Prediction Intervals for the Area Under the ROC Curve

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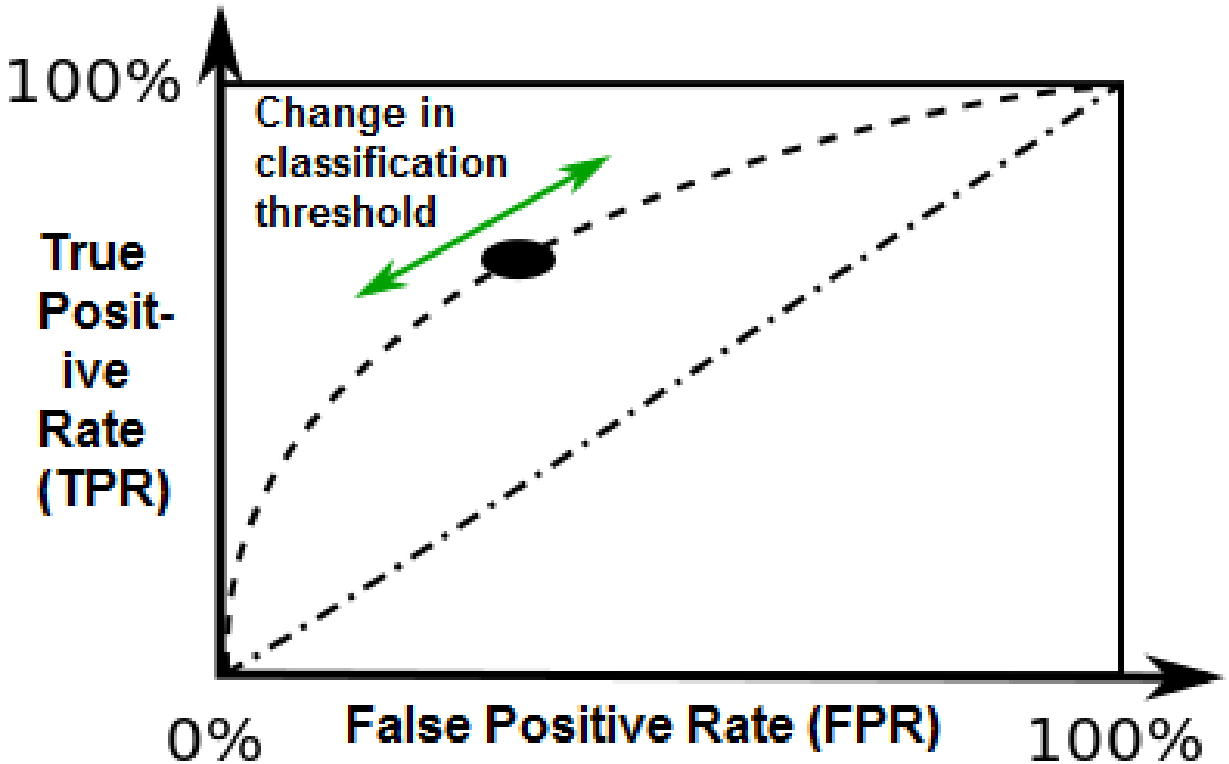
Predicting Performance of Classification Models

- **What:** Method for calculating a prediction interval for the Area Under the ROC curve (AUROC)
  - Area under the Receiver Operating Characteristic (ROC) curve is a measure of quality of a signal for a message
  - In predictive modeling, it is often used as a measure of performance of a classification model
- **Why:** Characterize the likely range of model performance when 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



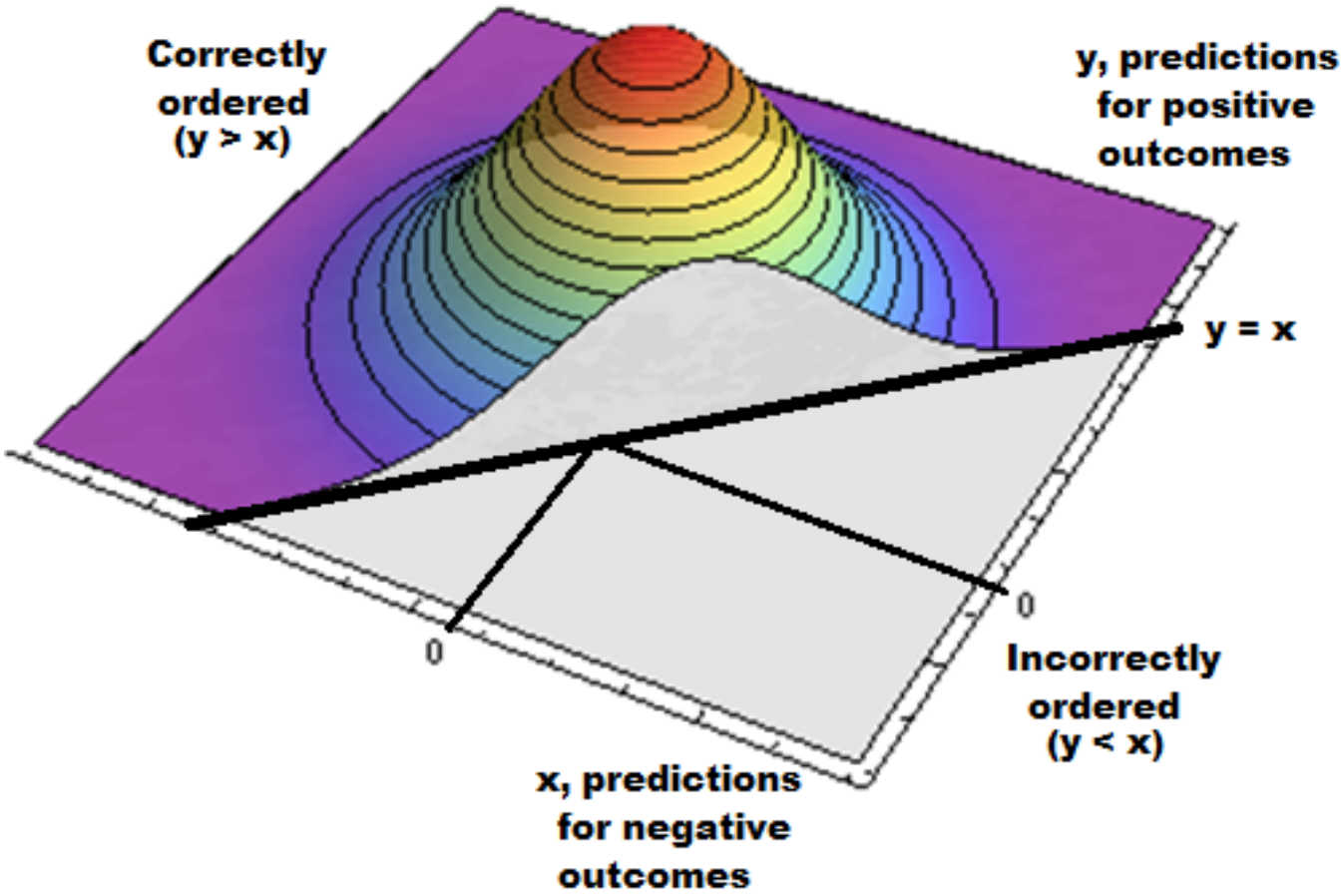
Measuring Predictive Value of Classification Models

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

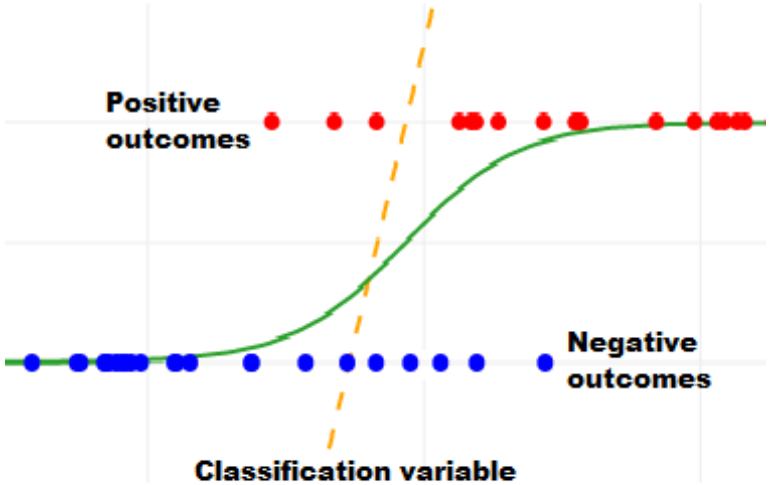


Figure: Predictive value of classification variables

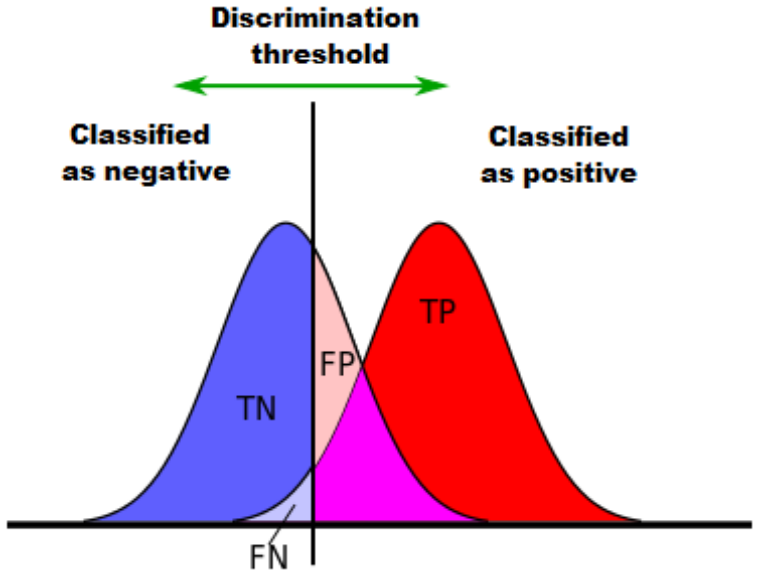


Figure: Difference in the distributions of variables

Performance of Classification Models

Conclusion: Variation of distributions of scores is of paramount importance

- In practice, track performance of model while in use
  - take AUROC measurements periodically
- Also, track evolution of distributions of predictions
  - take periodic measurements of changes in distributions from build sample
- Extreme changes in either would trigger rebuild of the model
- Prediction intervals should allow for this level of variability

Predicting Performance of Classification Models

Contribution:

- Existing literature seeks to characterize variability due to *sampling variation*
- In this paper, I allow for additional variation in the sample due to changes in the underlying distribution
- How far would the AUROC move before model rebuild is triggered?
- Method of calculation:
  1. Build model from entire sample and measure AUROC
  2. Measure distance between distributions in a series of subsamples
  3. Calculate extreme AUROC values that correspond to movements away from full dataset, using distances between observed distributions

Predicting Performance of Classification Models

Structure of Simulation

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

Simulation Results

Tables for first case

machine.learning()

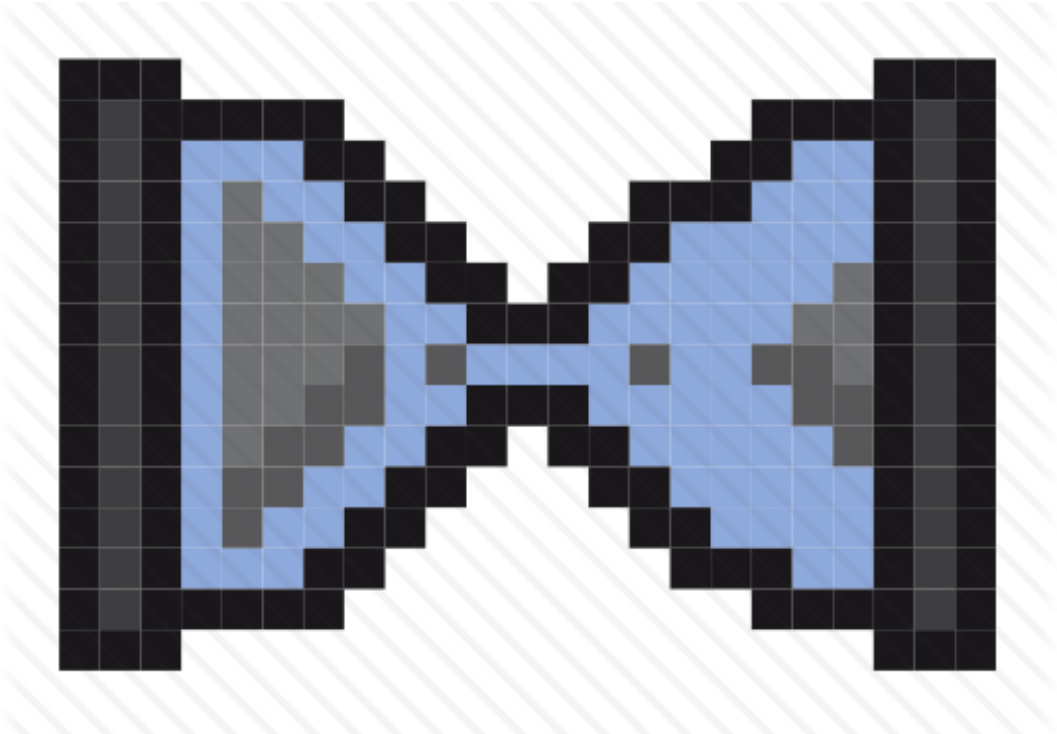
Competing Procedures

Confidence Intervals in Literature

- 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: $P_{yyx} = \frac{1}{mnn}\sum_i\sum_j\sum_k I_{\{y_j>x_i \cap y_k>x_i\}}$ and $P_{yyx} = \frac{1}{mmn}\sum_i\sum_j\sum_k I_{\{y_j>x_i \cap y_j>x_k\}}$
- 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: (next)

Competing Procedures

Plot confidence intervals for an example



Simulation Results

Tables for remaining cases

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machine.learning()
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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
- Change in distribution is summarized by a distance measurement
- Prediction interval: The set of all possible distributions this distance from the distributions in the sample

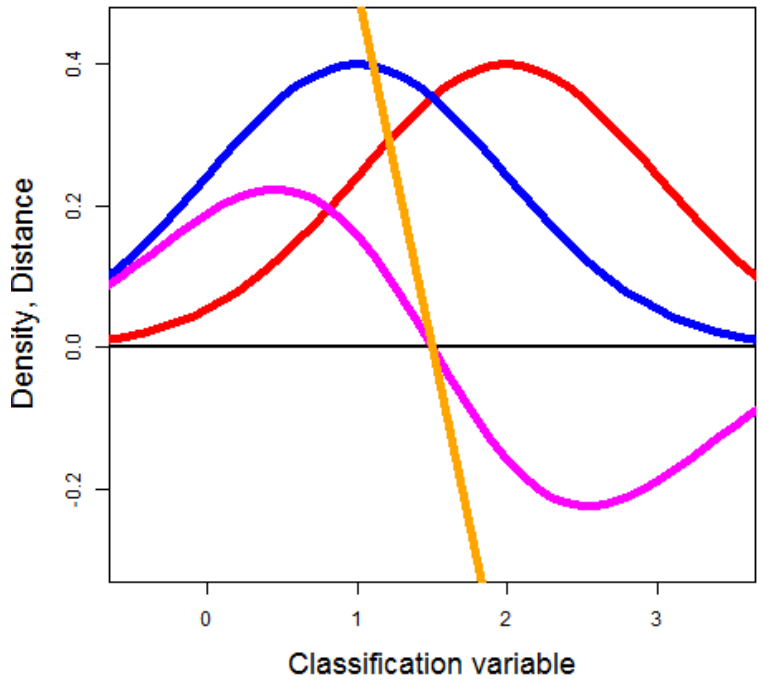
Distance Metric

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

Distance Metric

Why Kullback-Leibler Divergence?

- 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
- 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

Distance Metric

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

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 $\mathbf{f}$ and $\mathbf{g}$ are the observed distributions of classification variables for positive and negative cases, respectively, while $\mathbf{u}$ and $\mathbf{v}$ are the 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 via a switching algorithm with the recurrence relations
  - $u_i^{(t+1)} = k_x f_i^{1+u_i^{(t)}} \exp\left\{\lambda \sum_{j=1}^{n} v_j^{(t)} I_{\{y_j > x_i\}}\right\}$
  - $v_j^{(t+1)} = k_y g_j^{1+v_j^{(t)}} \exp\left\{\lambda \sum_{i=1}^{m} u_i^{(t)} I_{\{y_j > x_i\}}\right\}$
- k_x and k_y are normalizing constants and Lagrange multiplier λ is the step size.

Shifting distribution toward AUROC

Finding closest distribution with specified AUROC

machine.learning()

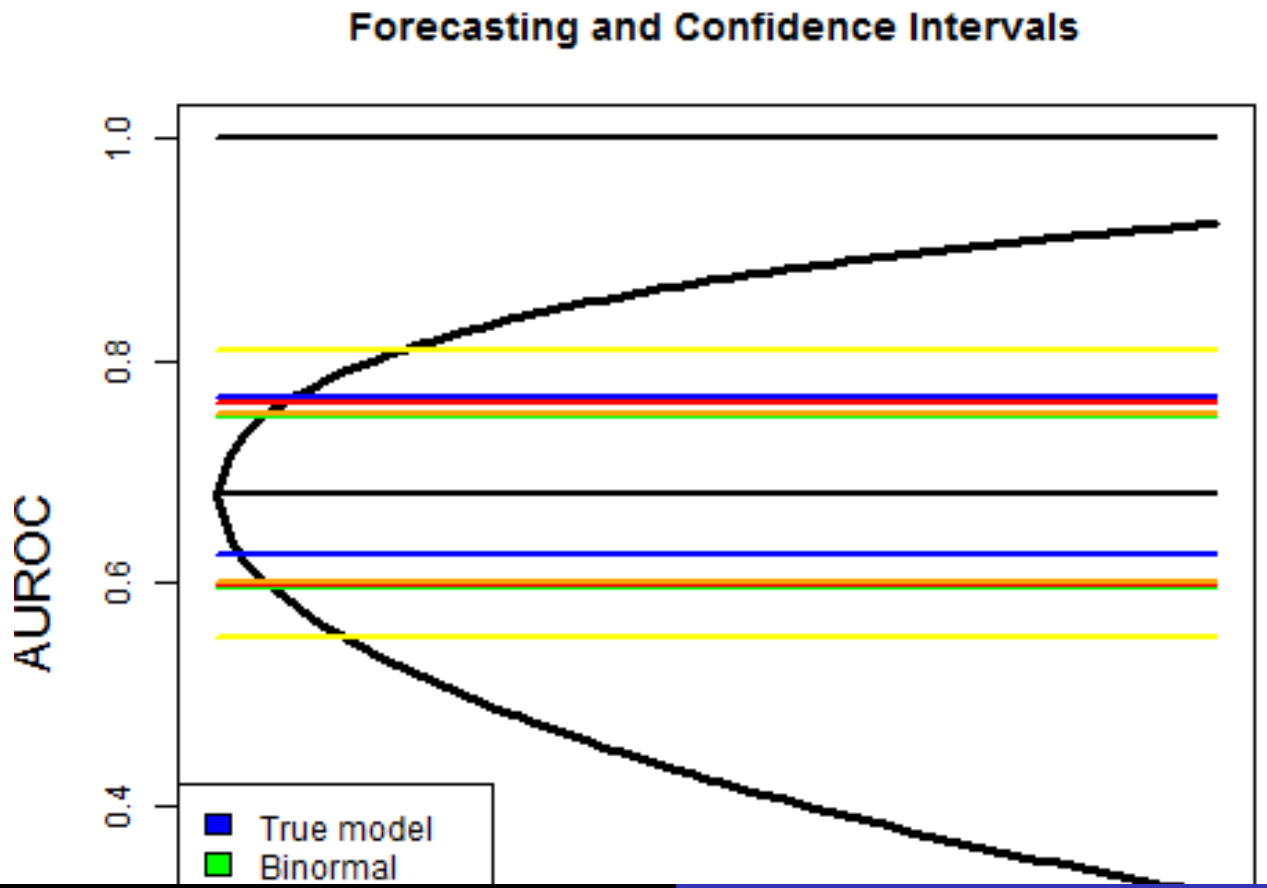
Prediction Intervals $[A_L, A_U]$

Solving for extreme values of A for a particular distance $\bar{D}$

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

Expanding Prediction Intervals

Expanding Prediction Intervals with Distance



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
- Question Answered here:
  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