Calibrated and Sharp Uncertainties in Deep Learning via Density Estimation

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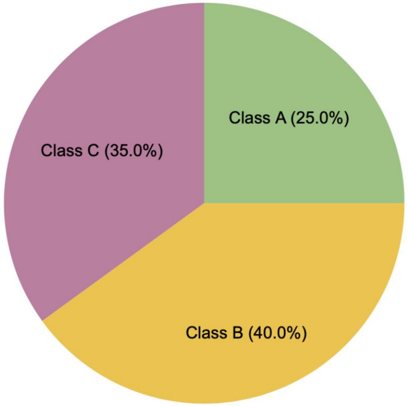
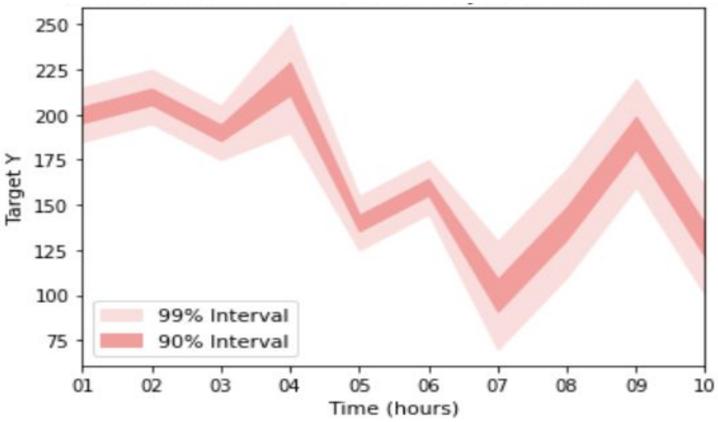
Machine Learning Models Output Probabilistic Predictions



Class membership probabilities



Raw confidence intervals from Bayesian Neural Network

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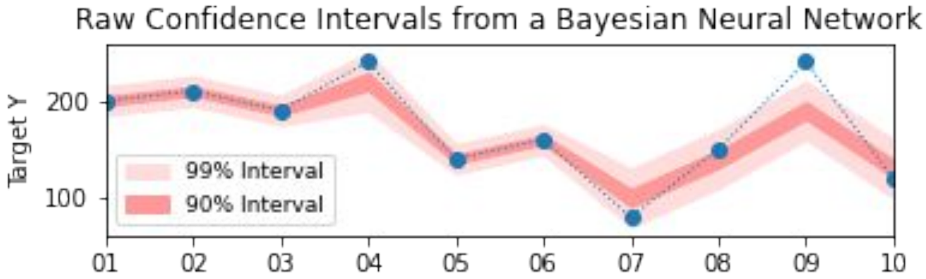
Machine Learning Models Output Probabilistic Predictions

Log-likelihood based training can give inaccurate probabilistic predictions!



Only **half** the points are within **90%** region!

Machine Learning Models Output Probabilistic Predictions

Accurate Probabilistic Forecast

Calibration

90% confidence interval contains the true outcome 90% times

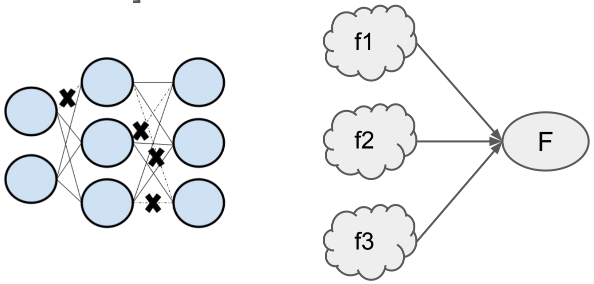
Sharpness

Narrow Confidence Intervals

Gneiting et al, 2007
Gneiting and Raftery, 2005; 2007

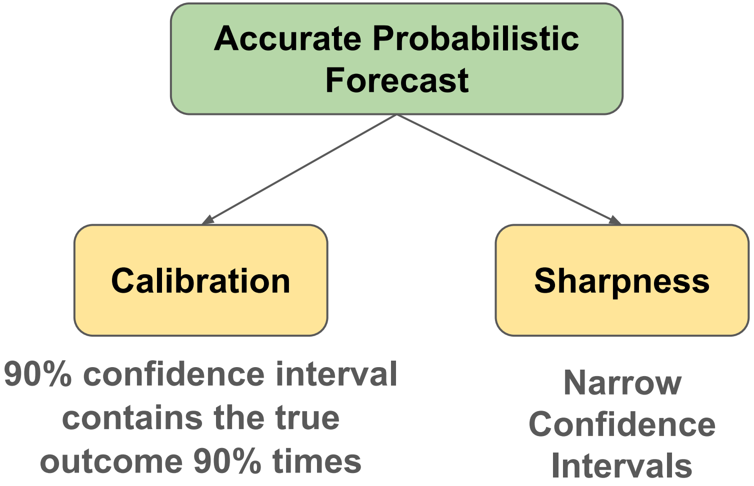
Solutions to improve probabilistic forecasts

- Dropout [Gal & Ghahramani, 2016] or ensembling [Lakshminarayanan et al,, 2017]



- Recalibration [Platt, 1999; Kuleshov et al. 2018; Song et al. 2019]

Calibration of Probabilistic Forecasts

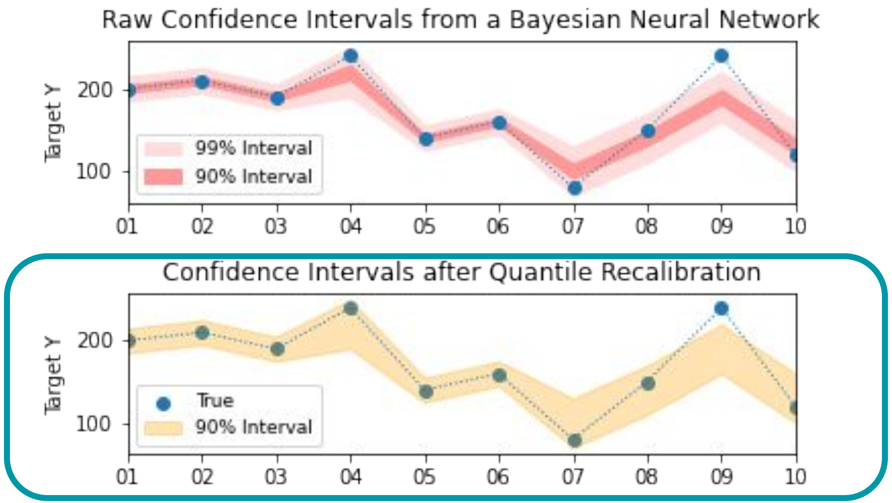


Gneiting et al, 2007
Gneiting and Raftery, 2005; 2007

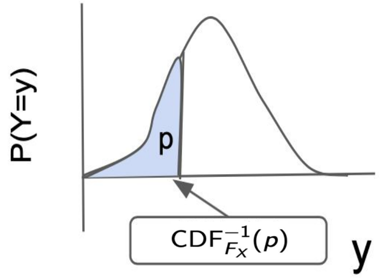
What we do

- **Simpler** techniques to obtain **distribution calibration** that are more broadly applicable
- Reason about uncertainty in terms of **calibration** and **sharpness**
- **Low-dimensional density estimation** to enforce distribution calibration
- **Theoretical analysis** to establish guarantees on calibration and vanishing regret

Quantile Calibration of Probabilistic Forecasts



Quantile Calibration



$$\mathbb{P}(Y \leq \mathrm{CDF}_{F_X}^{-1}(p)) = p \text{ for all } p \in [0,1],$$

9/10 points are within 90% region!

Quantile calibration re-labels 99% interval to 90% interval

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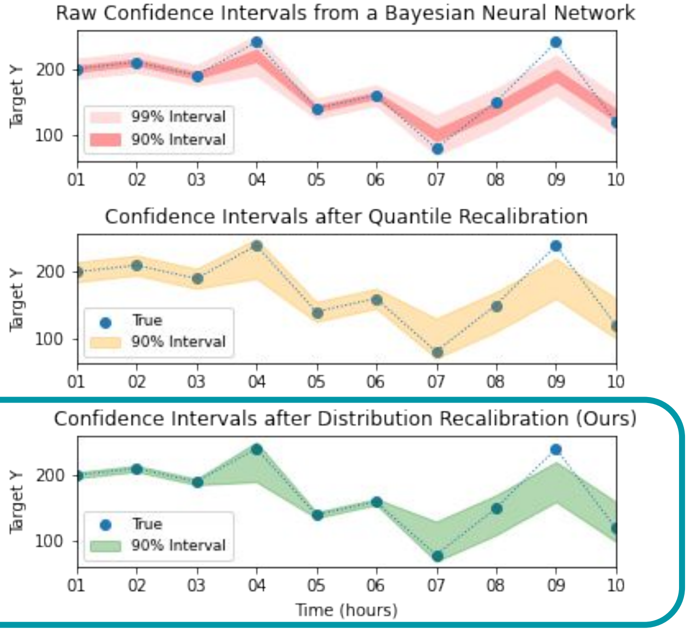
Distribution Calibration of Probabilistic Forecasts

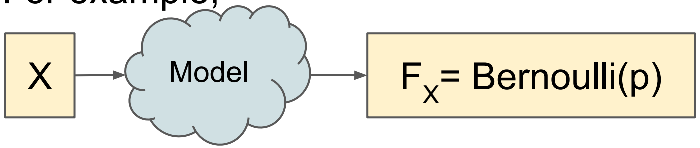


9/10 points are within 90% region and **tighter** confidence intervals after applying distribution calibration

Distribution Calibration

$\mathbb{P}(Y = y \mid F_X = F) = f(y)$ for all $y \in \mathcal{Y}, F \in \Delta_{\mathcal{Y}}$

For example,

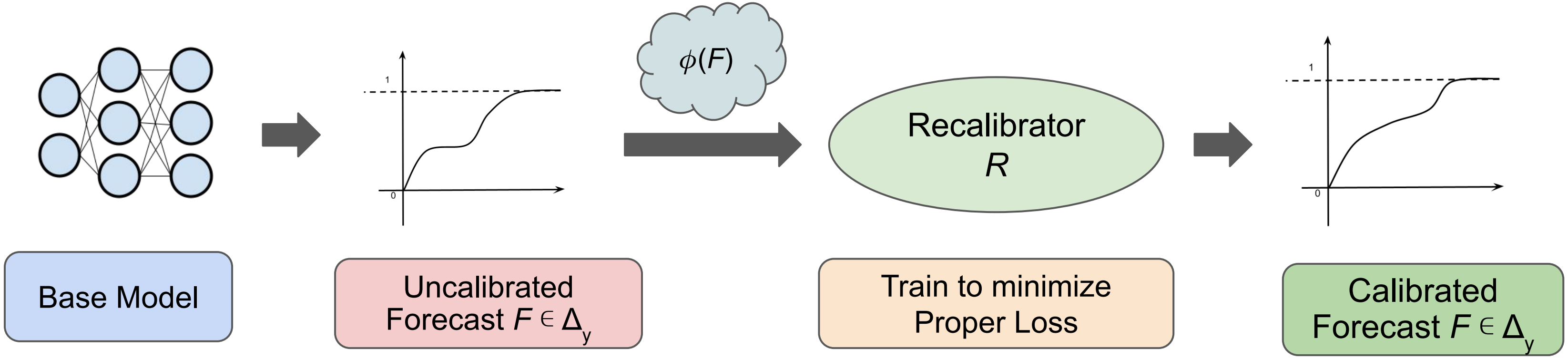


$P(Y=1|F_X=\text{Bern}(p)) = p$

Quantile Calibration

$\mathbb{P}(Y \leq \text{CDF}_{F_X}^{-1}(p)) = p$ for all $p \in [0, 1]$,

Training Distribution Calibrated Models



Recalibration as density estimation

$$R(F) = \mathbb{P}(Y \mid H(X) = F)$$

Challenge 1: Conditioning on *F*
(can be any arbitrary distribution)
Challenge 2: Learning objective for *R*

- Low dimensional density estimation (tractable)
- Proper Loss = **Calibration** - **Sharpness** + Irreducible term
- Quantile function regression when underlying model performs probabilistic regression
- Enforces stronger notion of calibration as compared to quantile calibration by Kuleshov et al. (2018)
- More broadly applicable as compared to distribution calibration by Song at al. (2019)

Theoretical Analysis and Experimental Results

- **Distribution Calibration**
  We prove that we can achieve distribution calibration via density estimation $P(Y| H(X)=F)$

- **Vanishing Regret**:
  We achieve calibration without degrading performance of baseline model (in terms of proper loss)

$$\text{ExpectedLoss}(R \circ H, Y) \leq \text{ExpectedLoss}(H, Y) + \delta_m$$

Experiments: UCI Regression benchmarks and Classification benchmarks
Key results:

- **Calibrated Regression**: Accuracies and uncertainties improve over Kuleshov et al. (2018) and in many cases over Song et al. (2019)
- **Calibrated Classification**: Best uncertainties are obtained via our method (compared with Platt scaling baseline) while accuracies remain similar

We test with a number of neural network base models. Please check our paper for more results!

Conclusions

- Reasoning about uncertainty in machine learning in terms of **calibration** and **sharpness**
- **Simple low-dimensional density estimation** to provably achieve distribution calibration
- Theoretical analysis to establish asymptotically distributionally calibrated forecasts while minimizing regret
- Calibration may be simpler than previously thought. Distribution calibration should be leveraged more broadly across machine learning

Thank you!