Tutorial 4 – Uncertainty & Bayesian Parameter Estimation

CSC2541 Neural Net Training Dynamics – Winter 2022

Slides adapted from CSC2541: Scalable and Flexible Models of Uncertainty – Fall 2017

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Motivation

Why model uncertainty?

- **Confidence calibration:** know how reliable a prediction is (e.g. so it can ask a human for clarification)
- **Regularization:** prevent your model from overfitting
- **Ensembling:** smooth your predictions by averaging them over multiple possible models
- **Model selection:** decide which of multiple plausible models best describes the data
- **Sparsification:** drop connections, encode them with fewer bits
- **Exploration:** decide which training examples are worth labeling (active learning), optimize an expensive black-box function (Bayesian optimization), estimating rewards from multi-armed bandits (reinforcement learning)
- **Robustness:** make good predictions when the data is either naturally perturbed or explicitly modified by an adversary

Bayesian Parameter Estimation: A Toy Example

- Motivating example: estimating the parameter of a biased coin
  - You flip a coin 100 times. It lands heads $N_H = 55$ times and tails $N_T = 45$ times.
  - What is the probability it will come up heads if we flip again?
- Model: observations x_i are independent and identically distributed (i.i.d.) Bernoulli random variables with parameter θ.
- The likelihood function is the probability of the observed data (the entire sequence of H's and T's) as a function of θ:

$$\begin{aligned} L(\theta) = p(\mathcal{D}) &= \prod_{i=1}^{N} \theta^{x_i}(1-\theta)^{1-x_i} \\ &= \theta^{N_H}(1-\theta)^{N_T} \end{aligned}$$

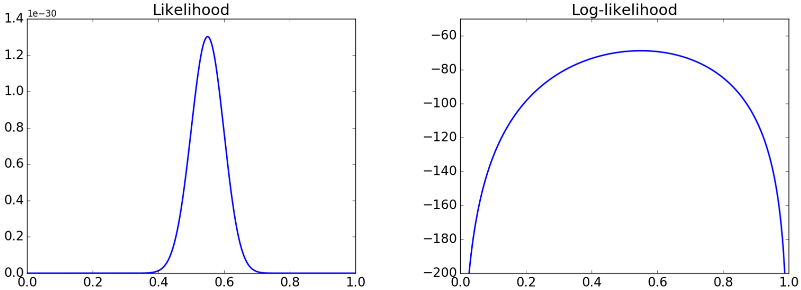
- N_H and N_T are sufficient statistics.

Bayesian Parameter Estimation: A Toy Example

- The likelihood is generally very small, so it's often convenient to work with log-likelihoods.

$$L(\theta) = \theta^{N_H}(1-\theta)^{N_T} \approx 7.9 \times 10^{-31}$$

$$\ell(\theta) = \log L(\theta) = N_H \log\theta + N_T \log(1-\theta) \approx -69.31$$



A Toy Example

- Good values of θ should assign high probability to the observed data. This motivates the maximum likelihood criterion.
- Solve by setting derivatives to zero:

$$\begin{aligned} \frac{\mathrm{d}\ell}{\mathrm{d}\theta} &= \frac{\mathrm{d}}{\mathrm{d}\theta}\left(N_H \log\theta + N_T \log(1-\theta)\right) \\ &= \frac{N_H}{\theta} - \frac{N_T}{1-\theta} \end{aligned}$$

- Setting this to zero gives the maximum likelihood estimate:

$$\hat{\theta}_{\mathrm{ML}} = \frac{N_H}{N_H + N_T},$$

- Normally there's no analytic solution, and we need to solve an optimization problem (e.g. using gradient descent).

Bayesian Parameter Estimation: A Toy Example

- Maximum likelihood has a pitfall: if you have too little data, it can overfit.
- E.g., what if you flip the coin twice and get H both times?

$$\theta_{\mathrm{ML}} = \frac{N_H}{N_H + N_T} = \frac{2}{2+0} = 1$$

- But even a fair coin has 25% chance of showing this result.
- Because it never observed T, it assigns this outcome probability 0. This problem is known as data sparsity.
- If you observe a single T in the test set, the likelihood is $-\infty$.

A Toy Example

- In maximum likelihood, the observations are treated as random variables, but the parameters are not.
- The Bayesian approach treats the parameters as random variables as well.
- To define a Bayesian model, we need to specify two distributions:
  - The prior distribution $p(\boldsymbol{\theta})$, which encodes our beliefs about the parameters *before* we observe the data
  - The likelihood $p(\mathcal{D} \mid \boldsymbol{\theta})$, same as in maximum likelihood
- When we update our beliefs based on the observations, we compute the posterior distribution using Bayes' Rule:

$$p(\boldsymbol{\theta} \mid \mathcal{D}) = \frac{p(\boldsymbol{\theta}) p(\mathcal{D} \mid \boldsymbol{\theta})}{\int p(\boldsymbol{\theta}') p(\mathcal{D} \mid \boldsymbol{\theta}') \, \mathrm{d}\boldsymbol{\theta}'}.$$

- We rarely ever compute the denominator explicitly due to intractability.

Bayesian Parameter Estimation: A Toy Example

- Let's revisit the coin example. We already know the likelihood:

$$L(\theta) = p(\mathcal{D}) = \theta^{N_H}(1-\theta)^{N_T}$$

- It remains to specify the prior $p(\theta)$.
  - We can choose an uninformative prior, which assumes as little as possible. A reasonable choice is the uniform prior.
  - But our experience tells us 0.5 is more likely than 0.99. One particularly useful prior that lets us specify this is the beta distribution:

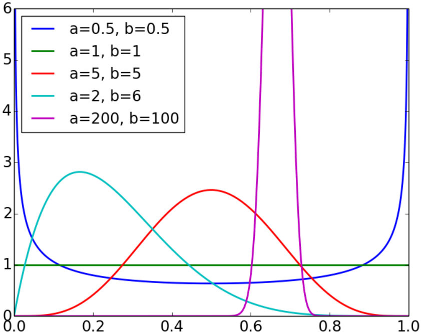
$$p(\theta; a, b) = \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} \theta^{a-1}(1-\theta)^{b-1}.$$

  - This notation for proportionality lets us ignore the normalization constant:

$$p(\theta; a, b) \propto \theta^{a-1}(1-\theta)^{b-1}.$$

Bayesian Parameter Estimation: A Toy Example

Beta distribution for various values of a, b:



- Some observations:
  - The expectation $\mathbb{E}[\theta] = a/(a+b)$.
  - The distribution gets more peaked when a and b are large.
  - The uniform distribution is the special case where $a = b = 1$.
- The main thing the beta distribution is used for is as a prior for the Bernoulli distribution.

Bayesian Parameter Estimation: A Toy Example

- Computing the posterior distribution:

$$\begin{aligned} p(\boldsymbol{\theta} \mid \mathcal{D}) &\propto p(\boldsymbol{\theta}) p(\mathcal{D} \mid \boldsymbol{\theta}) \\ &\propto \left[\theta^{a-1}(1-\theta)^{b-1}\right]\left[\theta^{N_H}(1-\theta)^{N_T}\right] \\ &= \theta^{a-1+N_H}(1-\theta)^{b-1+N_T}. \end{aligned}$$

- This is just a beta distribution with parameters $N_H + a$ and $N_T + b$.
- The posterior expectation of θ is:

$$\mathbb{E}[\theta \mid \mathcal{D}] = \frac{N_H + a}{N_H + N_T + a + b}$$

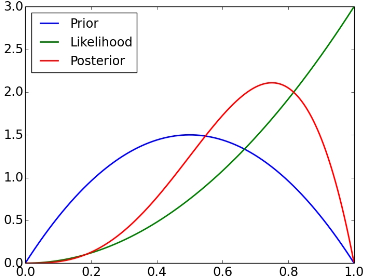
- The parameters a and b of the prior can be thought of as pseudo-counts.
  - The reason this works is that the prior and likelihood have the same functional form. This phenomenon is known as conjugacy, and it's very useful.

Bayesian Parameter Estimation: A Toy Example

Bayesian inference for the coin flip example:

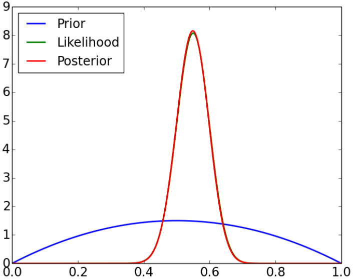
Small data setting

$N_H = 2, \ N_T = 0$



Large data setting

$N_H = 55, \ N_T = 45$



When you have enough observations, the data overwhelm the prior.

Bayesian Parameter Estimation: A Toy Example

- What do we actually do with the posterior?
- The posterior predictive distribution is the distribution over future observables given the past observations. We compute this by marginalizing out the parameter(s):

$$p(\mathcal{D}' \mid \mathcal{D}) = \int p(\boldsymbol{\theta} \mid \mathcal{D}) p(\mathcal{D}' \mid \boldsymbol{\theta}) \, \mathrm{d}\boldsymbol{\theta}. \tag{1}$$

- For the coin flip example:

$$\begin{aligned}
\theta_{\mathrm{pred}} &= \Pr(\mathbf{x}' = H \mid \mathcal{D}) \\
&= \int p(\theta \mid \mathcal{D}) \Pr(\mathbf{x}' = H \mid \theta) \, \mathrm{d}\theta \\
&= \int \mathrm{Beta}(\theta; N_H + a, N_T + b) \cdot \theta \, \mathrm{d}\theta \\
&= \mathbb{E}_{\mathrm{Beta}(\theta; N_H + a, N_T + b)}[\theta] \\
&= \frac{N_H + a}{N_H + N_T + a + b},
\end{aligned} \tag{2}$$

Bayesian Parameter Estimation: A Toy Example

- Maximum a-posteriori (MAP) estimation: find the most likely parameter settings under the posterior
- This converts the Bayesian parameter estimation problem into a maximization problem

$$
\begin{aligned}
\hat{\boldsymbol{\theta}}_{\mathrm{MAP}} &= \arg\max_{\boldsymbol{\theta}} \; p(\boldsymbol{\theta} \,|\, \mathcal{D}) \\
&= \arg\max_{\boldsymbol{\theta}} \; p(\boldsymbol{\theta}, \mathcal{D}) \\
&= \arg\max_{\boldsymbol{\theta}} \; p(\boldsymbol{\theta}) \, p(\mathcal{D} \,|\, \boldsymbol{\theta}) \\
&= \arg\max_{\boldsymbol{\theta}} \; \log p(\boldsymbol{\theta}) + \log p(\mathcal{D} \,|\, \boldsymbol{\theta})
\end{aligned}
$$

Bayesian Parameter Estimation: A Toy Example

- Joint probability in the coin flip example:

$$\begin{aligned}\log p(\theta, \mathcal{D}) &= \log p(\theta) + \log p(\mathcal{D} \,|\, \theta) \\ &= \mathrm{const} + (a-1)\log\theta + (b-1)\log(1-\theta) + N_H \log\theta + N_T \log(1-\theta) \\ &= \mathrm{const} + (N_H + a - 1)\log\theta + (N_T + b - 1)\log(1-\theta)\end{aligned}$$

- Maximize by finding a critical point

$$0 = \frac{\mathrm{d}}{\mathrm{d}\theta} \log p(\theta, \mathcal{D}) = \frac{N_H + a - 1}{\theta} - \frac{N_T + b - 1}{1 - \theta}$$

- Solving for θ,

$$\hat{\theta}_{\mathrm{MAP}} = \frac{N_H + a - 1}{N_H + N_T + a + b - 2}$$

Bayesian Parameter Estimation: A Toy Example

Comparison of estimates in the coin flip example:

	Formula	$N_H = 2, N_T = 0$	$N_H = 55, N_T = 45$
$\hat{\theta}_{\mathrm{ML}}$	$\frac{N_H}{N_H+N_T}$	1	$\frac{55}{100} = 0.55$
θ_{pred}	$\frac{N_H+a}{N_H+N_T+a+b}$	$\frac{4}{6} \approx 0.67$	$\frac{57}{104} \approx 0.548$
$\hat{\theta}_{\mathrm{MAP}}$	$\frac{N_H+a-1}{N_H+N_T+a+b-2}$	$\frac{3}{4} = 0.75$	$\frac{56}{102} \approx 0.549$

How many samples do we need for $\hat{\theta}_{\mathrm{ML}}$ to be a good estimate of θ? Use Hoeffding's Inequality for sampling complexity bound

$$p(|\hat{\theta}_{\mathrm{ML}} - \theta| \geq \varepsilon) \leq 2e^{-2N\varepsilon^2}$$

where $N = N_H + N_T$.

Bayesian Parameter Estimation: A Toy Example

Lessons learned

- Bayesian parameter estimation is more robust to data sparsity.
- Maximum likelihood is about optimization, while Bayesian parameter estimation is about integration.
- The Bayesian solution converges to the maximum likelihood solution as we observe more data.

Linear Regression as Maximum Likelihood

- We can give linear regression a probabilistic interpretation by assuming a Gaussian noise model:

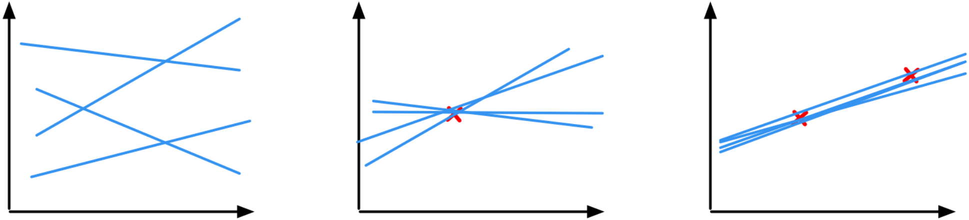
$$t \mid \mathbf{x} \sim \mathcal{N}(\mathbf{w}^\top \mathbf{x} + b,\ \sigma^2)$$

- Linear regression is just maximum likelihood under this model:

$$\begin{aligned}
\frac{1}{N}\sum_{i=1}^{N} \log p(t^{(i)} \mid \mathbf{x}^{(i)}; \mathbf{w}, b) &= \frac{1}{N}\sum_{i=1}^{N} \log \mathcal{N}(t^{(i)}; \mathbf{w}^\top \mathbf{x} + b, \sigma^2) \\
&= \frac{1}{N}\sum_{i=1}^{N} \log \left[\frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(t^{(i)} - \mathbf{w}^\top \mathbf{x} - b)^2}{2\sigma^2} \right) \right] \\
&= \mathrm{const} - \frac{1}{2N\sigma^2} \sum_{i=1}^{N} (t^{(i)} - \mathbf{w}^\top \mathbf{x} - b)^2
\end{aligned}$$

Bayesian Linear Regression

- Bayesian linear regression considers various plausible explanations for how the data points were generated.
- It makes predictions using all possible regression weights, weighted by their posterior probability.



no observations

one observation

two observations

Bayesian Linear Regression

- Leave out the bias for simplicity
- **Prior distribution:** a broad, spherical (multivariate) Gaussian centered at zero:

$$\mathbf{w} \sim \mathcal{N}(\mathbf{0}, \nu^2 \mathbf{I})$$

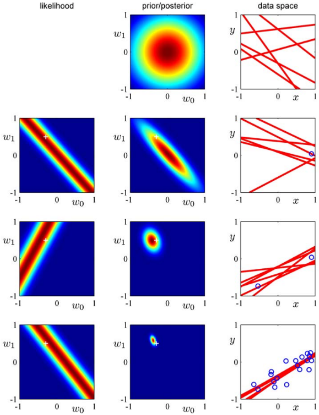
- **Likelihood:** same as in the maximum likelihood formulation:

$$t \,|\, \mathbf{x}, \mathbf{w} \sim \mathcal{N}(\mathbf{w}^\top \mathbf{x},\ \sigma^2)$$

- **Posterior:**

$$\mathbf{w} \,|\, \mathcal{D} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$$

$$\boldsymbol{\mu} = \sigma^{-2} \boldsymbol{\Sigma} \mathbf{X}^\top \mathbf{t} \qquad\qquad \boldsymbol{\Sigma}^{-1} = \nu^{-2} \mathbf{I} + \sigma^{-2} \mathbf{X}^\top \mathbf{X}$$



— Bishop, Pattern Recognition and Machine Learning

Bayesian Linear Regression

Posterior predictive distribution:

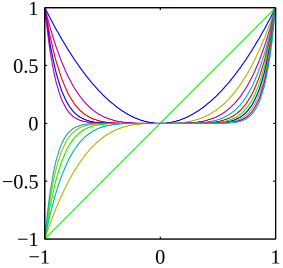
$$\begin{aligned} p(t \mid \mathbf{x}, \mathcal{D}) &= \int p(t \mid \mathbf{x}, \mathbf{w}) p(\mathbf{w} \mid \mathcal{D}) \, \mathrm{d}\mathbf{w} \\ &= \mathcal{N}(t \mid \boldsymbol{\mu}^\top \mathbf{x}, \sigma^2_{\mathrm{pred}}(\mathbf{x})) \\ \sigma^2_{\mathrm{pred}}(\mathbf{x}) &= \sigma^2 + \mathbf{x}^\top \boldsymbol{\Sigma} \mathbf{x}, \end{aligned}$$

where $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ are the posterior mean and covariance of $\boldsymbol{\Sigma}$.

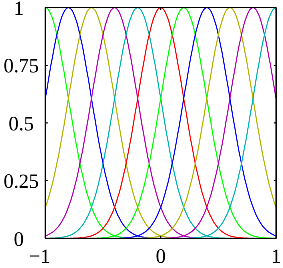
Bayesian Linear Regression

- We can turn this into nonlinear regression using basis functions.

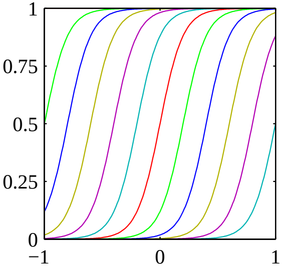
$$\phi_j(x) = x^j$$



$$\phi_j(x) = \exp\left(-\frac{(x-\mu_j)^2}{2s^2}\right)$$

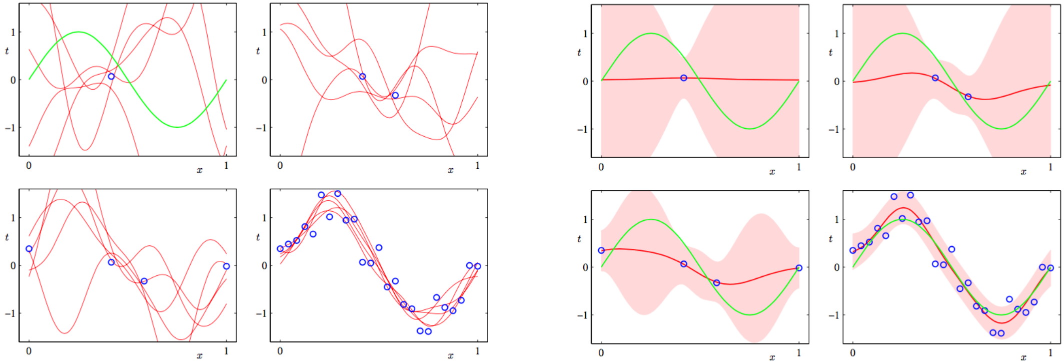


$$\phi_j(x) = \sigma\left(\frac{x-\mu_j}{s}\right)$$



— Bishop, Pattern Recognition and Machine Learning

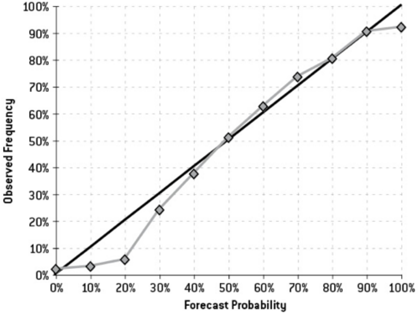
Bayesian Linear Regression



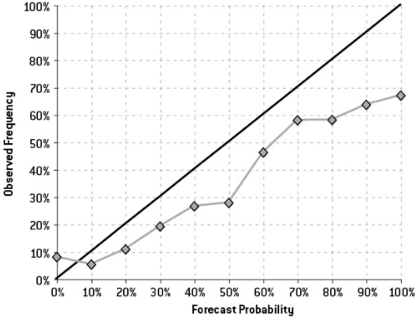
— Bishop, Pattern Recognition and Machine Learning

Calibration

- Calibration: of the times your model predicts something with 90% confidence, is it right 90% of the time?
- Example: calibration of weather forecasts



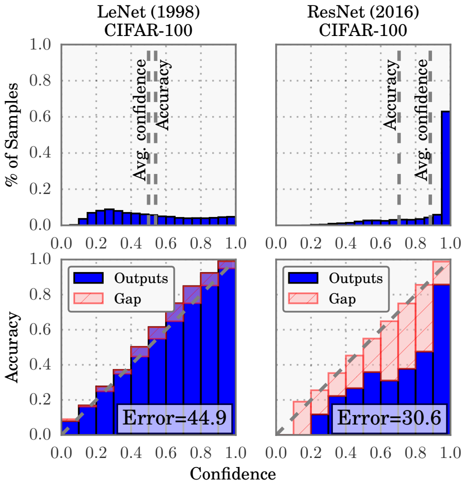
The Weather Channel



Local Weather Station

Calibration

- Most of our neural nets output probability distributions, e.g. over object categories. Are these calibrated?
- While more accurate, modern neural networks are overconfident in their decisions.



— Guo et al., 2017, On calibration of modern neural networks

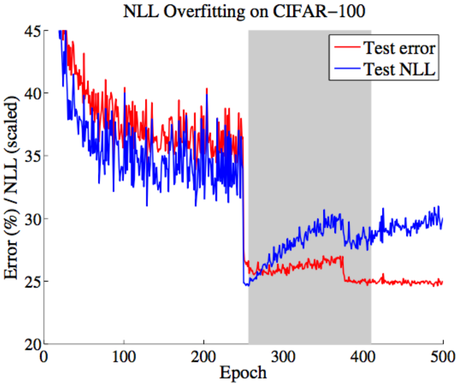
Calibration

- Suppose an algorithm outputs a probability distribution over targets, and gets a loss based on this distribution and the true target.
- A scoring rule is a numerical quantization of the calibration of a predictive distribution $p(y|x)$. If the underlying true distribution over data points is denoted $q(x, y)$, then the expected scoring rule is defined as $S(p, q) = \mathbb{E}_q[S(p, (x, y))]$ for a scoring function $S(p, (x, y))$.
- A proper scoring rule is a rule which ensures that $S(p, q) \leq S(q, q)$ with equality iff $p(y|x) = q(y|x)$.
- The canonical example is negative log-likelihood (NLL). If k is the category label, $\mathbf{t}$ is the indicator vector for the label, and $\mathbf{y}$ are the predicted probabilities,

$$L(\mathbf{y}, \mathbf{t}) = -\log y_k = -\mathbf{t}^\top(\log \mathbf{y})$$

Calibration

- Calibration failures show up in the test NLL scores:



— Guo et al., 2017, On calibration of modern neural networks

Calibration

- Guo et al. explored 7 different calibration methods, but the one that worked the best was also the simplest: temperature scaling.
- A classification network typically predicts $\sigma(\mathbf{z})$, where σ is the softmax function

  $$\sigma(\mathbf{z})_k = \frac{\exp(z_k)}{\sum_{k'} \exp(z_{k'})}$$

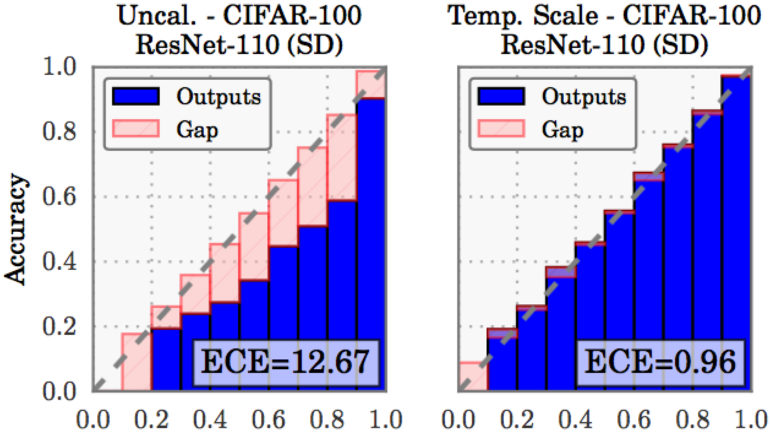
  and $\mathbf{z}$ are called the logits.
- They replace this with

  $$\sigma(\mathbf{z}/T),$$

  where T is a scalar called the temperature.
- T is tuned to minimize the NLL on a validation set.
- Intuitively, because NLL is a proper scoring rule, the algorithm is incentivized to match the true probabilities as closely as possible.

Calibration

- Before and after temperature scaling:



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- Chuan Guo, Geoff Pleiss, Yu Sun, and Kilian Q Weinberger, *On calibration of modern neural networks*, International Conference on Machine Learning, PMLR, 2017, pp. 1321–1330.

- Nate Silver, *The signal and the noise: Why so many predictions fail-but some don't*, Penguin, 2012.