

Logistic Regression

24.1 Geometric intuition of Logistic Regression.

→ classification Technique

→ Simple & elegant model

NB: Probabilistic model/Tech

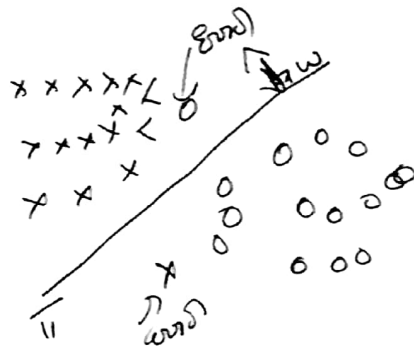
LR: geometric intuition.

Logistic Regression can be interpreted using below Techniques

↳ Geometry

↳ Probability

↳ Loss function.



x → +ve

o → -ve

2D: line } linear
nD: hyperplane } linear

If my data is linear separable

If the π passes through origin $\Rightarrow b=0$

$$w^T x + b = 0 \Rightarrow w^T x = 0$$

Assumption of Log Reg is class are almost/perfectly linearly separable

$$\pi = w^T x + b$$

$\pi = \begin{cases} +ve, & -ve \end{cases} \rightarrow$ given to us

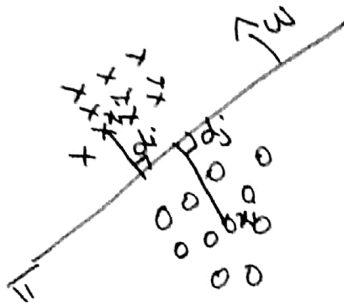
Task to
Find: w & b

Such that the line separates both +ve & -ve bts

Assumptions

NB: conditional independence of features

k-NN: Neighborhood.



$y_i = +1$: +ve pts

-1 : -ve pts

$$y_i \in \{-1, +1\}$$

d_i = distance of point from plane.

$$= \frac{w^T x_i}{\|w\|} ; w \text{ is normal to the plane}$$

$$\|w\| = 1 \Rightarrow \text{unit vector.}$$

$$d_j = w^T x_j$$

Since w & x_i are on the same side $d_i = w^T x_i > 0$

Since w & x_j are ^{not} on the same side $d_j = w^T x_j < 0$

classifier says is

If $w^T x_i > 0$ then $y_i = +1$

$w^T x_j < 0$ then $y_j = -1$

} line passes through origin.

→ Decision surface in LR is a plane

→ change to be v-good

4 min # misclassifications

4 max # correctly classified pts

← as many pts as possible to have $y_i \neq w^T x_i > 0$

$$\max \sum_{i=1}^n y_i w^T x_i$$

optimal w^* means best hyperplane.

$$w^* = \underset{(w)}{\operatorname{argmax}} \sum_{i=1}^n y_i w^T x_i \quad \left. \vphantom{\sum_{i=1}^n y_i w^T x_i} \right\} \text{Optimization problem}$$

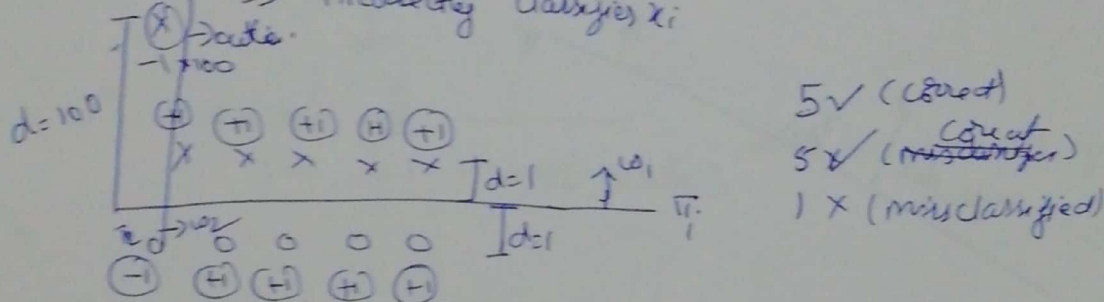
2.4.2 Sigmoid Function & Squashing

$$\operatorname{argmax} \sum_{i=1}^n y_i \underbrace{w^T x_i}_{\rightarrow \text{Signed distance.}}$$

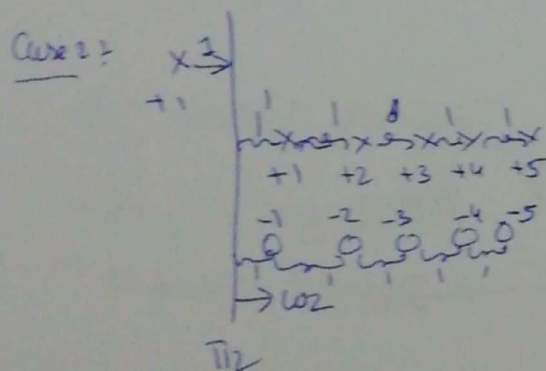
$w^T x_i$ distance from x_i to π (w is a unit vector)

$y_i w^T x_i = +ve \Rightarrow \pi$ as defined by w correctly classifies x_i

$\hookrightarrow -ve \Rightarrow$ incorrectly classifies x_i



Case 1: π_1 is my separator, $\sum y_i w^T x_i = 1+1+1+1+1+1+1+1+1+1-100$
 $\boxed{\dots -90}$



$$\sum_{i=1}^n y_i w_2^T x_i = 1+2+3+4+5 - 1-2-3-4-5 + 1 (\text{outlier})$$

$$= +1$$

$$5 \checkmark$$

$$5 \times$$

$$1 \checkmark$$

One single extreme/outlier pt is changing my model (hyperplane) in

Case 1 which is very bad.

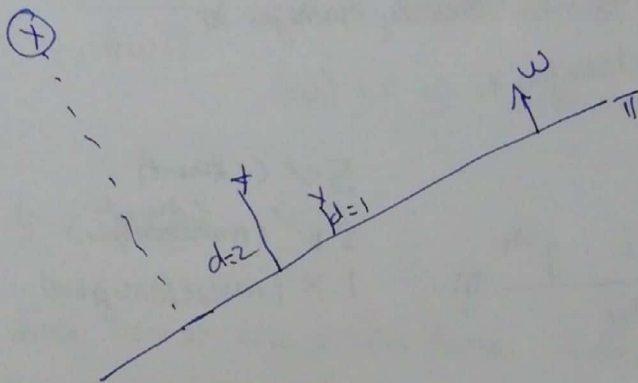
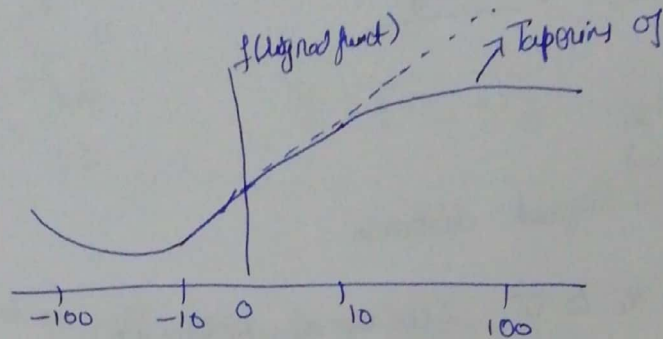
Max. sum. of signed distances not outlier ~~place~~ ^{poor}.

Squashing

idea: Instead of using signed distance.

If signed distance is small \rightarrow use it as is

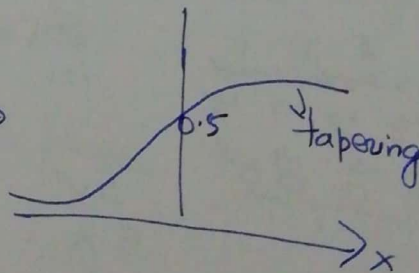
" " large \rightarrow make it smaller as possible.



$$\arg \max_w \sum_{i=1}^n \underbrace{f(y_i w^T x_i)}_{\text{signed distance.}}$$

Sigmoid function

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



\downarrow

max: 1

$$\sigma(0) = 0.5$$

min: 0

we will change our problem to

$$\arg \max_w \sum_{i=1}^n \sigma(y_i w^T x_i)$$

① \rightarrow w is very large $\rightarrow P(y=1) = 0.9999$
 $\rightarrow w^T x_i = 0 \rightarrow P(y=1) = 0.5$ } Probabilistic Interpretation.

Max. sum of signed dist \rightarrow outlier problem.

$\sigma(x) \rightarrow$ Sigmoid
 \hookrightarrow tapering linear
 \hookrightarrow probabilistic model.

max. sum of transformed signed interpretation.

$$w^* = \underset{(w)}{\operatorname{argmax}} \sum_{i=1}^n \sigma(y_i w^T x_i)$$

$$w^* = \underset{(w)}{\operatorname{argmax}} \sum_{i=1}^n \frac{1}{1 + \exp(-y_i w^T x_i)} \leftarrow \text{less impacted by outliers.}$$

disturb $\div (-\infty, \infty)$
 \hookrightarrow (squashing using σ function)
 $d(0 \text{ to } 1)$

why sigmoid function?

- \rightarrow Easy to differentiate
- \rightarrow probabilistic interpretation.

24.3 Mathematical formulation of objective function

$$w^* = \underset{(w)}{\operatorname{argmax}} \sum_{i=1}^n \frac{1}{1 + \exp(-y_i w x_i)} \rightarrow \text{optimization problem.}$$

→ monotonic functions : $g(x)$

$x \uparrow$; $g(x) \uparrow$ monotonically increasing fn.

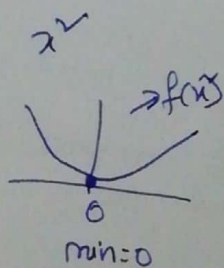
If $x_1 > x_2$ then $g(x_1) > g(x_2)$ then it is called monotonic function

e.g. $\log(x) > 0$; should be > 0

optimization problem:-

$$\rightarrow x = \underset{x}{\operatorname{argmin}} (x^v) = 0$$

best(x)



x^v is mono increasing when $x > 0$
 x^v is " decreasing when $x < 0$

$$g(x) = \log(x)$$

$$x^* = \underset{x}{\operatorname{argmin}} (f(x)) ; f(x) = x^v$$

$$x' = \underset{x}{\operatorname{argmin}} g(f(x))$$

$$x' = \underset{x}{\operatorname{argmin}} \log(x^v)$$

claim $x^* = x'$

If $g(x)$ is a monotonic function

$$\underset{x}{\operatorname{argmin}} f(x) = \underset{x}{\operatorname{argmin}} g(f(x))$$

$$\underset{x}{\operatorname{argmax}} f(x) = \underset{x}{\operatorname{argmax}} g(f(x))$$

$$x \uparrow \rightarrow g(x) \uparrow$$

$$x \uparrow \rightarrow g(x) \downarrow$$

$$w^* = \operatorname{argmax}_w \sum_{i=1}^n \frac{1}{1 + \exp(-y_i w^T x_i)}$$

$g(x) = \log(x)$: monotonic fn.

$$w^* = \operatorname{argmax}_w \sum_{i=1}^n \log \left(\frac{1}{1 + \exp(-y_i w^T x_i)} \right)$$

$$\log(1/x) = -\log(x)$$

$$w^* = \operatorname{argmax}_w \sum_{i=1}^n -\log(1 + \exp(-y_i w^T x_i)) \quad \left. \vphantom{\sum_{i=1}^n} \right\} \text{ geometry}$$

$$\boxed{\operatorname{argmax}_x f(x) = \operatorname{argmin}_x -f(x)}$$

$$w^* = \operatorname{argmin}_w \sum_{i=1}^n \log(1 + \exp(-y_i w^T x_i))$$

$\xrightarrow{\{ -1, 0, 1 \}}$
 $\underbrace{\hspace{2cm}}$
 Signed dist

$$\boxed{\log(e^x) = x}$$

$$\operatorname{argmin}_{(w)} \sum_{i=1}^n \log(1 + \exp(-y_i w^T x_i))$$

$$\operatorname{argmin}_{(w)} \sum_{i=1}^n -y_i w^T x_i$$

Probability
matrix

$$w^* = \operatorname{argmin}_{(w)} \sum_{i=1}^n -y_i \log p_i - (1 - y_i) \log(1 - p_i)$$

$$\boxed{p_i = \sigma(w^T x_i)}$$

24.4 Weight Vector

$$\omega^* = \underset{(\omega)}{\operatorname{argmax}} \sum_{i=1}^n \log(1 + \exp(-y_i \omega^T x_i))$$



$$\text{weight vector } (\omega) = \langle \omega_1, \omega_2, \omega_3, \omega_4, \dots, \omega_d \rangle$$

$\xrightarrow{\text{size}}$ $\rightarrow d$ features of weight vector ω

$$\omega = \langle \omega_1, \omega_2, \omega_3, \dots, \omega_d \rangle$$

$$\langle f_1, f_2, f_3, \dots, f_d \rangle$$

decision If $x_q \rightarrow y_q$

If $\omega^T x_q > 0$ Then $y_q = +1$

$\omega^T x_q < 0$ Then $y_q = -1$

Probabilistic function

$$\sigma(\omega^T x_q) = P(y_q = +1)$$

(0 to 1)

Interpretation of ω

$$\begin{array}{l} \text{If } \omega_i = +ve, x_{qi} \uparrow \Rightarrow (\omega_i x_{qi}) \uparrow \\ \uparrow \\ (f_i) \end{array} \quad \sum_{i=1}^d (\omega_i x_{qi}) \uparrow$$

$$\sigma(\omega^T x_q) \uparrow$$

$$P(y_q = +1) \uparrow$$

$$\text{If } \omega_i = -ve, x_{qi} \uparrow \Rightarrow (\omega_i x_{qi}) \downarrow$$

$$= \sum_{i=1}^d \omega_i x_{qi} \downarrow$$

$$= \sigma(\omega^T x_q) \downarrow$$

$$= P(y_q = +1) \downarrow \quad P(y_q = -1) \uparrow$$

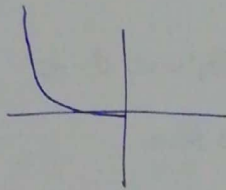
24.5 L2 Regularization: Overfitting & underfitting

$$\omega^* = \underset{(\omega)}{\operatorname{argmin}} \sum_{i=1}^n \log(1 + \exp(-y_i \omega^T x_i))$$

Let $z_i = y_i \omega^T x_i \rightarrow$ Signed distance.

$$= \underset{\omega}{\operatorname{argmin}} \sum_{i=1}^n \log(1 + \exp(-z_i))$$

$\log(\exp(-z))$ is always > 0



$$\sum_{i=1}^n \log(1 + \exp(-z_i)) \geq 0 \Rightarrow \log(1) = 0$$

$$\log(2) > \log(1)$$

$$\log(1+f) > \log(1) \quad f \geq 0$$

$$\omega^* = \underset{(\omega)}{\operatorname{argmin}} \sum_{i=1}^n (\log(1 + \exp(-z_i))) \geq 0$$

minimal value of $\sum_{i=1}^n \log(1 + \exp(-z_i))$ is zero

If $z_i = +ve$, $z_i \rightarrow +\infty$

Then $\exp(-z_i) \rightarrow 0$

$$\log(1 + \exp(-z_i)) = 0 \quad \text{Since } \log(1) = 0$$

If I pick my ω such that

(a) all training points are correctly classified

(b) $z_i \rightarrow \infty$

overfitting

Then that is called best ω .

If we make $\omega_i \rightarrow \infty$ or $-\infty$ we will reach minima $= 0$

Regularization (To avoid w^T to become $\rightarrow \infty$ or $-\infty$)

Regularization term

$$w^* = \underset{(w)}{\operatorname{argmin}} \sum_{i=1}^n \log(1 + \exp(-y_i w^T x_i)) + \lambda \underbrace{w^T w}_{\lambda \|w\|_2^2} = \lambda \sum_{j=1}^d w_j^2$$

$$\lambda w^T w = \lambda \sum_{j=1}^d w_j^2$$

$w^T w = 1$

When $\lambda = 0$, overfit \rightarrow high variance, by making $z_i \rightarrow \infty$ or $-\infty$
 $\lambda = \text{very large}$; underfit \rightarrow high bias, we are ignoring loss term

we have to find the right λ using CV

24.6 L1 regularization and Sparsity

$$w^* = \underset{(w)}{\operatorname{argmin}} \underbrace{\sum_{i=1}^n \log(1 + \exp(-y_i w^T x_i))}_{\text{Logistic loss}} + \underbrace{\lambda \|w\|_1}_{L_2 \text{-reg}}$$

$z_i \rightarrow \pm \infty$

Alternative to L_2 reg is L_1

$\|w\|_2^2$ for reg



$\|w\|_1$ for reg: $\|w\|_1 = \sum_{i=1}^d |w_i|$

$$w^* = \underset{(w)}{\operatorname{argmin}} (\text{Logistic loss for training data}) + \lambda \|w\|_1$$

hyper parameter

λ

L1-reg

will avoid $w_i \rightarrow \pm \infty$
 $w_i \rightarrow -\infty$

Sparcity :

$$w = \langle w_1, w_2, \dots, w_d \rangle$$

Solution to LR is said to be sparse if many w_i 's are zero

If we use L_1 reg in LR, all the unimportant (or) less important become zero

$$f_1, f_2, \dots, \underbrace{f_i}_{\text{less important}} \dots, f_d$$
$$w = \langle w_1, w_2, \dots, w_i, \dots, w_d \rangle$$

↓
Zero if L_1 is used.

If L_2 reg is used; w_i becomes a small value but not necessarily zero.

(Q) Why does L_1 reg create sparsity in w as compared to L_2 reg

ppb generally use L_1 than L_2

→ Elastic net : Either L_1 or L_2

$$w^+ = \underset{w}{\operatorname{argmin}} \sum_{i=1}^n \log(1 + \exp(-z_i)) + \lambda_1 \|w\|_1 + \lambda_2 \|w\|_2^2$$

We have to find two hyperparameters λ_1 & λ_2

24.7 Probabilistic Interpretation: Gaussian Naive Bayes

cs.cmu.edu/~tom/mlbook/NaBayesLogReg.pdf

LR \Rightarrow GRUB + Bernoulli

↓
 $p(x_i | y_i)$

↓
 $y_i \sim \text{Bernoulli}$

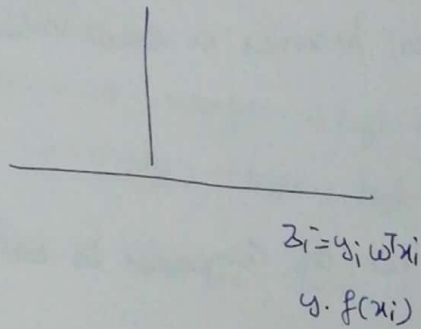
24.8 Loss minimization interpretation

$$w^+ = \underset{w}{\operatorname{argmin}} \sum_{i=1}^n \log(1 + \exp(-y_i w^T x_i))$$

$$z_i = y_i w^T x_i = y_i f(x_i)$$

If we build a ideal optimization model.

$$w^+ = \underset{w}{\operatorname{argmin}} (\text{num. of incorrectly classified pts})$$



function
+1: incorrectly classified
0: correctly classified
min: loss
max: profit

24.9 hyperparameter & random search

λ = hyper parameter

$\lambda = 0 \Rightarrow$ overfitting

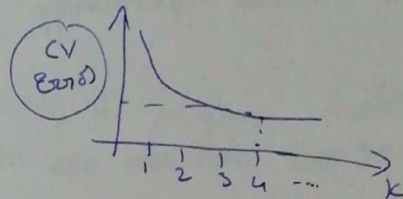
$\lambda = \infty \Rightarrow$ underfitting

(a) How to find the best λ

$$\lambda \in \mathbb{R}$$

$$K = \text{known}$$

$\alpha = \text{NB (Laplace smoothing)}$



K in known is an integer, which takes value $\{1, 2, 3, \dots, n\}$

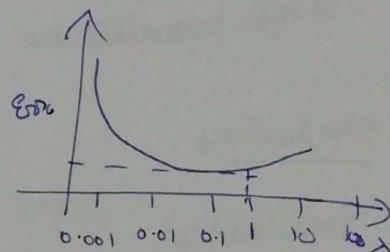
λ in LR is a real number.

$$\lambda \in \mathbb{R} \quad \begin{cases} \lambda = 0.1234 \\ \lambda = 0.2386 \end{cases}$$

\Rightarrow One technique to find λ is GRID Search.

Case 1: $\lambda = [0.001, 0.01, 0.1, 1, 10, 100, 1000]$

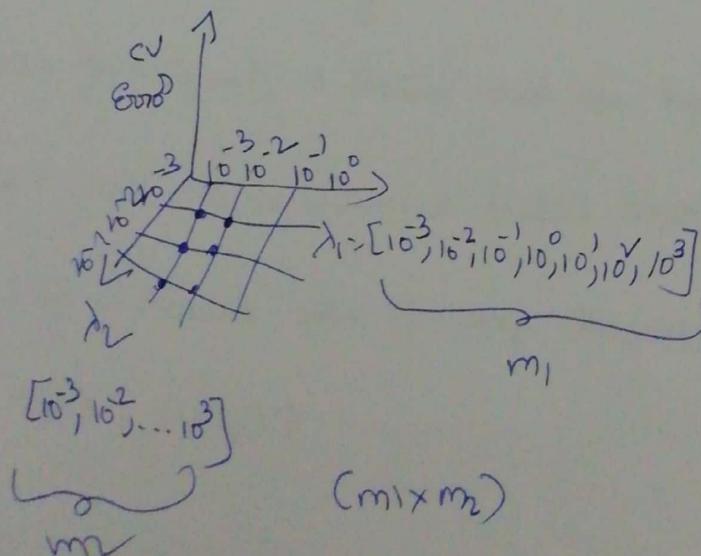
Case 2: $\lambda = [1, 2, 3, 4, 5, 6, 7, 8, 9, 10]$



\rightarrow Generally ppl select a large window.

$$\lambda = [10^{-4}, 10^{-3}, 10^{-2}, 10^{-1}, 10, 10^1, 10^2, 10^3, 10^4]$$

Elasticnet: $\lambda_1 \|w\|_1 + \lambda_2 \|w\|_2^2$



Grid search

λ : 1 hyperparameter + (m_1)

λ_1, λ_2 : 2 " $\div m_1 \times m_2$

$\lambda_1, \lambda_2, \lambda_3$: 3 " $\div m_1 \times m_2 \times m_3$

as # hyperparameters increase, the # times model needs to be trained increases exponentially

Grid Search

is not good when there are more hyperparameters

To overcome this issue we have another technique called

Random Search

$\lambda = [10^{-4}, 10^4] \leftarrow$ randomly pick values in the given interval

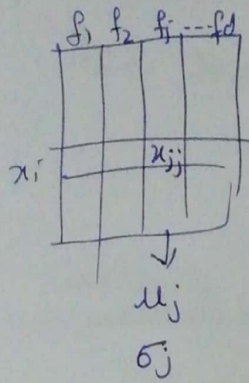
→ Random Search is almost as good as grid search especially when # hyperparameters are large.

Other functions

GridSearchCV

RandomizedSearchCV

24.10 Column Standardization (z-score)



$$x_i \in \mathbb{R}^d$$

$$x'_{ij} = \frac{x_{ij} - \mu_j}{\sigma_j} \quad \text{Standardization}$$

Even in Logistic Regression its mandatory to perform feature standardization before training

mean-centering
&
scaling } Standardization.

24.11 Feature Importance & model interpretability

$$\begin{array}{cccc} f_1 & f_2 & f_j & f_d \\ w \rightarrow & w_1 & w_2 & w_j & w_d \end{array}$$

assume all features are independent (Naive Bayes)

Feature Importance can be achieved based on the weights

In K-NN: Feature imp \rightarrow Forward Feature Selection.

\hookrightarrow we cannot get directly.

NB: $P(x_i | y=+1) \rightarrow$ features which are important.

LR: w_j 's \rightarrow to determine feature importance.

$|w_j|$ = absolute value of weight corresponding to f_j

$$|w_j| \uparrow ; (w^T x_j) \uparrow$$

Case 1 $w_j = +\text{ve \& large}$; $\sum_{j=1}^d w_j \cdot x_{qj} \Rightarrow w^T x_q$
 $L P(y_q = +1) \uparrow$

Case 2 $w_j = -\text{ve \& large}$; $\sum_{j=1}^d w_j x_{qj} \Rightarrow P(y_q = -1) \uparrow$

We can determine the important features in LP based on the weights

E.g. Predict the gender : male & female
 (+1) (-1)

1 feature: hair-length = $|w_{hl}|$ is large

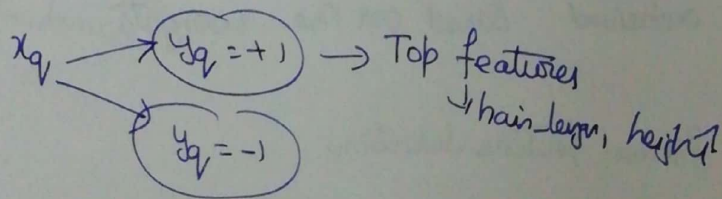
$\phi w_{hl} : -\text{ve}$

$w_{hl} \uparrow ; P(y_q = -1) \uparrow$

2 feature: height $\uparrow ; P(y_q = +1) \uparrow$
 \uparrow male

$w_h = +\text{ve}$

model interpretability



24.12 Collinearity of features

Feature Importance : features are independent
 $|w_j|$ as F.I values

Collinearity or multicollinearity

collinearity: f_i, f_j

$$\text{s.t. if } f_i = \alpha f_j + \beta$$

then f_i & f_j are collinear.

multicollinearity

If f_1, f_2, f_3 & f_4 such that

$$f_1 = \alpha_1 + \alpha_2 f_2 + \alpha_3 f_3 + \alpha_4 f_4$$

Then f_1, f_2, f_3 & f_4 are said to be multicollinearity

(Q) why does $|w_j|$ not be useful as f.i if features are collinear?

$$\mathcal{D} = \langle x_i, y_i \rangle_{i=1}^n$$

$$w^* = \begin{matrix} \langle 1, 2, 3 \rangle \\ f_1, f_2, f_3 \end{matrix} ; \quad x_q = \langle x_{q1}, x_{q2}, x_{q3} \rangle$$

$$w^{*T} x_q = x_{q1} + 2x_{q2} + 3x_{q3}$$

$$\text{If } f_2 = 1.5 f_1 \Rightarrow f_1 \text{ & } f_2 \text{ are collinear.}$$

$$w^T x_q = x_{q1} + 3x_{q2} + 3x_{q3} = 4x_{q1} + 3x_{q3}$$

$$w^* = \begin{matrix} \langle 1, 2, 3 \rangle \\ f_1, f_2, f_3 \end{matrix}$$

$$\begin{matrix} \langle 4, 0, 3 \rangle \\ \uparrow \quad \uparrow \quad \uparrow \\ x_{q1} \quad x_{q2} \quad x_{q3} \end{matrix}$$

$$\tilde{w} = \begin{matrix} \langle 4, 0, 3 \rangle \\ f_1 \text{ is imp} \end{matrix}$$

\therefore assumptions are completely changing
if features are collinear \Rightarrow weight vector can change arbitrarily $\Rightarrow |w_j|$ can be used for feature importance

$|w_j|$ as F.I

determine if features are multicollinear:

↑ Perturbation technique

↑ means to shake the values a little by adding a ϵ

f_1	f_2	f_3	y
	x_{ij}		y_i

→ $x_{ij} + \epsilon$
Standardized small noise
 $N(0, 0.01)$

Before Perturbation: $w = \langle w_1, w_2, \dots, w_j, \dots, w_d \rangle$

after " : $\tilde{w} = \langle \tilde{w}_1, \tilde{w}_2, \dots, \tilde{w}_j, \dots, \tilde{w}_d \rangle$

If w_i & \tilde{w}_i differ significantly then your features are collinear

$|w_j|$'s as F.I cannot be used

24.13 Test/Run time space & time complexity

Train LR: solving Logistic Regression problem.

Train time of LR is $O(nd)$

After this we get $w^* = \langle w_1, w_2, w_3, \dots, w_d \rangle$

$$w^{*T} x_q > 0 \rightarrow +ve$$

$$< 0 \rightarrow -ve.$$

At runtime we have to store w^T

Space = $O(d)$ → memory efficient as well

Time = $O(d)$

If d is small, LR is v good for low latency application

$$x_q \rightarrow (m) \rightarrow y_q$$

If d is large $d \approx 1000$

$w_{Tq} \div 1000$ mult & addition.

\rightarrow L1 reg \div Sparsity (w_j 's corresponding to less important features $= 0$)
 $\lambda \div$ reasonably

$\lambda \uparrow$; Sparsity \uparrow
more of $w_j = 0$ $\left\{ \begin{array}{l} 50 \text{ mult \& 30 additions} \\ \uparrow \text{ latency} \end{array} \right.$

Bias vs Latency

$\lambda \uparrow$; Bias \uparrow , Latency \downarrow

24.14 Real world cases

Decision Surfaces \div Linear / hyperplane. $\left\{ \begin{array}{l} + \\ - \end{array} \right.$

assumption \div data is linearly separable or almost linearly separable.

Imbalanced data: Upsampling or down sampling.

Outliers: less impact \because of $\sigma(x)$

\rightarrow $D_{\text{train}} \rightarrow w^*$

$\rightarrow x_i \rightarrow w^{*T} x_i \div$ distance from π to point x_i

\rightarrow remove points which are ~~are~~ very far away from π
from $D_{\text{train}} \rightarrow D'_{\text{train}}$

$\rightarrow D'_{\text{train}} \rightarrow \tilde{w}^*$
 \uparrow final solution.

mining \div Standard imputation.

multiclass \div one vs Rest \leftarrow typically

$\left\{ \begin{array}{l} \text{maxEnt model} \leftarrow \text{Extension to LR} \\ \text{softmax classifs} \leftarrow \text{deep learn} \\ \text{multinomial LR} \end{array} \right.$

Similarity matrix: Extension to LR \rightarrow Kernel LR

Best & worst cases

- \rightarrow almost ls separable
- \rightarrow low-latency requirement (L_1 reg)
- \rightarrow very fast to train.

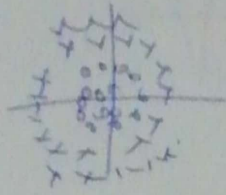
Large dimensionality

\rightarrow d is large, chance data is linearly separable is high

\downarrow

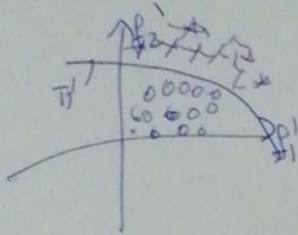
low-latency $\rightarrow L_1$ regularization.

24-15 Non-linearly separable data & feature Engineering



(a) Can we use LR to separate the classes

Feature Transform/Engineering
(FE)



$$\left\{ \begin{aligned} f_1' &= f_1^2 \\ f_2' &= f_2^2 \end{aligned} \right\} \rightarrow \text{FE}$$

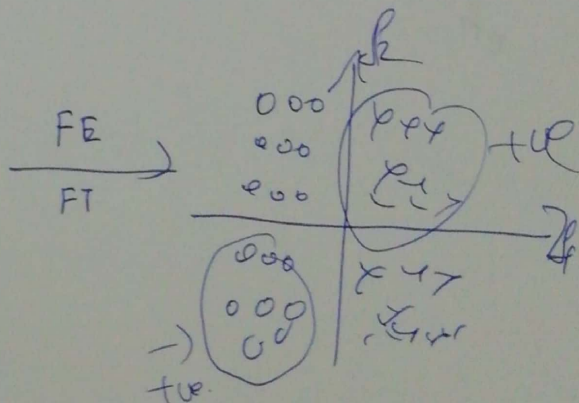
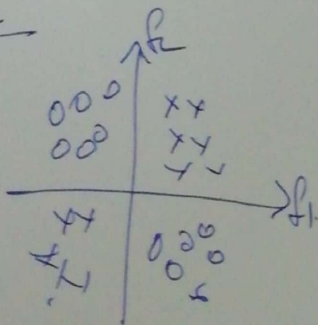
$$x_q = \langle x_{q1}, x_{q2} \rangle$$

J, FT or FE

$$x_q' = \langle x_{q1}', x_{q2}' \rangle \rightarrow \boxed{\text{LR}} \rightarrow y_q$$

(Q) how to know which transform to apply
↳ By experience.

Case 2

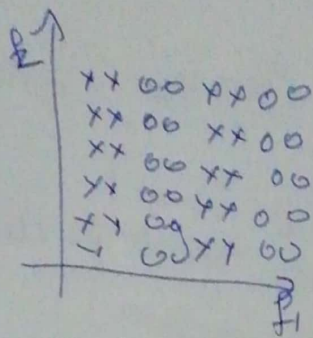


$$\begin{aligned} x_{q1} &= 0 & 1 \\ 0 & 0 & 1 \\ 1 & 1 & 0 \end{aligned}$$

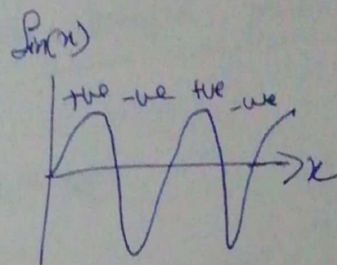
$$f_1' = f_1 \times f_2$$

$$f_2' = f_2$$

③

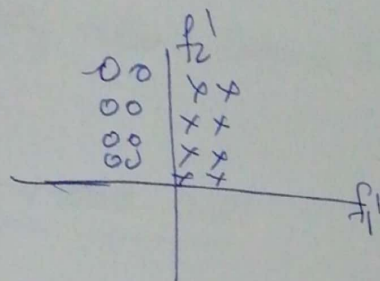


FE
FT



$$f_1' = \sin(f_1)$$

$$f_2' = f_2$$



Typical transform for real value features:

① $f_1 \times f_2, f_1^v, f_2^v, f_2^3, f_1^3$ } polynomial features

② Trigonometric features

$$\sin(f_1); \cos(f_1)$$

$$\sin(f_1) \times \cos(f_2)$$

$$\sin(f_1^v)$$

③ boolean features: OR, AND, XOR

④ Other

$$\log(f_1)$$

$$e^{f_1}$$