Evaluation metrics and proper scoring rules

Classifier Calibration Tutorial
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Expected/Maximum calibration error

- As seen in the previous Section, each notion of calibration is related to a reliability diagram
  - This can be used to visualise miscalibration on binned scores
- We will now see how these bins can be used to measure miscalibration

Toy example

- We start by introducing a toy example:

	$\hat{p}_1$	$\hat{p}_2$	$\hat{p}_3$	y
1	1.0	0.0	0.0	1
2	0.9	0.1	0.0	1
3	0.8	0.1	0.1	1
4	0.7	0.1	0.2	1
5	0.6	0.3	0.1	1
6	0.4	0.1	0.5	1
7	1/3	1/3	1/3	1
8	1/3	1/3	1/3	1
9	0.2	0.4	0.4	1
10	0.1	0.5	0.4	1

	$\hat{p}_1$	$\hat{p}_2$	$\hat{p}_3$	y
11	0.8	0.2	0.0	2
12	0.7	0.0	0.3	2
13	0.5	0.2	0.3	2
14	0.4	0.4	0.2	2
15	0.4	0.2	0.4	2
16	0.3	0.4	0.3	2
17	0.2	0.3	0.5	2
18	0.1	0.6	0.3	2
19	0.1	0.3	0.6	2
20	0.0	0.2	0.8	2

	$\hat{p}_1$	$\hat{p}_2$	$\hat{p}_3$	y
21	0.8	0.2	0.0	3
22	0.8	0.1	0.1	3
23	0.8	0.0	0.2	3
24	0.6	0.0	0.4	3
25	0.3	0.0	0.7	3
26	0.2	0.6	0.2	3
27	0.2	0.4	0.4	3
28	0.0	0.4	0.6	3
29	0.0	0.3	0.7	3
30	0.0	0.3	0.7	3

Binary-ECE

- We define the expected binary calibration error binary−ECE (Naeini et al., 2015) as the average gap across all bins in a reliability diagram, weighted by the number of instances in each bin:

$$\text{binary}-\text{ECE} = \sum_{i=1}^{M} \frac{|B_i|}{N} |\bar{y}(B_i) - \bar{p}(B_i)|,$$

- Where M and N are the numbers of bins and instances, respectively, B_i is the i-th probability bin, $|B_i|$ denotes the size of the bin, and $\bar{p}(B_i)$ and $\bar{y}(B_i)$ denote the average predicted probability and the proportion of positives in bin B_i

Binary-MCE

- We can similarly define the maximum binary calibration error binary$-$MCE as the maximum gap across all bins in a reliability diagram:

$$\text{binary}-\text{MCE} = \max_{i \in \{1,\ldots,M\}} |\bar{y}(B_i) - \bar{p}(B_i)|.$$

Binary-ECE using our example

- Let us pretend our example is binary by taking class 1 as positive

	$\hat{p}_1$	$\hat{p}_0$	y
1	1.0	0.0	1
2	0.9	0.1	1
3	0.8	0.2	1
4	0.7	0.3	1
5	0.6	0.4	1
6	0.4	0.6	1
7	1/3	2/3	1
8	1/3	2/3	1
9	0.2	0.8	1
10	0.1	0.9	1

	$\hat{p}_1$	$\hat{p}_0$	y
11	0.8	0.2	0
12	0.7	0.3	0
13	0.5	0.5	0
14	0.4	0.6	0
15	0.4	0.6	0
16	0.3	0.7	0
17	0.2	0.8	0
18	0.1	0.9	0
19	0.1	0.9	0
20	0.0	1.0	0

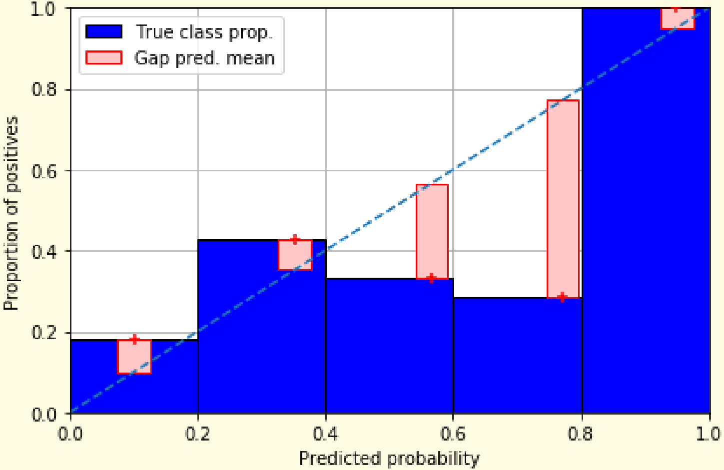
	$\hat{p}_1$	$\hat{p}_0$	y
21	0.8	0.2	0
22	0.8	0.2	0
23	0.8	0.2	0
24	0.6	0.4	0
25	0.3	0.7	0
26	0.2	0.8	0
27	0.2	0.8	0
28	0.0	1.0	0
29	0.0	1.0	0
30	0.0	1.0	0

Binary-ECE using our example

- We now separate class 1 probabilities and their corresponding instance labels into 5 bins: $[0, 0.2], (0.2, 0.4], (0.4, 0.6], (0.6, 0.8], (0.8, 1.0]$
- Then, we calculate the average probability and the frequency of positives at each bin

B_i	$\lvert B_i \rvert$		$\bar{p}(B_i)$		$\bar{y}(B_i)$
B_1	11	0.0, 0.0, 0.0, 0.0, 0.1, 0.1, 0.1, 0.2, 0.2, ...	1.1/11	0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 1	2/11
B_2	7	0.3, 0.3, 1/3, 1/3, 0.4, 0.4, 0.4	2.5/7	0, 0, 0, 0, 1, 1, 1	3/7
B_3	3	0.5, 0.6, 0.6	1.7/3	0, 0, 1	1/3
B_4	7	0.7, 0.7, 0.8, 0.8, 0.8, 0.8, 0.8	5.4/7	0, 0, 0, 0, 0, 1, 1	2/7
B_5	2	0.9, 1.0	1.9/2	1, 1	2/2

These same bins can be used to build a reliability diagram



Finally, we calculate the binary-ECE

B_i	$\bar{p}(B_i)$	$\bar{y}(B_i)$	$\|B_i\|$
B_1	0.10	0.18	11
B_2	0.35	0.43	7
B_3	0.57	0.33	3
B_4	0.77	0.29	7
B_5	0.95	1.00	2

$$\text{binary}-\text{ECE} = \sum_{i=1}^{M} \frac{|B_i|}{N} |\bar{y}(B_i) - \bar{p}(B_i)|$$

$$\text{binary}-\text{ECE} = \frac{11 \cdot 0.08 + 7 \cdot 0.08 + 3 \cdot 0.24 + 7 \cdot 0.48 + 2 \cdot 0.05}{30}$$

$$\text{binary}-\text{ECE} = 0.1873$$

Binary-MCE

- For the binary-MCE, we take the maximum gap between $\bar{p}(B_i)$ and $\bar{y}(B_i)$:

B_i	$\bar{p}(B_i)$	$\bar{y}(B_i)$	$\lvert B_i \rvert$
B_1	0.10	0.18	11
B_2	0.35	0.43	7
B_3	0.57	0.33	3
B_4	**0.77**	**0.29**	**7**
B_5	0.95	1.00	2

$$\text{binary}-\text{MCE} = \max_{i \in \{1,\ldots,M\}} \lvert \bar{y}(B_i) - \bar{p}(B_i) \rvert$$

$$\text{binary}-\text{MCE} = 0.48$$

Confidence-ECE

- Confidence-ECE (Guo et al., 2017) was the first attempt at an ECE measure for multiclass problems
- Here, confidence means the probability given to the winning class, i.e. the highest value in the predicted probability vector
- We calculate the expected confidence calibration error $\text{confidence}-\text{ECE}$ as the binary-ECE of the binned confidence values

Confidence-MCE

- We can similarly define the maximum confidence calibration error confidence$-$MCE as the maximum gap across all bins in a reliability diagram:

$$\text{confidence}-\text{MCE} = \max_{i \in \{1,\dots,M\}} |\bar{y}(B_i) - \bar{p}(B_i)|.$$

Confidence-ECE using our example

- First, let us determine the confidence values:

	$\hat{p}_1$	$\hat{p}_2$	$\hat{p}_3$	y
1	**1.0**	0.0	0.0	1
2	**0.9**	0.1	0.0	1
3	**0.8**	0.1	0.1	1
4	**0.7**	0.1	0.2	1
5	**0.6**	0.3	0.1	1
6	0.4	0.1	**0.5**	1
7	**1/3**	1/3	1/3	1
8	**1/3**	1/3	1/3	1
9	0.2	**0.4**	0.4	1
10	0.1	**0.5**	0.4	1

	$\hat{p}_1$	$\hat{p}_2$	$\hat{p}_3$	y
11	**0.8**	0.2	0.0	2
12	**0.7**	0.0	0.3	2
13	**0.5**	0.2	0.3	2
14	**0.4**	0.4	0.2	2
15	**0.4**	0.2	0.4	2
16	0.3	**0.4**	0.3	2
17	0.2	0.3	**0.5**	2
18	0.1	**0.6**	0.3	2
19	0.1	0.3	**0.6**	2
20	0.0	0.2	**0.8**	2

	$\hat{p}_1$	$\hat{p}_2$	$\hat{p}_3$	y
21	**0.8**	0.2	0.0	3
22	**0.8**	0.1	0.1	3
23	**0.8**	0.0	0.2	3
24	**0.6**	0.0	0.4	3
25	0.3	0.0	**0.7**	3
26	0.2	**0.6**	0.2	3
27	0.2	**0.4**	0.4	3
28	0.0	0.4	**0.6**	3
29	0.0	0.3	**0.7**	3
30	0.0	0.3	**0.7**	3

Confidence-ECE using our example

- We binarise the labels by checking if the classifier predicted the right class:

confidence	correct
1.00	1
0.90	1
0.80	1
0.70	1
0.60	1
0.50	0
0.33	1
0.33	1
0.40	0
0.50	0

confidence	correct
0.8	0
0.7	0
0.5	0
0.4	0
0.4	0
0.4	1
0.5	0
0.6	1
0.6	0
0.8	0

confidence	correct
0.8	0
0.8	0
0.8	0
0.6	0
0.7	1
0.6	0
0.4	0
0.6	1
0.7	1
0.7	1

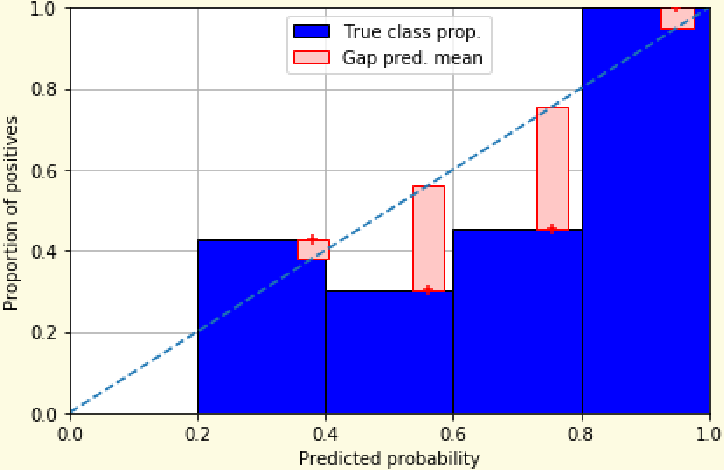
Confidence-ECE using our example

- We now separate the confidences into 5 bins:

B_i	$\lvert B_i \rvert$		$\bar{p}(B_i)$		$\bar{y}(B_i)$
B_1	0				
B_2	7	1/3, 1/3, 0.4, 0.4, 0.4, 0.4, 0.4	2.7/7	0, 0, 0, 0, 1, 1, 1	3/7
B_3	10	0.5, 0.5, 0.5, 0.5, 0.6, 0.6, 0.6, 0.6, 0.6, ...	5.6/10	0, 0, 0, 0, 0, 0, 0, 1, 1, 1	3/10
B_4	11	0.7, 0.7, 0.7, 0.7, 0.7, 0.8, 0.8, 0.8, 0.8, ...	8.3/11	0, 0, 0, 0, 0, 0, 1, 1, 1, 1, 1	5/11
B_5	2	0.9, 1.0	1.9/2	1, 1	2/2

- Note that bins that correspond to confidences **less than $1/K$** will always be **empty**

The corresponding reliability diagram



Finally, we calculate the confidence-ECE

B_i	$\bar{p}(B_i)$	$\bar{y}(B_i)$	$\lvert B_i \rvert$
B_1			0
B_2	0.38	0.43	7
B_3	0.56	0.30	10
B_4	0.75	0.45	11
B_5	0.95	1.00	2

$$\text{confidence}-\text{ECE} = \sum_{i=1}^{M} \frac{|B_i|}{N} |\bar{y}(B_i) - \bar{p}(B_i)|$$

$$\text{confidence}-\text{ECE} = \frac{0 + 7 \cdot 0.05 + 10 \cdot 0.26 + 11 \cdot 0.3 + 2 \cdot 0.05}{30}$$

$$\text{confidence}-\text{ECE} = 0.2117$$

Confidence-MCE

- For the confidence-MCE, we take the maximum gap between $\bar{p}(B_i)$ and $\bar{y}(B_i)$:

B_i	$\bar{p}(B_i)$	$\bar{y}(B_i)$	$\lvert B_i \rvert$
B_1			0
B_2	0.38	0.43	7
B_3	0.56	0.30	10
B_4	**0.75**	**0.45**	**11**
B_5	0.95	1.00	2

$$\text{confidence}-\text{MCE} = \max_{i \in \{1,\ldots,M\}} \lvert \bar{y}(B_i) - \bar{p}(B_i) \rvert$$

$$\text{confidence}-\text{MCE} = 0.3$$

Classwise-ECE

- Confidence calibration only cares about the winning class
- To measure miscalibration for all classes, we can take the average binary-ECE across all classes
- The contribution of a single class j to this expected classwise calibration error (classwise$-$ECE) is called **class-j-ECE**

Classwise-ECE

- Formally, classwise$-$ECE is defined as the average gap across all classwise-reliability diagrams, weighted by the number of instances in each bin:

$$\text{classwise}-\text{ECE} = \frac{1}{K}\sum_{j=1}^{K}\sum_{i=1}^{M}\frac{|B_{i,j}|}{N}|\bar{y}_j(B_{i,j}) - \bar{p}_j(B_{i,j})|,$$

- Where $B_{i,j}$ is the i-th bin of the j-th class, $|B_{i,j}|$ denotes the size of the bin, and $\bar{p}_j(B_{i,j})$ and $\bar{y}_j(B_{i,j})$ denote the average prediction of class j probability and the actual proportion of class j in the bin $B_{i,j}$

Classwise-MCE

- Similarly the maximum classwise calibration error (classwise$-$MCE) is defined as the maximum gap across all bins and all classwise-reliability diagrams:

$$\text{classwise}-\text{MCE} = \max_{j \in \{1,\ldots,K\}\, i \in \{1,\ldots,M\}} |\bar{y}_j(B_{i,j}) - \bar{p}_j(B_{i,j})|.$$

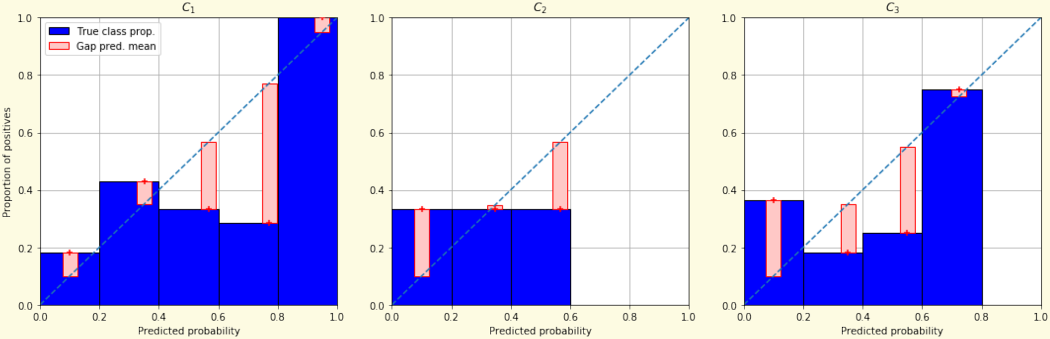
Classwise-ECE using our example

- We have already calculated class-1-ECE (0.1873) in our binary-ECE example
- Now we need to do the same for classes 2 and 3

$B_{i,2}$	$\|B_{i,2}\|$		$\bar{p}(B_{i,2})$		$\bar{y}(B_{i,2})$
$B_{1,2}$	15	0.0, 0.0, 0.0, 0.0, 0.0, 0.1, 0.1, 0.1, 0.1, ...	1.5/15	0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 1, 1, 1, 1	5/15
$B_{2,2}$	12	0.3, 0.3, 0.3, 0.3, 0.3, 1/3, 1/3, 0.4, 0.4...	4.2/12	0, 0, 0, 0, 0, 0, 0, 0, 1, 1, 1, 1	4/12
$B_{3,2}$	3	0.5, 0.6, 0.6	1.7/3	0, 0, 1	1/3
$B_{4,2}$	0				
$B_{5,2}$	0				

$B_{i,3}$	$\|B_{i,3}\|$		$\bar{p}(B_{i,3})$		$\bar{y}(B_{i,3})$
$B_{1,3}$	11	0.0, 0.0, 0.0, 0.0, 0.1, 0.1, 0.1, 0.2, 0.2, ...	1.1/11	0, 0, 0, 0, 0, 0, 0, 1, 1, 1, 1	4/11
$B_{2,3}$	11	0.3, 0.3, 0.3, 0.3, 1/3, 1/3, 0.4, 0.4, 0.4...	3.9/11	0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 1	2/11
$B_{3,3}$	4	0.5, 0.5, 0.6, 0.6	2.2/4	0, 0, 0, 1	1/4
$B_{4,3}$	4	0.7, 0.7, 0.7, 0.8	2.9/4	0, 1, 1, 1	3/4
$B_{5,3}$	0				

Each class has its own reliability diagram



Now we calculate class-2-ECE and class-3-ECE

$$\text{class}-2-\text{ECE} = \sum_{i=1}^{M} \frac{|B_{i,2}|}{N} |\bar{y}(B_{i,2}) - \bar{p}(B_{i,2})|$$

$$\text{class}-2-\text{ECE} = \frac{15 \cdot 0.23 + 12 \cdot 0.02 + 3\ \dot{0}.24 + 0 + 0}{30}$$

$$\text{class}-2-\text{ECE} = 0.147$$

$$\text{class}-3-\text{ECE} = \sum_{i=1}^{M} \frac{|B_{i,3}|}{N} |\bar{y}(B_{i,3}) - \bar{p}(B_{i,3})|$$

$$\text{class}-3-\text{ECE} = \frac{11 \cdot 0.26 + 11 \cdot 0.17 + 4 \cdot 0.3 + 4 \cdot 0.03 + 0}{30}$$

$$\text{class}-3-\text{ECE} = 0.2017$$

Finally, we take the mean of the 3 ECEs

$$\text{classwise}-\text{ECE} = \frac{1}{K}\sum_{j=1}^{K}\sum_{i=1}^{M}\frac{|B_{i,j}|}{N}|\bar{y}_j(B_{i,j}) - \bar{p}_j(B_{i,j})|$$

$$\text{classwise}-\text{ECE} = \frac{0.1873 + 0.147 + 0.2017}{3}$$

$$\text{classwise}-\text{ECE} = 0.1787$$

Classwise-MCE

- For the classwise-MCE, we take the maximum gap between $\bar{p}(B_{i,j})$ and $\bar{y}(B_{i,j})$ across all bins of all classes:

$B_{i,1}$	$\bar{p}(B_{i,1})$	$\bar{y}(B_{i,1})$	$\lvert B_{i,1}\rvert$
$B_{1,1}$	0.10	0.18	11
$B_{2,1}$	0.35	0.43	7
$B_{3,1}$	0.57	0.33	3
$B_{4,1}$	**0.77**	**0.29**	**7**
$B_{5,1}$	0.95	1.00	2

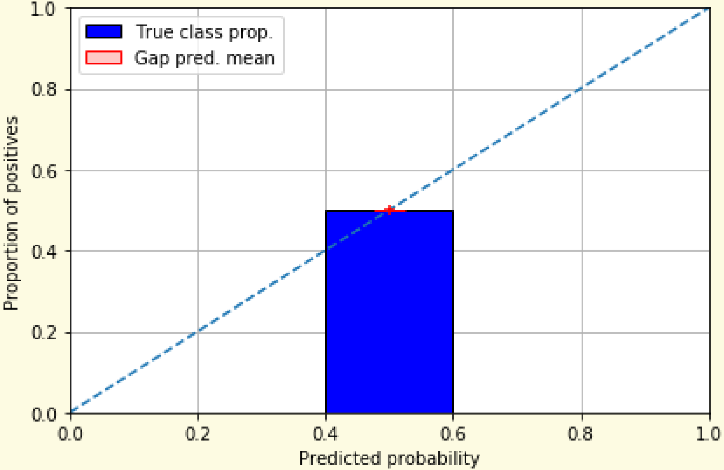
$B_{i,2}$	$\bar{p}(B_{i,2})$	$\bar{y}(B_{i,2})$	$\lvert B_{i,2}\rvert$
$B_{1,2}$	0.10	0.33	15
$B_{2,2}$	0.35	0.33	12
$B_{3,2}$	0.57	0.33	3
$B_{4,2}$			0
$B_{5,2}$			0

$B_{i,3}$	$\bar{p}(B_{i,3})$	$\bar{y}(B_{i,3})$	$\lvert B_{i,3}\rvert$
$B_{1,3}$	0.10	0.36	11
$B_{2,3}$	0.35	0.18	11
$B_{3,3}$	0.55	0.25	4
$B_{4,3}$	0.72	0.75	4
$B_{5,3}$			0

$$\text{classwise}-\text{MCE} = \max_{j\in\{1,\ldots,K\}\, i\in\{1,\ldots,M\}} |\bar{y}_j(B_{i,j}) - \bar{p}_j(B_{i,j})|$$

$$\text{classwise}-\text{MCE} = 0.48$$

Optimising ECE can be as simple as predicting the overall class distribution, regardless of the given instance



What about multiclass-ECE?

- True multiclass-ECE is still an open problem
- With large numbers of classes, the number of bins can be prohibitively high
  - Most bins would be empty
- Therefore, we turn to **proper scoring rules**

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Proper scoring rules

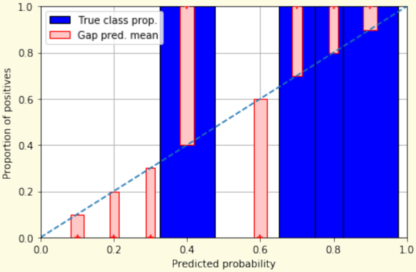
- We now talk about loss measures ($\breve{\phi}$) that prefer Bayes-optimal classifiers over other classifiers
- For any given $P(\mathbf{X}, Y)$, $\mathbf{x} \in \mathcal{X}$, the following is satisfied:

$$\mathbb{E}_{y \sim P(Y|\mathbf{X}=\mathbf{x})}\left[\breve{\phi}(\mathbf{q}, y)\right] \geq \mathbb{E}_{y \sim P(Y|\mathbf{X}=\mathbf{x})}\left[\breve{\phi}\left(P(Y \mid \mathbf{X} = \mathbf{x}), y\right)\right]$$

- And the left side is equal to right side if and only if $\mathbf{q} = P(Y \mid \mathbf{X} = \mathbf{x})$
- $P(Y \mid \mathbf{X} = \mathbf{x})$ is a vector with elements $P(Y = j \mid \mathbf{X} = \mathbf{x})$

Proper scoring rules

- Proper scoring rules are calculated at the item level, while ECE measures are averages across bins
- Think of them as putting **each item in its separate bin**, then computing the average of some **loss** for each **predicted probability** and its corresponding **observed label**
  - Instead of the absolute difference, as in ECE, this loss can be the quadratic error or the Kullback–Leibler divergence, which have better mathematical properties



Brier score/Quadratic error/Euclidean distance

$$\breve{\phi}_{\text{BS}}\left(\mathbf{Q}, \mathbf{y}\right) = \frac{1}{N}\sum_{n=1}^{N}\sum_{j=1}^{K}\left(\mathbb{I}(y_n = j) - q_{n,j}\right)^2$$

- We can easily see that this value is not minimised by constantly predicting the class distribution, as in ECE

$$\mathbf{Q} = \begin{bmatrix} 0.5 & 0.5 \\ 0.5 & 0.5 \end{bmatrix}$$

$$\mathbf{y} = [1, 2]$$

$$\breve{\phi}_{\text{BS}}\left(\mathbf{Q}, \mathbf{y}\right) = \frac{(1-0.5)^2 + (0-0.5)^2 + (0-0.5)^2 + (1-0.5)^2}{2}$$

$$\breve{\phi}_{\text{BS}}\left(\mathbf{Q}, \mathbf{y}\right) = 0.5$$

Log-loss/Cross entropy

$$\breve{\phi}_{\text{LL}}\left(\mathbf{Q}, \mathbf{y}\right) = -\frac{1}{N}\sum_{n=1}^{N}\sum_{j=1}^{K}\mathbb{I}(y_n = j) \cdot \log(q_{n,j})$$

- Frequently used to as the training loss of machine learning methods, such as neural networks
- Only penalises the probability given to the true class

$$\breve{\phi}_{\text{LL}}\left(\mathbf{Q}, \mathbf{y}\right) = -\frac{(1 \cdot \log(0.5) + 0 \cdot \log(0.5) + 0 \cdot \log(0.5) + 1 \cdot \log(0.5))}{2}$$

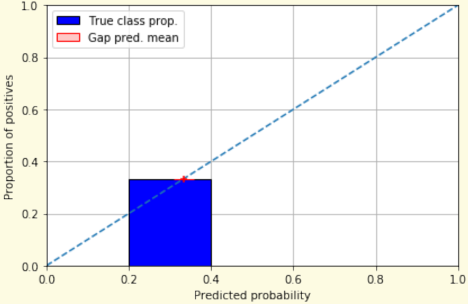
$$\breve{\phi}_{\text{LL}}\left(\mathbf{Q}, \mathbf{y}\right) = 0.6931$$

Let us rewind a bit

- As mentioned before, a model that always outputs the class proportion will have a perfect ECE of 0, but its log-loss is not 0 (in fact, it's 0.6365)

$$\mathbf{Q} = \begin{bmatrix} 2/3 & 1/3 \\ 2/3 & 1/3 \\ \vdots & \vdots \\ 2/3 & 1/3 \end{bmatrix}$$

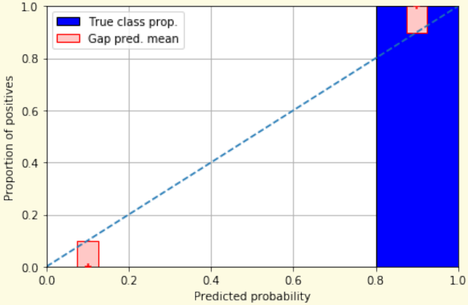
$$\begin{aligned}\mathbf{y} = [&1, 1, 1, 1, 1, 1, 1, 1, 1, 1,\\ &0, 0, 0, 0, 0, 0, 0, 0, 0, 0,\\ &0, 0, 0, 0, 0, 0, 0, 0, 0, 0]\end{aligned}$$



An evaluation trade-off

- What happens if our model gives 0.9 probability to the instances' true classes?

$$\text{accuracy} = 1$$
$$\text{ECE} = 0.1$$
$$\text{log-loss} = 0.1054$$



Proper scoring rule decomposition

- ECE increased (0 to 0.1), but log-loss decreased (0.6365 to 0.1054)
- So why did log-loss decrease?
  - Because proper scoring rules do not measure only calibration
  - In fact, they can be decomposed into terms with different interpretations (Kull and Flach, 2015)

Proper scoring rule decomposition

- An intuitive way to decompose proper scoring rules is into refinement and calibration losses: $\mathbb{E}\left[\breve{\phi}\right] = \mathsf{RL} + \mathsf{CL}$
  - Refinement loss: is the loss due to producing the same probability for instances from different classes
  - Calibration loss: is the loss due to the difference between the probabilities predicted by the model and the proportion of positives among instances with the same output

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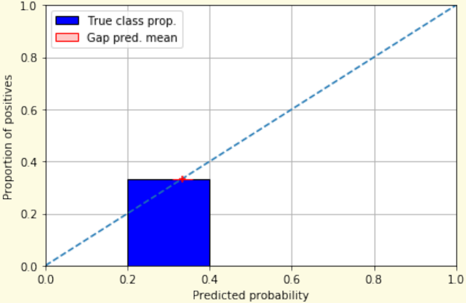

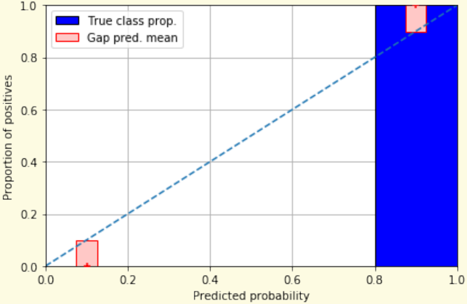

Proper scoring rule decomposition

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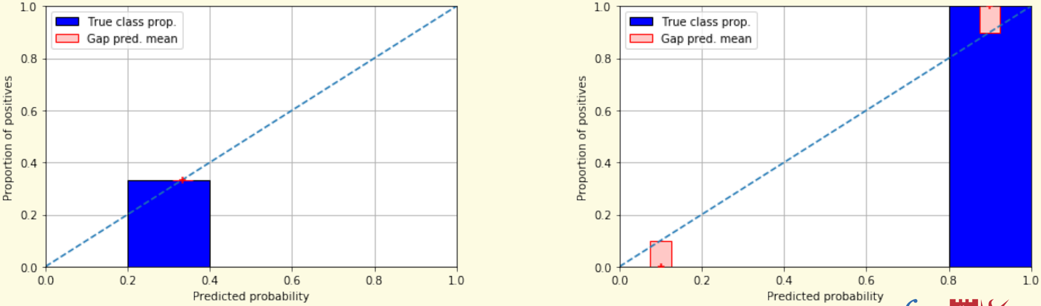

Proper scoring rule decomposition

- Since we don't usually know the real score distribution, we would need to once again rely on binning if we wanted to actually estimate refinement and calibration losses
- Additionally, the terms are calculated (estimated) differently, depending on the proper scoring rule
- **Fun fact:** the loss of the optimal classifier is not necessarily 0
  - This is due to irreducible loss, which is only 0 if the attributes provide enough information to uniquely determine the instances' right label Y, with probability 1 (Kull and Flach, 2015)

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Hypothesis test for calibration

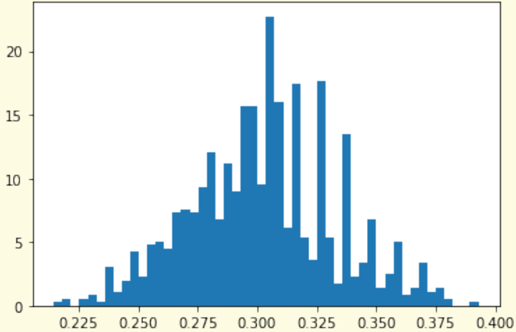
Summary

Hypothesis test for calibration

- Given a classifier $\hat{\boldsymbol{p}}$, we can check if its predictions for a test set $\{(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_N, y_N)\}$ are calibrated according to an arbitrary loss measure $\phi(\hat{\boldsymbol{p}}(X_{\text{test}}), \boldsymbol{y}_{\text{test}})$, such as ECE, log-loss or Brier score

Calculating the p-value

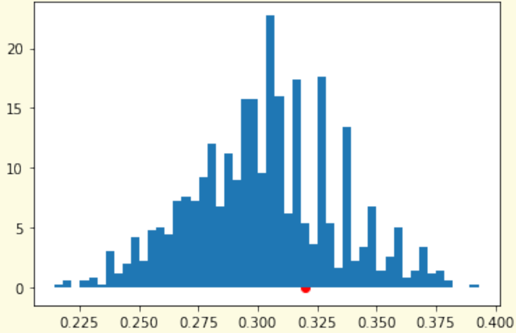
- We use a simple resampling-based hypothesis test under the null hypothesis that the classifier's outputs are calibrated (Vaicenavicius et al., 2019)
- First, we generate S bootstrapped label sets $\boldsymbol{y}_s$, $s \in \{1, \ldots, S\}$, such that each $y_{s,i}$ is sampled from $\hat{\boldsymbol{p}}(\hat{\boldsymbol{x}}_i)$
- Then we calculate $\phi(\hat{\boldsymbol{p}}(X_{\text{test}}), \boldsymbol{y}_s)$ for each label set s



Calculating the p-value

- We then calculate the p-value as:

$$P\Big(\phi(\hat{\boldsymbol{p}}(X_{\text{test}}), \boldsymbol{y}_s) > \phi(\hat{\boldsymbol{p}}(X_{\text{test}}), \boldsymbol{y}_{\text{test}})\Big) = P\Big(\phi(\hat{\boldsymbol{p}}(X_{\text{test}}), \boldsymbol{y}_s) > 0.32\Big) \tag{1}$$

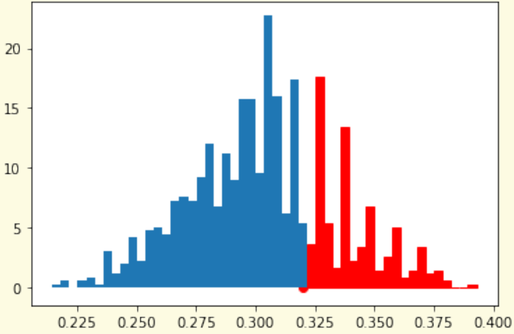


Calculating the p-value

- We then calculate the p-value as:

$$P\Big(\phi(\hat{\boldsymbol{p}}(X_{\text{test}}), \boldsymbol{y}_s) > 0.32\Big) \approx 0.26 \tag{2}$$

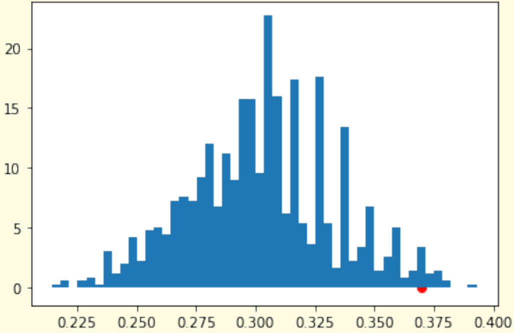
- We cannot reject the null hypothesis here



Calculating the p-value

- Now suppose the original labels were such that our classifier's classwise-ECE had a value of 0.37

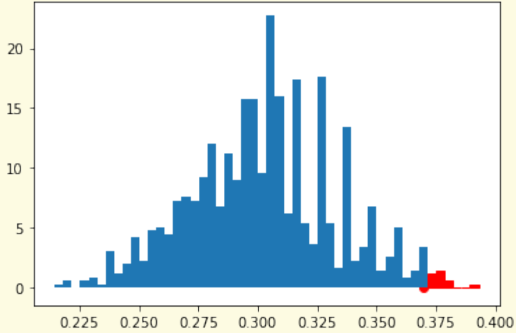
$$P\left(\phi(\hat{\boldsymbol{p}}(X_{\text{test}}), \boldsymbol{y}_s) > 0.37\right). \tag{3}$$



Calculating the p-value

- Now suppose that our classifier's classwise-ece had a value of 0.37

$$P\left(\phi(\hat{\boldsymbol{p}}(X_{\text{test}}), \boldsymbol{y}_s) > 0.37\right) \approx 0.01 \tag{4}$$

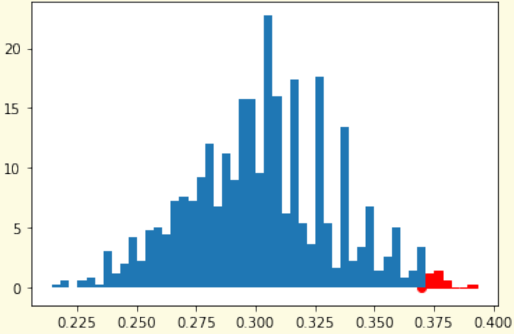


Calculating the p-value

- Now suppose the original labels were such that our classifier's classwise-ece had a value of 0.37

$$P\left(\phi(\hat{\boldsymbol{p}}(X_{\text{test}}), \boldsymbol{y}_s) > 0.37\right) \approx 0.01 \tag{5}$$

- We reject the null hypothesis: the model is **miscalibrated**



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Summary

Summary

- There are various ways to visualise and quantify calibration
- ECE measures aim at producing an aggregate measure of the visual information provided in reliability diagrams
  - Thus, their optimisation is **not** guaranteed to produce desirable classifiers
- Proper scoring rules measure different aspects of probability correctness
  - They have been used as training losses in classifier training for a while
  - But they cannot tell **“where”** the model is more miscalibrated
- Finally, the hypothesis test for calibration can help determine if a particular loss value means that the classifier is calibrated or not

What happens next

15.30 - Break and preparation for hands-on session

15.50 - Hao Song: Calibrators

Binary approaches; multi-class approaches;
regularisation and Bayesian treatments; implementation

16.50 - Miquel Perello-Nieto: Hands-on session

17.30 - Peter Flach, Hao Song: Advanced topics and conclusion

Cost curves; calibrating for F-score; regressor calibration

All times in CEST.

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Evaluation metrics and proper scoring rules

Classifier Calibration Tutorial
ECML PKDD 2020

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