Comparing binary classification rules. ROC curve and other methods

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Sections 9.2.5 in Hastie, Tibshirani, and Friedman (2009)

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The binary classification problem, or binary discrimation

- Let $(\boldsymbol{X}, Y)$ be a r.v. with support $\mathcal{X} \times \{0,1\} \subseteq \mathbb{R}^p \times \{0,1\}$.
- Binary classification problem, or binary prediction, or binary disrimination:
  - Training sample: $S = \{(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_n, y_n)\}$, i.i.d. from $(\boldsymbol{X}, Y)$.
  - The goal is to define a classification function (or discrimination rule) (depending on the sample)

$$h_S : \mathcal{X} \mapsto \{0,1\}$$

such that for a new independent observation $(\boldsymbol{x}_{n+1}, y_{n+1})$, from which we only know $\boldsymbol{x}_{n+1}$, it happens that

$$\Pr(h_S(\boldsymbol{x}_{n+1}) = y_{n+1}) \text{ is close to } 1.$$

A more general approach to the binary classification

- A more general goal in binary classification is to define a function $g_S : \mathcal{X} \mapsto [0,1]$ such that for a new independent observation $(\boldsymbol{x}_{n+1}, y_{n+1})$, from which we only know $\boldsymbol{x}_{n+1}$, $g_S(\boldsymbol{x}_{n+1})$ is close to y_{n+1} (in some sense).
- Observe that from such a function it is possible to define a classification function:
  - Let $c \in [0,1]$ be a cut point.
  - From $g_S : \mathcal{X} \mapsto [0,1]$ and c, define $h_S : \mathcal{X} \mapsto \{0,1\}$ as

$$h_S(\boldsymbol{x}) = \begin{cases} 0 & \text{if} \quad g_S(\boldsymbol{x}) \leq c, \\ 1 & \text{if} \quad g_S(\boldsymbol{x}) > c. \end{cases}$$

An example: Estimating $\Pr(Y = 1|\boldsymbol{X} = \boldsymbol{x})$

- Let $(\boldsymbol{X}, Y)$ be a r.v. with support $\mathcal{X} \times \mathcal{Y} \subseteq \mathbb{R}^p \times \{0, 1\}$.
- Let $(\boldsymbol{X}_1, Y_1), \dots, (\boldsymbol{X}_n, Y_n)$ i.i.d.r.v. distributed as $(\boldsymbol{X}, Y)$.
- Sample: $(\boldsymbol{x}_1, y_1), \dots, (\boldsymbol{x}_n, y_n)$, realizations of $(\boldsymbol{X}_1, Y_1), \dots, (\boldsymbol{X}_n, Y_n)$.
- Conditioning on $(\boldsymbol{X}_1 = \boldsymbol{x}_1, \dots, \boldsymbol{X}_n = \boldsymbol{x}_n)$, $Y_1, \dots, Y_n$ are independent random variables, each with distribution

$$(Y_i \mid \boldsymbol{X}_i = \boldsymbol{x}_i) \sim \text{Bernoulli}(p_i = \Pr(Y = 1 \mid \boldsymbol{X}_i = \boldsymbol{x}_i) = E(Y \mid \boldsymbol{X}_i = \boldsymbol{x}_i)).$$

- Let $p(\boldsymbol{x}) = \Pr(Y = 1 \mid \boldsymbol{X} = \boldsymbol{x})$.
- Given an estimation $\hat{p}(\boldsymbol{x})$ of the function $p(\boldsymbol{x})$, a classification rule $h_S : \mathcal{X} \mapsto \mathcal{Y}$ can be defined as

$$h_S(\boldsymbol{x}_{n+1}) = \begin{cases} 0 & \text{if} \quad \hat{p}(\boldsymbol{x}_{n+1}) \leq 1/2 \\ 1 & \text{if} \quad \hat{p}(\boldsymbol{x}_{n+1}) > 1/2 \end{cases}$$

- It is possible to use other cut point c different from $1/2$.

Evaluating a binary classification rule h_S.

Estimated value: $h_S(x)$

		1	0	Total
Real	Positive case: 1	p_{11}	p_{10}	$p_{1\cdot}$
value: y	Negative case: 0	p_{01}	p_{00}	$p_{0\cdot}$
	Total	$p_{\cdot 1}$	$p_{\cdot 0}$	$p_{\cdot\cdot} = 1$

- Eror rate, $p_{01} + p_{10}$: Probability of misclassification.
- Accuracy $=$ 1- Eror rate, $p_{00} + p_{11}$: Probability of right classification.
- Sensitivity, $p_{11}/p_{1\cdot}$: Probability of classifying correctly a positive case: True positive rate. Also known as Recall.
- Specificity, $p_{00}/p_{0\cdot}$: Probability of classifying correctly a negative case: True negative rate.
- Precision or Positive predicted value: $p_{11}/p_{\cdot 1}$, probability of having a true positive case among those classified as positive.
- F-score (or $F1$-score): combines Precision and Recall as their harmonic mean:

$$F = 2 \cdot \frac{\text{precision} \cdot \text{recall}}{\text{precision} + \text{recall}} = \frac{2p_{11}}{2p_{11} + p_{01} + p_{10}}.$$

A test sample or cross-validation techniques are required to estimate these quantities.

Evaluating a binary classification rule

From Wikipedia, the free encyclopedia

		Predicted condition			
	Total population $= P + N$	**Predicted Positive (PP)**	**Predicted Negative (PN)**	Informedness, bookmaker informedness (BM) $= TPR + TNR - 1$	Prevalence threshold (PT) $= \frac{\sqrt{TPR \times FPR} - FPR}{TPR - FPR}$
Actual condition	**Positive (P)**	**True positive (TP), hit**	**False negative (FN), type II error, miss, underestimation**	True positive rate (TPR), recall, sensitivity (SEN), probability of detection, hit rate, power $= \frac{TP}{P} = 1 - FNR$	False negative rate (FNR), miss rate $= \frac{FN}{P} = 1 - TPR$
	Negative (N)	**False positive (FP), type I error, false alarm, overestimation**	**True negative (TN), correct rejection**	False positive rate (FPR), probability of false alarm, fall-out $= \frac{FP}{N} = 1 - TNR$	True negative rate (TNR), specificity (SPC), selectivity $= \frac{TN}{N} = 1 - FPR$
	Prevalence $= \frac{P}{P + N}$	Positive predictive value (PPV), precision $= \frac{TP}{PP} = 1 - FDR$	False omission rate (FOR) $= \frac{FN}{PN} = 1 - NPV$	Positive likelihood ratio (LR+) $= \frac{TPR}{FPR}$	Negative likelihood ratio (LR−) $= \frac{FNR}{TNR}$
	Accuracy (ACC) $= \frac{TP + TN}{P + N}$	False discovery rate (FDR) $= \frac{FP}{PP} = 1 - PPV$	Negative predictive value (NPV) $= \frac{TN}{PN} = 1 - FOR$	Markedness (MK), deltaP (Δp) $= PPV + NPV - 1$	Diagnostic odds ratio (DOR) $= \frac{LR+}{LR-}$
	Balanced accuracy (BA) $= \frac{TPR + TNR}{2}$	F_1 score $= \frac{2 PPV \times TPR}{PPV + TPR} = \frac{2TP}{2TP + FP + FN}$	Fowlkes–Mallows index (FM) $= \sqrt{PPV \times TPR}$	Matthews correlation coefficient (MCC) $= \sqrt{TPR \times TNR \times PPV \times NPV} - \sqrt{FNR \times FPR \times FOR \times FDR}$	Threat score (TS), critical success index (CSI), Jaccard index $= \frac{TP}{TP + FN + FP}$

https://en.wikipedia.org/wiki/Template:Diagnostic_testing_diagram

Error rate, sensitivity and specificity. Estimation

- Apparent error rate. The training data are used twice: first for estimating the classification rule $h_S(\boldsymbol{x})$, and then to validate it. Too optimistic. Biased estimation.
- Error rate in a test set. Unbiased estimation, because the test set is independent from the training set used to estimate $h_S(\boldsymbol{x})$.
- k-fold cross-validation. Almost unbiased estimation.
  - The sample (of size n) is randomly divided into k parts.
  - The model is fitted with $(k-1)$ parts and the other one is used as validation sample.
  - The k possible combinations are done.
  - At the end, a classification is obtained for each element in the sample. The cross table of these n estimated classes and the true ones provide estimations for p_{00}, p_{01}, p_{10} and p_{11}.
- Leave-one-out. It coincides with n-fold cross-validation.
- It is also possible to take m random sample divisions into two set (training and test) and then average the m cross tables.

Different cut points lead to different classification rules

- In practice, the ususal classification rules (logistic regression, k nearest neighbors, neural netwotks for binary classification, etc.) provide an estimation of the probability of being in the class 1:

$$g_S(\boldsymbol{x}) = \widehat{\Pr}(Y = 1|\boldsymbol{X} = \boldsymbol{x}).$$

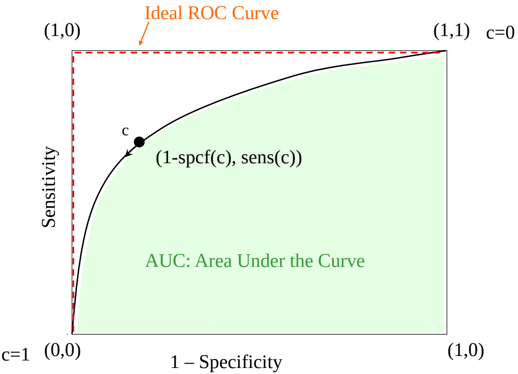
- Given a cut point $c \in [0, 1]$, which divide the range of these estimated probabilities into two parts, a classification rule is obtained: $h_c(\boldsymbol{x}) = \mathbb{I}_{(c,1]}(\widehat{\Pr}(Y = 1|\boldsymbol{X} = \boldsymbol{x}))$.
- So each cut point $c \in [0, 1]$ defines a *Sensitivity(c)* and a *Specificity(c)*.

ROC Curve (Receiver Operating Characteristic Curve)

The ROC curve is a parametric curve,

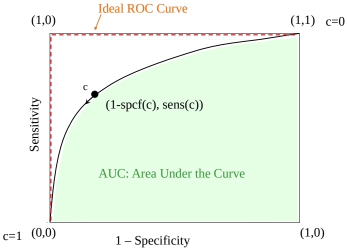
$$\{(1 - \text{Specificity}(c), \text{Sensitivity}(c)) : \; c \in [0,1]\} \in [0,1] \times [0,1],$$

starting at $(1,1)$ when $c = 0$ and finishing at $(0,0)$ when $c = 1$.



ROC Curve: A way to evaluate a rule $g_S : \mathcal{X} \to [0, 1]$.

- It does not depend on the cut point c.
- Summary measure: AUC, Area Under the Curve.
- We are proving that AUC coincides with the probability that, given two new independent cases, one negative $(-)$ and the other positive $(+)$, the classification rule assigns a greater probability of being positive to the true positive case than to the negative one.



AUC = probability or rightly order two cases, + and −

- Remember that $g_S(\boldsymbol{x}) = \widehat{\Pr}(Y = 1|\boldsymbol{X} = \boldsymbol{x})$.
- Let G_0 and G_1 be two independent random variables, with

$$G_0 \sim g_S(\boldsymbol{X}|Y = 0),\ G_1 \sim g_S(\boldsymbol{X}|Y = 1).$$

- The binary classification rule $h_c(\boldsymbol{x}) = \mathbb{I}_{(c,1]}(g_S(\boldsymbol{x}))$ has (1 - specificity) and sensitivity values, respectively,

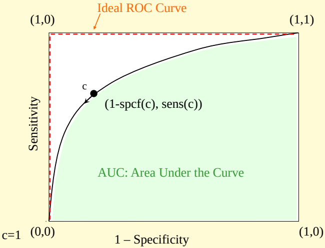
$$u = 1 - \text{spcf}(c) = \Pr(g_S(\boldsymbol{X}) > c|Y = 0) = 1 - F_{G_0}(c),$$

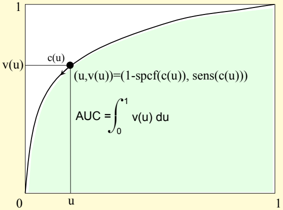
$$v = \text{sens}(c) = \Pr(g_S(\boldsymbol{X}) > c|Y = 1) = 1 - F_{G_1}(c),$$

where F_{G_0} and F_{G_1} are the distribution functions of G_0 and G_1, respectively, which we assume to be continuous with densities f_{G_0} and f_{G_1}.

AUC = probability or rightly order two cases, + and −

$$u = 1 - \mathrm{spcf}(c) = 1 - F_{G_0}(c) \Rightarrow c = F_{G_0}^{-1}(1-u),\ v = \mathrm{sens}(c) = 1 - F_{G_1}(c) = \Pr(G_1 > F_{G_0}^{-1}(1-u))$$





$$\mathrm{AUC} = \int_0^1 v(u)du = \int_0^1 \Pr(G_1 > F_{G_0}^{-1}(1-u))du \overset{(1-u=F_{G_0}(t))}{=}$$

$$-\int_1^0 \Pr(G_1 > t) f_{G_0}(t)dt = \int_0^1 \int_0^1 \mathbb{I}_{\{s>t\}} f_{G_1}(s) f_{G_0}(t) ds\, dt = \Pr(G_1 > G_0)$$

Estimating the ROC curve and the AUC

- If a test sample is available, AUC can be estimated by the Mann-Whitney-Wilcoxon test statistic value, used to test the null hypothesis that the medians of G_0 and G_1 are equal, from the data $g_S(\boldsymbol{x}_i^0)$, $i = 1, \ldots, n_0$, and $g_S(\boldsymbol{x}_j^1)$, $j = 1, \ldots, n_1$.
- The Mann-Whitney-Wilcoxon test statistic estimates the probability $\Pr(G_0 \leq G_1) = \Pr(g_S(\boldsymbol{X}|Y = 0) \leq g_S(\boldsymbol{X}|Y = 1))$.

Estimating the ROC curve and the AUC

- The full estimation of the ROC curve requires the estimation of probabilities $p_{00}(c_j)$, $p_{01}(c_j)$, $p_{10}(c_j)$ y $p_{11}(c_j)$ for a large number J of evenly spaced values c_j, $j = 0, \ldots, J$, $c_0 = 0$, $c_J = 1$.
- This problem is analogous to that of estimating the error rate $p_{01}(c_j) + p_{10}(c_j)$.
- The same techniques are used: test sample, k-fold cross validation.
- Once the ROC curve has been estimated, the AUC is computed by numerical integration:

$$\widehat{\text{AUC}} = \sum_{j=1}^{J} \frac{1}{2}(\widehat{\text{sens}}(c_j) + \widehat{\text{sens}}(c_{j+1}))(\widehat{\text{spcf}}(c_{j+1}) - \widehat{\text{spcf}}(c_j)),$$

where

$$\widehat{\text{sens}}(c_j) = \frac{\hat{p}_{11}(c_j)}{\hat{p}_{10}(c_j) + \hat{p}_{11}(c_j)}, \quad \widehat{\text{spcf}}(c_j) = \frac{\hat{p}_{00}(c_j)}{\hat{p}_{00}(c_j) + \hat{p}_{01}(c_j)}.$$

Some R implementations:

- `roc` function in package `pROC`,
- `ROC` function in package `ROC632`.

They plot the ROC curve and compute the AUC, among other.

Other ways to evaluate rules $g_S : \mathcal{X} \to [0,1]$

- We assume that the rule $g_S : \mathcal{X} \to [0,1]$ provides an estimation for the probability that a case belongs to class 1 when the explanatory variable takes the valuer $\boldsymbol{x}$ at this case:

$$g_S(\boldsymbol{x}) = \widehat{\Pr}(Y = 1 | \boldsymbol{X} = \boldsymbol{x}).$$

- Therefore, the logarithm of the likelihood function for the observed data $(y_i, \boldsymbol{x}_i)$, $i = 1, \ldots, n$, divided by n, is

$$\frac{1}{n} \log \left(\prod_{i=1}^{n} g_S(\boldsymbol{x}_i)^{y_i} (1 - g_S(\boldsymbol{x}_i))^{1-y_i} \right) =$$

$$\frac{1}{n} \sum_{i=1}^{n} \left(y_i \log g_S(\boldsymbol{x}_i) + (1 - y_i) \log(1 - g_S(\boldsymbol{x}_i)) \right).$$

- This measure, as it happens for the apparent error rate, is an optimistic estimation of the expected value of the random variable

$$\log \widehat{\Pr}(Y = Y_{n+1}|\boldsymbol{X}_{n+1}) = Y_{n+1} \log g_S(\boldsymbol{X}_{n+1}) + (1-Y_{n+1}) \log(1-g_S(\boldsymbol{X}_{n+1})),$$

  with $(Y_{n+1}, \boldsymbol{X}_{n+1})$ independent from the first n observations, which were used to estimate the rule $g_S(\boldsymbol{x})$.
- An unbiased estimation is achieved if a validation sample is available: $(y_j^v, \boldsymbol{x}_j^v)$, $j = 1, \ldots, m$, independent from the training sample.
- In this case,

$$\ell_{\mathrm{val}}(g_S) = \frac{1}{m} \sum_{j=1}^{m} \left(y_j^v \log g_S(\boldsymbol{x}_j^v) + (1 - y_j^v) \log(1 - g_S(\boldsymbol{x}_j^v)) \right).$$

- k-fold cross-validation or leave-one-out cross-validation can also be used.

SPAM E-mail Database

- From the description file: *The "spam" concept is diverse: advertisements for products/web sites, make money fast schemes, chain letters, pornography... Our collection of spam e-mails came from our postmaster and individuals who had filed spam. Our collection of non-spam e-mails came from filed work and personal e-mails, and hence the word 'george' and the area code '650' are indicators of non-spam. These are useful when constructing a personalized spam filter. One would either have to blind such non-spam indicators or get a very wide collection of non-spam to generate a general purpose spam filter.*
- Attribute Information:
  - The last column of 'spambase.data' denotes whether the e-mail was considered spam (1) or not (0), i.e. unsolicited commercial e-mail.
  - Most of the attributes indicate whether a particular word or character was frequently occuring in the e-mail.
  - The run-length attributes (55-57) measure the length of sequences of consecutive capital letters.

Practice:

- Use the script `spam.R` to read the data from the SPAM e-mail database.
- Divide the data into two parts: 2/3 for the training sample, 1/3 for the test sample. You should do it in a way that 2/3 of the SPAM e-mails are in the training sample and 1/3 in the test sample, and that the same happens for NO SPAM e-mails.
- Consider the following three classification rules:
  - Logistic regression fitted by maximum likelihood (IRWLS, `glm`).
  - Logistic regression fitted by Lasso (`glment`).
  - k-nn binary regression (you can use your own implementation or functions `knn` and `knn.cv` from the R package `class`).

  Use the training sample to fix the tuning parameters (when needed) and to estimate the model parameters (when needed).
- Use the test sample to compute and plot the ROC curve for each rule.
- Compute also the confusion matrix and the misclassification rate for each rule when using the cut point $c = 1/2$.
- Compute ℓ_{val} for each rule.

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