

### Matlab / Python Logit-Related Functions and References

Matlab Functions: <fitglm, predict> <mnrfit, mnrval>

#### Overall

- http://www.mathworks.com/help/stats/generalized-linear-regression.html
- http://www.mathworks.com/help/stats/generalized-linear-regression-2.html

### Generalized LinearModel class

- http://www.mathworks.com/help/stats/generalizedlinearmodel-class.html
- http://www.mathworks.com/help/stats/examples/fitting-data-with-generalized-linear-models.html
- Multinomial logistic regression https://www.mathworks.com/help/stats/mnrfit.html#namevaluepairarguments

### Python scikit-learn, logistic regression

- $\bullet \qquad http://scikit-learn.org/stable/modules/generated/sklearn.linear\_model.LogisticRegression.html\\$
- http://scikit-learn.org/0.15/modules/generated/sklearn.linear\_model.LogisticRegression.html
- L1 Penalty & Sparsity <a href="http://scikit-learn.org/stable/auto\_examples/linear\_model/plot\_logistic\_l1\_l2\_sparsity.html">http://scikit-learn.org/stable/auto\_examples/linear\_model/plot\_logistic\_l1\_l2\_sparsity.html</a>
- LogisticRegressionCV <a href="http://scikit-learn.org/stable/modules/generated/sklearn.linear\_model.LogisticRegressionCV.html">http://scikit-learn.org/stable/modules/generated/sklearn.linear\_model.LogisticRegressionCV.html</a>
- Multiclass and multilabel algorithms <a href="http://scikit-learn.org/stable/modules/multiclass.html">http://scikit-learn.org/stable/modules/multiclass.html</a>

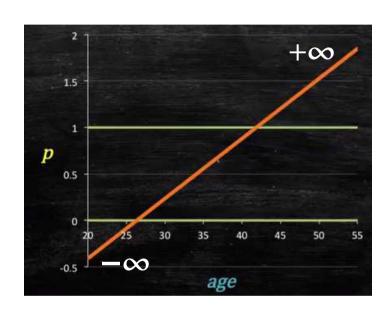
### Outline

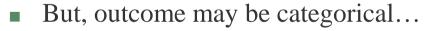
- How it works? Matlab / Python functions.
- Diagnoses / Visualization.
- Prediction and Quality.
- Outliers.
- Multiclasses Prediction.
- Nonlinearity / High Dimensionality / Visualization.
- Regularization.
- Cost Function.

## Why Not Just Linear Regression?

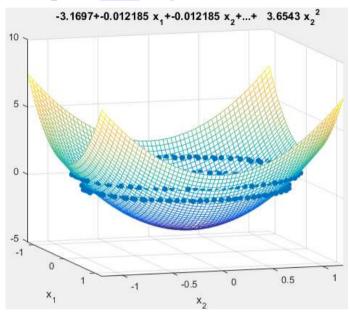
Linear Regression

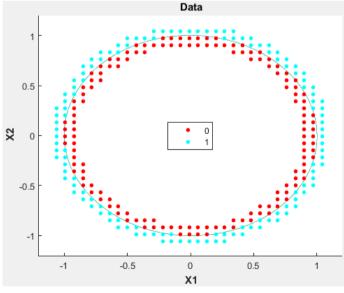
$$h_{\theta}(x) = \theta^{\mathrm{T}} X \in [-\infty .. + \infty]$$
 (i.e. ANY range in R).





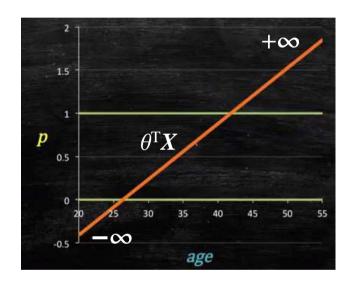
- Gender, Rank, City...
- Buy or no buy...

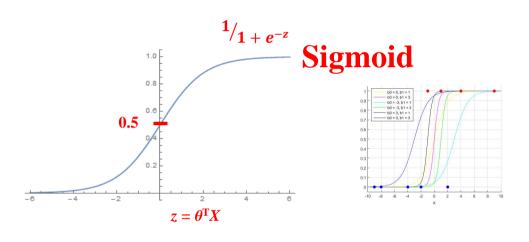




## Logistic Regression...Why Not Just Linear Regression?

- Linear Regression  $h_{\theta}(x) = z = \theta^{T}X \in [-\infty .. +\infty]$  (i.e. ANY range in R).
  - But, outcome may be categorical... Gender, Diseases, Rank, ...

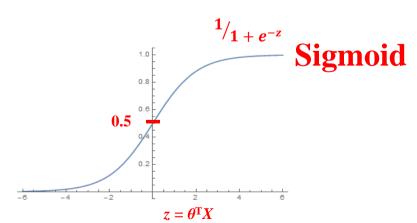




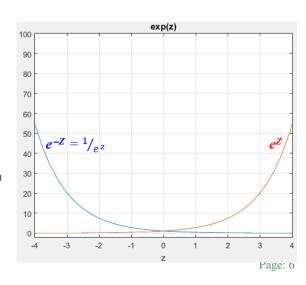
- Logistic (or logit) regression is a model where the dependent var is **categorical**.
  - Predict classes by *linking*  $\theta^T X$  to probabilities [0..1].

### Link Categorical Response to Continuous Probability

- Logistic (or logit) regression is a model where the dependent var is categorical.
  - Predict classes by *linking*  $\theta^T X$  to *likelihood* [0..1] via *logistic function*.
    - <a href="https://en.wikipedia.org/wiki/Logistic\_regression">https://en.wikipedia.org/wiki/Logistic\_regression</a>
  - Also refer to as generalized linear model (GLM).
- Why  $P = \frac{1}{1 + e^{-z}}$ ?  $\rightarrow$  guarantee  $0 \le P \le 1$ 
  - $e^z \ge 0$  for  $z \in [-\infty, \infty]$ , no matter what is z.
  - $\frac{P}{1-P} = e^{\theta^{T}X} = e^{Z}$   $P = \frac{1}{1+e^{-Z}}$ 
    - $\frac{P}{1-P}$  is *odds* = prob. of "true" over prob. of "not true".



syms z y ezplot('exp(-z)', [-4 4 -2 100]) hold on ezplot('exp(z)', [-4 4 -2 100]) hold off grid on



### Logistic Regression and Interpretation

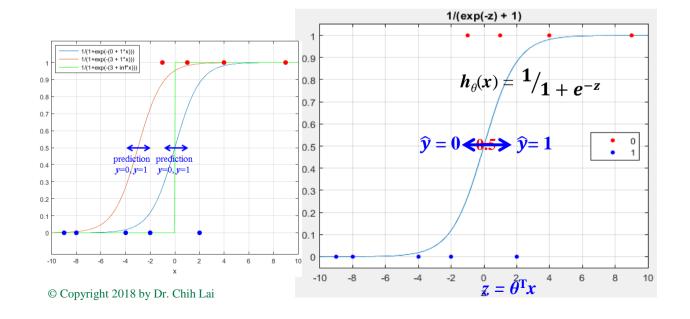
- Logistic regression  $\rightarrow$   $0 \le h(\theta^T x) = h(z) = \frac{1}{1+e^{-z}} \le 1$ , asymptotes at 1 or 0.
  - $\frac{1}{1+e^{-z}}$  is referred to as **Sigmoid function** or logistic function.

• If 
$$\theta \uparrow \rightarrow \theta^T X \uparrow \rightarrow z \uparrow \rightarrow h_{\theta}(x) = \frac{1}{1 + e^{-z}} \approx 1$$
. predict  $\hat{y} = 1$ .

• If 
$$\theta \downarrow \rightarrow \theta^T X \downarrow \rightarrow z \downarrow \rightarrow h_{\theta}(x) = \frac{1}{1+e^{-z}} \approx 0$$
. predict  $\hat{y} = 0$ .

• If 
$$z = 0 \rightarrow h_{\theta}(x) = \frac{1}{1 + e^{-z}} \approx ??$$

•  $\theta$ s tell us which attributes have **positive** or **negative impact** on **P**, or classification.

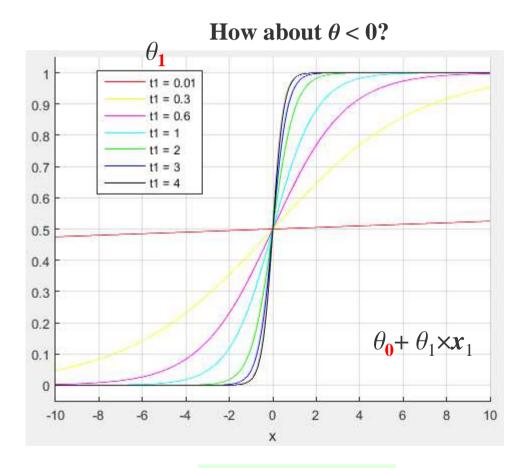


```
syms z
figure,
ezplot(1 / (1 + exp(-z)), [-10 10])

red = [-1 1; 1 1; 4 1; 9 1];
blue = [2 0; -2 0; -4 0; -8 0; -9 0];
data = [red; blue];
Y = [zeros(size(red, 1), 1); ...
ones(size(blue, 1), 1)];
hold on
gscatter(data(:, 1), data(:, 2), Y, 'rb')
hold off
ylim([-0.05 1.05])
grid on
```

## Logistic Function– Changing $\theta_1$

- Logistic (sigmoid) function  $\sigma$  takes LR output  $(\hat{y})$  as input & convert to P[0..1].
  - For smaller  $\theta_1$ , x must be very large to reach P = 1.



See Appendix for changing both  $\theta_0 \& \theta_1$ 

```
syms x
t0 = 0:
                                      \theta_0
t1_arr = [0.01, 0.3, 0.6, 1, 2, 3, 4]; % \theta_1 slope
fstr = \frac{1}{1+exp(-(t0 + t1*x))};
                           % line colors
c = ['rymcgbk'];
figure, hold on
loops = 0; legendStr = [];
for t1 = t1 arr
  fstrX = strrep(fstr, 't0', num2str(t0));
  fstrX = strrep(fstrX, 't1', num2str(t1));
  h = ezplot(fstrX, [-10 10]);
  loops = loops + 1;
  set(h, 'color', c(loops));
  legendStr\{loops\} = ['t1 = 'num2str(t1)];
end
legend(legendStr), title("), grid on,
ylim([-0.05 \ 1.05]), hold off
```

## Matlab fitglm() Functions

- Matlab fitglm() functions.
  - GLM– Generalized Linear Model.
- fitglm().
  - mdl = **fitglm**(X, Y, 'distr', '**binomial**', 'link', '**logit'**)

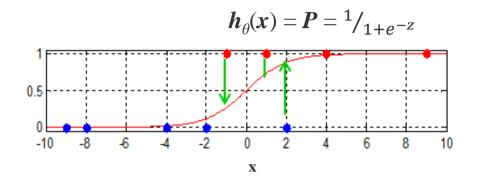
### See **Appendix** for

- 1. Different distributions,
- 2. Different link functions.



Link Function Name	Link Function	Mean (Inverse) Function	
'log'	$f(\mu) = \log(\mu)$	$\mu = \exp(Xb)$	
'logit'	$f(\mu) = \log(\mu/(1-\mu))$	$ \mu = \exp(Xb) / (1 + \exp(Xb)) \qquad \frac{e^z}{1 + e^z} = $	$= \frac{1}{1+e^{-2}}$
'probit'	$f(\mu) = \Phi^{-1}(\mu)$	$\mu = \Phi(Xb)$	
'comploglog'	$f(\mu) = \log(-\log(1 - \mu))$	$\mu = 1 - \exp(-\exp(Xb))$	
'reciprocal'	$f(\mu) = 1/\mu$	$\mu = 1/(Xb)$	

## Main Output from fitglm()



Estimated Coefficients:				
	Estimate	SE	tStat	pValue
	$\underline{\hspace{1cm}}$			
(Intercept) $\theta_0$	-0.0146	0.9583	-0.015235	0.98784
$\mathbf{x}_1$ $\theta_1$	0.51551	0.35954	1.4338	0.15162

- How do we decide best  $\theta$ ?
- Class probability of each instance?

### sklearn Logistic Regression

- 0.5 0.5 0.6 4 -2 0 2 4 6 8 10 X
- sklearn logistic regression requires <u>at least</u> 2-D data.
  - So we copy 1<sup>st</sup>-D data into 2<sup>nd</sup>-D.

```
import numpy as np
from sklearn import linear_model

X = [[-1, -1], [1, 1], [4, 4], [9, 9], [-9, -9], [-8, -8], [-4, -4], [-2, -2], [2, 2]]
Y = [1, 1, 1, 1, 0, 0, 0, 0]

# Inverse of regularization strength; ↓C ==> ↑regularization
# LOSS = C * E + theta, default C = 1
logreg = linear_model.LogisticRegression(C = 90)

logreg.fit(X, Y)  # fit the data
print(logreg.intercept_, logreg.coef_)
```

%%%% Matlab logistic regression, 2-D X = [-1, -1; 1, 1; 4, 4; 9, 9; -9, -9; -8, -8; ... -4, -4; -2, -2; 2, 2]; Y = [1, 1, 1, 1, 0, 0, 0, 0, 0]; mdl = fitglm(X, Y, 'distr', 'binomial', 'link', 'logit')

# [-0.01457369] [[ 0.25773197, 0.25773197]]



## Detailed Information Returned from Matlab Logistic Regression

- Model info returned from fitglm()
  - Use workspace to exam info in the model.

http://www.mathworks.com/help/stats/generalizedlinearmodel-class.html

- Coefficients .Estimate  $(\theta)$
- Fitted
  - .Response (P) = .Probability (P)
  - .LinearPredictor  $(z = \theta^T X)$
- Residuals, .Raw
- SSE, SST, SSR
- Diagnostics, .Leverage .CooksDistance
- Rsquared
- LogLikelihood



### Predicted Response (Probability)

■ mdl.**Fitted.Response** = mdl.**Fitted.Probability** = probability =  $\frac{1}{1+e^{-z}}$  = 1 ./ (1+exp(-Z))

 $\boldsymbol{\theta}$ 

 $\mathbf{Z} = \text{mdl.}$  Fitted.LinearPredictor =  $\theta^{T}X$ .

(Intercept)  $\theta_0$  -0.0146 x1  $\theta_1$  0.51551

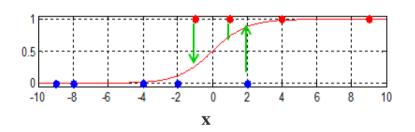
#### mdl.Fitted.Response

= probability

 $= 1 . / (1 + \exp(-Z))$ 

X		Re	1 sponse		Y	$\widehat{Y}$
-9	1	111	0.0094		0	
-8	2		0.0157		0	
-4	3		0.1114		0	
-2	4		0.2601		0	
2	5		0.7343		0	1
-1	6		0.3705	П	1	0
1	7		0.6227		1	
4	8		0.8857		1	
9	9		0.9903		1	

Residual =  $(Y - \widehat{Y})$ 



mdl = **fitglm**(X, Y, 'distr', 'binomial', 'link', 'logit')

B = mdl.Coefficients.Estimate;  $\% \theta = -0.0146 \quad 0.5155$ 

XX = [ones(length(X), 1) X];

Z = XX \* B; %  $\theta^T X$ 

[Z mdl.Fitted.LinearPredictor]  $\% \theta^{T}x = z$ 

[1 ./ (1+exp(-Z)) **predict**(mdl, X) ... % **probability** 

mdl.Fitted.Probability, mdl.Fitted.Response]

# Plotting Probability = $\frac{1}{1+e^{-z}}$ Against X or Z

```
red = [-11; 1 1; 4 1; 9 1];

blue =[-90; -80; -40; -20; 20];

X = [blue(:, 1); red(:, 1);];

Y = [blue(:, 2); red(:, 2)];

mdl = fitglm(X, Y, 'distr', 'binomial', 'link', 'logit')

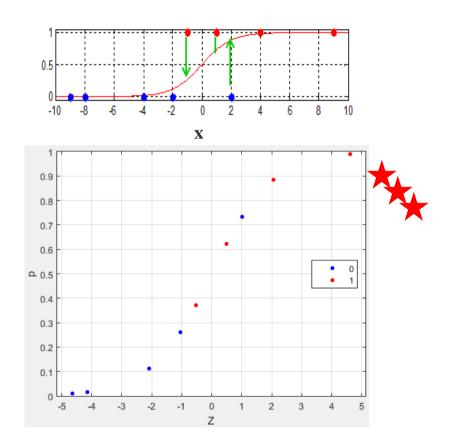
%% Plot Z wrt P

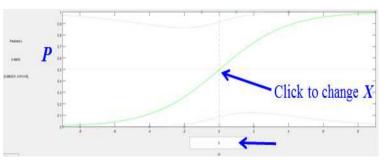
p = mdl.Fitted.Response; % probability

Z = mdl.Fitted.LinearPredictor; % Z = \theta^T X

figure, gscatter(Z, p, Y, 'br'); grid on

plotSlice(mdl)
```

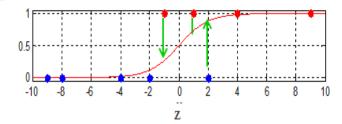


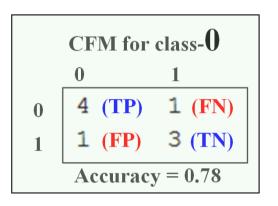


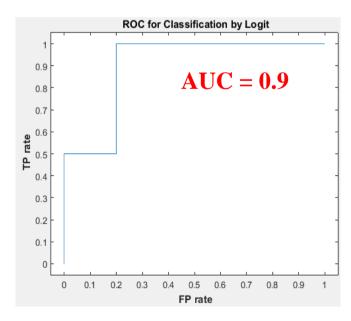
### Accuracy & Confusion Matrix

• Class prediction =  $P \ge 0.5$ 

```
red = [-1 1; 1 1; 4 1; 9 1];
blue = [-9 0; -8 0; -4 0; -2 0; 2 0];
X = [blue(:, 1); red(:, 1);];
Y = [blue(:, 2); red(:, 2)];
mdl = fitglm(X, Y, 'distr', 'binomial', 'link', 'logit')
scores = predict(mdl, X)
P_Labels = double(scores >= 0.5); ◀
CFM = confusionmat(Y, P_Labels)
[xpos, ypos, T, AUC] = perfcurve(Y, scores, 1);
figure,
          plot(xpos, ypos) % plot ROC
xlim([-0.05 1.05]), ylim([-0.05 1.05])
xlabel('\bf FP rate'), ylabel('\bf TP rate')
title('\bf ROC for Classification by Logit')
```

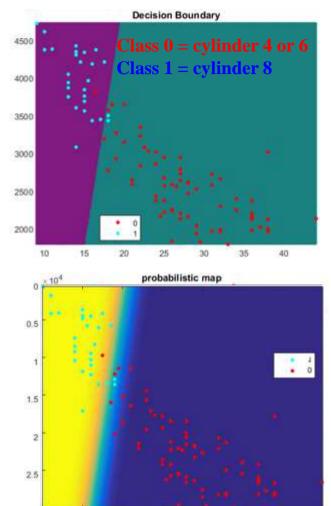




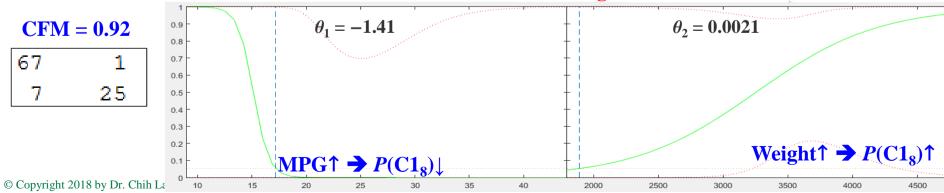


### Fuzzy Probability Boundary

■ Predicting Car's Cylinder from **MPG** + **Weight** 



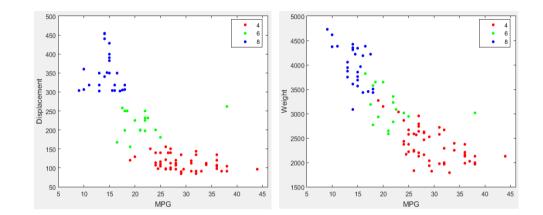
**MPG** + Weight

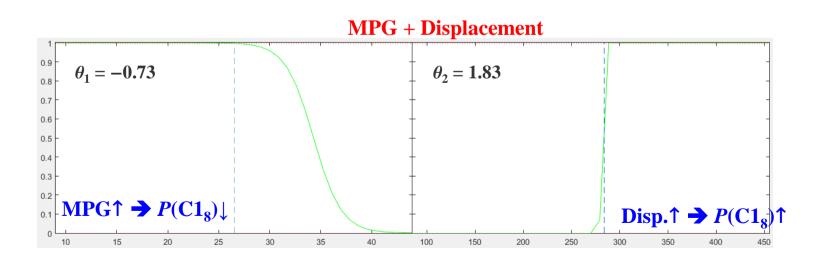


# Predicting Car's Cylinder from **MPG** + **Displacement**

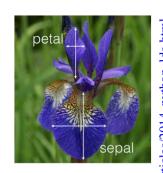
Displacement is a sensitive predictor in predicting cylinder.

- Class 0
  - Cylinder 4 or 6.
- Class 1
  - Cylinder 8.





### Visualizing High Dimension Data



load fisheriris

X = meas(51:end,:); % 100×4, 4-dimension  $\leftarrow \leftarrow$ 

% Next, create 100×1 BINARY class

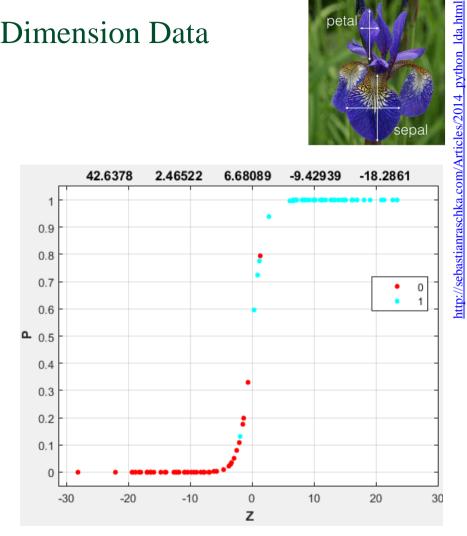
Y = strcmp('versicolor', species(51:end)); mdl = **fitglm**(X, Y, 'distr', 'binomial', 'link', 'logit') plotSlice(mdl)

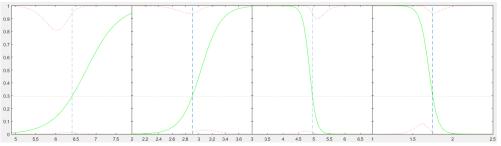
p = mdl.Fitted.Response;

**Z** = mdl.Fitted.LinearPredictor;

figure, gscatter(Z, p, Y); grid on

```
zmin = min(Z);
                   zmax = max(Z);
ylim([-0.05 \ 1.05]), xlabel('\bf Z'),
ylabel('\bf P'),
title(num2str(mdl.Coefficients.Estimate'));
```



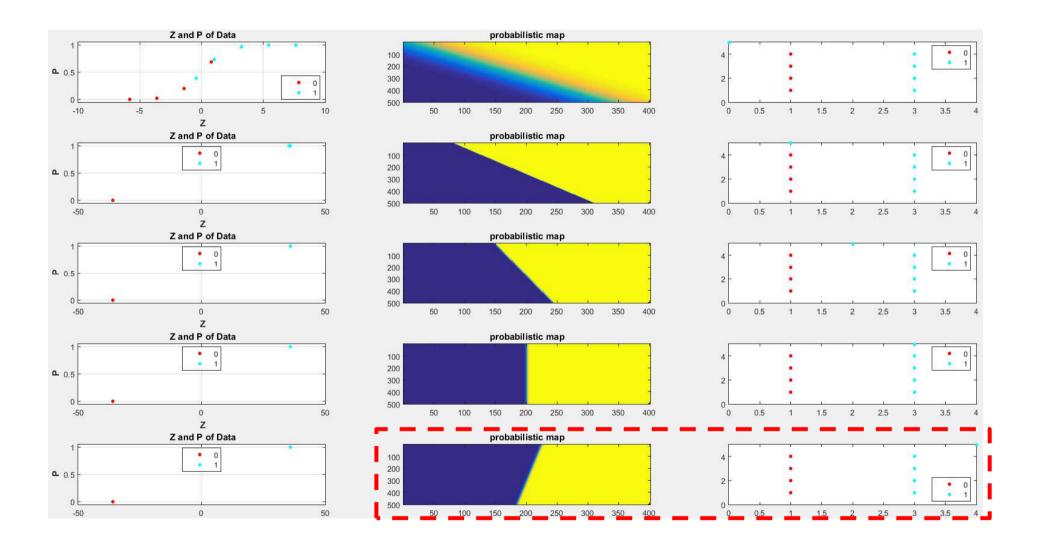


### **Python Logistic Regression**

```
import numpy as np
from sklearn import linear_model, datasets
# import data, and use some
iris = datasets.load iris()
#X = iris.data[:, :2] # use all records from first two features.
X = iris.data[50:, :2] # use records 51 to end from first two features.
#X = iris.data # use all 4 features.
Y = iris.target;
Y = Y[50:] # use only records 51 to end, so only 2 classes
# Inverse of regularization strength; smaller C ==> stronger regularization.
\# LOSS = C * E + theta, default C = 1
logreg = linear model.LogisticRegression()
                                                      print(logreg.intercept , logreg.coef , '\n')
                                                      print(logreg.predict(X), '\n')
# fit the data.
logreg.fit(X, Y)
                                                      print(logreg.predict_proba(X), '\n')
logreg.predict(X) # predicted classes
                                                      print(logreg.predict_log_proba(X))
```

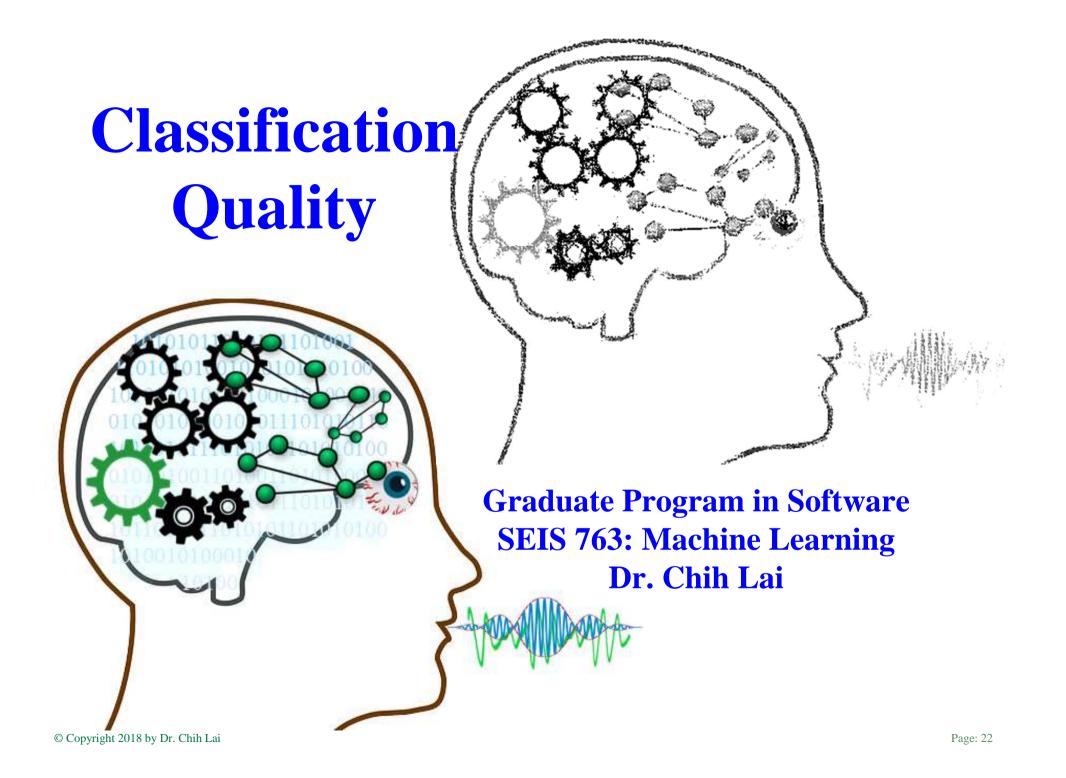
- In the multiclass case, the training algorithm uses the one-vs-rest (OvR) scheme if the 'multi\_class' option is set to 'ovr', and ...
  - It uses the cross- entropy loss if the 'multi\_class' option is set to 'multinomial'. (Currently the 'multinomial' option is supported only by the 'lbfgs', 'sag' and 'newton-cg' solvers.)

# Visualizing Outlier Impacts



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- How it works? Matlab / Python functions.
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- Cost Function.

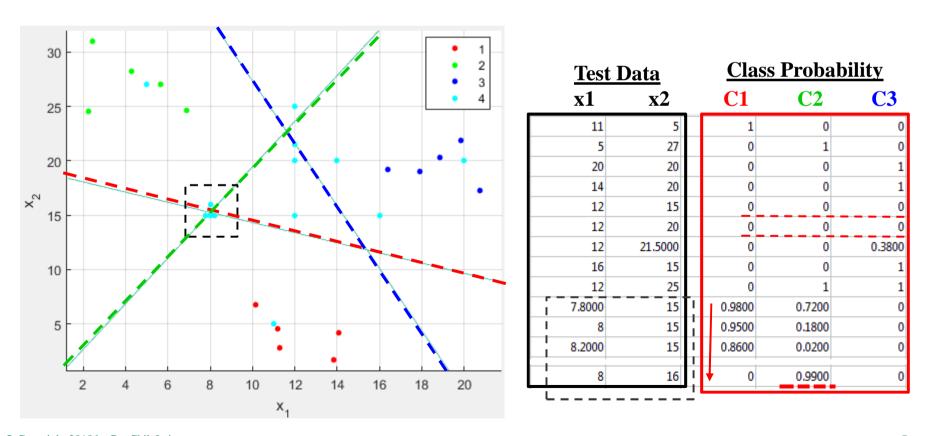


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### One-vs-All (Rest) Prediction

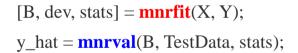
- Train multiple binary models.
  - One for each class *i* against rest of records of other classes.
  - Feed a test data X to **EVERY** classifier, predict X as class i that has maximum P.
- There can be a region that cannot be classified.

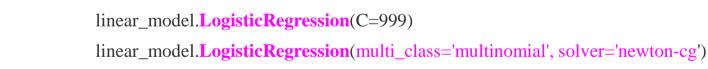


### One vs. Reference

- Multinomial logistic regression, 3 classes.
  - Compute  $\theta$  for red & green classes
  - vs the 3<sup>rd</sup> class (**blue**)

heta for	heta for		
red vs blue	green vs blue		
$\theta_0$ 56.5740	37.2130		
$\theta_1^{-2.4661}$	-3.1063		
$\theta_{2}^{-1}$ -1.6311	-0.0493		





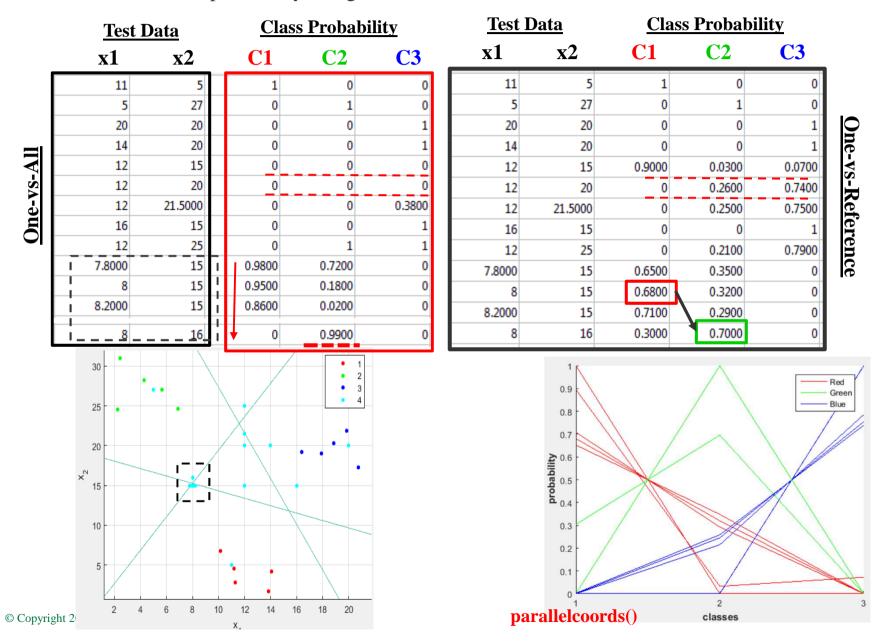
- Matlab functions for <u>multinomial</u> logistic regression → mnrfit(), mnrval().
  - https://www.mathworks.com/help/stats/mnrfit.html#namevaluepairarguments
  - http://www.mathworks.com/help/stats/mnrval.html
  - $http://scikit-learn.org/stable/modules/generated/sklearn.linear\_model. Logistic Regression. html \#sklearn.linear\_model. Logistic Regression. predict\_probation and the probation of the probati$
  - http://scikit-learn.org/stable/modules/multiclass.html

30 25 20 15 10 5 12 20 22 2 8 10 14 16 18

MNLR, Red vs Blue, Green vs Blue

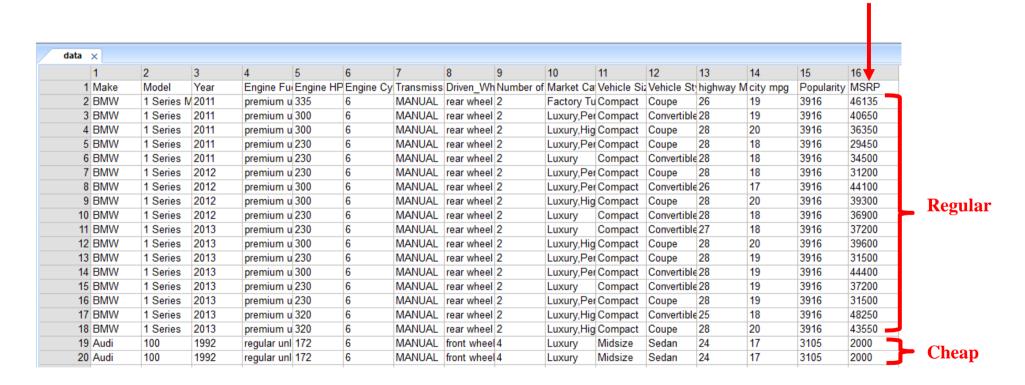
### Multinomial Logistic Regression, Compare to One-vs-All

• Not sure how the probability being normalized in the One-vs-Reference method.



### Case Study–Predicting Car Prices

- From many predictors in training cases, want to build a model to predict car \$\$.
- Is this problem always a regression problem?
- OK, how many classes do we have?

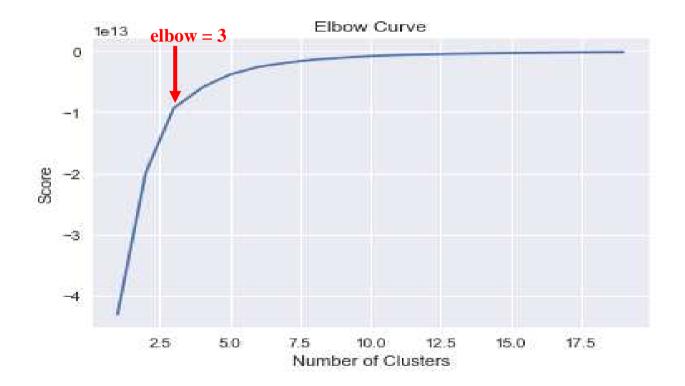


#### Predicting Car Prices, MDL-01 2018 spring

Saleh Alkadayar , Rathana Sorn Jose Rodriguez, Julie Flater, Gassan Zaid

## Deciding # of Classes

- How many classes?
  - Do some kind of clustering (i.e. k-means).
  - How do we do classification on more than 2 classes?



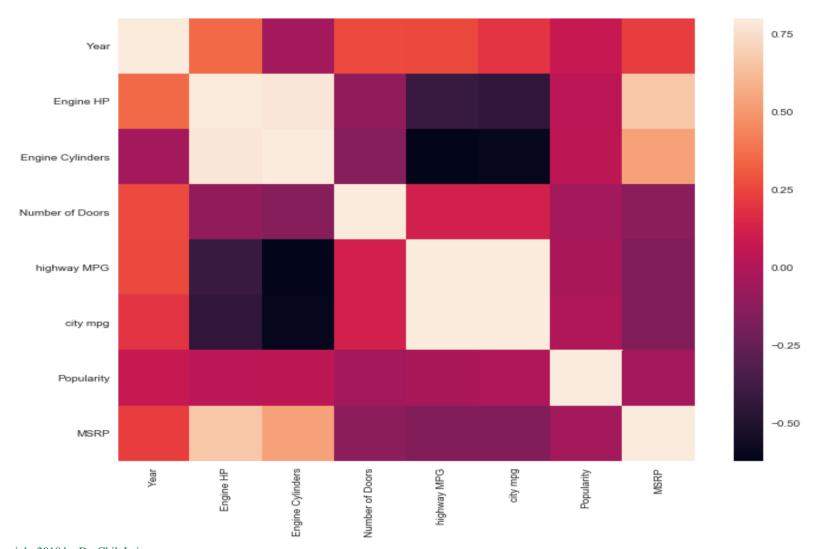
#### Predicting Car Prices, MDL-01 2018 spring

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# Data Leaking Problem??

#### Predicting Car Prices, MDL-01 2018 spring

Saleh Alkadayar , Rathana Sorn Jose Rodriguez, Julie Flater, Gassan Zaid

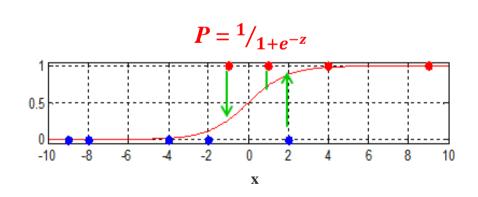


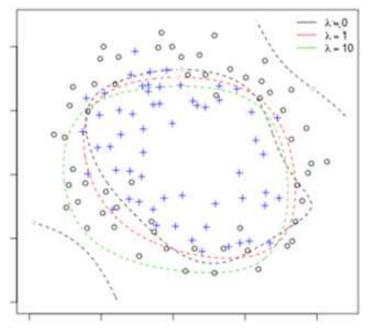
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- Cost Function, Other Issues / Examples / Demos.

### Regularize Logistic Regression

- Regularization.
  - Reduce the number of predictors and identify important ones.
  - Shrink  $\theta$ s, potentially avoid *overfitting* problem.
- **Assume** the cost function for logistic regression:
  - $J(\theta) \approx E + \lambda \text{Complexity} \approx E + \lambda \sum_{i=1}^{n} |\theta_i| \approx P_{\text{joined}} + \lambda \text{Complexity}$
  - $\lambda \uparrow \rightarrow$  simpler model  $\rightarrow$  smoother decision boundary.





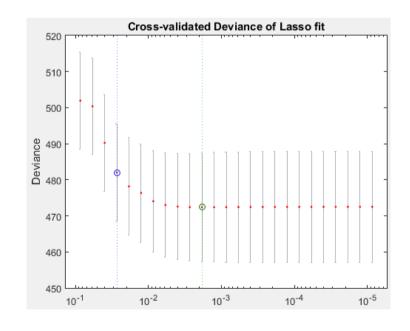
## Regularizing Logistic Regression—lassoglm()

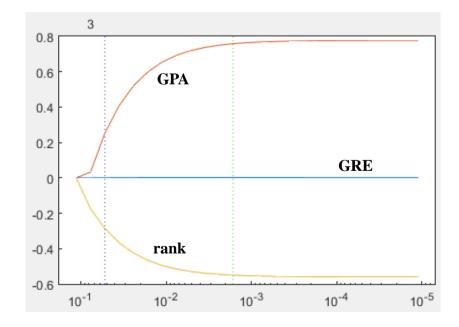
- Graduate school admission prediction from 400 applications.
  - 3 predictors: GRE, GPA, Institute rank
  - Response: admit or not.
  - Do we need any preprocessing?

$\theta$
-3.4495
0.0023
0.7770
-0.5600

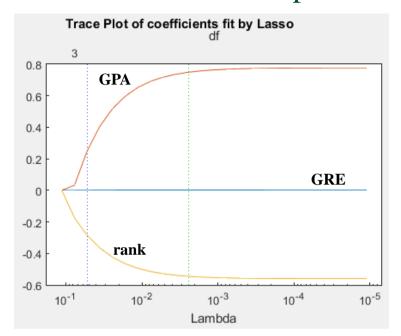
- CFM = (71%)
  - 254 19
  - 97 30

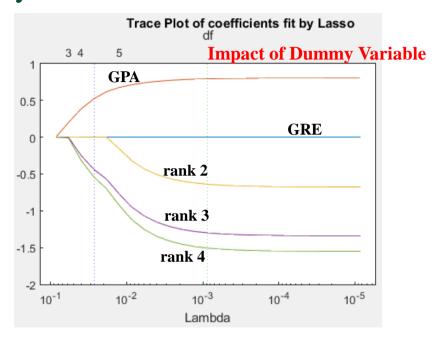
[LB, FitInfo] = lassoglm(X, Y, 'binomial', 'NumLambda', 25, 'CV', 10); lassoPlot(LB, FitInfo, 'PlotType', 'CV'); lassoPlot(LB, FitInfo, 'PlotType', 'Lambda', 'XScale', 'log');

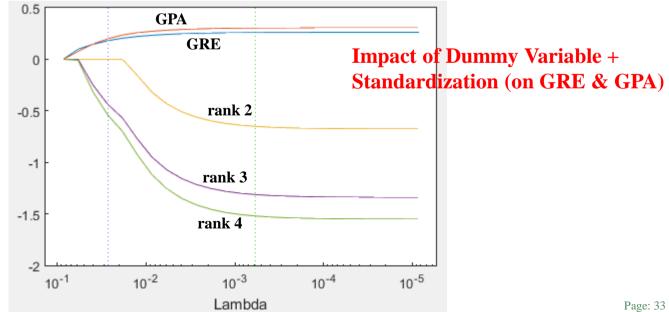




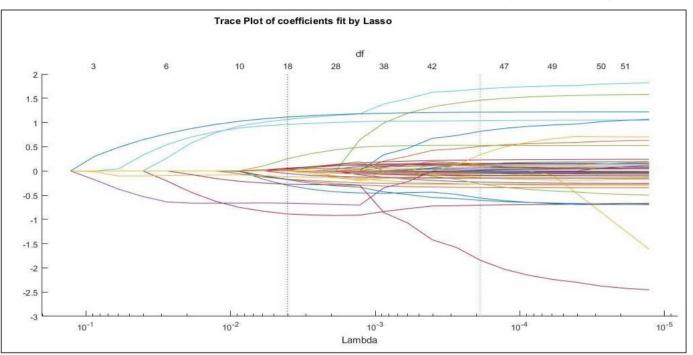
### Impact of Dummy Variable







# Bank's Marketing Strategy



#### MDL-01 2018S, Bank Marketing

Terrence White Ronald E Twite Leela Sowjanya Chippada Ahmad K Lubnani Mowlid Abdillahi Nathan Adams

Predictor	Description (likely to open an account)		
Month - August	Month of campaign		
Duration	Contact durations (seconds) (longer better)		

Predictor	<b>Description</b> (unlikely to open an account)		
Employment Rate	Quarterly employment index		
Month - September	Month of campaign		

## Regularization = Identifying Important Predictors

- Application or implication of "important" predictors?
- Couple previous student projects on Chicago or SF crime data...
  - If race is an important predictors in predicting arrest after a traffic stop, does it imply "bias"?

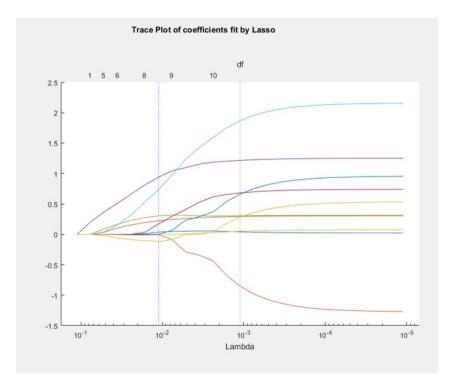
# Regularization in the Logistic Regression Model

Any comment?

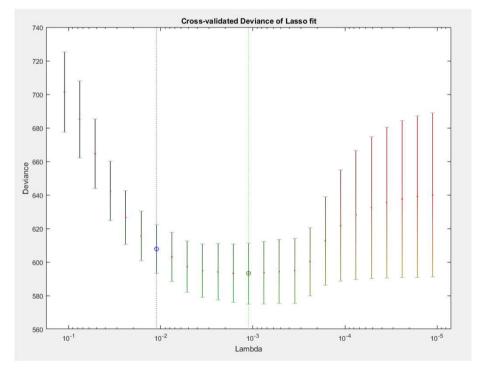
 $J(\theta) \approx E + \lambda \theta$ 

#### Predicting Liver Disease, MDL-01 2018 S

Abdulaziz Alreshedi, Beau Birkholz, Matt Conroy, Adam Grams, Dorothy Lesher, Don Stryker



Significant reduction between the minimum MSE and 1 standard deviation from the minimum MSE

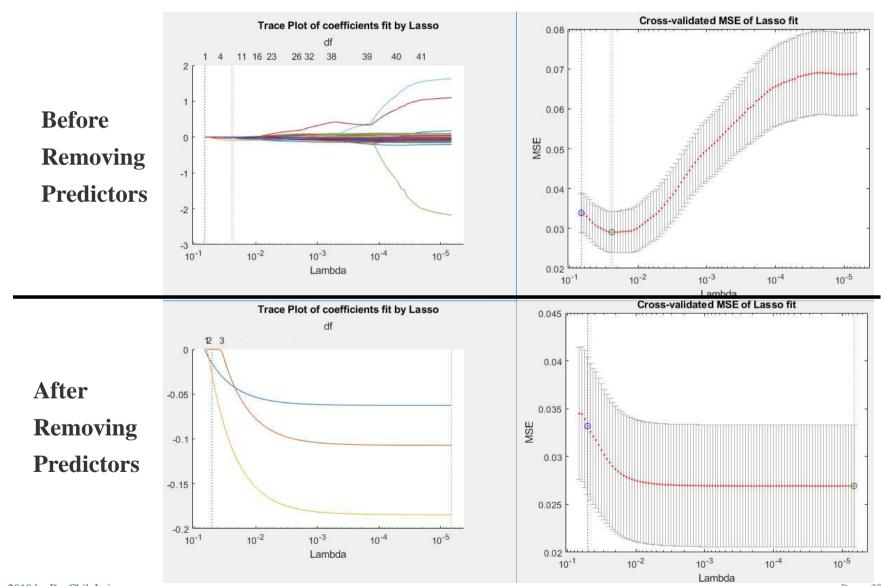


Models built with theta values at the minimum MSE and at 1 standard deviation.

#### $J(\theta) \approx MSE + \lambda \theta$

### Interpreting This Result??

91 records of 53 predictors to predict software readability.



# Regularization "MAY" Improve Minority Class Prediction

#### **Lasso Regularization Applied to**

- Minimum MSE
- $\triangle$  MSE + 1 SD

#### **Lasso Regularization Effects**

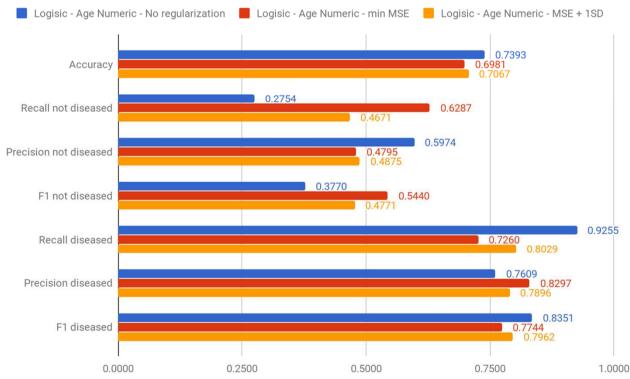
- Not Diseased Class
  - Improved: Recall & F1
  - ♣ Reduced: Precision
- A Diseased Class
  - + Improved: Precision
  - + Reduced: Recall & F1

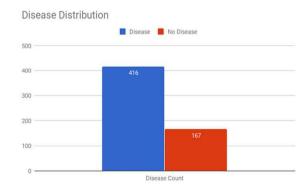
#### Predicting Liver Disease, MDL-01 2018 S

Abdulaziz Alreshedi, Beau Birkholz, Matt Conroy, Adam Grams.

Dorothy Lesher, Don Stryker

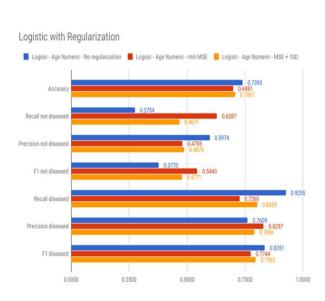






# Visualizing Quality

- CFM tells us if our dataset has class-balancing issue.
- So, please always include CFM.



Training Dataset		Test Dataset					
CFM	Precision Recall F	Target Class	Precision Recall F	CFM			
104015 0 366 84 0 81030 83 5 280 52 71675 10 61 58 9 142272	0.9967 0.9957 <b>0.9962</b>	1 (1234)	0.9955 0.9947 <b>0.9951</b>	26051 0 104 14	0 20206 22 13	116 20 17818 3	22 5 2 35604
81030 0 83 5 0 104015 366 84 52 280 71675 10 58 61 9 142272	0.9986 0.9989 <b>0.9988</b>	2 (2134)	0.9983 0.9988 <b>0.9985</b>	20206 0 22 13	0 26051 104 14	20 116 17818 3	5 22 2 35604
71675 280 52 10 366 104015 0 84 83 0 81030 5 9 61 58 142272	0.9937 0.9953 <b>0.9945</b>	3 (3124)	0.9923 0.9929 <b>0.9926</b>	17818 116 20 3	104 26051 0 14	22 0 20206 13	2 22 5 35604
142272     61     58     9       84     104015     0     366       5     0     81030     83       10     280     52     71675	0.9993 0.9991 <b>0.9992</b>	4 (4123)	0.9992 0.9992 <b>0.9992</b>	35604 22 5 2	14 26051 0 104	13 0 20206 22	3 116 20 17818

#### Predicting Liver Disease, MDL-01 2018 S

Abdulaziz Alreshedi, Beau Birkholz, Matt Conroy, Adam Grams, Dorothy Lesher, Don Stryker

#### **Satillite Image Classification**

MDL-01, 2018 S

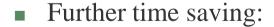
Erin Jacot, Jared Gilbert Khaled Mahmud Laura Nicla, Lydia Xu

# Regularize Wide Data in Parallel

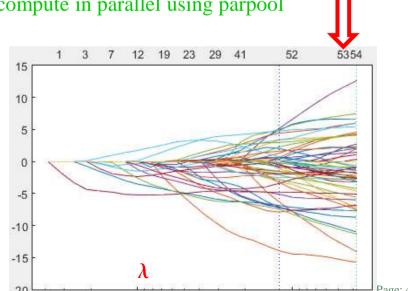
Ovarian cancer data.

- load ovariancancer
- 216 observations and 4,000 predictors.
- Wide data # predictors >> records.
- Use <u>lasso</u> to screen & select a smaller set of important predictors from wide data.
- Use parallel computing to speed up cross validation &  $\lambda$  testing.
- Parallel processing using Matlab
  - opt = statset('UseParallel',true); % Set options to use parallel computing.
  - parpool()

% Prepare to compute in parallel using parpool



- Fewer cross-validation folds.
- Fewer  $\lambda$  testing.
- $\alpha \uparrow \rightarrow$  more lasso than ridge.
  - Remove more predictors.  $(1-\alpha) \times \mathbf{R} + \alpha \times \mathbf{L}$



Waltinger

# **Python Logistic Regression + Regularization**

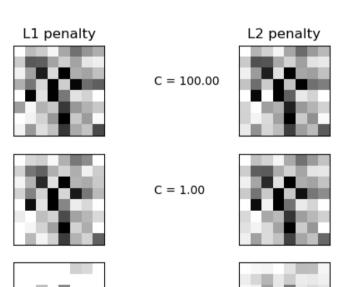
- Logistic regression + regularization
  - Classify 8x8 images of digits into two classes: 0-4 against 5-9.
  - Figures show coefficients of the models for varying *C*.
  - C = Inverse of regularization strength.
  - http://scikit-learn.org/stable/auto\_examples/linear\_model/plot\_logistic\_l1\_l2\_sparsity.html

```
J(\theta) \approx E + \lambda \times \thetaJ(\theta) \approx C \times E + \theta
```

```
C\uparrow \rightarrow MSE\downarrow \rightarrow \theta\uparrow
C\downarrow \rightarrow MSE\uparrow \rightarrow \theta\downarrow
```

```
for i, Cx in enumerate((100, 1, 0.01)):
    # turn down tolerance for short training time
    clf_11_LR = LogisticRegression(C= Cx, penalty = '11', tolerance=0.01)
    clf_12_LR = LogisticRegression(C= Cx, penalty = '12', tolerance=0.01)
    clf_11_LR.fit(X, y)
    clf_12_LR.fit(X, y)

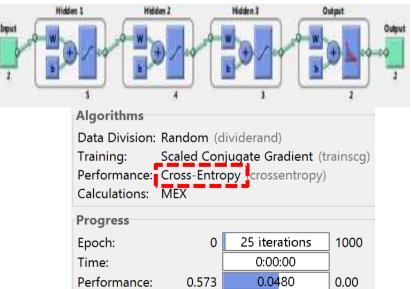
    coef_12_LR = clf_11_LR.coef_  # .ravel()
    coef_12_LR = clf_12_LR.coef_  # .ravel()
# ...
```



#### Outline

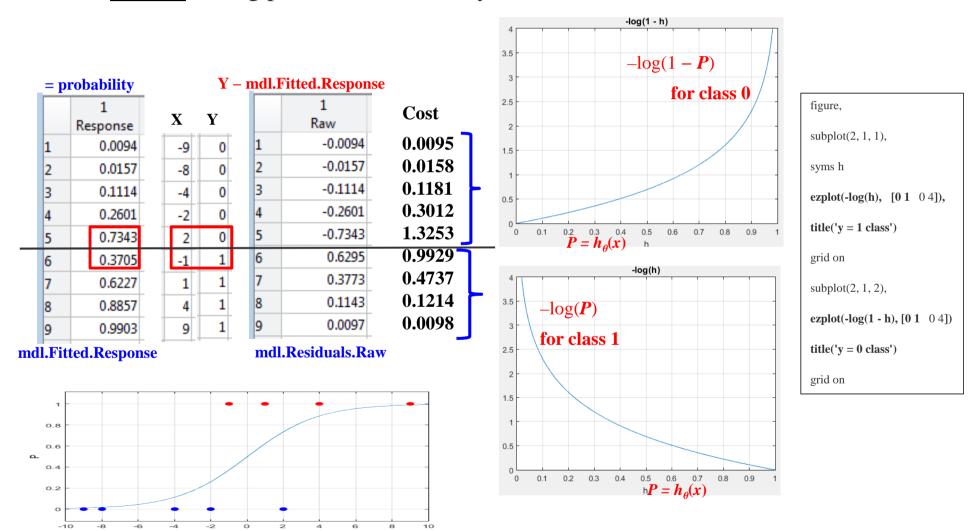
- How it works? Matlab / Python functions.
- Diagnoses / Visualization.
- Prediction and Quality.
- Outliers.
- Multiclasses Prediction.
- Nonlinearity / High Dimensionality / Visualization.
- Regularization.
- Cost Function.





# Cost Function? Why Not Just Residual?

- Residual = (Y Response) = (Y Probability)
- For <u>VERY</u> wrong prediction → Penalty ↑↑



# Logistic Regression Cost Function $P = h_{\theta}(x) = \frac{1}{1+e^{-z}}$

$$P = h_{\theta}(x) = \frac{1}{1 + e^{-z}}$$

• If y = 1 and  $P \approx 1$ , then  $-\log(P) \approx 0$ .

Correct prediction wo/ penalty.

• If y = 1 and  $P \approx 0$ , then  $-\log(P) \approx \infty$ .

Error prediction w/ huge penalty.

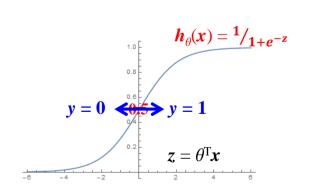
If y = 0 and  $P \approx 0$ , then  $-\log(1 - P) \approx 0$ .

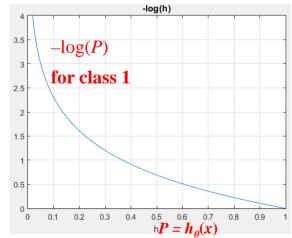
Correct prediction wo/penalty.

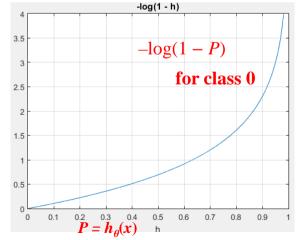
• If  $\mathbf{v} = 0$  and  $\mathbf{P} \approx 1$ , then  $-\log(1 - \mathbf{P}) \approx \infty$ .

Error prediction w/ huge penalty.

- Logistic regression cost function  $\Rightarrow J(\theta) = \begin{cases} -\log(P) & \text{if } Y_i = 1\\ -\log(1-P) & \text{if } Y_i = 0 \end{cases}$ 
  - It is **convex**!!!







# Logistic Regression Cost Function, Cross-Entropy

■ Logistic regression cost function 
$$\Rightarrow$$
  $J(\theta) = \begin{cases} -\log(P) & \text{if } Y_i = 1 \\ -\log(1-P) & \text{if } Y_i = 0 \end{cases}$ 

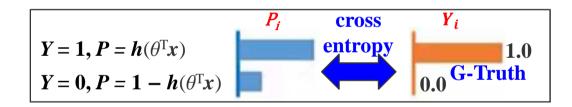
• Put together for  $y \in \{0, 1\}$ ,

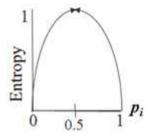
• 
$$J(\theta) = \frac{-1}{m} \sum_{i=1}^{m} [Y_i log(P_i) + (1 - Y_i) log(1 - P_i)]$$

"cross-entropy" cost function

$$y \log \frac{1}{1 + e^{-\theta^T x}} + (1 - y) \log(1 - \frac{1}{1 + e^{-\theta^T x}})$$

NOTE:  $0 \le P \le 1 \rightarrow -\infty \le \log(P) \le 0$ .





Entropy( $p_1, p_2$ ) =  $-p_1 \log_2 p_1 - p_2 \log_2 p_2$ 

■ Why this cost function? *maximum likelihood*.

# Why That Cost Function? → Maximum Likelihood

- How do we decide best  $\theta$ ? The answer is...
- Select  $\theta$  to maximize the *joined probability* of each prediction.
  - Maximize multiplications of all predicted probabilities.
  - That is, for Y = 1, maximize  $P_i^{Yi}$ . for Y = 0, maximize  $(1 P_i)^{(1 Yi)}$ .
  - Put together, maximize  $L = \prod_{i=1}^{m} P_i^{Yi} \times (1 P_i)^{(1 Yi)}$ . Solve it by set  $\frac{\partial L}{\partial P} = 0$ .
  - Difficult to solve (chain rule), but we know  $log(a \times b) = log(a) + log(b)$ .
  - =  $\underset{i=1}{\text{maximize}} \log liklihood \log(L) = \log(\prod_{i=1}^{m} P_i^{Y_i} \times (1 P_i)^{(1 Y_i)}) = \sum_{i=1}^{m} \log(P_i^{Y_i} \times (1 P_i)^{(1 Y_i)})$ =  $\sum_{i=1}^{m} [Y_i \log P_i + (1 - Y_i) \log(1 - P_i)]$

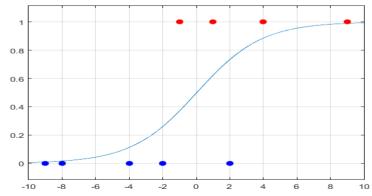
$$y \log \frac{1}{1 + e^{-\theta^T x}} + (1 - y) \log(1 - \frac{1}{1 + e^{-\theta^T x}})$$

NOTE: 
$$0 \le P \le 1 \implies -\infty \le \log(P) \le 0$$
.

• Same as to minimize negative log likelihood

$$\frac{-1}{m} \sum_{i=1}^{m} [Y_i log(P_i) + (1 - Y_i) log(1 - P_i)]$$





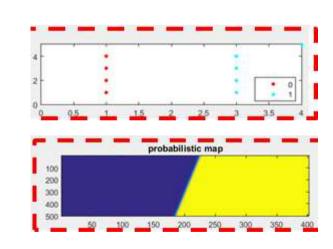
#### Maximize Likelihood = Minimize Negative Log-Likelihood

- Maximize joined probability → Maximize Log Likelihood → Minimize Negative Log Likelihood.
  - Access it from the model returned in Matlab:
    - mdl = fitglm(X, Y, 'distr', 'binomial', 'link', 'logit')
    - mdl.LogLikelihood % this is a log likelihood, NOT negative log likelihood
    - To **compare performance** between different logistic models.

See Appendix for detail matlab code

$$y \log \frac{1}{1 + e^{-\theta^T x}} + (1 - y) \log(1 - \frac{1}{1 + e^{-\theta^T x}})$$

NOTE: 
$$0 \le P \le 1 \implies -\infty \le \log(P) \le 0$$
.



$$\frac{d}{dt} \left( \log \left( \frac{1}{1 + e^{-t}} \right) \right) = \frac{1}{e^t + 1}$$

$$\frac{\partial}{\partial t} \left( \log \left( \frac{1}{1 + e^{-tx}} \right) \right) = \frac{x}{e^{tx} + 1}$$

$$\frac{\partial}{\partial t} \left( \log \left( \frac{1}{1 + e^{-tx}} \right) \right) = \frac{x}{e^{tx} + 1}$$

$$\frac{d}{dt} \left( \log \left( 1 - \frac{1}{1 + e^{-t}} \right) \right) = -\frac{e^t}{e^t + 1} \qquad x \left( \frac{1}{e^{tx} + 1} - 1 \right)$$

$$\frac{\partial}{\partial t} \left( \log \left( 1 - \frac{1}{1 + e^{-tx}} \right) \right) = -\frac{x e^{tx}}{e^{tx} + 1} \qquad \frac{x}{e^{tx} + 1} - x$$

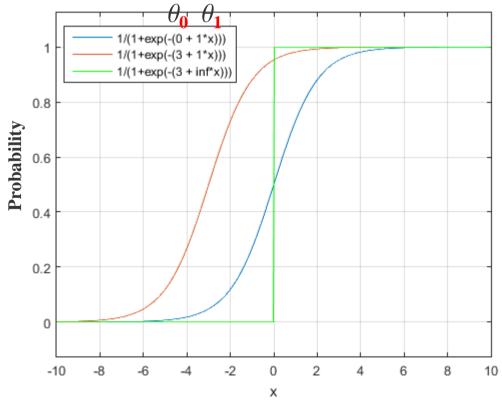
# Appendix

# Shifting in Logistic Function – Changing $\theta_0$

- Logistic Regression  $h_{\theta}(x) = h(\theta^{T}x) = h(z) = \frac{1}{1+e^{-z}}$ 
  - $z = \theta^{\mathrm{T}} x = \theta_0 \times x_0 + \theta_1 \times x_1 + \dots + \theta_n \times x_n$ .

 $z = \theta^{\mathrm{T}} x = \theta_0 \times x_0 + \theta_1 \times x_1.$ 

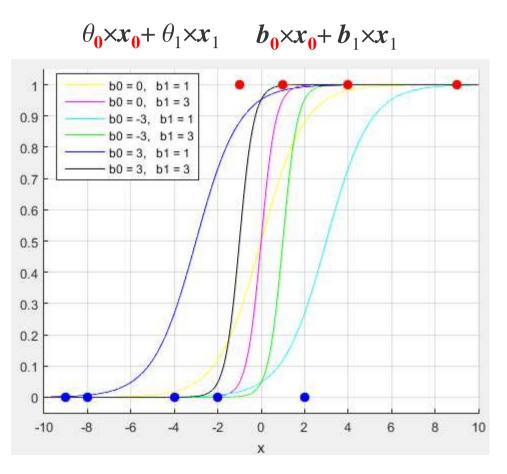
• What will be the curve if we set  $\theta_1 \approx \infty$ ?



```
syms x
fstr1 = \frac{1}{1+exp(-(0+1*x))};
fstr2 = \frac{1}{1+exp(-(3+1*x))};
fstr3 = \frac{1}{1 + exp(-(3 + inf * x))};
ezplot(fstr1, [-10 10]);
hold on
ezplot(fstr2, [-10 10]);
h3 = ezplot(fstr3, [-10 10]);
set(h3, 'color', 'g')
hold off
grid on
legend({fstr1, fstr2, fstr3})
title(")
```

# Logistic Function– Changing Both $\theta_0$ and $\theta_1$

■ Logistic (sigmoid) function  $\sigma$  takes LR output  $(\hat{y})$  as input & convert to P[0..1].



```
syms x
b0 arr = [0 -3 3]; b1 arr = [1 3];
fstr = \frac{1}{1+exp(-(b0 + b1*x))};
c = ['ymcgbk'];
figure, hold on
loops = 0; legendStr = [];
for b0 = b0_arr
  for b1 = b1 arr
     fstrX = strrep(fstr, 'b0', num2str(b0));
     fstrX = strrep(fstrX, 'b1', num2str(b1));
     h = ezplot(fstrX, [-10 10]);
     loops = loops + 1;
     set(h, 'color', c(loops));
     legendStr{loops} = \lceil b0 = ' num2str(b0) ', b1 = ' num2str(b1) \rceil;
  end
end
legend(legendStr), title("), grid on, ylim([-0.05 1.05])
red = [-1 \ 1; 1 \ 1; 4 \ 1; 9 \ 1];
blue = [2 0; -2 0; -4 0; -8 0; -9 0];
data = [red; blue];
Y = [zeros(size(red, 1), 1); ones(size(blue, 1), 1)];
gscatter(data(:, 1), data(:, 2), Y, 'rb', '..', 25, 'off')
hold off
```

#### **Binomial Distribution**

- A **binomial experiment** has the following properties:
  - The experiment consists of *n* repeated trials of two outcomes: a success & a failure.
  - The probability of success, denoted by *P*, is the same on every trial.
  - The trials are independent: one trial does not affect the outcome on other trials.
  - http://stattrek.com/probability-distributions/binomial.aspx
- Binomial experiment Example: flip a coin *N* times and count the # of heads.
  - Repeated trials of flipping a coin *N* times with outcomes heads or tails: 0.5.
  - The trials are independent; getting heads on one trial does not affect results of others.

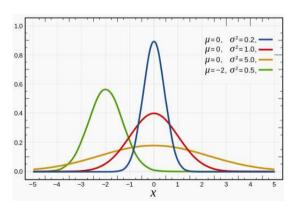
#### Different Distributions

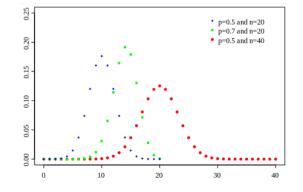
http://www.mathworks.com/help/stats/generalizedlinearmodel-class.html

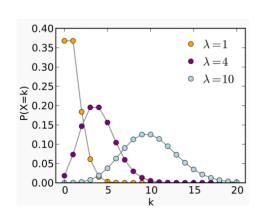
$$h_{\theta}(x) = P = \frac{e^z}{1+e^z} = \frac{1}{1+e^{-z}}$$

$$\frac{P}{1-P} = e^z.$$

Distribution	Link Function Name	Link Function	Mean (Inverse) Function
'normal'	'identity'	$f(\mu) = \mu$	$\mu = Xb$
'binomial'	'logit'	$f(\mu) = \log(\mu/(1-\mu))$	$\mu = \exp(Xb) / (1 + \exp(Xb))$
'poisson'	'log'	$f(\mu) = \log(\mu)$	$\mu = \exp(Xb)$
'gamma'	-1	$f(\mu) = 1/\mu$	$\mu = 1/(Xb)$
'inverse gaussian'	-2	$f(\mu) = 1/\mu^2$	$\mu = (Xb)^{-1/2}$

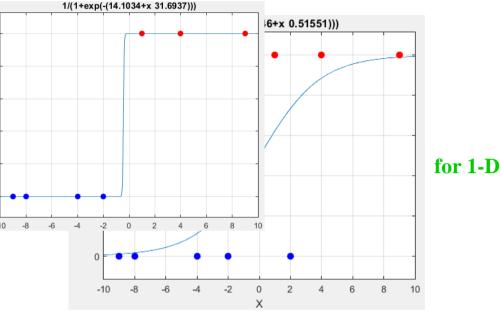


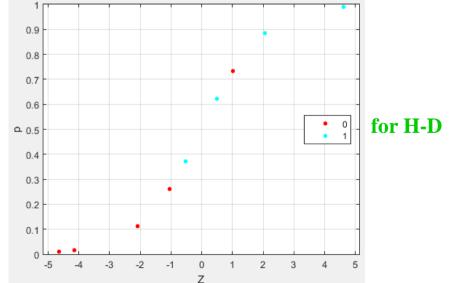




# Plotting *X* against Response (Probability = $\frac{1}{1+e^{-z}}$ )

```
red = [-1 \ 1; 1 \ 1; 4 \ 1; 9 \ 1];
blue = [-9 0; -8 0; -4 0; -2 0; 2 0];
X = [blue(:, 1); red(:, 1);];
Y = [blue(:, 2); red(:, 2)];
mdl = fitglm(X, Y, 'distr', 'binomial', 'link', 'logit')
B = mdl.Coefficients.Estimate;
                                          %% θ
Bstr = num2str(B);
Zstr = [Bstr(1,:) '+x*' Bstr(2,:)]; \frac{\%}{\%} = \theta^{T}x
syms x,
figure, ezplot(['1/(1+exp(-(' Zstr ')))'], [-10 10])
hold on.
           gscatter(X(:, 1), Y, Y, 'br', '..', 25, 'off')
hold off, grid on
xlabel('X'), ylabel('P')
mdl.LogLikelihood
```



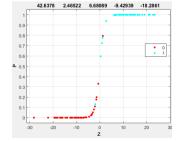


#### %% Plot Z wrt P (much easier)

**p** = **mdl.Fitted.Response**;

**Z** = mdl.Fitted.LinearPredictor;

figure, gscatter(Z, p, Y); grid on



#### Some Matlab Link Functions

mdl = fitglm(X, Y, 'distr', 'binomial', 'link', 'logit')

Link Function Name	Link Function	Mean (Inverse) Function		
'log'	$f(\mu) = \log(\mu)$	$\mu = \exp(Xb)$		
'logit'	$f(\mu) = \log(\mu/(1-\mu))$	$ \mu = \exp(Xb) / (1 + \exp(Xb)) \qquad \frac{e^z}{1 + e^z} $		
'probit'	$f(\mu) = \Phi^{-1}(\mu)$	$\mu = \Phi(Xb)$		
'comploglog'	$f(\mu) = \log(-\log(1 - \mu))$	$\mu = 1 - \exp(-\exp(Xb))$		
'reciprocal' $f(\mu) = 1/\mu$		$\mu = 1/(Xb)$		

$$\Phi(x) = \int_{-\infty}^{x} \frac{1}{\sqrt{2\pi}} e^{-t^{2}/2} dt$$

normal distribution function

- Logit function  $\log(\frac{P}{1-P}) = z = \theta^{T}x$ .
  - <u>Inverse</u> of the sigmoidal "<u>logistic</u>" function.
  - It gives the log-odds (log of odds).
  - $\frac{P}{1-P}$  is refer to as *odds*.
  - $\frac{P}{1-P} = e^z \rightarrow P = e^z e^z P \rightarrow P = \frac{e^z}{1+e^z} = \frac{1}{1+e^{-z}} = h_{\theta}(x)$ .

#### Logit Function (Visualize in Mathematica)

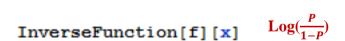
$$f[x_{-}] := 1 / (1 + Exp[-x]) \frac{1}{1 + e^{-z}}$$
  
Plot[f[x], {x, -6, 6}]

f[x\_]:=1/(1+Exp[-x]) Plot[f[x], {x, -6, 6}]

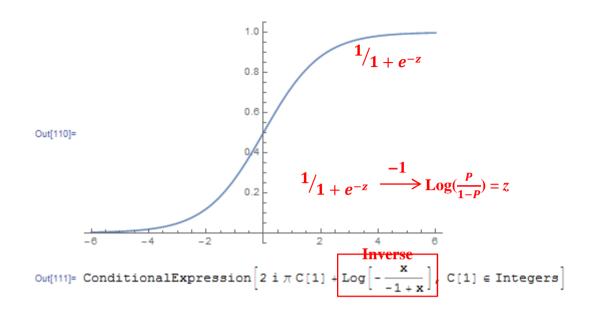
InverseFunction[f][x]

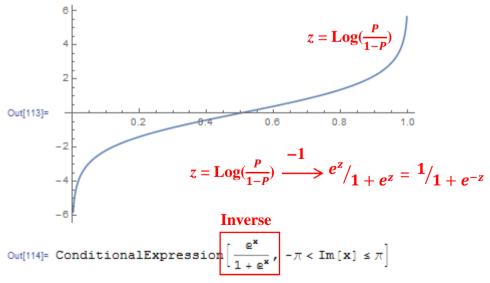
 $fi[x_]:=Log[x/(1-x)]$ Plot[fi[x], {x, 0, 1}]

InverseFunction[fi][x]



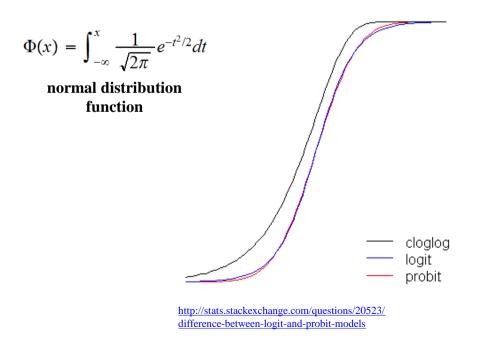
InverseFunction[fi][x]

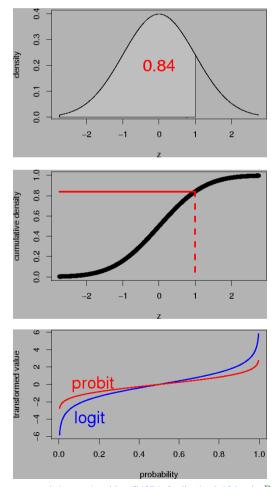




# Logit and Probit

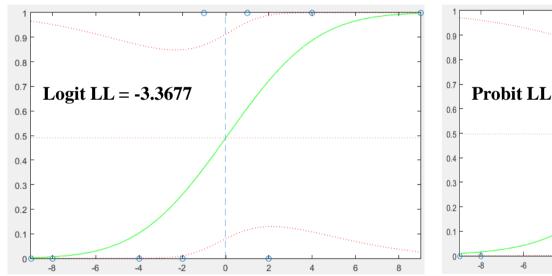
- The probit function is the inverse of the standard cumulative normal distribution.
- Logit and Probit generate very similar curves.
  - Logit has slightly fatter tails than probit, making it slightly more 'robust'.
  - For 2 classes, undifferentiated between logit & probit.
  - For 3+ classes, harder to apply probit.
  - Use **likelihood** value to decide logit or probit.





### Logit and Probit Comparison, Likelihood

- Logit has slightly longer tails than probit → logit is slightly more robust.
- In binary response, probit & logit are largely the same.
- Use **log likelihood** (larger → better) value to decide logit or probit.



```
red = [-11; 1 1; 4 1; 9 1];
blue = [-9 0; -8 0; -4 0; -2 0; 20];
X = [blue(:, 1); red(:, 1);];
Y = [blue(:, 2); red(:, 2)];

mdl = fitglm(X, Y, 'distr', 'binomial', 'link', 'logit')
plotSlice(mdl)
mdl.LogLikelihood
% -3.3677 equal to following
sum(Y.*log(mdl.Fitted.Response) + (1-Y).*log(1 - mdl.Fitted.Response))
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```

```
red = [ -1 1; 1 1; 4 1; 9 1];
blue = [-9 0; -8 0; -4 0; -2 0; 2 0];
X = [blue(:, 1); red(:, 1);];
Y = [blue(:, 2); red(:, 2)];
mdl = fitglm(X, Y, 'distr', 'binomial', 'link', 'probit')
plotSlice(mdl)
mdl.LogLikelihood
% -3.3153
```

#### Total Cost = $-1 \times \text{Log Likelihood}$

$$y \log \frac{1}{1 + e^{-\theta^T x}} + (1 - y) \log(1 - \frac{1}{1 + e^{-\theta^T x}})$$

- $Cost(h(\theta^{T}x), y) = \frac{-1}{m} \sum_{i=1}^{m} [Y_{i}log(P_{i}) + (1 Y_{i})log(1 P_{i})]$ 
  - Total cost = -1 \* mdl.LogLikelihood (negative log likelihood)

H LogLikelihood 🛑 -3.3677

C0 = log(1 - mdl.Fitted.Response(1:5))

 $C1 = \log(\text{mdl.Fitted.Response}(6:9))$ 

-1 \* sum([C0;C1]) **% Total Cost = 3.367** 

= <u>r</u>	pro	ba	bi	lity
	_			

V - mdl Fitted Response

- probability				1 - 1	IIuI.I	ritteu.Kesponse	
	1 Response		X	Y		1 Raw	Cost
1	0.0094		-9	0	1	-0.0094	0.0095
2	0.0157		-8	0	2	-0.0157	0.0158
3	0.1114	-	-4	0	3	-0.1114	0.1181
4	0.2601	1	-2	0	4	-0.2601	0.3012
5	0.7343		2	0	5	-0.7343	1.3253
6	0.3705		-1	1	6	0.6295	0.9929
7	0.6227		1	1	7	0.3773	0.4737
8	0.8857	1	4	1	8	0.1143	0.1214
9	0.9903	1	9	1	9	0.0097	0.0098

mdl.Fitted.Response

mdl.Residuals.Raw

