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

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Notion of Calibration

A probabilistic classifier p^ is:

- Multiclass-calibrated if for any prediction vector $q = (q_1, \ldots, q_k) \in \nabla_k$, proportions of classes

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

- Classwise-calibrated if

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

- Confidence-calibrated if $P\Big(Y = argmax\big(\hat{\mathbf{p}}(X)\big) \;\Big|\; max\big(\hat{\mathbf{p}}(X)\big) = c\Big) = c.$

Evaluation of Calibration

Some empirical measures of calibration are

confidence-ECE (place here equation)

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

Ever proper loss is minimised by the canonical calibration function

P-test versions for conf-ECE and cw-ECE

Temperature Scaling

Temperature scaling proposed by [9] learns a temperature-parameter t > 0 wich decreases (t > 1) or increases (t < 1) the confidence of a model with softmax output.

$$\sigma_{\mathrm{SM}}(\mathbf{z}_i)^{(k)} = \frac{\exp(z_i^{(k)})}{\sum_{j=1}^{K} \exp(z_i^{(j)})}, \quad \hat{p}_i = \max_k \sigma_{\mathrm{SM}}(\mathbf{z}_i)^{(k)}$$

$$\hat{q}_i = \max_k \sigma_{\mathrm{SM}}(\mathbf{z}_i/T)^{(k)}.$$

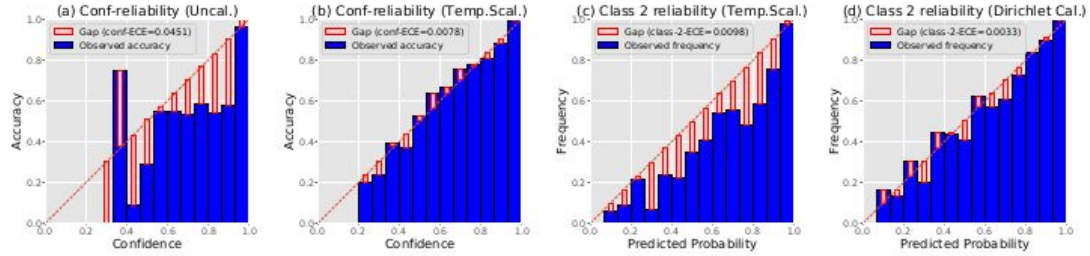

Figure 1: Reliability diagrams of `c10_resnet_wide32` on CIFAR-10: (a) confidence-reliability before calibration; (b) confidence-reliability after temperature scaling; (c) classwise-reliability for class 2 after temperature scaling; (d) classwise-reliability for class 2 after Dirichlet calibration.

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Dirichlet Calibration

We consider the distribution of prediction vectors p^(x) separately on instances of each class, and assume these are Dirichlet distributions with different parameters:

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

generative parametrisation: $\hat{\mu}_{DirGen}(\mathbf{q};\alpha,\pi) = (\pi_1 f_1(\mathbf{q}),\ldots,\pi_k f_k(\mathbf{q}))/z$

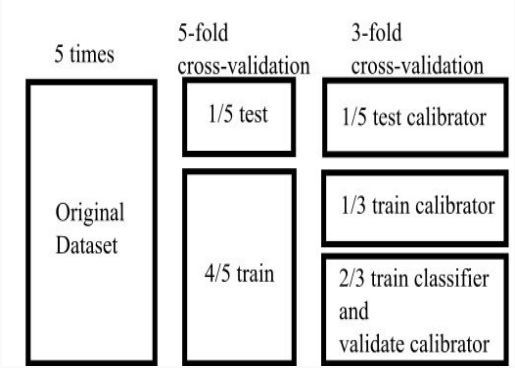
linear parametrisation: $\hat{\mu}_{DirLin}(\mathbf{q};\mathbf{W},\mathbf{b}) = \sigma(\mathbf{W}\ln\mathbf{q}+\mathbf{b})$

canonical parametrisation: $\hat{\mu}_{Dir}(\mathbf{q};\mathbf{A},\mathbf{c}) = \sigma(\mathbf{A}\ln\frac{\mathbf{q}}{1/k}+\ln\mathbf{c})$

All parameterizations are equal, i.e. they contain exactly the same calibration maps.

Experiment non-neural: Setting

- 21 datasets and 11 classifiers = 231 settings
  - Logistic, nbayes, forest, adas, lda, qda, tree, knn, mlp, svc-linear, svc-rbf
- 6 calibration methods:
  - OvR_Isotonic, OvR_Width_Bin, OvR_Freq_Bin, OvR_Beta, Temp_Scaling, Dirichlet_L2
- 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

Experiment non-neural: Results

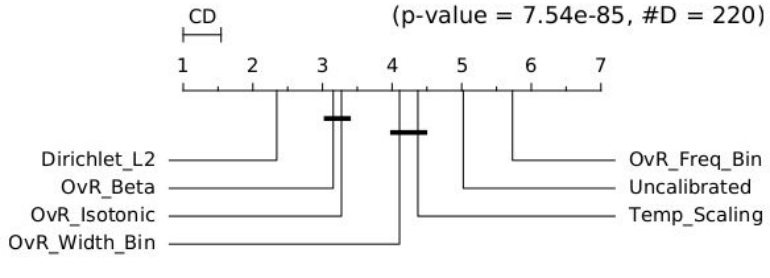
Table 1: Ranking of calibration methods for **p-cw-ECE** (Friedman's test significant with p-value $7.54e^{-85}$).

	DirL2	Beta	FreqB	Isot	WidB	TempS	**Uncal**
adas	**2.4**	3.2	4.1	4.2	3.9	5.0	5.2
forest	3.5	**2.3**	5.7	3.0	3.6	5.0	5.0
knn	2.5	4.0	4.5	**2.1**	3.2	5.8	6.0
lda	**1.9**	3.1	5.8	3.0	3.5	5.0	5.8
logistic	**2.2**	2.8	6.4	3.0	4.2	3.9	5.5
mlp	**2.2**	2.9	6.7	4.0	5.2	3.0	4.1
nbayes	**1.4**	3.6	4.8	2.6	4.2	5.3	6.1
qda	**2.2**	2.8	6.3	2.5	3.8	4.8	5.6
svc-linear	**2.3**	2.7	6.7	3.8	4.0	3.7	4.8
svc-rbf	**2.9**	3.0	6.3	3.5	4.1	3.9	4.3
tree	**2.4**	4.3	5.9	4.2	5.2	3.0	3.0
avg rank	**2.34**	3.15	5.73	3.27	4.11	4.37	5.02

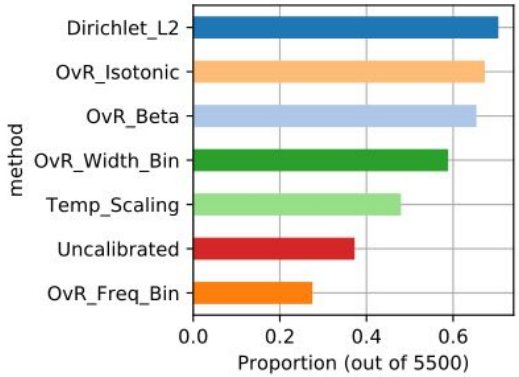
Table 2: Ranking of calibration methods for **log-loss** (p-value $4.39e^{-77}$).

DirL2	Beta	FreqB	Isot	WidB	TempS	**Uncal**
1.4	3.1	3.2	4.3	3.5	5.9	6.6
4.2	**1.9**	4.7	4.1	2.9	5.2	5.2
3.8	4.8	3.0	**1.6**	2.0	6.5	6.5
1.6	2.2	5.2	5.2	3.5	4.6	5.7
1.3	2.1	5.8	6.1	3.5	3.6	5.6
2.2	2.3	6.5	6.2	4.7	2.9	3.4
1.1	3.4	3.4	4.0	4.4	5.5	6.3
1.7	2.7	5.6	4.6	3.4	4.2	5.8
1.3	2.3	6.1	6.1	4.3	3.0	4.8
2.6	**2.2**	4.3	4.8	4.5	4.0	5.6
3.9	5.1	3.4	**2.1**	2.4	5.6	5.6
2.25	2.92	4.66	4.48	3.54	4.61	5.54

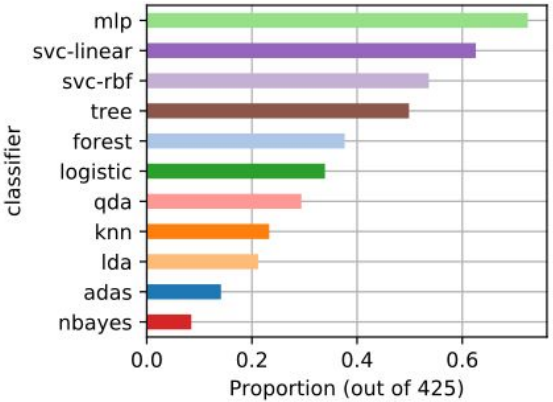
Experiment non-neural: Results



(a) p-cw-ECE critical difference



(b) p-cw-ECE for calibrators



(c) p-cw-ECE for classifiers

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Experiment Deep Neural Networks: Setting

- 3 datasets
  - CIFAR-10, CIFAR-100, SVHN
- 11 convolutional NNs
  - ResNet 110, ResNet 110 SD, ResNet 152 SD, WideNet 32, LeNet 5
- 3 pretrained CNNs
- 5 calibration methods:
  - TempS, Dir-L2, Dir-ODIR, VecS, MS-ODIR
- 8 evaluation measures
- 5-fold-crossval.
  - Optimal regularisation parameters

Experiment Deep Neural Networks: Results

Table 3: Scores and ranking of calibration methods for **cw-ECE**.

		general-purpose calibrators			calibrators using logits	
	Uncal	TempS	Dir-L2	Dir-ODIR	VecS	MS-ODIR
c10_convnet	0.104_6	0.044_4	0.043_2	0.045_5	$\mathbf{0.043_1}$	0.044_3
c10_densenet40	0.114_6	0.040_5	$\mathbf{0.034_1}$	0.037_4	0.036_2	0.037_3
c10_lenet5	0.198_6	0.171_5	$\mathbf{0.052_1}$	0.059_4	0.057_2	0.059_3
c10_resnet110	0.098_6	0.043_5	$\mathbf{0.032_1}$	0.039_4	0.037_3	0.036_2
c10_resnet110_SD	0.086_6	0.031_4	0.031_5	0.029_3	0.027_2	$\mathbf{0.027_1}$
c10_resnet_wide32	0.095_6	0.048_5	0.032_3	0.029_2	0.032_4	$\mathbf{0.029_1}$
c100_convnet	0.424_6	$\mathbf{0.227_1}$	0.402_5	0.240_3	0.241_4	0.240_2
c100_densenet40	0.470_6	0.187_2	0.330_5	$\mathbf{0.186_1}$	0.189_3	0.191_4
c100_lenet5	0.473_6	0.385_5	0.219_4	0.213_2	$\mathbf{0.203_1}$	0.214_3
c100_resnet110	0.416_6	0.201_3	0.359_5	$\mathbf{0.186_1}$	0.194_2	0.203_4
c100_resnet110_SD	0.375_6	0.203_4	0.373_5	0.189_3	$\mathbf{0.170_1}$	0.186_2
c100_resnet_wide32	0.420_6	0.186_4	0.333_5	0.180_2	$\mathbf{0.171_1}$	0.180_3
SVHN_convnet	0.159_6	0.038_4	0.043_5	0.026_2	$\mathbf{0.025_1}$	0.027_3
SVHN_resnet152_SD	0.019_2	$\mathbf{0.018_1}$	0.022_6	0.020_3	0.021_5	0.021_4
Average rank	5.71	3.71	3.79	2.79	2.29	2.71

Table 4: Scores and ranking of calibration methods for **log-loss**.

		general-purpose calibrators			calibrators using logits	
	Uncal	TempS	Dir-L2	Dir-ODIR	VecS	MS-ODIR
c10_convnet	0.391_6	$\mathbf{0.195_1}$	0.197_4	0.195_2	0.197_5	0.196_3
c10_densenet40	0.428_6	0.225_5	$\mathbf{0.220_1}$	0.224_4	0.223_3	0.222_2
c10_lenet5	0.823_6	0.800_5	0.744_2	0.744_3	0.747_4	$\mathbf{0.743_1}$
c10_resnet110	0.358_6	0.209_5	$\mathbf{0.203_1}$	0.205_3	0.206_4	0.204_2
c10_resnet110_SD	0.303_6	0.178_5	0.177_4	0.176_3	0.175_2	$\mathbf{0.175_1}$
c10_resnet_wide32	0.382_6	0.191_5	0.185_4	0.182_2	0.183_3	$\mathbf{0.182_1}$
c100_convnet	1.641_6	$\mathbf{0.942_1}$	1.189_5	0.961_2	0.964_4	0.961_3
c100_densenet40	2.017_6	1.057_2	1.253_5	1.059_4	1.058_3	$\mathbf{1.051_1}$
c100_lenet5	2.784_6	2.650_5	2.595_4	2.490_2	2.516_3	$\mathbf{2.487_1}$
c100_resnet110	1.694_6	1.092_3	1.212_5	1.096_4	1.089_2	$\mathbf{1.074_1}$
c100_resnet110_SD	1.353_6	0.942_3	1.198_5	0.945_4	$\mathbf{0.923_1}$	0.927_2
c100_resnet_wide32	1.802_6	0.945_3	1.087_5	0.953_4	0.937_2	$\mathbf{0.933_1}$
SVHN_convnet	0.205_6	0.151_5	0.142_3	0.138_2	0.144_4	$\mathbf{0.138_1}$
SVHN_resnet152_SD	0.085_6	$\mathbf{0.079_1}$	0.085_5	0.080_2	0.081_4	0.081_3
Average rank	6.0	3.5	3.79	2.93	3.14	1.64

Conclusion

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

Future work

1. Which neural architectures and training methods have temperature scaling as a canonical calibration function
2. Use other distributions of the exponential family
3. Investigate scores coming from mixtures of distributions per class

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

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