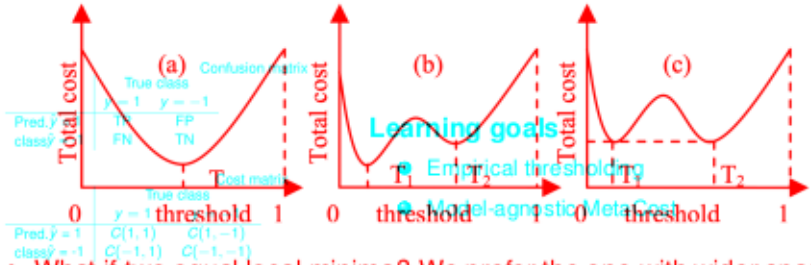
EMPIRICAL THRESHOLDING: BINARY CASE

- Theoretical threshold from MECP not always best, due to e.g. wrong model class, finite data, etc.
- Simply measure costs on data with different thresholds
- Then pick best threshold (Fig.1 in Sheng et al. 2006):



Learning goals

- Empirical thresholding
- Model-agnostic MetaCost

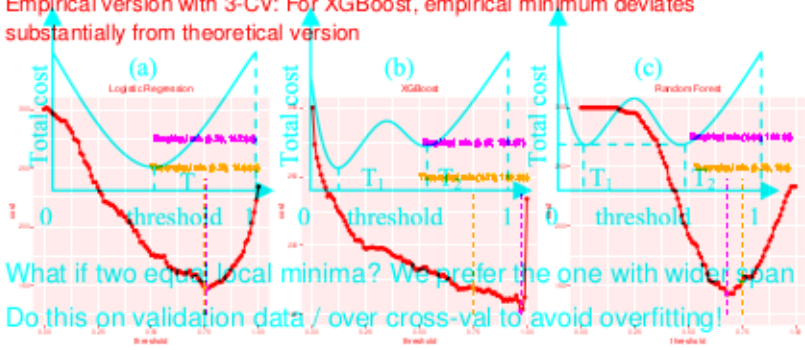
- What if two equal local minima? We prefer the one with wider span
- Do this on validation data / over cross-val to avoid overfitting!

EMPIRICAL THRESHOLDING: BINARY CASE

- Example: German Credit task
- Theoretical threshold from MECP not always best, due to e.g. wrong model class, finite data, etc.
- Simply measure costs on data with different thresholds
- Then pick best threshold (Fig. 1 in Sheng et al. 2006):

		True class $y = good$	True class $y = bad$
Pred. $\hat{y}$	$= good$	0	3
class	$= bad$	1	0

- Theoretical: $C(good, bad)/(C(bad, good) + C(good, bad)) = 3/4 = c^*$
- Empirical version with 3-CV: For XGBoost, empirical minimum deviates substantially from theoretical version



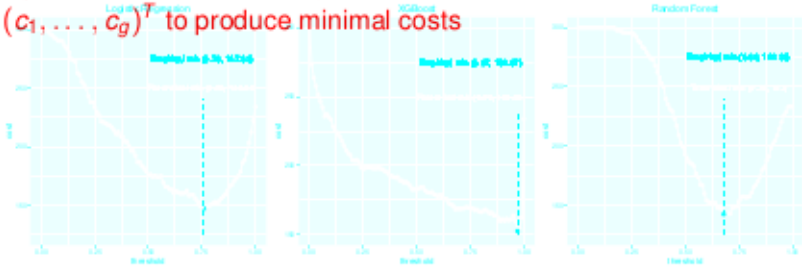
- What if two equal local minima? We prefer the one with wider span
- Do this on validation data / over cross-val to avoid overfitting!

EMPIRICAL THRESHOLDING: MULTICLASS

- In the standard setting, we predict class $h(\mathbf{x}) = \arg\max_k \pi_k(\mathbf{x})$.
- Let's use g thresholds c_k now

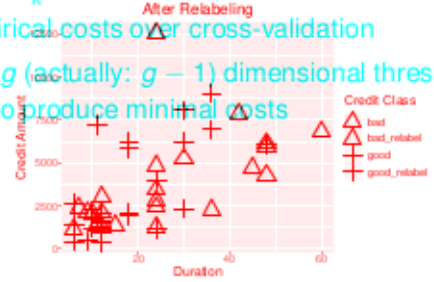
		True class	
		$y = \text{good}$	$y = \text{bad}$
Pred. class	$\hat{y} = \text{good}$	0	3
	$\hat{y} = \text{bad}$	1	0

- Re-scale scores $\mathbf{s} = \left(\frac{\pi(\mathbf{x})_1}{c_1}, \ldots, \frac{\pi(\mathbf{x})_g}{c_g}\right)^\top$,
- Predict class $\arg\max_k \pi_k(\mathbf{x})$
- Theoretical optimum: $c^* = (C(bad, bad) + C(bad, good)) = 3/4 = c^*$
- Empirical version with 3-CV: For XGBoost, empirical minimum deviates substantially from theoretical version
- Compute empirical costs over cross-validation
- Optimize over g (actually: $g - 1$) dimensional threshold vector $(c_1, \ldots, c_g)^\top$ to produce minimal costs



METACOST: OVERVIEW

- Model-agnostic wrapper technique
- General idea:
  1. Relabel train obs with their low expected cost classes
  2. Apply classifier to relabeled data
- Example German Credit task:



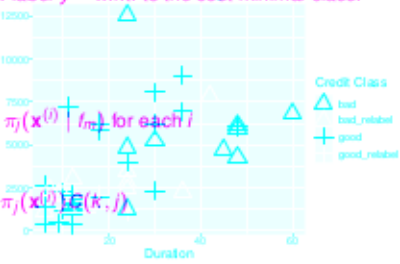
- Relabeled instances colored red
- Relabeling from good to bad more common because of costs

METACOST: ALGORITHM

Input: $\mathcal{D} = \{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^{n}$ training data, B number of bagging iterations, $\pi(\mathbf{x})$ probabilistic classifier, $\mathbf{C}$ cost matrix, empty dataset $\tilde{\mathcal{D}} = \emptyset$

# Bagging: Classifiers trained on different bootstrap samples.
for $b = 1, \ldots, B$ **do**
  $\mathcal{D}_b \leftarrow$ Bootstrap version of $\mathcal{D}$
  $\pi_b \leftarrow$ train classifier on $\mathcal{D}_b$
end for
# Relabeling: Find classifiers for which $\mathbf{x}^{(i)}$ is OOB and compute π_b by averaging over predictions. Determine new label $\tilde{y}^{(i)}$ w.r.t. to the cost minimal class.
for $i = 1, \ldots, n$ **do**
  $\tilde{M} \leftarrow \bigcup_{m \mathbf{x}^{(i)} \notin \mathcal{D}_m} \{m\}$
end for
for $j = 1, \ldots, g$ **do**
  $\pi_j(\mathbf{x}^{(i)}) \leftarrow \frac{1}{|\tilde{M}|} \sum_{m \in \tilde{M}} \pi_j(\mathbf{x}^{(i)} \mid f_m)$ for each i
end for
for $i = 1, \ldots, n$ **do**
  $\tilde{y}^{(i)} \leftarrow \arg\min_k \sum_{j=1}^{g} \pi_j(\mathbf{x}^{(i)}) C(k, j)$
  $\tilde{\mathcal{D}} \leftarrow \tilde{\mathcal{D}} \cup \{(\mathbf{x}^{(i)}, \tilde{y}^{(i)})\}$
end for
# Cost Sensitivity: Train on relabeled data.
$f_{meta} \leftarrow$ train f on $\tilde{\mathcal{D}}$

- Model-agnostic wrapper technique
- General idea:
  1. Relabel train obs with their low expected cost classes
  2. Apply classifier to relabeled data
- Example German Credit task:



- Relabeled instances colored red
- Relabeling from good to bad more common because of costs

METACOST: ALGORITHM

Input: $\mathcal{D} = \{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^{n}$ training data, B number of bagging iterations, $\pi(\mathbf{x})$ probabilistic classifier, $\mathbf{C}$ cost matrix, empty dataset $\tilde{\mathcal{D}} = \emptyset$

\# Bagging: Classifier is trained on different bootstrap samples.

for $b = 1, \ldots, B$ **do**

  $\mathcal{D}_b \leftarrow$ Bootstrap version of $\mathcal{D}$

  $\pi_b \leftarrow$ train classifier on $\mathcal{D}_b$

end for

\# Relabeling: Find classifiers for which $\mathbf{x}^{(i)}$ is OOB and compute π_b by averaging over predictions. Determine new label $\tilde{y}^{(i)}$ w.r.t. to the cost minimal class.

for $i = 1, \ldots, n$ **do**

  $\tilde{M} \leftarrow \bigcup_m \mathbf{x}^{(i)} \notin \mathcal{D}_m \{m\}$

end for

for $j = 1, \ldots, g$ **do**

  $\pi_j(\mathbf{x}^{(i)}) \leftarrow \frac{1}{|\tilde{M}|} \sum_{m \in \tilde{M}} \pi_j(\mathbf{x}^{(i)} \mid t_m)$ for each i

end for

for $i = 1, \ldots, n$ **do**

  $\tilde{y}^{(i)} \leftarrow \arg\min_k \sum_{j=1}^{g} \pi_j(\mathbf{x}^{(i)}) C(k, j)$

  $\tilde{\mathcal{D}} \leftarrow \tilde{\mathcal{D}} \cup \{(\mathbf{x}^{(i)}, \tilde{y}^{(i)})\}$

end for