langle x^{(i)},x^{(j)}\rangle\\ s.t.\quad & \alpha_i\geq 0,\quad i=1,\ldots,m\\ & \sum_{i=1}^{m}\alpha_i y^{(i)}=0\end{aligned}$$

The optimal margin classifier(7)

Having found w^*,then we can get b^* as:

$$b^* = -\frac{\max_{i:y^{(i)}=-1} w^{*T} + \min_{i:y^{(i)}=1} w^{*T} x^{(i)}}{2}$$

Suppose we've fit our model's parameters to a training set ,and now wish to make a prediction at a new point x.We would calculate $w^T x + b$,and do prediction.But using (1), this quantity can also be written:

$$w^T x + b = \sum_{i=1}^{m} \alpha_i y^{(i)} \langle x^{(i)}, x \rangle + b$$

Using (2) we saw that the α_i's will all be zero except for the support vector.

Kernels

Define **Kernel** to be:

$$K(x,z) = \phi(x)^T \phi(z)$$

we let ϕ denote the **feature mapping**, which maps from the original input value (**attributes**) to the features in higher dimensional.

Let's see an example. Suppose $x, z \in \mathbb{R}^n$, and consider:

$$K(x,z) = (x^T z)^2 = \sum_{i,j=1}^{n} (x_i x_j)(z_i z_j) = \phi(x)^T \phi(z)$$

Thus, we can see feature mapping ϕ is given by (shown here for the case of $n = 3$)

$$\phi(x) = (x_1 x_1, x_1 x_2, \ldots, x_3 x_3)^T$$

Kernels(2)

Another example:

$$\begin{aligned} K(x,z) &= (x^T z + c)^2 \\ &= \sum_{i,j=1}^{n} (x_i x_j)(z_i z_j) + \sum_{i=1}^{n} (\sqrt{2c} x_i)(\sqrt{2c} z_i) + c^2 \end{aligned}$$

feature mapping:(Again shown for $n = 3$)

$$\phi(x) = (x_1 x_1, x_1 x_2, \ldots, x_3 x_3, \sqrt{2c} x_1, \sqrt{2c} x_2, \sqrt{2c} x_3, c)^T$$

More broadly, the kernel $K(x,z) = (x^T z + c)^d$ corresponds to a feature mapping to an $\binom{n+d}{d}$ feature space.
Map attribute to infinity dimension **Gaussian kernel**:

$$K(x,z) = \exp\left(-\frac{\|x-z\|^2}{2\sigma^2}\right)$$

Kernels(3)

More broadly, given some function K, how can we tell if it's a valid kernel; i.e., can we tell if there is some feature mapping ϕ so that $K(x, z) = \phi(x)^T\phi(z)$ for all x, z?
Consider some finite set of m points $\{x^{(1)}, x^{(2)}, \dots, x^{(m)}\}$, and let a m-by-m matrix K be defined as

$$K_{ij} = K(x^{(i)}, y(i))$$

K is called the **Kernel matrix**.
Now, if K is a valid Kernel, then

$$K_{ij} = \phi(x^{(i)})^T\phi(x^{(j)}) = \phi(x^{(j)})^T\phi(x^{(i)}) = K_{ji}$$

Hence, K must be symmetric.

Kernels(4)

More over, letting $\phi_k(x)$ denote the k-th coordinate of the vector $\phi(x)$,we find that for any vector z, we have

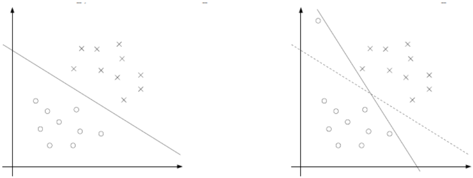
$$\begin{aligned}
z^T K z &= \sum_i \sum_j z_i K_{ij} z_j \\
&= \sum_i \sum_j z_i \phi(x^{(i)})^T \phi(x^{(j)}) z_j \\
&= \sum_i \sum_j z_i \sum_k \phi_k(x^{(i)})^T \phi_k(x^{(j)}) z_j \\
&= \sum_k \sum_i \sum_j z_i \phi_k(x^{(i)})^T \phi_k(x^{(j)}) z_j \\
&= \sum_k \left(\sum_i z_i \phi_k(x^{(i)}) \right)^2 \geq 0
\end{aligned}$$

This shows that K is positive semi-definite

Kernels(5)

Theorem (Mercer). Let $K : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ be given. Then for K to be a valid (Mercer) Kernel, it is necessary and sufficient that for any $\{x^{(1)}, \ldots, x^{(m)}\}, (m < \infty)$,the corresponding kernel matrix is symmetric positive semi-definite.

Regularization and the non-separable case



To make the algorithm work for non-linearly separable datasets as well as be less sensitive to outliers, we reformulate our optimization (l_1 **regularization**):

$$\begin{aligned} \min_{\gamma,w,b} \quad & \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{m}\xi_i \\ s.t \quad & y^{(i)}(w^T x^{(i)} + b) \geq 1 - \xi_i, i = 1, \ldots, m \\ & \xi_i \geq 0, i = 1, \ldots, m \end{aligned}$$

Regularization and the non-separable case(2)

As before, we can form the Lagrangian:

$$\mathcal{L}(w,b,\xi,\alpha,\gamma) = \frac{1}{2}w^Tw + C\sum_{i=1}^{m}\xi_i - \sum_{i=1}^{m}\alpha_i\left(y^{(i)}(x^Tw+b)-1+\xi_i\right) - \sum_{i=1}^{m}\gamma_i\xi_i$$

Here, the α_i's and γ_i's are our Lagrangian multipliers.
After some work,we obtain the dual form of the problem:

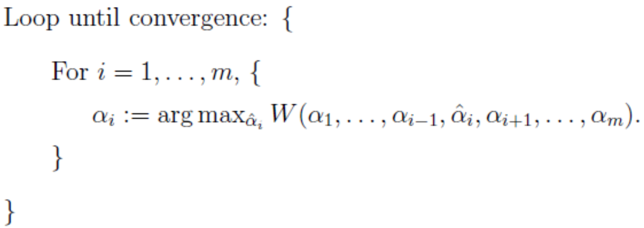
$$\begin{aligned} \max_{\alpha} \quad & W(\alpha) = \sum_{i=1}^{m}\alpha_i - \frac{1}{2}\sum_{i,j=1}^{m} y^{(i)}y^{(j)}\alpha_i\alpha_j\langle x^{(i)}, x^{(j)}\rangle \\ s.t. \quad & 0 \leq \alpha_i \geq C, i = 1, \ldots, m \\ & \sum_{i=1}^{m}\alpha_i y^{(i)} = 0 \end{aligned}$$

The SMO algorithm

Consider trying to solve the unconstrained optimization problem

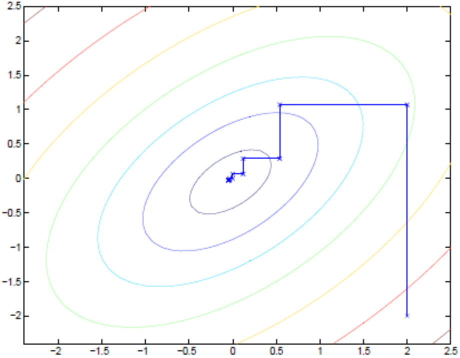
$$\max_{\alpha} W(\alpha_1, \alpha_2, \ldots, \alpha_m).$$

The algorithm here is called **coordinate ascent**:



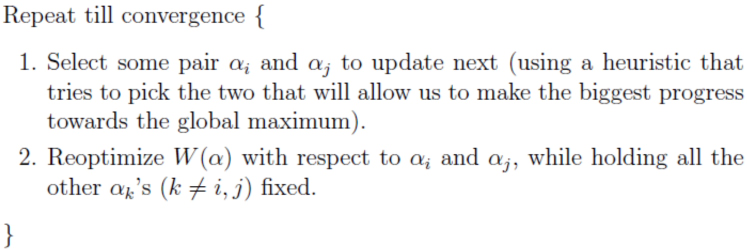
```
Loop until convergence: {
    For $i = 1, \ldots, m$, {
        $\alpha_i := \arg\max_{\hat{\alpha}_i} W(\alpha_1, \ldots, \alpha_{i-1}, \hat{\alpha}_i, \alpha_{i+1}, \ldots, \alpha_m)$.
    }
}
```

The SMO algorithm(2)



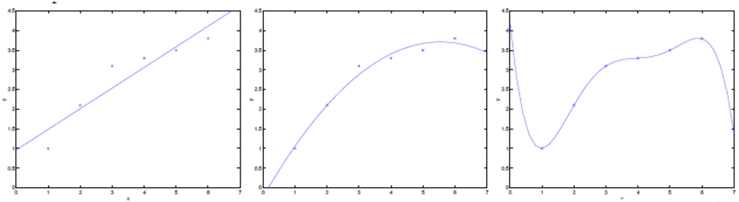
The ellipses in the figure are the contours of a quadratic function that we want to optimize.

The SMO algorithm(3)



```
Repeat till convergence {
    1. Select some pair $\alpha_i$ and $\alpha_j$ to update next (using a heuristic that
       tries to pick the two that will allow us to make the biggest progress
       towards the global maximum).
    2. Reoptimize $W(\alpha)$ with respect to $\alpha_i$ and $\alpha_j$, while holding all the
       other $\alpha_k$'s $(k \neq i, j)$ fixed.
}
```

Bias/variance tradeoff



$y = \theta_0 + \theta_1 x$ $y = \theta_0 + \theta_1 x + \theta_2 x^2$ $y = \theta_0 + \theta_1 x + \cdots \theta_5 x^5$

- The linear model suffers from large bias, and may underfit the data.
- The 5th order polynomial model suffers from large variance, and may overfit the data.

Preliminaries

Lemma. (The union bound). Let $A_1, A_2, \ldots, A_k$ be k different events (that may not be independent). Then

$$P(A_1 \cup \ldots \cup A_k) \leq P(A_1) + \ldots + P(A_k)$$

Lemma. (Hoeffding inequality) Let $Z_1, \ldots, Z_m$ be the m independent and identically distributed (iid) random variables drawn from a $\mathrm{Bernoulli}(\phi)$ distribution. I.e., $P(Z_i = 1) = \phi$, and $P(Z_i = 0) = 1 - \phi$. Let $\hat{\phi} = (1/m)\sum_{i=1}^{m} Z_i$ be the mean of these random variables, and let any $\gamma > 0$ be fixed. Then

$$P(|\phi - \hat{\phi}| > \gamma) \leq 2\exp(-2\gamma^2 m)$$

Preliminaries(2)

We assume we are given a training set $S = \{(x^{(i)}, y^{(i)}); i = 1, \ldots, m\}$ of size m, where the training examples $(x^{(i)}, y^{(i)})$ are drawn iid from some probability distribution $\mathcal{D}$. For a hypothesis h, we define the **training error** (also called the **empirical risk** or **empirical error** in learning theory) to be

$$\hat{\varepsilon}(h) = \frac{1}{m} \sum_{i=1}^{m} 1\{h(x^{(i)}) \neq y^{(i)}\}$$

Here $1\{condition\}$ means, if condition is true then $1\{condition\} = 1$, otherwise $1\{condition\} = 0$.
Define **generalization error** to be

$$\varepsilon(h) = P_{(x,y)\sim\mathcal{D}}(h(x) \neq y)$$

Empirical risk minimization (ERM)

We define the **hypothesis class** $\mathcal{H}$ used by a learning algorithm to be the set of all classifiers considered by it. For linear classification, $\mathcal{H} = \{h_w : h_w(x) = 1\{w^T x \geq 0\}, w \in \mathbb{R}^{n+1}\}$.
Empirical risk minimization can now be thought of as a minimization over the class of functions $\mathcal{H}$:

$$\hat{h} = \arg\min_{h \in \mathcal{H}} \hat{\varepsilon}(h)$$

Let's consider the case of finite $\mathcal{H} = \{h_1, \dots, h_k\}$. Take any one, fixed, $h_i \in \mathcal{H}$. Consider a Bernoulli random variable $Z_j = 1\{h_i(x^{(i)}) \neq y^{(j)}\}$, then the training error can be written

$$\hat{\varepsilon}(h_i) = \frac{1}{m} \sum_{j=1}^{m} Z_j$$

Since our training set was drawn idd from $\mathcal{D}$

$$\varepsilon(h_i) = E[Z_j] = P(Z_j = 1)$$

Empirical risk minimization (ERM)(2)

We can apply the Hoeffding inequality, and obtain

$$P(|\varepsilon(h_i) - \hat{\varepsilon}(h_i)| > \gamma) \leq 2\exp(-2\gamma^2 m)$$

Let A_i denote the event that $|\varepsilon(h_i) - \varepsilon(\hat{h}_i)| > \gamma$. Using the union bound, we have

$$\begin{aligned} P(\exists h \in \mathcal{H}. |\varepsilon(h_i) - \hat{\varepsilon}(h_i)| > \gamma) &= P(A_1 \cup \ldots \cup A_k) \\ &\leq \sum_{i=1}^{k} P(A_i) \\ &\leq \sum_{i=1}^{k} 2\exp(-2\gamma^2 m) \\ &= 2k\exp(-2\gamma^2 m) \end{aligned}$$

Empirical risk minimization (ERM)(3)

Subtract both sides from 1, we obtain

$$\begin{aligned} P(\neg\exists h \in \mathcal{H}.|\varepsilon(h_i) - \hat{\varepsilon}(h_i)| > \gamma) &= P(\forall \in \mathcal{H}.|\varepsilon(h_i) - \hat{\varepsilon}(h_i)| \leq \gamma) \\ &\geq 1 - 2k\exp(-2\gamma^2 m) \end{aligned}$$

So, with probability at least $1 - 2k\exp(-2\gamma^2 m)$ we have that $\varepsilon(h)$ will be within γ of $\varepsilon(\hat{h})$ for all $h \in \mathcal{H}$. This is called a **uniform convergence result**.

Given γ and some $\delta > 0$, by setting $\delta = 2k\exp(-2\gamma^2 m)$,we find that if

$$m \geq \frac{1}{2\gamma^2}\log\frac{2k}{\delta},$$

then with probability at least $1-\delta$, we have that $|\varepsilon(h) - \hat{\varepsilon}(h)| \leq \gamma$ for all $h \in \mathcal{H}$.

The training set size m that a certain method or algorithm requires in order to achieve a certain level if performance is also called the algorithm's **sample complexity**.

Empirical risk minimization (ERM)(4)

Similarly,we can also hold m and δ fixed and solve for γ.

$$|\varepsilon(\hat{h}) - \varepsilon(h)| \leq \gamma \leq \sqrt{\frac{1}{2m} \log \frac{2k}{\delta}}$$

Define $h^* = \arg\min_{h \in \mathcal{H}} \varepsilon(h)$. We have:

$$\varepsilon(\hat{h}) \leq \hat{\varepsilon}(\hat{h}) + \gamma \leq \hat{\varepsilon}(h^*) + \gamma \leq \varepsilon(h^*) + 2\gamma$$

Theorem. Let $|\mathcal{H}| = k$, and let any m, δ be fixed. Then with probability at least $1 - \delta$, we have that

$$\varepsilon(\hat{h}) \leq \left(\min_{h \in \mathcal{H}} \varepsilon(h) \right) + 2\sqrt{\frac{1}{2m} \log \frac{2k}{\delta}}$$

Empirical risk minimization (ERM)(5)

Given a set $S = \{x^{(1)}, \dots, x^{(d)}\}$, we say that $\mathcal{H}$ **shatters** S if $\mathcal{H}$ can realize any labelling on S. I.e., if for any set of labels $\{y^{(1)}, \dots, y^{(d)}\}$, there exists some $h \in \mathcal{H}$ so that $h(x^{(i)}) = y^{(i)}$ for all $i = 1, \dots, d$.

Given a hypothesis class $\mathcal{H}$, we can define its **Vapnik-Chervonenkis dimension**, written $VC(\mathcal{H})$, to be the size of the largest set that is shattered by $\mathcal{H}$.

Theorem. Let $\mathcal{H}$ be given, and let $d = VC(\mathcal{H})$. Then with probability at least $1 - \delta$, we have that for all $h \in \mathcal{H}$,

$$|\epsilon(h) - \hat{\epsilon}(h)| \leq O\left(\sqrt{\frac{d}{m}\log\frac{m}{d} + \frac{1}{m}\log\frac{1}{\delta}}\right).$$

Empirical risk minimization (ERM)(6)

Thus, with probability at least $1-\delta$, we also have that:

$$\epsilon(\hat{h}) \leq \epsilon(h^*) + O\left(\sqrt{\frac{d}{m}\log\frac{m}{d} + \frac{1}{m}\log\frac{1}{\delta}}\right).$$

Corollary. For $|\epsilon(h) - \hat{\epsilon}(h)| \leq \gamma$ to hold all $h \in \mathcal{H}$ with probability at least $1-\delta$, it suffices that $m = O_{\gamma,\delta}(d)$.

In Mixture densities we have some assumptions.

1. The samples come from a known number of classes.
2. The prior probabilities $P(\omega_j)$ for each class are known, $j = 1, \ldots, c$.
3. The forms for the class-conditional probability densities $p(x|\omega_j, \theta_j)$ are known, $j = 1, \ldots, c$.
4. The values for the c parameter vectors. $\theta_1, \ldots, \theta_c$ are unknown.
5. The category labels are unknown.

Samples are assumed to be obtained by selecting state if nature ω_j with probability $P(\omega_j)$ and then selecting an x according to the probability law $p(x|\omega_j, \theta_j)$. Thus probability density function for the samples is given by

$$p(x|\theta) = \sum_{j=1}^{c} p(x|\omega_j, \theta_j) P(\omega_j)$$

Definition: A density $p(x|\theta)$ is said to be *identifiable* if $\theta \neq \theta'$ implies that there exists an x such that $p(x|\theta) \neq p(x|\theta')$.
Or put another way, a density $p(x|\theta)$ is *not identifiable* if we cannot recover a unique θ.
A example for unidentifiable:

$$\begin{aligned} P(x|\theta) &= \frac{1}{2}\theta_1^x(1-\theta_1)^{1-x} + \frac{1}{2}\theta_2^x(1-\theta_2)^{1-x} \\ &= \begin{cases} \frac{1}{2}(\theta_1+\theta_2) & \text{if } x = 1; \\ 1 - \frac{1}{2}(\theta_1+\theta_2) & \text{if } x = 0. \end{cases} \end{aligned}$$

Suppose, for example, that we know for our data that P(x = 1—) = 0.6, and hence that $P(x=0|\theta) = 0.4$. Then we know the function $P(x|\theta)$, but we cannot determine θ, and hence cannot extract the component distributions. The most we can say is that $\theta_1 + \theta_2 = 1.2$. Thus, here we have a case in which the mixture distribution is completely unidentifiable.

Suppose now that we are given a set $\mathcal{D} = \{x_1, \ldots, x_n\}$ of n unlabeled samples drawn independently from mixture density.

$$p(x|\theta) = \sum_{j=1}^{c} p(x|\omega_j, \theta_j) P(\omega_j)$$

where the full parameter vector θ is fixed but unknown. The likelihood of the observed samples is, by definition, the joint density

$$p(\mathcal{D}|\theta) \equiv \prod_{k=1}^{n} p(x_k|\theta)$$

The maximum-likelihood estimate $\hat{\theta}$ is that value of θ that maximizes $p(\mathcal{D}|\theta)$.

The Log maximum-likelihood:

$$l = \sum_{k=1}^{n} \log p(x_k|\theta)$$

and

$$\begin{aligned} \nabla_{\theta_i} l &= \sum_{k=1}^{n} \frac{1}{p(x_k|\theta)} \nabla_{\theta_i} \left(\sum_{j=1}^{c} p(x_k|\omega_j, \theta_j) P(\omega_j) \right) \\ &= \sum_{k=1}^{n} \frac{1}{p(x_k|\theta)} \nabla_{\theta_i} p(x_k|\omega_i) P(\omega_i) \end{aligned}$$

Here we assume that θ_i and θ_j are independent if $i \neq j$.

According the Bayes' formula,

$$P(\omega_i|x_k,\theta)=\frac{p(x_k|\omega_i,\theta_i)P(\omega_i)}{p(x_k|\theta)}$$

Hence,

$$\nabla_{\theta_i} l=\sum_{k=1}^{n} P(\omega_i|x_k,\theta)\nabla_{\theta_i}\log p(x_k|\omega_i,\theta_i)$$

and $P(\omega_i)$ can be estimate by $P(\omega_i|x_k)$:

$$p(\omega_i)=\frac{1}{n}\sum_{k=1}^{n} P(\omega_i|x_k,\theta)$$

Mixtures of Gaussians and the EM algorithm

Suppose that we are given a training set $\{x^{(1)}, \ldots, x^{(m)}\}$, we wish to model the data by specifying a joint distribution $p(x^{(1)}, z^{(i)}) = p(x^{(i)}|z^{(i)})$. Here,

$$\begin{aligned} z^{(i)} \in \{1, \ldots, k\} &\sim \text{Multinomial}(\phi), \\ x^{(i)}|z^{(i)} = j &\sim \mathcal{N}(\mu_j, \Sigma_j) \end{aligned}$$

This is call the **mixture of Gaussians** model, and $z^{(i)}$'s are **latent** random variables. To estimate ϕ, μ and Σ, we can write down the likelihood of our data.

$$\begin{aligned} l(\phi, \mu, \Sigma) &= \sum_{i=1}^{m} \log p(x^{(i)}; \phi, \mu, \Sigma) \\ &= \sum_{i=1}^{m} \log \sum_{z^{(i)}=1}^{k} p(x^{(i)}|z^{(i)}; \mu, \Sigma) p(z^{(i)}; \phi) \end{aligned}$$

Mixtures of Gaussians and the EM algorithm(2)

Note that if we knew what the $z^{(i)}$'s were, the maximum likelihood problem would have been easy. Specifically, we could then write down the likelihood as

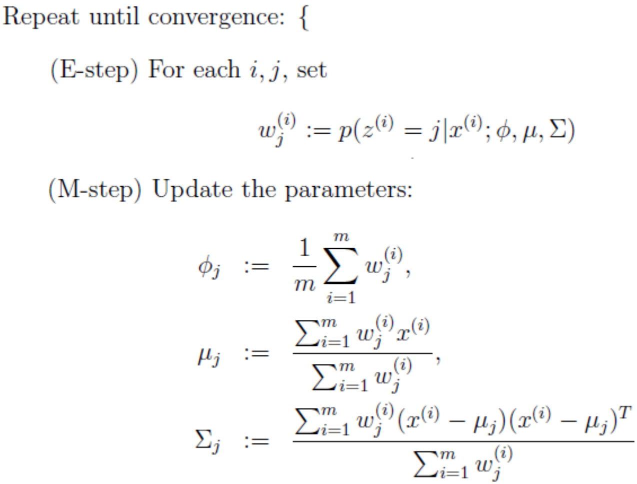
$$l(\phi, \mu, \Sigma) = \sum_{i=1}^{m} \log p(x^{(i)} | z^{(i)}; \mu, \Sigma) + \log p(z^{(i)}; \phi)$$

Maximizing this with respect to ϕ, μ and Σ gives the parameters.

$$\begin{aligned}
\phi_j &= \frac{1}{m} \sum_{i=1}^{m} 1\{z^{(i)} = j\} \\
\mu_j &= \frac{\sum_{i=1}^{m} 1\{x^{(i)} = j\} x^{(i)}}{\sum_{i=1}^{m} 1\{z^{(i)} = j\}} \\
\Sigma_j &= \frac{\sum_{i=1}^{m} 1\{z^{(i)} = j\} (x^{(i)} - \mu_j)(x^{(i)} - \mu_j)^T}{\sum_{i=1}^{m} 1\{z^{(i)} = j\}}
\end{aligned}$$

Mixtures of Gaussians and the EM algorithm(3)

The EM algorithm is an iterative algorithm that has two main step.



Repeat until convergence: {

(E-step) For each i, j, set

$$w_j^{(i)} := p(z^{(i)} = j | x^{(i)}; \phi, \mu, \Sigma)$$

(M-step) Update the parameters:

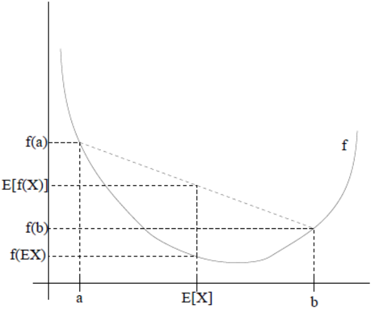
$$\begin{aligned} \phi_j &:= \frac{1}{m} \sum_{i=1}^{m} w_j^{(i)}, \\ \mu_j &:= \frac{\sum_{i=1}^{m} w_j^{(i)} x^{(i)}}{\sum_{i=1}^{m} w_j^{(i)}}, \\ \Sigma_j &:= \frac{\sum_{i=1}^{m} w_j^{(i)} (x^{(i)} - \mu_j)(x^{(i)} - \mu_j)^T}{\sum_{i=1}^{m} w_j^{(i)}} \end{aligned}$$

Jensens inequality

Theorem. Let f be a convex(concave) function, and let X be a random variable. Then:

$$E[f(X)] \geq f(EX) \quad \text{(Concave case is } E[f(X)] \leq f(EX) \text{)}$$

Moreover, if f is strictly convex(concave), then $E[f(X)] = f(EX)$ holds true if and only if $X = E[X]$ with probability 1.



The EM algorithm

Suppose we have a training set $\{x^{(i)}, \ldots, x^{(m)}\}$. We wish to fit the parameters of a model p(x,z) to the data, where the likelihood is given by

$$l(\theta) = \sum_{i=1}^{m} \log p(x;\theta) = \sum_{i=1}^{m} \log \sum_{z} p(x,z;\theta).$$

For each i, let Q_i be some distribution over the z's($\sum_z Q_i(z) = 1, Q_i(z) \geq 0$. Consider:

$$\begin{aligned}
\sum_i \log p(x^{(i)};\theta) &= \sum_i \log \sum_{z^{(i)}} p(x^{(i)}, z^{(i)};\theta) && (3)\\
&= \sum_i \log \sum_{z^{(i)}} Q_i(z^{(i)}) \frac{p(x^{(i)}, z^{(i)};\theta)}{Q_i(z^i)} && (4)\\
&= \sum_i \log E_{z^{(i)} \sim Q_i}[\frac{p(x^{(i)}, z^{(i)};\theta)}{Q_i(z^{(i)})}] && (5)\\
&\geq \sum_i \sum_{z^{(i)}} Q_i(z^{(i)}) \log \frac{p(x^{(i)}, z^{(i)};\theta)}{Q_i(z^{(i)})} && (6)
\end{aligned}$$

The EM algorithm(2)

To make the bound tight,we need Jensen's inequality to hold equality.we require that

$$\frac{p(x^{(i)}, z^{(i)})}{Q_i(z^{(i)})} = c$$

for some constant c that not depend on $z^{(i)}$

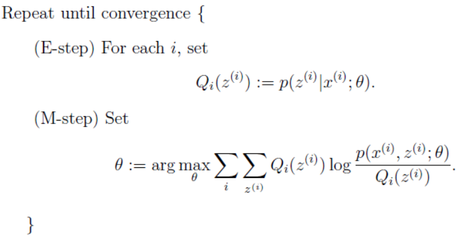
$$Q_i(z^{(i)}) \propto p(x^{(i)}, z^{(i)}; \theta)$$

Actually,since $\sum_z Q_i(z^{(i)}) = 1$:

$$\begin{aligned} Q_i(z^{(i)}) &= \frac{p(x^{(i)}, z^{(i)}; \theta)}{\sum_z p(x^{(i)}, z; \theta)} \\ &= \frac{p(x^{(i)}, z^{(i)}; \theta)}{p(x^{(i)}; \theta)} = p(z^{(i)}|x^{(i)}; \theta) \end{aligned}$$

The EM algorithm(3)

Generalized EM algorithm:



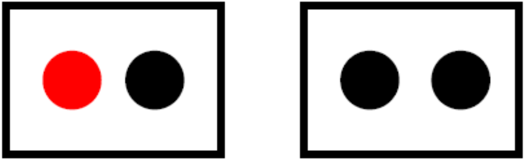
```
Repeat until convergence {
    (E-step) For each $i$, set
        $Q_i(z^{(i)}) := p(z^{(i)}|x^{(i)};\theta).$
    (M-step) Set
        $\theta := \arg\max_\theta \sum_i \sum_{z^{(i)}} Q_i(z^{(i)}) \log \frac{p(x^{(i)}, z^{(i)}; \theta)}{Q_i(z^{(i)})}.$
}
```

If we define

$$J(Q,\theta) = \sum_i \sum_{z^{(i)}} Q_i(z^{(i)}) \log \frac{p(x^{(i)}, z^{(i)}; \theta)}{Q_i(z^{(i)})}.$$

the EM can also be viewed a coordinate ascent on J.

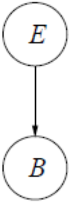
The envelope quiz



- red ball is goal
- You randomly picked an envelop randomly took out a ball and it was black
- Should you choose this envelope or the other envelope?

The envelope quiz(2)

- Probabilistic inference
  - Joint distribution on $E \in \{1, 0\}, B \in \{r, b\}$: $P(E, B) = P(E)P(B|E)$
  - $P(E = 1) = P(E = 0) = \frac{1}{2}$
  - $P(B = r|E = 1) = \frac{1}{2}, P(B = r|E = 0) = 0$
  - The graphical model:



- Statistical decision theory: switch if $P(E = 1|B = b) < \frac{1}{2}$
- $P(E = 1|B = b) = \frac{P(B=b|E=1)P(E=1)}{P(B=b)} = \frac{1}{3}$

Some concepts

- The world is reduced to a set of random variables $x_1, \dots, x_d$
  - e.g. $(x_1, \dots, x_{d-1})$ is a feature vector, $x_d \equiv y$ is the class label.
- Inference: given joint distribution $p(x_1, \dots, x_d)$, compute $p(X_Q | X_E)$ where $X_Q \cup X_E \subseteq \{x_1, \dots, x_d\}$
  - e.g. $Q = \{x_d\}, E = \{x_1, \dots, x_{d-1}\}$, by the definition of conditional

$$p(x_d | x_1, \dots, x_{d-1}) = \frac{p(x_1, \dots, x_d)}{\sum_v p(x_1, \dots, x_{d-1}, x_d = v)}$$

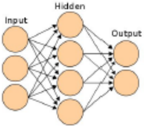
- Learning estimate $p(x_1, \dots, x_d)$ from training data $\{x^{(1)}, \dots, x^{(m)}\}$

What are graphical models?

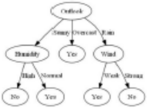
- Graphical model = joint distribution $p(x_1, \ldots, x_d)$
  - Bayesian network
  - Markov random field
- Inference $= p(X_Q|X_E)$, in general $X_Q \cup X_E \subseteq \{x_1, \ldots, x_d\}$
- If $p(x_1, \ldots, x_d) notgiven, estimateitfromdata$
  - parameter and structure learning

What are graphical models?(2)

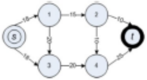
- Graphical model is the study of probabilistic models
- Just because there are nodes and edges doesn't mean it's a graphical model
- These are not graphical models:



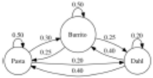
neural network



decision tree



network flow



HMM template
(but HMMs are!)

Directed graphical models

- Also called Bayesian networks
- A directed graph has nodes $x_1, \ldots, x_d$, some of them connected by directed edges $x_i \to x_j$
- A cycle is a directed path $x_1 \to \ldots \to x_k$ where $x_1 = x_k$
- A directed acyclic graph (DAG) contains no cycles

Directed graphical models(2)

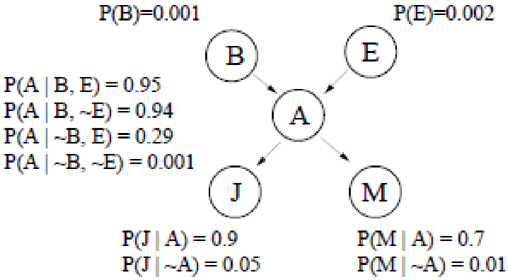
- A Bayesian network on the DAG is a family of distributions satisfying

$$p|p(x_1, \dots, x_d) = \prod_i p(x_i|Pa(x_i))$$

where $Pa(x_i)$ is the set of parents of x_i

- $p(x_i|Pa(x_i))$ is the conditional probability distribution (CPD) at x_i
- By specifying the CPDs for all i, we specify a joint distribution $p(x_1, \dots, x_d)$

Example:Burglary, Earthquake, Alarm, John and Marry



P(B)=0.001

P(E)=0.002

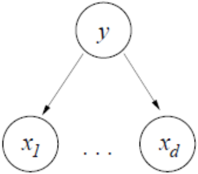
P(A | B, E) = 0.95
P(A | B, ~E) = 0.94
P(A | ~B, E) = 0.29
P(A | ~B, ~E) = 0.001

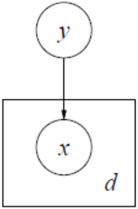
P(J | A) = 0.9
P(J | ~A) = 0.05

P(M | A) = 0.7
P(M | ~A) = 0.01

$$P(B, \sim E, A, J, \sim M) = P(B)P(\sim E)P(A|B, \sim E)P(J|A)P(\sim M|A)$$

Example: Naive Bayes



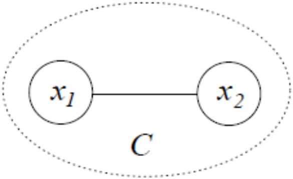


- $p(y, x_1, \ldots, x_d) = p(y) \prod_{i=1}^{d} p(x_i|y)$
- Plate representation on the right
- $p(y)$ multinomial
- $p(x_i|y)$ depends on the feature type.

Undirected graphical models

- Also known as Markov Random Fields
- A clique C in an undirected graph is a set of fully connected nodes (full of loops!)
- Define a nonnegative potential function $\psi_C : X_C \to \mathbb{R}_+$
- An undirected graphical model is a family of distributions satisfying
$$\left\{ p | p(X) = \frac{1}{Z} \prod_C \psi_C(X_c) \right\}$$
- $Z = \int \prod_C \psi_C(X_C) dX$

A Tiny Markov Random Field



- $x_1, x_2 \in \{-1, 1\}$
- A single clique $\psi_C(x_1, x_2) = e^{ax_1x_2}$
- $p(x_1, x_2) = \frac{1}{Z} e^{ax_1x_2}$
- $Z = (2e^a + 2e^{-a})$
- $p(1, 1) = p(-1, -1) = \frac{e^a}{2e^a + 2e^{-a}}$

Topic Model

- A topic is defined as a probability distribution over terms or a cluster of weighted terms.
- A document is defined as a set of words generated from a mixture of latent topics.

Various topic modeling methods, such as PLSI, LDA, LSI, NMF, and RLSI have been proposed and successfully applied to different applications.

Probabilistic Topic Models

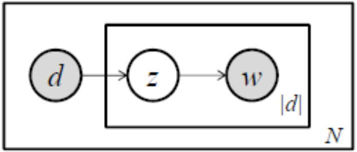
Suppose that $\mathcal{D} = \{d_1, d_2, \ldots, d_N\}$ is a set of documents with size N and $\mathcal{V}$ is a set of terms or words with size M, i.e., the vocabulary. A document $d \in \mathcal{D}$ consists of $|d|$ words from the vocabulary, denoted as $d = (w_1, w_2, \ldots, w_{|d|})$. Suppose that there are K topics in the document collection.
PLSI is one of the widely used probabilistic topic models. One can generate the documents in the collection in the following way.

- select a document d from the collection with probability $P(d)$
- select a latent topic z with probability $P(z|d)$
- generate a word w with probability $P(w|z)$

Here $z \in \{z_1, \ldots, z_K\}$ is a latent variable representing a topic.

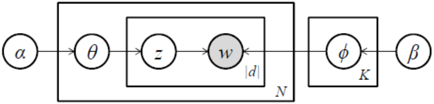
Probabilistic Topic Models(2)

The parameters of $P(d)$, $P(w|z)$, and $P(z|d)$ can be estimated by EM algorithm.



Probabilistic Topic Models(3)

LDA Model:



1. for each topic $k = 1, \ldots, K$
   (a) draw word distribution ϕ_k according to $\phi_k|\beta \sim \mathrm{Dir}(\beta)$
2. for each document d in the collection
   (a) draw topic distribution θ according to $\theta|\alpha \sim \mathrm{Dir}(\alpha)$
   (b) for each word w in the document d
      i. draw a topic z according to $z|\theta \sim \mathrm{Mult}(\theta)$
      ii. draw a word w according to $w|z \sim \mathrm{Mult}(\phi_z)$

Non-probabilistic Topic Models

Non-probabilistic topic models are usually obtained by matrix factorization.Suppose that $\mathcal{D}$ is a set of document with size N, and $\mathcal{V}$ is a vocabulary with size M.The document collection $\mathcal{D}$ is represented as an $M \times N$ matrix $D = (d_1, \ldots, d_N)$.
Suppose that there are K topics represented as an $M \times K$ term-topic matrix $U = (u_1, \ldots, u_K)$. $V^T = (v_1, \ldots, v_N)$ is an $K \times N$ topic-document matrix.
Our goal is to factor matrix D by U and V^T.

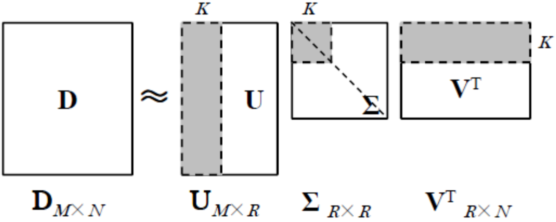
$$D \approx UV^T$$

Non-probabilistic Topic Models(2)

LSI assumes that the K columns of matrix U as well as the K columns of matrix V are orthonormal. LSI amounts to minimizing the following objective function with the orthonormal constraints.

$$\min_{U,V} \|D - U\Sigma V^T\|_F$$

$$s.t. \quad U^T \times U = I, V \times V^T = I, \text{and } \Sigma \text{ is diagonal}$$



What is entropy

In thermodynamics, entropy (usual symbol S) is a measure of the number of specific ways in which a thermodynamic system may be arranged, commonly understood as a measure of disorder.

$$\Delta = \int \frac{dQ_{rev}}{T}$$

In information theory, **Entropy** is a measure of unpredictability of information content. Shannon defined the entropy H of a discrete random variable X with possible values $x1, ..., xn$ and probability mass function P(X) as:

$$H(X) = E[I(X)] = E[-\ln(P(X))]$$

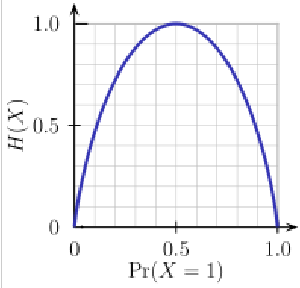
Here I is the information content of X.

What is entropy(2)

When taken from a finite sample, the entropy can explicitly be written as

$$H(X) = \sum_i P(x_i) I(x_i) = -\sum_i P(x_i) \log_b P(x_i)$$

Common values of b are 2, e, and 10, and the unit of entropy is bit for $b = 2$, nat for $b = e$, and dit (or digit) for $b = 10$.



Whis is entropy(3)

According the definition of $H(X)$, we can define **Joint Entropy** as:

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

and define **Conditional Entropy** to measure unpredictability of random variable Y given random variable X as:

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

The entropy or the amount of information revealed by evaluating (X,Y) (that is, evaluating X and Y simultaneously) is equal to the information revealed by conducting two consecutive experiments: first evaluating the value of Y, then revealing the value of X given that you know the value of Y. This may be written as

$$H(X,Y) = H(X|Y) + H(Y) = H(Y|X) + H(X) \tag{7}$$

Whis is entropy(4)

We can get (7) by:

$$\begin{aligned}
& H(X,Y) - H(X) \\
= & -\sum_{x,y} p(x,y)\log p(x,y) + \sum_{x} p(x)\log p(x) \\
= & -\sum_{x,y} p(x,y)\log p(x,y) + \sum_{x}\left(\sum_{y} p(x,y)\right)\log p(x) \\
= & -\sum_{x,y} p(x,y)\log p(x,y) + -\sum_{x,y} p(x,y)\log p(x) \\
= & -\sum_{x,y} p(x,y)\log \frac{p(x,y)}{p(x)} \\
= & -\sum_{x,y} p(x,y)\log p(y|x) = H(Y|X)
\end{aligned}$$

Whis is entropy(5)

Another useful measure of entropy that works equally well in the discrete and the continuous case is the **Relative Entropy** of a distribution. It is also called as the **Kullback-Leibler Divergence**.

$$D(p||q) = \sum_x p(x) \log \frac{p(x)}{q(x)} = E_{p(x)} \log \frac{p(x)}{q(x)}$$

To some extent, Relative Entropy can be the measure of the distance between two random variables.
Mutual Information can be defined as:

$$I(X,Y) = \sum_{x,y} \log \frac{p(x,y)}{p(x)p(y)}$$

What is entropy(6)

Let's consider

$$
\begin{aligned}
& H(Y) - I(X,Y) \\
= \quad & -\sum_{y} p(y) \log p(y) - \sum_{x,y} \log \frac{p(x,y)}{p(x)p(y)} \\
= \quad & -\sum_{y} \left(\sum_{x} p(x,y) \right) \log p(y) - \sum_{x,y} p(x,y) \log \frac{p(x,y)}{p(x)p(y)} \\
= \quad & -\sum_{x,y} p(x,y) \log p(y) - \sum_{x,y} \log \frac{p(x,y)}{p(x)p(y)} \\
= \quad & -\sum_{x,y} p(x,y) \log \frac{p(x,y)}{p(x)} \\
= \quad & -\sum_{x,y} p(x,y) \log p(y|x) = H(Y|X)
\end{aligned}
$$

According the formula (7):

$$I(X,Y) = H(X) + H(Y) - H(X,Y)$$