

# Machine Learning

Supervised

Unsupervised

Active

Collaborative filtering

Machine Translation

out of many approaches in ML, this course will focus on probabilistic (Bayesian) methods

Textbook - Bishop 2006

Terminology

model

sample

likelihood, max likelihood

prior

posterior

MAP

predictive distribution

Model a coin flip

$$P(\text{Head}) = p$$

$$P(\text{Tail}) = 1 - p$$

assumption: no. of flips  $\rightarrow \infty$   
 $\Rightarrow$  consecutive flips are independent

Model explains how data is generated.

Sample (Sample Data)

H T H H T H T T

$x_1, x_2, x_3, \dots$   
 $i^{\text{th}}$  coin flip  $x_i$

$$x_i = \begin{cases} 1 & \text{Head} \\ 0 & \text{Tail} \end{cases}$$

bernoulli variable

$$P(\text{Head}) = P(x_i = 1) = p$$

Scenario 1      200 H      300 T

Scenario 2      2 H      3 T

Scenario 3      15 H      0 T

$$\text{likelihood} = P(\text{data} | \text{model})$$

H T H H T

$$p(1-p) p p (1-p)$$
$$p^3 (1-p)$$

if data  $x_1, x_2, x_3, \dots, x_n$

$$P(x_i) = p^{x_i} (1-p)^{1-x_i}$$

$$= \begin{cases} p & x_i = 1 \\ 1-p & x_i = 0 \end{cases}$$

$$\text{likelihood} = L = \prod_{i=1}^n P(x_i)$$

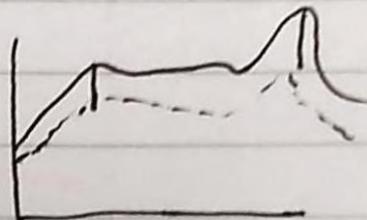
$$= \prod_{i=1}^n p^{x_i} (1-p)^{1-x_i}$$

$$= p^{\sum x_i} (1-p)^{n - \sum x_i}$$

max likelihood: pick the model that maximizes the value of likelihood.

$$L = p^{\sum x_i} (1-p)^{n - \sum x_i}$$

find  $p$  s.t.  $L$  is max.



To maximize  $f$

maximize  $\log f$  instead (monotonic transformation)

$$L = p^{\#H} (1-p)^{\#T}$$

Take log on both sides

$$\log L = \#H \cdot \log p + \#T \log(1-p)$$

Differentiate wrt  $p$ .

$$\frac{d \log L}{dp} = \frac{\#H}{p} + \frac{\#T}{1-p} (-1)$$

set derivative to 0.

$$\frac{\#H}{p} = \frac{\#T}{1-p}$$

$$\frac{\#H}{1-p} = \frac{\#T}{p}$$

$$\#H(1-p) = p \cdot \#T$$

$$\#H - \#H p = p \cdot \#T$$

$$\#H = p(\#H + \#T)$$

$$p = \frac{\#H}{\#H + \#T} = \frac{\#H}{N}$$

max. likelihood estimate of  $p$

$$\hat{p} = \frac{\#H}{N}$$

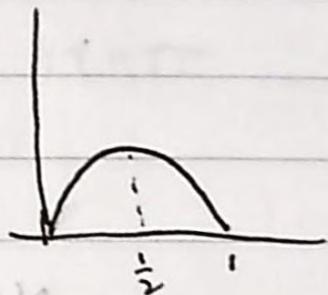
prior = distribution over possible models.

distribution in game over p. choices

choice of prior should reflect our belief / knowledge about the problem.

Choose  $p, C(p) \sim C p^2 (1-p)^2$

arbitrarily



$$\int_0^1 C p^2 (1-p)^2 dp = 1$$

$$C \int_0^1 p^2 (1-p)^2 dp = 1$$

$$C \int_0^1 (p^2 + p^4 - 2p^3) dp = 1$$

$$C \left[ \frac{p^3}{3} + \frac{p^5}{5} - 2 \frac{p^4}{4} \right]_0^1 = 1$$

$$C = 30$$

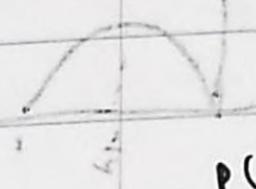
Posterior = distribution over a model - that reflects our belief on probability of models, after having seen data.

$$P(A|B) = \frac{P(B|A) P(A)}{P(B)}$$

↑ Bayes theorem  
↑ model data  
↑ P(B)

$$P(A|B) = P(A) P(B|A)$$

$$\Rightarrow P(B) P(A|B)$$



$$P(\text{model} | \text{data}) = \frac{\overset{\text{prior}}{P(\text{model})} \overset{\text{likelihood}}{P(\text{data} | \text{model})}}{P(\text{data})}$$

$$\propto P(\text{model}) P(\text{data} | \text{model})$$

$$\propto \text{prior} \times \text{likelihood}$$

here,

$$P(\text{model} | \text{data}) \propto 30p^2(1-p)^2 p^n(1-p)^T$$

$$\propto p^{n+2} (1-p)^{T+2}$$

$$P(\text{Data}) = A \int_0^1 30 p^2 (1-p)^2 p^{200} (1-p)^{200} dp$$

$\uparrow$  All possible ways to generate  $\uparrow$  for each test

2<sup>nd</sup> possible prior (discrete)

$P_i$	Head		Data
$\frac{1}{2}$	0.9		HTHTT
$\frac{1}{4}$	0.05		
$\frac{3}{4}$	0.05		

$$P(\text{Data}) = 0.9 \binom{5}{2} \left(\frac{1}{2}\right)^5 + 0.05 \binom{5}{1} \left(\frac{1}{4}\right) \left(\frac{3}{4}\right)^4 + 0.05 \binom{5}{4} \left(\frac{3}{4}\right)^4 \left(\frac{1}{4}\right)$$

$p = \frac{1}{2}$                        $p = \frac{1}{4}$                        $p = \frac{3}{4}$

next flip  
Data H T H T H ...

Data H H H H H ...

(next flip)

Prior - distribution over model which expresses our belief (before seeing data) about what are likely models.

choosing arbitrary prior  $Pr(P) = 30p^2(1-p)^2$

How to predict without data?

Predicting with data

$$P(\text{model} | \text{Data}) = \frac{P(\text{Data} | \text{model}) P(\text{Model})}{P(\text{Data})}$$
$$\propto P(\text{Data} | \text{model}) P(\text{model})$$

$$\text{Prior} \propto p^2(1-p)^2$$

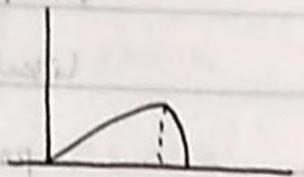
$$\text{Likelihood} = p^3(1-p)^2$$

$$\text{prior} \times \text{likelihood} \propto 15p^5(1-p)^4$$

Situation - H T H T H

NOTE: If we know the functional form of a distribution then we can calculate its normalizing constant.

$$\text{Posterior} = C_2 p^5 (1-p)^4$$



Maximum A Posteriori (MAP): Pick the model ( $\theta$ ) which maximizes the posterior.

$$\text{Posterior} = C_2 p^5 (1-p)^4$$

$$\begin{aligned} \log \text{posterior} &= \log C_2 + \log p^5 + \log (1-p)^4 \\ &= \log C_2 + 5 \log p + 4 \log (1-p) \end{aligned}$$

Differentiate wrt  $p$  on both sides

$$\frac{d}{dp} \log \text{posterior} = 0 + \frac{5}{p} + \frac{4}{1-p}$$

set derivative to zero.

$$\frac{5}{p} + \frac{4}{1-p} = 0$$

$$5(1-p) = 4p$$

$$\frac{5}{9} = p$$

vis  $\frac{3}{5}$  from max likelihood

situation HHHHH

$$\text{prior } p^2(1-p)^2$$

$$\text{likelihood } = p^5$$

$$\text{posterior} = C_3 p^7(1-p)^2$$

log & d/dp

$$\frac{d}{dp} \log \text{posterior} = \frac{d}{dp} \log C_3 + 7 \frac{d}{dp} \log p + 2 \frac{d}{dp} \log (1-p)$$

$$= 0 + \frac{7}{p} + \frac{2}{1-p}(-1)$$

set derivative to zero.

$$\frac{7}{p} = \frac{2}{1-p}$$

$$7(1-p) = 2p$$

$$\frac{7}{9} = \hat{p}$$

vis  $\hat{p} = \frac{7}{9}$  from  
maximum  
likelihood

Given my current belief:  $\Pr(p)$

what is the prob. that next coin is H.

Ex. current belief  $\Pr(p) = \begin{cases} 0.9 & p=0.2 \\ 0.1 & p=0.3 \end{cases}$

$$0.9 \times 0.2 + 0.1 \times 0.3 = 0.2$$

Predictive Distribution:

$$P(\text{next head} | \text{data}) =$$

$$\int_P \Pr(p | \text{Data}) P(\text{Next head} | p) dp$$

*posterior* *likelihood*

Coin Problem:

H Heads

$$\text{Prior} \propto p^2 (1-p)^2$$

T Tails.

$$\text{Posterior} \propto p^{H+2} (1-p)^{T+2}$$

$$\hat{P}_{\text{predictive}} = \int C p^{H+2} (1-p)^{T+2} p dp$$

Probability that  $\Pr(\text{next head}) = p$  given data.

prob. that next flip is head given prob head is  $p$ .

Conjugate prior : prior and posterior have the same type of dependence on the parameters.

(belong to same family of distributions)

Model - say how data was generated ; prior + dist. over model

Sample - subset of data

method of prediction - max. likelihood

max. a posteriori

predictive dist.

prior :

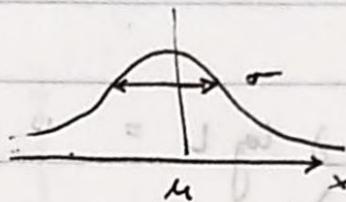
do not rule out options

as the amount of data increases, impact of prior goes down

prior  $\neq$  bias.

Normal Distribution.

$$f(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2\sigma^2}(x-\mu)^2}$$



precision  
 $\beta = \frac{1}{\sigma^2}$

$$f(x) = \frac{\beta}{\sqrt{2\pi}} e^{-\frac{\beta}{2}(x-\mu)^2}$$

Assume that each  $x_i$  is drawn from

$N(\mu, \frac{1}{\beta})$  and that different  $x_i$ 's are independent

Data: 10.3 5.1 12.6 11.1 2.5

Estimation: pick mean & precision.

$$L = \text{Likelihood} = P(\text{Data} | \text{model})$$

$$= p(x_1) \cdot p(x_2) \cdot p(x_3) \cdot p(x_4) \cdot p(x_5)$$

$$= \prod_i \frac{\beta}{\sqrt{2\pi}} e^{-\frac{\beta}{2}(x_i - \mu)^2}$$

$$\log L = \sum \log \left( \frac{\beta}{\sqrt{2\pi}} e^{-\frac{\beta}{2}(x_i - \mu)^2} \right)$$

$$= \sum \left[ -\frac{1}{2} \log 2\pi + \frac{1}{2} \log \beta - \frac{\beta}{2} (x_i - \mu)^2 \right]$$

$$= \frac{N}{2} \log 2\pi + \frac{N}{2} \log \beta - \frac{\beta}{2} \sum (x_i - \mu)^2$$

$$\frac{\partial \log L}{\partial \mu} = 0 + 0 - \beta \sum_i z(x_i - \mu) (-1) = 0$$

$$\sum_i x_i = \sum_i \mu = N\mu$$

$$\hat{\mu}_{ML} = \frac{\sum x_i}{N} \quad \left\| \begin{array}{l} \text{max likelihood} \\ \text{estimator} \end{array} \right.$$

Estimator is a function of random variable(s)

$\Rightarrow$  it is a random variable

- ① unbiased  $E[\hat{\mu}] = \mu$   
 ② Prefer low variance
- } properties of good estimator

$$\frac{\partial \log L}{\partial \beta} = \frac{N}{2} \frac{1}{\beta} - \frac{1}{2} \sum (x_i - \mu)^2 = 0$$

$$\frac{1}{\beta_{ML}} = \frac{1}{N} \sum (x_i - \mu)^2 \quad \leftarrow \text{replace with } \hat{\mu}_{ML}$$

$$\frac{1}{\beta_{ML}} = \frac{1}{N} \sum (x_i - \mu)^2 \quad \leftarrow \text{biased estimator}$$

$$E(\hat{\mu}_{ML}) = \frac{N\mu}{N}$$

$$\frac{1}{\beta} = \frac{1}{N-1} \sum (x_i - \hat{\mu}_{ML})^2 \quad \leftarrow \text{corrected unbiased}$$

$$E[\hat{\mu}_n] = E\left[\frac{1}{n} \sum x_i\right]$$

$$= \frac{1}{n} \sum E[x_i]$$

$$= \frac{1}{n} \cdot \sum \mu$$

$$= \frac{1}{n} \cdot n \mu = \mu$$

∴ it is an unbiased estimator

# Machine Learning

- ① A model explains how data is generated
- ② We estimate the concrete model (parameters) using data

① Maximum Likelihood - non bayesian

② Prior + data  $\rightarrow$  posterior  $\rightarrow$  MAP

all information  $\rightarrow$  Predictive distribution } bayesian

prior protects against overfitting

coin model :  $p$

$$L = p^{\#H} (1-p)^{\#T}$$

$$\text{prior } \beta(a, b) = \frac{p^{a-1} (1-p)^{b-1}}{\int_0^1 p^{a-1} (1-p)^{b-1} dp} = \frac{\Gamma(a)\Gamma(b)}{\Gamma(a+b)}$$

Used  $\beta(3, 3)$  in example

$$\text{posterior} \propto \text{prior} \times L \propto p^{\#H + a - 1} (1-p)^{\#T + b - 1}$$

$$\text{dist.} \propto p^2 (1-p)^2$$

must be

$$Pr(p) = \frac{\Gamma(3+3)}{\Gamma(3)\Gamma(3)} p^2 (1-p)^2 = \frac{6!}{3!3!} p^2 (1-p)^2$$

$$= \frac{720}{36} p^2 (1-p)^2$$

$$= 20 p^2 (1-p)^2$$

$$\int p^3 (1-p)^7 dp \times \frac{\Gamma(4+8)}{\Gamma(4)\Gamma(8)} = \frac{\Gamma(6)\Gamma(8)}{\Gamma(4+8)}$$

$$\downarrow$$

$$\frac{\Gamma(4)\Gamma(8)}{\Gamma(4+8)} \int \beta(4,8) dp$$

$$\frac{4!7!}{12!}$$

Normal distribution

$$p(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2\sigma^2}(x-\mu)^2}$$

$$= \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2\sigma^2}x^2} e^{\frac{x\mu}{\sigma^2}} e^{-\frac{\mu^2}{2\sigma^2}}$$

$$\propto e^{\frac{2\mu x - x^2}{2\sigma^2}}$$

"completing the squares"

$$p(x) \propto e^{-16x^2 + 8x}$$

← normal distribution

$$\frac{2\mu x - x^2}{2\sigma^2} = -16x^2 + 8x$$

$$\frac{+1}{2\sigma^2} = +16 \quad \text{and} \quad \frac{\mu}{\sigma^2} = 8$$

$$8/32 = \frac{1}{4}$$

$$\sigma^2 = 32$$

$$\mu = 8 \times 32$$

Model 2: independent samples from Normal( $\mu, \frac{1}{\beta}$ )

$$L = \prod_i \sqrt{\frac{\beta}{2\pi}} e^{-\frac{\beta}{2}(x_i - \mu)^2}$$

$$\hat{\mu}_{ML} = \frac{\sum x_i}{N}$$

What would a conjugate prior for  $\mu$  look like?

prior  $\times$  L  $\propto$  posterior

$$L = \prod_i \sqrt{\frac{\beta}{2\pi}} e^{-\frac{\beta}{2}(x_i - \mu)^2}$$

$$= \prod_i \sqrt{\frac{\beta}{2\pi}} e^{-\frac{\beta}{2} x_i^2} e^{-\beta \mu \sum x_i} e^{\frac{\beta}{2} \mu^2 \sum 1}$$

exponential quadratic  $\mu$

Prior  $P(\mu | \mu_0, \beta_0) = \sqrt{\frac{\beta_0}{2\pi}} e^{-\frac{\beta_0}{2}(\mu - \mu_0)^2}$

$$= \sqrt{\frac{\beta_0}{2\pi}} e^{-\frac{\beta_0}{2}\mu^2 + \beta_0 \mu \mu_0 - \frac{\beta_0 \mu_0^2}{2}}$$

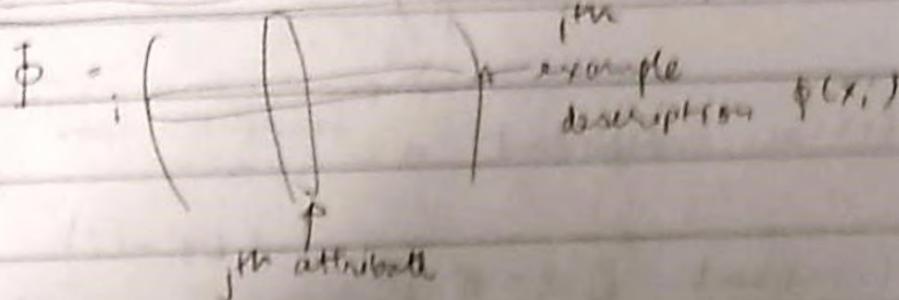
$$= \sqrt{\frac{\beta_0}{2\pi}} e^{-\frac{\beta_0 \mu_0^2}{2}} \left( e^{-\frac{\beta_0}{2}\mu^2 + \beta_0 \mu \mu_0} \right)$$

What are mean & precisions ( $= \frac{1}{\sigma^2}$ ) for posterior?  
 (Todo)

House

	Age	Size	Condition	Centrality	Price
House 1	2	1000	10	-1000	10
House 2	100	500	8	1	15
					?

output



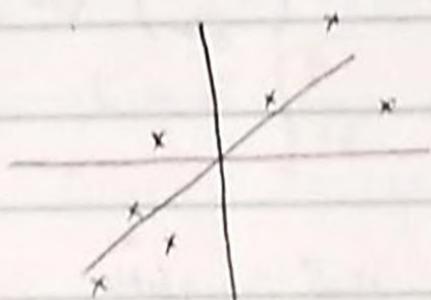
$t =$  vector of values we want to predict,  
 one for each example.

NOTE: All vectors are column vectors

$x_i =$   $i$ th example

$\phi(x_i) =$  representation of  $i$ th example

## Linear regression



$x_i$ 's are arbitrary

$$y_i = \bar{w}^T \phi(x_i)$$

$$y_i = \sum_j w_j \phi_j(x_i)$$

True

$$t_i \sim N(y_i, \frac{1}{\beta})$$

observed

$t_i$ 's are independent of each other  
 assume variance of all examples is same.

$$\text{Likelihood } L = \prod_i \frac{\beta}{\sqrt{2\pi}} e^{-\frac{\beta}{2}(y_i - t_i)^2}$$

$$L = \prod_i \frac{\beta}{\sqrt{2\pi}} e^{-\frac{\beta}{2}(w^T \phi(x_i) - t_i)^2}$$

$$\log L = \frac{N}{2} \log \frac{\beta}{2\pi} - \frac{\beta}{2} \sum_{i=1}^N (w^T \phi(x_i) - t_i)^2$$

Max. likelihood for  $w$

$$\max \log L \text{ is same as } \max - \sum_{i=1}^N (w^T \phi(x_i) - t_i)^2$$

$$\text{or } \min \sum_{i=1}^N (w^T \phi(x_i) - t_i)^2$$

A matrix vector product is the  
 Linear combination of the column vectors of  
 matrix.

$$\min \sum (w^T \phi(x_i) - t_i)^2 \quad \text{Least Squares.}$$

$$\begin{bmatrix} | & | & | \\ A & & \\ | & | & | \\ a_i & & \end{bmatrix} \begin{bmatrix} | \\ b \\ | \end{bmatrix} = \begin{bmatrix} | & | & | \\ \sum a_i b_i & & \\ | & | & | \end{bmatrix}$$

$$\begin{pmatrix} a & b & c \\ d & e & f \\ g & h & i \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix} = \begin{pmatrix} a\alpha \\ d\alpha \\ h\alpha \end{pmatrix} + \begin{pmatrix} b\beta \\ e\beta \\ i\beta \end{pmatrix} + \begin{pmatrix} c\gamma \\ f\gamma \\ j\gamma \end{pmatrix}$$

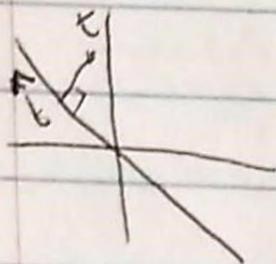
$$\left( \begin{array}{l} \leftarrow \\ \leftarrow \end{array} \right) \begin{array}{l} w^T \phi(x_i) \\ = \phi(x_i)^T w \end{array}$$

$$\begin{aligned} \min \sum (w^T \phi(x_i) - t_i)^2 \\ \min \| \Phi w - t \|^2 \end{aligned}$$

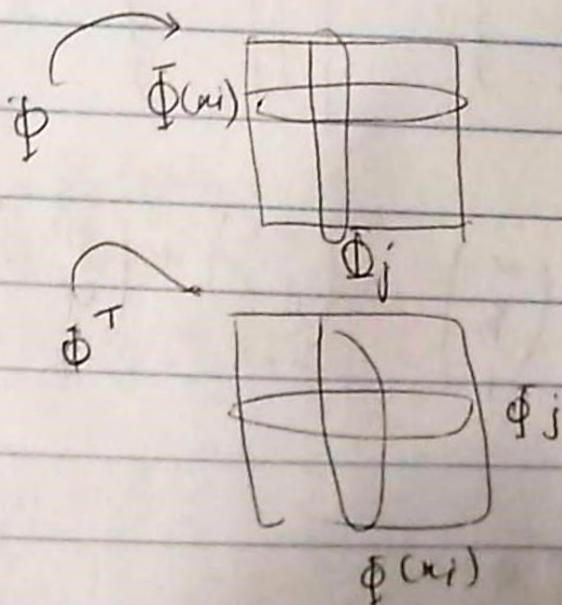
Find  $\hat{w}$  such that  $\| \hat{t} - t \|^2$  is

minimized where  $\hat{t} = \Phi \hat{w}$  prediction parameter

$\hat{t}$  is a linear combination of columns of  $\Phi$



~~$t$~~  +  $\hat{t}$  is perpendicular to columns of  $\Phi$



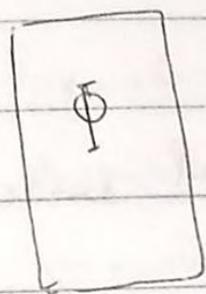
$$\Phi^T (t - \hat{t}) = 0$$

$$\Phi^T (t - \Phi \hat{w}) = 0$$

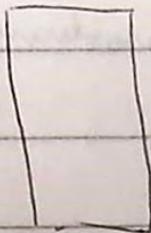
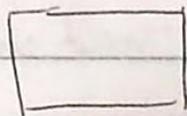
$$\cancel{\Phi^T t} = \Phi^T \Phi \hat{w}$$

$$\Phi^T t = \Phi^T \Phi \hat{w}$$

$$\hat{w} = (\Phi^T \Phi)^{-1} \Phi^T t$$



$$\Phi^T \Phi$$



=



correlation  
b/w elements

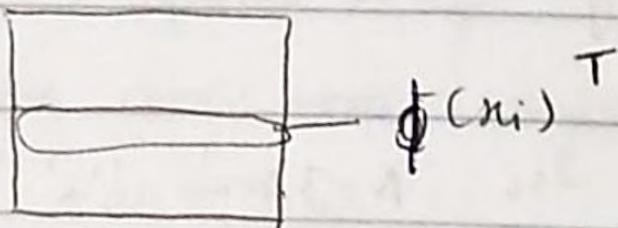
must be invertible.

For any  $A$

$A^T A$  has an inverse

iff. col of  $A$  are independent

# Machine Learning.



$x_i$  example

$\phi(x_i)$  column vector, represents the example

true hidden value

$$y_i = w^T \phi(x_i)$$

observe

$$t_i \sim N(y_i, \frac{1}{\beta})$$

Every example is drawn independently

$$L = \prod_i \frac{\beta}{\sqrt{2\pi}} e^{-\frac{\beta}{2} (\sum w^T \phi(x) - t_i)^2}$$

⋮

Maximum likelihood :

$$\text{Max } \frac{N}{2} \log \beta - \frac{\beta}{2} \sum_{i=1}^N (w^T \phi(x_i) - t_i)^2$$

max L for w

is same as

$$\min_i \sum (w^T \phi(x_i) - t_i)^2$$
$$\min \| \Phi w - t \|^2$$

Soln #1 Geometric

$$\hat{w}_{ML} = (\bar{\Phi}^T \Phi)^{-1} \bar{\Phi}^T t$$

Soln #2 Using Derivatives

$$\min \sum (w^T \phi(x_i) - t_i)^2$$

$$w^T \phi(x_i) = \sum_{k=1}^K w_k \phi_{ik}(x_k)$$

$$\frac{\partial}{\partial w} \sum_i (w^T \phi(x_i) - t_i)^2 = \sum_i 2(w^T \phi(x_i) - t_i) \phi(x_i)$$

= let A

$$\frac{\partial A}{\partial w} = \begin{pmatrix} \frac{\partial A}{\partial w_1} \\ \frac{\partial A}{\partial w_2} \\ \vdots \\ \frac{\partial A}{\partial w_K} \end{pmatrix} = 2 \sum (w^T \phi(x_i) - t_i) \phi(x_i) = \bar{0} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

what is the vector whose entries are  $\phi_k(x_i)$ :  $\begin{pmatrix} \phi_1(x_i) \\ \vdots \\ \phi_k(x_i) \end{pmatrix}$

$\phi(x_i)$

$$\sum (w^T \phi(x_i)) \phi(x_i) = \sum t_i \phi(x_i)$$

$$\phi^T \phi w \quad \phi^T t$$

vector whose entries are  $\sum w^T \phi(x_i) = \sum \phi(x_i)^T w$

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$$a^T b = \sum_k a_k b_k$$

$$\Rightarrow \Phi^T \Phi w = \Phi^T t$$

$$\Rightarrow \hat{w}_{ML} = (\Phi^T \Phi)^T \Phi^T t$$

Soln #3 Vector derivatives

$$\text{Min } \|\Phi w - t\|^2$$

$$\|\Phi w - t\|^2 = (\Phi w - t)^T (\Phi w - t) \quad \text{scalar}$$

$$= w^T \Phi^T \Phi w - w^T \Phi^T t - t^T \Phi w + t^T t$$

$$= w^T \Phi^T \Phi w - 2w^T \Phi^T t + t^T t$$

(Assuming  $A$  is symmetric)

$$\left\| \frac{\partial w^T A w}{\partial w} = 2Aw \right.$$

$$\left\| \frac{\partial w^T b}{\partial w} = b \right.$$

$$\frac{\partial \|\Phi w - t\|^2}{\partial w} = 2\Phi^T \Phi w - 2\Phi^T t = 0$$

$$\Rightarrow \Phi^T \Phi w = \Phi^T t$$

$$\Rightarrow \hat{w} = (\Phi^T \Phi)^{-1} \Phi^T t$$

Regularization : trick to restrict  $W$  from getting arbitrary values & therefore overfitting the data.

New objective :  $\min \|\Phi W - t\|^2 + \lambda \|W\|^2$

regularization parameter

penalty for increase in norm of  $W$ .

$$\lambda \|W\|^2 = \lambda W^T W$$

$$\frac{d \lambda \|W\|^2}{dW} = 2\lambda W$$

$$\therefore \frac{d \|\Phi W - t\|^2 + \lambda \|W\|^2}{dW}$$

$$= 2\Phi^T \Phi W - 2\Phi^T t + 2\lambda W$$

$$\frac{d \text{objective}}{dW} = 0$$

$$\Phi^T \Phi W + \lambda W - 2\Phi^T t = 0$$

$$\Phi^T \Phi W + \lambda I W - 2\Phi^T t = 0$$

$$(\Phi^T \Phi + \lambda I) W = \Phi^T t$$

$$\hat{W}_R = (\Phi^T \Phi + \lambda I)^{-1} \Phi^T t$$

$$\log L = -\frac{N}{2} \log 2\pi + \frac{N}{2} \log \beta - \frac{\beta}{2} \mathbf{1}^T \Phi \mathbf{W} - \mathbf{t} \mathbf{1}^T$$

compute MLE for  $\beta$

$$\frac{d \log L}{d \beta} = \frac{N}{2\beta} - \frac{1}{2} \mathbf{1}^T \Phi \mathbf{W} - \mathbf{t} \mathbf{1}^T$$

$$\sigma^2 = \frac{1}{\beta} = \frac{1}{N} \mathbf{1}^T \Phi \mathbf{W} - \mathbf{t} \mathbf{1}^T$$

conjugate prior for  $\mathbf{W}$ ?

Prior  $\times$  Likelihood  $\rightarrow$  posterior

$$L \propto \pi \left( \frac{\beta}{2\pi} \right)^{\frac{1}{2}} e^{-\frac{\beta}{2} (\mathbf{w}^T \Phi(\mathbf{x}_i) - t)^2}$$

$$\propto e^{-\frac{\beta}{2} \mathbf{1}^T \Phi \mathbf{W} - \mathbf{t} \mathbf{1}^T}$$

$$\propto e^{-\frac{\beta}{2} \mathbf{1}^T \Phi \mathbf{W} \mathbf{1}^T} e^{\frac{\beta}{2} \mathbf{1}^T \Phi \mathbf{W} \mathbf{1}^T \mathbf{t}} e^{-\frac{\beta}{2} \mathbf{t}^T \mathbf{t}}$$

$$\propto e^{-\frac{\beta}{2} \mathbf{W}^T \Phi^T \mathbf{1} \mathbf{1}^T \mathbf{W}} e^{\frac{\beta}{2} \mathbf{1}^T \Phi^T \mathbf{t}} e^{-\frac{\beta}{2} \mathbf{t}^T \mathbf{t}}$$

$$\propto e^{-\frac{\beta}{2} \mathbf{W}^T \Phi^T \mathbf{1} \mathbf{1}^T \mathbf{W}} e^{\frac{\beta}{2} \mathbf{1}^T \Phi^T \mathbf{t}} \quad \text{ignore}$$

$e^{-\frac{\beta}{2} \mathbf{W}^T \Phi^T \mathbf{1} \mathbf{1}^T \mathbf{W}}$  is quadratic  
 $e^{\frac{\beta}{2} \mathbf{1}^T \Phi^T \mathbf{t}}$  is linear

~~Note~~ Multivariate Gaussian Distribution

↳ looks like a gaussian in  $n$ -dimensions

\* Read Linear Algebra review

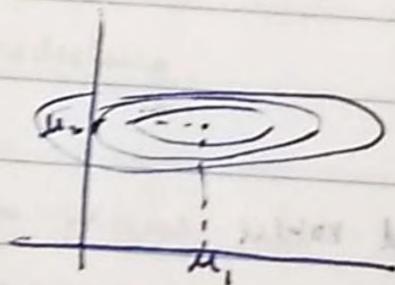
# Machine Learning

Independent  $x_1, x_2$

$$x_1 \sim N(\mu_1, \sigma_1^2)$$

$$x_2 \sim N(\mu_2, \sigma_2^2)$$

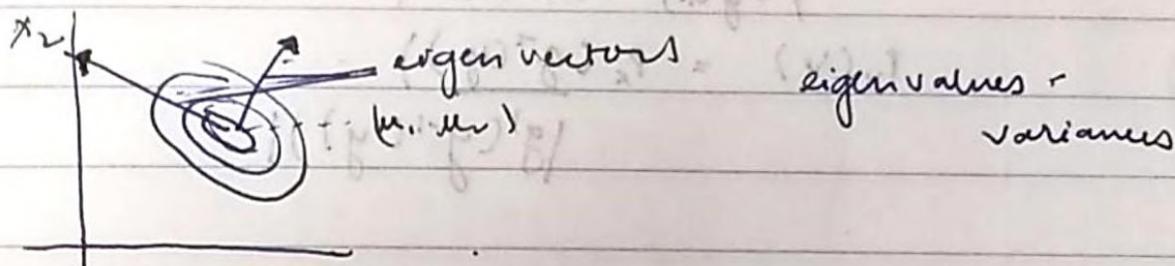
$$p(x_1, x_2) = \frac{1}{\sqrt{2\pi}\sigma_1} e^{-\frac{1}{2\sigma_1^2}(x_1 - \mu_1)^2} \times \frac{1}{\sqrt{2\pi}\sigma_2} e^{-\frac{1}{2\sigma_2^2}(x_2 - \mu_2)^2}$$



$$p(x_1, x_2) = \left(\frac{1}{\sqrt{2\pi}}\right)^2 \frac{1}{\sigma_1 \sigma_2} e^{-\frac{1}{2} \frac{(x_1 - \mu_1)^2}{\sigma_1^2} - \frac{1}{2} \frac{(x_2 - \mu_2)^2}{\sigma_2^2}}$$
$$= \left(\frac{1}{\sqrt{2\pi}}\right)^2 \frac{1}{\sigma_1 \sigma_2} e^{-\frac{1}{2} \begin{pmatrix} x_1 - \mu_1 & x_2 - \mu_2 \end{pmatrix} \begin{pmatrix} \frac{1}{\sigma_1^2} & 0 \\ 0 & \frac{1}{\sigma_2^2} \end{pmatrix} \begin{pmatrix} x_1 - \mu_1 \\ x_2 - \mu_2 \end{pmatrix}}$$

$$P(x) = \left(\frac{1}{2\pi}\right)^{m/2} \frac{1}{\sigma_1 \dots \sigma_m} e^{-\frac{1}{2} (x-\mu)^T \Sigma^{-1} (x-\mu)}$$

Direction and width of ellipse is determined by the eigen decomposition of  $\Sigma$



$$\Sigma = V \Lambda V^T$$

$$y = V^T (x - \mu)$$

①  $X \in \{0, 1\}$  coin

$$Y = 3 + X$$

$$P(X=1) = 0.7$$

$$P(X=0) = 0.3$$

$$Y \in \{3, 4\}$$

$$P(Y=4) = 0.7$$

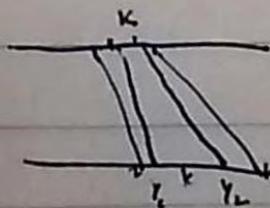
$$P(Y=3) = 0.3$$

②  $X \in [1, 2]$   $Y = 2X$

$$P_x(x) = 1$$

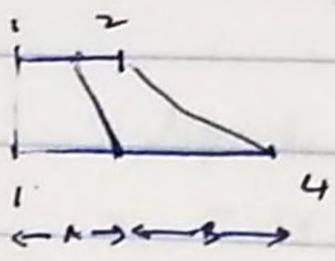
$$\int_0^1 1 dx = x \Big|_0^1 = 1$$

$P_x(x)$



$$y_1 = x_1 \quad y_2 = x_2$$

③  $X \in [1, 2]$   $P_X(x) = 1$   $Y = X^2$



$$\sum_A P_X(x) > \sum_B P_Y(y)$$

$Y = g(X)$  one one & invertible.

$$P_Y(y) = P_X(g^{-1}(y)) |g'(g^{-1}(y))|$$

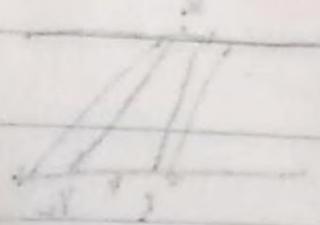
change of variable for variables in 1D

④  $P_Y(y) = \frac{P_X(x)}{g'(g^{-1}(y))} = \frac{1}{2}$

slope of transformation at its image at  $y$ .

⑤  $P_Y(y) = \frac{1}{2\sqrt{y}}$

$$\begin{aligned}
 Y = g(x) &= x^2 \\
 g'(x) &= 2x \\
 g^{-1}(y) &= \sqrt{y} \\
 g'(g^{-1}(y)) &= 2\sqrt{y}
 \end{aligned}$$



$$\textcircled{4} \quad x \in [1, 2]$$

$$y = g(x) = x^2$$

$$y \in [1, 4]$$

$$p_y(y) = \text{uniform } [1, 4]$$

$$= \frac{1}{3}$$

$$p_x(x) = ?$$

$$x = f(y) = \sqrt{y}$$

$$p_x(x) = \frac{p_y(f^{-1}(x))}{|f'(f^{-1}(x))|}$$

$$= \frac{p_y(x^2)}{|f'(x^2)|}$$

$$= \frac{p_y(x^2)}{\left| \frac{-1}{2x} \right|}$$

$$= \frac{1/3}{\frac{1}{2|x|}}$$

$$= \frac{1/3}{\frac{1}{2|x|}}$$

$$= \frac{2}{3} |x| = \frac{2x}{3}$$

$$f^{-1}(x) = x^2$$

$$f'(y) = \frac{-1}{2\sqrt{y}}$$

$$f'(f^{-1}(x))$$

$$= \frac{-1}{2\sqrt{x^2}}$$

$$= \frac{-1}{2x}$$

$$P_x(g^{-1}(y)) \cdot |J_{g^{-1}}(y)| = P_x(g^{-1}(y)) \cdot |J_{g^{-1}}(g^{-1}(y))|$$

$$P_x(g^{-1}(y)) (g^{-1})'(y) = \frac{P_x(g^{-1}(y))}{|g'(g^{-1}(y))|}$$

Multivariate

$$y = g(x) \quad Y = g(x) \quad x \in \mathbb{R}^k \quad y \in \mathbb{R}^k$$

$$P_Y(Y) = \frac{P_x(g^{-1}(Y))}{|J_Y(g^{-1}(Y))|}$$

Jacobians

output

$$\begin{pmatrix} y_1 \\ \vdots \\ y_k \end{pmatrix}$$

input  $(x_1 \dots x_k)$

$$J = \begin{pmatrix} \frac{\partial y_1}{\partial x_1} & \dots & \frac{\partial y_k}{\partial x_1} \\ \frac{\partial y_1}{\partial x_2} & \dots & \frac{\partial y_k}{\partial x_2} \\ \vdots & \ddots & \vdots \\ \frac{\partial y_1}{\partial x_k} & \dots & \frac{\partial y_k}{\partial x_k} \end{pmatrix}$$

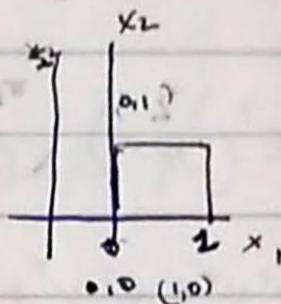
linear transform.

$$\textcircled{5} Y = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = \begin{pmatrix} 2 & 2 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = g(x)$$

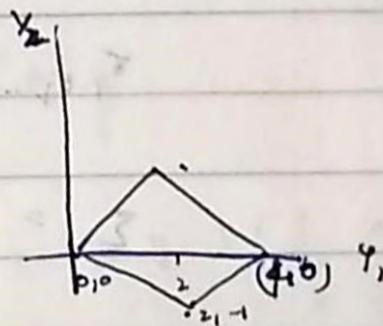
$$X \sim \text{Uniform} [0, 1]$$

$$P_X(X) = 1$$

$$P_Y(Y) = ?$$



$$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = g^{-1}(y) = \frac{1}{4} \begin{pmatrix} 1 & 2 \\ 1 & -2 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}$$



$$J = \begin{pmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_2}{\partial x_1} \\ \frac{\partial y_1}{\partial x_2} & \frac{\partial y_2}{\partial x_2} \end{pmatrix} = \begin{pmatrix} 2 & 2 \\ 1 & -1 \end{pmatrix} \quad \text{(Jacobian transform)}$$

$$\text{abs}(|J|) = |2 \cdot (-2) - 2 \cdot 1| = |-4 - 2| = 6$$

$$P_Y(Y) = \frac{P_X(g^{-1}(Y))}{|J(g^{-1}(Y))|} = \frac{1}{4}$$

is diagonal.

$$\Sigma = \begin{pmatrix} \sigma_1^2 & & & \\ & \sigma_2^2 & & \\ & & \dots & \\ & & & \sigma_n^2 \end{pmatrix}$$

$$|\Sigma| = \prod_{i=1}^m \sigma_i$$

$$\sigma_1 \sigma_2 \dots \sigma_m = |\Sigma|^{1/2}$$

$$\Sigma = V \Lambda V^T$$

Capital Lambda.

special linear transform

$$Y = V^T (X - \mu) = g(X)$$

$$X = g^{-1}(Y) = VY + \mu$$

orthonormal.  
 $V = (V^T)^{-1}$   
 or  $V^{-1} = V^T$

$$P_Y(y) = \frac{P_X(g^{-1}(y))}{|J|}$$

$$\Sigma = V \Lambda V^T$$

$$\Sigma^{-1} = V \Lambda^{-1} V^T$$

(see Linear Algebra notes)

$$p_x(x) = (2\pi)^{-m/2} \frac{1}{|\Sigma|^{1/2}} e^{-\frac{1}{2}(x-\mu)^T \Sigma^{-1}(x-\mu)}$$

$$p_x(g^{-1}(y)) = (2\pi)^{-m/2} |\Sigma|^{1/2} e^{-\frac{1}{2}(Vy + \mu - \mu)^T V \Lambda^{-1} V^T (Vy + \mu - \mu)}$$

$$p_x(g^{-1}(y)) = (2\pi)^{-m/2} |\Sigma|^{1/2} e^{-\frac{1}{2}(Vy) \Lambda^{-1} y^T V^T V \Lambda^{-1} V^T Vy}$$

$$\text{exponent} = -\frac{1}{2} y^T \Lambda^{-1} y$$

var of  $y$  is the  $\Lambda^{-1}$  eigenvalues of  $\Sigma \Rightarrow \frac{1}{2} (y_1, y_2) \begin{pmatrix} \frac{1}{\lambda_1} & 0 \\ 0 & \frac{1}{\lambda_2} \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}$

$$E[x] = \int p_x(x) x dx$$

$$z = x - \mu = Vy$$

$$dz = dx$$

$$E[x] = \int \left( \frac{1}{2\pi} \right)^{m/2} \frac{1}{|\Sigma|^{1/2}} e^{-\frac{1}{2}(x-\mu)^T \Sigma^{-1}(x-\mu)} dx$$

$$= \int e^{-\frac{1}{2} z^T z^{-1} z} (z + \mu) dz$$

symmetric  $\times$  asymmetric  $\Rightarrow 0$

(symmetric  $\times$  asymmetric  $\Rightarrow 0$ )

$$Z = \int \beta(u) g(u) du$$

$$u = -z$$

$$du = -dz$$

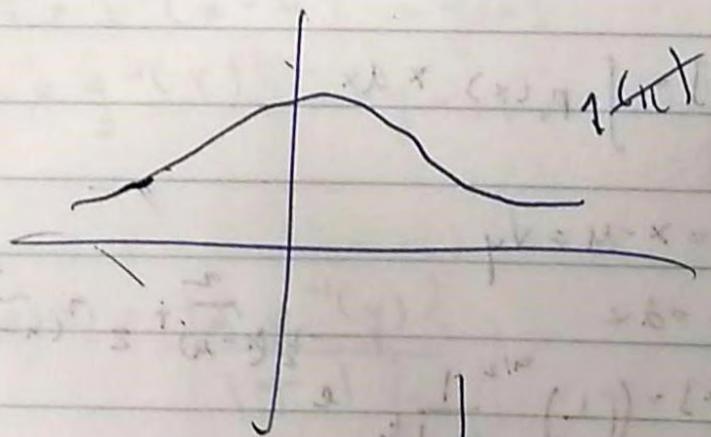
$$I = \int \beta(-z) g(-z) dz$$

$$= \int \beta(z) g(-z) dz$$

$$= \int \beta(z) g(z) dz$$

$$2I = \int \beta(u) g(u) du - \int \beta(u) g(u) du = 0$$

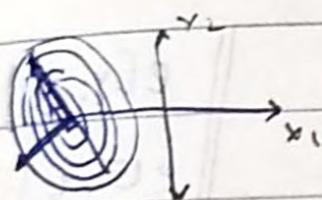
$$g(-u) = -g(u)$$



~~$$g(u) = -g(-u)$$~~

# Machine Learning.

$$P(x) = \frac{1}{(2\pi)^{d/2}} \frac{1}{|\Sigma|^{1/2}} e^{-\frac{1}{2} (x-\mu)^T \Sigma^{-1} (x-\mu)}$$



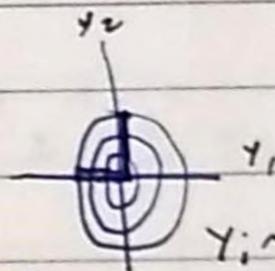
$$Y = V^T (x - \mu)$$

$$x = VY + \mu \Leftrightarrow$$

where

$$\Sigma = V \Lambda V^T$$

$$\Lambda = \begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_d \end{pmatrix}$$



$$Y_i \sim N(0, \lambda_i)$$

$Y_i$ 's are independent

mean  $\mathbb{E}(Y_i) = 0$

Variance  $\lambda_i$

$$E[x] = \int x \frac{1}{(2\pi)^{d/2}} \frac{1}{|\Sigma|^{1/2}} e^{-\frac{1}{2} (x-\mu)^T \Sigma^{-1} (x-\mu)} dx$$

let  $x - \mu = z \Rightarrow x = z + \mu$

$$= \int \frac{1}{(2\pi)^{d/2}} \frac{1}{|\Sigma|^{1/2}} e^{-\frac{1}{2} z^T \Sigma^{-1} z} (z + \mu) dz$$

$$= \int z P(z + \mu) dz + \int \mu P(z + \mu) dz$$

$$\because f(-z) = -f(z)$$

$$1 \times \mu$$

$$I = 0$$

$$\Rightarrow E(x) = \mu$$

$$\text{Cov}(x) = E[(x - \mu)(x - \mu)^T]$$

$$= E[zz^T] = E[VY(VY)^T]$$

$$= E[VY Y^T V^T]$$

$$= V E[YY^T] V^T$$

$$= V \begin{bmatrix} \lambda_1 & & \\ & \lambda_2 & \\ & & \ddots \\ & & & \lambda_p \end{bmatrix} V^T$$

$$= V \Lambda V^T = \Sigma$$

$$E[y_1 y_3] = ?$$

$$= E[y_1] E[y_3]$$

$$0 \quad 0$$

$$= 0$$

$$E[y_i^2] = E[y_i^2] = ?$$

$$\text{var} = \lambda_i = E[y_i^2] - (E[y_i])^2$$

$$E[y_i] = \lambda_i$$

diagonals

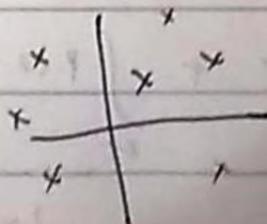
Exercise

independently

Data is generated by a multivariate normal

distribution. Estimate parameters  $\mu, \Sigma$

using Maximum likelihood



data: ~~z~~,  $z^{(1)}, z^{(2)}, \dots, z^{(N)}$

Likelihood =

$$\pi(z; \mu, \Sigma) = \prod_{i=1}^N \frac{1}{(2\pi)^{d/2} |\Sigma|^{1/2}} e^{-\frac{1}{2} (z^i - \mu)^T \Sigma^{-1} (z^i - \mu)}$$

$$\log L = \sum_i \left[ -\frac{d}{2} \log 2\pi - \frac{1}{2} \log |\Sigma| - \frac{1}{2} (z^i - \mu)^T \Sigma^{-1} (z^i - \mu) \right]$$

$$\frac{\partial a^T B a}{\partial a} = ? \quad \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \quad B \text{ symmetric}$$

$$a^T B a = \sum_i \sum_j a_i a_j B_{ij}$$

$$\frac{\partial (a^T B a)}{\partial a_k} = \sum_j a_j B_{kj} + \sum_i a_i B_{ik}$$

$$= \sum_j a_j B_{kj} + \sum_i a_i B_{ik}$$

$$= \sum_j B_{kj} a_j + \sum_i B_{ki} a_i$$

$$= 2 (\text{kth row of } B) a$$

$$\frac{\partial (a^T B a)}{\partial a_k} = 2 b_k^T a$$

$\frac{\partial}{\partial a_k}$

$b_k = k^{\text{th}} \text{ col of } B.$

$$\frac{\partial (a^T B a)}{\partial a} = 2 B a.$$

$\frac{\partial}{\partial a}$

$$\frac{\partial}{\partial \mu} \left( \frac{-1}{2} \sum_i (z^i - \mu)^T \Sigma^{-1} (z^i - \mu) \right) \quad \frac{\partial (a^T b)}{\partial a} = 2b$$

$$\frac{\partial}{\partial \mu} \left[ \frac{-1}{2} \left( \sum_i z^i \Sigma^{-1} z^i - 2\mu^T \Sigma^{-1} \sum_i z^i + \mu^T \Sigma^{-1} \mu \right) \right]$$

$$= \begin{matrix} 0 \\ 0 \end{matrix} - \sum_i z^i \Sigma^{-1} \sum_i z^i + \sum_i \Sigma^{-1} \mu = 0$$

$$-\sum_i z^i + \Sigma \mu = 0$$

$$\mu = \frac{\sum_i z^i}{N}$$

$$\frac{\partial \log |A|}{\partial A} = (A^{-1})^T$$

$$\frac{\partial (a^T A^{-1} b)}{\partial A} = -A^{-T} a b^T A^{-1}$$

$$\log L = \sum_i \underbrace{-\frac{1}{2} \log 2\pi}_{\text{constant}} - \frac{1}{2} \sum_i \log |\Sigma| - \frac{1}{2} \sum_i (z^i - \mu)^T \Sigma^{-1} (z^i - \mu)$$

$$\frac{\partial \log L}{\partial \Sigma} = \frac{1}{2} \cdot N (\Sigma^{-1})^T$$

~~constant~~

$$-\frac{1}{2} \sum_i (z^i - \mu) (\Sigma^{-1})^T (z^i - \mu) (\Sigma^{-1})^T$$

w

$$\frac{d \log L}{d \Sigma} = \frac{1}{2} (\Sigma^{-1})^T + \frac{1}{2} \Sigma (\Sigma^{-1})^T (Z^i - \mu) (Z^i - \mu)^T (\Sigma^{-1})^T = 0$$

multiply on right by  $\Sigma^T$

$$\frac{N}{2} \Sigma = \frac{1}{2} \Sigma (\Sigma^{-1})^T \sum_i (Z^i - \mu) (Z^i - \mu)^T$$

$$\Sigma^T = \frac{1}{N} \sum_i \underbrace{(Z^i - \mu) (Z^i - \mu)^T}_{\text{Symmetric}}$$

$$\Rightarrow \Sigma^T = \Sigma = \frac{1}{N} \sum_i (Z^i - \mu) (Z^i - \mu)^T$$

Develop derivative identities

ex. 1

$\frac{d}{dx} (AB)_{ij}$   
 ← matrices  
 ← scalar

$$C = AB$$

$$C_{ij} = \sum_k A_{ik} B_{kj}$$

$$\left( \begin{array}{c} i \\ \hline \end{array} \right) \left( \begin{array}{c} | \\ j \end{array} \right)$$

$$\frac{d}{dx} C_{ij} = \sum_k \frac{\partial A_{ik}}{\partial x} B_{kj} + \frac{\partial B_{kj}}{\partial x} A_{ik}$$

$$\left( \frac{\partial C}{\partial x} \right)_{ij} = \left( \frac{\partial A}{\partial x} B \right)_{ij} + \left( A \frac{\partial B}{\partial x} \right)_{ij}$$

$$\frac{\partial C}{\partial x} = \frac{\partial A}{\partial x} B + A \frac{\partial B}{\partial x} \quad (\text{matrix product rule})$$

$$0 = \frac{\partial}{\partial x} (A^{-1}) (A^{-1})^T (I) = \frac{\partial}{\partial x} (A^{-1} A^{-1}^T I)$$

$$\frac{\partial}{\partial x} (A^{-1} A) = \frac{\partial}{\partial x} (I)$$

$$= \frac{\partial A^{-1}}{\partial x} A + A^{-1} \frac{\partial A}{\partial x} = 0$$

$$\frac{\partial A^{-1}}{\partial x} = -A^{-1} \frac{\partial A}{\partial x} A^{-1}$$

ex. 3

$$\frac{\partial A^{-1}}{\partial x_{kl}} = -A^{-1} \frac{\partial A}{\partial x_{kl}} A^{-1}$$

$$= A^{-1} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} A^{-1}$$

$$\frac{\partial}{\partial d} \begin{pmatrix} a & b & c \\ d & e & f \\ g & h & i \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

ex. 4

$$\frac{\partial a^T A^{-1} b}{\partial x_{kl}} \quad \left. \begin{array}{l} \text{scalar} \\ \text{scalar} \end{array} \right\}$$

$$= a^T \frac{\partial A^{-1}}{\partial x_{kl}} b$$

$$= -a^T A^{-1} \begin{pmatrix} \dots & 0 \\ \dots & 1 & \dots \\ \dots & \dots & 0 \end{pmatrix} A^{-1} b$$

$$A^T \begin{pmatrix} \text{all zeros} \\ \text{except } k\text{-th} \\ \text{which is } 1 \end{pmatrix} = \begin{pmatrix} \text{zeros except} \\ \text{the } k\text{-th column} \end{pmatrix}$$

The diagram shows a column vector with a '1' in the \$k\$-th row and zeros elsewhere. To its right is a matrix with a single column highlighted, representing the \$k\$-th column of the matrix \$A\$.

$k$ th column of  $A^{-1}$  moves to  $k$ th column of result

$$\begin{pmatrix} 1 \\ \vdots \\ 0 \end{pmatrix} \begin{pmatrix} A^{-1} \end{pmatrix} = \begin{pmatrix} i \\ \vdots \\ 1 \end{pmatrix} A^{-1}_{ik} A^{-1}_{kj}$$

$\hat{A}$  = Matrix whose  $ij$  entry is  $A^{-1}_{ik} A^{-1}_{kj}$

$$\frac{\partial a^T A^{-1} b}{\partial A} = -a^T \hat{A} b$$

$$\frac{\partial A}{\partial A}$$

$$= -\sum_i \sum_j a_i b_j \hat{A}_{ij}$$

$$= -\sum_i \sum_j a_i b_j A^{-1}_{ik} A^{-1}_{kj}$$

$$\Rightarrow \frac{\partial a^T A^{-1} b}{\partial A} = \mathbf{0}$$

where entries in  $\hat{A}$  are

$$\frac{\partial (a^T A^{-1} b)}{\partial A} = -A^{-1T} a b^T A^{-1T}$$

Linear Regression

$$L = p(t|w)$$

$$t|w \sim N(\phi w, \frac{1}{\beta} \sigma^2)$$

$$t_i|w \sim N(w^T \phi(x_i), \frac{1}{\beta} \sigma^2) \quad t_i\text{'s are independent}$$

Normal prior for  $w$ :

$$w \sim N(m_0, S_0)$$

$m_0$  is the mean of the prior

= mean after seeing 0 observations

$S_0$  is the covariance matrix of prior

cov. after seeing 0 observations.

$$\rightarrow w|t \propto p(t|w) p(w)$$

$$\frac{1}{\sigma^2} (t - \phi w)^T \left(\frac{1}{\beta} \sigma^2\right)^{-1} (t - \phi w) \quad \frac{1}{2} (w - m_0)^T S_0^{-1} (w - m_0)$$

multiply & see what this looks like in terms of  $w$

# Machine Learning

## Linear Regression

$$t_i \sim N(w^T \phi(x_i), \frac{1}{\beta})$$

$t_i$  independent

$$t|w \sim N(\Phi w, \frac{1}{\beta} I)$$

$$\left\| \begin{bmatrix} \frac{1}{\beta} \\ \frac{1}{\beta} \\ \dots \end{bmatrix} \right\|$$

$$w \sim N(m_0, S_0) \quad (\text{gaussian prior})$$

$$x \sim N(\mu_x, S_x)$$

$$y|x \sim N(Ax + b, S_y)$$

observe  $y$  & want  $P(w | y = y)$

$$\begin{array}{l} t \equiv y \\ w \equiv x \end{array}$$

Generic MVN,  $z \sim N(\mu, \Sigma)$

$$\propto \left(\frac{1}{2\pi}\right)^{d/2} \frac{1}{|\Sigma|^{1/2}} e^{-\frac{1}{2}(z-\mu)^T \Sigma^{-1} (z-\mu)}$$

$$e^{-\frac{1}{2} z^T \Sigma^{-1} z} \underbrace{e^{-\frac{1}{2} \mu^T \Sigma^{-1} \mu}}_{\text{does not depend on } z} e^{\mu^T \Sigma^{-1} z}$$

does not depend on  $z$   
 $\rightarrow$  ignore

$$P(z) \propto e^{-\frac{1}{2} z^T \Sigma^{-1} z} e^{\mu^T \Sigma^{-1} z}$$

$$P(X, Y) = P(X) P(Y|X) = ?$$

$$= \left( e^{-\frac{1}{2} x^T S_x x} \quad e^{x^T S_x^{-1} m_x} \right) \left( e^{-\frac{1}{2} (y - (Ax+b))^T S_y^{-1} (y - (Ax+b))} \right)$$

consider exponents of second term

$$-\frac{1}{2} y^T S_y^{-1} y - \frac{1}{2} (Ax+b)^T S_y^{-1} (Ax+b) + (Ax+b)^T S_y^{-1} y$$

$$\textcircled{3} -\frac{1}{2} x^T A^T S_y^{-1} A x$$

$$-x^T A^T S_y^{-1} b$$

$$\textcircled{4} -\frac{1}{2} b^T S_y^{-1} b$$

$$\textcircled{5} x^T A^T S_y^{-1} y + b^T S_y^{-1} y$$

① & ③ quadratic terms

$$-\frac{1}{2} x^T (S_x^{-1} + A^T S_y^{-1} A) x \Rightarrow \Sigma^{-1} = S_x^{-1} + A^T S_y^{-1} A$$

on comparison

②, ④ & ⑤

$$x^T (S_x^{-1} m_x - A^T S_y^{-1} b + A^T S_y^{-1} y)$$

$$= x^T (S_x^{-1} m_x + A^T S_y^{-1} (y - b))$$

$$\Rightarrow \Sigma^{-1} \mu = S_x^{-1} m_x + A^T S_y^{-1} (y - b)$$

on comparison

$$\Rightarrow \mu = (S_x^{-1} + A^T S_y^{-1} A)^{-1} (S_x^{-1} m_x + A^T S_y^{-1} (y - b))$$

$$\left(\frac{1}{\beta} I\right)^T = \beta I$$

Posterior

$$w|t \sim N(\mu^*, \Sigma^*)$$

$$m_y = m_0, S_y = S_0$$

$$K = \Phi, b = 0$$

$$S_y = \frac{1}{\beta} I$$

$$\Sigma^* = \left( S_0^{-1} + \Phi^T \left( \frac{1}{\beta} I \right) \Phi \right)^{-1}$$

$$\begin{aligned} \mu^* &= \Sigma^* \left( S_0^{-1} m_0 + \Phi^T \beta I \Phi \right) \\ &= \Sigma^* \left( S_0^{-1} m_0 + \beta \Phi^T \Phi \right) \end{aligned}$$

MAP = ~~maximum~~ input that maximizes posterior  
(in normal dist., it is same as mean)  
=  $\mu^*$ .

$$w|t \sim N(\mu_N, S_N)$$

$$S_N = \left( S^{-1} + \beta \Phi^T \Phi \right)^{-1}$$

$$\mu_N = S_N \left( \beta \Phi^T t + S_0^{-1} m_0 \right)$$

'no information prior' (fall back to MLE)

$$\text{variance} \rightarrow \infty \quad S_0 = \begin{pmatrix} \infty & & \\ & \infty & \\ & & \ddots \end{pmatrix} \quad S_0^{-1} = \begin{pmatrix} 0 & & \\ & 0 & \\ & & \ddots \end{pmatrix}$$

$$S_N = \left( \beta \Phi^T \Phi \right)^{-1}$$

$$\mu_N = \left( \beta \Phi^T \Phi \right)^{-1} \left( \beta \Phi^T t + 0 \right)$$

$$= \left( \beta \Phi^T \Phi \right)^{-1} \left( \beta \Phi^T t \right)$$

$$= \frac{1}{\beta} \left( \Phi^T \Phi \right)^{-1} \beta \left( \Phi^T t \right) = \left( \Phi^T \Phi \right)^{-1} \left( \Phi^T t \right)$$

$$w \sim N(0, \frac{1}{\alpha} I)$$

$\alpha$   
alpha

$$S_N = \left( \frac{1}{\alpha} I + \beta \Phi^T \Phi \right)^{-1}$$

$$w_N = \left( \frac{1}{\alpha} I + \beta \Phi^T \Phi \right)^{-1} (\beta \Phi^T t + 0)$$

$$= \left( \frac{1}{\alpha} I + \Phi^T \Phi \right)^{-1} (\Phi^T t)$$

$$= \left( \frac{1}{\beta} I + \Phi^T \Phi \right)^{-1} (\Phi^T t)$$

$$\text{let } \lambda = \frac{\alpha}{\beta}$$

$$w_N = (\lambda I + \Phi^T \Phi)^{-1} (\Phi^T t)$$

regularized linear regression

Predictive distribution

$$P(t_{N+1} | w) \sim N(\Phi(x_{N+1})^T w, \frac{1}{\beta})$$

$$P(t_{N+1} | t) \sim ?$$

$$w \sim N(\mu_N, \Sigma_N)$$

$$t_{n+1} | w \sim N(\phi(x_{n+1})^T w, \frac{1}{\beta})$$

$$a = \phi^T$$

$$b = 0$$

$$t_{n+1} \sim N(\phi(x_{n+1})^T \mu_N,$$

$$\frac{1}{\beta} + \phi(x_{n+1})^T \Sigma_N \phi(x_{n+1}))$$

What if  $\beta$  is not known?

conjugate prior/posterior for  $(w, \beta)$

Likelihood

$$\prod_{n=1}^N \frac{1}{\sqrt{2\pi}} \frac{1}{\beta} e^{-\frac{1}{2\beta} (\phi w - t)^T (\phi w - t)}$$

$$\left( \frac{1}{2\pi} \right)^{N/2}$$

$$\beta^{-N} e^{-\frac{1}{2\beta} (\phi w - t)^T (\phi w - t)}$$

$$\left\| \begin{array}{l} \Sigma = \frac{1}{\beta} \Sigma \\ |Z| \propto \left(\frac{1}{\beta}\right)^N \\ \frac{1}{|\Sigma|} = \beta^N \end{array} \right.$$

What would be a conjugate prior for  $\beta$ ?

$$\beta \propto \beta^{-p}$$

$$\left\| \begin{array}{l} \text{Gamma dist.} \\ \text{Gamma}(x | a, b) \\ = \frac{1}{\Gamma(a)} b^a x^{a-1} e^{-bx} \end{array} \right.$$

(ay)

$$X \begin{cases} w \sim N(\mu_0, \Sigma_0) \\ \beta \sim \text{Gamma}(\beta, a, b) \end{cases} \quad \left. \begin{array}{l} \text{independent} \\ \text{independent} \end{array} \right\}$$

$$p(\beta, w | t)$$

$$S_w = (\Sigma_0^{-1} + \beta \phi^T \phi)^{-1} \quad \text{dependent}$$

$$(1000) \quad \text{unstable} \quad S_w = \frac{1}{\beta} \Sigma_0$$

# Machine Learning

Goal: use bayesian solution for both  $w, \beta$ .

Problem:  $\left\{ \begin{array}{l} \text{even if we start with independent } P(w) \& P(\beta) \\ \text{in prior,} \\ \text{posterior will have } P(w, \beta) \text{ with } w, \beta \text{ correlated} \end{array} \right.$

$$t_i \sim N(w^T \phi(x_i), \frac{1}{\beta})$$

$$t \sim N(\Phi w, \frac{1}{\beta} I)$$

Gamma Distribution

$$P(x|a, b) = \frac{1}{\Gamma(a)} b^a x^{a-1} e^{-bx} \quad a, b, x > 0$$

Distribution over positive random variable

Prior

$$P(\beta | a_0, b_0) = \text{Gamma}(\beta, a_0, b_0) \quad \dots \text{marginal}$$

$$P(w | m_0, s_0, \beta) = N(m_0, \frac{1}{\beta} s_0) \quad \dots \text{conditional}$$

Hope for posterior

$$P(\beta | a_N, b_N) = \text{Gamma}(\beta | a_N, b_N)$$

$$P(w | m_N, s_N, \beta) = N(m_N, \frac{1}{\beta} s_N)$$

Posterior  $\propto$  Prior  $\times$  Likelihood

$\beta$  prior  $\dots \frac{1}{\Gamma(a_0)} b_0^{a_0} \beta^{a_0-1} e^{-b_0 \beta}$

$w$  prior  $\dots \left(\frac{1}{2\pi}\right)^{d/2} \frac{1}{|\frac{1}{\beta} S_0|}^{1/2} e^{-\frac{1}{2} (w-m_0)^T (\frac{1}{\beta} S_0)^{-1} (w-m_0)}$

Likelihood  $\dots \left(\frac{1}{2\pi}\right)^{N/2} \frac{1}{\sqrt{|\frac{1}{\beta} I|}} e^{-\frac{1}{2} (t-\Phi w)^T \beta I (t-\Phi w)}$

$\sqrt{\left(\frac{1}{\beta}\right)^N} = \left(\frac{1}{\beta}\right)^{N/2}$

Param	$(w, \beta)$	prior $(w, \beta)$
data	$t$	
posterior	$p(w   t)$	

$\frac{1}{|\frac{1}{\beta} S_0|}^{1/2} = \left(\frac{1}{\beta}\right)^{d/2} |S_0|^{-1/2} \Rightarrow \frac{1}{\sqrt{|\frac{1}{\beta} S_0|}} = \beta^{d/2} \frac{1}{\sqrt{|S_0|}}$

ignoring constant terms

$\beta^{a_0-1} e^{-b_0 \beta} e^{-\frac{\beta}{2} w^T S_0^{-1} w} e^{-\frac{\beta}{2} m_0^T S_0^{-1} m_0} \beta w^T S_0^{-1} m_0$

$\beta^{N/2} e^{-\frac{\beta}{2} t^T t} e^{-\frac{\beta}{2} w^T \Phi^T \Phi w} \beta w^T \Phi^T t$

Quadratic term

$$-\frac{\beta}{2} w^T (\beta_0^{-1} + \Phi^T \Phi) w \quad \text{v/s} \quad -\frac{1}{2} z^T \Sigma^{-1} z$$

$$\Rightarrow \Sigma^{-1} = \beta_0^{-1} + \Phi^T \Phi$$

$$\Sigma = \frac{1}{\beta} \underbrace{(\beta_0^{-1} + \Phi^T \Phi)^{-1}}_{S_N} \quad S_N = (\beta_0^{-1} + \Phi^T \Phi)^{-1}$$

Linear term

$$w^T (\beta_0^{-1} m_0 + \beta \Phi^T t) \quad \text{v/s} \quad z^T \Sigma^{-1} \mu$$

$$\boxed{w} = \Sigma^{-1} \mu$$

$$\Sigma^{-1} \mu = \square$$

$$\mu = \Sigma \square$$

$$\mu = \Sigma(\beta) (\beta_0^{-1} m_0 + \Phi^T t)$$

$$\mu = \frac{1}{\beta} (\beta_0^{-1} + \Phi^T \Phi)^{-1} \beta (\beta_0^{-1} m_0 + \Phi^T t)$$

$$\boxed{\mu = (\beta_0^{-1} + \Phi^T \Phi)^{-1} (\beta_0^{-1} m_0 + \Phi^T t)}$$

next work on  $\beta$

but

look at posterior on  $w$ .

$$\frac{1}{(2\pi)^{d/2}} \frac{1}{\sqrt{\frac{1}{\beta} S_N}} e^{-\frac{1}{2} (w^T (\frac{1}{\beta} S_N)^{-1} w - \frac{1}{2} m_N^T (\frac{1}{\beta} S_N)^{-1} m_N)} \frac{1}{\beta} \frac{1}{\sqrt{|S_0|}} e^{-\frac{1}{2} m_N^T (\frac{1}{\beta} S_N)^{-1} m_N}$$

not accounted for

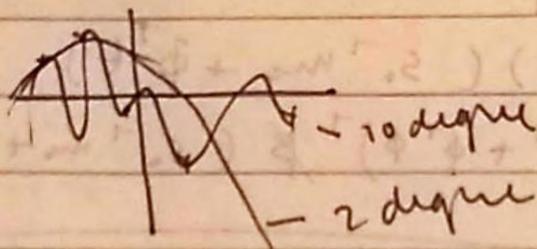
$$\text{Gamma}(x | a, b) \propto x^{a-1} e^{-bx}$$

$$\beta^{a_0 + \frac{N}{2} - 1} \Rightarrow a_N = a_0 + \frac{N}{2}$$

$$e^{-\frac{1}{2} \left( b_0 + \frac{1}{2} m_0^T S_0^{-1} m_0 + \frac{1}{2} t^T t - \frac{1}{2} m_N^T S_0^{-1} m_N \right)}$$

$\beta_N$

$\therefore$  no term remains, by completing the squares the form of the posterior is Normal  $\times$  Gamma.



$$\Phi = \begin{pmatrix} 1 & x & x^2 & \dots & x^{10} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \vdots & \vdots & \vdots & \ddots & \vdots \end{pmatrix}$$

$$\Phi = \begin{pmatrix} 1 & x & x^2 \\ \vdots & \vdots & \vdots \end{pmatrix}$$

$$\begin{pmatrix} 1 \\ x \\ x^2 \\ \vdots \end{pmatrix}$$

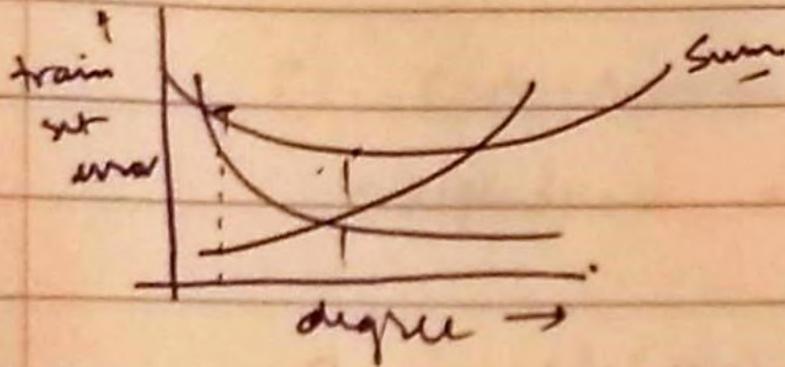
Model Selection

How to pick extra parameters

$\hat{=}$  param of prior

# Simple intuition

Bayesian information criteria



Size of confidence interval grows with complexity of model class

# Evidence maximization

# Machine Learning

## Model Selection

$$P(w) = N(0, \frac{1}{\alpha} \Sigma)$$

$$P(t|w) = N(\Phi w, \frac{1}{\beta} \Sigma)$$

Posterior  $P(w|t) \sim N(m_N, S_N)$

$$m_N = \beta S_N \Sigma^{-1} t$$

$$S_N = (\alpha \Sigma + \beta \Phi^T \Phi)^{-1}$$

what values of  $\alpha, \beta$ ?

hyper-parameters

polynomial regression

$$\phi(x) = \begin{pmatrix} 1 \\ x \\ \dots \\ x^d \end{pmatrix}$$

what value of  $d$ ?

Problem 1

fixed  $d$

pick  $\alpha, \beta$

So as to get "best" posterior

Problem 2

pick  $\alpha, \beta, d$

!

Problem

$\theta$  parameters

$\gamma$  hyperparameters

prior  $P(\theta|\gamma)$

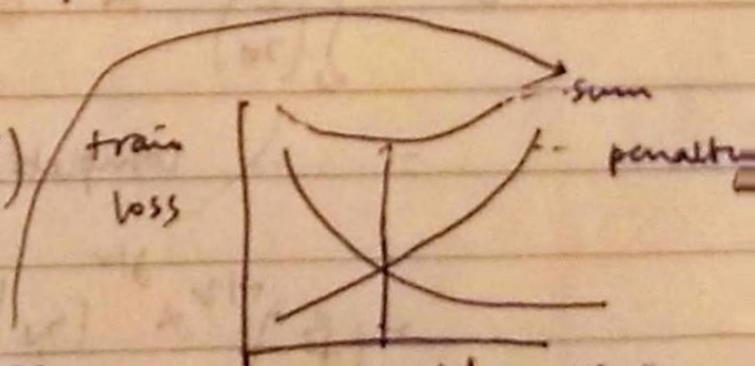
Likelihood  $P(t|\theta)$

find  $P(\theta|t, \gamma)$

what value for  $\gamma$

Standard trick

min  $Loss(\gamma) + Penalty(\gamma)$   
to pick  $\gamma$ .



BIC, AIC, MDL, SRM

Pick  $\gamma$  using evidence function  
 Evidence  $P(t | Y)$   
 $\equiv$  max. likelihood on hyper parameters  
 $\equiv$  2nd level max. L  
 $\equiv$  Empirical Bayes  
 $\equiv$  Evidence approximation.

Bishop: ① intuitive arguments that this works  
 ② rough calculation shows that we get BIC as a special case.

$$\text{Evidence } (Y) = \int_{\theta} \underbrace{P(\theta | Y)}_{\text{prior}} \underbrace{P(t | \theta)}_L d\theta$$

pick hyper param to max

Model 1

$$E_V = \int_w \left( \frac{1}{2\pi} \right)^{d/2} \alpha^{d/2} e^{-\frac{\alpha}{2} w^T w} \left( \frac{1}{2\pi} \right)^{N/2} \beta^{N/2} e^{-\frac{\beta}{2} (\phi w - t)^T (\phi w - t)}$$

.. completing the square to normal

$$= \left( \frac{\beta}{2\pi} \right)^{N/2} \alpha^{N/2} |\Sigma| e^{-\frac{\beta}{2} u^T \Sigma^{-1} u - t^T u}$$

1. Calculate Log Likelihood
2. Take derivative
3. Solve for  $\lambda, \beta$ .

Solution gives an iterative algorithm:

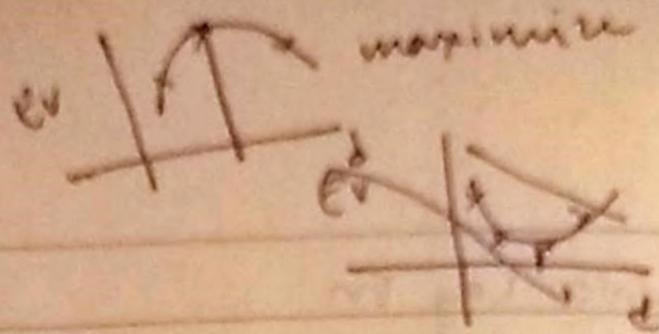
1. Calc.  $\lambda_i$  - eigenvalues of  $\beta \Phi^T \Phi$
2. Calc.  $\gamma = \sum_{i=1}^d \frac{\lambda_i}{\lambda_i + \beta}$

3. Update  $\alpha = \frac{\gamma}{\|\mathbf{m}_N\|^2}$

$$\frac{1}{\beta} = \frac{1}{N-1} \|\Phi \mathbf{m}_N - \mathbf{t}\|^2$$

Model Selection Algorithm

1. Initialize  $\lambda, \beta$
2. Repeat until convergence
  - Calculate  $\mathbf{m}_N, \mathbf{s}_N$
  - Update  $\lambda, \beta$



Model 2,

alg. 10 Select  $\alpha, \beta, d$   
for  $d = 1, \dots, D$

run alg. for Model Selection #1 ~~to pick~~  $\alpha, \beta$

Calculate evidence using  $d, \alpha, \beta$

Pick  $d, \alpha_d, \beta_d$  which ~~max~~ <sup>max</sup> Evidence.

	eigenvalues
$\Phi^T \Phi$	$\hat{\lambda}_i$
$\beta \Phi^T \bar{q}$	$\lambda_i = \beta \hat{\lambda}_i$
$\alpha \Gamma + \beta \bar{q}^T \Phi$	$\alpha + \beta \hat{\lambda}_i$
$S_N$	$\frac{1}{\lambda_i + \alpha} = \frac{1}{\beta \hat{\lambda}_i + \alpha}$

$$\lambda_i \rightarrow \infty \Rightarrow \text{var in direction} \approx 0$$

$$\lambda_i \rightarrow 0 \Rightarrow \text{var} \approx \infty$$

$$\frac{\lambda_i}{\lambda_i + \alpha} \begin{cases} (\lambda_i \rightarrow \infty) \rightarrow 1 \\ (\lambda_i \rightarrow 0) \rightarrow 0 \end{cases}$$

$$r = \sum \frac{\lambda_i}{\lambda_i + \alpha} \approx \text{no. of determined dimensions}$$

# Machine Learning

## Linear Regression

Limitations - model is linear

predicting  $t \in \mathbb{R}$

Classification: when  $t$  is discrete

$$\left( \begin{array}{c} \Phi \\ \vdots \\ \vdots \end{array} \right) \quad \left( \begin{array}{c} x \\ \vdots \\ \vdots \end{array} \right) \quad \left( \begin{array}{c} t \\ \vdots \\ \vdots \end{array} \right) \quad \left( \begin{array}{c} 1 \\ 0 \\ \vdots \\ 1 \end{array} \right)$$

↑ multiclass  
↑ binary  
target value = label.

Simplest Soln for 2 class

Use linear regression

$$Y \leftrightarrow 1$$

$$N \leftrightarrow -1$$

use  $\max L \rightarrow W$

for new example  $x$ ,

compute  $a = w^T x$

if  $a \geq 0 \Rightarrow$  say yes  
otherwise  $\Rightarrow$  no

## Methodology

Specify a model that explains how data is generated

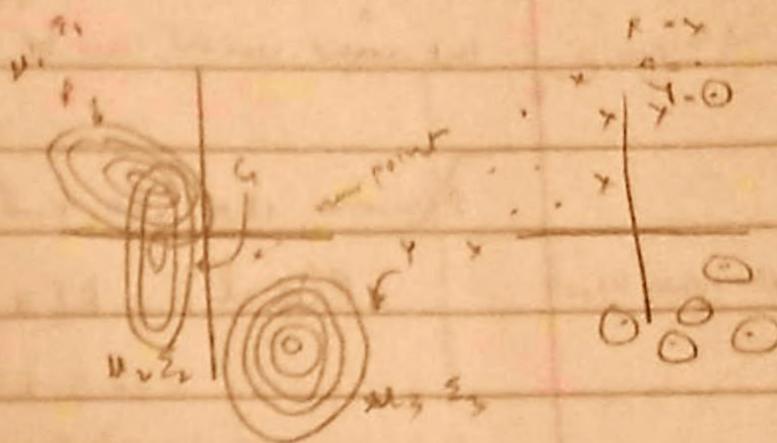
Then given data learn parameters of that model. (or a posterior over parameters)

### Example

$$P(c=1) \quad P(P) = 0.5$$

$$P(c=2) \quad P(G) = 0.4$$

$$P(c=3) \quad P(Y) = 0.1$$



$$P(x|P)$$

$$P(x|G)$$

$$P(x|Y)$$

To generate data

for each  $i$

pick class  $c_i \in \{1, 2, 3\}$

pick  $x$  from  $P(x|c = c_i)$

We also want to include cases where features are discrete

$$x = \begin{pmatrix} 0 & 1 & 1 \\ 0 & 0 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 1 \end{pmatrix}$$

We will need a different  $P(x|C=l)$   
but some model can be used

Assume that we know

$$P(C=l) \quad P(x|C=l)$$

How is a new example classified?

compute  $P(C=j|x)$

$$P(C=j|x) = \frac{P(x|C=j) P(C=j)}{P(x)}$$

$$= \frac{P(C=j) P(x|C=j)}{\sum_i P(x|C=i) P(C=i)}$$

$$= \frac{P(C=j) P(x|C=j)}{\sum_i P(x|C=i) P(C=i)}$$

$$\text{Define } a_j = \log [P(C=j) P(x|C=j)]$$

$$e^{a_j}$$

$$\sum_i e^{a_i}$$

← Softmax

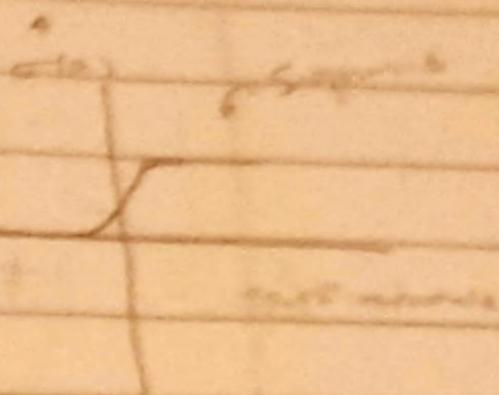
In 2 class case

$$P(c=1) = \frac{e^{a_1}}{e^{a_1} + e^{a_2}}$$

$$= \frac{1}{1 + e^{a_2 - a_1}}$$

Define  $a$  to be  $a_1 - a_2$

$$\Rightarrow \frac{1}{1 + e^{-a}}$$



with equal costs, predict  $c=1$

$$\Leftrightarrow P(c=1) \geq 1/2$$

$$\Leftrightarrow a \geq 0$$

What does prediction look like in geometric space  
when  $P(y|c_j) = N(\mu_j, \Sigma_j)$

Consider cost with  $\mu=2$ ,  $\Sigma_1 = \Sigma_2 = \Sigma$

When do we predict class = 1

$$P = a_1 - a_2$$

$$= \log \frac{P(c=1) P(x|c=1)}{P(c=2) P(x|c=2)}$$



$$\begin{aligned}
 a &= \log P(c=1) - \log P(c=2) \\
 &= \frac{d}{2} \log(2\pi) - \frac{1}{2} \log |\Sigma| - \frac{1}{2} (x - \mu_1)^T \Sigma^{-1} (x - \mu_1) \\
 &\quad + \frac{d}{2} \log(2\pi) + \frac{1}{2} \log |\Sigma| + \frac{1}{2} (x - \mu_2)^T \Sigma^{-1} (x - \mu_2) \\
 &\geq \frac{1}{2}
 \end{aligned}$$

$$\frac{1}{2} x^T \Sigma^{-1} x - \frac{1}{2} \mu_1^T \Sigma^{-1} \mu_1 \neq x^T \Sigma^{-1} \mu_1 \quad \text{linear in } x$$

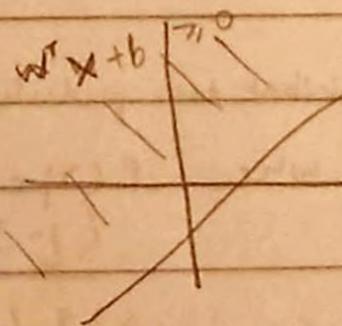
Cancel out

$$\frac{1}{2} x^T \Sigma^{-1} x + \frac{1}{2} \mu_2^T \Sigma^{-1} \mu_2 + x^T \Sigma^{-1} \mu_2 \geq \frac{1}{2}$$

$$w = \Sigma^{-1} (\mu_2 - \mu_1)$$

$$b = \frac{1}{2} + \log \left( \frac{P(c=1)}{P(c=2)} \right) - \frac{1}{2} \mu_1^T \Sigma^{-1} \mu_1 - \frac{1}{2} \mu_2^T \Sigma^{-1} \mu_2$$

$$x^T w + b \geq 0$$

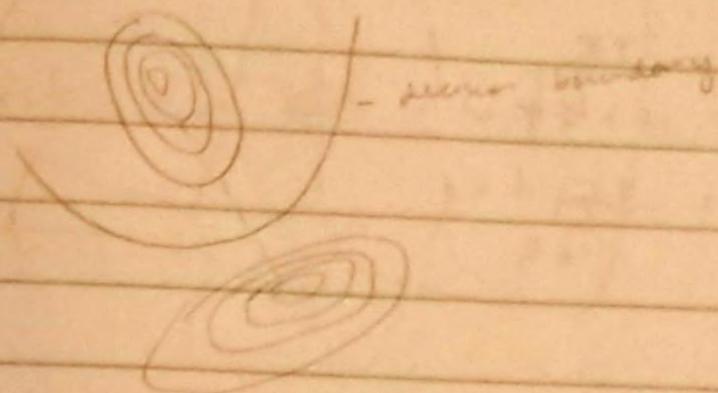


When  $\Sigma_1 \neq \Sigma_2$

only one step in the derivation changes

$$\frac{1}{2} x^T \Sigma_2^{-1} x - \frac{1}{2} x^T \Sigma_1^{-1} x = x^T \left( \frac{1}{2} (\Sigma_2^{-1} - \Sigma_1^{-1}) \right) x$$

Quadratic



or

4 classes

Max likelihood estimate

$$\{ \mu_i, \Sigma_i \}$$

$$P_i = \pi(\omega_i)$$

$$\text{Likelihood} = \left[ \prod_{i \in A} P_A N(x_i | \mu_A, \Sigma_A) \right]$$

$$\left[ \prod_{i \in B} P_B N(x_i | \mu_B, \Sigma_B) \right]$$

$$\left[ \prod_{i \in Y} P_Y N(x_i | \mu_Y, \Sigma_Y) \right]$$

$$\left[ \prod_{i \in B} P_B N(x_i | \mu_B, \Sigma_B) \right]$$

each  $\mu_j$  is independent of  $\mu_i$ .

$$\text{Log } L = \left( \sum_{i \in A} \log P_A + \sum_{i \in G} \log N(x_i | \mu_G, \Sigma_G) \right)$$

$$+ \sum_{i \in B} \left( \dots \right)$$

$$+ \sum_{i \in Y} \left( \dots \right)$$

$$+ \sum_{i \in B} \left( \dots \right)$$

For  $\mu_i, \Sigma_i$  same as above  $L$  for MVM parameters

$$\text{For } P_A + P_B + P_Y = 1$$

$$P_A = \frac{\# \text{ points } G}{\text{total \# of points}}$$

$$\bar{\Sigma} = \frac{1}{N} \sum (x_i - \mu) (x_i - \mu)^T$$

Grand covariance

$$\bar{\Sigma} = \frac{1}{N} \left( \sum_G (x_i - \mu_G) (x_i - \mu_G)^T \right.$$

$$+ \sum_B (x_i - \mu_B) (x_i - \mu_B)^T$$

$$\left. + \dots \right)$$

data  $\approx$  lot of params

$\{ \mu, \Sigma, \gamma, \dots \}$

1000 + 1000 params

param  $\approx$   $w, b$

Predict (a)  $\odot$   $w^{-1}$   $\approx 10^7$

1000 params

# Machine Learning

$$P(c=c)$$
$$P(x|c=c)$$

observed  $x_1, \dots, x_n$

$\Rightarrow$  Max L for param of  $P(c=c) P(x|c=c)$

$$\{\mu_i, \Sigma_i\}_{i=1, \dots, K}$$

To predict on new example

$$w = f(\{\mu_i, \Sigma_i\})$$
$$b = g(\dots)$$

$$Z \text{ is yes} \Leftrightarrow w^T \phi(x) + b \geq 0$$

instead of writing  $w^T \phi(x) + b$

$$w = (w_1, \dots, w_d)$$
$$v = (\underbrace{w_0}_{\text{representable}}, w_1, \dots, w_d)$$

$$\hat{\phi}(x) = (1, \phi_1(x), \dots, \phi_d(x))$$

$$v^T \hat{\phi}(x) = w_0 + w^T \phi(x)$$

$$\text{set } w_0 = b$$

linear regression

$$a_i = w^T \phi(x_i)$$

$$y_i = a_i$$

$$t_i \sim N(y_i, \frac{1}{\beta})$$

logistic regression

$$a_i = w^T \phi(x_i)$$

$$y_i = \sigma(a_i)$$

Sigmoid

$$t_i \sim \text{Bernoulli}(y_i)$$

drawn independently

random variable

$$\Phi = \begin{pmatrix} \text{---} \\ \text{---} \\ \text{---} \end{pmatrix}$$

$$t = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 1 \end{pmatrix}$$

Prob that  
label of ith  
example is 1  
 $= y_i$

$$\Rightarrow w_{max} L$$

$$L = \prod_i y_i^{t_i} (1-y_i)^{1-t_i}$$

take log

$$\log L = \sum_i t_i \log y_i + (1-t_i) \log(1-y_i)$$

diff wrt  $w$ ,

$$\frac{d \log L}{d w} = \sum_i t_i \frac{1}{y_i} \frac{\partial y_i}{\partial w} + (1-t_i) \left( \frac{-1}{1-y_i} \right) \frac{\partial y_i}{\partial w}$$

$$\frac{\partial y_i}{\partial w} = \frac{\partial y_i}{\partial a_i} \frac{\partial a_i}{\partial w}$$

$$y = \sigma(a)$$

$$\frac{dy}{da} = \frac{d}{da} \left( \frac{1}{1+e^{-a}} \right)$$

$$= (-1) \frac{1}{(1+e^{-a})^2} (e^{-a})(-1)$$

$$= \frac{1}{1+e^{-a}} \cdot \frac{e^{-a}}{1+e^{-a}}$$

$$= \sigma(a) (1 - \sigma(a))$$

$$\frac{\partial a_i}{\partial w} = \frac{d}{dw} w^T \phi(x_i) = \phi(x_i)$$

$$\frac{d \log L}{dw} = \sum_i t_i \frac{1}{y_i} \frac{dy_i}{da_i} \frac{\partial a_i}{\partial w} + \sum_i (1-t_i) \frac{1}{1-y_i} \frac{dy_i}{da_i} \frac{\partial a_i}{\partial w} (-1)$$

$$= \sum_i \frac{t_i}{y_i} y_i (1-y_i) \phi(x_i) - \sum_i \left( \frac{1-t_i}{1-y_i} \right) y_i (1-y_i) \phi(x_i)$$

$$= \sum_i \left[ t_i \phi(x_i) - t_i y_i \phi(x_i) - y_i \phi(x_i) + t_i y_i \phi(x_i) \right]$$

$$= \sum_i \left[ (t_i - y_i) \phi(x_i) \right] = \phi^T (t - y)$$

$$\frac{d \log L}{dw} = 0$$

vector elements      matrix columns

$$\sum_i (t_i \phi(x_i)) - \sum_i y_i \phi(x_i) = 0$$

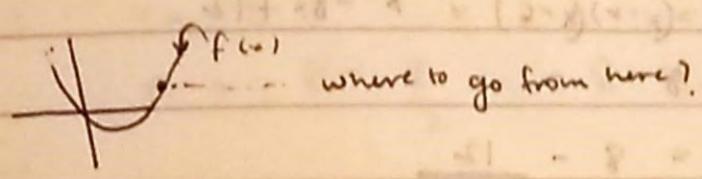
$$\phi^T (t - y) = 0$$

log L is concave and has only one maxima. So, GD will converge.

$$\sum_i t_i \Phi(x_i) = \sum_i y_i \Phi(x_i) \\ = \sum \sigma(w^T \Phi(x_i)) \Phi(x_i)$$

No simple "closed form solutions" for  $w$ .

optimize directly.



- if  $f$  is increasing go left
- if  $f$  is decreasing go right

To maximize, go with gradient  
To minimize, go against gradient

### Gradient Descent:

initialize  $x$

Repeat

$$x \leftarrow x - \eta \cdot f'(x)$$

### Gradient Descent for Logistic Regression

$$w \leftarrow w + \eta \underbrace{\Phi^T(Lt - y)}_{\frac{d}{dw} \log L}$$

$$\equiv w \leftarrow w + \eta \frac{d}{dw} \log L$$

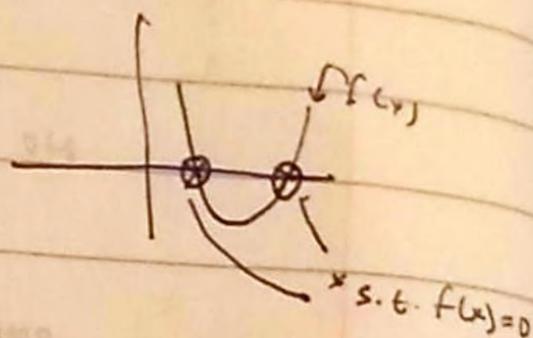
Maximize log likelihood.

if fn. is linear  
this method terminates in  
1 step and is exact

Newton's method.

To find a zero of  $f(x)$

$$x_{n+1} \leftarrow x_n - \frac{f(x_n)}{f'(x_n)}$$



ex.  $f(x) = (x-2)(x-6) = x^2 - 8x + 12$

$$x_0 = 8$$

$$x_1 = 8 - \frac{12}{8}$$

why?

$$f(x_0+h) \approx f(x_0) + f'(x_0)h + \left\{ \frac{1}{2} f''(x_0)h^2 + \dots \right.$$

Taylor  
expansion

$$\approx f(x_0) + f'(x_0)h$$

higher order terms  
are small; ignore  
them

$$\text{if } f(x_0+h) = 0$$

$$\Rightarrow f(x_0) + f'(x_0)h = 0$$

$$\Rightarrow h = \frac{-f(x_0)}{f'(x_0)}$$

if this quadratic  
this method terminates in 1 step  
and is exact

Newton's method for finding extremum of a function  
[find zero of  $f'(x)$ ]

$$x_{n+1} \leftarrow x_n - \frac{f'(x_n)}{f''(x_n)}$$

ex.  $f(x) = (x-2)(x-6) = x^2 - 8x + 12$

$$x_0 = 8$$

$$x_1 = 8 - \frac{8}{2} = 8 - 4 = 4 \leftarrow \text{minimum at point. this}$$

consider  $F: \mathbb{R}^k \rightarrow \mathbb{R}$

$$F(x_0+h) = F(x_0) + \left( \frac{\partial F}{\partial x} \Big|_{x_0} \right)^T h + \dots$$

ignore higher order terms

$$F: \mathbb{R}^k \rightarrow \mathbb{R}$$

$$J = \begin{pmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_1}{\partial x_2} & \dots & \frac{\partial y_1}{\partial x_k} \\ \vdots & \vdots & & \vdots \\ \frac{\partial y_k}{\partial x_1} & \frac{\partial y_k}{\partial x_2} & & \frac{\partial y_k}{\partial x_k} \end{pmatrix} \quad \left\| \begin{array}{l} J \text{ is different} \\ \text{from change} \\ \text{of p.v.} \end{array} \right.$$

$$h = \begin{pmatrix} h_1 \\ \vdots \\ h_k \end{pmatrix}$$

To find zero of  $F$

$$0 = F(x_0+h) \approx F(x_0)$$

$$+ J|_{x_0} \cdot h$$

$$h = -J|_{x_0}^{-1} F(x_0)$$

To find min of  $G: \mathbb{R}^n \rightarrow \mathbb{R}$

and zero of  $f = \frac{\partial G}{\partial x}$

In this case  $J(G) =$  Matrix of 2nd derivatives

$$\text{Hessian} = \begin{pmatrix} \frac{\partial^2 G}{\partial x_1^2} & \frac{\partial^2 G}{\partial x_1 \partial x_2} & \dots & \frac{\partial^2 G}{\partial x_1 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 G}{\partial x_2 \partial x_1} & \dots & \dots & \frac{\partial^2 G}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \vdots & \vdots \\ \frac{\partial^2 G}{\partial x_n \partial x_1} & \dots & \dots & \frac{\partial^2 G}{\partial x_n \partial x_n} \end{pmatrix}$$

$$x_{n+1} \leftarrow x_n - H|_{x_n}^{-1} \frac{\partial G}{\partial x} \Big|_{x_n}$$

$$g(x) = 5x_1^2 + 6x_1x_2 + 5x_2^2$$

find minimum of  $g$

$$\frac{\partial g}{\partial x} = \begin{pmatrix} 10x_1 + 6x_2 \\ 6x_1 + 10x_2 \end{pmatrix}$$

$$H = \begin{pmatrix} 10 & 6 \\ 6 & 10 \end{pmatrix}$$

$$H^{-1} = \frac{1}{24} \begin{pmatrix} 6 & -6 \\ -6 & 10 \end{pmatrix}$$

$$h(x) = 5x_1^3 + 6x_1x_2 + 3x_2^2$$

$$\frac{\partial h}{\partial x} = \begin{pmatrix} 15x_1^2 + 6x_2 \\ 6x_1 + 6x_2 \end{pmatrix}$$

$$H = \begin{pmatrix} 30x_1 & 6 \\ 6 & 6 \end{pmatrix}$$

logistic regression

Also called

iterative reweighted  
least squares  
(IRLS)

$$\frac{\partial \log L}{\partial w} = \sum_i (b_i - y_i) \phi(x_i)$$

$$\frac{\partial \log L}{\partial w \partial w^T} = - \sum_i \left( \frac{\partial y_i}{\partial w} \right) \phi(x) \frac{\partial y_i}{\partial w^T}$$

$$= - \sum_i \phi(x_i) \frac{\partial y_i}{\partial w^T}$$

$$A_i \begin{pmatrix} \downarrow \\ \sum a_i b_i^T \\ = A^T B^T \end{pmatrix}$$

$$= - \sum_i \phi(x_i) y_i (1 - y_i) \phi(x_i)^T$$

almost  
same as calculated  
earlier

$$= - \sum_i \phi(x_i) y_i (1 - y_i) \phi(x_i)^T$$

$$= - \Phi^T R \Phi$$

$$R = \text{diag} \left\{ y_i (1 - y_i) \right\}_i$$

$R \equiv$  positive (semi) definite

$$w \leftarrow w + (\Phi^T R \Phi)^{-1} \Phi^T (t y)$$

$$\text{or } w \leftarrow w - (\Phi^T R \Phi)^{-1} \Phi^T (y - t)$$

Proof that our function is concave (i.e. has 1 maximum)

~~or guarantee that~~

we need  $H \preceq 0$

negative

positive definite

$$c^T H c \preceq 0$$

$c$  - arbitrary vector

$$-c^T \Phi^T R \Phi c < 0$$

$c \neq 0$

$$-c^T (\Phi^T R^{1/2}) (R^{1/2} \Phi c) < 0$$

$$-\underbrace{(R^{1/2} \Phi^T c)^T (R^{1/2} \Phi c)}_{\text{norm}} < 0$$

this holds if  $R^{1/2} \Phi$  is full rank

i.e. if columns in data matrix are linearly independent

Trade off

Newton

optimal step size

but compute hessian

GD

fixed non optimal

step size

but ~~need~~

no additional

computation

# Machine Learning

Generative model

K classes  $c=1, \dots, c=K$

Prob. of class  $k$ :  $P(c_k)$

Prob. of generating data:  $P(X|c_k)$

Given model.

prediction

$$\text{Softmax} = \frac{e^{a_k}}{\sum_j e^{a_j}}$$

$$\text{sigmoid}, \sigma = \frac{1}{1 + e^{-(a_1 - a_2)}}$$

$$a_j = \ln \frac{P(c_j)}{P(c_k)} + P(X|c_k)$$

When  $X|c_j \sim N(\mu_j, \Sigma_j)$

Shared  $\Sigma = \Sigma_j \forall j$

Distinct  $\Sigma_j$

Shared  $\Sigma$ , 2 class

$$\text{Prediction } P(c=1) = \sigma(w^T X + w_0)$$

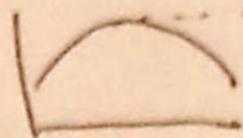
$$\text{let } w = \Sigma^{-1}(\mu_1 - \mu_2)$$

$$w_0 = \ln \frac{P(c_1)}{P(c_2)} - \frac{1}{2} \mu_1^T \Sigma^{-1} \mu_1 + \frac{1}{2} \mu_2^T \Sigma^{-1} \mu_2$$

use  $\Sigma^{-1}$  is easy

(from data dist. to model)

-ve definite hessian  
⇒ concave fn.



Single max pt

Discriminative model

Logistic Regression

$$P(c=1 | x) = \sigma(w^T \phi(x_i))$$

absorbed bias term  $w_0$  into extra dimension

for analogy  $\phi(x) = x$

$$a_i = w^T \phi(x_i)$$

$$y_i = \sigma(a_i)$$

$$t_i \sim \text{Bernoulli}(y_i)$$

Max<sup>m</sup> likelihood  
is hard

No closed form solution

⇒ Optimization: Gradient ascent or Newton's method

$$\frac{\partial \log L}{\partial w} = \sum_i \phi(x_i) [t_i - y_i]$$

$$\frac{\partial^2 \log L}{\partial w^2} = -\Phi^T R \Phi$$

$$R = \text{diag} \{y_i (1 - y_i)\}$$

# Naive Bayes

Generative model for discrete data.

Say Binary features.

$$\Phi = \begin{pmatrix} 0 & 1 & 1 \\ 0 & 1 & 1 \\ 0 & \dots & \dots \end{pmatrix}$$

$$P(X|c_k) = ?$$

How to write a compact prob. dist.?

- Given Ex
- $P(000)$
  - $P(001)$
  - $P(010)$
  - $P(011)$
  - $P(100)$
  - $P(101)$
  - $P(110)$
  - $P(111)$

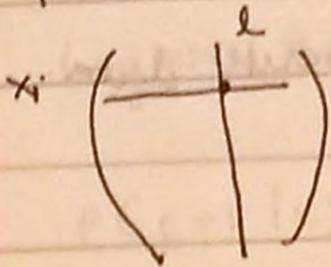
$2^n$ -exponential  
for general dist.

Specifying a general dist.  
requires too much time/space

A very simple restriction:  
assume that features are  
conditionally independent  
given the label.

$$P(x_i | x_j | c)$$

# Notation



$x_{il}$  =  $l$ th bit of  $i$ th example.

$$P(x_i | C_k) = \prod_{l=1}^d \mu_{kl}^{x_{il}} (1 - \mu_{kl})^{1-x_{il}}$$

$\mu_{kl}$  = parameter for  $l$ th bit given that label =  $k$ th class

Let first label example have label 3

$$P(C_3) P(x_1 | C_3) = P(C_3) \prod_{l=1}^d \mu_{3l}^{x_{1l}} (1 - \mu_{3l})^{1-x_{1l}}$$

$$L = \prod_i \prod_k \left[ P(C_k) \prod_l \mu_{kl}^{x_{il}} (1 - \mu_{kl})^{1-x_{il}} \right]$$

boolean  $\sum_{l=1}^d$

$$\log L = \sum_i \sum_k \left[ \ln P(C_k) + \sum_l x_{il} \ln \mu_{kl} + \sum_l (1-x_{il}) \ln (1 - \mu_{kl}) \right]$$

$\sum_{l=1}^d$

MLE for  $P(C_k)$  is same as general case

$$\frac{\partial \log L}{\partial \mu_{kl}} = \sum_i \left[ \frac{x_{il}}{\mu_{kl}} - \frac{L x_{il}}{1 - \mu_{kl}} \right] = 0$$

such that

$$\Rightarrow \sum_{i=1}^n x_{i1}(1 - \mu_{k1}) - \sum_{i=1}^n \mu_{k1}(1 - x_{i1}) = 0$$

$$\sum_{i=1}^n x_{i1} - \sum_{i=1}^n \mu_{k1} - \sum_{i=1}^n \mu_{k1} + \sum_{i=1}^n \mu_{k1} x_{i1} = 0$$

$$\sum_{i=1}^n x_{i1} - N_k \mu_{k1} = 0$$

$$\sum_{i=1}^n x_{i1} = N_k \mu_{k1}$$

$$\mu_{k1} = \frac{\sum_{i=1}^n x_{i1}}{N_k} = \frac{\text{no. of examples in } P^{\text{th}} \text{ test set}}{\text{no. of examples of class } k}$$

It can be shown that

$$P(c_k | x) = \frac{e^{a_k}}{\sum_j e^{a_j}}$$

$$a_j = w_j^T x + w_{j0}$$

$$\exists w, w_0$$

for some

1<sup>st</sup> order

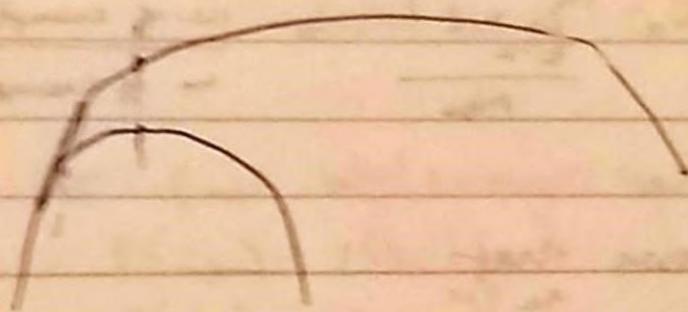
gradient ascent  
move with gradient  
 $w \leftarrow w + \eta \frac{\partial \log L}{\partial w}$

gradient descent  
move against gradient  
 $w \leftarrow w - \eta \frac{\partial \log L}{\partial w}$

0<sup>th</sup> order

Newton's method.

assume that the function is quadratic  
and jump to the location that gives the  
maximum of the quadratic fn.



2<sup>nd</sup> order

$$w \leftarrow w + H^{-1} \frac{\partial \log L}{\partial w}$$

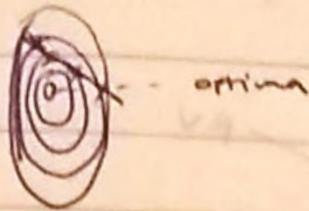
ⓐ compute hessian

ⓑ invert hessian

$$H = \frac{\partial^2 \log L}{\partial w \partial w^T}$$

alternative: approximate hessian in linear time

Line search. to choose  $\eta$



want to find ideal  $\eta$

① Brute force search (expensive)

② backtracking line search

Backtracking Line search  
for minimization

initialize  $\eta = 1$

$$\text{while } f(w + \eta \frac{\partial f}{\partial w}) > f(w) - \frac{\eta}{2} \left\| \frac{\partial f}{\partial w} \right\|^2$$

$$\eta \leftarrow \frac{\eta}{2}$$

Compromise backtracking line search  $\hat{w}$  gradient ascent/descent

What if computing derivative is expensive?

$$\frac{\partial L}{\partial w} = \sum_{i=1}^N \phi(x_i) (f_i - y_i)$$

Sum over

all data points  
expensive

## Stochastic Gradient Descent

$$GD: w \leftarrow w - \eta G$$

$$G = \frac{\partial f}{\partial w}$$

if  $w$  can get  $\hat{G}$  ← RV

$$s.t. E[\hat{G}] = G \quad // \text{ unbiased estimator}$$

then we can use  $\hat{G}$  instead of  $G$

$\rightarrow w \leftarrow w - \eta_t \hat{G}$  converges to the  $\min^m$  of  $f$ .

where  $\eta_t$  must satisfy some conditions

$$\eta_t = \frac{1}{t}$$

\* Cheap random estimate of gradient for logistic regression

To get  $\hat{G}$

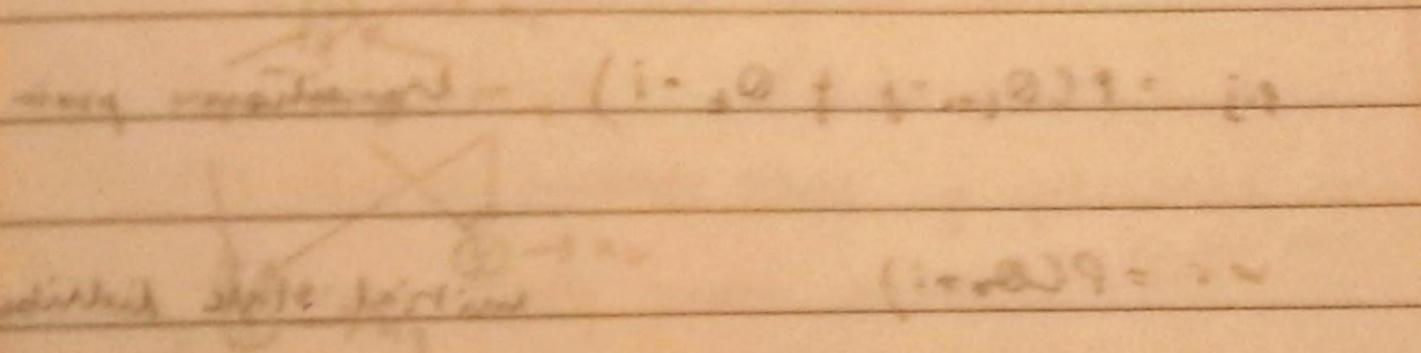
pick  $i \in 1 \dots N$  at random (uniformly)

$$\hat{G} = N \phi(x_i) (t_i - y_i)$$

$$E(\hat{G}) = \frac{1}{N} \sum_i N \phi(x_i) (t_i - y_i) = \sum \phi_i (t_i - y_i)$$

Alternative minibatch SGD

take  $k$  examples and take mean  
instead of 1 example



$(i-1) \cdot \theta + (i-k) \cdot \theta = (i-k) \cdot \theta$

for a particular day  
(margin)

with some error all day  
(MSE)

# Machine Learning

## Exponential family of distributions

Any distribution that can be written in form  $p(x) = h(x) g(\eta) e^{\eta^T U(x)}$  is a member of exponential family

\* constrain the form of PDF.

$$\eta^T U(x) = A(\eta)$$
$$A(\eta) = -\log g(\eta) \Rightarrow p(x) = h(x) e^{\eta^T U(x) - A(\eta)}$$

Bernoulli  $\in$  exp. family

$$p(x) = \mu^x (1-\mu)^{1-x}$$
$$= e^{(\log \mu)x + (\log(1-\mu))(1-x)}$$
$$= e^{(\log \mu)x + \log(1-\mu) - \log(1-\mu)x}$$
$$= \frac{e^{(\log \mu)x}}{e^{\log(1-\mu)x}}$$
$$= (1-\mu) e^{x \log \frac{\mu}{1-\mu}}$$

$h(x) =$  base measure

$g(\eta) =$  log normalizer

$\eta =$  Natural parameters  
canonical parameters

$U(x) =$  Sufficient Statistics

dim.  $\eta = 1$        $\eta = \log \frac{\mu}{1-\mu}$        $h(x) = 1$

$g(\eta) = ? = 1 - \mu$

$\mu = \log \frac{\mu}{1-\mu} \Rightarrow e^\eta = \frac{\mu}{1-\mu} \Rightarrow e^\eta - \mu e^\eta - \mu = 0$

$\Rightarrow \frac{e^\eta}{1+e^\eta} = \mu$

$g(\eta) = \frac{e^\eta}{1+e^\eta} = \frac{1}{1+e^{-\eta}}$

$\mu = \frac{1}{1+e^{-\eta}} = \sigma(\eta)$   
sigmoid

$P(x) = \frac{1}{1+e^\eta} \cdot e^{\eta x}$   
 $U(x) = x$   
 $g(\eta) = \frac{1}{1+e^{-\eta}}$   
 $h(\eta) = 1$

$E[U(x)] = \text{mean parameter} = \theta$        $\eta = \mu$  for bernoulli

if entries of  $U(x)$  are linearly independent

then  $\theta \xleftrightarrow{1-1} \eta$

Normal

$$f(x) = (2\pi)^{-1/2} \sigma^{-1} \exp\left\{-\frac{1}{2\sigma^2}(x-\mu)^2\right\}$$
$$= (2\pi)^{-1/2} \sigma^{-1} \exp\left\{\frac{-x^2}{2\sigma^2}\right\} \exp\left\{\frac{-\mu}{\sigma^2}x + \frac{\mu^2}{2\sigma^2}\right\}$$

$$h(x) = 1 \quad u(x) = \begin{pmatrix} x \\ x^2 \end{pmatrix} \quad \eta = \begin{pmatrix} \eta_1 \\ \eta_2 \end{pmatrix} = \begin{pmatrix} \mu/\sigma^2 \\ -1/2\sigma^2 \end{pmatrix}$$

$$g(\eta) = (2\pi)^{-1/2} \sigma^{-1} \exp\left\{\frac{-\eta^2}{4\eta_2}\right\}$$
$$= \frac{\sqrt{2\pi}}{\sqrt{\pi}} \exp\left\{-\eta_1^2 / 4\eta_2\right\}$$

Poisson

$$p(x) = \lambda^x e^{-\lambda} \frac{1}{x!}$$
$$\frac{1}{x!} = \frac{1}{g(\eta) h(x)}$$

$$\frac{1}{x!} \rightarrow \frac{(\log \lambda)^x}{e^x}$$

$$\dim = 1 \quad \eta = \log \lambda \quad \lambda = e^\eta$$

$$h(x) = \frac{1}{x!} \quad u(x) = x$$

Fact 1 If  $x_1, \dots, x_n$  are iid sampled from an exp. family distribution then

$$P(x_1, \dots, x_n) = \left( \prod_i h(x_i) \right) (g(\eta))^n e^{\eta^T \sum_{i=1}^n U(x_i)}$$

$U$ : Sufficient stats since only sum is needed for MLE and not each  $x_i$ .

Fact 2:  $E[U(x)] = \frac{\partial}{\partial \eta} \log g(\eta)$

$$\text{cov}(U(x)) = E \left[ (U(x) - E[U(x)]) (U(x) - E[U(x)])^T \right]$$

$$= - \frac{\partial^2}{\partial \eta \partial \eta^T} \log g(\eta)$$

Fact 3: (S1) If we have one sample from exp. <sup>family</sup> dist. Max likelihood solution is obtained when

$$U(x) = \frac{\partial}{\partial \eta} \log g(\eta)$$

(S2) For iid samples

$$\frac{1}{N} \sum_i U(x_i) = \frac{\partial}{\partial \eta} \log g(\eta)$$

$$\rightarrow \text{Max } L = \frac{1}{N} \sum U(x_i) = E[U(x)]$$

Max L for Bernoulli dist

Use fact 3

$$p(x) = \frac{\lambda^x e^{-\lambda}}{x!}$$

$$h(\lambda) = -\log p(x) = -\log \frac{\lambda^x e^{-\lambda}}{x!} = -x \log \lambda + \lambda - \log x!$$

~~max L~~

$$p(x) = \mu^x (1-\mu)^{1-x}$$

$$\eta = \log \frac{\mu}{1-\mu} \quad h(\eta) = 1$$

$$\frac{\partial}{\partial \eta} g(\eta)$$

$$g(\eta) = 1 - \mu = \frac{1 - e^{\eta}}{1 + e^{\eta}}$$

$$\begin{aligned} &= \frac{\partial}{\partial \eta} \left( \frac{1}{1 + e^{\eta}} \right) \\ &= \frac{-e^{\eta}}{(1 + e^{\eta})^2} \cdot e^{\eta} \end{aligned}$$

$$= \frac{1}{1 + e^{\eta}}$$

$$\frac{\partial}{\partial \eta} \log g(\eta)$$

$$\bar{x} = - \frac{1}{g(\eta)} \frac{\partial}{\partial \eta} g(\eta)$$

$$\bar{x} = \frac{e^{\eta}}{(1 + e^{\eta})^2} (1 + e^{\eta})$$

$$\bar{x} = \frac{e^{\eta}}{1 + e^{\eta}}$$

$$\eta = \log \frac{\bar{x}}{1 - \bar{x}}$$

Sanity check.

$$\mu = \frac{1}{1+e^{-\eta}} = \frac{1}{1+\frac{1-\mu}{\mu}} = \mu$$

Solving using fact 2 + fact 3 together.

$$E[\mu(x)] = \bar{x}$$

$$\Rightarrow \mu = \bar{x}$$

$$E[U(x)] = \frac{1}{N} \sum U(x_i)$$

$$\begin{pmatrix} E[x] \\ E[x^2] \end{pmatrix} = \frac{1}{N} \begin{pmatrix} \sum x_i \\ \sum x_i^2 \end{pmatrix}$$

$$\begin{pmatrix} E[x] \\ E[x^2] \end{pmatrix} = \frac{1}{N} \begin{pmatrix} \sum x_i \\ \sum x_i^2 \end{pmatrix}$$

$$\mu = \frac{1}{N} \sum x_i$$

$$\mu^2 + \sigma^2 = \frac{1}{N} \sum x_i^2$$

$$\sigma^2 = \frac{1}{N} \sum (x_i - \hat{\mu}_{ML})^2$$

Proof of Fact 3.1

$$L = h(x) g(\eta) e^{\eta^T U(x)}$$

$$\log L = \log h(x) + \log g(\eta) + \eta^T U(x)$$

$$\frac{\partial \log L}{\partial \eta} = \frac{\partial}{\partial \eta} \log g(\eta) + U(x) = 0$$

$$U(x) = -\frac{\partial}{\partial \eta} \log g(\eta)$$

Fact 3.2

$$L = \prod_i h(x_i) g(\eta)^N e^{\eta^T \sum U(x_i)}$$

$$\log L = \sum \log h(x_i) + N \log g(\eta) + \eta^T \sum U(x_i)$$

$$\frac{\partial \log L}{\partial \eta} = \left( N \frac{\partial}{\partial \eta} \log g(\eta) + \sum U(x_i) \right) = 0$$

Proof of fact 2

$$\int h(x) g(\eta) e^{\eta^T U(x)} dx = 1$$

$$g(\eta) \int h(x) e^{\eta^T U(x)} dx = 1$$

$$\frac{\partial}{\partial \eta} (g(\eta)) \left( \int h(x) e^{\eta^T U(x)} dx \right) = 0$$

product rule

$$\frac{\partial}{\partial \eta} g(\eta) \int h(x) e^{\eta^T U(x)} dx + g(\eta) \frac{\partial}{\partial \eta} \left( \int h(x) e^{\eta^T U(x)} dx \right) = 0$$

$$\int h(x) e^{\eta^T U(x)} dx = \frac{1}{g(\eta)} \quad \text{and} \quad \int h(x) e^{\eta^T U(x)} U(x) dx = \frac{E[U(x)]}{g(\eta)}$$

$$\frac{\partial g(\eta)}{\partial \eta} \frac{1}{g(\eta)} + \cancel{g(\eta)} \frac{E[U(x)]}{\cancel{g(\eta)}} = 0$$

$$\frac{1}{g(\eta)} \frac{\partial g(\eta)}{\partial \eta} + E[U(x)] = 0$$

$$\frac{\partial \log g(\eta)}{\partial \eta} + E[U(x)] = 0 \quad \Rightarrow \quad E[U(x)] = -\frac{\partial \log g(\eta)}{\partial \eta}$$

$$\text{cov}(U(x_i), U(x_j)) = E[(U(x_i) - E[U(x_i)])(U(x_j) - E[U(x_j)])]$$

$$\frac{\partial \log g(\eta)}{\partial \eta} + g(\eta) \int h(x) e^{\eta^T U(x)} U(x) dx = 0$$

$$\frac{\partial \log g(\eta)}{\partial \eta_i} + g(\eta) \int h(x) e^{\eta^T U(x)} U_i(x) dx = 0$$

$$\frac{\partial^2 \log g(\eta)}{\partial \eta_i \partial \eta_j} + g(\eta) \int h(x) e^{\eta^T U(x)} U_i(x) U_j(x) dx = 0$$

$$+ \frac{\partial g(\eta)}{\partial \eta_j} \int h(x) e^{\eta^T U(x)} U_i(x) dx = 0$$

$$\frac{\partial}{\partial \eta_k} (\log g(\eta)) + E(U_k(x)) = 0$$

$$E(U_k(x)) = - \frac{\partial}{\partial \eta_k} (\log g(\eta))$$

$$= - \frac{g(\eta)}{g(\eta)} + \frac{1}{g(\eta)} \frac{\partial g(\eta)}{\partial \eta_k}$$

$$\frac{\partial}{\partial \eta_k} g(\eta) = E(U_k(x)) g(\eta)$$

$$\int h(x) e^{\eta^T U(x)} U_i(x) dx = \frac{E[U_i(x)]}{g(\eta)}$$

$$\int h(x) e^{\eta^T U(x)} U_i(x) U_k(x) dx = \frac{E[U_i(x) U_k(x)]}{g(\eta)}$$

$$\frac{\partial^2 \log g(\eta)}{\partial \eta_i \partial \eta_k} = E[U_i(x)] E[U_k(x)] + E[U_i(x) U_k(x)] = 0$$

$$- E[U_i(x)] E[U_k(x)] + E[U_i(x) U_k(x)] = 0$$

$$= \frac{\partial^2}{\partial \eta_i \partial \eta_k} [\log g(\eta)]$$

$$L \propto g(\eta)^N e^{\eta^T \sum_i U(x_i)}$$

no. of obs-  $\swarrow$

$\searrow$  sum of sufficient stats

Conjugate prior should have

$$p(\eta) \propto g(\eta)^{\nu} e^{\eta^T g}$$

$$= g(\eta)^{\nu} e^{g^T \eta} = g(\eta)^{\nu} e^{(\nu \bar{g})^T \eta}$$

$\nu \equiv$  pretend  
to have seen  
 $\nu$  no. of  
examples

$\bar{g} =$  mean  
of such  
pseudo  
observations

added  
counts

mean  
for newer  
obs.

$$p(x|y) \propto \frac{1}{z} e^{-\beta \phi(x)}$$

## Machine Learning

Quiz 3 model selection - GLM, HW3.

### Generalised Linear Models

Linear Regression

$$a_i = w^T \phi(x_i)$$

$$t_i \sim N(a_i, \frac{1}{\beta})$$

Logistic Regression

$$a_i = w^T \phi(x_i)$$

$$y_i = \sigma(a_i)$$

$$t_i \sim \text{Bernoulli}(y_i)$$

Poisson Regression

$$a_i = w^T \phi(x_i)$$

$$y_i = e^{a_i}$$

$$t_i \sim \text{Poisson}(y_i)$$

$$\frac{\partial \log L}{\partial w} = \sum (t_i - y_i) \phi(x_i)$$

$$\frac{\partial^2 \log L}{\partial w^2} = - \sum y_i (1 - y_i) \phi(x_i) \phi(x_i)^T$$

$$R = - \Phi^T R \Phi$$

$$R = \text{diag}(y_i (1 - y_i))$$

Poisson Regression

$$L = \prod_i y_i^{t_i} e^{-y_i} \frac{1}{t_i!}$$

$$\log L = \sum t_i \log y_i - y_i - \log t_i!$$

$$= \sum t_i (\log e^{a_i}) - y_i - \log t_i!$$

$$= \sum t_i a_i - y_i - \log t_i!$$

$$\frac{\partial \log L}{\partial w} = \sum t_i \phi(x_i) - e^{a_i} \phi(x_i)$$

$$= \sum (t_i - y_i) \phi(x_i)$$

same form.

$$\begin{aligned}
 \frac{\partial \log L}{\partial \omega^T} &= \sum_i \phi(x_i) \frac{\partial y_i}{\partial \omega^T} \\
 &= \sum_i \phi(x_i) e^{a_i} \phi(x_i)^T \\
 &= \sum_i e^{a_i} \phi(x_i) \phi(x_i)^T \\
 &= \sum_i y_i \phi(x_i) \phi(x_i)^T \\
 &= \Phi^T R \Phi \quad R = \text{diag}(y_i)
 \end{aligned}$$

$$\mu \leftarrow \omega = (\Phi^T R \Phi)^{-1} \Phi^T (y - t)$$

Exponential Family of Distributions

$$P(x|\eta) = h(x) g(\eta) e^{\eta^T U(x)}$$

$\eta$ : natural parameter

$g$ : normalizer

$U$ : sufficient statistics

$\mu = E[U(x)]$ : mean parameter

If  $U$  is linearly independent then

we can write PDF in 2 ways (given + with  $\mu$ )

$$\mu = \Psi(\eta)$$

$$\eta = \Psi^{-1}(\mu)$$

Bernoulli

$$P(x|\eta) = \eta^x (1-\eta)^{1-x}$$

$$P(x|\eta) = \frac{1}{1+e^\eta} e^{\eta x}$$

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

$$\eta = \log \frac{\mu}{1-\mu}$$

Poisson

$$P(x|\eta) = \frac{1}{x!} e^{-e^\eta} e^{\eta x}$$

$$\eta = \log \lambda$$

$$\lambda = e^\eta$$

Any PDF  $f(x)$  can be changed to add a scale parameter.

$$\textcircled{1} P(x) = \frac{1}{s} f\left(\frac{x}{s}\right)$$

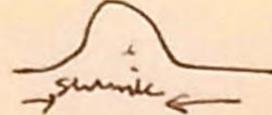
Apply to an 1D exp. family dist.  $U(x) = x$

$$P(x) = \frac{1}{s} h\left(\frac{x}{s}\right) g(\eta) e^{\frac{1}{s} \eta \cdot x}$$

For any exp family dist.

$$E[U(x)] = -s \frac{\partial}{\partial \eta} \log g(\eta)$$

$$\textcircled{2} E[x] = -s \frac{\partial}{\partial \eta} \log g(\eta)$$

scale (  , s )  $\rightarrow$  

$$\text{cov}(U(\eta)) = -\frac{\partial^2}{\partial \eta \partial \eta^T} \log g(\eta)$$

$$\textcircled{3} \text{ var}(x) = -s^2 \frac{\partial^2}{\partial \eta^2} \log g(\eta)$$

$$p(x) = (2\pi)^{-1/2} \sigma^{-1/2} \exp\left\{ -(2\sigma^2)^{-1} (x^2 - 2\mu x + \mu^2) \right\}$$

$$\stackrel{\text{---}}{\approx} \underbrace{(2\pi\sigma^2)^{-1/2} e^{-\frac{(2\sigma^2)^{-1}\mu^2}{2}}}_{g(\eta)} \underbrace{e^{-\frac{(2\sigma^2)^{-1}x^2}{2}}}_{h(x/s)} \underbrace{e^{\frac{(2\sigma^2)^{-1}\mu x}{2}}}_{e^{\frac{1}{2}\mu x}}$$

in this representation  $\eta = \mu$   $\Psi = \text{identity}$

### Generalized Linear Model

$$a_i = w^T \phi(x_i)$$

$y_i = f(a_i)$   $\leftarrow$  mean parameter and mean of  $t_i$

$f$ : activation

$$\eta_i = \Psi(y_i) \text{ natural parameter}$$

$f^{-1}$ : link function.

$$t_i \sim P(t_i | \eta_i) \text{ (exp. family dist.)}$$

'D exp family dist.

Canonical link function picks  $f(a) = \psi^{-1}(a)$

$$\eta_i = \sum \psi(y_i) = \psi(\psi^{-1}(a_i)) = a_i$$

for linear regression,  $\psi = \text{identity}$ .

for logistic regression

$$t_i \sim \text{Bernoulli}(y_i) \\ \sim \text{Ber.}^{\text{natural}}(t_i | a_i)$$

for poisson

$$t_i \sim \text{Poisson}(y_i) \\ \sim \text{natural poisson}(t_i | a_i)$$

GLM

$$L = \prod_i \frac{1}{s} h\left(\frac{t_i}{s}\right) g(\eta_i) e^{\frac{1}{s} \eta_i t_i}$$

$\psi(a) = x$   
 $t_i \sim \text{ID exp. family dist.}$   
 $\eta$  scale

$$\log L = \sum_i \log s + \log h\left(\frac{t_i}{s}\right) + \log g(\eta_i) + \frac{1}{s} \eta_i t_i$$

$$\frac{\partial \log L}{\partial \omega} = \sum_i \frac{1}{g(\eta_i)} \frac{\partial g(\eta_i)}{\partial \omega} + \frac{1}{s} \frac{\partial \eta_i}{\partial \omega} t_i$$

$$= \sum_i \frac{1}{g(\eta_i)} \frac{\partial g(\eta_i)}{\partial \eta} \cdot \frac{\partial \eta_i}{\partial y} \frac{\partial y_i}{\partial a_i} \frac{\partial a_i}{\partial \omega}$$

$$+ \frac{1}{s} \frac{\partial \eta_i}{\partial y} \frac{\partial y_i}{\partial a_i} \frac{\partial a_i}{\partial \omega}$$

$$= \sum_i \frac{\partial \log g(\eta_i)}{\partial \eta_i} \eta_i f'(a_i) \phi(x_i) + \frac{1}{s} t_i \psi(y_i) f'(a_i)$$

Canonical link

$$\eta_i = a_i$$

$$\frac{\partial \eta_i}{\partial w} = \phi(x_i)$$

$$\Rightarrow \frac{\partial \log L}{\partial w} = \frac{\partial \log g(\eta_i)}{\partial \eta_i} \phi(x_i) + \frac{1}{S} t_i \phi(x_i)$$

$$E[U(x)] = - \frac{\partial \log g(\eta)}{\partial \eta}$$

$$E[x] = -S \frac{\partial \log g(\eta)}{\partial \eta}$$

$$\frac{\partial \log g(\eta)}{\partial \eta} = -\frac{1}{S} E[x]$$

$$\Rightarrow \frac{\partial \log L}{\partial w} = -\frac{1}{S} E[t] \phi(x_i) + \frac{1}{S} t_i \phi(x_i)$$

$$= -\frac{1}{S} y_i \phi(x_i) + \frac{1}{S} t_i \phi(x_i)$$

$$= \frac{1}{S} \sum_i (t_i - y_i) \phi(x_i)$$

choose  $f$

$\psi$  is determined by exp-family dist. type

$t_i$  describes data-generation

$$\frac{\partial \log L}{\partial w} = -\frac{1}{S} \sum f'(a_i) \phi(x_i) \phi(x_i)^T$$

$$= -\frac{1}{S} \phi^T R \phi$$

$$R = \text{diag}(r_i) \quad r_i = f'(a_i)$$

$$\frac{\partial \log L}{\partial w} = \sum_i \frac{\partial \log g(y_i)}{\partial \eta_i} \psi'(y_i) f'(a_i) \phi(x_i)$$

$$= \sum_i \frac{1}{s} (t_i - y_i) \psi'(y_i) f'(a_i) \phi(x_i)$$

$\phi^T$

$$\frac{\partial \log L}{\partial w \partial w^T} = \sum_i \frac{1}{s} (t_i - y_i) [\psi'(y_i) f''(a_i) \phi(x_i) \phi(x_i)^T$$

$$+ f'(a_i)^2 \psi''(y_i) \phi(x_i) \phi(x_i)^T]$$

$$- \frac{1}{s} \psi'(y_i) f'(a_i)^2 \phi(x_i) \phi(x_i)^T$$

$$\text{let } r_i = (t_i - y_i) [\psi'(y_i) f''(a_i) + f'(a_i)^2 \psi''(y_i) - \psi'(y_i) f'(a_i)^2]$$

$$\Rightarrow \sum_i \frac{1}{s} r_i \phi(x_i) \phi(x_i)^T = -\frac{1}{s} \Phi^T R \Phi$$

$$w \leftarrow w + s (\Phi^T R \Phi)^{-1} \frac{1}{s} \Phi^T (t - y)$$

} Canonical  
link

$$R = \text{diag}(f'(a_i))$$

Normal  $f(a) = a$      $f'(a) = 1$      $R = I$

Bernoulli  $f(a) = \sigma(a)$      $f'(a) = y_i(1-y_i)$

Poisson  $f(a) = e^a$      $f'(a) = e^a$

# Machine Learning.

## Logistic Regression

$$a_i = w^T \phi(x_i)$$

$$y_i = \sigma(a_i)$$

$$L = \prod_i \sigma(w^T \phi(x_i))^{t_i} (1 - \sigma(w^T \phi(x_i)))^{1-t_i}$$

$$\frac{\partial \log L}{\partial w} = \Phi^T (t - y)$$

$$\frac{\partial^2 \log L}{\partial w \partial w^T} = -\Phi^T R \Phi \quad R = \text{diag}(y_i (1 - y_i))$$

$$w \leftarrow w - (\Phi^T R \Phi)^{-1} \Phi^T (t - y)$$

iterative method

what would be a conjugate prior for  $w$ ?

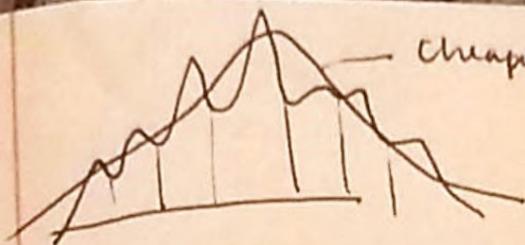
prior  $\times$  likelihood  $\propto$  posterior

same form

No known PDF satisfies conjugate requirement

Let's use a normal prior,  $w \sim N(\mu_0, \Sigma_0)$

(since it's most convenient)



Cheapest approx. by gaussian

This model is not conjugate

$$t_i | w \sim \text{Bernoulli}(w^T \phi(x_i), \frac{1}{\beta})$$

Posterior  $\propto$  prior  $\times$  likelihood

$$\text{also, posterior} \propto \prod y_i^{t_i} (1-y_i)^{1-t_i} \left(\frac{1}{2\pi}\right)^{d/2} \frac{1}{|S_0|^{d/2}} e^{-\frac{1}{2}(w-w_0)^T S_0^{-1} (w-w_0)}$$

No known form for posterior

Sol 1: Maybe we can represent it "indirectly"  
(typically via sampling)

Sol 2: Approximate posterior "as well as we can"

Before Posterior, let's compute MAP.

$$\log \text{Posterior} = \text{const} + \sum t_i \ln y_i + \sum (1-t_i) \ln(1-y_i) - \frac{1}{2} (w-w_0)^T S_0^{-1} (w-w_0)$$

diff wrt  $w$ .

$$\frac{d}{dw} \log \text{Posterior} = 0 + \phi^T (t-y) - S_0^{-1} (w-w_0)$$

(no closed form solution for  $w$ )

$$\frac{d^2}{dw dw^T} \log \text{Posterior} = -\phi^T R \phi - S_0^{-1}$$

$$\frac{d^2}{dw dw^T} \left( \frac{1}{N} \sum \phi \phi^T \right) = \frac{1}{N} \sum \phi \phi^T$$

$$w \leftarrow w - H^{-1} G$$

$$= w - (H^{-1}) G$$

$$= w - (\phi^T R \phi + S_0^{-1})^{-1} (\phi^T (y-t) + S_0^{-1} (w-w_0))$$

finds  $w_{MAP}$

## Laplace Approximation

1D case:

want to approximate  $f(x)$  as  $\mathcal{N}$

$$f(x) \propto e^{-\frac{1}{2} \frac{(x-\mu)^2}{\sigma^2}}$$

So, approx.  $g(x) = \log f(x)$  as a quadratic fn.

$$x = x_0 + h$$

Taylor expansion  $\rightarrow$

$$g(x) \approx g(x_0) + \underbrace{g'(x_0) \cdot h}_0 + \frac{1}{2} g''(x_0) h^2 + \dots$$

ignore higher order terms

$$= g(x_0) + \frac{1}{2} g''(x_0) (x-x_0)^2$$

$$g'(x_0) = 0 \Rightarrow x_0 = \mu$$

$$A = \frac{1}{\sigma^2} = -g''(x_0)$$

point of i.e. mean of normal = point of curvature at mean (maxima of  $g$  is same)

$$f(x) \propto e^{-\frac{A}{2} (x-x_0)^2} = e^{-\frac{1}{2\sigma^2} (x-\mu)^2}$$

Multivariate case

$$A = -H^{-1}$$

$$f(x) \propto e^{-\frac{1}{2} (x-x_0)^T H (x-x_0)}$$

$$= e^{-\frac{1}{2} (x-x_0)^T A^{-1} (x-x_0)}$$

$A$  is known as covariance matrix

Coming back to Logistic Regression

$$x_0 = w_{\text{MAP}}$$

$$H = -(\Phi^T R \Phi + S_0^{-1})$$

$$\Rightarrow m_N = w_{\text{MAP}}$$

$$S_N = (\Phi^T R \Phi + S_0^{-1})^{-1}$$

$$w_{\text{MAP}} \sim N(m_N, S_N)$$

How to predict?

Using  $w_{\text{MAP}}$ : Given  $x_{N+1}$  predict  $p(c=1) = \sigma(w_{\text{MAP}}^T \Phi(x_{N+1}))$

For Bayesian Solution

$$P(c=1) = \int_w P(w | m_N, S_N) p(c=1 | w) dw$$

$$\int_w N(w | m_N, S_N) \sigma(w^T \Phi(x_{N+1})) dw$$

Approximate  $\sigma(a)$  as  $\phi(\lambda a)$   $\phi = \text{PDF of normal dist}$   
mean = 0, variance = 1

$$\lambda = \sqrt{\frac{\pi}{8}}$$

$$\sigma(a) \approx \phi(\lambda a)$$

$$a = w^T \Phi(x_{n+1})$$

$$a \sim N(\Phi(x_{n+1})^T \mu_N, \Phi(x_{n+1})^T \Sigma_N \Phi(x_{n+1}))$$

if  $w$  is gaussian, a linear transform of  $w$  is also gaussian

$$P(c=1) = \int N(a | \mu_a, \sigma_a^2) \sigma(a) da$$
$$= \int N(a | \mu_a, \sigma_a^2) \Phi(\lambda a) da$$

Final result

$$\sigma \left( \frac{\mu_a}{\sqrt{1 + \frac{\pi}{8} \sigma_a^2}} \right)$$

$$\sigma: \quad x > 0 \Rightarrow 1$$

$$x < 0 \Rightarrow 0$$

(+ same cost of +ve & -ve labels)

$P(c=1)$  depends only on sign of  $\mu_a$

# Machine Learning

## Applying ML Algorithms,

Nearest neighbours and decision trees,

KNN algorithm for classification

store all examples

find  $k$  nearest neighbours

predict label based on voting for each neighbour

can be for regression

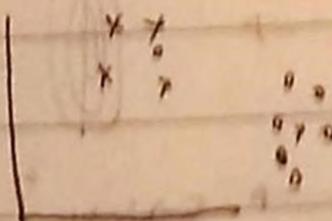
take mean of  $k$  nearest neighbours.

\* NON PARAMETRIC METHOD.

no prior commitment to hypothesis

complexity increases w/ more data

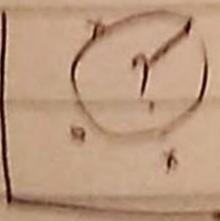
! noise



increase value of  $k$  for random noise

! query by example

Search is expensive



use distance inequality

geometric D.P. ( $k$  nearest)

$k$  is free parameter

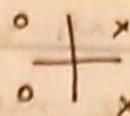
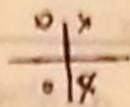
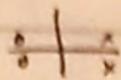
how to choose  $k$ ?

use validation data to evaluate how each  $k$  performs  
model selection

! sensitivity to how data is presented (scale)

since it depends on distance

normalize  $\rightarrow$  linear  $\rightarrow$  Z scaling



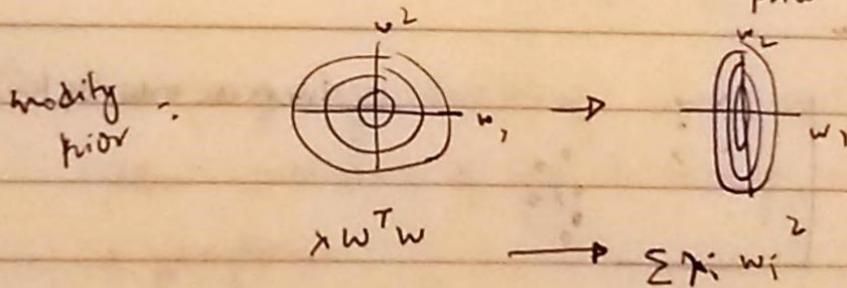
Sensitive to irrelevant features

irrelevant features dominate relevant features

apply dimensionality reduction

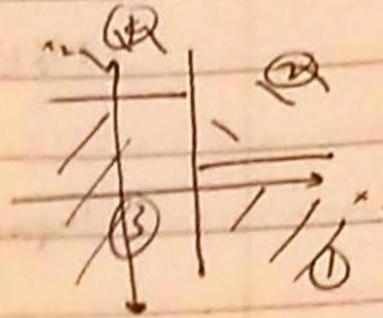
Bayes-LP

$$\sum (t_i - u^T \phi(x_i))^2 + \underbrace{\lambda W^T W}_{\text{prior}}$$

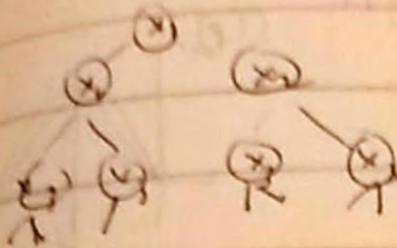


# Decision Trees.

non-parametric and non-probabilistic classifier.



recursively split feature space



! tree can be very large (exponential)  
! it may overfit

how to build a good tree (best tree = NP hard)

Splitting criteria.

algorithm:

if data has pure class

make leaf

else:

pick feature to split on

split data into subsets

apply algorithm recursively for each subset

Measure uncertainty

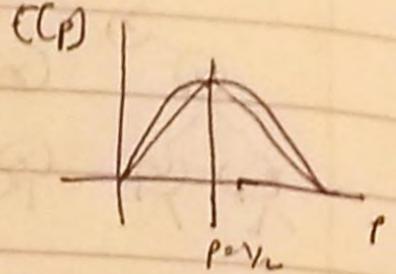
entropy - classification

MSE - regression

(accuracy does not work as well)

Information gain = reduction in uncertainty due to split.

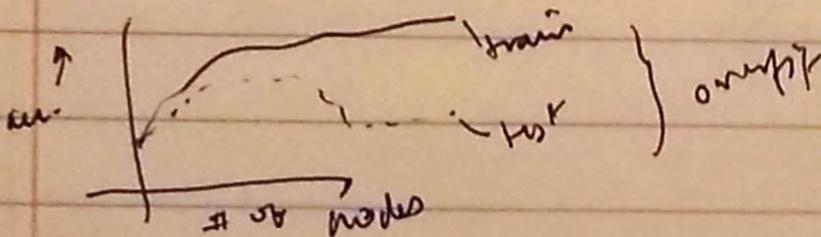
$$\text{Entropy}(P_1, \dots, P_n) = -\sum P_i \log P_i$$



$$\text{Gain}(\text{split}) = \text{Ent}(S) - \sum \frac{|S_j|}{|S|} \text{Ent}(S_j)$$

Real valued Attributes.

$x_1$									} expanded overfit
2.3	T	2.3	3.5	1.6	2.7	8.3	...		
3.5	-								
1.6	-	-	+	+	-	+	-		
2.7	+	1.6	2.3	2.7	3.5	6.5	8.3		
8.3	-	① only finite # points make d'Hermite							
6.5	+	② no need to test values in [2.3, 2.7]							



solutions to overfitting  
prevent -

min # points at any level

min. information gain

grow tree to full size.

then prune use valid. set

} best

ex. Reduced error pruning

# App Machine Learning

## Applying ML

individual feature preprocessing

linear scaling to  $[0, 1]$

$$x \leftarrow \frac{x - x_{\min}}{x_{\max} - x_{\min}}$$

normal scaling

$$x \leftarrow \frac{x - \mu}{\sigma}$$

## Discretizing features

unsupervised

1. equal bin size      predetermined by range
2. equal frequency      adapts to data
3. cluster

Supervised.

use labels. Run decision tree on single feature  
most helpful after pruning

discrete to numerical

unit vector      0000, 0100, 0010, 0001

increasing weight vectors

1000, 1100, 1110, 1111

## Manifold methods

data resides on a "manifold"

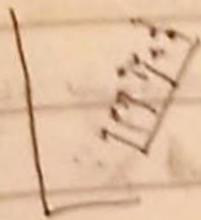
embed data in low dim space, preserving local distances.

process "embedding"

### PCA - Principal Component Analysis

linear dim. reduction

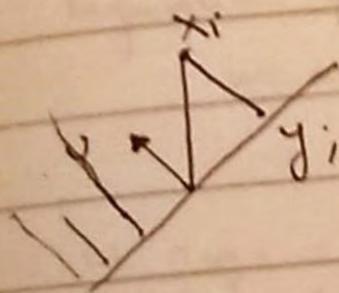
project data onto  $k$  dim. with max variance



center data matrix

$$\Phi^T \Phi = V \Lambda V^T \quad \text{eigen decomposition}$$

take top  $k$  eigenvectors.



$$\text{Data} = x_1 \dots x_N$$

$$y = u^T x_i$$

$$\bar{x} = \frac{1}{N} \sum x_i$$

$$\bar{y} = \frac{1}{N} \sum y_i$$

$$\bar{y} = \frac{1}{N} \sum u^T x_i = \frac{1}{N} u^T \bar{x}$$

Projected variance

$$J = \frac{1}{N} \sum (y_i - \bar{y})^2$$

want to max  $J$

vector

scalar

$$\begin{aligned}
 \text{also, } \bar{S} &= \frac{1}{N} \sum_i [U^T (x_i - \bar{x})]^2 \\
 &= \frac{1}{N} \sum_i U^T (x_i - \bar{x}) (x_i - \bar{x})^T U \\
 &= U^T \left[ \frac{1}{N} \sum_i (x_i - \bar{x}) (x_i - \bar{x})^T \right] U \\
 &= U^T \Sigma U
 \end{aligned}$$

constraint norm  $U = 1$

Use Lagrange Multiplier

objective +  $\lambda$ (constraint) = new objective  
 solve for original vars. and  $\lambda$

$$\max U^T S U \quad \text{s.t. } U^T U = 1$$

$$\equiv U^T S U + \lambda (U^T U - 1)$$

$$\frac{\partial \mathcal{L}(U, \lambda)}{\partial \lambda} = 1 - U^T U = 0 \Rightarrow \|U\| = 1$$

$$\frac{\partial \mathcal{L}(U, \lambda)}{\partial U} = 2SU - 2\lambda U = 0$$

$$S U = \lambda U \quad \begin{array}{l} \text{eigenvalue} \\ \text{eigenvector} \end{array} \quad \|U\| = 1$$

which eigenvector?

$$S = U^T S U \Rightarrow U^T \lambda U = \lambda \|U\|^2$$

pick max eigen value

Projection =  $\Phi U$

Feature Selection.

Filter method

calculate score (ex. info gain, correlation w/ label)

for each feature

we pick top  $k$

Issue - may end up choosing same / similar duplicate features

L1 Regularization

Regularized linear regression

$$w = \arg \min \underbrace{\frac{1}{2} \sum (\omega^T \phi(x_i) - t_i)^2}_{\text{loss}} + \underbrace{\lambda \sum_{k=1}^K \omega_k^2}_{\text{regularization}}$$

L1 reg.

$$w = \arg \min \frac{1}{2} \text{LOSS} + \lambda \sum_{k=1}^K |w_k|$$

use Laplace distribution

instead of gaussian for prior

Evaluating ML outcomes.

what to measure?

Regression, Classification

MSE

acc.

Confusion matrix

	+	-	← classified as
+	TP	FN	
-	FP	TN	

$$acc = \frac{TP + TN}{TP + TN + FN + FP}$$

IR terminology

Ignore  
true  
negative

$$Precision = \frac{TP}{TP + FP}$$

of those that I predicted,  
how many are POSITIVE

$$Recall = \frac{TP}{TP + FN}$$

of the ones that I should've  
found how many did I find

$$F = \frac{2 \cdot PR}{R + P}$$

medical terminology

$$sensitivity = recall$$

accuracy in + class

$$Specificity = \frac{TN}{TN + FP}$$

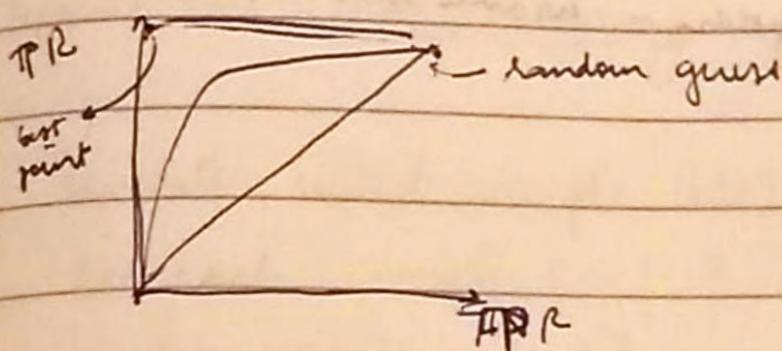
accuracy in - class

signal detection

$$TP_{rate} = Recall$$

$$FP_{rate} = 1 - Specificity$$

ROC (receiver operator characteristic) curve



get points by changing threshold

area under ROC curve

( $< 1 \sim$  probability)

$\neq$  that random example from test set is classified correctly

How to measure?

validation set method

+ unbiased estimate of data

- variance due to choice of valid set

- wastes data

do many times and take average

(-introduces bias)

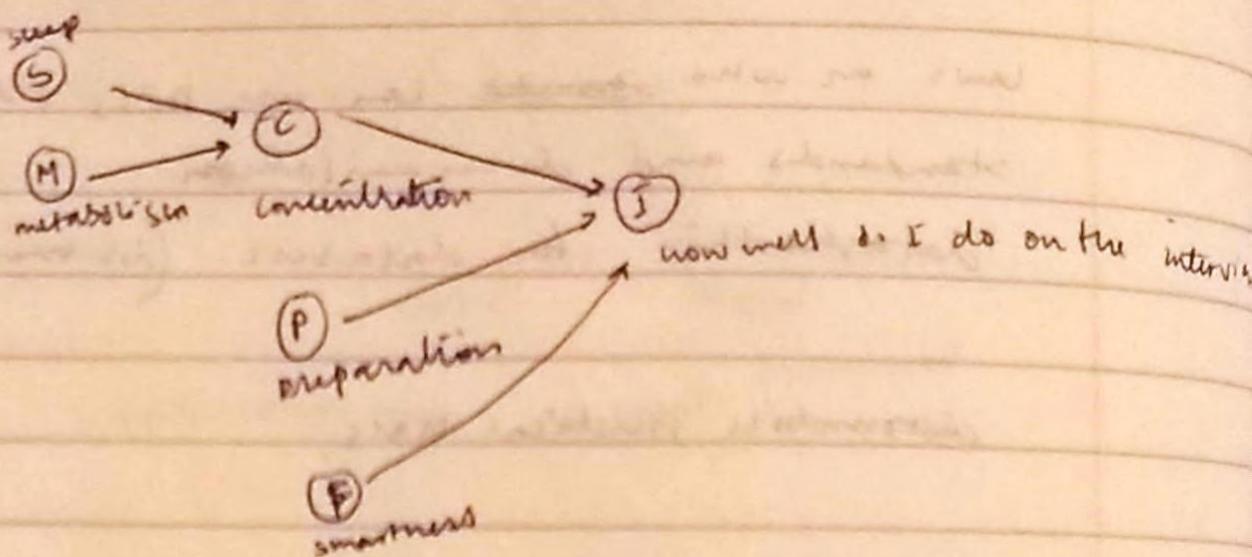
$\rightarrow$  k fold cross validation (disjoint)

(= class label dist. same)

$\rightarrow$  stratified CV

# Machine Learning

## Graphical Models



## Bayesian network

a directed acyclic graph  
probabilistic relationship b/w variables  
for every node  $v$ :  $P(v | \text{parents}(v))$

## General form

Nodes are  $X_1, \dots, X_N$

$$P(X_i | \text{Pa}(X_i))$$

## Joint Dist

$$P(X_1, \dots, X_N) = \prod_i P(X_i | \text{Pa}(X_i))$$

Undirected Graphical models

(Markov Random Fields)

Graphs with no edges

For every clique in graph  
potential function  $\psi(x_c)$



$$P(x_1, \dots, x_n) \propto \prod_c \psi_c(x_c)$$

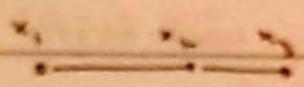
$$c_1 = 1, 2, 3, 4$$

$$c_2 = 2, 5$$

$$c_3 = 5, 4, 7$$

$$c_4 = 7, 8$$

or



$$c_1 = 1, 2$$

$$c_2 = 2, 3$$

	$x_1$	$x_2$	$\psi_c$
$\psi_{c_1}$	0	0	5
	0	1	1
	1	0	3
	1	1	100
	$x_2$	$x_3$	
$\psi_{c_2}$	0	0	1
	0	1	1
	1	0	2
	1	1	2

$$P(x_1, \dots, x_n) = \frac{1}{Z} \prod_c \psi_c(x_c)$$

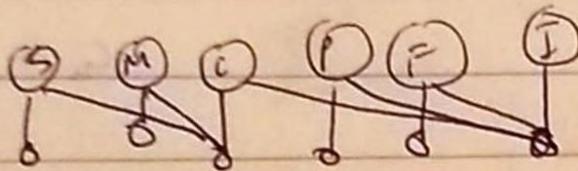
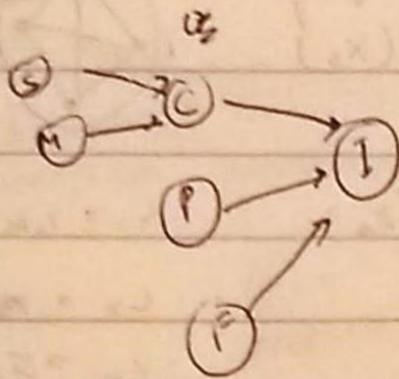
$$Z = \sum_{x_1, \dots, x_n} \prod_c \psi_c(x_c)$$

a generalization  
of binary net  
 $c_i = i$  and parents  
 $\psi(x_i, p_i(x_i))$

More general  $\rightarrow$  factor graph.

Random Variables  $(x_1, \dots, x_n)$

and functions of R.V.s.



in linear regression

in Bayesian linear regression

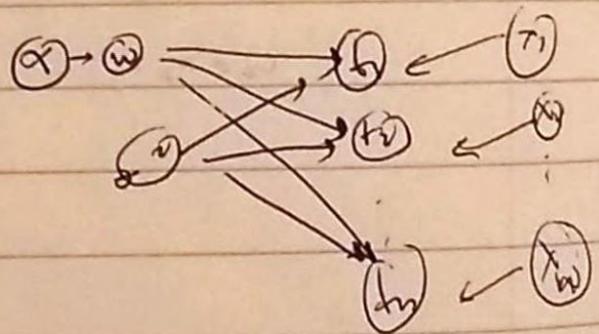
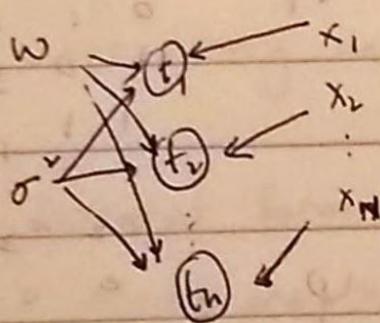
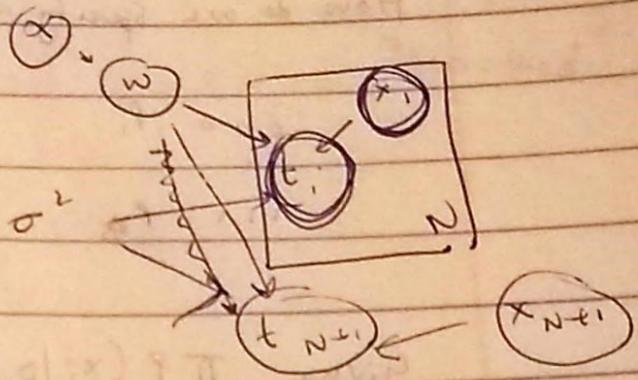
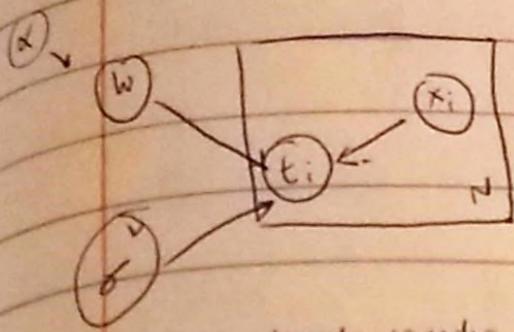


Plate notation.



observe some nodes,  
ML, MAP:

find assignment to some variable ( $w$ )  
s.t.  $P(\text{evidence} | w)$  is Max.

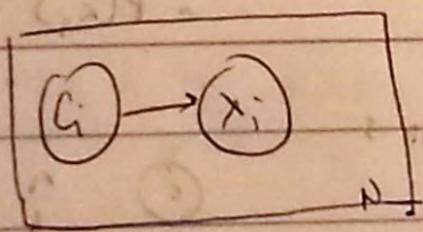
PA

Predictive distribution

find  $P(t_{N+1} | \text{Evidence})$

Generative model:

$$P(c_i) \cdot P(x_i | c_i)$$



How do we specify a dist. over 3 binary r.v.?

$$\begin{matrix} 000 & p_1 \\ \vdots & \\ \dots & p_8 \end{matrix} \quad \sum p_i = 1$$

Given  $\prod P(x_i | p_i(x_i))$

Q obs  ~~$x_3 = 1$~~   $x_3 = 1$

$$P(x_2 = 1) = ?$$

$$P(x_2 = 1) = \sum_{x_1, x_3} P(x_1, x_2 = 1, x_3)$$

(Can ~~not~~ first write a full table of joint dist. and marginalize variables not of interest ( $x_1, x_3$ ))

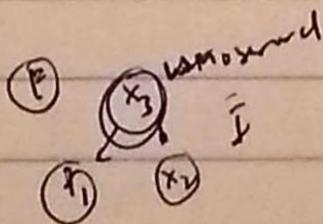
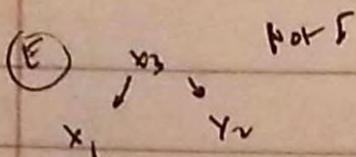
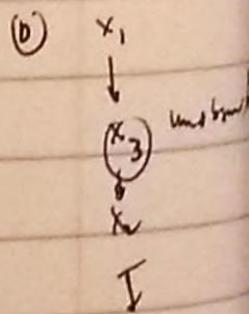
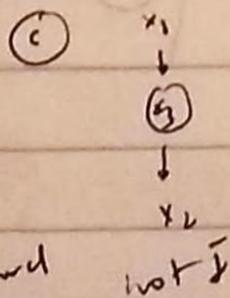
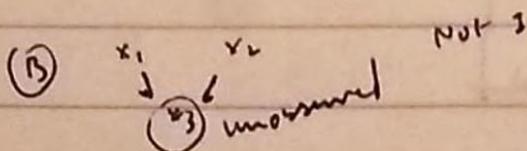
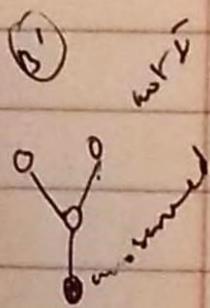
$J = x_1, x_2$

(A)  $x_1, x_2, x_3$   $\downarrow$   $x_3$

$$P(x_1, x_2, x_3) = P(x_1) P(x_2) P(x_3 | x_1, x_2)$$

$$P(x_1, x_2) = \sum P(x_1) P(x_2) P(x_3 | x_1, x_2)$$

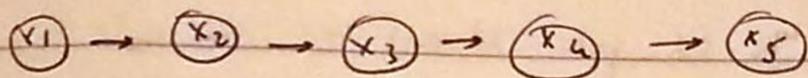
$$= P(x_1) P(x_2) \sum \underbrace{P(x_3 | x_1, x_2)}_{= 1}$$



head to head assumed  
 incoming outgoing assumed  
 tail to tail assumed

Theorem:  $v$  is independent of  $U$

$\Leftrightarrow$  every path from  $v \in V$  to  $u \in U$  is "blocked"



$$P(x_1 = 1) = 0.7$$

$$P(x_i = 1 | x_{i-1} = 1) = 0.9$$

$$P(x_i = 1 | x_{i-1} = 0) = 0.3$$

①  $P(x_3 = 1)$

no witness.

②  $P(x_3 = 1 | x_1 = 1)$

parent to children

③  $P(x_3 = 1 | x_5 = 1)$

children to parent

$$P(x_3) = \sum_{x_1, x_2, x_4, x_5} P(x_1) P(x_2 | x_1) P(x_3 = 1 | x_2) P(x_4 | x_3 = 1) P(x_5 | x_4)$$

$$P(x_1 = 1) = 0.7$$

$$P(x_2 = 1) = \sum_{v \in \{0,1\}} P(x_1 = v) P(x_2 = 1 | x_1 = v)$$

$$= 0.72$$

$$P(x_3 = 1) = \sum_{x_2 = v} P(x_2 = v) P(x_3 = 1 | x_2 = v)$$

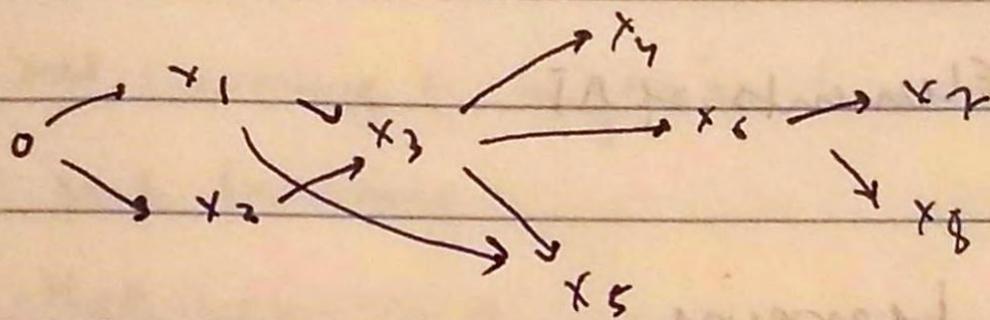
$$\begin{aligned}
 P(X_3=1) &= \sum_{x_1, x_2, x_4, x_5} P(x_1) P(x_2|x_1) P(x_3=1|x_2) P(x_4|x_3) P(x_5|x_4) \\
 &= \sum_{x_1, x_2, x_4} P(x_1) P(x_2|x_1) P(x_3=1|x_2) P(x_4|x_3) \sum_{x_5} P(x_5|x_4) \\
 &= \sum_{x_1, x_2} P(x_1) P(x_2|x_1) P(x_3=1|x_2) \sum_{x_4} P(x_4|x_3) \\
 &= \sum_{x_2} P(x_3=1|x_2) \sum_{x_1} P(x_1) P(x_2|x_1) \\
 &= P(x_3=1)
 \end{aligned}$$

$$(2) \quad P(X_1=1 | X_3=1) = \frac{P(X_1=1, X_3=1)}{P(X_3=1)}$$

$$(3) \quad P(X_3=1 | X_5=1) = \frac{P(X_3=1, X_5=1)}{P(X_5=1)}$$

$$P(X_3=1, X_5=1) = \sum_{x_1, x_2, x_4, x_5} P(x_1) P(x_2|x_1) P(x_3=1|x_2) P(x_4|x_3) P(x_5=1|x_4)$$

$$= \sum_{x_1, x_2} P(x_1) P(x_2|x_1) P(x_3=1|x_2) \sum_{x_4, x_5} P(x_4|x_3) P(x_5=1|x_4)$$

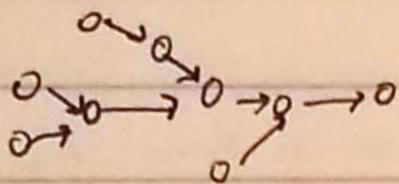


Sum  $x_7$   $\Rightarrow$  result depends on

$x_1, x_2, x_3, x_4, x_5, x_6$

## Machine Learning

If Bayesian net is a polytree  
then, var. elimination produces tables  
which are  $\leq$  tables in original B.N.



if Bayesian net is not polytree,  
tables could be  $>$  than size of tables in B.N.

$$\sum_{x_i} f(x_1, x_2, x_3) g(x_1, x_5, x_6)$$

= function of  $(x_2, x_3, x_5, x_6)$

for continuous R.V.,

$$P(x_1) = \int_{x_2} P(x_1 | x_2) P(x_2) dx$$

integrations should be simple

var. elim. is NP hard. for non polytrees

Belief Propagation (loopy B.P.)

assume graph is polytree  
approximate inference.

Alternate idea:

instead of computing marginals exactly,  
try to sample from the marginal  
distribution.

\*x:

logistic regression

$P(w | \text{data})$

Previously, we computed a wrong

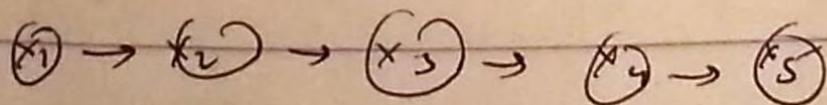
posterior  $\hat{P}(w | \text{data})$

instead, try to sample  $w_1, w_2, \dots, w_k$

$w_i \sim P(w | \text{data})$

- To predict instead of  $\int P(w | \text{data}) P(y_{\text{next}} | w) dw$  pred dist.

compute  $\frac{1}{k} \sum_i P(y_{\text{next}} | w_i)$



$P(x_2)$

$P(x_3 | x_1=1)$

$P(x_3 | x_5=1)$

sample  $x_1$ , then  $x_2 | x_1$ , then  $x_3 | x_2 \dots$

fix  $x_1=1 \dots$

@ rejection sampling

Sampling  $\equiv$  monte-carlo.

Ⓐ Rejection Sampling

take sample, discard if  $x_5 \neq 1$   
correct but slow (wastes sampling time)

Ⓑ Likelihood weighting

instead of sampling and rejecting  
stop after 1100 and force  $x_5 = 1$   
and use with weight of 0.3.  $= P(x_5=1 | x_4=1)$

11001 .3

10101 .3

00101 .3

0.9 total sample

does not waste samples. still slow.

For these algorithms, we must be able to  
sample from  $P(x_i | P_a(x_i))$

Easy for discrete. Various methods & tricks  
for continuous variables.

## Monte Carlo Markov Chain

Sample entire string at once.

$(101 \rightarrow) 10111 \rightarrow) 00101 \rightarrow) \dots$

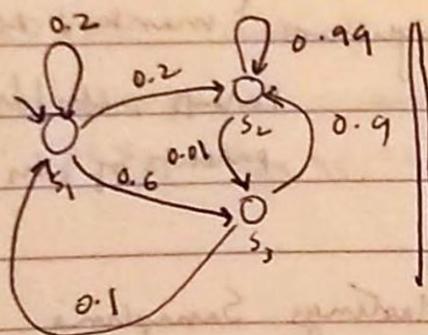
define a random process

in limit, the distribution is same as exactly what we want.

## Markov Chain

Nodes are states.

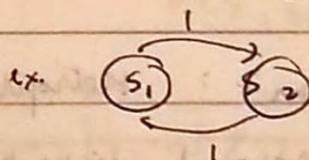
Edges are probabilistic transitions.



stationary distribution over states

$$\forall s \quad P(s) = P(\text{arrive in } s \text{ in next step})$$

$$\forall i \quad P(s_i) = \sum_j P(s_j) P(s_i | s_j)$$



ex. does not have s.p.

We will build a Markov chain s.t. states are value configurations of Bayes net and its stationary distribution is  $P(\text{unobserved vars.} | \text{observed vars.})$

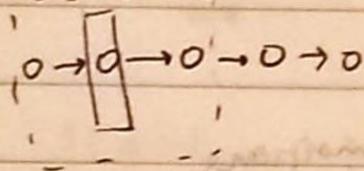
Transitions in the MC go from  $x_1, \dots, x_n$  to  
(11001)

another valuation (01001)

Option 1: Gibbs Sampling

Pick  $i \in \{1, \dots, N\}$  at random (uniformly)

Pick  $x_i$  from dist  $P(x_i | x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_n)$



need only neighbours "Markov blanket"

parents, children,  
parents of children

Option 2: Metropolis's Hastings Sampling

\* Proposal distribution  $q(y|x)$

repeat ① Pick  $y$  from  $q(y|x)$

② compute accept. probability  $A = \min\left(1, \frac{P(y)q(x|y)}{P(x)q(y|x)}\right)$

③ Accept  $y$  i.e.  $x \leftarrow y$  with prob  $A$

or stationary dist

### Detailed Balance

Markov Chain with Transition prob  $T$

has Detailed Balance relative to  $P$

$$P(a) T(b|a) = P(b) T(a|b)$$

Fact 1 DB  $\rightarrow P$  is stationary for MC

Fact 2 MH has DB for  $P$ .

Fact 3 Gibbs is special case of MH where  $A=1$ .

00100 current state

resample  $x_2$  using Gibbs.

$$P(x_2 | x_{1,3,4,5} = 0100) = \frac{P(x_2 = v \text{ and } x_{1,3,4,5} = 0100)}{P(x_{1,3,4,5} = 0100)}$$

~~$$P(x_1=0) P(x_2=v | x_1=0) P(x_3=1) P(x_4=0) P(x_5=0)$$~~

numerator:  $P(x_1=0) P(x_2=v | x_1=0) P(x_3=1 | x_2=v)$

$$P(x_4=0 | x_3=1) P(x_5=0 | x_4=0)$$

$$v = \{0, 1\}$$

$$P(x_2=0 \text{ and } x_{1,3,4,5} = 0100)$$

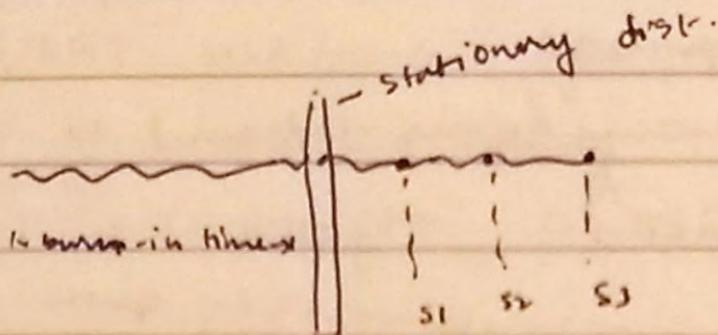
$$P(x_2=1 \text{ and } x_{1,3,4,5} = 0100)$$

$$P(x_2=0 | x_1=0) P(x_3=1 | x_2=0)$$

$$P(x_2=1 | x_1=0) P(x_3=1 | x_2=1)$$

# Machine Learning

## Markov Chain Monte Carlo.



$s_1, s_2, s_3$  are not independent  
but we assume so.

Gibbs sampling

MH sampling

$$p(v_i | v_1, \dots, v_{i-1}, v_{i+1}, \dots, v_n) \quad \text{— can't compute for undirected models}$$
$$\min \left( 1, \frac{p(v') q(v|v')}{p(v) q(v'|v)} \right)$$

use MH

Fact 1: DB implies PC is stationary.

Fact 2: MH satisfies DB for PC.

Fact 3: Gibbs is MH G and.

proof in slides

# Latent Dirichlet Allocation.

completely unsupervised text learning.

Dirichlet

constraint  $\sum \alpha_i = 1$

$$\alpha = (\alpha_1, \dots, \alpha_k)^T \quad \alpha_i = \sum d_i \quad \alpha_i - 1$$

$$p(w|d) = \text{Dir}(M|d) = \frac{\prod (d_{oi}) M_i}{\prod \Gamma(\alpha_i)}$$

Dirichlet list

$$p(\text{structure}) = \prod M_i (M_i | \alpha + m)$$

"topic" : dist over words.

each doc. is about multiple topics.

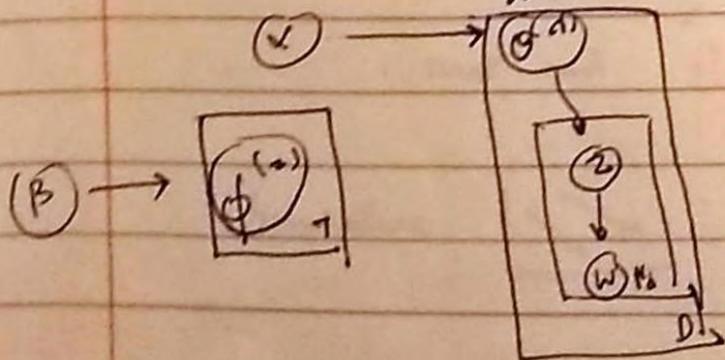
~~each~~ each doc. draws topic from dir.

each topic draws word from dir.

For each doc, for each iteration

decide topic

draw word from topic



LDA - matrix of doc/w. w.s.

Topic model - matrix of probs.

$N$  : total # of words

$N_d$  : # of words in doc  $d$ .

$N_{k,d}$  : # of ~~times~~ times a topic occurred.

$N_{k,d,i}$  : # of times topic  $k$  appeared in  $d$ .

$N_{i,k}$  : # of times word  $i$  occurred in topic  $k$ .

prior:  $\prod_{d=1}^D \text{Dir}(\theta_d | \alpha)$

$\prod_{k=1}^K \text{Dir}(\phi_k | \beta)$

posterior: -

but we do not know topics  $(z_i)$

Gibbs sampling

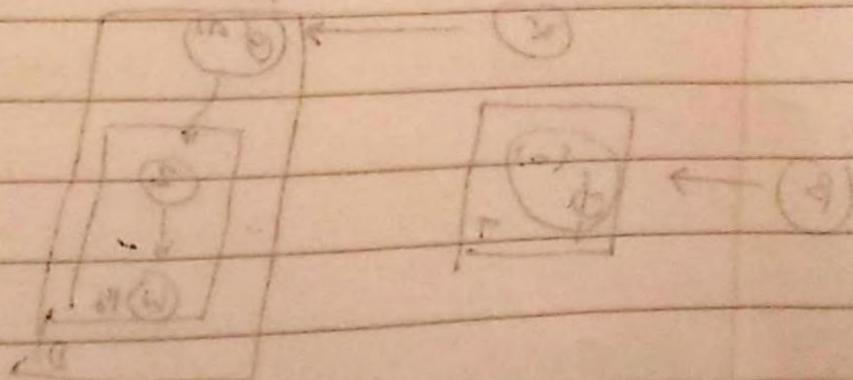
remove word.

Learning  $\alpha$  and  $\beta$ .

Evidence Maximization

direct  $\rightarrow$  exponential

use sum of log of samples



# Machine Learning

$Y$  observed variables

$Z$  hidden variables

want to max.  $P(Y|\theta) = \int P(Y, Z|\theta) dz$

$$Q(\theta^{new}, \theta^{old}) = E_{P(Z|Y, \theta^{old})} [\ln P(Y, Z|\theta^{new})]$$

EM Algorithm

init  $\theta^{old}$

repeat

+ E step: calculate  $Q(\theta^{new}, \theta^{old})$

\* M step: pick  $\theta^{new}$  to max  $Q(\theta^{new}, \theta^{old})$

what does this mean?

Mixture of coin models

for each  $i$

pick  $z_i \in \{1, \dots, k\}$  from discrete  $\{P_1, \dots, P_k\}$

ex.  $k=3$   $z = \{1, 2, 3\}$

$p = \{0.7, 0.1, 0.2\}$

$z_i = 1 \Leftrightarrow 100$

$2 \Leftrightarrow 010$

$3 \Leftrightarrow 001$

flip coin  $z_i$   $T$  times to get  $y_i$

ex.  $T=6$   $Y_i = UHTHTH$

coin  $i$  has  $P(H) = \mu_i$

likelihood =  $\mu_i^{\#H} (1-\mu_i)^{\#T}$

Complete data likelihood

$$L = \prod_i \prod_j \left[ p_j \prod_t \mu_j^{y_{it}} (1-\mu_j)^{1-y_{it}} \right]^{z_{ij}}$$

coins  $\uparrow$   
 labels  $\uparrow$

$$\theta = \{(p_j), \{\mu_j\}\}$$

$$\ln(P(Y, Z | \theta^{new})) = \sum_i \sum_j z_{ij} \left[ \ln p_j + \sum_t y_{it} \ln \mu_j + (1-y_{it}) \ln (1-\mu_j) \right]$$

Next figure out  $Q$ .

$$Q(\theta^{new}, \theta^{old}) = \sum_i \sum_j E_{P(Z|Y, \theta^{old})} [z_{ij}] \dots$$

fn. of new  
params

let  $\alpha_{ij} = p_j P(Y_i | \theta_j) = p_j \prod_t \mu_j^{y_{it}} (1-\mu_j)^{1-y_{it}}$

fn. of old  
params

let  $\gamma_{ij} = E_{P(Z|Y, \theta^{old})} [z_{ij}] = \gamma_{ij}$

$$Q(\theta^{new}, \theta^{old}) = \sum_i \sum_j \gamma_{ij} \ln \alpha_{ij}$$

$$Y_{ij} = E_{P(z|Y, \theta^{old})} [z_{ij}] = P(z_{ij}=1 | Y, \theta^{old})$$

$$= \frac{P(z_{ij}=1, y_i | Y^i, \theta^{old})}{P(y_i | Y^i, \theta^{old})}$$

$$= \frac{P(z_{ij}=1, y_i | \theta^{old})}{P(y_i | \theta^{old})} \quad \text{because } y_i \perp Y^{-i} | \theta^{old}$$

$$\text{Numerator} = P(z_i=j) P(y_i | z_i=j)$$

$$= p_j P(y_i | \theta_j)$$

$$= \underset{\text{binomial}}{\alpha_{ij}} \underset{\text{assumed}}{P(y_i | \theta_j)}$$

$$\Rightarrow Y_{ij} = \frac{\alpha_{ij}}{\sum_k \alpha_{ik}} \quad \text{I}$$

$$Q = \sum_i \sum_j Y_{ij} [\ln p_j + \sum_t y_{it} \ln m_j + (1 - y_{it}) \ln (1 - m_j)]$$

$p_j, m_j$  are new.

$$\text{Must satisfy } \sum_j p_j = 1 \quad \left\| \begin{array}{l} \text{use Lagrange} \\ \text{multipliers} \end{array} \right.$$

$$Q = \text{Const}(p_j) + \sum_i \sum_j Y_{ij} \ln p_j$$

$$L = \sum_i \sum_j Y_{ij} \ln p_j + \lambda (\sum_j p_j - 1)$$

No. of examples in class j

$$\frac{\partial}{\partial \lambda} \sum p_j - 1 = 0; \quad \frac{\partial}{\partial p_j} \sum_i \sum_t r_{ij} \cdot \frac{1}{p_j} + \lambda = 0$$

$$\Rightarrow p_j = -\frac{1}{\lambda} \sum_i r_{ij}$$

$$= -\frac{1}{\lambda} N_j$$

$$N_j = \sum_i r_{ij}$$

$$\sum_j p_j = 1 \Rightarrow \sum_j -\frac{1}{\lambda} N_j = 1 \Rightarrow N = \lambda$$

$$p_j = \frac{N_j}{N} \quad \text{II}$$

$$\frac{\partial}{\partial \mu_j} = \sum_i \sum_t \left[ \frac{y_{it}}{\mu_j} - \frac{1-y_{it}}{1-\mu_j} \right] r_{ij} = 0$$

$$\sum_i \sum_t (y_{it}(1-\mu_j) - \mu_j(1-y_{it})) r_{ij} = 0$$

$$\sum_i \sum_t r_{ij} (y_{it} - y_{it} \mu_j - \mu_j + \mu_j y_{it}) = 0$$

$$\sum_i \sum_t r_{ij} \mu_j = \sum_i \sum_t r_{ij} y_{it}$$

$$\Rightarrow \mu_j \sum_i \sum_t r_{ij} = \sum_i r_{ij} \left( \sum_t y_{it} \right)$$

$$\Rightarrow \mu_j T N_j = \sum_i r_{ij} \left( \sum_t y_{it} \right)$$

$$\Rightarrow \mu_j = \frac{\sum_i r_{ij} \left( \sum_t y_{it} \right)}{T N_j} \quad \text{III}$$

EM for Mixture of Gauss

init  $\{\mu_j, \sigma_j\}$

Repeat

Calculate  $\gamma_{ij}$  using I

Calculate  $\{\mu_j, \sigma_j\}$  using II, III

EM does marginal likelihood estimation when one or more parameters are not observed.

Why does it work?

Fact if  $Q(\theta^{new}, \theta^{old}) > Q(\theta^{old}, \theta^{old})$

then  $P(Y|\theta^{new}) > P(Y|\theta^{old})$

Proof  $0 < Q(\theta^{new}, \theta^{old}) - Q(\theta^{old}, \theta^{old})$

$$= E_{P(z|Y, \theta^{old})} [\ln P(Y, z|\theta^{new}) - \ln P(Y, z|\theta^{old})]$$

$$= E_{P(z|Y, \theta^{old})} \left[ \ln \frac{P(Y|\theta^{new}) P(z|Y, \theta^{new})}{P(Y|\theta^{old}) P(z|Y, \theta^{old})} \right]$$

$$= E_{P(z)} \left[ \ln \frac{P(Y|\theta^{new})}{P(Y|\theta^{old})} + E_{P(z)} \left[ \ln \frac{P(z|Y, \theta^{new})}{P(z|Y, \theta^{old})} \right] \right]$$

no 2 term

$$0 \leq \ln \frac{P(Y|\theta^{new})}{P(Y|\theta^{old})} \Rightarrow \frac{P(Y|\theta^{new})}{P(Y|\theta^{old})} \geq 1$$

less than 0  
down

Jensen's inequality: concave  $f$

ex. variance

$$E[X]^2 - E[X^2] \geq 0$$



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

$P_1(v)$   $P_2(v)$

$k_L$  divergence  
not symmetric

$$d_{k_L}(P_1 \parallel P_2) = \int P_1(v) \ln \frac{P_1(v)}{P_2(v)} dv$$

$$= E_{P_1(v)} \left[ \ln \frac{P_1(v)}{P_2(v)} \right] \geq 0$$

$$-d_{k_L}(P_1 \parallel P_2) = E_{P_1(v)} \ln \frac{P_2(v)}{P_1(v)}$$

$$\leq \ln E_{P_1(v)} \frac{P_2(v)}{P_1(v)}$$

$$= \ln \int P_1(v) \frac{P_2(v)}{P_1(v)} dv = \ln 1 = 0$$

# Machine Learning

**Kernel Function** : Fast way to compute inner product in some feature space

$$k(x_i, x_j) = \phi(x_i)^T \phi(x_j)$$

For ex. euclidean  $\frac{(x_i^T x_j)}{\frac{1}{2} \|x_i - x_j\|^2}$ , quadratic  $(x_i^T x_j + 1)^2$ , polynomial  $(x_i^T x_j + 1)^d$

int. polynomial  $\rightarrow$  RBF (e) Alg  $\leftarrow$  kernel  $\leftarrow$  para

**Kernel Method** : Learning algorithm that works with kernels

For ex. Perceptron, SVM, Regularized Linear Regression.

**Merker's Theorem** :  $k(\cdot, \cdot)$  is a kernel  $\Leftrightarrow$

- ①  $k$  is symmetric    ② kernel matrix is Positive Semidefinite  $\forall$  finite points

All eigenvalues  $\geq 0 \Leftrightarrow \forall c \ c^T K c \geq 0$

Proof one dim. if  $k(a, b) = \phi(a)^T \phi(b)$  then  $c^T K c \geq 0$

$$\begin{aligned} c^T K c &= \sum_i \sum_j c_i c_j k(x_i, x_j) \\ &= \sum_i \sum_j c_i c_j \phi(x_i)^T \phi(x_j) \\ &= \left[ \sum_i c_i \phi(x_i)^T \right] \left[ \sum_j c_j \phi(x_j) \right] \\ &= \left\| \sum_i c_i \phi(x_i) \right\|^2 \geq 0 \end{aligned}$$

**Fact** if  $k_1$  is a kernel,  $k_2$  is a kernel

then ①  $k_3 = k_1 + k_2$  is a kernel

②  $k_4 = k_1 \times k_2$  is a kernel.

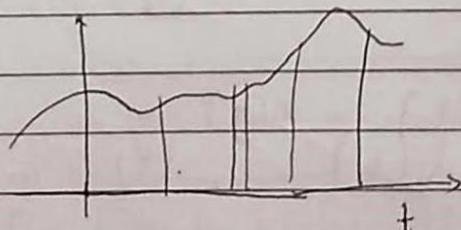
Proof of ①  $c^T k_3 c = c^T (k_1 + k_2) c = c^T k_1 c + c^T k_2 c \geq 0$

After  $k_3(x_i, x_j) = k_1(x_i, x_j) + k_2(x_i, x_j)$

$$\begin{aligned} &= \phi_1^T(x_i) \phi_1(x_j) + \phi_2^T(x_i) \phi_2(x_j) \\ &= \hat{\phi}(a)^T \hat{\phi}(b) \quad \left| \begin{array}{l} \hat{\phi}(a) = \text{concat} \ \phi_1(a) \\ \phi_2(a) \end{array} \right. \end{aligned}$$

## Gaussian Process

A distribution over functions such that for any finite set of inputs  $x_1, \dots, x_N$  the vector of function values



$f = (f(x_1), \dots, f(x_N))^T \sim N((m(x_1), \dots, m(x_N))^T, C)$

is distributed normally

it is specified by mean fn. and covariance

$$C_{ij} = \begin{pmatrix} & j \\ i & \end{pmatrix} = k(x_i, x_j)$$

next point is first in  
covariance matrix

Given  $x_1 \dots x_N$   
 $f_1 \dots f_N$   
 $x_{N+1}$

$$C_{N+1} = \begin{pmatrix} C & v^T \\ v & C_N \end{pmatrix} \quad \begin{matrix} 0 = C(x_{N+1}, x_{N+1}) \\ v = C(x_1, x_{N+1}) \\ \vdots \\ C(x_N, x_{N+1}) \end{matrix}$$

Predict  $f_{N+1}$

$$\bar{f}_{N+1} = (f_1 \dots f_N) \quad C_N = C \text{ applied to } x_1 \dots x_N$$

Assume  $m(x) = 0 \quad \forall x$

$$\bar{f}_{N+1} = (f_{N+1} \quad (\bar{f}_N)^T)^T \sim N(0, C_{N+1})$$

observe  $\bar{f}_N$

$p(f_{N+1})$

$$\Sigma = C - v^T C_N^{-1} v$$

$$M = 0 + v^T C_N^{-1} (\bar{f}_N)$$

Application  
of MVN  
conditional  
template

$$\begin{pmatrix} x_a \\ x_b \end{pmatrix} \sim N \left( \begin{pmatrix} \mu_a \\ \mu_b \end{pmatrix}, \begin{pmatrix} \Sigma_{aa} & \Sigma_{ab} \\ \Sigma_{ba} & \Sigma_{bb} \end{pmatrix} \right)$$

$$\Sigma_{a|b} = \Sigma_{aa} - \Sigma_{ab} \Sigma_{bb}^{-1} \Sigma_{ba}$$

$$M_{a|b} = \mu_a + \Sigma_{ab} \Sigma_{bb}^{-1} (x_b - \mu_b)$$

Bayes LR.

$$p(w) = N(0, \frac{1}{\alpha} I) ; y = \Phi w ; t \sim N(y, \frac{1}{\beta} I)$$

$$t_i \sim N(w^T \phi(x_i), \frac{1}{\beta})$$

(Claim:  $t$  is sampled from gaussian process.

$$E[y] = \Phi E[w] = 0$$

$$E[y y^T] = E[\Phi w w^T \Phi^T]$$

$$= \Phi E[w w^T] \Phi^T$$

$$= \Phi \left[ \frac{1}{\alpha} I \right] \Phi^T = \frac{1}{\alpha} \Phi \Phi^T$$

$$\Phi = \begin{pmatrix} \phi(x_1) \\ \vdots \\ \phi(x_N) \end{pmatrix}_{N \times D}$$

$$\Phi^T \Phi = \begin{pmatrix} \phi(x_1)^T \\ \vdots \\ \phi(x_N)^T \end{pmatrix} \begin{pmatrix} \phi(x_1) \\ \vdots \\ \phi(x_N) \end{pmatrix}$$

$$= K \quad N \times N$$

$$E[t] = E[y] = 0$$

$$E[t t^T] = \text{cov}(y) + \text{cov}(t|y)$$

$$= \frac{1}{\alpha} K + \frac{1}{\beta} I$$

$$\Phi \Phi^T = \begin{pmatrix} \phi(x_1) \phi(x_1)^T \\ \vdots \\ \phi(x_N) \phi(x_N)^T \end{pmatrix}$$

$$= \begin{pmatrix} \phi(x_1) \\ \vdots \\ \phi(x_N) \end{pmatrix} \begin{pmatrix} \phi(x_1)^T \\ \vdots \\ \phi(x_N)^T \end{pmatrix}$$

inner product

For any  $x_1 \dots x_N$

$$t = (t(x_1) \dots t(x_N)) \sim N(0, C)$$

$$C = \frac{1}{\alpha} K + \frac{1}{\beta} I$$

$$C = \frac{1}{\alpha} K + \frac{1}{\beta} I$$

$$K_{ij} = e^{-\frac{1}{2}(x_i - x_j)^2 / s^2}$$

$$\text{Evidence} = P(t | \alpha, \beta) = N(0, C_N)$$

$$\log \tilde{E} = -\frac{N}{2} \log 2\pi - \frac{1}{2} \log |C_N| - \frac{1}{2} t^T C_N^{-1} t$$

= Marginal Likelihood.

$$\frac{\partial}{\partial \alpha} \quad \frac{\partial}{\partial \beta} \quad \frac{\partial}{\partial s} \quad \Rightarrow \text{Gradient Descent}$$

Logistic - Bernoulli?  
if  $m \neq 0$  then?