MODELASSESSMENT

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COMPARING MODELS

Purpose of Modeling

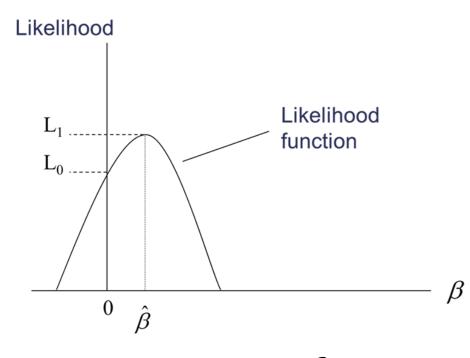
- Statistical models are created for two different purposes estimation and prediction.
 - Estimation: Quantifying the expected change in response associated with predictors (relationships).
 - Prediction: Use the model to predict new response.
- Won't necessarily agree!

Deviance/Likelihood Measures

- AIC and BIC approximate out-of-sample prediction error by applying a penalty for model complexity:
 - AIC crude, large-sample approximation of leave-oneout cross-validation.
 - BIC favors smaller models/penalizes model complexity more.
- Lower values "better" than higher.
- No amount of lower is "better" enough.
- May not always agree, but neither is necessarily better.

Deviance/Likelihood Measures

- Number of "pseudo"-R² quantities for logistic regression.
- Higher values indicate "better" model.
- Generalized / Nagelkerke
 R² how much better than intercept only model?
- Unlike linear regression, there is no interpretation on these.



$$R_G^2 = 1 - \left(\frac{L_0}{L_1}\right)^{\frac{2}{n}}$$

Generalized R² – SAS

Generalized R² – SAS

Model Fit Statistics				
Criterion	Intercept Only	Intercept and Covariates		
AIC	236.672	225.015		
SC	239.914	241.223		
-2 Log L	234.672	215.015		

R-Square	0.0988	Max-rescaled R-Square	0.1389	
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Generalized R² – R

Generalized R² – R

```
AIC(logit.model)
## [1] 225.0147
BIC(logit.model)
## [1] 241.2234
PseudoR2(logit.model, which = "Nagelkerke")
## Nagelkerke
## 0.1389144
```



ASSESSING PREDICTIVE POWER

What is a Good Logistic Model?

- Logistic regression is a model for probability of an event – NOT the occurrence of an event.
- Logistic regression can be a classification model as well.
- Good model should reflect both of these, but importance of one over the other depends on the problem.

Discrimination vs. Calibration

- Discrimination ability to separate the events from the non-events. How good is model at distinguishing the 1's from the 0's.
- Calibration how well predicted probabilities agree with the actual frequency of the outcomes. Are predicted probabilities systematically too low/high?
- May not agree with each other!



ASSESSING PREDICTIVE POWER

Probability Based Metrics

Coefficient of Discrimination

- Want model to assign a higher probability to events and lower probability to non-events.
- Coefficient of discrimination (or discrimination slope)
 is the difference in average predicted probability between
 1's and 0's:

$$D = \bar{\hat{p}}_1 - \bar{\hat{p}}_0$$

Able to compare with histograms as well.

Discrimination Slope – SAS

```
proc logistic data=logistic.lowbwt noprint;
   class race(ref='white') / param=ref;
   model low(event='1') = race lwt smoke;
   output out=predprobs p=phat;
run;
proc sort data=predprobs;
   by descending low;
run;
proc ttest data=predprobs order=data;
   ods select statistics summarypanel;
   class low;
   var phat;
   title 'Coefficient of Discrimination and Plots';
run;
```

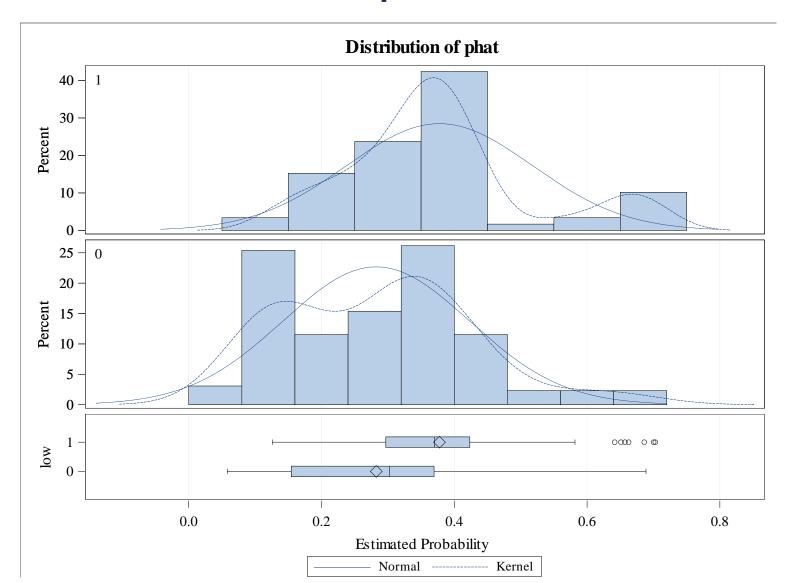
Discrimination Slope – SAS

Coefficient of Discrimination and Plots The TTEST Procedure

Variable: phat (Estimated Probability)

low	Method	N	Mean	Std Dev	Std Err	Minimum	Maximum
1		59	0.3776	0.1401	0.0182	0.1258	0.7028
0		130	0.2825	0.1407	0.0123	0.0580	0.6887
Diff (1-2)	Pooled		0.0952	0.1405	0.0221		
Diff (1-2)	Satterthwaite		0.0952		0.0220		

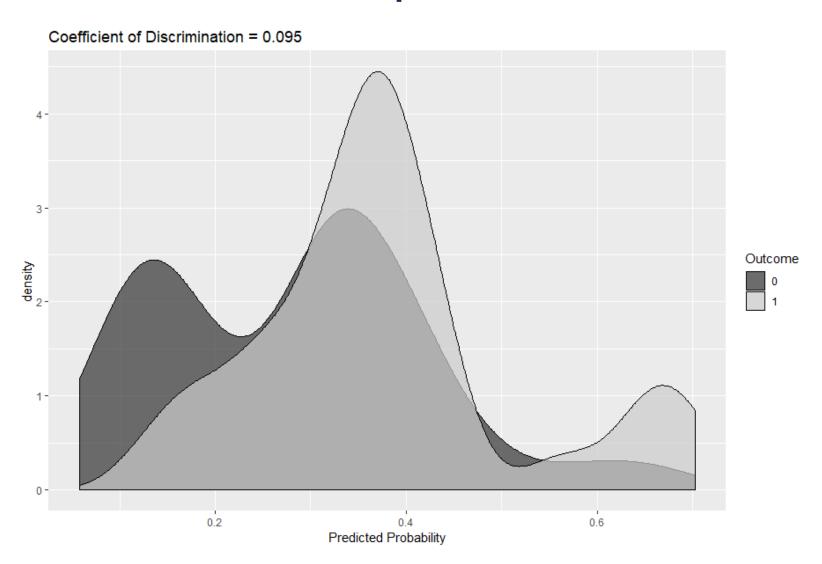
Discrimination Slope – SAS



Discrimination Slope – R

```
bwt$p_hat <- predict(logit.model, type = "response")</pre>
p1 <- bwt$p hat[bwt$low == 1]
p0 <- bwt$p hat[bwt$low == 0]
coef_discrim <- mean(p1) - mean(p0)</pre>
ggplot(bwt, aes(p_hat, fill = factor(low))) +
  geom_density(alpha = 0.7) +
  scale fill grey() +
  labs(x = "Predicted Probability",
       fill = "Outcome",
       title = paste("Coefficient of Discrimination = ",
                      round(coef discrim, 3), sep = ""))
```

Discrimination Slope – R



Rank-order Statistics

- How well does the model order predictions?
- Concordance: for a pair of subjects with and without the event, the one with the event had the higher predicted probability.
- Discordance: for a pair of subjects with and without the event, the one with the event had the lower predicted probability.
- Tied: for a pair of subjects with and without the event, they both have the same predicted probability.

Concordance

- Interpretation For all possible (1,0) pairs, the model assigned the higher predicted probability to the observation with the event concordance% of the time.
- Common metrics based on concordance:

• c-statistic:
$$c = Concordance \% + \frac{1}{2}Tied \%$$

• Somers' D:
$$D_{xy} = 2c - 1$$

• Kendall's
$$\tau_a$$
: $\tau_a = \frac{\# concordant - \# discordant}{\frac{n(n-1)}{2}}$

Rank-order Statistics – SAS

Rank-order Statistics – SAS

Association of Predicted Probabilities and Observed Responses				
Percent Concordant	68.3	Somers' D	0.371	
Percent Discordant	31.2	Gamma	0.373	
Percent Tied	0.5	Tau-a	0.160	
Pairs	7670	С	0.686	

Rank-order Statistics – R

```
Concordance(bwt$low, bwt$p hat)
## $Concordance
## [1] 0.6831812
##
## $Discordance
## [1] 0.3168188
##
## $Tied
## [1] 5.551115e-17
##
## $Pairs
## [1] 7670
somersD(bwt$low, bwt$p_hat)
## [1] 0.3663625
```



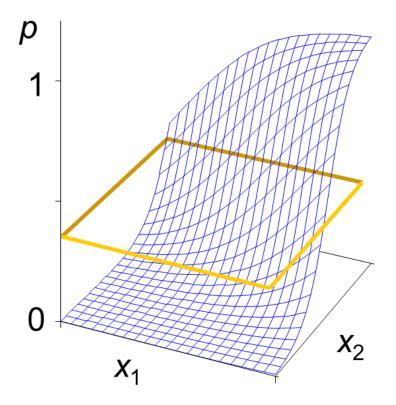
ASSESSING PREDICTIVE POWER

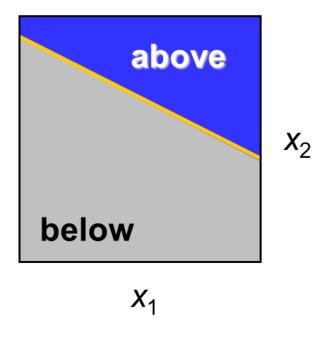
Classification Based Metrics

Classification

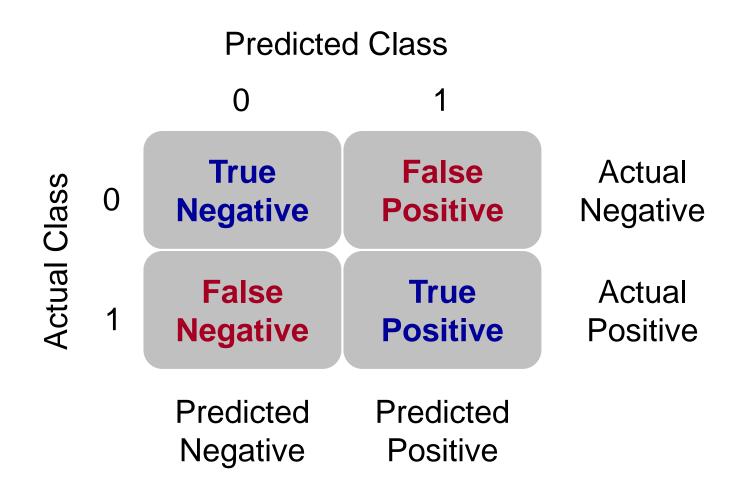
- Want model to correctly classify events and non-events.
- Classification forces the model to predict $\hat{y}_i = 1$ or $\hat{y}_i = 0$ based on whether the predicted probability exceeds some threshold for example, $\hat{y}_i = 1$ if $\hat{p}_i > 0.5$.
- Strict classification-based measures completely discard any information about the actual quality of the model's predicted probabilities.

Logistic Discrimination

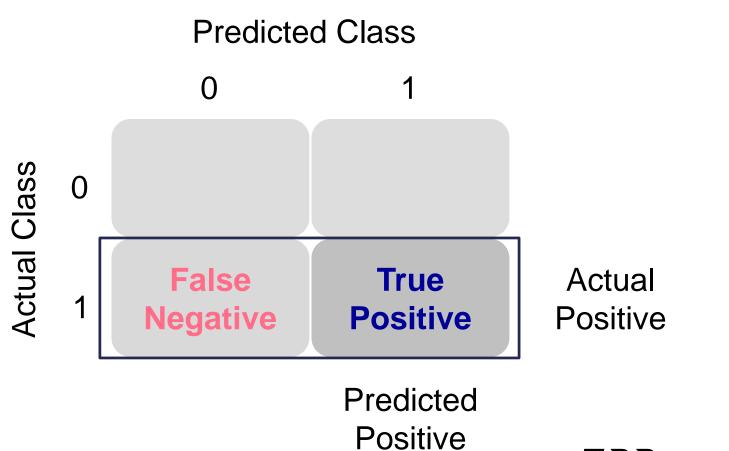




Classification Table

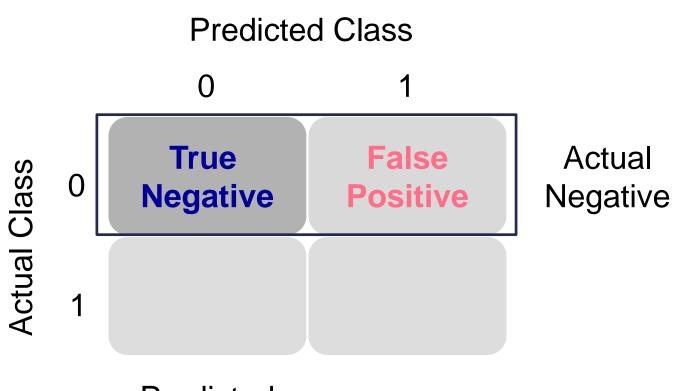


Sensitivity / Recall



$$TPR = \frac{TP}{TP + FN}$$

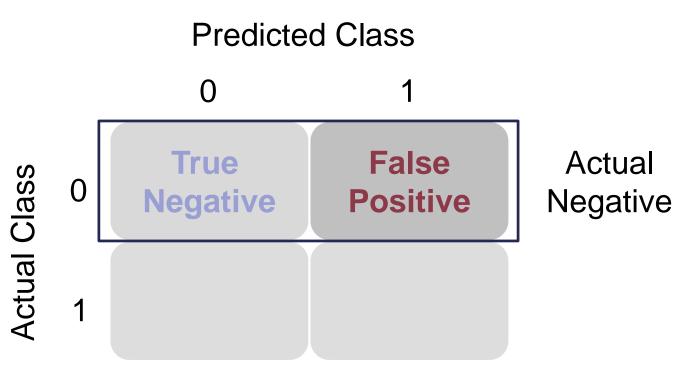
Specificity



Predicted Negative

$$TNR = \frac{TN}{TN + FP}$$

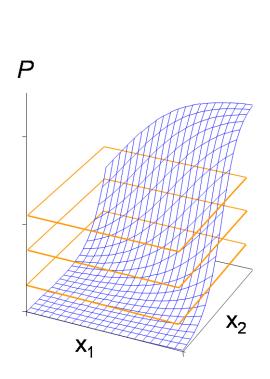
1 – Specificity



Predicted Negative

$$FPR = \frac{FP}{TN + FP}$$

Classification Changes with Cut-off



	<u> </u>		
<u>response</u>	<u>P</u>	cutoff=.5	cutoff=.25
0	.32	0	1
1	.40	0	1
1	.92	1	1
0	.06	0	0
1	.52	1	1
1	.39	0	1
1	.22	0	0
0	.17	0	0
0	.13	0	0
:	:	:	:
1	.75	1	1
-		-	-

Best Cut-off?

- Always consider the cost of false positives and false negatives when doing classification.
- When NOT considering costs, many different techniques to "optimal" cut-off.
- Youden J statistic (or Youden's index):

```
J = \text{sensitivity} + \text{specificity} - 1
```

 "Optimal" – false positives and false negatives are weighed equally, so select cut-off that produces highest Youden J statistic.

Classification Table – SAS

Classification Table – SAS

Classification Table										
Prob	Correct		Incorrect		Percentages					
Level	Event	Non- Event	Event	Non- Event	Correct	Sensi- tivity	Speci- ficity	Pos Pred	Neg Pred	
0.000	59	0	130	0	31.2	100.0	0.0	31.2	•	
0.020	59	0	130	0	31.2	100.0	0.0	31.2	-	
0.040	59	0	130	0	31.2	100.0	0.0	31.2	•	
0.060	59	1	129	0	31.7	100.0	0.8	31.4	100.0	
0.080	59	4	126	0	33.3	100.0	3.1	31.9	100.0	
0.100	59	10	120	0	36.5	100.0	7.7	33.0	100.0	
0.120	58	15	115	1	38.6	98.3	11.5	33.5	93.8	
0.140	57	26	104	2	43.9	96.6	20.0	35.4	92.9	
0.160	54	35	95	5	47.1	91.5	26.9	36.2	87.5	
0.180	53	43	87	6	50.8	89.8	33.1	37.9	87.8	

Youden's Index – SAS

```
data classtable;
   set classtable;
   youden = sensitivity + specificity - 100;
   drop PPV NPV Correct;
run;
proc sort data=classtable;
      by descending youden;
run;
proc print data=classtable;
run;
```

Youden's Index – SAS

Obs	ProbLevel	Sensitivity	Specificity	FalsePositive	FalseNegative	youden
1	0.200	89.8	34.6	61.6	11.8	24.4459
2	0.180	89.8	33.1	62.1	12.2	22.9074
3	0.220	86.4	36.2	61.9	14.5	22.5945
4	0.240	81.4	39.2	62.2	17.7	20.5867
5	0.300	72.9	47.7	61.3	20.5	20.5737



Classification Table – R

```
confusionMatrix(bwt$low, bwt$p_hat, threshold = 0.5)
## 0 1
## 0 122 50
## 1 8 9
```

Classification & Youden Index – R

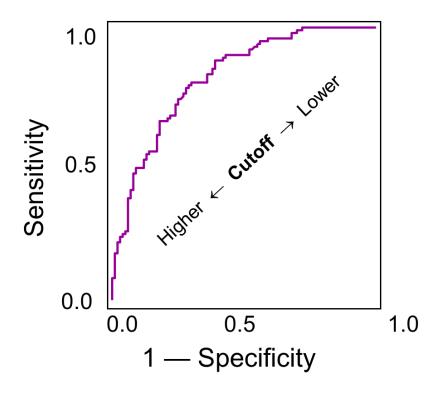
```
sens <- NULL
spec <- NULL
youden <- NULL
cutoff <- NULL
for(i in 1:49){
  cutoff = c(cutoff, i/50)
  sens <- c(sens, sensitivity(bwt$low, bwt$p_hat,</pre>
            threshold = i/50)
  spec <- c(spec, specificity(bwt$low, bwt$p hat,</pre>
            threshold = i/50)
  youden <- c(youden, youdensIndex(bwt$low, bwt$p_hat,</pre>
              threshold = i/50)
ctable <- data.frame(cutoff, sens, spec, youden)
```

Classification & Youden Index – R

```
cutoff
##
                                          youden
                   sens
                               spec
## 1
        0.02 1.00000000 0.000000000 0.000000000
## 2
        0.04 1.00000000 0.000000000 0.000000000
## 3
        0.06 1.00000000 0.007692308 0.007692308
## 4
        0.08 1.00000000 0.030769231 0.030769231
## 5
        0.10 1.00000000 0.084615385 0.084615385
## 6
        0.12 1.00000000 0.123076923 0.123076923
## 7
        0.14 0.96610169 0.230769231 0.196870926
## 8
        0.16 0.96610169 0.284615385 0.250717080
## 9
        0.18 0.93220339 0.330769231 0.262972621
        0.20 0.89830508 0.353846154 0.252151239
## 10
## 11
        0.22 0.89830508 0.369230769 0.267535854
## 12
        0.24 0.86440678 0.400000000 0.264406780
## 13
        0.26 0.81355932 0.415384615 0.228943937
```

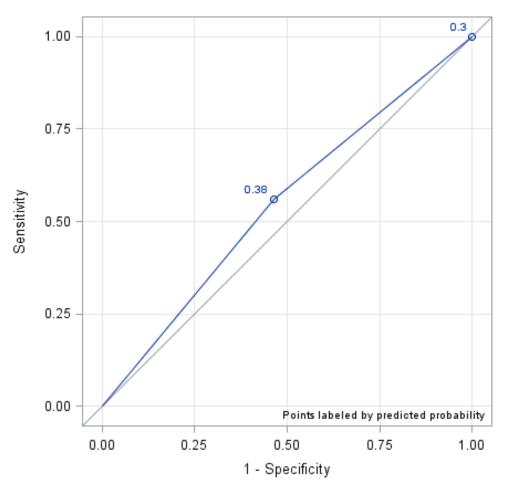
=

ROC Curve

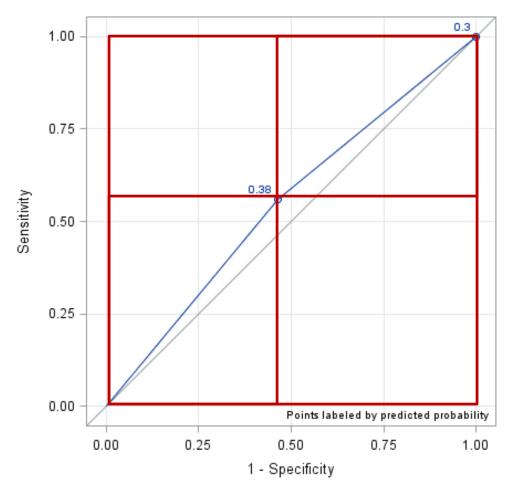


- ROC curve plots TPR vs.
 FPR for a grid of thresholds.
- Area under the curve (AUC or AUROC) summarizes the overall quality of ROC curve – equivalent to c-statistic.
- Want high sensitivity and high specificity.

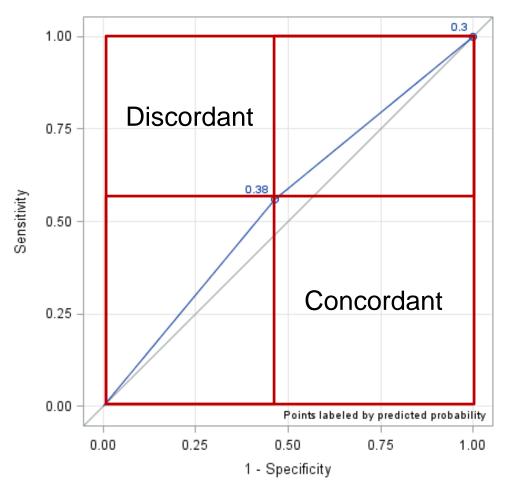
$$AUC = \% Concordant + \frac{1}{2}(\% Tied)$$



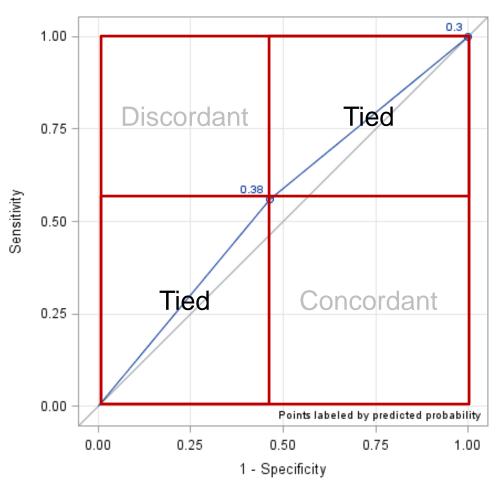
$$AUC = \% Concordant + \frac{1}{2}(\% Tied)$$



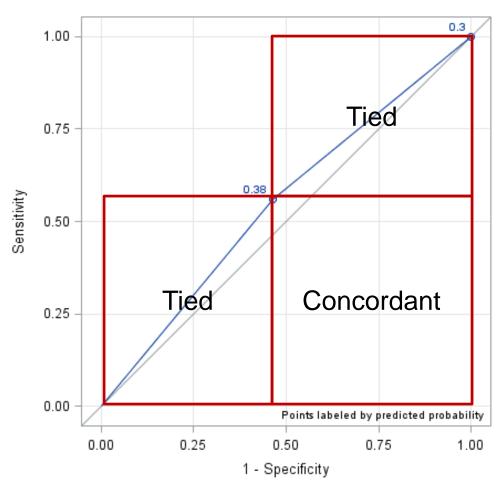
$$AUC = \% Concordant + \frac{1}{2}(\% Tied)$$



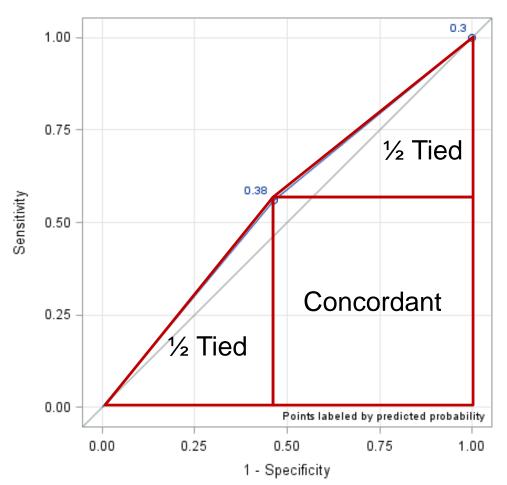
$$AUC = \% Concordant + \frac{1}{2}(\% Tied)$$



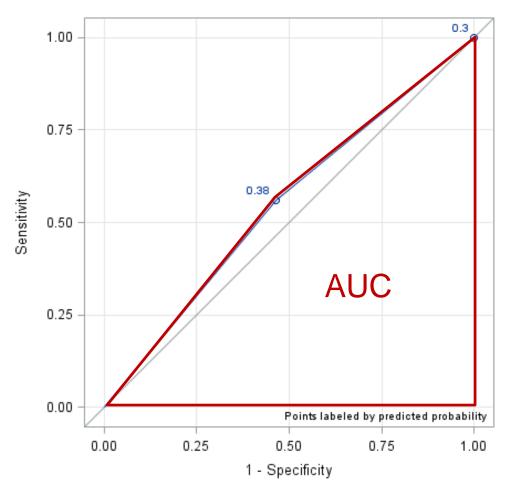
$$AUC = \% Concordant + \frac{1}{2}(\% Tied)$$



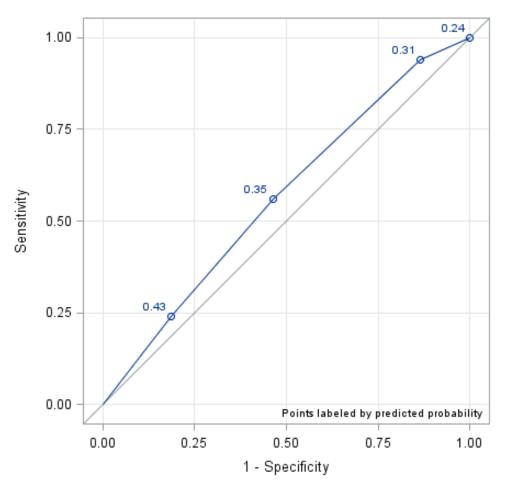
$$AUC = \% Concordant + \frac{1}{2}(\% Tied)$$



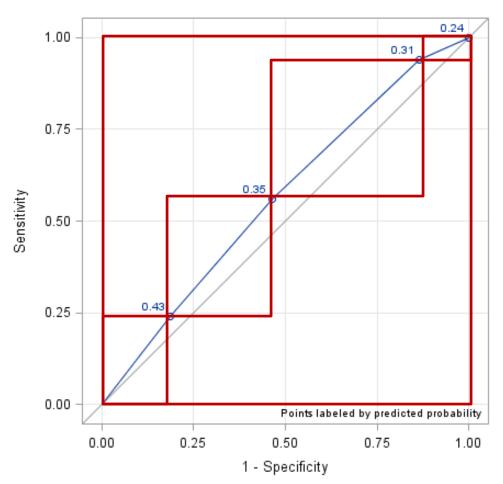
$$AUC = \% Concordant + \frac{1}{2}(\% Tied)$$



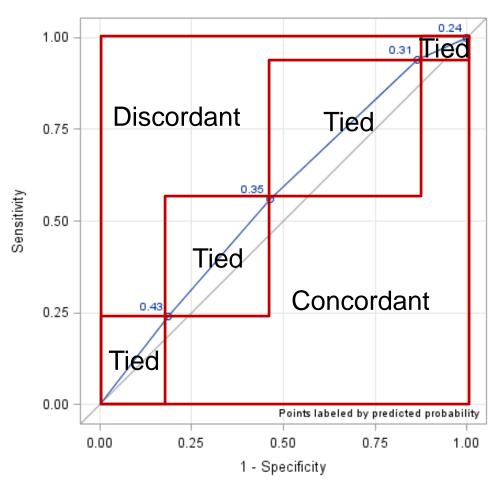
$$AUC = \% Concordant + \frac{1}{2}(\% Tied)$$



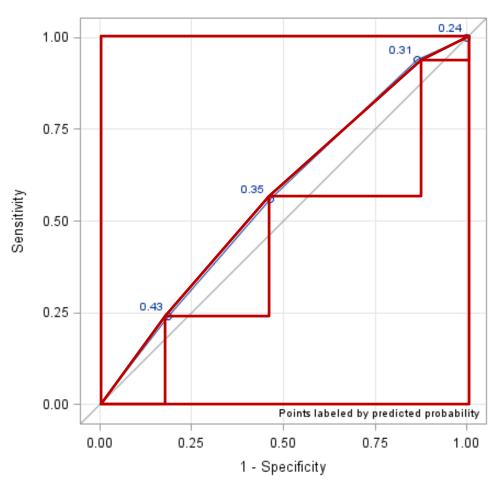
$$AUC = \% Concordant + \frac{1}{2}(\% Tied)$$



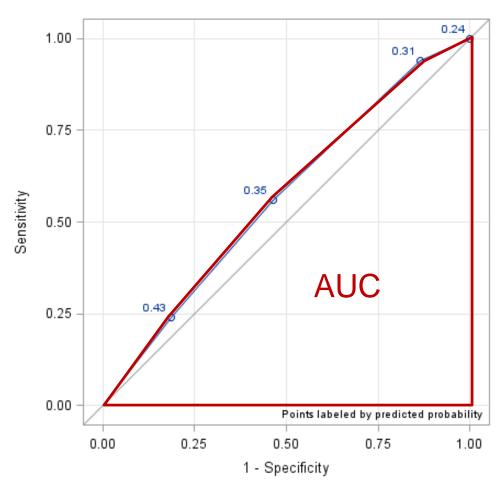
$$AUC = \% Concordant + \frac{1}{2}(\% Tied)$$



$$AUC = \% Concordant + \frac{1}{2}(\% Tied)$$

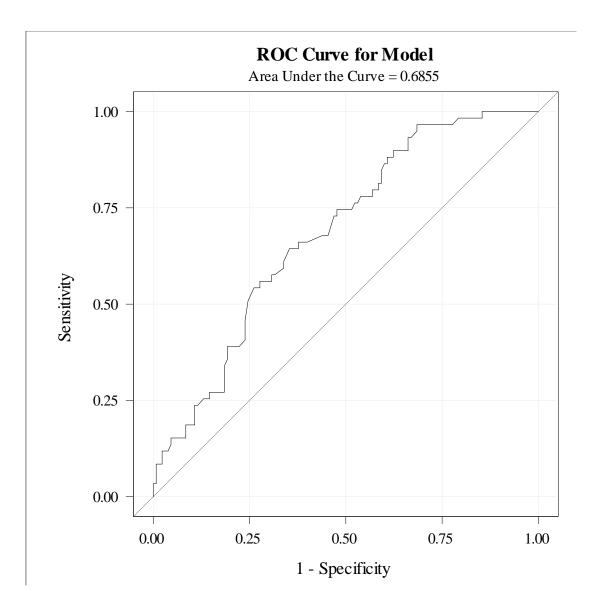


$$AUC = \% Concordant + \frac{1}{2}(\% Tied)$$



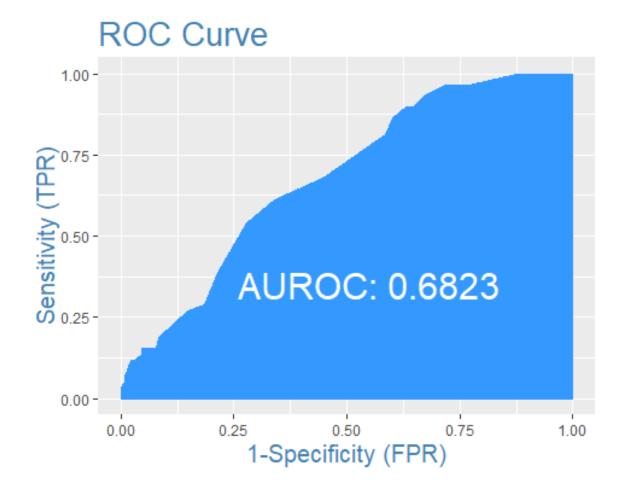
ROC Curve – SAS

ROC Curve – SAS



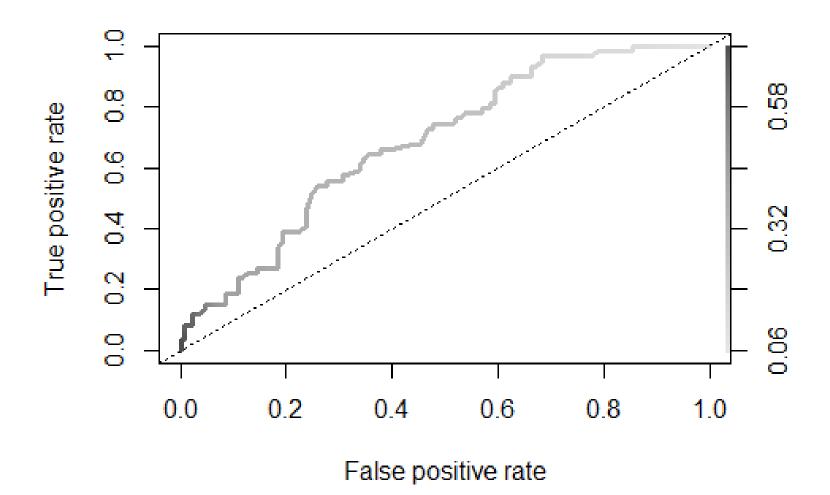
ROC Curve – R

plotROC(bwt\$low, bwt\$p_hat)



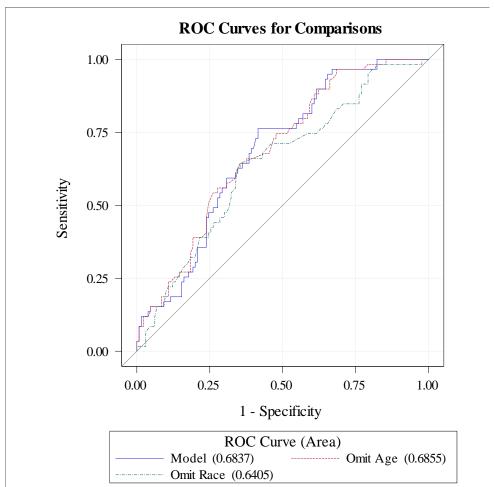
ROC Curve – R

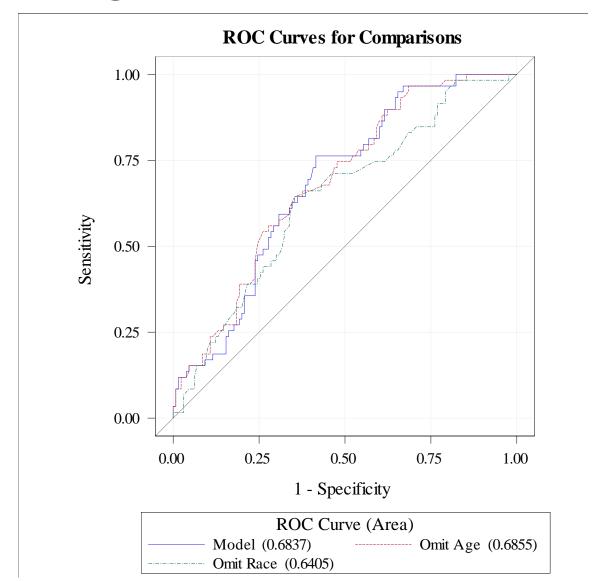
ROC Curve – R



Comparing ROC Curves

Can compare different ROC curves statistically by their AUC.



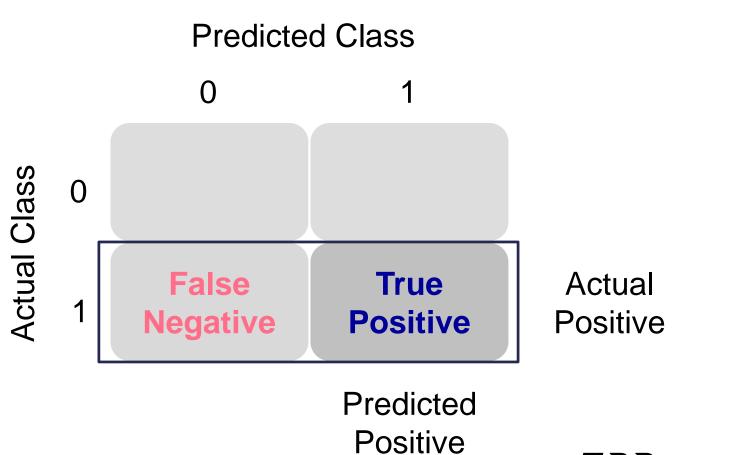


ROC Association Statistics									
ROC Model		Mann-V	Vhitney	Somers'	Gamma	Tau-a			
	Area	Standard Error	95% Wald Confidence Limits				D		
Model	0.6837	0.0393	0.6068	0.7606	0.3674	0.3675	0.1586		
Omit Age	0.6855	0.0395	0.6081	0.7630	0.3711	0.3728	0.1602		
Omit Race	0.6405	0.0428	0.5567	0.7243	0.2810	0.2843	0.1213		

ROC Contrast Test Results							
Contrast DF Chi-Square Pr > ChiSq							
Reference = Model	2	1.7008	0.4273				

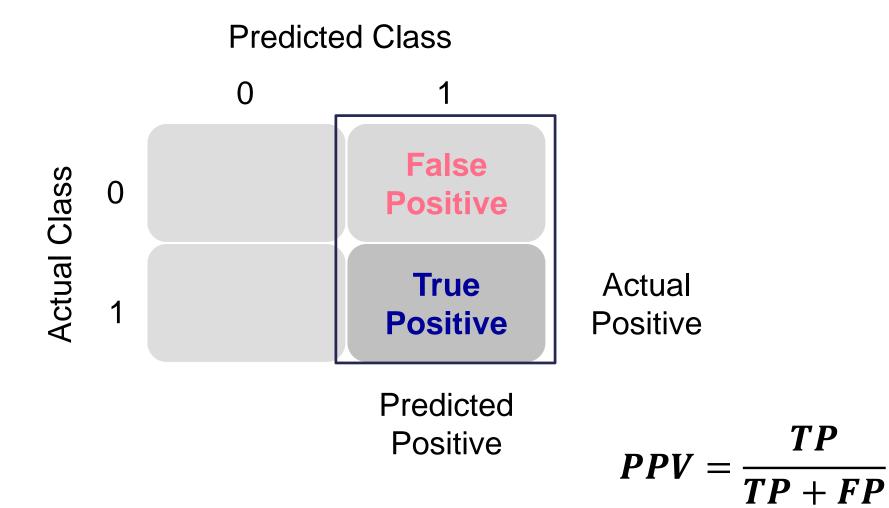
ROC Contrast Estimation and Testing Results by Row								
Contrast	Estimate	Standard Error	95% Confiden	Wald ce Limits	Chi- Square	Pr > ChiSq		
Model - Omit Age	-0.00183	0.00940	-0.0202	0.0166	0.0377	0.8460		
Model - Omit Race	0.0432	0.0344	-0.0242	0.1107	1.5772	0.2092		
Omit Age - Omit Race	0.0450	0.0345	-0.0227	0.1127	1.7008	0.1922		

Sensitivity / Recall



$$TPR = rac{TP}{TP + FN}$$

Precision



Best Cut-off?

- Always consider the cost of false positives and false negatives when doing classification.
- When NOT considering costs, many different techniques to "optimal" cut-off.
- F₁ score (precision-recall version of Youden's Index):

$$F_1 = 2 \left(\frac{\text{precision} \times \text{recall}}{\text{precision} + \text{recall}} \right)$$

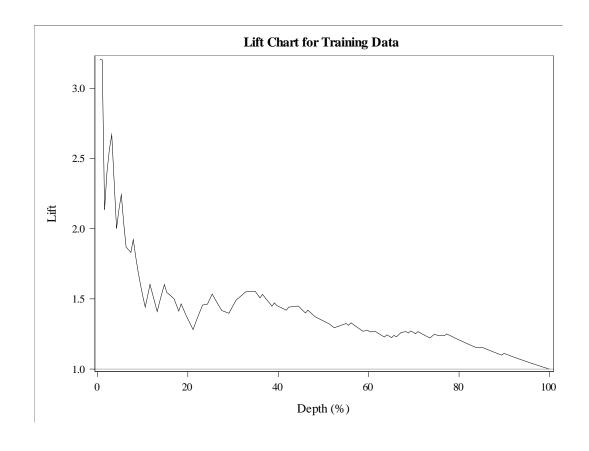
• "Optimal" – precision and recall are weighed equally, so select cut-off that produces highest F_1 score.

Precision & Lift

$$PPV = rac{TP}{TP + FP}$$

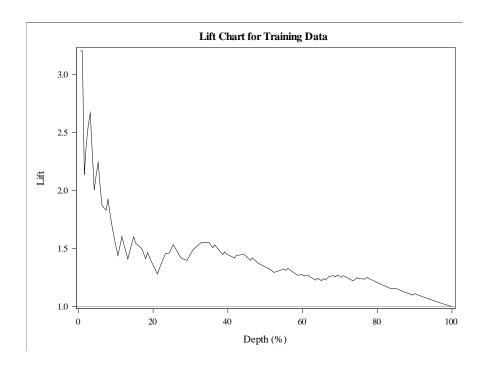
$$\downarrow$$
 $PPV = rac{TP}{Depth}$

$$\downarrow$$
 $Lift = rac{PPV}{\pi_1}$



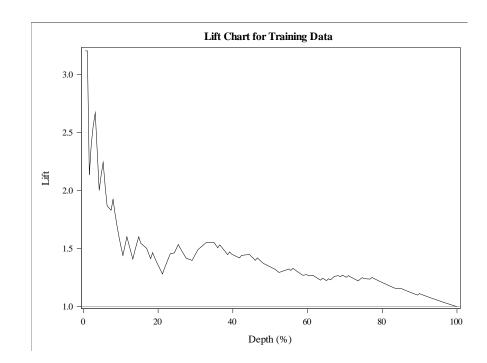
Lift Interpretation

 The top <u>depth</u>% of your customers, based on predicted probability, you get <u>lift</u> times as many responses compared to targeting a random sample of <u>depth</u>% of your customers.



Lift Interpretation

- The top <u>depth</u>% of your customers, based on predicted probability, you get <u>lift</u> times as many responses compared to targeting a random sample of <u>depth</u>% of your customers.
- Careful, in oversampled data, you need to readjust your predicted probabilities!



Precision, Recall, F_1 – SAS

```
data classtable;
   set classtable;
   F1 = 2*(PPV*Sensitivity)/(PPV + Sensitivity);
   drop Specificity NPV Correct;
run;
proc sort data=classtable;
   by descending F1;
run;
proc print data=classtable;
run;
```

Precision, Recall, F_1 – SAS

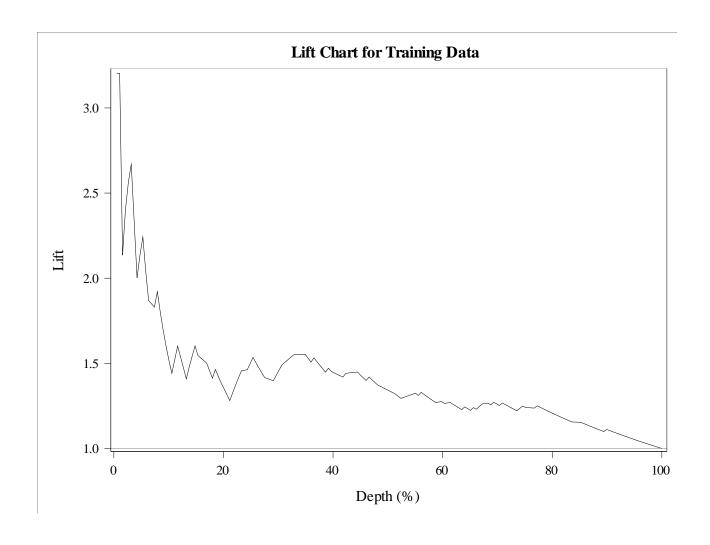
Obs	ProbLevel	Sensitivity	PPV	F1
1	0.200	89.8	38.4	53.8071
2	0.180	89.8	37.9	53.2663
3	0.220	86.4	38.1	52.8497
4	0.160	91.5	36.2	51.9231
5	0.140	96.6	35.4	51.8182
6	0.240	81.4	37.8	51.6129

-

Lift Chart – SAS

```
proc logistic data=logistic.lowbwt plots(only)=(oddsratio);
   class race(ref='white') / param=ref;
   model low(event='1') = race lwt smoke / clodds=pl clparm=pl;
   score data=logistic.lowbwt fitstat outroc=roc;
   title 'Modeling Low Birth Weight';
run;
quit;
data work.roc;
   set work.roc;
   cutoff = PROB;
   specif = 1 - 1MSPEC ;
   depth=(POS + FALPOS)/189*100;
   precision= POS / ( POS + FALPOS );
   acc= POS + NEG ;
   lift=precision/0.3122;
run;
```

Lift Chart – SAS



Precision, Recall, $F_1 - R$

```
prec <- NULL
reca <- NULL
f1 <- NULL
cutoff <- NULL
for(i in 1:49){
  cutoff = c(cutoff, i/50)
  reca <- c(reca, sensitivity(bwt$low, bwt$p hat,
            threshold = i/50)
  prec <- c(prec, precision(bwt$low, bwt$p_hat,</pre>
            threshold = i/50)
  f1 <- c(f1, 2*((prec[i]*reca[i])/(prec[i]+reca[i])))</pre>
ctable <- data.frame(cutoff, reca, prec, f1)
```

Precision, Recall, $F_1 - R$

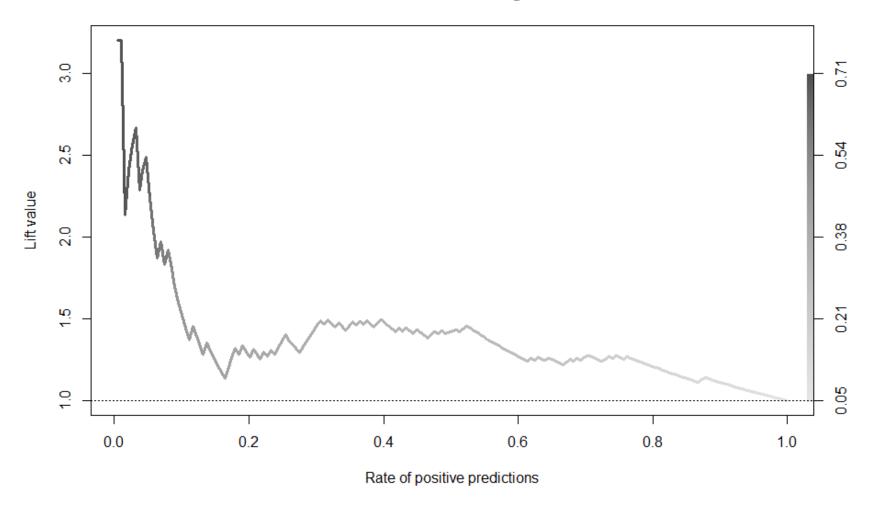
```
##
      cutoff
                                           f1
                   reca
                              prec
        0.02 1.00000000 0.3121693 0.47580645
## 1
        0.04 1.00000000 0.3121693 0.47580645
## 2
## 3
        0.06 1.00000000 0.3138298 0.47773279
## 4
        0.08 1.00000000 0.3189189 0.48360656
## 5
        0.10 1.00000000 0.3314607 0.49789030
## 6
        0.12 1.00000000 0.3410405 0.50862069
## 7
        0.14 0.96610169 0.3630573 0.52777778
## 8
        0.16 0.96610169 0.3800000 0.54545455
## 9
        0.18 0.93220339 0.3873239 0.54726368
## 10
        0.20 0.89830508 0.3868613 0.54081633
## 11
        0.22 0.89830508 0.3925926 0.54639175
## 12
        0.24 0.86440678 0.3953488 0.54255319
## 13
        0.26 0.81355932 0.3870968 0.52459016
```



Lift Chart – R

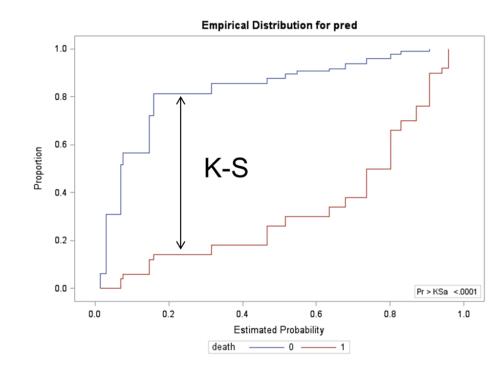
Lift Chart – R

Lift Chart for Training Data



K-S Statistic

- The Two-Sample K-S statistic can determine if there is a difference between two cumulative distribution functions.
- Has a corresponding hypothesis test, with D test statistic, and p-value.



Best Cut-off?

- Always consider the cost of false positives and false negatives when doing classification.
- When NOT considering costs, many different techniques to "optimal" cut-off.
- KS statistic D (maximum difference between TPR and FPR):

$$D = \max_{depth} (TPR - FPR)$$

"Optimal" – select cut-off that produces highest D statistic.

K-S Statistic – SAS

```
proc logistic data=logistic.lowbwt noprint;
   class race(ref='white') / param=ref;
   model low(event='1') = race lwt smoke;
   output out=predprobs p=phat;
run;

proc nparlway data=predprobs d plot=edfplot;
   class low;
   var phat;
run;
```

K-S Statistic – SAS

The NPAR1WAY Procedure

Kolmogorov-Smirnov Te	est for Variable phat			
Classified by Variable low				

Classifica by Variable 1011				
low	N	EDF at Maximum	Deviation from Mean at Maximum	
0	130	0.646154	1.032979	
1	59	0.355932	-1.533336	
Total	189	0.55556		

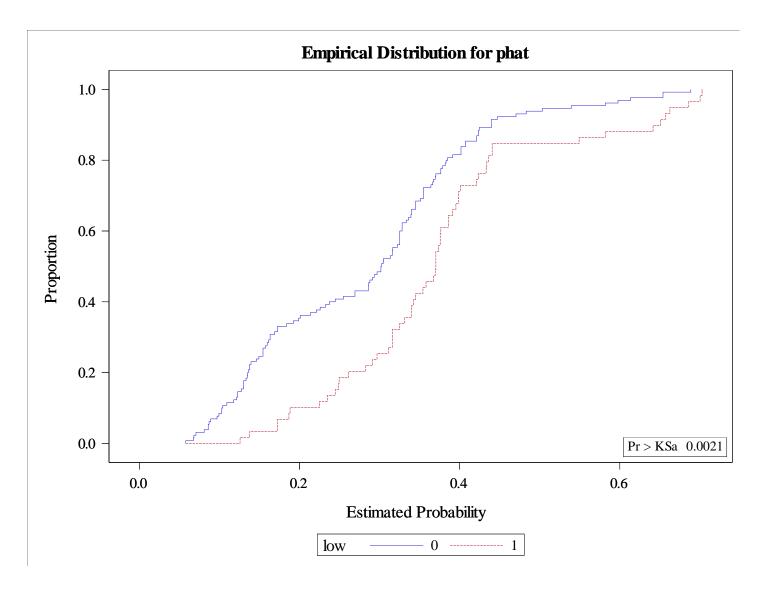
Maximum Deviation Occurred at Observation 27

Value of phat at Maximum = 0.339202

Kolmogorov-Smirnov Two-Sample Test (Asymptotic)

D = max F1 - F2	0.2902
Pr > D	0.0021

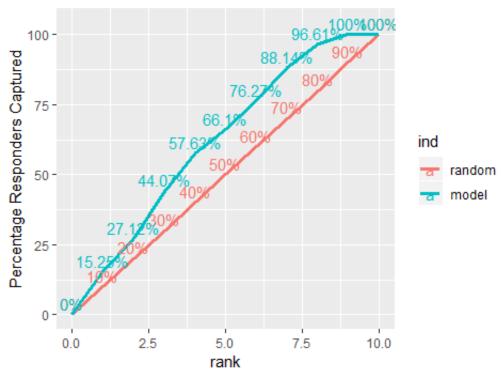
K-S Statistic – SAS



K-S Statistic – R

```
ks_stat(bwt$low, bwt$p_hat)
## [1] 0.2583
ks_plot(bwt$low, bwt$p_hat)
```

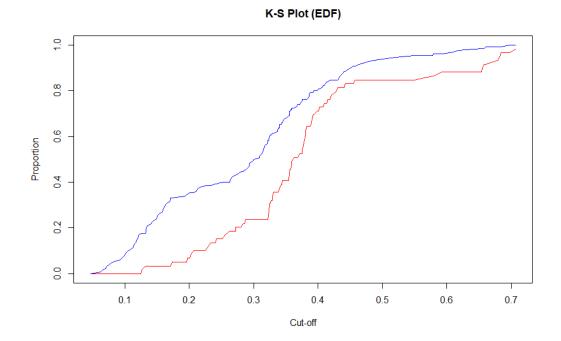
KS Plot



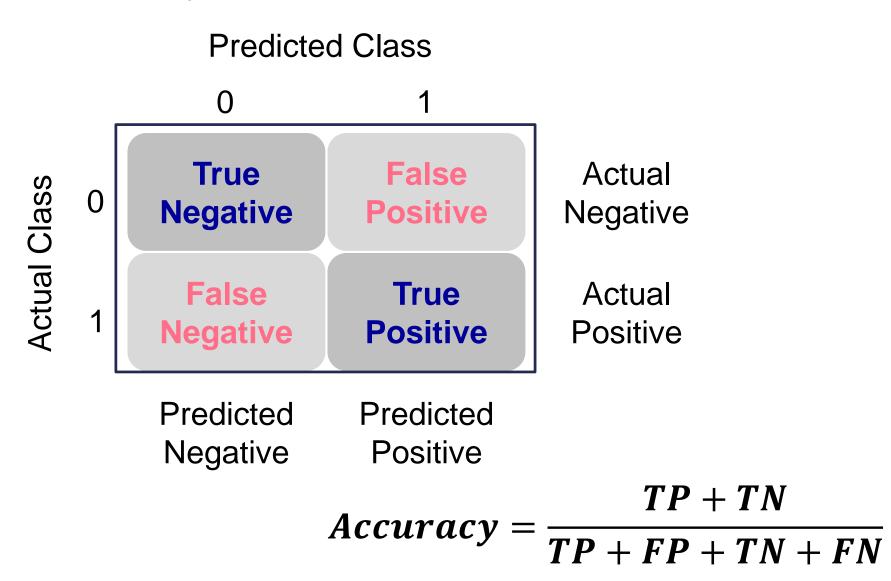
K-S Statistic – R

K-S Statistic – R

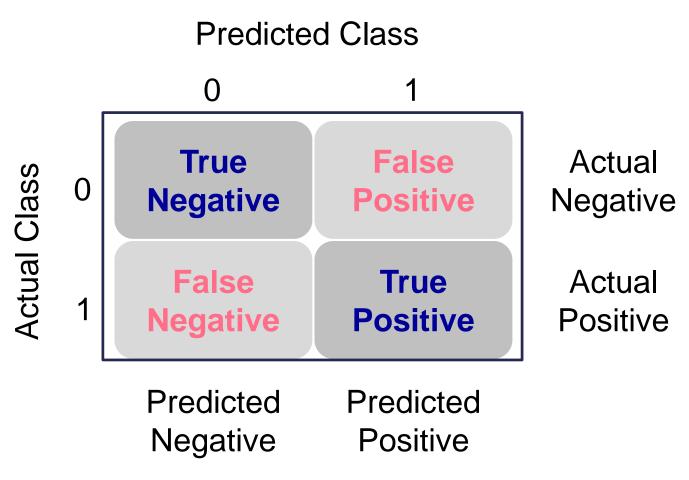
```
plot(x = unlist(perf@alpha.values), y = (1-unlist(perf@y.values)),
    type = "l", main = "K-S Plot (EDF)",
    xlab = 'Cut-off',
    ylab = "Proportion",
    col = "red")
lines(x = unlist(perf@alpha.values), y = (1-unlist(perf@x.values)),
    col = "blue")
```



Accuracy

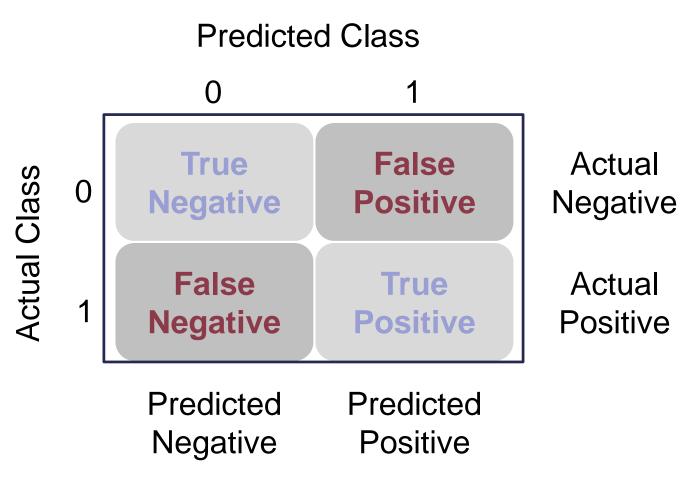


Accuracy



$$Accuracy = \frac{TP + TN}{n}$$

Misclassification (Error) Rate



$$Error = rac{FP + FN}{n}$$

Accuracy and Error

- Accuracy and error can be easily fooled so careful focusing only on them.
- If your data has 10% events and 90% non-events, you can have a 90% accurate model by guessing non-events for every observation.
- There is more to model building than simply maximizing overall classification accuracy.
- Good numbers to report, but not necessarily to choose models on.

Closing Thoughts on Classification

- Classification is a decision that is extraneous to statistical modeling.
- Although logistic regression tends to work well in classification, it is a probability model and does not output 1's and 0's.
- Classification assumes cost for each individual is the same.
 - Useful for groups.
 - Careful about single observation decisions.

