Paper Notes: Proper Scoring Rules and Cost Weighted Loss Functions for Binary Classification

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Notations: in binary classification

- We are interested in fitting a model $q(\mathbf{x})$ for the true conditional class 1 probability

$$\eta(\mathbf{x}) = P(Y = 1 \mid \mathbf{X} = \mathbf{x})$$

- Two types of problems
  - Classification: estimating a region of the form $\{\eta(\mathbf{x}) > c\}$
  - Class probability estimation: approximate $\eta(\mathbf{x})$, by fitting a model $q(\mathbf{x}, \beta)$, where β are parameters to be estimated
- Surrogate criteria for estimation, e.g.,
  - Log-loss: $L(y \mid q) = -y \log(q) - (1 - y) \log(1 - q)$
  - Squared error loss: $L(y \mid q) = (y - q)^2 = y(1 - q)^2 + (1 - y)q^2$
- Surrogate criteria of classification are exactly the primary criteria of class probability estimation

Proper scoring rule

- Fitting a binary model is to minimize a loss function

$$\mathcal{L}\left(q()\right) = \frac{1}{N}\sum_{n=1}^{N} L(y_n \mid q_n)$$

- In game theory, the agent's goal is to maximize expected score (or minimize expected loss)
  - A scoring rule is proper if truthfulness maximizes expected score
  - It is strictly proper if truthfulness uniquely maximizes expected score

- In the context of binary response data, Fisher consistency holds pointwise if

$$\arg\min_{q\in[0,1]} E_{Y\sim\text{Bernoulli}(\eta)} L(Y \mid q) = \eta, \quad \forall \eta \in [0,1]$$

- Fisher consistency is the defining property of proper scoring rules

Bernoulli related simplification on the scoring rules

- Because Y takes only two values, 0 and 1, $L(y \mid q)$ consists only two "partial losses", $L(1 \mid q)$ and $L(0 \mid q)$
- For simplicity, we prefer to express both in term of increasing functions

$$L_1(1-q) = L(1 \mid q), \quad L_0(q) = L(0 \mid q)$$

- Pointwise expected loss is defined as

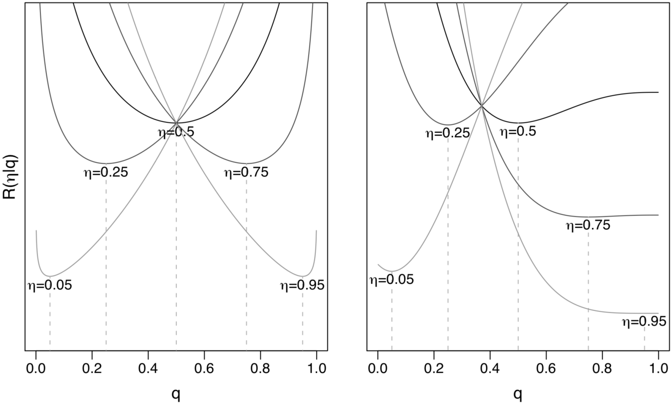
$$R(\eta \mid q) = E_Y L(Y \mid q) = \eta L_1(1-q) + (1-\eta) L_0(q)$$

- Fisher consistency becomes

$$\arg\min_q R(\eta \mid q) = \eta$$

Visualization of two proper scoring rules

- Left: log-loss, or Beta loss with $\alpha = \beta = 0$
- Right: Beta loss with $\alpha = 1, \beta = 3$
  - Tailored for classification with false positive cost $c = \frac{\alpha}{\alpha+\beta} = 0.25$ and false negative cost $1 - c = 0.75$



How to check property of a scoring rule for binary response data

- Suppose the partial losses $L_1(1-q), L_0(q)$ are smooth, then the proper scoring rule property implies

$$\begin{aligned} 0 &= \left.\frac{\partial}{\partial q}\right|_{q=\eta} R(\eta \mid q) \\ &= -\eta L_1'(1-\eta) + (1-\eta) L_0'(\eta) \end{aligned}$$

- Therefore, a scoring rule is proper if

$$\eta L_1'(1-\eta) = (1-\eta) L_0'(\eta)$$

- A scoring rule is strictly proper if

$$\left.\frac{\partial^2}{\partial q^2}\right|_{q=\eta} R(\eta \mid q) > 0$$

Log-loss

- Log-loss is the negative log likelihood of the Bernoulli distribution

$$\mathcal{L} = \frac{1}{N} \sum_{n=1}^{N} \left[-y_n \log(q_n) - (1 - y_n) \log(1 - q_n) \right]$$

- Partial losses for log-loss

$$L_1(1 - q) = -\log(q), \quad L_0(q) = -\log(1 - q)$$

- Expected loss for log-loss

$$R(\eta \mid q) = -\eta \log(q) - (1 - \eta) \log(1 - q)$$

- Log-loss is a strictly proper scoring rule

Squared error loss

- Squared error loss is also known as Brier score

$$\mathcal{L} = \frac{1}{N} \sum_{n=1}^{N} \left[y_n (1 - q_n)^2 - (1 - y_n) q_n^2 \right]$$

- Partial losses for squared error loss

$$L_1(1 - q) = (1 - q)^2, \quad L_0(q) = q^2$$

- Expected loss for squared error loss

$$R(\eta \mid q) = \eta (1 - q)^2 + (1 - \eta) q^2$$

- Squared error loss is a strictly proper scoring rule

Misclassification loss

- Usually, misclassification loss uses $c = 0.5$ as the cutoff

$$\mathcal{L} = \frac{1}{N} \sum_{n=1}^{N} \left[y_n \mathbf{1}_{\{q_n \leq 0.5\}} + (1 - y_n) \mathbf{1}_{\{q_n > 0.5\}} \right]$$

- Partial losses for misclassification loss

$$L_1(1 - q) = \mathbf{1}_{\{q_n \leq 0.5\}}, \quad L_0(q) = \mathbf{1}_{\{q_n > 0.5\}}$$

- Expected loss for misclassification loss

$$R(\eta \mid q) = \eta \mathbf{1}_{\{q \leq 0.5\}} + (1 - \eta) \mathbf{1}_{\{q > 0.5\}}$$

- Since any $q > 0.5$ for events and any $q \leq 0.5$ for non-events minimize the misclassification loss, misclassification loss is a proper score rule, but it is not strictly proper

A counter-example of proper scoring rule: absolute loss

- Because $y \in \{0, 1\}$, the absolute deviation $L(y \mid q) = |y - q|$ becomes

$$L(y \mid q) = y(1 - q) + (1 - y)q$$
$$R(\eta \mid q) = \eta(1 - q) + (1 - \eta)q$$

- Absolute deviation is not a proper scoring rule, because $R(\eta \mid q)$ is minimized by $q = 1$ for $\eta > 1/2$, and $q = 0$ for $\eta < 1/2$

Structure of proper scoring rules

- **Theorem**: Let $\omega(dt)$ be a positive measure on $(0, 1)$ that is finite on intervals $(\epsilon, 1-\epsilon), \forall\epsilon > 0$. Then the following defines a proper scoring rule:

$$L_1(1-q) = \int_q^{f_1} (1-t)\omega(dt), \quad L_0(q) = \int_{f_0}^q t\omega(dt)$$

- The proper scoring rule is strict iff $\omega(dt)$ has non-zero mass on every open interval of (0, 1)
- The fixed limits $f_0 \geq 0$ and $f_1 \leq 1$ are somewhat arbitrary
- Note that for log-loss, $L_1(1-q)$ is unbounded (goes to infinity) below near $q = 1$, and $L_0(q)$ is unbounded below near $q = 0$
- Except for log-loss, all other common proper scoring rules seem to satisfy

$$\int_0^1 t(1-t)\omega(dt) < \infty$$

Connection between the false positive (FP) / false negative (FN) costs and the classification cutoff

- Suppose the costs of FP and FN sum up to 1:
  - FP: has a cost c, and expected cost $cP(Y = 0) = c(1 - \eta)$
  - FN: has a cost $1 - c$, and expected cost $(1 - c)P(Y = 1) = (1 - c)\eta$
- The optimal classification is therefore class 1 iff

$$(1 - c)\eta \geq c(1 - \eta) \iff \eta \geq c$$

  - Since we don't know the truth η, we classify as class 1 when $q \geq c$
- Therefore, the classification cutoff equals

$$\frac{\text{cost of FP}}{\text{cost of FP} + \text{cost of FN}}$$

  - Standard classification assumes costs of FP and FN are the same, so the classification cutoff is 0.5

Cost-weighted misclassification errors

- Cost-weighted misclassification errors:

$$L_c(y \mid q) = y(1-c)\cdot \mathbf{1}_{\{q\le c\}} + (1-y)c\cdot \mathbf{1}_{\{q>c\}}$$
$$L_{1,c}(1-q) = (1-c)\cdot \mathbf{1}_{\{q\le c\}}, \quad L_{0,c}(q) = c\cdot \mathbf{1}_{\{q>c\}}$$

- **Shuford-Albert-Massengil-Savage-Schervish theorem**: an intergral representation of proper scoring rules

$$L(y \mid q) = \int_0^1 L_c(y \mid q)\omega(dc) = \int_0^1 L_c(y \mid q)\omega(c)dc$$

  – The second equality holds if $w(dc)$ is absolutely continuous wrt Lebesgue measure
  – This can be used to tailor losses to specific classification problems with cutoffs other than $1/2$ of $\eta(x)$, by designing suitable weight functions $\omega()$

- The paper proposes to use Iterative Reweighted Least Squares (IRLS) to fit linear models with proper scoring rules

Beta family of proper scoring rules

- This paper introduced a flexible 2-parameter family of proper scoring rules

$$\omega(t) = t^{\alpha-1}(1-t)^{\beta-1}, \quad \text{where } \alpha > -1, \beta > -1$$

- **Loss function of the Beta family proper scoring rules**

$$\begin{aligned} L(y \mid q) &= y \int_q^1 t^{\alpha-1}(1-t)^{\beta} dt + (1-y) \int_0^q t^{\alpha}(1-t)^{\beta-1} dt \\ &= yB(\alpha, \beta+1)\left[1 - I_q(\alpha, \beta+1)\right] \\ &\quad + (1-y)B(\alpha+1, \beta)I_q(\alpha+1, \beta) \end{aligned}$$

  – See the definitions of $B(a, b)$ and $I_x(a, b)$ in the next page

- Log-loss and squared error loss are special cases
  – Log-loss: $\alpha = \beta = 0$
  – Squared error loss: $\alpha = \beta = 1$
  – Misclassification loss: $\alpha = \beta \to \infty$

Special functions and Python / R implementations

- Beta function

$$B(a,b) = \int_0^1 t^{a-1}(1-t)^{b-1}dt$$

  – Python implementation: `scipy.special.beta(a,b)`
  – R implementation: `beta(a, b)`

- Incomplete Beta function

$$I_x(a,b) = \frac{1}{B(a,b)} \int_0^x t^{a-1}(1-t)^{b-1}dt$$

  – Python implementation: `scipy.special.betainc(a, b, x)`
  – R implementation: `pbeta(x, a, b)`

Tailor proper scoring rules for cost-weighted misclassification

- We can use $\alpha \neq \beta$ when FP and FN costs are not viewed equal
- Since Beta family proper scoring rule is like adding a Beta distribution on the FP cost c, we can use mean/variance matching to elicit α and β

$$\mu = \frac{\alpha}{\alpha + \beta} = c$$

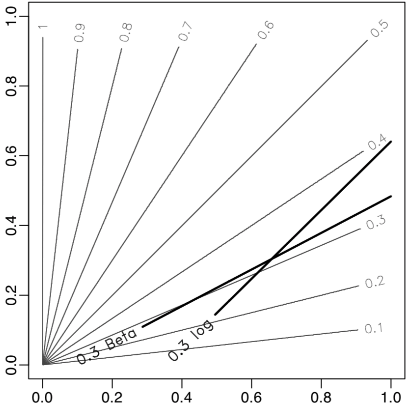
$$\sigma^2 = \frac{\alpha\beta}{(\alpha+\beta)^2(\alpha+\beta+1)} = \frac{c(1-c)}{\alpha+\beta+1}$$

- Alternatively, we can match the mode

$$c = q_{\text{mode}} = \frac{\alpha - 1}{\alpha + \beta - 2}$$

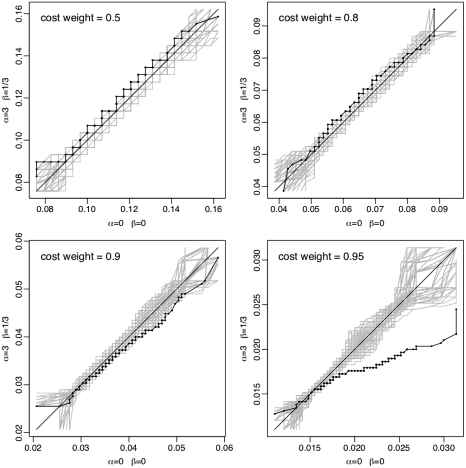
A simulation example

- In the simulation data with bivariate x, where decision boundaries of different η are not in parallel (grey lines)
- The logit link Beta family linear model with $\alpha = 6, \beta = 14$ estimates the $c = 0.3$ classification boundary better than the logistic regression



On the Pima Indians diabetes data

- Comparing logistic regression with a proper scoring rule tailored for high class 1 probabilities: $\alpha = 9, \beta = 1$.
- Black lines: empirical QQ curves of 200 cost-weighted misclassification costs computed on randomly selected test sets



References

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- For a game theory definition of proper scoring rule, see https://www.cis.upenn.edu/~aaroth/courses/slides/agt17/lect23.pdf
- Fitting linear models with custom loss functions in Python: https://alex.miller.im/posts/linear-model-custom-loss-function-regularization-python/
- Fitting XGBoost with custom loss functions in Python: https://xgboost.readthedocs.io/en/latest/tutorials/custom_metric_obj.html