On Calibration of Modern **Neural Networks**

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Presented by Lukas Fluri

Introduction

VERY DEEP CONVO

Deep Networks with Stochastic Depth

Deen Regid

Densely Connected Convolutional Networks

New state of the art results
For CIFAR 10/10+/100/100+

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Under certain assumptions

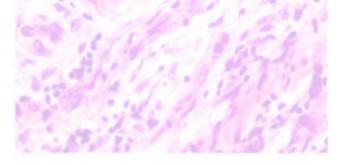
As of 2020

Introduction

Neural networks must not only be accurate, they must also provide a reliable estimation about how confident they are about the prediction!

Cancer detection

Survey: [Daoud Artif. Intell. Med. 2019]



Overview

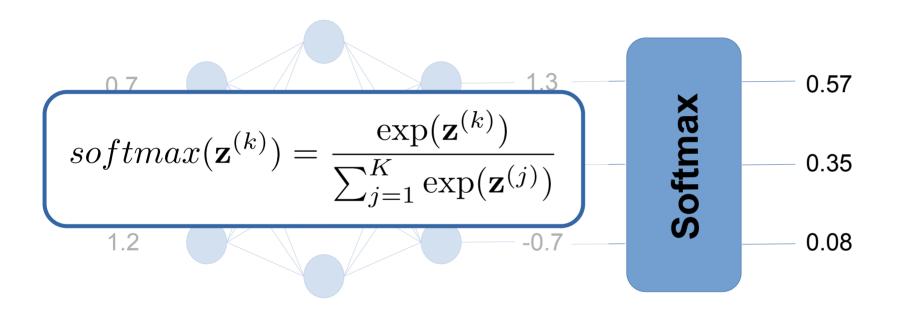
- Introduction: It's important for neural networks to be well-calibrated.
- **Definition**: How to measure model calibration?

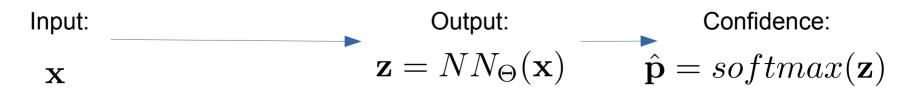
- Problem: Modern neural networks are no longer calibrated!
- Analysis: Which factors might influence model calibration?

Mitigation: How to calibrate neural networks?

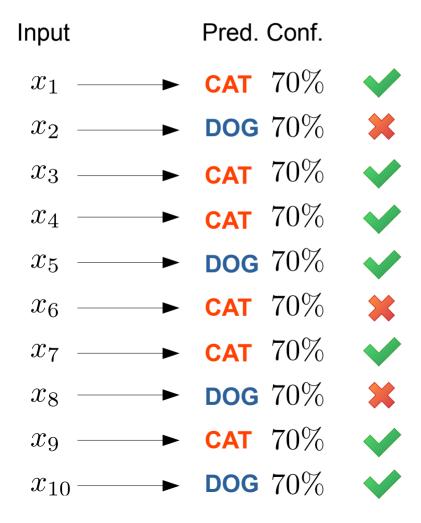
• Experiments: Which calibration methods perform best?

How to create confidence estimates





How to interpret calibration



Different sources of error

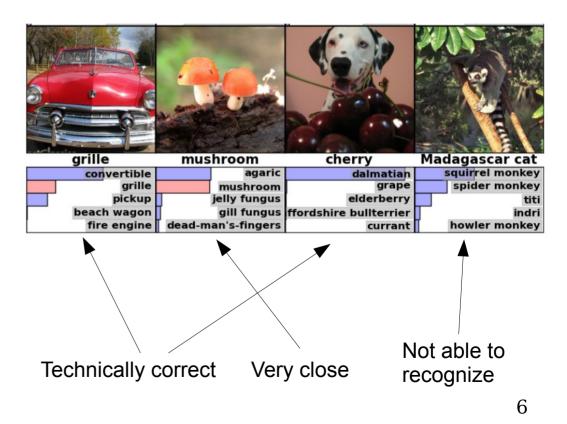
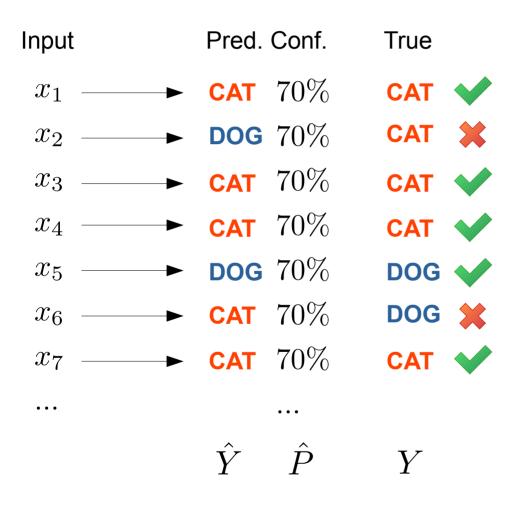


Image source: Krizhevsky et al. "ImageNet Classification...", 2012



Perfect calibration

A neural network has perfect calibration if for all $p \in [0,1]$:

$$\mathbb{P}\left(\hat{Y} = Y | \hat{P} = p\right) = p$$

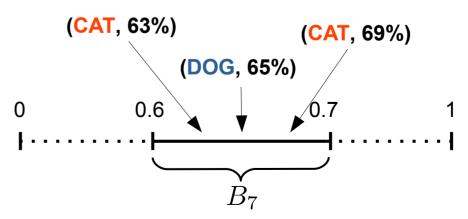
• Perfect calibration:
$$\mathbb{P}\left(\hat{Y}=Y|\hat{P}=p\right) = p \quad \forall p \in [0,1]$$

• Model calibration:
$$\mathbb{E}\left[\left|\mathbb{P}\left(\hat{Y}=Y|\hat{P}=p\right)-p\right|
ight]$$

Problem: In practice we only have finite data! We need to approximate the model calibration

- Expected Calibration Error (ECE):
 - 1. Train neural network on training data
 - 2. Create predictions and confidence estimates using the test data
 - 3. Group the predictions into M bins. Define bin B_m to be the set of all predictions (\hat{y}_i, \hat{p}_i) for which it holds that

$$\hat{p_i} \in \left(\frac{m-1}{M}, \frac{m}{M}\right]$$



- Expected Calibration Error (ECE):
 - 4. Compute the accuracy and confidence of bin B_m as:

$$acc(B_m) = \frac{1}{|B_m|} \sum_{i \in B_m} \mathbf{1}(\hat{y}_i = y_i)$$
 $conf(B_m) = \frac{1}{|B_m|} \sum_{i \in B_m} \hat{p}_i$

5. Compute the expected calibration error as:

$$ECE = \sum_{m=1}^{M} \frac{|B_m|}{n} |acc(B_m) - conf(B_m)|$$

• Perfect calibration:
$$\mathbb{P}\left(\hat{Y}=Y|\hat{P}=p\right) = p \quad \forall p \in [0,1]$$
 • Model calibration:
$$\mathbb{E}\left[\left|\mathbb{P}\left(\hat{Y}=Y|\hat{P}=p\right)-p\right|\right]$$

- **Expected Calibration Error:**

Finite approximation

$$ECE = \sum_{m=1}^{M} \frac{|B_m|}{n} |acc(B_m) - conf(B_m)|$$

Expected Calibration Error:

$$ECE = \sum_{m=1}^{M} \frac{|B_m|}{n} |acc(B_m) - conf(B_m)|$$

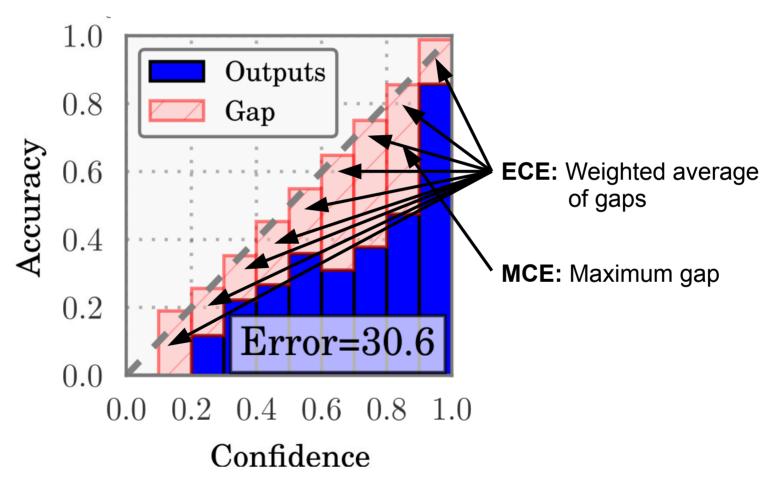
Computes weighted average of mis-calibration

Maximum Calibration Error: Useful for high risk applications

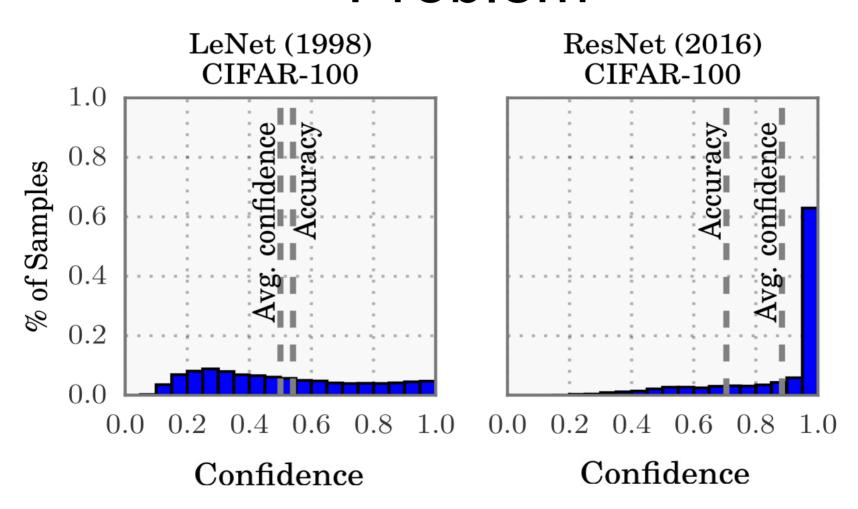
$$MCE = \max_{m \in \{1, \dots, M\}} |acc(B_m) - conf(B_m)|$$

Computes maximum mis-calibration

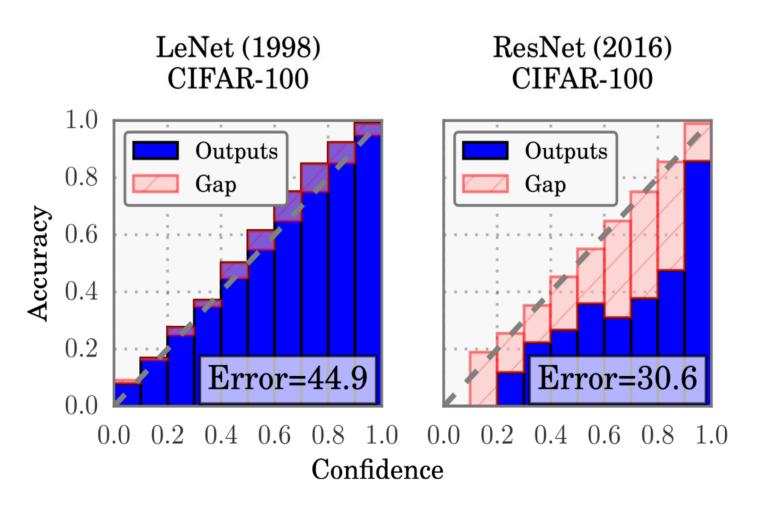
Reliability Diagram



Problem



Problem



Goal

 Understand why neural networks have become miscalibrated

2) Identify and compare methods to alleviate this problem

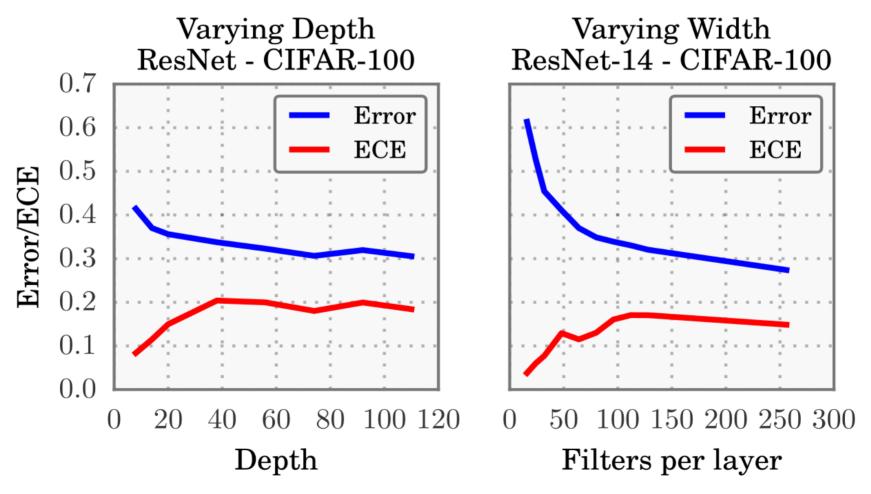
Overview

- Introduction: It's important for neural networks to be well-calibrated.
- **Definition**: How to measure model calibration?
 - ECE, MCE, Reliability diagrams
- Problem: Modern neural networks are no longer calibrated!
- Analysis: Which factors might influence model calibration?

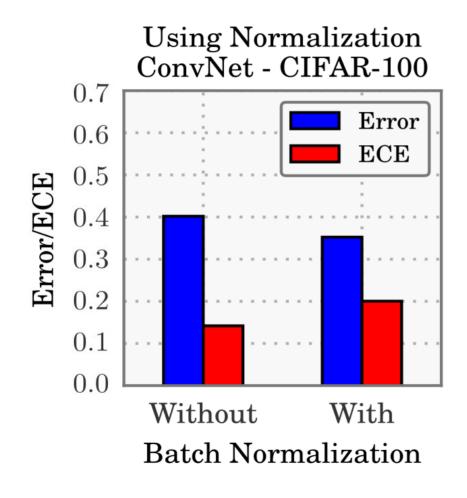
Mitigation: How to calibrate neural networks?

• Experiments: Which calibration methods perform best?

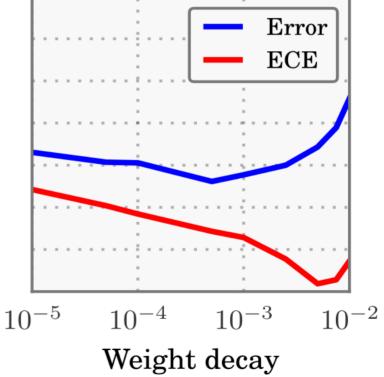
1. Model capacity: Depth & Width of network



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- 2. Batch normalization
- 3. Weight decay

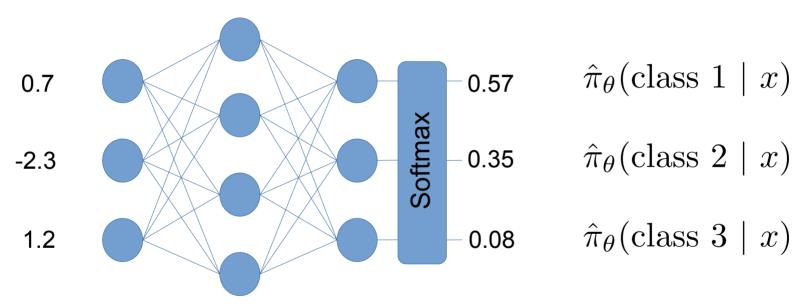


Varying Weight Decay ResNet-110 - CIFAR-100



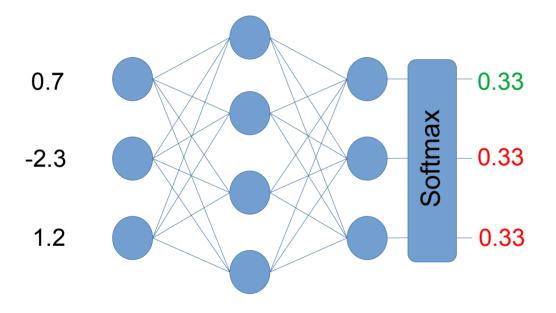
- 1. Model capacity: Depth & Width of network
- 2. Batch normalization
- 3. Weight decay
- 4. Training using negative log-likelihood / cross-entropy loss

Training using negative log-likelihood / cross-entropy loss



$$NLL(\theta) = \arg\max_{\theta} \prod_{i=1}^{n} \hat{\pi}_{\theta}(y_i \mid x_i) = \arg\min_{\theta} - \sum_{i=1}^{n} \log(\hat{\pi}_{\theta}(y_i \mid x_i))$$

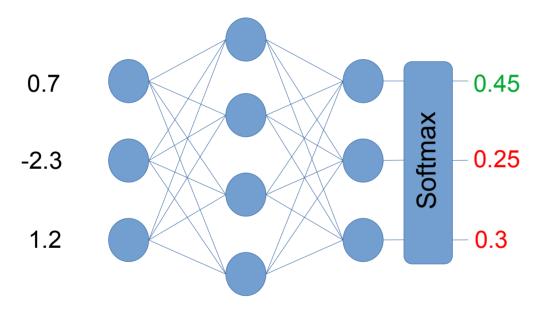
Training using negative log-likelihood / cross-entropy loss



How to minimize NLL:

$$NLL(\theta) = \arg\max_{\theta} \prod_{i=1}^{n} \hat{\pi}_{\theta}(y_i \mid x_i) = \arg\min_{\theta} - \sum_{i=1}^{n} \log(\hat{\pi}_{\theta}(y_i \mid x_i))$$

Training using negative log-likelihood / cross-entropy loss



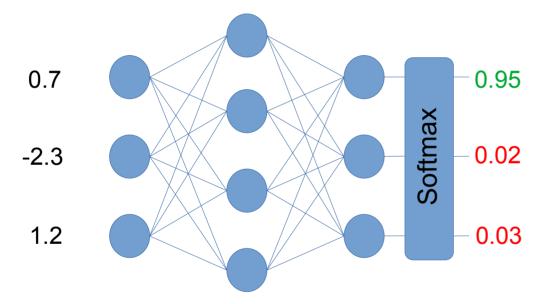
How to minimize NLL:

1) Predict the correct classes:

$$\hat{\pi}_{\theta}(y_i \mid x_i) \geq \hat{\pi}_{\theta}(y' \mid x_i) \quad \forall y' \in \mathcal{Y}$$

$$NLL(\theta) = \arg \max_{\theta} \prod_{i=1}^{n} \hat{\pi}_{\theta}(y_i \mid x_i) = \arg \min_{\theta} - \sum_{i=1}^{n} \log(\hat{\pi}_{\theta}(y_i \mid x_i))$$

Training using negative log-likelihood / cross-entropy loss

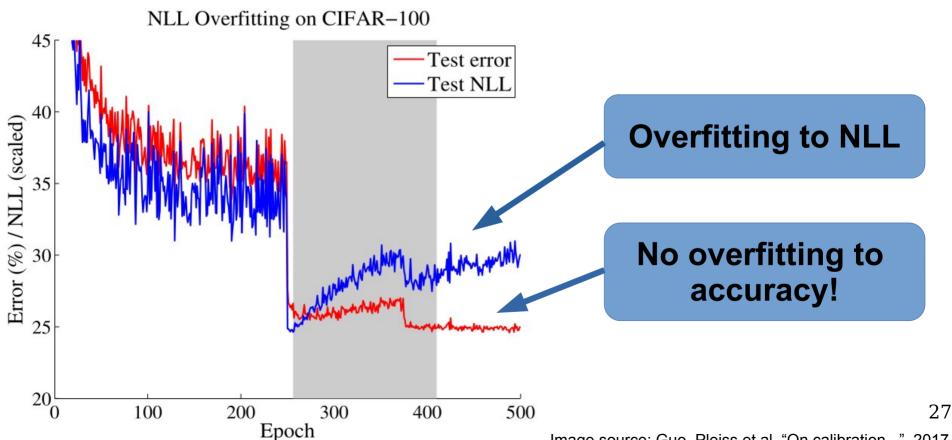


How to minimize NLL:

- 1) Predict the correct classes: $\hat{\pi}_{\theta}(y_i \mid x_i) \geq \hat{\pi}_{\theta}(y' \mid x_i) \quad \forall y' \in \mathcal{Y}$
- 2) Increase confidence in correct classes!

$$NLL(\theta) = \arg\max_{\theta} \prod_{i=1}^{n} \hat{\pi}_{\theta}(y_i \mid x_i) = \arg\max_{\theta} \mathbf{Overfitting to NLL!}$$

Training using negative log-likelihood / cross-entropy loss

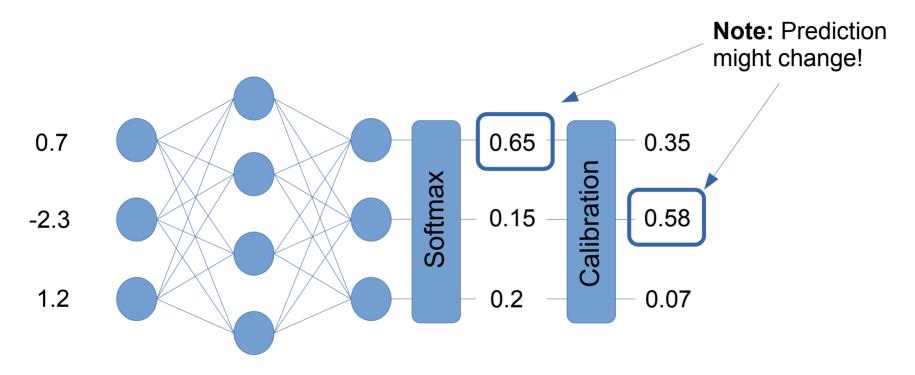


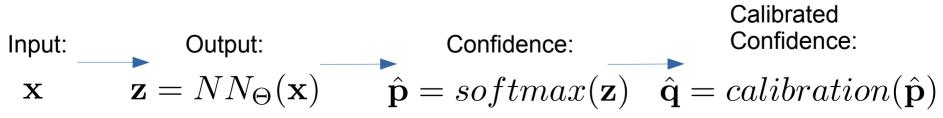
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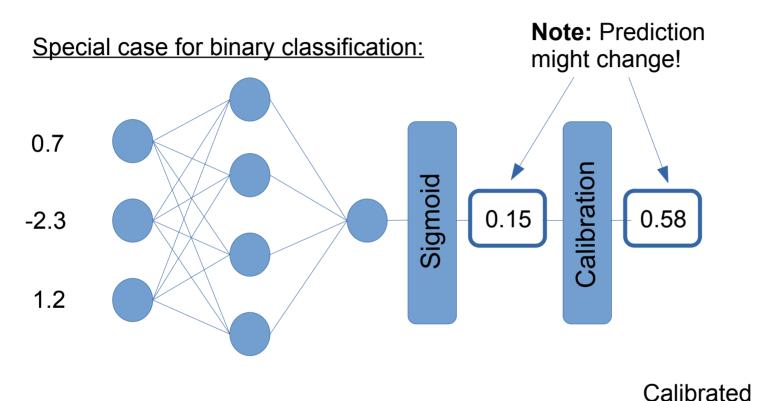
Experiments: Which calibration methods perform best?

Calibration of neural networks





Calibration of neural networks



Input: Output: Confidence: Confidence: $\hat{\mathbf{x}} = NN_{\Theta}(\mathbf{x})$ $\hat{\mathbf{p}} = \sigma(\mathbf{z})$ $\hat{\mathbf{q}} = calibration(\hat{\mathbf{p}})$

Histogram Binning

[Zadrozny et al. ICML 2001]

1. Group the predictions into M bins. Define bin B_m to be the set of all predictions (\hat{y}_i, \hat{p}_i) for which it holds that:

$$\hat{p_i} \in \left(\frac{m-1}{M}, \frac{m}{M}\right]$$

2. For all predictions in bin B_m output the probability θ_m

(63%) (65%) 0.6 0.7 1

3. For each bin B_m find θ_m which minimizes

$$\sum_{y_i: \hat{p}_i \in B_m} (y_i - \theta_m)^2$$

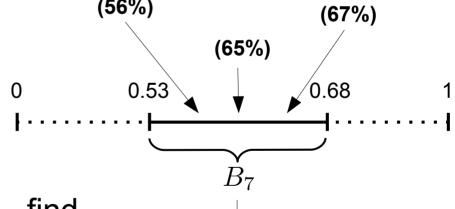
Isotonic Regression

[Zadrozny et al. KDD 2002]

1. Group the predictions into M bins. Define bin B_m to be the set of all predictions (\hat{y}_i, \hat{p}_i) for which it holds that:

$$\hat{p_i} \in \left(\frac{m-1}{M}, \frac{m}{M}\right]$$

2. For all predictions in bin $\,B_m\,$ 0 output the probability θ_m



3. For each bin $B_m = (a_m, a_{m+1}]$ which minimize

$$\sum_{y_i:\hat{p}_i\in B_m} (y_i - \theta_m)^2 \qquad \theta_7 = 55\%$$

$$\theta_7 = 55\%$$

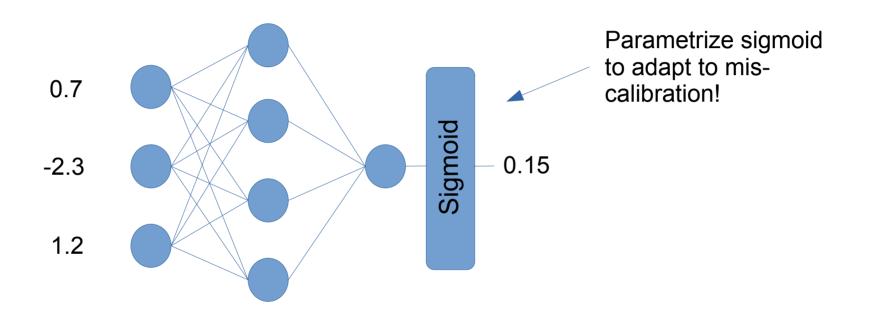
Bayesian Binning into Quantiles (BBQ) [Naeini et al. AAAI 2015]

- Look at all possible binning schemes at the same time!
- For a given validation set \mathcal{D} let \mathcal{S} be the set of all possible binning schemes for this data set.
- Previous models: Fix one principles and compute optimal parameters θ for each data sample Sum over all binning schemes θ for each f how probable the model f is given the data f
- Bayesian Binning into Quantiles:

$$\hat{q}_i = \mathbb{P}(y_i = 1 \mid \hat{p}_i) = \sum_{s \in \mathcal{S}} \mathbb{P}(y_i = 1 \mid \hat{p}_i, S = s, \mathcal{D}) \cdot \mathbb{P}(S = s \mid \mathcal{D})$$

Platt scaling

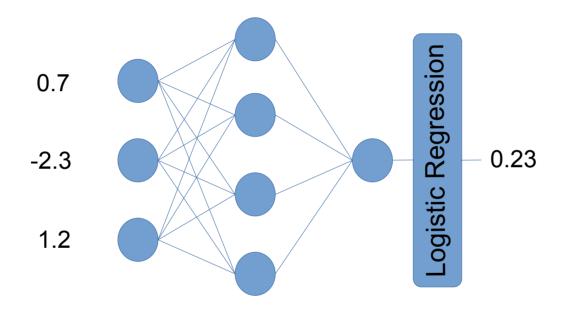
[Platt et al. Advances in large margin classifiers 1999]



Input: Output: Confidence:
$$\mathbf{x} \qquad \mathbf{z} = NN_{\Theta}(\mathbf{x}) \qquad \hat{\mathbf{p}} = \sigma(\mathbf{z})$$

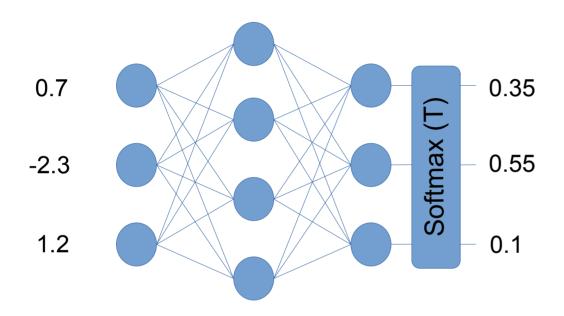
Platt scaling

[Platt et al. Advances in large margin classifiers 1999]



Input: Output: Confidence:
$$\mathbf{x} \quad \mathbf{z} = NN_{\Theta}(\mathbf{x}) \quad \hat{\mathbf{q}} = \sigma(a \cdot \mathbf{z} + b) \quad a, b \in \mathbb{R}$$

Temperature scaling

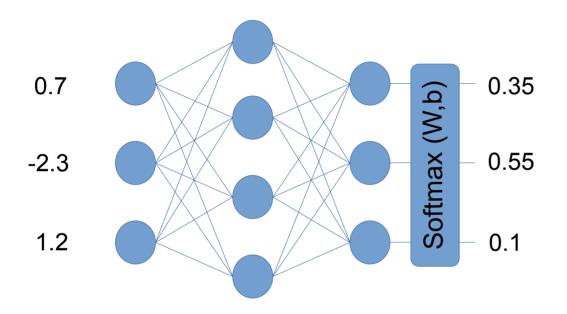


Temperature scaling

- Number of parameters is constant!
- This method doesn't change the predictions! => Accuracy stays the same
- Very easy to implement
- Fast to compute

Input: Output: Confidence:
$$\mathbf{x} \quad \mathbf{z} = NN_{\Theta}(\mathbf{x}) \quad \hat{\mathbf{q}} = softmax(\mathbf{z}/T) \qquad T \in \mathbb{R}$$

Matrix and Vector scaling



Matrix scaling

- No restrictions on W
- Number of parameters grows quadratically!

Vector scaling

- Restrict W to be a diagonal matrix
- Number of parameters grows linearly

Input: Output: Confidence:
$$\mathbf{x} = NN_{\Theta}(\mathbf{x}) \qquad \hat{\mathbf{q}} = softmax(\mathbf{W} \cdot \mathbf{z} + \mathbf{b}) \qquad \mathbf{b} \in \mathbb{R}^{k \times k}$$

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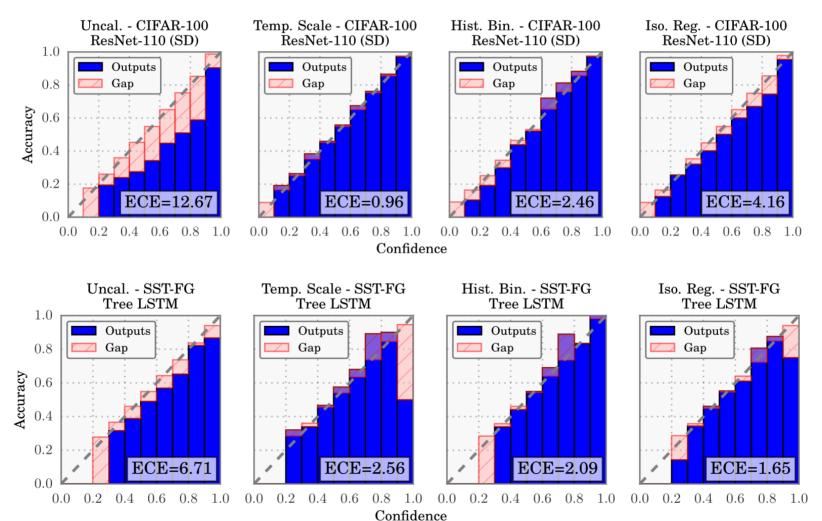
Experiments: Results ECE

| Dataset | Model | Uncalibrated | Hist. Binning | Isotonic | BBQ | Temp. Scaling | Vector Scaling | Matrix Scaling |
|------------------|-----------------|--------------|---------------|----------|-------|---------------|----------------|----------------|
| Birds | ResNet 50 | 9.19% | 4.34% | 5.22% | 4.12% | 1.85% | 3.0% | 21.13% |
| Cars | ResNet 50 | 4.3% | 1.74% | 4.29% | 1.84% | 2.35% | 2.37% | 10.5% |
| CIFAR-10 | ResNet 110 | 4.6% | 0.58% | 0.81% | 0.54% | 0.83% | 0.88% | 1.0% |
| | | | | | | | | |
| CIFAR-10 | ResNet 110 (SD) | 4.12% | 0.67% | 1.11% | 0.9% | 0.6% | 0.64% | 0.72% |
| CIFAR-10 | Wide ResNet 32 | 4.52% | 0.72% | 1.08% | 0.74% | 0.54% | 0.6% | 0.72% |
| CIFAR-10 | DenseNet 40 | 3.28% | 0.44% | 0.61% | 0.81% | 0.33% | 0.41% | 0.41% |
| CIFAR-10 | LeNet 5 | 3.02% | 1.56% | 1.85% | 1.59% | 0.93% | 1.15% | 1.16% |
| CIFAR-100 | ResNet 110 | 16.53% | 2.66% | 4.99% | 5.46% | 1.26% | 1.32% | 25.49% |
| CIFAR-100 | ResNet 110 (SD) | 12.67% | 2.46% | 4.16% | 3.58% | 0.96% | 0.9% | 20.09% |
| CIFAR-100 | Wide ResNet 32 | 15.0% | 3.01% | 5.85% | 5.77% | 2.32% | 2.57% | 24.44% |
| CIFAR-100 | DenseNet 40 | 10.37% | 2.68% | 4.51% | 3.59% | 1.18% | 1.09% | 21.87% |
| CIFAR-100 | LeNet 5 | 4.85% | 6.48% | 2.35% | 3.77% | 2.02% | 2.09% | 13.24% |
| ImageNet | DenseNet 161 | 6.28% | 4.52% | 5.18% | 3.51% | 1.99% | 2.24% | - |
| ImageNet | ResNet 152 | 5.48% | 4.36% | 4.77% | 3.56% | 1.86% | 2.23% | - |
| SVHN | ResNet 152 (SD) | 0.44% | 0.14% | 0.28% | 0.22% | 0.17% | 0.27% | 0.17% |
| 20 News | DAN 3 | 8.02% | 3.6% | 5.52% | 4.98% | 4.11% | 4.61% | 9.1% |
| Reuters | DAN 3 | 0.85% | 1.75% | 1.15% | 0.97% | 0.91% | 0.66% | 1.58% |
| SST Binary | TreeLSTM | 6.63% | 1.93% | 1.65% | 2.27% | 1.84% | 1.84% | 1.84% |
| SST Fine Grained | TreeLSTM | 6.71% | 2.09% | 1.65% | 2.61% | 2.56% | 2.98% | 2.39% |

Experiments: Results Error

| Dataset | Model | Uncalibrated | Hist. Binning | Isotonic | BBQ | Temp. Scaling | Vector Scaling | Matrix Scaling |
|------------------|-----------------|--------------|---------------|----------|--------|---------------|----------------|----------------|
| Birds | ResNet 50 | 22.54% | 55.02% | 23.37% | 37.76% | 22.54% | 22.99% | 29.51% |
| Cars | ResNet 50 | 14.28% | 16.24% | 14.9% | 19.25% | 14.28% | 14.15% | 17.98% |
| CIFAR-10 | ResNet 110 | 6.21% | 6.45% | 6.36% | 6.25% | 6.21% | 6.37% | 6.42% |
| CIFAR-10 | ResNet 110 (SD) | 5.64% | 5.59% | 5.62% | 5.55% | 5.64% | 5.62% | 5.69% |
| CIFAR-10 | Wide ResNet 32 | 6.96% | 7.3% | 7.01% | 7.35% | 6.96% | 7.1% | 7.27% |
| CIFAR-10 | DenseNet 40 | 5.91% | 6.12% | 5.96% | 6.0% | 5.91% | 5.96% | 6.0% |
| CIFAR-10 | LeNet 5 | 15.57% | 15.63% | 15.69% | 15.64% | 15.57% | 15.53% | 15.81% |
| CIFAR-100 | ResNet 110 | 27.83% | 34.78% | 28.41% | 28.56% | 27.83% | 27.82% | 38.77% |
| CIFAR-100 | ResNet 110 (SD) | 24.91% | 33.78% | 25.42% | 25.17% | 24.91% | 24.99% | 35.09% |
| CIFAR-100 | Wide ResNet 32 | 28.0% | 34.29% | 28.61% | 29.08% | 28.0% | 28.45% | 37.4% |
| CIFAR-100 | DenseNet 40 | 26.45% | 34.78% | 26.73% | 26.4% | 26.45% | 26.25% | 36.14% |
| CIFAR-100 | LeNet 5 | 44.92% | 54.06% | 45.77% | 46.82% | 44.92% | 45.53% | 52.44% |
| ImageNet | DenseNet 161 | 22.57% | 48.32% | 23.2% | 47.58% | 22.57% | 22.54% | - |
| ImageNet | ResNet 152 | 22.31% | 48.1% | 22.94% | 47.6% | 22.31% | 22.56% | - |
| SVHN | ResNet 152 (SD) | 1.98% | 2.06% | 2.04% | 2.04% | 1.98% | 2.0% | 2.08% |
| 20 News | DAN 3 | 20.06% | 25.12% | 20.29% | 20.81% | 20.06% | 19.89% | 22.0% |
| Reuters | DAN 3 | 2.97% | 7.81% | 3.52% | 3.93% | 2.97% | 2.83% | 3.52% |
| SST Binary | TreeLSTM | 11.81% | 12.08% | 11.75% | 11.26% | 11.81% | 11.81% | 11.81% |
| SST Fine Grained | TreeLSTM | 49.5% | 49.91% | 48.55% | 49.86% | 49.5% | 49.77% | 48.51% |

Results



Overview

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- Experiments: Which calibration methods perform best?
 - Temperature scaling

My Take

- Interesting paper
- Well-written
- More data to show correlation between optimization techniques and ECE would have been appreciated

Takeaways

- Fact: Neural Networks are increasingly used in high risk decision making applications
- Problem: Modern neural networks are miscalibrated
- Solution: Performing Post-processing like for example temperature scaling to adjust confidence estimates helps to mitigate the problem

Appendix

Experiments: Datasets

| Table | Description | # of classes | Train/Validation/Test |
|-------------------------------------|----------------------|--------------|--|
| Caltech-UCSD | Bird images | 200 | 5,994 / 2,897 / 2,897 |
| Stanford Cars | Car images | 196 | 8,041 / 4,020 / 4,020 |
| ImageNet 2012 | Natural scene images | 1000 | 1.3M /25,000 / 25,000 |
| CIFAR-10/CIFAR-100 | Color images | 10 / 100 | 45,000 / 5,000 / 10,000 |
| Street View House Numbers (SVHN) | House number images | 10 | 598,388 / 6,000 / 26,032 |
| 20 News | News articles | 20 | 9,034 / 2,259 / 7,528 |
| Reuters | News articles | 8 | 4,388 / 1,097 / 2,189 |
| Stanford Sentiment Treebank | Movie reviews | 2/5 | 6,920 / 872 / 1,821 544 / 1,101 / 2,210 |

Experiments: Networks

- Image classification tasks:
 - ResNets [He et al. CVPR 2016]
 - ResNets with stochastic depth [Huang et al. ECCV 2016]
 - Wide ResNets [Zagoruyko et al. BMVC 2016]
 - DenseNets [Huang et al. CVPR 2017]
- Document classification tasks:
 - Deep Averaging Networks [lyyer et al. ACL 2015]
 - TreeLSTMs [Tai et al. ACL 2015]

Experiments: Results MCE

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| Cars | ResNet 50 | 41.55% | 5.16% | 15.23% | 9.31% | 20.23% | 8.59% | 29.65% |
| CIFAR-10 | ResNet 110 | 33.78% | 26.87% | 7.8% | 72.64% | 8.56% | 27.39% | 22.89% |
| CIFAR-10 | ResNet 110 (SD) | 34.52% | 17.0% | 16.45% | 19.26% | 15.45% | 15.55% | 10.74% |
| CIFAR-10 | Wide ResNet 32 | 27.97% | 12.19% | 6.19% | 9.22% | 9.11% | 4.43% | 9.65% |
| CIFAR-10 | DenseNet 40 | 22.44% | 7.77% | 19.54% | 14.57% | 4.58% | 3.17% | 4.36% |
| CIFAR-10 | LeNet 5 | 8.02% | 16.49% | 18.34% | 82.35% | 5.14% | 19.39% | 16.89% |
| CIFAR-100 | ResNet 110 | 35.5% | 7.03% | 10.36% | 10.9% | 4.74% | 2.5% | 45.62% |
| CIFAR-100 | ResNet 110 (SD) | 26.42% | 9.12% | 10.95% | 9.12% | 8.85% | 8.85% | 35.6% |
| CIFAR-100 | Wide ResNet 32 | 33.11% | 6.22% | 14.87% | 11.88% | 5.33% | 6.31% | 44.73% |
| CIFAR-100 | DenseNet 40 | 21.52% | 9.36% | 10.59% | 8.67% | 19.4% | 8.82% | 38.64% |
| CIFAR-100 | LeNet 5 | 10.25% | 18.61% | 3.64% | 9.96% | 5.22% | 8.65% | 18.77% |
| ImageNet | DenseNet 161 | 14.07% | 13.14% | 11.57% | 10.96% | 12.29% | 9.61% | - |
| ImageNet | ResNet 152 | 12.2% | 14.57% | 8.74% | 8.85% | 12.29% | 9.61% | - |
| SVHN | ResNet 152 (SD) | 19.36% | 11.16% | 18.67% | 9.09% | 18.05% | 30.78% | 18.76% |
| 20 News | DAN 3 | 17.03% | 10.47% | 9.13% | 6.28% | 8.21% | 8.24% | 17.43% |
| Reuters | DAN 3 | 14.01% | 16.78% | 44.95% | 36.18% | 25.46% | 18.88% | 19.39% |
| SST Binary | TreeLSTM | 21.66% | 3.22% | 13.91% | 36.43% | 6.03% | 6.03% | 6.03% |
| SST Fine Grained | TreeLSTM | 27.85% | 28.35% | 19.0% | 8.67% | 44.75% | 11.47% | 11.78% |

Paper Impact

On calibration of modern neural networks

C Guo, G Pleiss, Y Sun... - ... Conference on Machine ..., 2017 - proceedings.mlr.press Confidence calibration—the problem of predicting probability estimates representative of the true correctness likelihood—is important for classification models in many applications. We discover that modern neural networks, unlike those from a decade ago, are poorly calibrated. Through extensive experiments, we observe that depth, width, weight decay, and Batch Normalization are important factors influencing calibration. We evaluate the performance of various post-processing calibration methods on state-of-the-art architectures ...

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Paper impact

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- Learning Confidence for Out-of-Distribution Detection in Neural Networks: https://arxiv.org/pdf/1802.04865.pdf
- Deep anomaly detection with outlier exposure: https://arxiv.org/pdf/1812.04606.pdf
- Why ReLU networks yield high-confidence predictions far away fromthe training data and how to mitigate the problem:
 https://openaccess.thecvf.com/content_CVPR_2019/papers/Hein_Why_ReLU_Networks_Yield_High-Confidence_Predictions_Far_Away_From_the_CVPR_2019_paper.pdf

Application of paper:

- A Clinically Applicable Approach to Continuous Prediction of Future Acute Kidney Injury: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC6722431/
- Deep k-Nearest Neighbors: Towards Confident,Interpretable and Robust Deep Learning: https://arxiv.org/pdf/1803.04765.pdf?fbclid=lwAR2D5gqQf9SL0xRWBctEVrUCL9uUilf9lZrpPN83YZYbiCGdLAlMlhhaVns

Comparison and Critique:

- Can you trust your model's uncertainty? Evaluating predictive uncertainty under dataset shift: https://arxiv.org/pdf/1906.02530.pdf
- Measuring calibration in deep learning:
 https://openaccess.thecvf.com/content_CVPRW_2019/papers/Uncertainty%20and%20Robustness%20in%20Deep%20Visual%20Learning/Nixon_Measuring_Calibration_in_Deep_Learning_CVPRW_2019_paper.pdf

Calibration and fairness:

- On fairness and calibration: https://arxiv.org/pdf/1709.02012.pdf