Forecast Intervals for the Area Under the ROC Curve with a Time-varying Population

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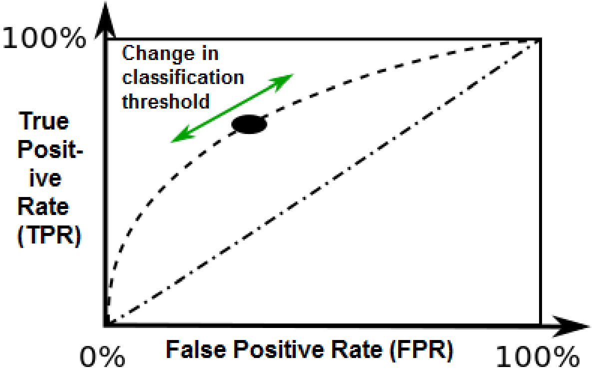
Predicting Performance of Classification Models

- **What:** Method for calculating a forecast interval for the Area Under the ROC curve (AUROC)
  - Area under the Receiver Operating Characteristic (ROC) curve: quality of a signal for predicting an outcome
  - Predictive modeling: performance of a classification model
- **Why:** Characterize the likely range of model performance while a model is used for prediction
  - In practice, businesses will use model until:
    - Performance (AUROC) degrades
    - Population changes
- **How:** Measure the variation in AUROC in terms of the variation in the underlying distribution of predictive variables
  - Not only from sampling variation from a fixed distribution

Measuring Predictive Value of Classification Models

Receiver Operating Characteristic Curve:
True Positive Rate vs. False Positive Rate



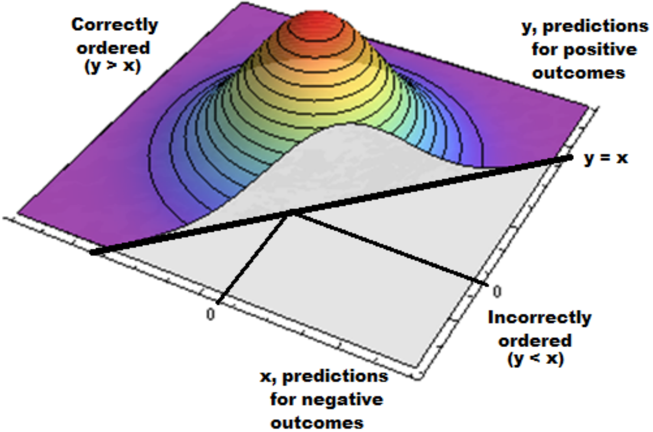
Measuring Predictive Value of Classification Models

Definition of AUROC

- Direct definition: Calculation of area by integration
  - $\int_{-\infty}^{\infty} TPR(t)[-FPR'(t)]dt$
- Direct definition: Pairwise comparison of correct ordering of predictions for all pairs of predictions
  - $\hat{A} = \hat{\Pr}\{y > x\} = \frac{1}{mn}\sum_{i=1}^{m}\sum_{j=1}^{n} I_{\{y_j > x_i\}}$
- In words: If you were to pick a pair of predictions, drawn randomly from predictions corresponding to pairs of the positive (y) and negative (x) outcomes, the AUROC is the probability that these predictions are correctly ordered.

Graphical Interpretation of AUROC

Volume Under the Joint distribution of Predictor Variables



An Important Correspondence for Classification Models

Predicting Outcomes vs. Measuring Difference

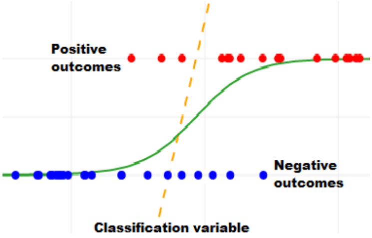


Figure: Predictive value of classification variables

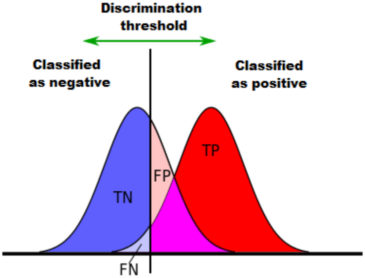


Figure: Difference in the distributions of variables

Predicting Performance of Classification Models

Conclusion: Variation of distributions is of paramount importance

- AUROC statistic is closely related to the pairs of distributions
- In practice, track performance of model while in use
  - take AUROC measurements periodically
  - take periodic measurements of changes in distributions to measure deviations from build sample
- Extreme changes in either would trigger rebuild of the model
- Forecast intervals should allow for this level of variability

Predicting Performance of Classification Models

Calculation of forecast intervals:

1. Build model from entire sample and measure AUROC
2. Measure distance between distributions
   - by dividing sample into a series of subsamples
   - by specifying a model for the evolution of the distributions
3. Calculate extreme AUROC values that correspond to movements a specified distance away from the full sample

Optimization Problem

Find the highest value of the AUROC, $A^{(U)}$, a specified distance from observed distribution

$\max_{\mathbf{u},\mathbf{v}} \frac{1}{mn} \sum_{i=1}^{m} \sum_{j=1}^{n} u_i v_j I_{\{y_j > x_i\}}$

- subject to $D(\mathbf{u} \otimes \mathbf{v}, \mathbf{f} \otimes \mathbf{g}) = \bar{D}$,
- unit mass constraints $\sum_{i=1}^{m} u_i = 1, \quad \sum_{j=1}^{n} v_j = 1$,
- nonnegativity constraints $\{u_i \geq 0\}_{i=1}^{m}, \quad \{v_j \geq 0\}_{j=1}^{n}$
- where $\mathbf{f}$ and $\mathbf{g}$ are the observed distributions of classification variables for positive and negative cases, respectively, while $\mathbf{u}$ and $\mathbf{v}$ are the weights with distance $\bar{D}$

Dual Problem

Find *minimum* distance from observed distribution and a distribution with a particular AUROC
$\min_{\mathbf{u},\mathbf{v}} KLD(\mathbf{u} \otimes \mathbf{v}, \mathbf{f} \otimes \mathbf{g})$

- subject to $\frac{1}{mn} \sum_{i=1}^{m} \sum_{j=1}^{n} u_i v_j I_{\{y_j > x_i\}} = A_0$,
- unit mass constraints $\sum_{i=1}^{m} u_i = 1, \quad \sum_{j=1}^{n} v_j = 1$,
- nonnegativity constraints $\{u_i \geq 0\}_{i=1}^{m}, \quad \{v_j \geq 0\}_{j=1}^{n}$
- where **f** and **g** are the observed distributions of classification variables for positive and negative cases, respectively, while **u** and **v** are the closest weights that satisfy $A = A_0$

Optimum

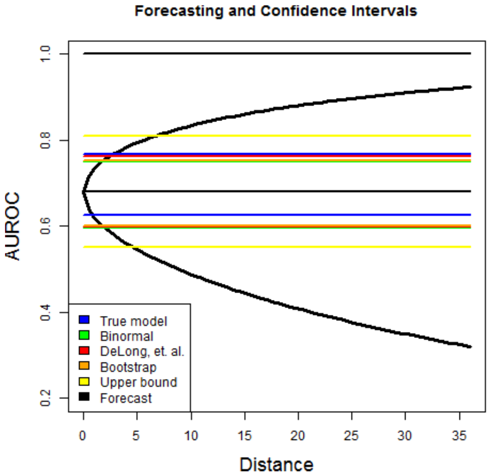
Fixed points from first order conditions

- $\frac{dD(\mathbf{u},\mathbf{f})}{du_i} = \lambda \sum_{j=1}^{n} v_j I_{\{y_j > x_i\}} + \gamma_x + \delta_{x,i}, i = 1, \ldots, m$
- $\frac{dD(\mathbf{v},\mathbf{g})}{dv_j} = \lambda \sum_{i=1}^{m} u_i I_{\{y_j > x_i\}} + \gamma_y + \delta_{y,i}, j = 1, \ldots, n$
- Solved with the recurrence relations (for a particular distance function)
    - $u_i^{(t+1)} = k_x f_i^{1+u_i^{(t)}} \exp\left\{\lambda \sum_{j=1}^{n} v_j^{(t)} I_{\{y_j > x_i\}}\right\}$
    - $v_j^{(t+1)} = k_y g_j^{1+v_j^{(t)}} \exp\left\{\lambda \sum_{i=1}^{m} u_i^{(t)} I_{\{y_j > x_i\}}\right\}$
- k_x and k_y are normalizing constants and Lagrange multiplier λ is the step size.

Competing Procedures

- Parametric models:
  - Binormal model: $[\Phi(\tilde{z}_{\alpha/2}), \Phi(\tilde{z}_{1-\alpha/2})]$
  - Biexponential model: $[\hat{A} \pm z_{1-\alpha/2}\hat{\sigma}_A]$, with
    $\sigma_A^2 = \frac{1}{mn}\{A(1-A) + (n-1)(P_{yyx} - A^2) + (m-1)(P_{yxx} - A^2)\}$,
    $P_{yyx} = A/(2-A)$, $P_{yxx} = 2A^2/(1+A)$
- Empirical distribution (DeLong et. al.):
  $P_{yyx} = \frac{1}{mnn}\sum_i \sum_j \sum_k I_{\{y_j > x_i \cap y_k > x_i\}}$
  $P_{yxx} = \frac{1}{mmn}\sum_i \sum_j \sum_k I_{\{y_j > x_i \cap y_j > x_k\}}$
- Bootstrap: $[\hat{A}^*_{\alpha/2}, \hat{A}^*_{1-\alpha/2}]$
- Upper bound of variance: $\sigma^2_{max} = \frac{A(1-A)}{\min\{m,n\}} \left(\leq \frac{1}{4\min\{m,n\}} \right)$
- Fixed error rate: Interval depends on a specified error rate.

Prediction Intervals Expanding with Distance



Predicting Performance of Classification Models

Structure of Simulation

- Regime-switching model
  - 2 states, high- and low-AUROC regimes, equally probable
  - past regimes known, future unknown
- Measure AUROC from both regimes
- Measure distance between distributions in regimes and full sample
- Calculate extreme AUROC values that correspond to movements away from full sample, using distances between distributions

Simulation Results

Coverage Rates

True values: $A_L = 0.68, A_H = 0.72$

Method	Coverage Rate	Correct Forecast Rate
Bi-normal	0.8265	0.6612
DeLong et. al.	0.8395	0.6689
Bootstrap	0.8310	0.6616
Upper Bound	0.9885	0.9074
Forecast	0.9955	0.9600

Simulation Results

Coverage Rates

True values: $A_L = 0.65, A_H = 0.75$

Method	Coverage Rate	Correct Forecast Rate
Bi-normal	0.2360	0.3427
DeLong et. al.	0.2470	0.3515
Bootstrap	0.2455	0.3453
Upper Bound	0.7725	0.6615
Forecast	0.9795	0.9259

Simulation Results

Coverage Rates
True values: $A_L = 0.75, A_H = 0.80$

Method	Coverage Rate	Correct Forecast Rate
Bi-normal	0.6805	0.5912
DeLong et. al.	0.6845	0.5979
Bootstrap	0.6730	0.5889
Upper Bound	0.9665	0.8654
Forecast	0.9940	0.9451

Simulation Results

Coverage Rates
True values: $A_L = A_H = 0.70$

Method	Coverage Rate	Correct Forecast Rate
Bi-normal	0.951	0.7402
DeLong et. al.	0.944	0.7477
Bootstrap	0.941	0.7386
Upper Bound	1.000	0.9464
Forecast	0.999	0.9702

A "Non-parametric" Solution

- AUROC is inherently nonparametric measure of performance
  - General distaste for parametric assumptions, particularly when not supported by the data
  - Little justification to impose parametric specification for variation in distributions, when parametric distributions are not used for the distributions themselves
  - Still, parametric specification would work
- Change in distribution is summarized by a distance measurement
  - Forecast interval is a function of the distance measurement

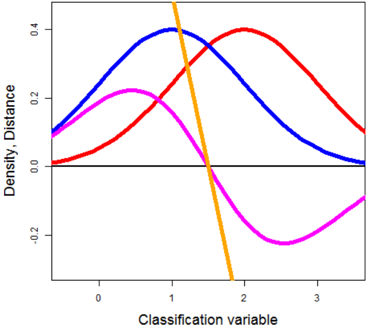
Distance Function

Kullback-Leibler Divergence Criterion

- A criterion for discriminating between distributions
- Definition
  - $KLD(f_1, f_2) = \sum_{k=1}^{K} \left\{ \left(f_1(t_k) - f_2(t_k) \right) \log \left(\frac{f_1(t_k)}{f_2(t_k)} \right) \right\}$
  - where f_1 and f_2 are two density functions

Kullback-Leibler Divergence

Difference and Log-difference for Two Normal Densities



Terms in $KLD(f_1, f_2) = \sum_{k=1}^{K} \left\{ (f_1(t_k) - f_2(t_k)) \log \left(\frac{f_1(t_k)}{f_2(t_k)} \right) \right\}$

Distance Function

Why Kullback-Leibler Divergence?

- More weight on tails: Penalty for deviations in low density has more influence on variation of AUROC, since the variation in AUROC is generated where the densities overlap
- Information-theoretic justification: Measures quality of information for discriminating between pairs of distributions
- Relation to MLE: $KLD(f_1, f_2)$ is the second term in the asymptotic distribution of the MLE (the first is the information from f_1), where f_2 is the distribution fitted to data from true distribution f_1

Distance Function

Why not χ^2?

- Equal weight on equal deviations at all points in the distribution
- Overlapping tails of distributions is where discriminating power is greatest
- Computationally, requires additional constraints to impose non-negativity of densities when shifting distributions

Prediction Intervals $[A_L, A_U]$

Solving for extreme values of A for a particular distance $\hat{D}$ (measured from sample)

- Record estimate of AUROC ($\rightarrow \hat{A}$)
- Solve distance minimization problem for a particular candidate A_0 ($\rightarrow \bar{D}$)
- Search on A_0 above $\hat{A}$ until $\bar{D} = \hat{D}$ ($\rightarrow A_U$)
- Repeat for A_0 below $\hat{A}$ ($\rightarrow A_L$)

A Practical Solution

In practice

- Appetite to compare AUROC stats for classification models
  - between samples: indicate drop potential
  - between models: comparison of predictive value
- Often surprising how far AUROC can move over time
- Answered the question:
  Can we predict likely range for *future* AUROC?

Future Research

Next steps:

- Using distance to specify a confidence interval
  - requires mapping to 95% confidence interval
- Bootstrap test statistic
  - Shift weight to closest distribution with $A = A_0$
  - Simulating from this distribution will satisfy the null hypothesis
  - Reject null if actual statistic is in tails of simulated distribution
- Extend to multiple samples
  - Classification variables from same population
  - Need to account for covariance