Beyond temperature scaling: Obtaining well-calibrated multiclass probabilities with Dirichlet calibration

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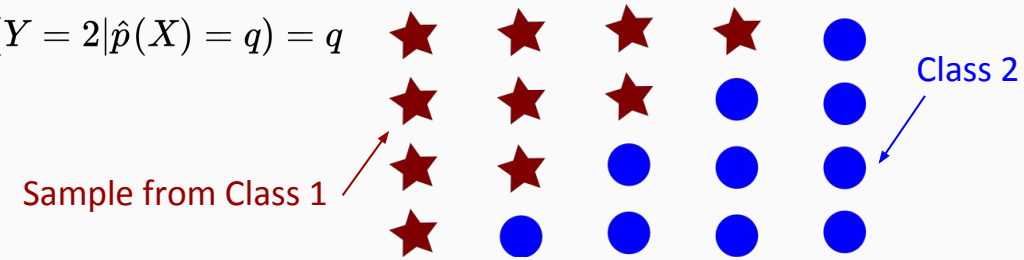
What is Classification Calibration?

A probabilistic classifier $\hat{\mathbf{p}}$ is:

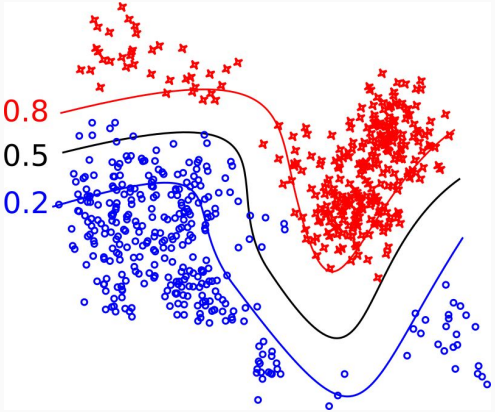
- Binary-calibrated if for any prediction q the proportion of positives among all instances x getting the same prediction $\hat{p}(x) = q$ are:

$$P(Y = 2|\hat{p}(X) = q) = q$$

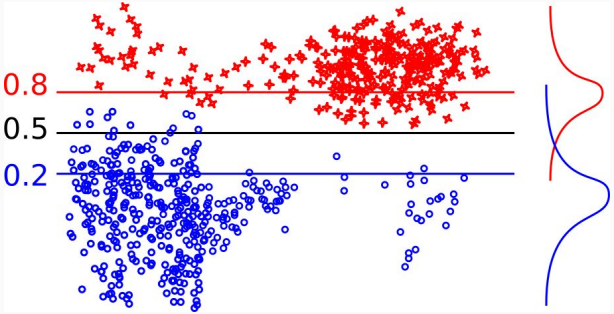


Empirical proportion Class 2:	0%	25%	50%	75%	100%
Calibrated classifier:	0%	25%	50%	75%	100%
Uncalibrated classifier:	9%	34%	70%	99%	100%

What is Classification Calibration?

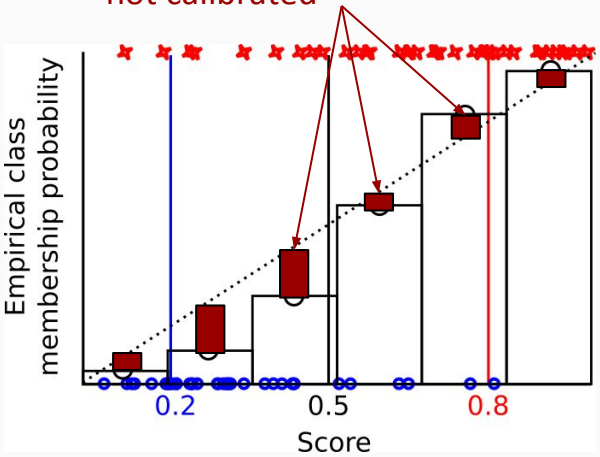


Decision boundary and parallel hyperplanes



Projection to an orthogonal vector

Deviation to diagonal indicates not calibrated



Model scores and empirical probabilities

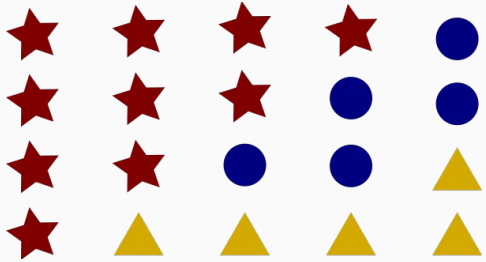
Multiclass Classification Calibration

A probabilistic classifier $\hat{\mathbf{p}}$ is:

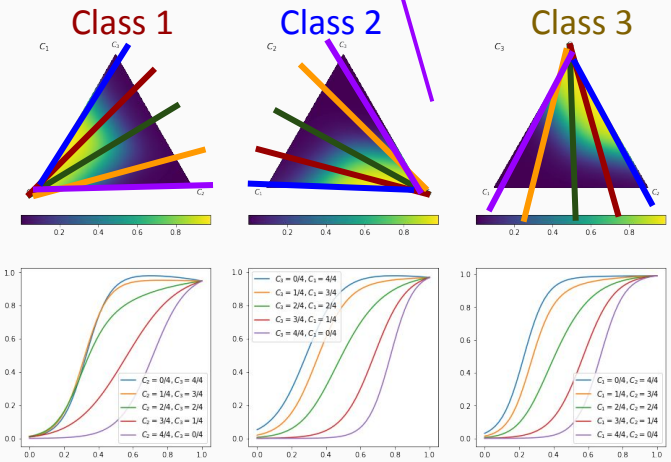
- Multiclass-calibrated if for any prediction vector $\mathbf{q} = (q_1, \ldots, q_k) \in \Delta_k$, the proportions of classes among all possible instances $\mathbf{x}$ getting the same prediction $\hat{\mathbf{p}}(\mathbf{x}) = \mathbf{q}$ are:

$$P(Y = i \mid \hat{\mathbf{p}}(X) = \mathbf{q}) = q_i \quad \text{for } i = 1, \ldots, k.$$

Multiclass example



Empirical proportions Class 1:	100%	75%	50%	25%	0%
Class 2:	0%	0%	25%	50%	50%
Class 3:	0%	25%	25%	25%	50%



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Why is calibration important? Optimal decision making

Cost Matrix	Predicted True	Predicted False
Actual True	-1£	100£
Actual False	50£	0£

Population proportion
50%
50%

Changes on costs

Changes on proportions

It also allows the decision to abstain

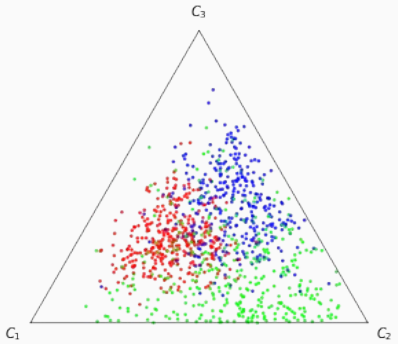
Cost Matrix	Predicted True	Predicted False
Actual True	-10£	90£
Actual False	40£	-5£

Population proportion
70%
30%

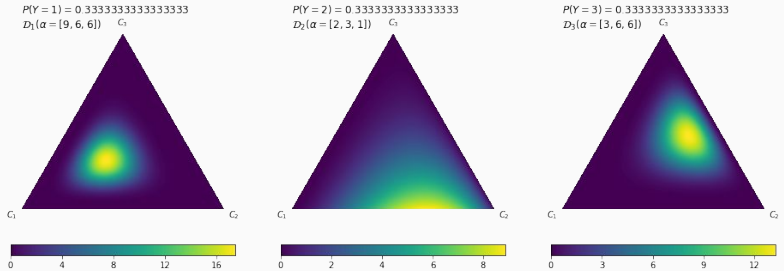
Dirichlet Calibration

We consider the distribution of prediction vectors $\hat{p}(\mathbf{x})$ separately on instances of each class, and assume these are Dirichlet distributions with different parameters:

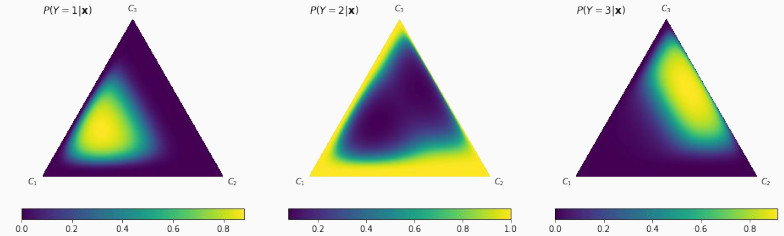
$$\hat{\mathbf{p}}(X) \mid Y = j \sim \text{Dir}(\alpha^{(j)})$$



True density



True posterior probabilities



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Evaluation of multiclass calibration is critical

Confidence-calibrated if

$$P\Big(Y = argmax\big(\hat{\mathbf{p}}(X)\big) \,\Big|\, max\big(\hat{\mathbf{p}}(X)\big) = c\Big) = c.$$

Empirically measured as

$$\text{confidence-ECE} = \sum_{i=1}^{m} \frac{|B_i|}{n} |y_j(B_i) - \hat{p}_j(B_i)|$$

Classwise-calibrated if

$$P(Y = i \mid \hat{p}_i(X) = q_i) = q_i.$$

Empirically measured as

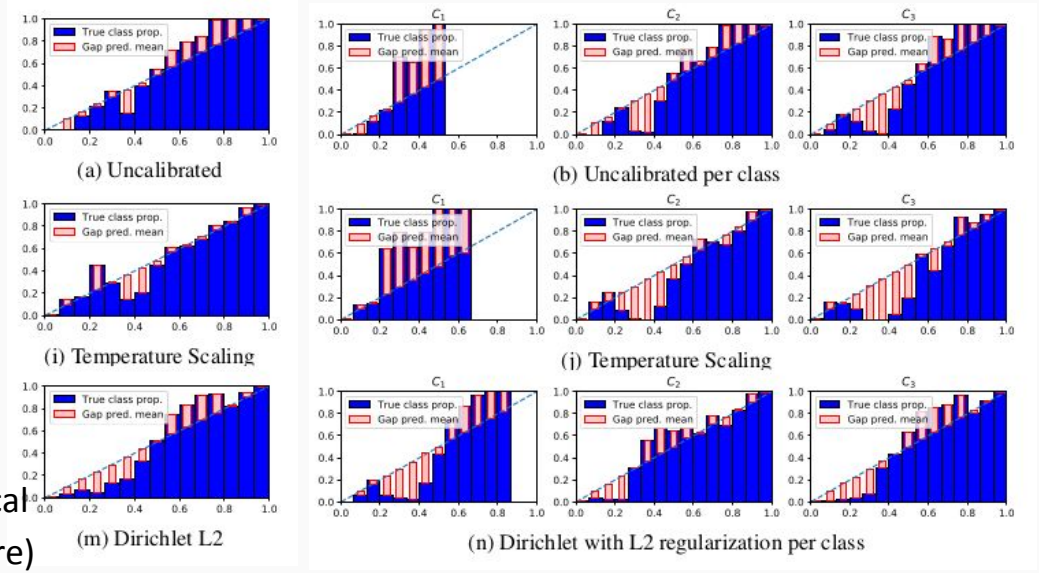
$$\text{classwise}-\text{ECE} = \frac{1}{k} \sum_{j=1}^{k} \sum_{i=1}^{m} \frac{|B_{i,j}|}{n} |y_j(B_{i,j}) - \hat{p}_j(B_{i,j})|$$

Every proper loss is minimised by the canonical calibration function (eg. log-loss and Brier score)

Confidence Calibration Error

Calibration Error Per class

Class 1 Class 2 Class 3



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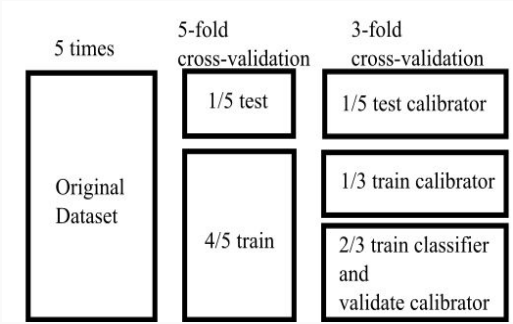
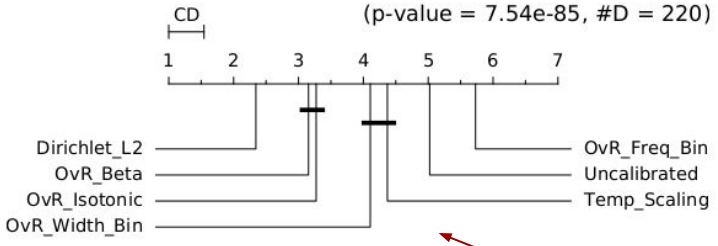
Non-neural Experiments: Settings

- 21 datasets and 11 classifiers = 231 settings
  - Logistic, nbayes, forest, adas, lda, qda, tree, knn, mlp, svc-linear, svc-rbf
- 8 calibration methods (for each of the 231 settings):
  - OvR_Isotonic, OvR_Width_Bin, OvR_Freq_Bin, OvR_Beta, Temp_Scaling, Vect_Scaling, Dirichlet_L2, Dirichlet_ODIR
- 8 evaluation measures
- 5 times 5-fold-crossval.
  - Inner 3-fold-crossval.

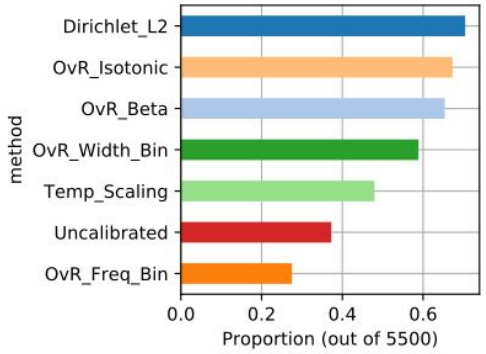


dataset	n_samples	n_features	n_classes
abalone	4177	8	3
balance-scale	625	4	3
car	1728	6	4
cleveland	297	13	5
dermatology	358	34	6
glass	214	9	6
iris	150	4	3
landsat-satellite	6435	36	6
libras-movement	360	90	15
mfeat-karhunen	2000	64	10
mfeat-morphological	2000	6	10
mfeat-zernike	2000	47	10
optdigits	5620	64	10
page-blocks	5473	10	5
pendigits	10992	16	10
segment	2310	19	7
shuttle	101500	9	7
vehicle	846	18	4
vowel	990	10	11
waveform-5000	5000	40	3
yeast	1484	8	10

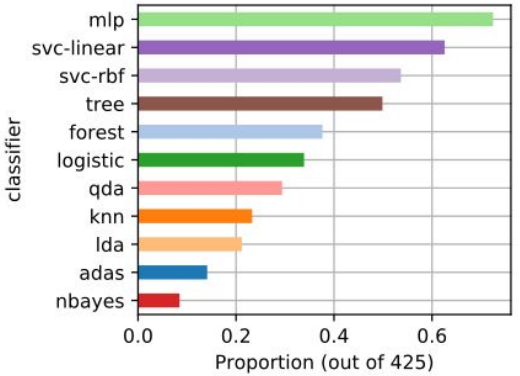
Non-neural Experiments: Results



(a) p-cw-ECE critical difference



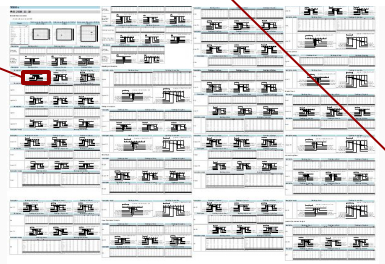
(b) p-cw-ECE for calibrators

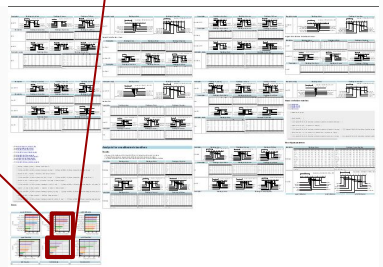


(c) p-cw-ECE for classifiers

These are just 3 figures out of 30 pdf pages of results.

And the 30 pages are only a subset of the generated results.





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Conclusion

1. Dirichlet calibration: New parametric general-purpose multiclass calibration method
    a. Natural extension of the two-class Beta calibration
    b. Easy to implement with multinomial logistic regression on log-transformed class probabilities
2. Our experiments show
    a. Best or tied best performance with 21 datasets x 11 classifiers
    b. Advances state-of-the-art on Neural Networks by introducing ODIR regularisation

For more details check https://dirichletcal.github.io/

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Extra 1: Experimental considerations

- Use random seeds everywhere (models, data partitions, data shuffling)
  - These can be the iteration number
- If comparing two models, train and test in the exact same data partitions
- Use arguments in a user-friendly command-line interface
- Parallelize everything that can be parallelizable (with common sense)
- Store raw results for all executions **before plotting**
- Create a code to summarize all results from raw (csv) files
- Use statistical tests to compare the proposed method

Extra 2: Statistical comparison

- Choose your objective metric based on your problem requirements
  - accuracy, log-loss, mean squared error, expected calibration error…
- Test the compared methods in several scenarios:
  - 21 datasets each one with 11 classifiers = 231 combinations
- Repeat experiments changing dataset partitions and model initializations
  - In my case 5 times 5-fold-cross-validation and inner 3-fold-cross-validation
  - This results in 25 metrics per method that we will use to estimate the expected performance
  - Use the resulting expected values to rank the methods to be compared
- Use the rankings of the compared methods (8) in all combinations (231)
- Use Friedman test statistic to see significance levels between all methods
- Use Bonferroni-Dunn one-tailed statistical test to compute minimum ranking distance to see the Critical Difference Diagram