02477 – Bayesian Machine Learning: Lecture 7

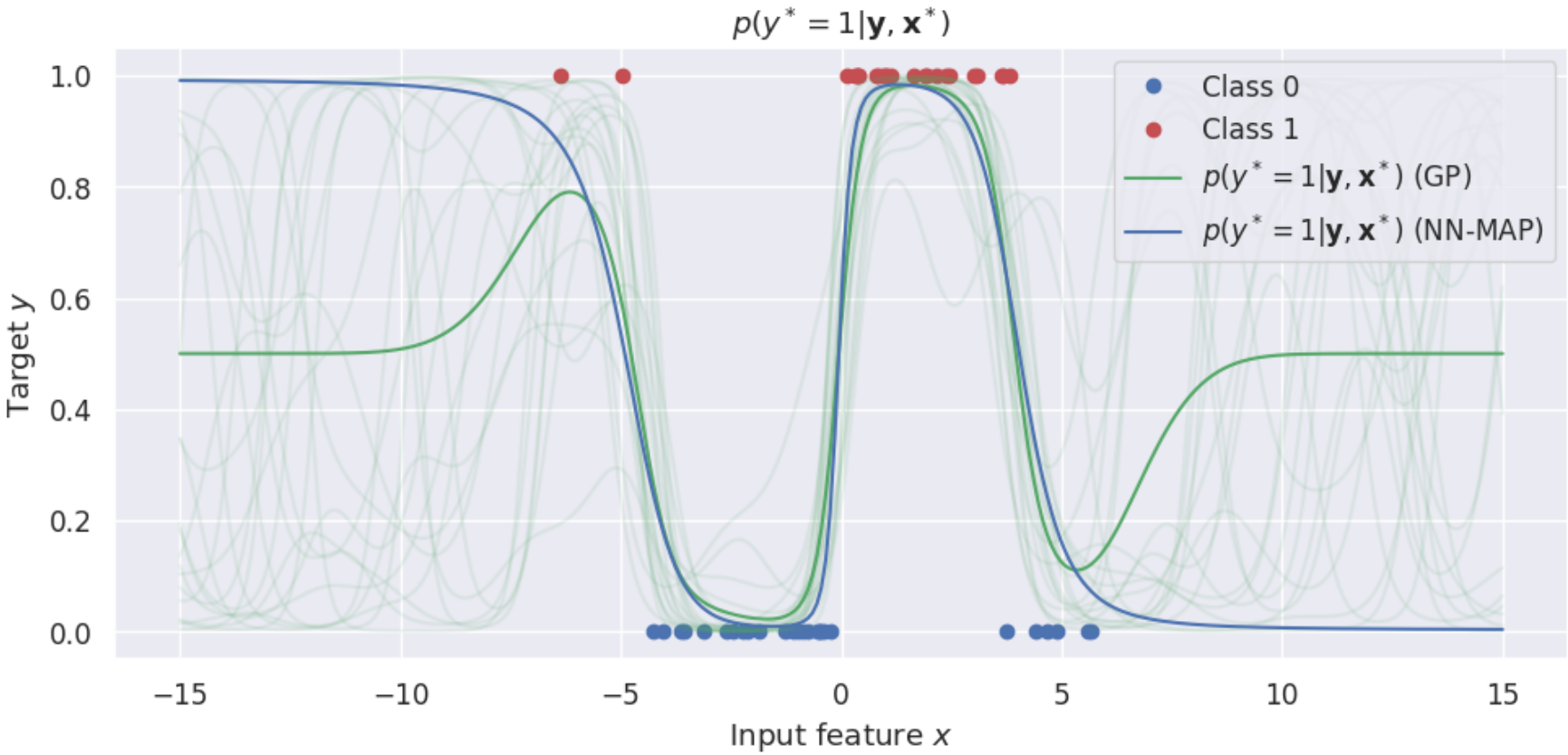
Michael Riis Andersen

Technical University of Denmark,
DTU Compute, Department of Applied Math and Computer Science

Outline

Gaussian processes and neural networks

From last week's exercise



- Some NN researchers are striving to make NNs behave more like Gaussian processes
- Some GP researchers are striving to make GPs flexible and as easy to scale as NNs
- Exploring relationships between GPs and NNs

Infinitely wide neural networks I

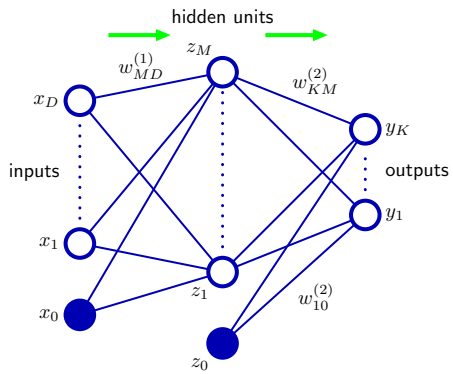
Exploring connections between GPs and NNs

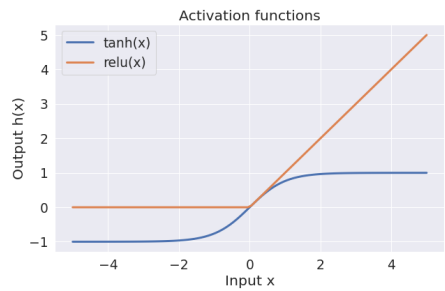
- Consider a network with a single hidden layer with H neurons and one output

$$\boldsymbol{z}(\boldsymbol{x}) = h(\boldsymbol{W}_1\boldsymbol{x} + \boldsymbol{b}_1)$$
$$f(\boldsymbol{x}) = \boldsymbol{W}_2\boldsymbol{z}(\boldsymbol{x}) + \boldsymbol{b}_2$$

- For $\boldsymbol{x} \in \mathbb{R}^D$, then $\boldsymbol{W}_1 \in \mathbb{R}^{H\times D}$ and $\boldsymbol{W}_2 \in \mathbb{R}^{H\times 1}$

- *Universal approximators* for many classes of functions





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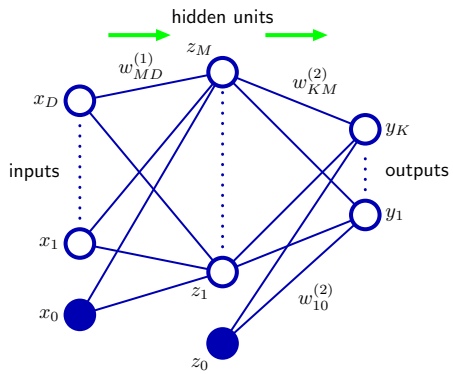

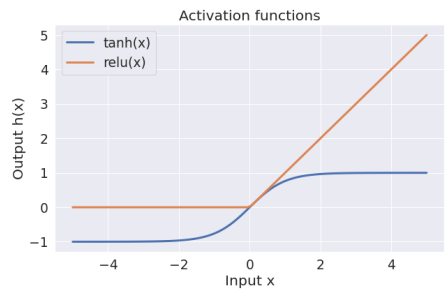

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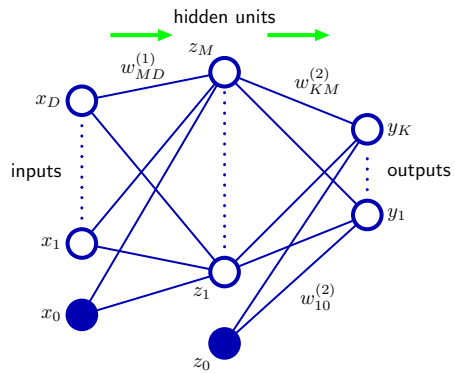

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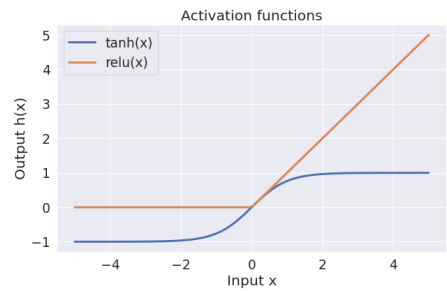

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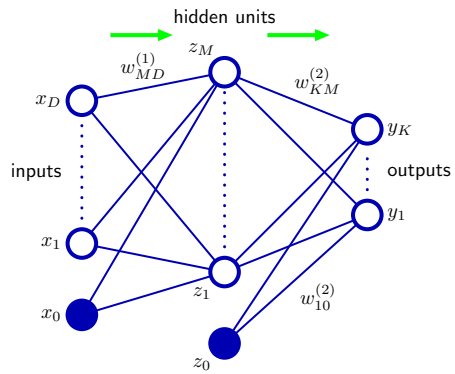

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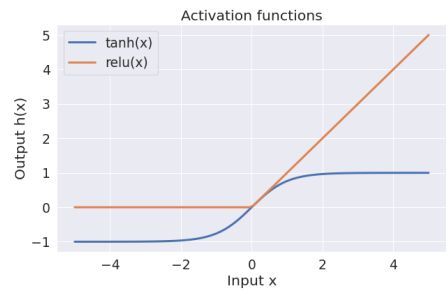

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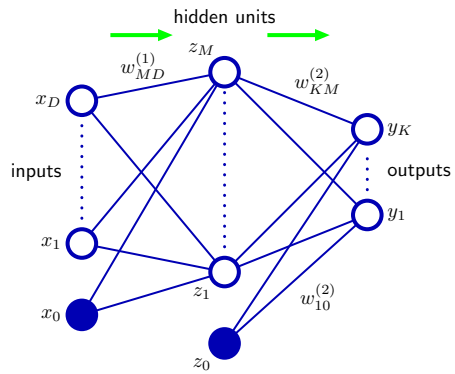

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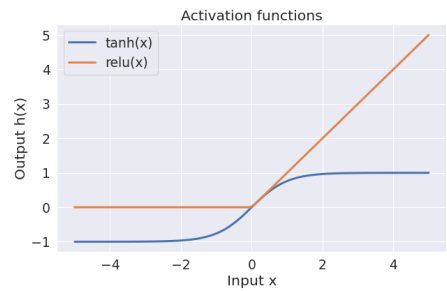

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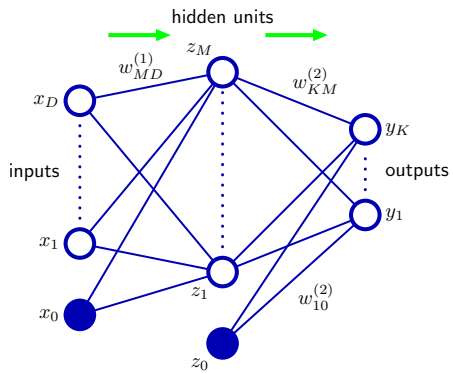

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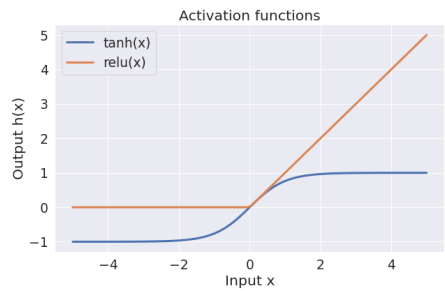

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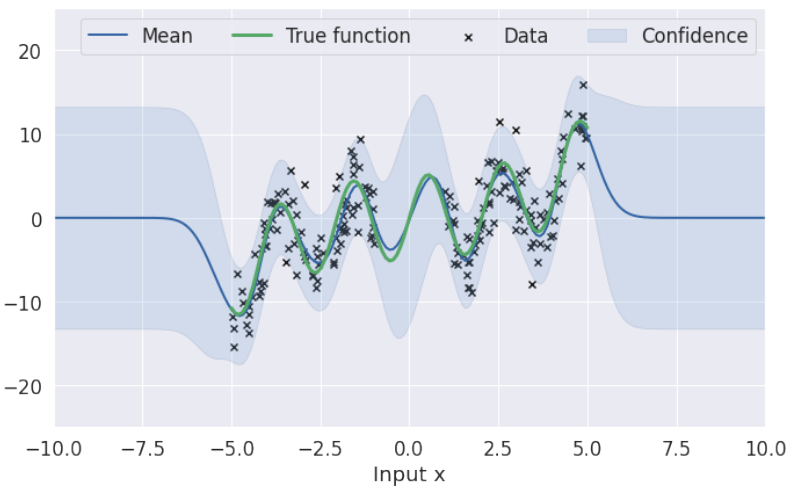
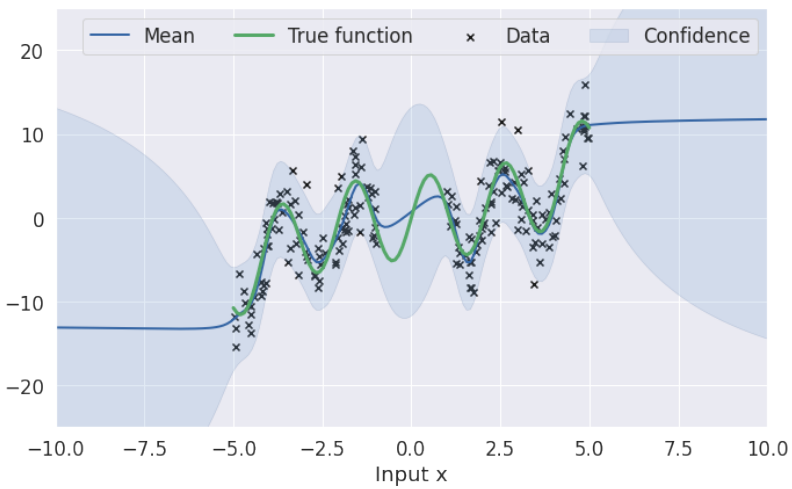
- Comparing *squared exponential* and *neural network kernels*





Generalized linear models and non-Gaussian likelihoods

Likelihoods as observation models: Why bother?

- Consider a linear model

$$f(\boldsymbol{x}) = \boldsymbol{\phi}(\boldsymbol{x})^T \boldsymbol{w}$$

- Regression using Gaussian likelihood

$$y_n | f_n \sim \mathcal{N}(y_n | f_n, \beta^{-1})$$

- Binary classification with sigmoid function $\sigma(\cdot)$

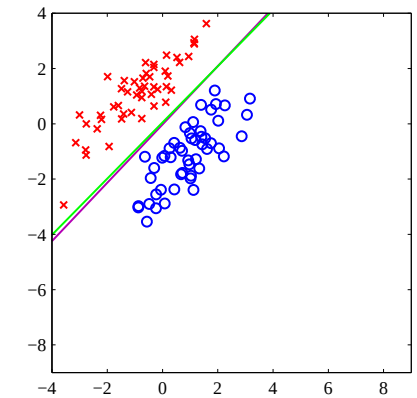
$$y_n | f_n \sim \text{Ber}(y_n | \sigma(f_n))$$

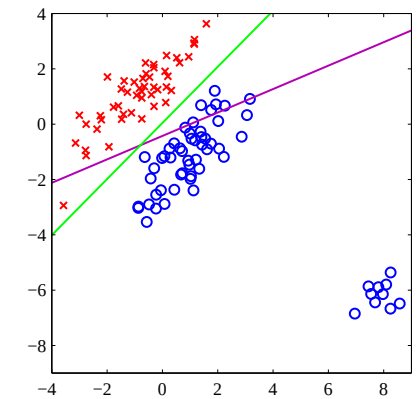
- ..., but why not just use regression for everything?

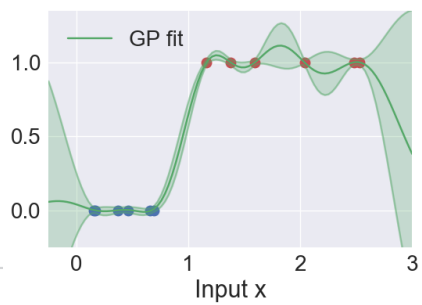
- More general setting: *generalized linear models* GLMs

$$y_n | f_n \sim p(y_n | f_n)$$

Least squared vs logistic regression







Common likelihoods in machine learning

Likelihood	**Support**	**Example**
Gaussian	$y_n \in \mathbb{R}$	Standard regression
Student's t	$y_n \in \mathbb{R}$	Standard regression with heavier tails
Exponential	$y_n \in (0, \infty)$	Strictly positive target values
Gamma	$y_n \in (0, \infty)$	Strictly positive target values
Bernoulli	$y_n \in \{0, 1\}$	Binary classification
Binomial	$y_n \in \{0, 1, \ldots, N\}$	Sequence of Bernoulli trials
Poisson	$y_n \in \{0, 1, 2, 3, \ldots, \}$	Count data
Categorial	$y_n \in \{0, 1, 2, \ldots, K\}$	Multi-class classification (requires K latent fucntions)

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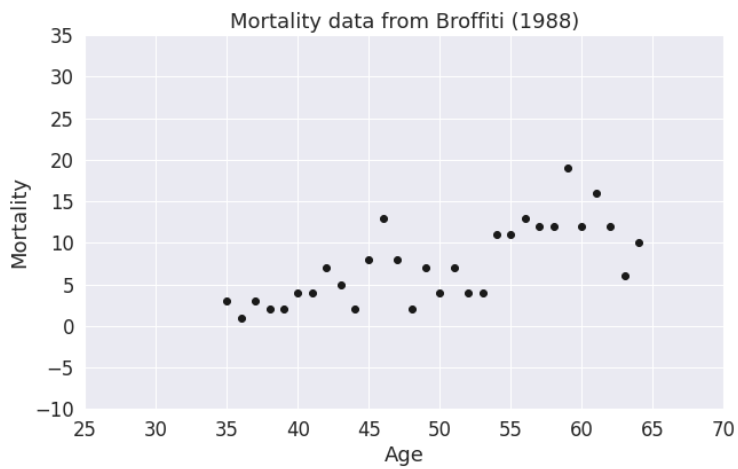
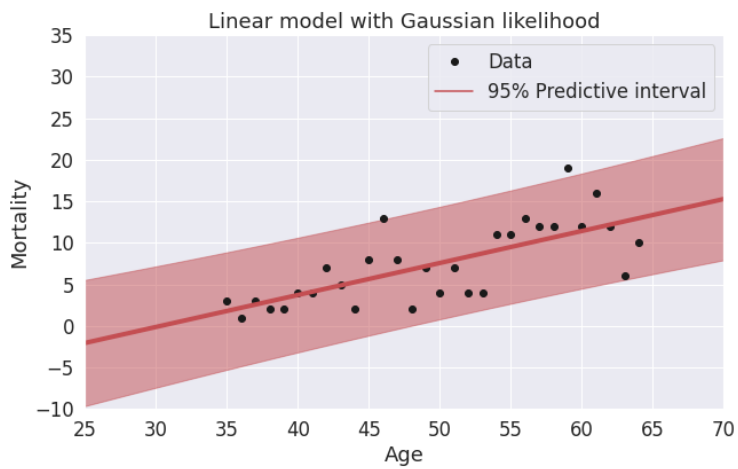
Example: analyzing mortality as a function of age





Under this model, the posterior predictive distribution for age $= 25$ is $\mathcal{N}(-2.61, 14.76)$ meaning that $p(\text{mortality} < 0 | \text{age} = 25) \approx 0.75$

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Spend 5 minutes on the DTU Learn quiz: "Lecture 7a: Common likelihoods in machine learning."

Discuss what type of observation model might be appropriate for ...

1. Predicting whether a student will pass a course (based on the student's previous grades)
2. Predicting the time it takes to finish a written exam
3. Predicting number of errors in a multiple choice exam
4. Predicting whether the student will fill out the exam with a blue, red or black pen

Generalized linear models in three steps

The components of a generalized linear model (GLM)

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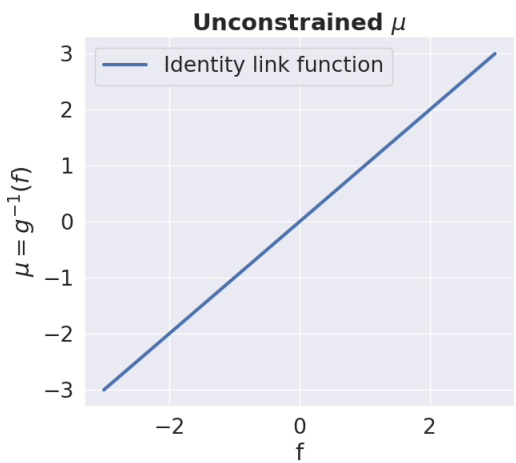
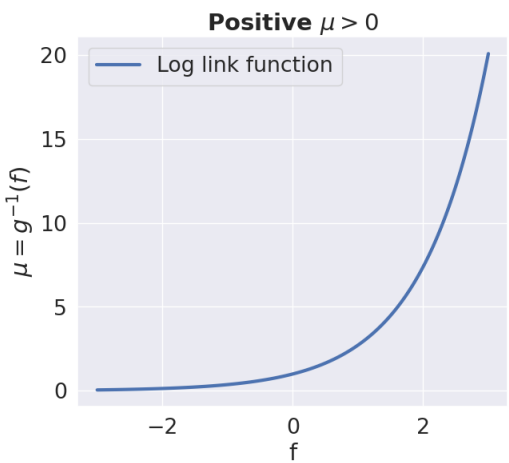
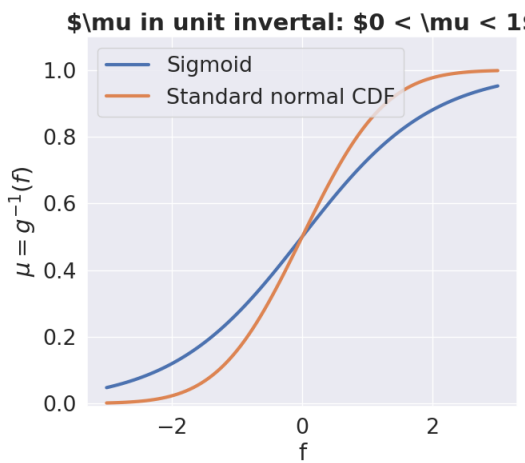


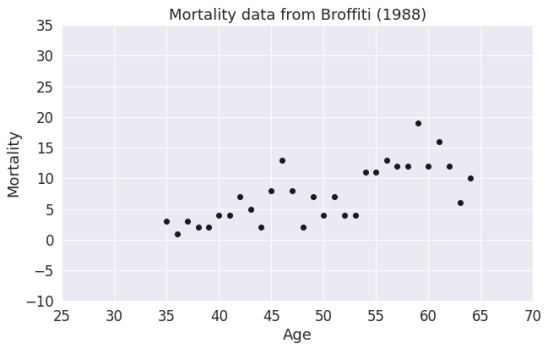




Example: Bayesian Poisson Regression I

- Step 1: We assume a linear model with $\boldsymbol{x} = [1 \quad \text{age}]^T$

$$f(\text{age}) = w_0 + w_1 \text{age} \quad \Longleftrightarrow \quad f(\boldsymbol{x}) = \boldsymbol{x}^T \boldsymbol{w}$$



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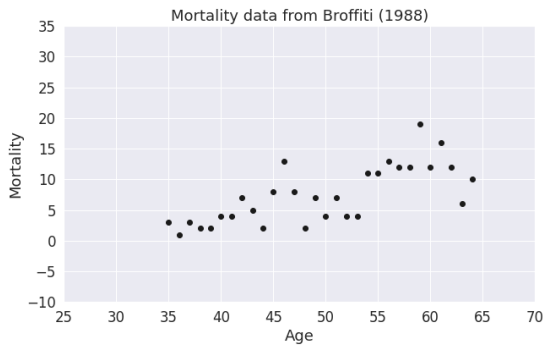

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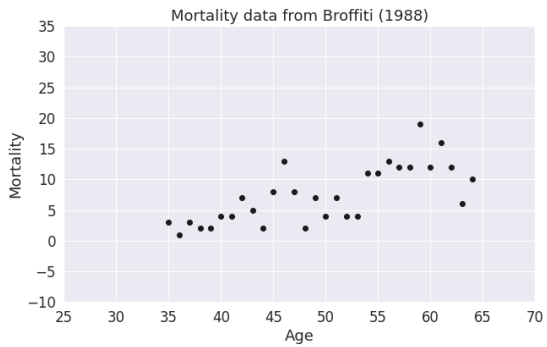

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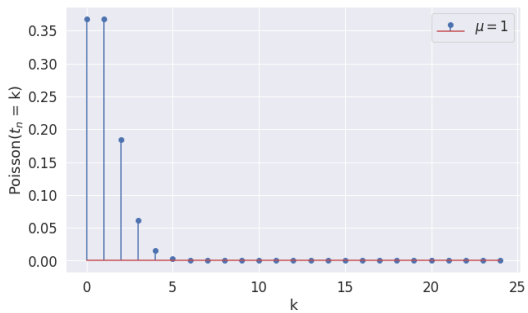

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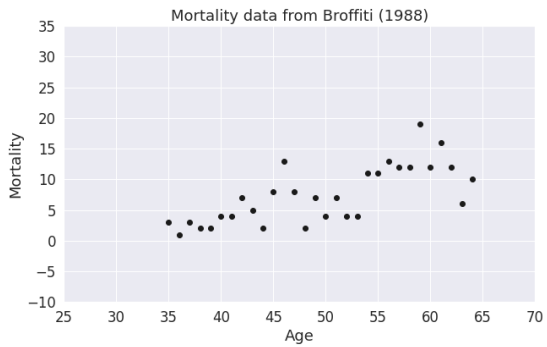

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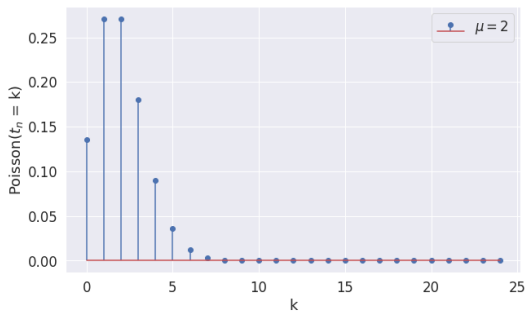

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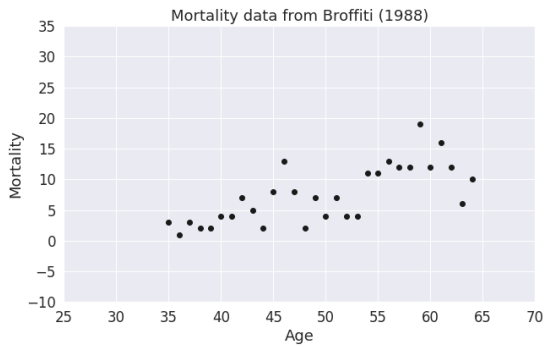

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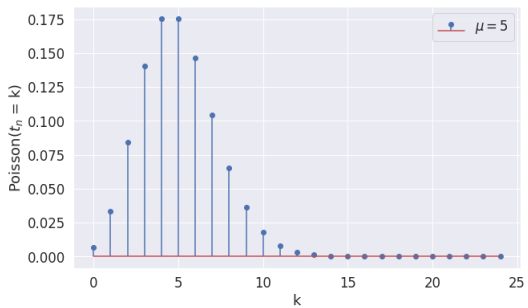

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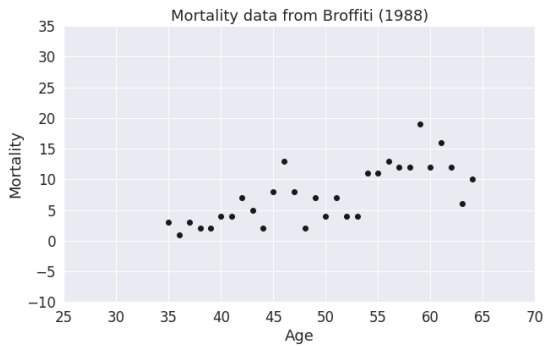

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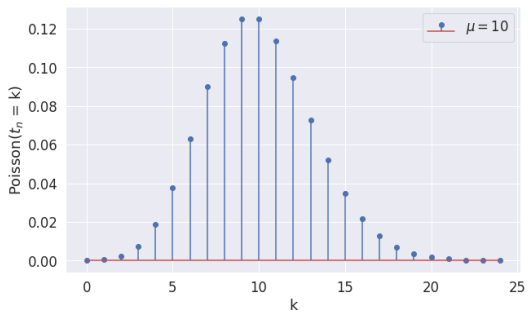

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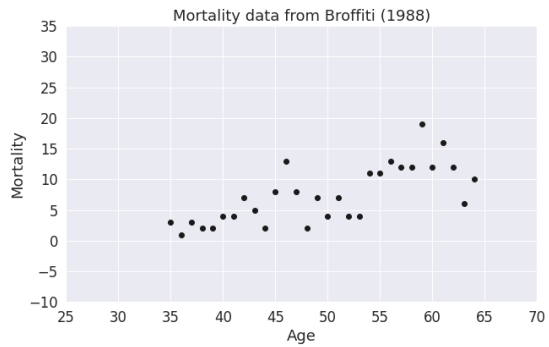

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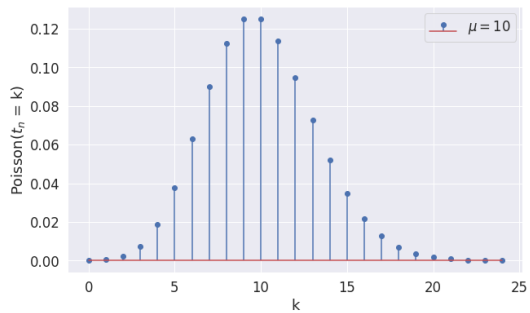

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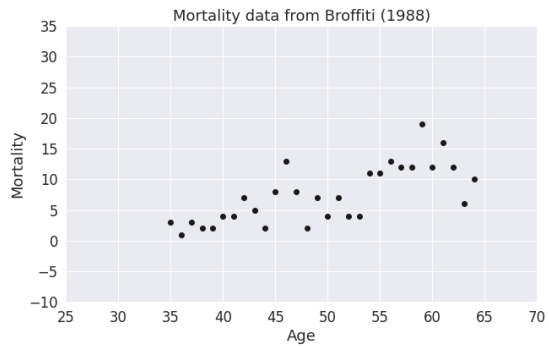

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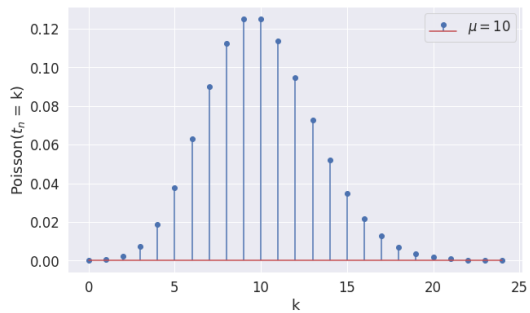

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- We use a Gaussian prior for $\boldsymbol{w}$

$$p(\boldsymbol{w}) = \mathcal{N}(\boldsymbol{w}|\boldsymbol{0}, \boldsymbol{I})$$

Example: Bayesian Poisson Regression II

- Using $\mu_n = \mu(\boldsymbol{x}) = \exp(\boldsymbol{x}_n^T \boldsymbol{w})$, the joint model becomes

$$p(\boldsymbol{y}, \boldsymbol{w}) = p(\boldsymbol{y}|\boldsymbol{w})p(\boldsymbol{w}) = \prod_{n=1}^{N} \text{Poisson}(y_n|\mu_n)\mathcal{N}(\boldsymbol{w}|\boldsymbol{0}, \boldsymbol{I})$$

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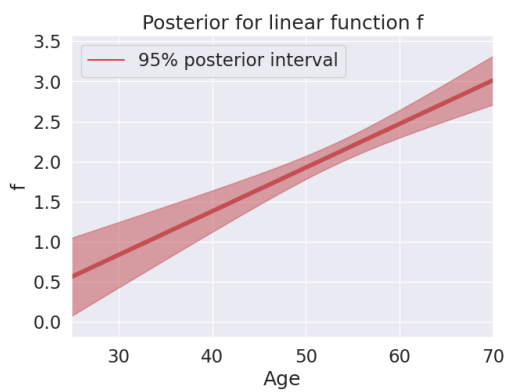

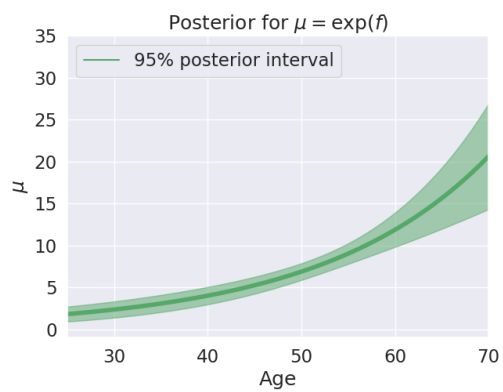

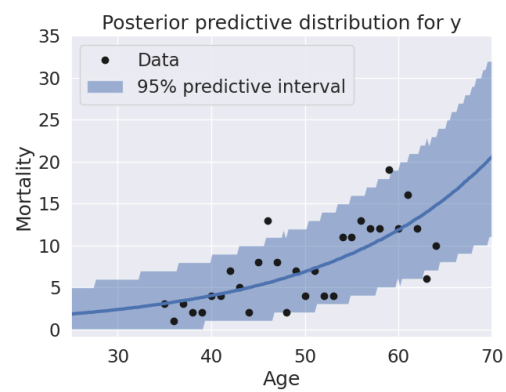

Example: Bayesian Poisson Regression III

- The (approximate) posterior predictive distribution for a new point $\boldsymbol{x}_*$ with $\mu_* = g^{-1}(\boldsymbol{x}_*^T \boldsymbol{w})$

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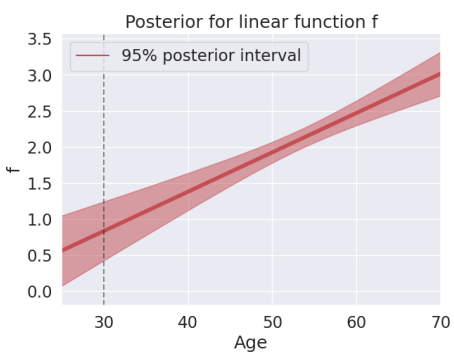

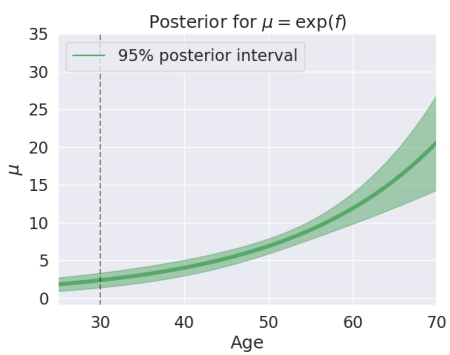

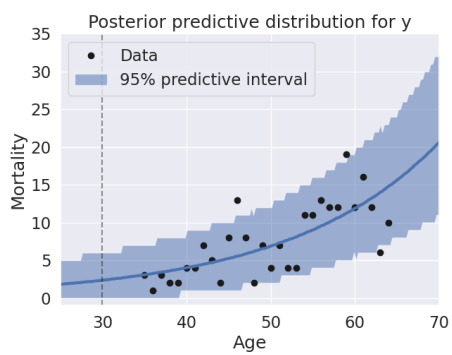

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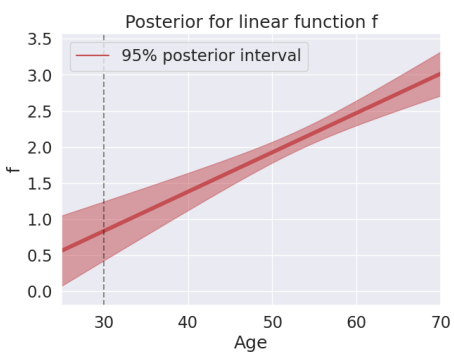
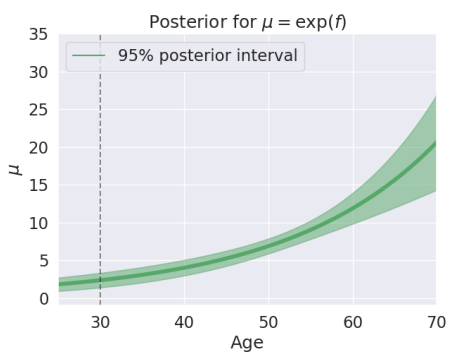
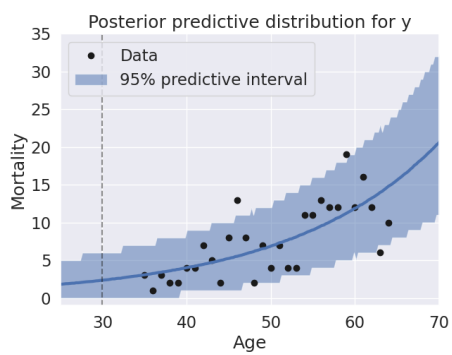
- Calculating predictions for age $= 30$. Let $\boldsymbol{x}_* = [1 \quad 30]$, then $f_* = \boldsymbol{x}_*^T \boldsymbol{w}$

$$p(f_*|\boldsymbol{y}) = \mathcal{N}(f_*|\boldsymbol{x}_*^T \boldsymbol{m}, \boldsymbol{x}_*^T \boldsymbol{S}\boldsymbol{x}_*) \approx \mathcal{N}(f_*|0.8, 0.2^2)$$







Example: Bayesian Poisson Regression III

- The (approximate) posterior predictive distribution for a new point $\boldsymbol{x}_*$ with $\mu_* = g^{-1}(\boldsymbol{x}_*^T \boldsymbol{w})$

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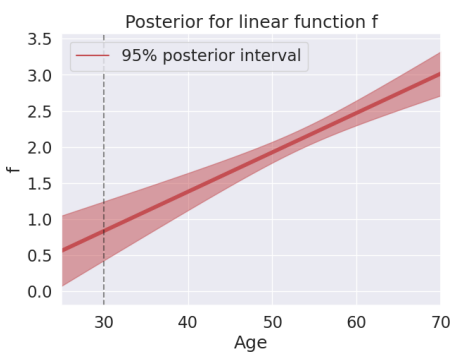

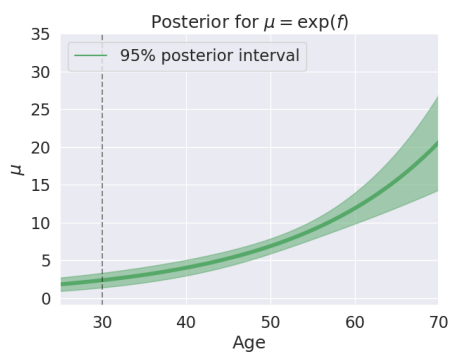

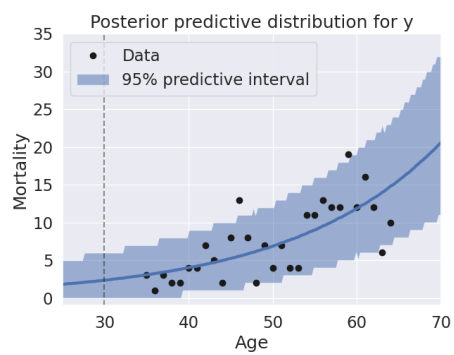

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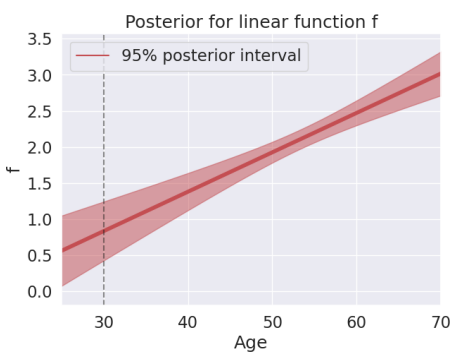
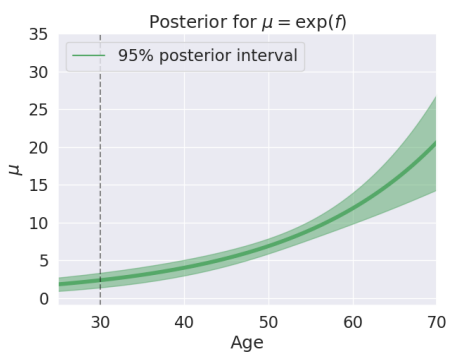
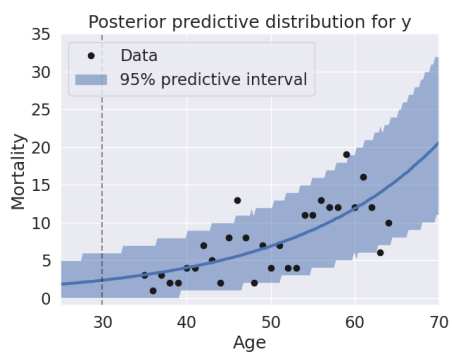
- Finally, we calculate the sample means (or variances, percentiles etc)

$$\mathbb{E}\left[\mu_*^{(s)}|\boldsymbol{y}\right] \approx \frac{1}{S}\sum_{s=1}^{S} \mu_*^{(s)} = 2.34 \qquad \mathbb{E}\left[y_*^{(s)}|\boldsymbol{y}\right] \approx \frac{1}{S}\sum_{s=1}^{S} y_*^{(s)} = 2.34$$







Generalized GP/NN models in three steps

The components of a generalized model

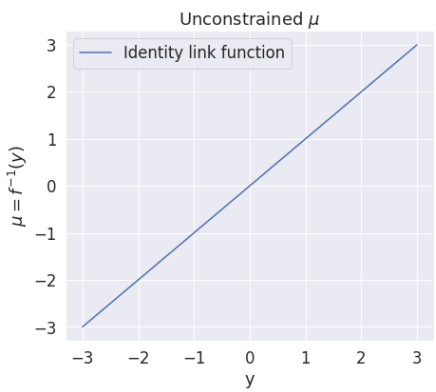
1. We replace the linear model with a Gaussian process (or a NN)

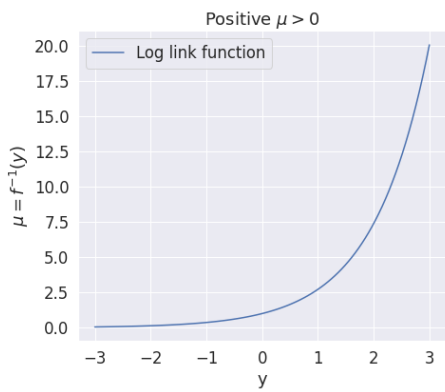
$$f(\boldsymbol{x}) \sim \mathcal{GP}(0, k(\boldsymbol{x}, \boldsymbol{x}'))$$

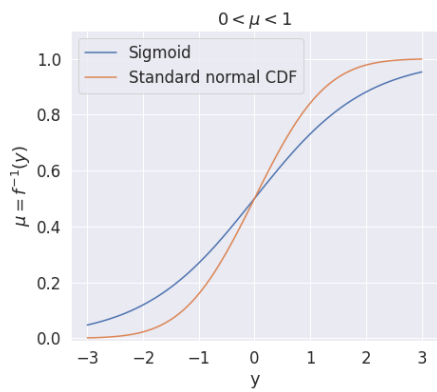
2. The *link function* f that related the mean of the linear model to the mean of the response variable $t(\boldsymbol{x})$

$$g\left[\mu(\boldsymbol{x})\right] = f(\boldsymbol{x}) \qquad \Longleftrightarrow \qquad \mathbb{E}\left[y|\boldsymbol{x}\right] = \mu(\boldsymbol{x}) = g^{-1}\left[f(\boldsymbol{x})\right]$$

3. The distribution $p(y|\boldsymbol{x})$ for the response variable $y(\boldsymbol{x})$, e.g. Poisson, binomial, gamma etc.







Adapting GP models to different likelihoods

- From last weeks' exercise: Laplace approximation GP for classification

$$p(\mathbf{f}|\mathbf{y}) = \frac{p(\mathbf{y}|\mathbf{f})p(\mathbf{f})}{p(\mathbf{y})} \approx q(\mathbf{f}) = \mathcal{N}(\mathbf{f}|\mathbf{m}, \mathbf{S}),$$

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- The log joint of the target $\mathbf{y}$ and latent function values $\mathbf{f}$

$$\log p(\mathbf{y}, \mathbf{f}) = \log p(\mathbf{y}|\mathbf{f}) + \log p(\mathbf{f}) = \sum_{n=1}^{N} \log p(y_n|f_n) - \frac{N}{2}\log(2\pi) - \frac{1}{2}|\mathbf{K}| - \frac{1}{2}\mathbf{f}^T\mathbf{K}^{-1}\mathbf{f}$$

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- The gradient and Hessian of the log joint

$$\nabla_{\mathbf{f}} \log p(\mathbf{y}, \mathbf{f}) = \sum_{n=1}^{N} \nabla_{\mathbf{f}} \log p(y_n|f_n) - \mathbf{K}^{-1}\mathbf{f},$$

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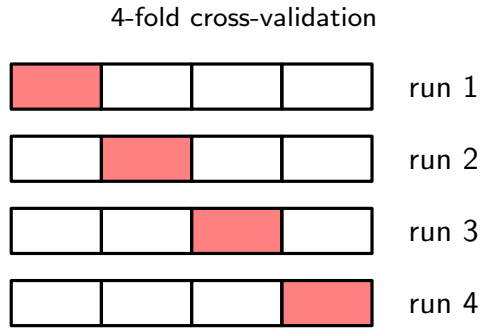
- Hence, all we need to change is the first and second order derivative of log likelihood

Generalization and evaluation

Generalization error and model evaluation

- Consider a supervised problem with $\mathcal{D} = \{\boldsymbol{x}_i, y_i\}_{i=1}^N$
- We measure performance of models using *cross-validation*
  1. Held-out test set
  2. K-fold
  3. Leave-one-out
  4. Split-half
  5. ...
- Goal: assess the *generalization error* of the model, i.e. how well can we expected the model to perform on a new, unseen test example?
- We use cross-validation to *estimate* the generalization error
- Parameter tuning: training/validation/test or nested cross-validation



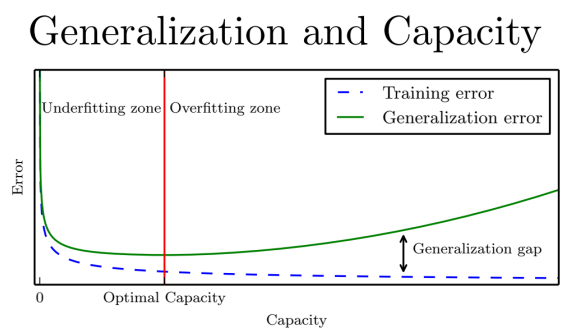


Figure from Goodfellow 2016

Generalization error and loss functions

- Let y be the target value for a input vector $\boldsymbol{x}$ and let $\hat{y} \equiv \hat{y}(\boldsymbol{x})$ be a prediction

- The *loss function* $\mathcal{L}(y, \hat{y})$ define the cost of predicting $\hat{y}$ when the true value is y

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- We rarely know the *true data generating mechanism* $p(\boldsymbol{x}, y)$ in practice

Estimating the generalization

- The *exact* generalization error

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- For ERM, one can show that the training error is *optimistic*

$$\mathbb{E}\left[\widehat{\mathcal{R}}_{\hat{y}}^{\text{train}}\right] \leq \mathbb{E}\left[\widehat{\mathcal{R}}_{\hat{y}}^{\text{test}}\right]$$

Example: the expected generalization error wrt. to the squared loss

- Consider the following (very simple) linear regression model (no slope, only intercept)

$$y = w_{\text{true}} + e, \qquad e \sim \mathcal{N}(0, \sigma^2)$$

- We will use some estimator $\hat{w}$ for w_{true} (fixed) as a prediction for a new y, i.e. $y^* = \hat{w}$.

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- What is the *generalization error* wrt. *squared loss*?

$$\begin{aligned}
\mathcal{R}_{\hat{w}} = \mathbb{E}\left[\mathcal{L}\right] &= \iint (t - \hat{w})^2 p(y, \boldsymbol{x}) \mathrm{d}y \mathrm{d}\boldsymbol{x} \\
&= \int (y - \hat{w})^2 p(y) \mathrm{d}y \\
&= \int (y - \hat{w})^2 \mathcal{N}(y | w_{\text{true}}, \sigma^2) \mathrm{d}y \\
&= \int (y^2 + \hat{w}^2 - 2y\hat{w}) \mathcal{N}(y | w_{\text{true}}, \sigma^2) \mathrm{d}y \\
&= \int y^2 \mathcal{N}(y | w_{\text{true}}, \sigma^2) \mathrm{d}y + \hat{w}^2 \int \mathcal{N}(y | w_{\text{true}}, \sigma^2) \mathrm{d}y - 2\hat{w} \int y \mathcal{N}(y | w_{\text{true}}, \sigma^2) \mathrm{d}y \\
&= (w_{\text{true}} - \hat{w})^2 + \sigma^2
\end{aligned}$$

- Unsurprisingly, the generalization error is minimized when $\hat{w} = w_{\text{true}}$, which leads to $\mathbb{E}\left[\mathcal{L}\right] = \sigma^2$.

What is the expected generalization error for a given dataset size?

- The generalization error

$$\mathcal{R}_{\hat{w}} = (w - \hat{w})^2 + \sigma^2$$

- Suppose we observe a dataset $\mathcal{D} = \{y_n\}_{n=1}^N$ with the goal of estimating the parameter w_{true}

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- The *expected generalization error* for the maximum likelihood estimator for a dataset of size N is

$$\left\langle \mathcal{R}_{w_{\text{MLE}}} \right\rangle_N = \int \left[(w_{\text{true}} - \hat{w}_{\text{ML}})^2 + \sigma^2\right] \mathcal{N}\left(w_{\text{ML}} | w_{\text{true}}, \frac{\sigma^2}{N}\right) \mathrm{d}w_{\text{ML}} = \frac{\sigma^2}{N} + \sigma^2$$

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- Interpretation
  1. Average excess error due to finite training data
  2. Inherent noise in the data

Decision theory

Uncertainty in multi-class classification

- Categorical distributions for multi-class classification with K classes

$$y_n|\mathbf{f}_n \sim \text{Categorical}\left[\text{softmax}(\mathbf{f}_n)\right]$$

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- Example

$$\begin{aligned} p(y^* = \text{cat}|\text{img}) &= 0.36 \\ p(y^* = \text{dog}|\text{img}) &= 0.34 \\ p(y^* = \text{bird}|\text{img}) &= 0.30 \end{aligned} \qquad \begin{aligned} p(y^* = \text{healthy}|\text{x-ray}) &= 0.36 \\ p(y^* = \text{pre-phase cancer}|\text{x-ray}) &= 0.34 \\ p(y^* = \text{severe cancer}|\text{x-ray}) &= 0.30 \end{aligned}$$

Quantifying uncertainty for multi-class classification

- The *confidence* of the posterior predictive distribution is defined as

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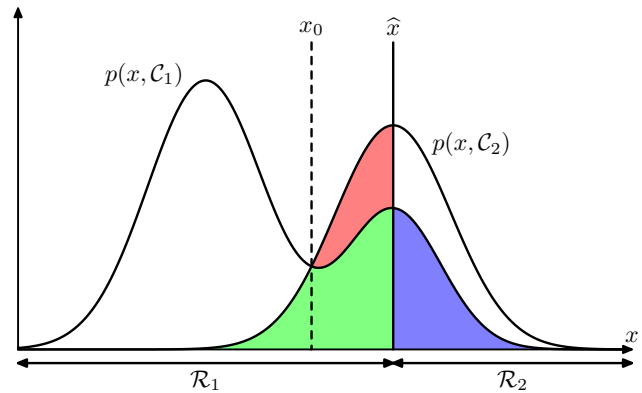
- Examples

$p(y^* = \text{cat}\|\text{img})$	$= 0.50$	$p(y^* = \text{healthy}\|\text{x-ray})$	$= 0.50$
$p(y^* = \text{dog}\|\text{img})$	$= 0.50$	$p(y^* = \text{pre-phase cancer}\|\text{x-ray})$	$= 0.25$
$p(y^* = \text{bird}\|\text{img})$	$= 0.0$	$p(y^* = \text{severe cancer}\|\text{x-ray})$	$= 0.25$
$\mathcal{C} = 0.5$		$\mathcal{C} = 0.5$	
$\mathcal{H} \approx 0.69$		$\mathcal{H} \approx 1.04$	

Reject option: I don't know?

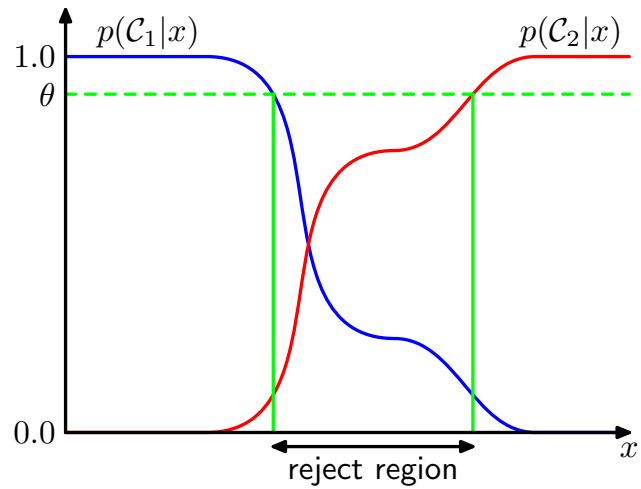
- For applications in medicin etc. it may be better to say "I don't know" rather than provide a prediction we don't really trust

- *Reject option*: Avoid making a decision if the uncertainty is too large



- Reject to make decision if

$$\mathcal{C} = \max_k p(y^* = i|\boldsymbol{y}, \boldsymbol{x}^*) < \theta_{\text{reject}}$$



- If $\theta_{\text{reject}} = 1$, then all samples will get rejected

- If $\theta_{\text{reject}} \leq \frac{1}{K}$, then no samples will get rejected

Decision theory: a more formal approach

- In Bayesian modelling we strive to represent all unknown quantities (parameters, predictions etc.) using *probability distributions*

- Yet, we are often forced to reduce these to single decisions/predictions

  1. Cancer or not cancer?
  2. Which online campaign is better? A, B or C etc?
  3. How many airline passengers in year 2025?
  4. Which model best describes the data?
  5. ...

- *Statistical decision theory* tells us to make optimal decisions under uncertainty

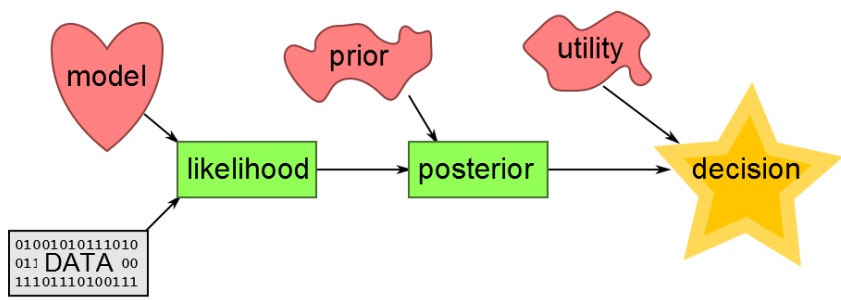


Figure from https://www.azimuthproject.org

Bayesian decision theory in a nutshell

- A decision maker has a set of actions/choices $a \in \mathcal{A}$ to choose from
- The optimal action depends on the true state $s \in \mathcal{S}$ of the system of interest
- The *loss function* $\mathcal{L}(s, a)$ determines the cost for choice a when the true state is s. We can also use a *utility function* $\mathcal{U}(s, a) = -\mathcal{L}(s, a)$

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- Example: assigning medical treatment to potential Covid19 patient

$\mathcal{L}(s, a)$	Do nothing	Isolate at home	Hospitalization
Healthy	0	10	50
Covid19, mild symptoms	10	0	20
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- In practice, we do not know the true state s. What to do?
- *Bayesian decision theory*
  1. Compute posterior of the state s given data $\boldsymbol{y}$, i.e. $p(s|\boldsymbol{y})$
  2. Choose the action that minimizes the posterior extected loss

$$\hat{a} = \arg\min_{a \in \mathcal{A}} \mathbb{E}_{p(s|\boldsymbol{y})} \left[\mathcal{L}(s, a)\right]$$

5 minutes exercise

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- Suppose a medical doctor collected data about a patient and arrived at the following posterior predictions for whether the patient will get Covid19 or not

State s	Healthy	Mild symptoms	Severe symptoms
$p(s\|\boldsymbol{y})$	0.65	0.3	0.05

Questions

- What is the posterior expected loss for each action, i.e. $\mathbb{E}_{p(s|\boldsymbol{y})}\left[\mathcal{L}(s, a)\right]$?

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$$a_1 : 0.65 \cdot 0 + 0.3 \cdot 10 + 0.05 \cdot 100 = 8$$
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  The best action is a_2 (to isolate at home) because it minimizes the posterior expected loss

Decision theory for classification I

- Consider a binary classification problem with $\mathcal{D} = \{\boldsymbol{x}_i, y_i\}_{i=1}^N$ for $y_i \in \{0, 1\}$
- The *0/1 utility function* is given by $\mathcal{U}(y, \hat{y}(\boldsymbol{x})) = \mathbb{I}[y = \hat{y}(\boldsymbol{x})]$

$\mathcal{U}(y, \hat{y}(\boldsymbol{x}))$	$\hat{y} = 0$	$\hat{y} = 1$
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- Picking the class with largest posterior pred. probability is *Bayes optimal* under the 0/1-loss function

Decision theory for classification II

- Consider a binary classification problem with $\mathcal{D} = \{\boldsymbol{x}_i, y_i\}_{i=1}^N$ for $y_i \in \{0, 1\}$
- Example: classifying cancer from medical imagery $\boldsymbol{x}$

$\mathcal{U}(y, \hat{y}(\boldsymbol{x}))$	$\hat{y} = 0$(not cancer)	$\hat{y} = 1$(cancer)
$y = 0$(not cancer)	1	-10
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$$\Rightarrow (1-p)\mathcal{U}_{00} + p\mathcal{U}_{10} \geq (1-p)\mathcal{U}_{01} + p\mathcal{U}_{11}$$

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&\Rightarrow (1-p)\mathcal{U}_{00} + p\mathcal{U}_{10} \geq (1-p)\mathcal{U}_{01} + p\mathcal{U}_{11} \\
&\Rightarrow p \leq \frac{\mathcal{U}_{01} - \mathcal{U}_{00}}{\mathcal{U}_{10} - \mathcal{U}_{11} + \mathcal{U}_{01} - \mathcal{U}_{00}}
\end{aligned}$$

- We have

$$p \leq \frac{\mathcal{U}_{01} - \mathcal{U}_{00}}{\mathcal{U}_{10} - \mathcal{U}_{11} + \mathcal{U}_{01} - \mathcal{U}_{00}} = \frac{-10 - 1}{-100 - 1 - 10 - 1} \approx 0.099$$

Decision theory for classification II

- Consider a binary classification problem with $\mathcal{D} = \{\boldsymbol{x}_i, y_i\}_{i=1}^N$ for $y_i \in \{0, 1\}$
- Example: classifying cancer from medical imagery $\boldsymbol{x}$

$\mathcal{U}(y, \hat{y}(\boldsymbol{x}))$	$\hat{y} = 0$(not cancer)	$\hat{y} = 1$(cancer)
$y = 0$(not cancer)	1	-10
$y = 1$(cancer)	-100	1

- How certain do we need to be before we "dare" to predict $\hat{y}^* = 0$?

$$\begin{aligned}
&\mathbb{E}\left[\mathcal{U}(y^*, 0)\right] \geq \mathbb{E}\left[\mathcal{U}(y^*, 1)\right] \\
&\Rightarrow (1-p)\mathcal{U}_{00} + p\mathcal{U}_{10} \geq (1-p)\mathcal{U}_{01} + p\mathcal{U}_{11} \\
&\Rightarrow p \leq \frac{\mathcal{U}_{01} - \mathcal{U}_{00}}{\mathcal{U}_{10} - \mathcal{U}_{11} + \mathcal{U}_{01} - \mathcal{U}_{00}}
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- That is, if $p(y^* = 0|\boldsymbol{x}) = 1 - p > 0.901$, we predict "No cancer"

Decision theory for regression I

- Consider a regression problem with $\mathcal{D} = \{\boldsymbol{x}_i, y_i\}_{i=1}^N$ for $y_i \in \mathbb{R}$

- The most common loss function for regression is the *quadratic loss*

$$\mathcal{L}(y, y(\boldsymbol{x})) = (y - \hat{y}(\boldsymbol{x}))^2$$

- The expected loss for a complete probabilistic description $p(\boldsymbol{x}, y)$ is

$$\mathbb{E}\left[\mathcal{L}(y, y(\boldsymbol{x}))\right] = \iint (y - \hat{y}(\boldsymbol{x}))^2 p(\boldsymbol{x}, y) \mathrm{d}\boldsymbol{x} \mathrm{d}y$$

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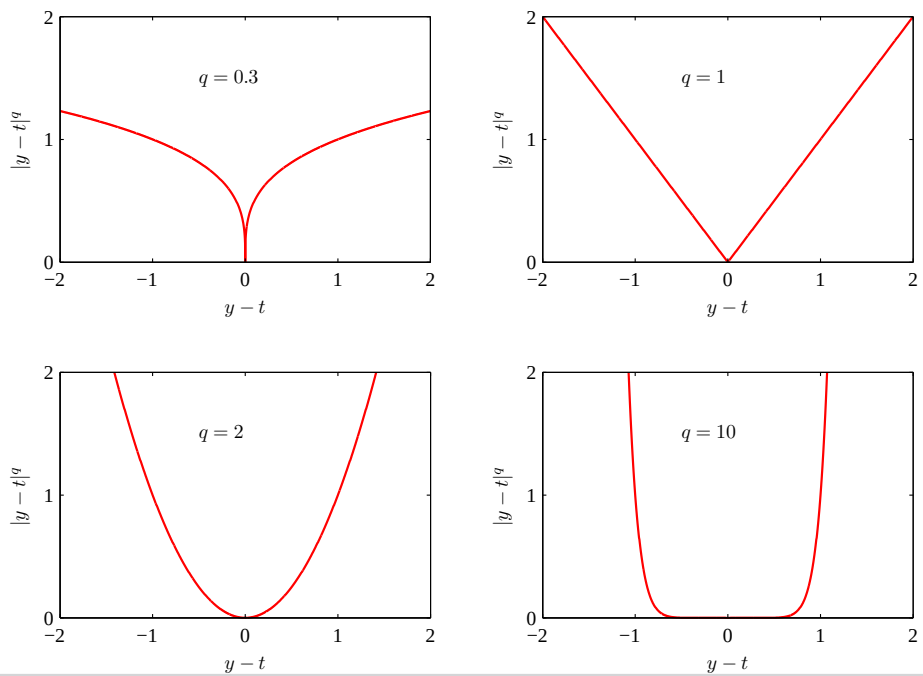
- The *posterior predictive mean* is *optimal* wrt. the quadratic loss

Decision theory for regression II

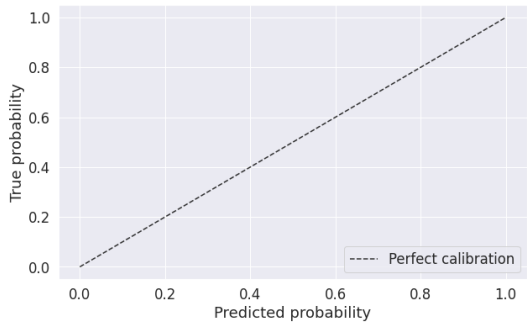
- The *Minkowski loss* is a generalization of the quadractic loss and is given by $\mathcal{L} = (\hat{y}(\boldsymbol{x}) - y)^q$
- One can show that ...
  - the posterior mean is optimal for $q = 2$
  - the posterior median is optimal for $q = 1$
  - the posterior mode is optimal for $q \to 0$
- $q = 2$ can be sensitive to outliers because of the quadratic form, while $q = 1$ is more robust



Calibration

Calibration for classification models

- We have seen that probabilities play an important role in decision-making, but how do we know if the probabilities are accurate?
- Training models via maximum likelihood or Bayesian methods should in theory yield calibrated models, however, in practice, models are rarely perfectly calibrated
- If we have an independent validation/test set, we can quantify the degree of calibration or miscalibration
- Among all the example in the test set, where the predictive probability is approximately 80% we expect roughly 80% of the corresponding examples to belong to the positive class.
- Metrics for quantifying degree of miscalibration for classification
    1. Expected calibration error (ECE)
    2. Maximum calibration error
    3. Marginal calibration error
    4. Brier score



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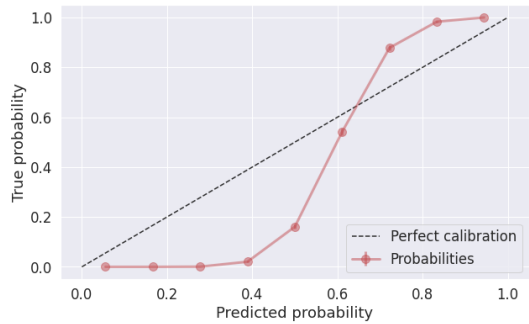
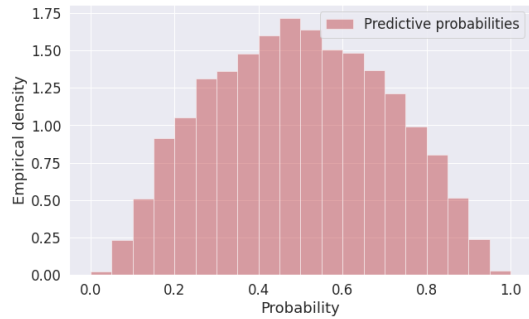


Expected calibration error (ECE)

- Compute predictions for validation set $\mathcal{D}_{\text{val}} = \{\mathbf{x}_m^*, y_m^*\}_{m=1}^M$



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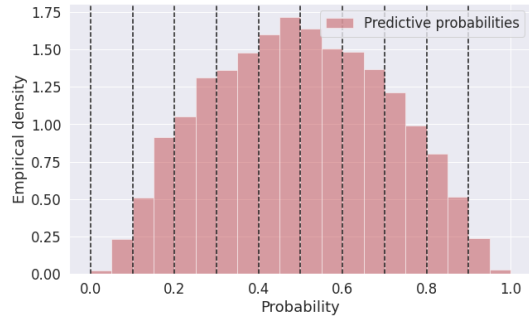

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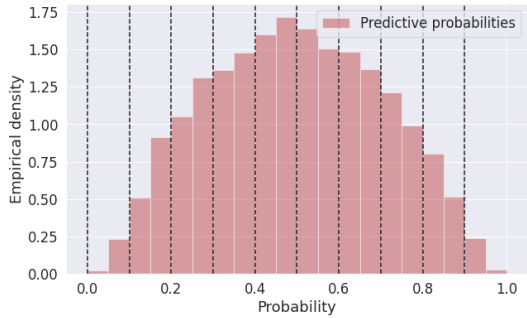

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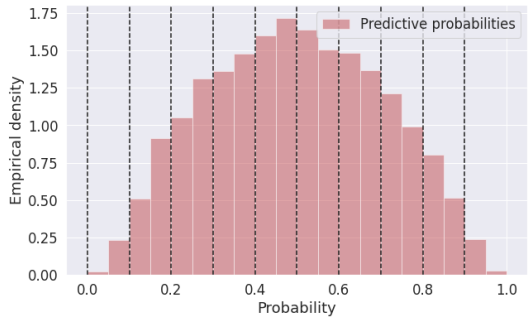

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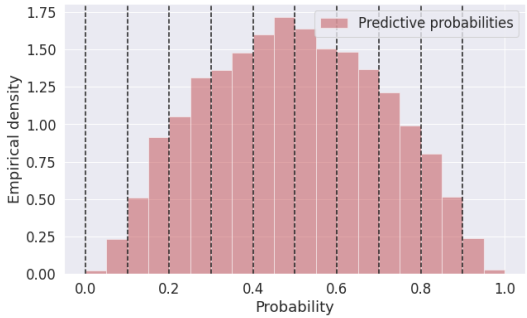

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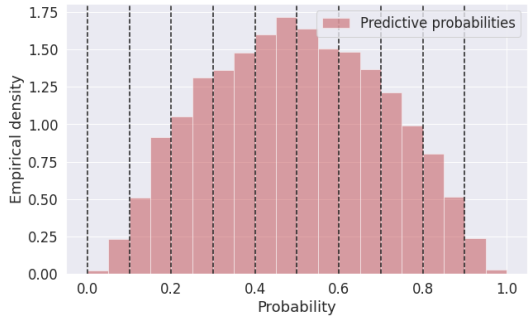

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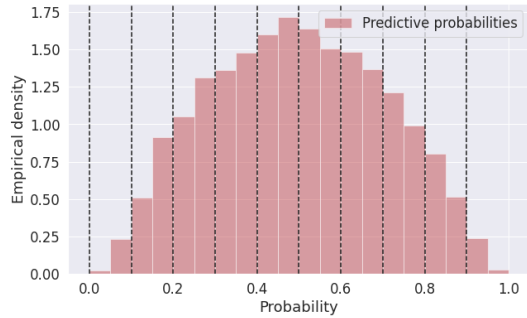

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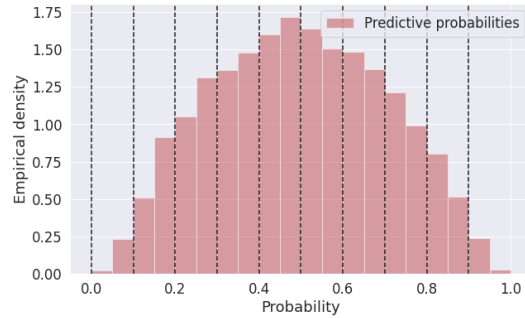
$$\text{ECE} = \sum_{b=1}^{B} \frac{|\mathcal{B}_b|}{M} |\text{acc}(\mathcal{B}_b) - \text{conf}(\mathcal{B}_b)|$$



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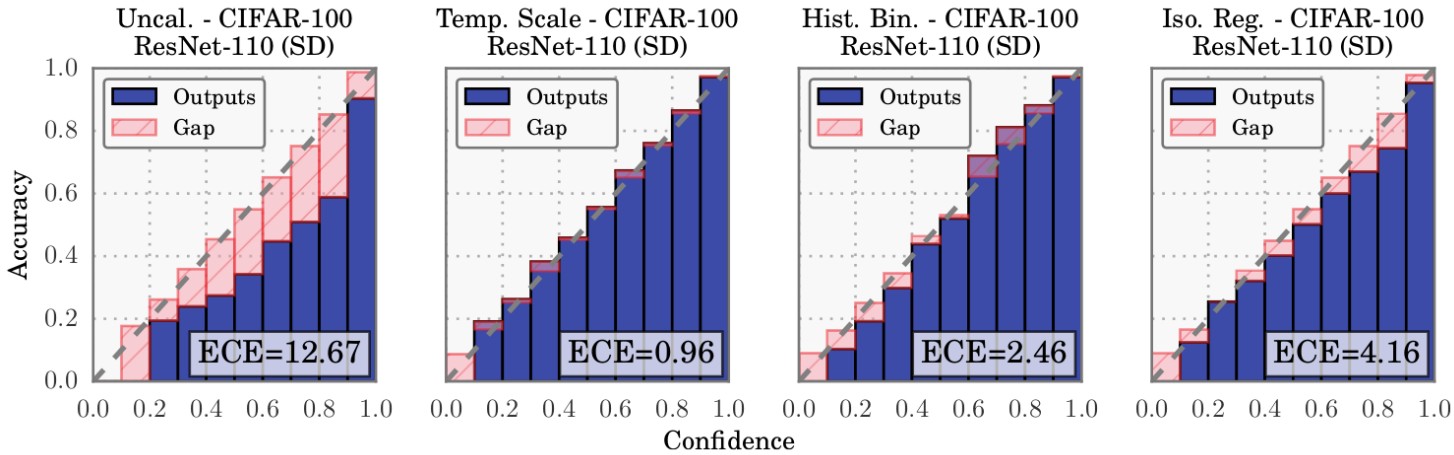

- Results on CIFAR-100 dataset from Guo et al, 2017 (and page 573 in Murphy2)
- Several methods for recalibration:
  1. Platt scaling
  2. Temperature scaling
  3. Histogram binning
  4. Isotonic regression
- In *temperature scaling*, we introduce a temperature parameter $T > 0$ in the softmax-function:

$$p(y|f(\mathbf{x}), T) = \text{Cat}(y|\text{softmax}(f(\mathbf{x})/T))$$

- T is estimated using a validation set.

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- We talked about how we can use *confidence* and *entropy* to quantify the uncertainty for multi-class classification
- Bayesian decision theory: Uncertainties are crucial for optimal decision-making and therefore *calibration* becomes important
- The calibration error can be assessed via the *expected calibration error* (ECE) metric or *reliability curves*

$$\text{ECE} = \sum_{b=1}^{B} \frac{|\mathcal{B}_b|}{M} |\text{acc}(\mathcal{B}_b) - \text{conf}(\mathcal{B}_b)|$$