CS5014 Machine Learning

Lecture 5 Maximum Likelihood Estimation (MLE)

Lei Fang

School of Computer Science, University of St Andrews

Spring 2021

University of St Andrews

Motivation

Objective: **probabilistic perspective** of linear regression

- justify least squared error: $(\boldsymbol{y} - \boldsymbol{X\theta})^T(\boldsymbol{y} - \boldsymbol{X\theta})$
- maximum likelihood estimator: $\boldsymbol{\theta}_{\text{ML}}$
- BUT nothing new: $\boldsymbol{\theta}_{\text{ML}} = \boldsymbol{\theta}_{\text{LS}} = (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}\boldsymbol{y}$

So why bother ?

- MLE: very general model
- lots of ML algorithms fit in MLE category
  - linear regression, logistic regression, k-means, mixture model, neural nets, discriminant analysis, naive Bayes ...
- large number theory for MLE (next time)
  - $P(\theta_{\text{ML}})$? or *sampling distribution*
  - does θ_{ML} change much given another $\mathcal{D}_k = \{\boldsymbol{X}_k, \boldsymbol{y}_k\}$?

Motivation

Objective: **probabilistic perspective** of linear regression

- justify least squared error: $(\boldsymbol{y} - \boldsymbol{X\theta})^T(\boldsymbol{y} - \boldsymbol{X\theta})$
- maximum likelihood estimator: $\boldsymbol{\theta}_{\text{ML}}$
- BUT nothing new: $\boldsymbol{\theta}_{\text{ML}} = \boldsymbol{\theta}_{\text{LS}} = (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}\boldsymbol{y}$

So why bother ?

- MLE: very general model
- lots of ML algorithms fit in MLE category
  - linear regression, logistic regression, k-means, mixture model, neural nets, discriminant analysis, naive Bayes ...
- large number theory for MLE (next time)
  - $P(\boldsymbol{\theta}_{\text{ML}})$? or *sampling distribution*
  - does $\boldsymbol{\theta}_{\text{ML}}$ change much given another $\mathcal{D}_k = \{\boldsymbol{X}_k, \boldsymbol{y}_k\}$?

Topics of today

Review of probability theory

- univariate Gaussian

Maximum likelihood estimation in general

- MLE for Gaussian
- MLE for Bernoulli/Binomial

Linear regression revisit: MLE

Logistic regression and MLE

Review: Random variable

Random variable X

- opposite to deterministic variable: X can take a range of value associated with some probability $P(X)$
- discrete r.v.: if X can only take discrete values
  - e.g. $X \in \{T, F\}$, $X \in \{1, 2, 3, \ldots\}$ etc.
- otherwrise X is continuous r.v.
  - e.g. $X \in [0, 1]$, $X \in R^2$

Random variable - discrete r.v.

If r.v. X's target space $\mathcal{T}$ is discrete

- X is a **discrete random variable**
- the probability distribution P is called **probability mass function** (p.m.f.)
- and

$$0 \leq P(X = x) \leq 1, \text{ and } \sum_{x \in T} P(X = x) = 1$$

Example - discrete r.v.

Bernoulli distribution Tossing a coin , $\mathcal{T} = 1, 0$ (1 is H, 0 is T),

$$P(X = 1) = p, P(X = 0) = 1 - p, 0 \leq p \leq 1$$

or

$$P(X = x) = p^x (1 - p)^{1-x}$$

Example - discrete r.v.

Multinoulli distribution

X can take $\{1, 2, \ldots, k\}$, its probability mass function is

$$P(X) = \begin{cases} p_1 & X = 1 \\ p_2 & X = 2 \\ \vdots & \\ p_k & X = k \end{cases}$$

$$P(x) = \prod_{i=1}^{k} p_i^{I(x=i)}$$

$$I(x = i) = 1 \text{ if } x = i \text{ or } 0 \text{ if } x \neq i$$

E.g. throw a fair 6-facet die, $\mathcal{T} = 1, 2, \ldots, 6$, the distribution is

$$P(X = i) = 1/6$$

Random variable - continuous r.v.

If r.v. X's target space $\mathcal{T}$ is continuous

- X is a **continuous random variable**
- the probability distribution p is called **probability density function** (p.d.f.): note we use p
- and satisfies

$$p(x) \geq 0, \text{ and } \int_{x \in T} p(x)dx = 1$$

- pdf is not probability as $p(x)$ can be greater 1;
- calculate probability over an interval: e.g.

$$0 \leq P(X \in [a, b]) = \int_a^b p(x)dx \leq 1$$

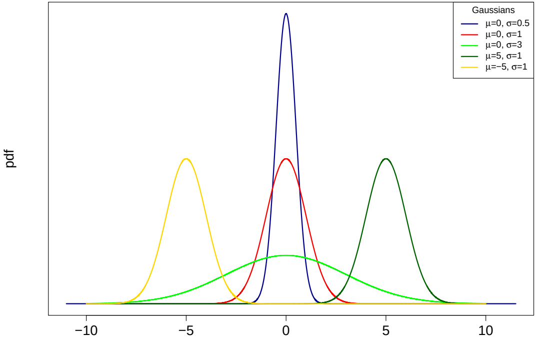
- for $\forall a \in \mathcal{T}$ $P(X = a) = P(X \in [a, a]) = \int_a^a p(x)dx = 0$

Example - continuous r.v.

Gaussian distribution $\mathcal{T} = R$, or $X \in R$ the pdf is

$$p(x) = \mathcal{N}\left(x; \mu, \sigma^2\right) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}$$

$\left(\frac{x-\mu}{\sigma}\right)^2$ is a distance measure: how far x is away from μ (measured by σ as a unit)



Joint distribution

Ramdom variable $\boldsymbol{X} = [X_1, X_2, \ldots, X_n]^T$ can be multidimensional (each X_i is r.v.)

- essentially a *random vector*

Still satisfies the same requirements

$$\forall \boldsymbol{x}, 0 < P(\boldsymbol{X} = \boldsymbol{x}) < 1, \sum_{x_1} \sum_{x_2} \ldots \sum_{x_n} P(\boldsymbol{X} = [x_1, x_2, \ldots, x_n]) = 1$$

- means the probability that $X = \boldsymbol{x}$ is jointly true

For bivariate case, i.e. $n = 2$, X_1, X_2 are **independent** (e.g. rolling two dice independently) if

$$P(\boldsymbol{X}) = P(X_1)P(X_2)$$

Example: joint distribution

The joint distribution of X snow or not, $Y \in \{$spring, summer, autumn, winter$\}$ represents the season that x belongs to :

	$y =$ Spring	$y =$ Summer	$y =$ Autumn	$y =$ winter
$x = F$	0.05	0.25	0.075	0
$x = T$	0.2	0	0.175	0.25

It is easy to verify that

$$\sum_x \sum_y p(x, y) = 1$$

Probability rules

There are only two probability rules (integration for continuous r.v.):

1. product rule:

$$p(x, y) = p(y|x)p(x) = p(x|y)p(y)$$

2. sum rule (marginalisation):

$$p(x) = \sum_y p(x, y),\ p(y) = \sum_x p(x, y)$$

Conditional probability

Conditional probability distribution (by product rule):

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

- probability distribution of x conditional on the value of y

	$y =$ Spring	$y =$ Summer	$y =$ Autumn	$y =$ winter
$x = F$	0.05	0.25	0.075	0
$x = T$	0.2	0	0.175	0.25

- $P(Y = \text{Spring})$? use sum rule

$$P(Y = \text{Spring}) = \sum_{x=\{T,F\}} P(X = x, Y = \text{Spring}) = 0.05 + 0.2 = \frac{1}{4}$$

- $P(X = T|Y = \text{Spring})$?
  $P(X = T|y = \text{Spring}) = \frac{P(x=T, y=\text{Spring})}{P(y=\text{Spring})} = \frac{0.2}{0.25} = 0.8$

Parameter estimation problem

Given dataset $\mathcal{D} = \{y^{(1)}, y^{(2)}, \ldots, y^{(m)}\}$, and assume

$$y^{(i)} \sim P(y^{(i)}|\theta), \; i = 1, \ldots, m$$

- *parameter estimation*: given $\mathcal{D}$, what is θ?

For example, throw the same coin n times and record value $y^{(i)} \in \{1, 0\}, i = 1, \ldots, m$

$$P(y^{(i)}|\theta) = Ber(\theta)$$

- $y^{(i)} \overset{iid}{\sim} Ber(\theta)$: independent and identically distributed
- θ: the probability that head turns up

Maximum Likelihood Estimation

Likelihood function: $P(\mathcal{D}|\theta) = \prod_i^m p(y^{(i)}|\theta)$

- the probability of observing data $\mathcal{D}$ given θ
- it is not a probability distribution for θ: $\int p(\mathcal{D}|\theta)d\theta \neq 1$
- but it is a function of θ (given $\mathcal{D}$)

Maximum likelihood estimation:

$$\theta_{ML} = \underset{\theta}{\text{argmax}}\, P(\mathcal{D}|\theta)$$

- the value θ most likely to have generated the data

We usually deal with log-likelihood, denoted as $\mathcal{L}(\theta)$

$$\theta_{ML} = \underset{\theta}{\text{argmax}}\, \underbrace{\log P(\mathcal{D}|\theta)}_{\mathcal{L}(\theta)} = \underset{\theta}{\text{argmax}}\, P(\mathcal{D}|\theta)$$

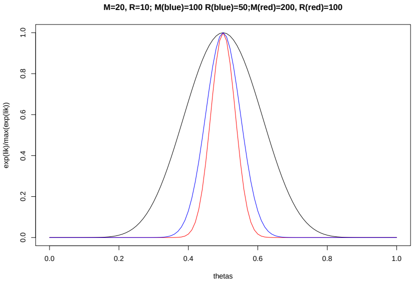
MLE for Bernoulli

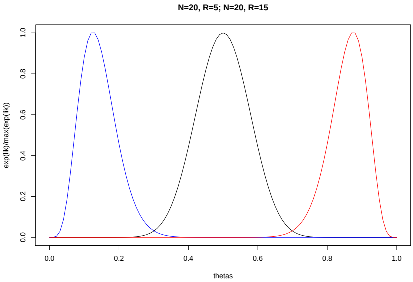
For the Bernoulli case: $y^{(i)} \in \{1, 0\}$

$$\begin{aligned}
\mathcal{L}(\theta) &= \log P(\mathcal{D}|\theta) = \log \prod_{i=1}^{m} P(y^{(i)}; \theta) \\
&= \log \prod_{i=1}^{m} \theta^{y^{(i)}} (1-\theta)^{1-y^{(i)}} \\
&= \log(\theta^{\sum_{i=1}^{m} y^{(i)}} (1-\theta)^{\sum_{i=1}^{m}(1-y^{(i)})}) \\
&= \sum_{i=1}^{m} y^{(i)} \log\theta + (m - \sum_{i=1}^{m} y^{(i)}) \log(1-\theta) \\
&= R\log\theta + (m-R)\log(1-\theta)
\end{aligned} \tag{1}$$

- $R = \sum_{i}^{m} y^{(i)}$: the total count of heads
- we will use the likelihood function eq.(1) for logistic regression later

Some plots of (scaled) likelihood





$m = 20; R = \sum x_i = 10$

$m = 100; R = \sum x_i = 50$

$m = 200; R = \sum x_i = 100$

$m = 40; R = \sum x_i = 20$

$m = 40; R = \sum x_i = 5$

$m = 40; R = \sum x_i = 35$

MLE for Bernoulli

Take the derivative $\frac{d\mathcal{L}(\theta)}{d\theta}$ and set it to zero

$$\mathcal{L}(\theta) = R\log\theta + (m-R)\log(1-\theta)$$
$$\frac{dL}{d\theta} = \frac{R}{\theta} - \frac{m-R}{1-\theta} = 0$$
$$\Rightarrow \theta_{ML} = \frac{R}{m}$$

- note $R = \sum_{i=1}^{m} y^{(i)}$ is the count of heads;
- m is the total count
- θ_{ML} is just the relative frequency

Gradient ascent (descent) ?

We can also apply gradient **ascent** (why ascent?):
loop until converge:

$$\theta_{t+1} \leftarrow \theta_t + \alpha \nabla_\theta \mathcal{L}(\theta_t)$$

- where

$$\nabla_\theta \mathcal{L}(\theta) = \frac{R}{\theta} - \frac{m - R}{1 - \theta}$$

or gradient descent with negative log likelihood $N\mathcal{L}(\theta) = -\mathcal{L}(\theta)$:

$$\theta_{t+1} \leftarrow \theta_t - \alpha \nabla_\theta (N\mathcal{L}(\theta_t))$$

- but $\theta \in [0, 1]$: constrained optimisation
- the gradient $\nabla_\theta \mathcal{L}(\theta)$ is not defined at $\theta = 0, 1$!
- difficult to converge if step outside: $\theta_t \geq 1; \theta_t \leq 0$

Reparameterisation trick for gradient descent (ascent)

Reparameterisation trick: find f

$$\theta = f(\beta), \text{ such that}$$

- $\beta \in R$ and write $\mathcal{L}(\theta) = \mathcal{L}(f(\beta))$
- use chain rule to find $\nabla_\beta \mathcal{L}(\beta) = \nabla_\theta \mathcal{L} \cdot \nabla_\beta f(\beta)$
- gradient ascent against β; then transform back

$$\beta_{t+1} \leftarrow \beta_t + \alpha \nabla_\beta \mathcal{L}(\beta_t); \;\; \theta_{t+1} \leftarrow f(\beta_{t+1})$$

For example, if $\theta > 0$, then

$$\theta = f(\beta) = e^\beta, \text{ the new gradient is then}$$

$$\nabla_\beta \mathcal{L}(\beta) = \nabla_\theta \mathcal{L} \cdot e^\beta$$

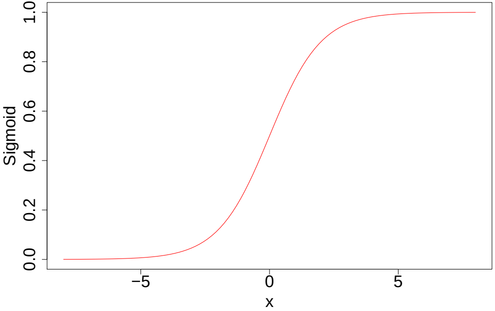
Reparameterisation trick for Bernoulli MLE

For $\theta \in [0, 1]$, such a function is sigmoid:

$$\sigma(x) = \frac{1}{1 + e^{-x}} = \frac{e^x}{e^x + 1};$$

The derivative:

$$\frac{d\sigma(x)}{dx} = \sigma(x)(1 - \sigma(x))$$



Reparameterisation trick for Bernoulli MLE

For the Bernoulli case, reparameterize θ:

$$\theta = \sigma(\beta);$$

Rewrite the log likelihood $\mathcal{L}$ as a function of β:

$$\mathcal{L}(\beta) = \log \prod_{i=1}^{m} \theta^{y^{(i)}} (1-\theta)^{1-y^{(i)}} = \log \prod_{i=1}^{m} \sigma(\beta)^{y^{(i)}} (1-\sigma(\beta))^{1-y^{(i)}}$$

The gradient of L w.r.t β is

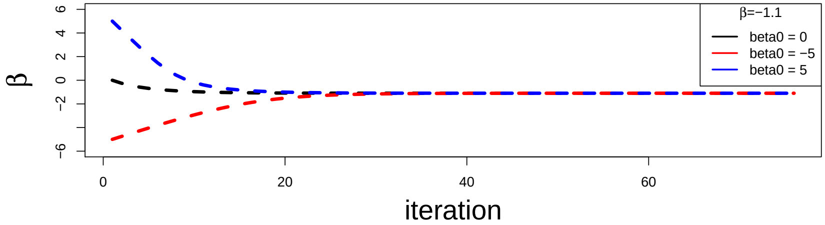
$$\nabla_\beta \mathcal{L}(\beta) = \nabla_\theta \mathcal{L} \cdot \nabla_\beta \theta = \left(\frac{R}{\sigma} - \frac{m-R}{1-\sigma} \right) \sigma(1-\sigma)$$

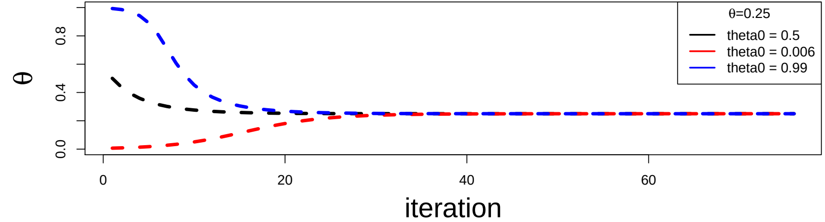
Code (R like syntax)

```
grad <- function(m,r,beta){
  sig <- sigmoid(beta)
  g <- (r/sig - (m-r)/(1-sig))*sig*(1-sig)
  return(g)
}

berGAscent <- function(alpha, iter, m, r, beta0){
  betas <- vector(mode="numeric", length = iter+1)
  betas[1] <- beta <- beta0
  for(i in 1:iter){
    g <- grad(m,r,beta)
    betas[i+1] <- beta <- beta + alpha*g
  }
  return(betas)
}
```

Example with $m = 100, R = 25, \theta_{ML} = 0.25, \alpha = 0.01$





MLE for Gaussian

Similarly, for Gaussian $\mathcal{D} = \{y^{(1)}, \ldots, y^{(m)}\}$, the parameters are $\boldsymbol{\theta} = \{\mu, \sigma^2\}$ and

$$p(y^{(i)}; \mu, \sigma^2) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left\{-\frac{1}{2\sigma^2}(y^{(i)} - \mu)^2\right\}$$

therefore, the log likelihood for $y^{(i)}$ is:

$$\log p(y^{(i)}; \mu, \sigma^2) = -\frac{1}{2}\log(2\pi\sigma^2) - \frac{1}{2\sigma^2}\underbrace{(y^{(i)} - \mu)^2}_{\text{squared error!}}$$

$$\mathcal{L}(\mu, \sigma^2) = \log p(\mathcal{D}|\mu, \sigma^2) = \log \prod_{i=1}^{m} p(y^{(i)}; \mu, \sigma^2) = \sum_{i=1}^{m} \log p(y^{(i)}; \mu, \sigma^2)$$

$$= \sum_{i=1}^{m} \left(-\frac{1}{2} \log(2\pi\sigma^2) - \frac{(y^{(i)} - \mu)^2}{2\sigma^2} \right)$$

$$= -\frac{m}{2} \log(2\pi\sigma^2) - \frac{1}{2\sigma^2} \underbrace{\sum_{i=1}^{m} (y^{(i)} - \mu)^2}_{\text{sum of squared error}}$$

Take (partial) derivative and set to zero (verify yourself!):

$$\frac{\partial L}{\partial \mu} = \frac{1}{\sigma^2} \left(\sum_{i=1}^{m} (y^{(i)} - \mu) \right) = 0; \;\; \frac{\partial L}{\partial \sigma^2} = -\frac{m}{2\sigma^2} + \frac{\sum_{i=1}^{m} (y^{(i)} - \mu)^2}{2(\sigma^2)^2} = 0$$

$$\Rightarrow \begin{cases} \mu_{ML} = \frac{1}{m} \sum_{i=1}^{m} y^{(i)} & \leftarrow \text{ sample mean!} \\ \sigma^2_{ML} = \frac{1}{m} \sum_{i=1}^{m} (y^{(i)} - \mu_{ML})^2 \end{cases}$$

Linear regression: revisit

Linear regression model:

$$y^{(i)} = \boldsymbol{\theta}^T \boldsymbol{x}^{(i)} + e^{(i)}$$

- $i = 1, \ldots, m$: index of data samples (row index),
- $\boldsymbol{x}^{(i)} = [1, x_1^{(i)}, \ldots, x_n^{(i)}]^T$ is a $(n+1) \times 1$ vector:
  - n: number of predictors (columns)
- $\boldsymbol{\theta}$ is the model parameter
- $e^{(i)}$ is the prediction difference

Assume

$$e^{(i)} \sim \mathcal{N}\left(0, \sigma^2\right)$$

- the prediction error is Gaussian distributed
- the mean of the error is 0
- the variance is σ^2, which needs to be estimated

Linear regression: revisit

$$e^{(i)} \sim \mathcal{N}\left(0, \sigma^2\right)$$

$$\Downarrow$$

$$y^{(i)} = \boldsymbol{\theta}^T \boldsymbol{x}^{(i)} + e^{(i)} \sim \mathcal{N}\left(\boldsymbol{\theta}^T \boldsymbol{x}^{(i)}, \sigma^2\right)$$

$$\Downarrow$$

$$p(y^{(i)}|\boldsymbol{\theta}, \sigma^2, \boldsymbol{x}^{(i)}) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(y^{(i)} - \boldsymbol{\theta}^T \boldsymbol{x}^{(i)})^2}{2\sigma^2}\right)$$

$$\Downarrow$$

$$\mathcal{L}(\boldsymbol{\theta}, \sigma^2) = \log p(\mathcal{D}|\boldsymbol{\theta}, \sigma^2) = \log p(\boldsymbol{y}|\boldsymbol{\theta}, \sigma^2, \boldsymbol{X}) = \log \prod_{i=1}^{m} p(y^{(i)}; \boldsymbol{\theta}, \boldsymbol{x}^{(i)})$$

Linear regression: maximum likelihood estimation

The log likelihood function is:

$$\begin{aligned}
\mathcal{L}(\boldsymbol{\theta}, \sigma^2) &= \log \prod_{i=1}^{m} p(y^{(i)}; \boldsymbol{\theta}, \boldsymbol{x}^{(i)}) \\
&= \sum_{i=1}^{m} \log p(y^{(i)}; \boldsymbol{\theta}, \boldsymbol{x}^{(i)}) \\
&= -\frac{m}{2} \log(2\pi\sigma^2) - \frac{1}{2\sigma^2} \sum_{i=1}^{m} (y^{(i)} - \boldsymbol{\theta}^T \boldsymbol{x}^{(i)})^2
\end{aligned}$$

Maximising $\mathcal{L}$ w.r.t $\boldsymbol{\theta}$ is the same as minimising loss function

$$L(\boldsymbol{\theta}) = \sum_{i=1}^{m} (y^{(i)} - \boldsymbol{\theta}^T \boldsymbol{x}^{(i)})^2$$

$$\Rightarrow \boldsymbol{\theta}_{ML} = \boldsymbol{\theta}_{LS}$$

Logistic regression

Let's consider binary classification $y^{(i)} \in \{1, 0\}$, assume Bernoulli likelihood

$$P(y^{(i)} = 1) = \sigma\left(\boldsymbol{\theta}^T \boldsymbol{x}^{(i)}\right)$$

- $i = 1, \ldots, m$: index of data samples (row index)
- $\boldsymbol{\theta}^T \boldsymbol{x}^{(i)} = \theta_0 + \theta_1 x_1^{(i)} + \ldots + \theta_n x_n^{(i)} \in R$
- $\sigma(x) \in [0, 1]$
- $\boldsymbol{\theta}$ is the model parameter

The log likelihood function is

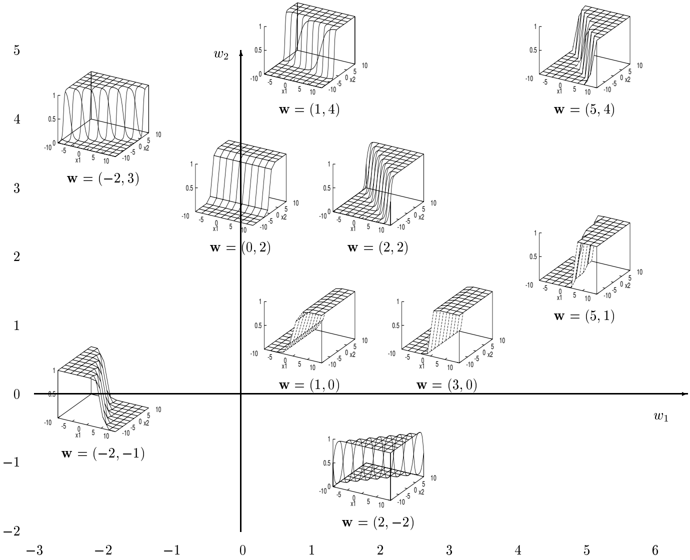
$$\mathcal{L}(\boldsymbol{\theta}) = \underbrace{\log \prod_{i=1}^{m} \sigma^{y^{(i)}} (1 - \sigma)^{1 - y^{(i)}}}_{\text{the same as Bernoulli model with } \theta}$$

- replace single parameter $\sigma(\beta)$ with $\sigma(\boldsymbol{\theta}^T \boldsymbol{x}^{(i)})$
- β serves the same purpose as θ_0: the intercept (cf. page 22)

Logistic regression: geometric view

$$\sigma(\boldsymbol{\theta}^T \boldsymbol{x})$$

- $\boldsymbol{\theta}^T \boldsymbol{x}$ is a hyperplane
- $\sigma(\boldsymbol{\theta}^T \boldsymbol{x})$ squeeze the plane between $(0, 1)$
- $\boldsymbol{\theta}$ determines the direction of surface facing
- $||\boldsymbol{\theta}||_2^2$ determines the steepness



[1]

[1] Information theory, inference and learning algorithms, David MacKay

Summary

Maximum likelihood estimation

- gives rise to squared error loss function for regression
  - sample mean is the simplest kind of linear regression where $x^{(i)} = 1$ for all $i = 1, \dots, m$
- gives rise to logistic error (cross-entropy) for classification
  - relative frequency is the simpliest kind of logistic regression where $x^{(i)} = 1$ for all $i = 1, \dots, m$

Suggested reading and exercises

Reading

- MLAPP 2.2, 2.3.1, 2.3.2, 2.4.1, 7.3, 8.1-8.3.1
- DL 3, 5.5, 5.7.1
- Information theory, inference and learning algorithms by David MacKay, chapter 2, 22.1, 39.1, 39.2

Exercise

- go through the equations
- write gradient descent for Gaussian model's likelihood function
  - generate some artifical data
  - workout the gradients
  - use the reparameterisation trick to treat $\sigma^2 > 0$
  - check whether they converge
- derive the gradient for logistic regression's log likelihood function

Next time

- Large number theory of MLE

$$\theta_{ML} \to \mathcal{N}(\theta, I_m^{-1}(\theta))$$

  - ML estimator can recover the true parameter θ
  - as data size $m \to \infty$
- gradient descent of logistic regression
- Newton's method for optimisation

*Random variable: formal aspects

Formally, r.v. X is a mapping from *sample space* Ω to *target space* $\mathcal{T}$

- Ω: all possible outcomes of an experiment
- $\mathcal{T}$: possible values X can take
- events $E \subseteq \Omega$
- $X(\omega) \in \mathcal{T}, \forall \omega \in \Omega$
- X^{-1} defines a partition of Ω

Example: toss a fair coin twice, r.v. X: # of heads turned up

- the *sample space* is $\Omega = \{HH, TT, HT, TH\}$
- *target space* is $T = \{0, 1, 2\}$
- $X(HH) = 2; X(HT) = X(TH) = 1; X(TT) = 0$
- $X^{-1} = \{E_0, E_1, E_2\}$ defines a parition of Ω:
  $E_0 = \{TT\}, E_1 = \{TH, HT\}, E_2 = \{HH\}$
  - disjoint: $E_0 \cap E_1 = E_0 \cap E_2 = E_1 \cap E_2 = \emptyset$
  - complete: $E_0 \cup E_1 \cup E_2 = \Omega$