Machine Intelligence:: Deep Learning
Week 5

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Probabilistic Prediction Models

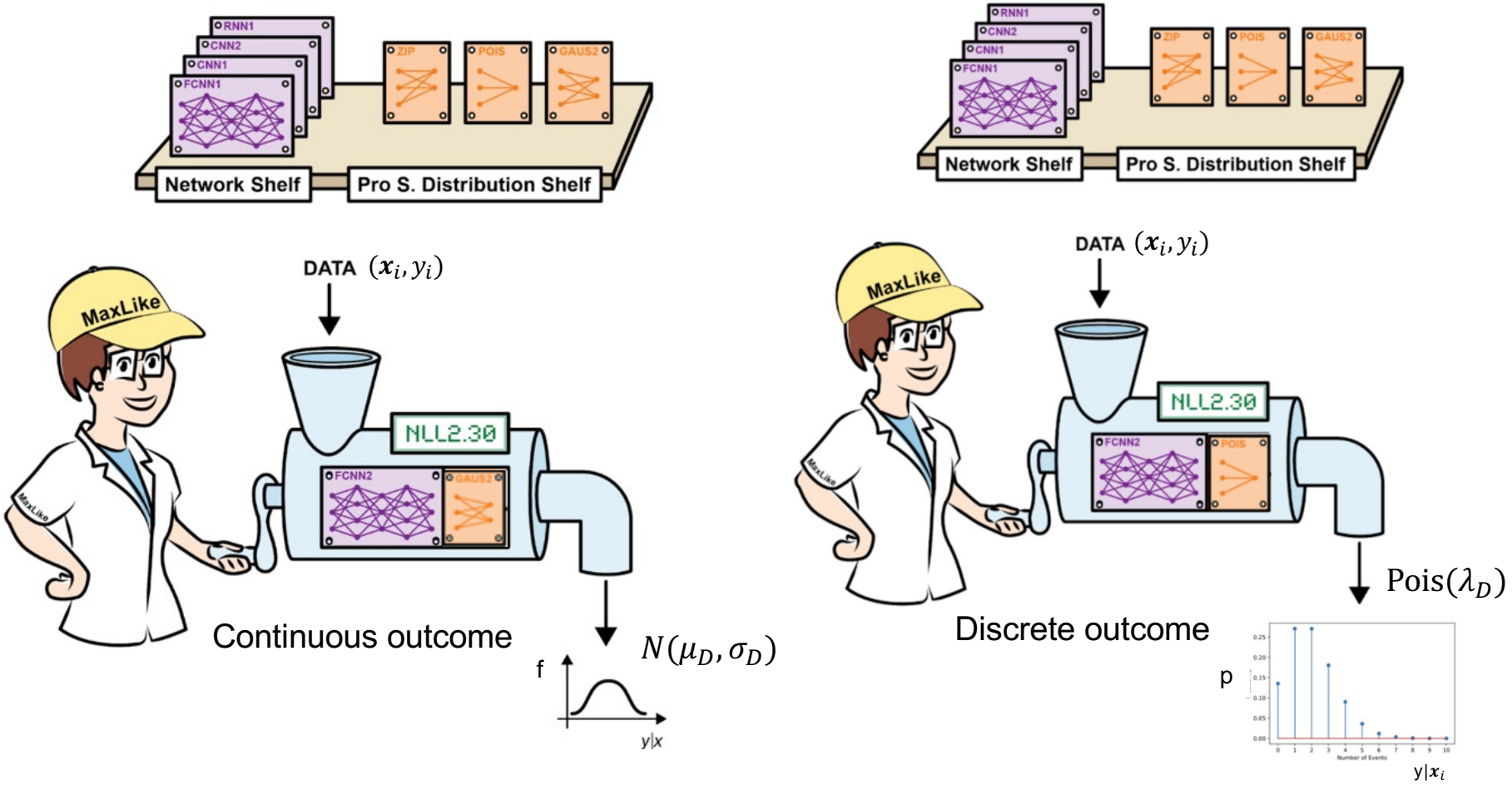
First Version, might change slightly before lecture

Outline of the DL Module (tentative)

- Day 1: Jumpstart to DL
  - What is DL
  - Basic Building Blocks
  - Keras
- Day 2: CNN I
  - ImageData
- Day 3: CNN II and RNN
  - Tips and Tricks
  - Modern Architectures
  - 1-D Sequential Data
- Day 4: Looking at details
  - Linear Regression
  - Backpropagation
    - Resnet
  - Likelihood principle
- Day 5: Probabilistic Aspects
  - Likelihood principle (cont'd)
  - TensorFlow Probability (TFP)
  - Negative Loss Likelihood NLL
  - Count Data
- Day 6: Probabilistic models in the wild
  - Complex Distributions
  - Generative modes with normalizing flows
- Day 7: Uncertainty in DL
  - Bayesian Modeling
- Day 8: Uncertainty cont'd
  - Bayesian Neural Networks
  - Projects

Projects please register (see website)

Probabilistic DL Models for continuous or discrete outcomes



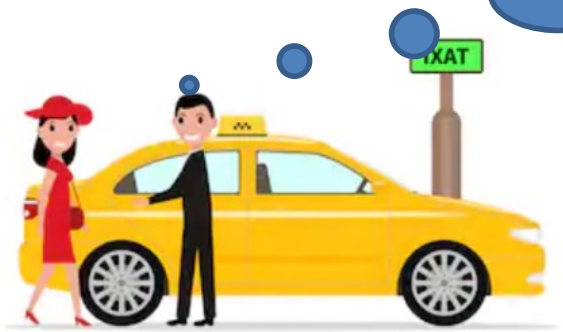
Probabilistic prediction models predict conditional probability distributions (CPDs), rather than only a point estimate.

What is a probabilistic model good for?

Probabilistic travel time prediction (cost)

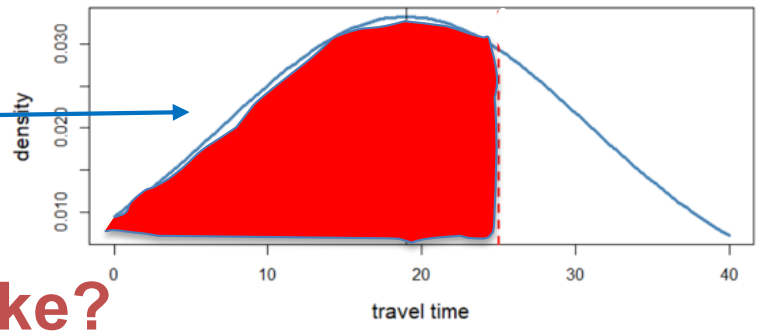
You'll get 500$ tip if I arrive at MOMA within 25 minutes!

Let's use my probabilistic travel time gadget!

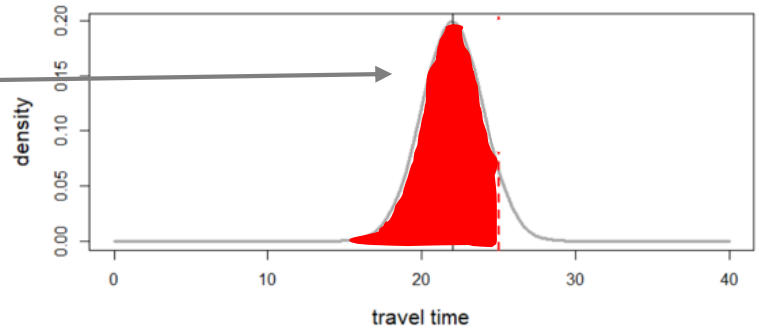


Which way would you take?

Chance to get tip: 69%



Chance to get tip: 93%

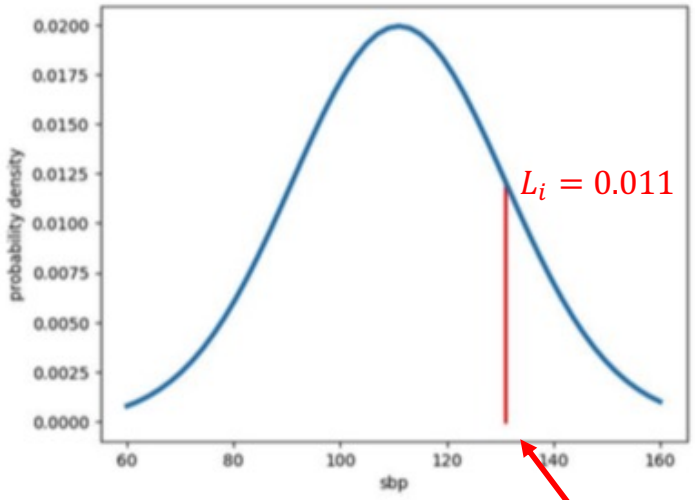


How is a probabilistic model trained via the Maximum Likelihood principle?

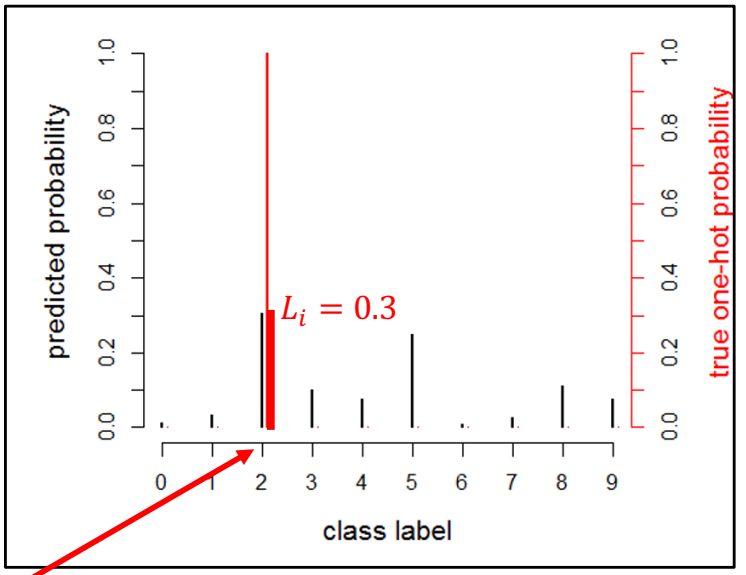
Likelihood L_i of the i-th observation (x_i, y_i)

- Based on the features $\boldsymbol{x_i}$ a CPD for the outcome is predicted
- The likelihood L_i of the observed y_i under the CPD is density of the CPD at the position y_i : $L_i = f_{\text{pred}}(y_i)$

CPD for a continuous outcome

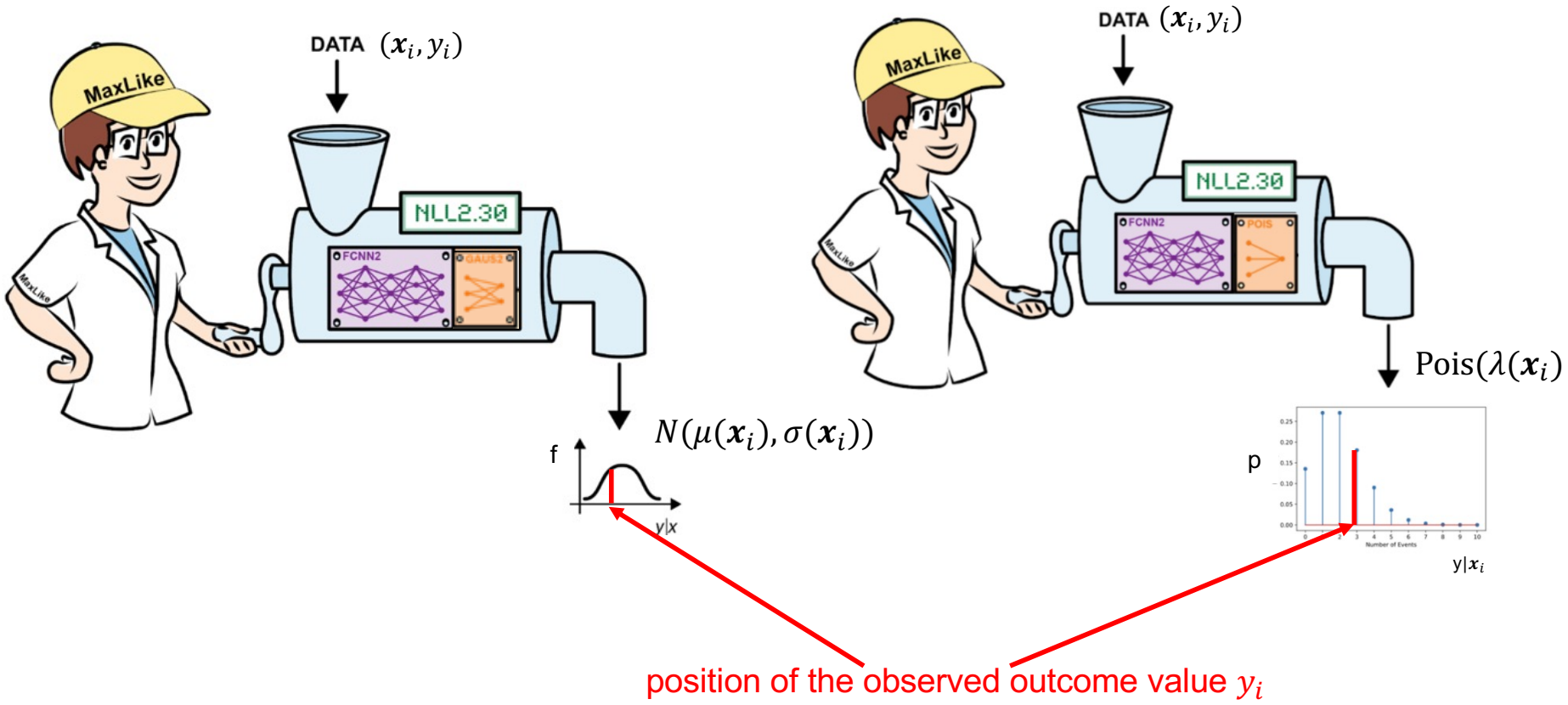


CPD for a discrete outcome



position of the observed outcome value

We use the NLL as loss to train probabilistic models



$$\text{NLL} = -\frac{1}{n}\sum_{i=1}^{n}\log(L_i) = -\frac{1}{n}\sum_i \log f(y_i|\boldsymbol{x}_i) = -\frac{1}{n}\sum_i \log p(y_i|\boldsymbol{x}_i)$$

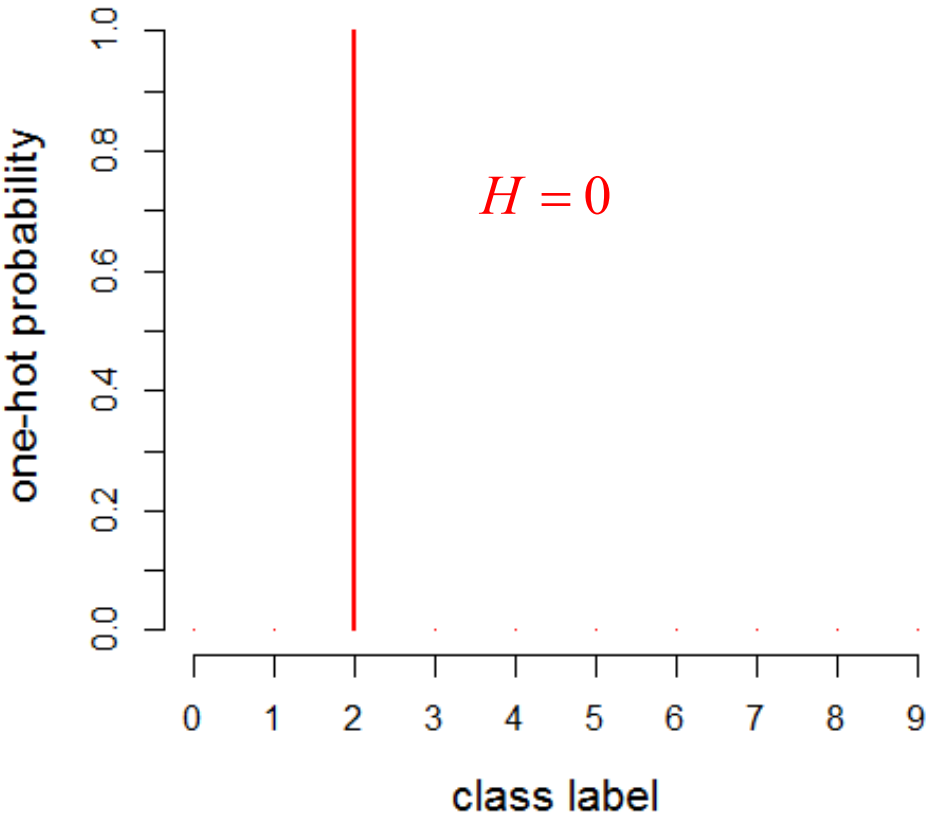
Side track:

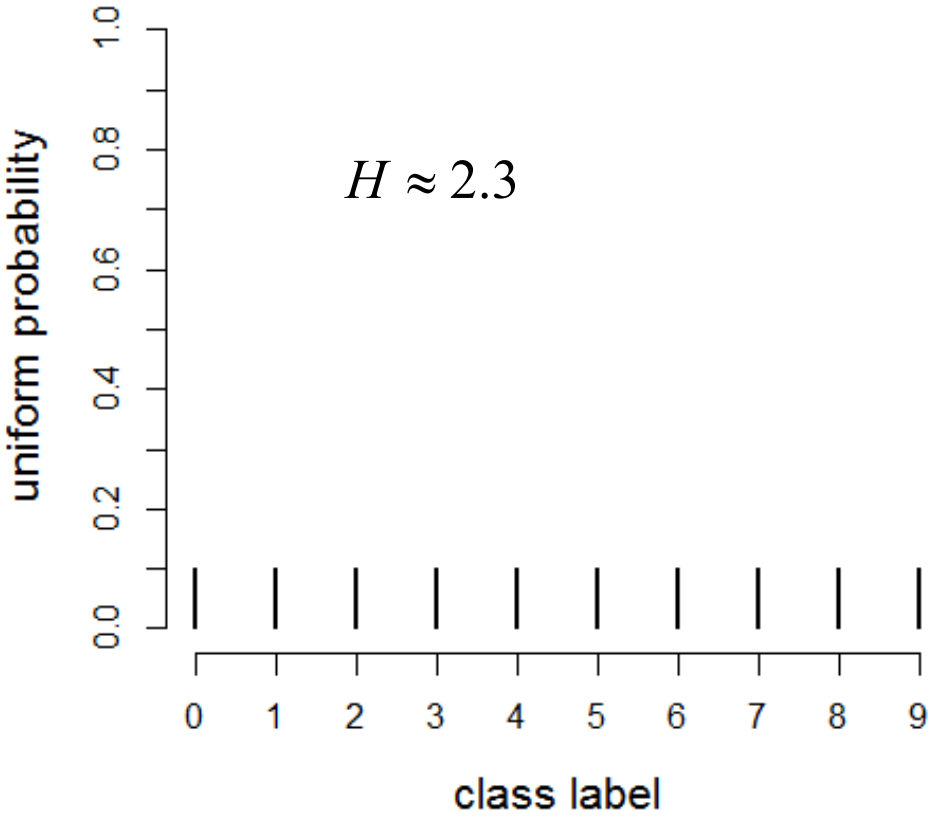
Why the name X-entropy?

Side track: Entropy

$$H(P) = -\sum_i p_i \cdot \log(p_i)$$

Entropy is a measure for “untidyness”.
If a distribution has only one peak, it is tidy and H=0
If all outcomes are equally probable it is maximal untidy

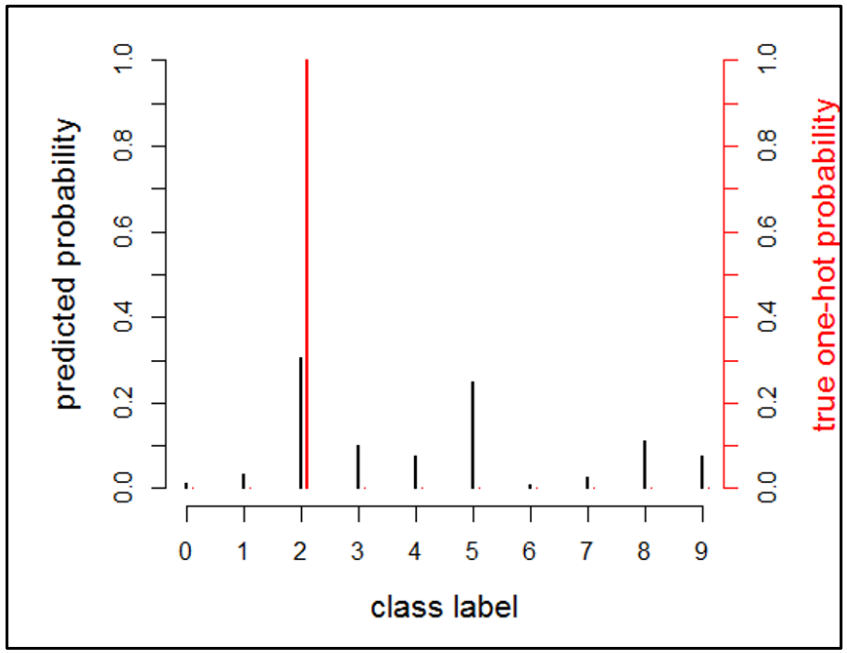




X-entropy

Cross-entropy of ${}^{true}\mathrm{p}$ and ${}^{true}\mathrm{q}$

$$\text{X-entropy} = \sum_i \mathrm{H}({}^{true}\mathrm{p}_i, {}^{pred}\mathrm{q}_i) = -\sum_i {}^{true}\mathrm{p}_i \cdot \log({}^{pred}\mathrm{q}_i) = \mathrm{NLL}$$



The cross-entropy is the same as the NLL, if the true probability distribution puts the whole weight on one class.

Looking back at homework

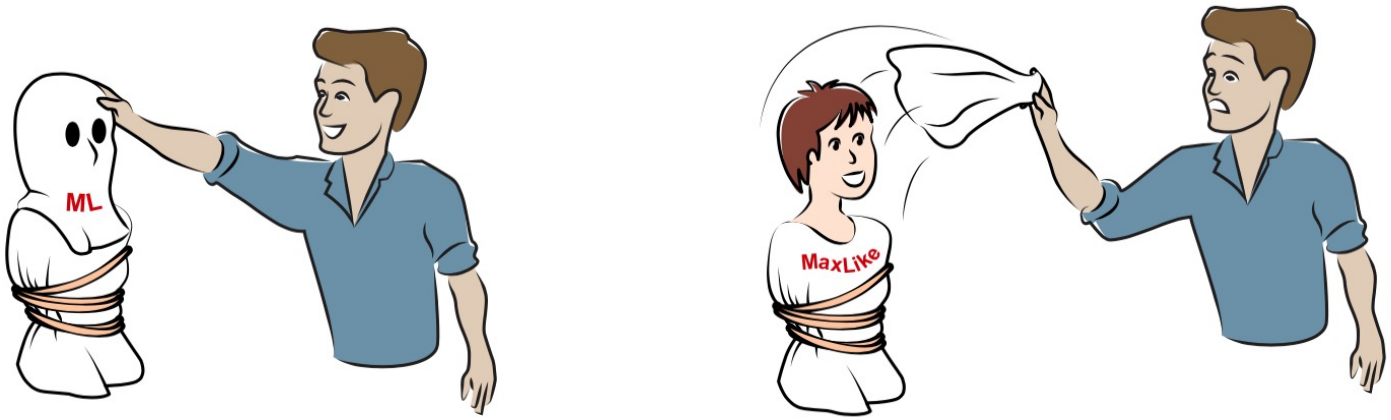
Task:

- Calculate (with calculator or numpy) the excepted cross-entropy for the MNIST example if you just guess, each class with p=1/10.

- Load MNIST and make a small CNN without training and calculate the loss

- See NB 12b_mnist_loglike (Scroll down)

Machine Learning based on the Maximum Likelihood principle



Unmasking the secrets of almost all loss functions in machine learning (ML in figure) and deep learning. After: https://www.instagram.com/neuralnetmemes/

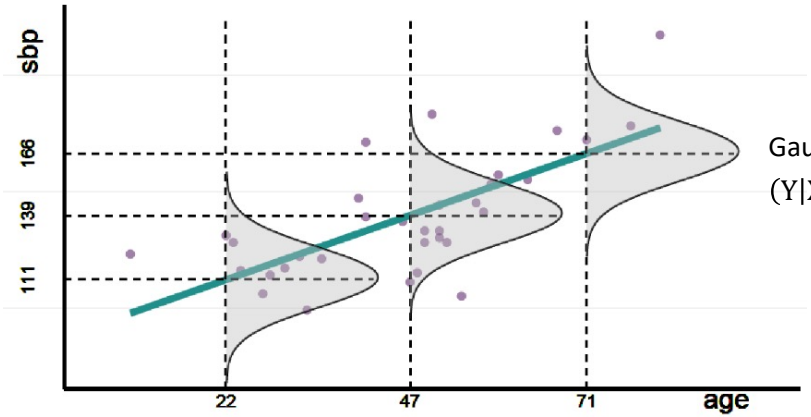
Tune the parameters weights of the network, so that observed data (training data) is most likely under the predicted conditional probability distribution (CPD).

Practically: Minimize Negative Log-Likelihood:

$$\hat{w} = \underset{w}{\operatorname{argmin}} \frac{1}{n} \sum_{i=i}^{N} -\log(p(y_i|x_i, w))$$

Modeling continuous outcomes:

M1: Linear regression

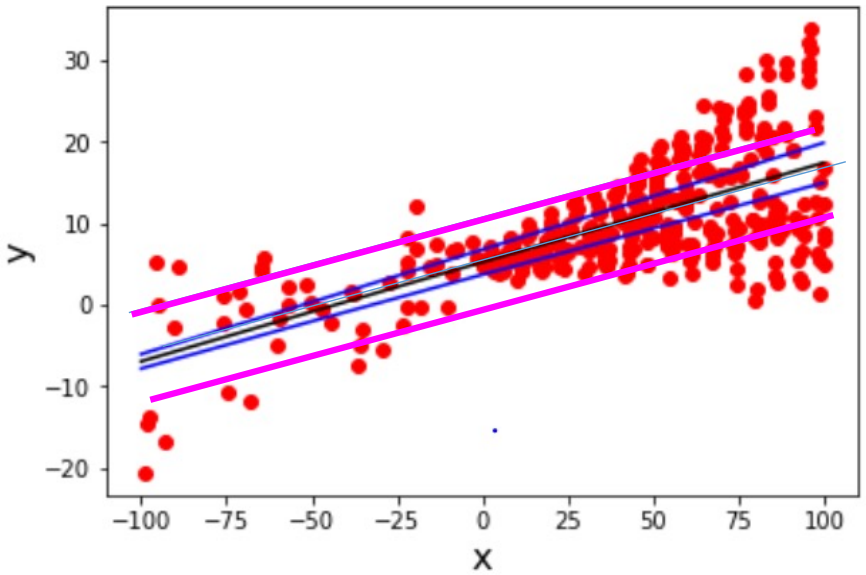


Gaussian CPD

$(\mathrm{Y}|\mathrm{X}_i) \sim \mathrm{N}(\mu(x), \sigma)$

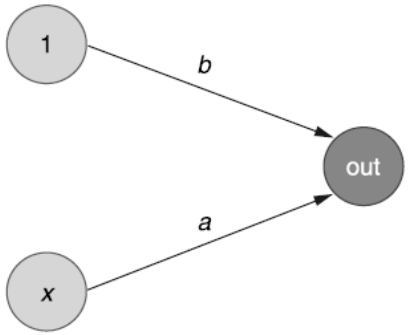
Fit a probabilistic regression with constant variance

$$(Y|x_i) \sim \mathrm{N}(\mu_{x_i}, \sigma)$$



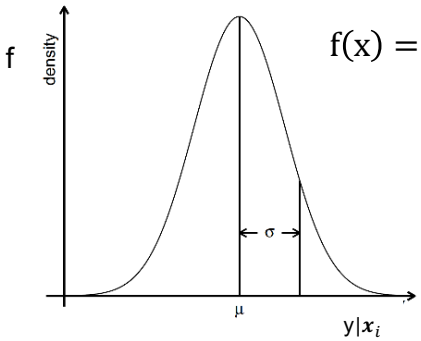
$$(Y|x_i) \sim \mathrm{N}(\mu_{x_i} = ax_i + b, \sigma)$$

b



$\mu_{x_i} = \mathrm{out}_i$

Gaussian CPD



$$f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \cdot e^{-\frac{(y_i-\mu_{x_i})^2}{2\sigma^2}}$$

$$\hat{w} = \underset{w}{\operatorname{argmin}} \sum_{i=1}^{n} -\log\left(\frac{1}{\sqrt{2\pi\sigma^2}}\right) + \frac{(y_i - \mu_{x_i})^2}{2\sigma^2}$$

$$= \underset{w}{\operatorname{argmin}} \sum_{i=1}^{n} (y_i - \mu_{x_i})^2$$

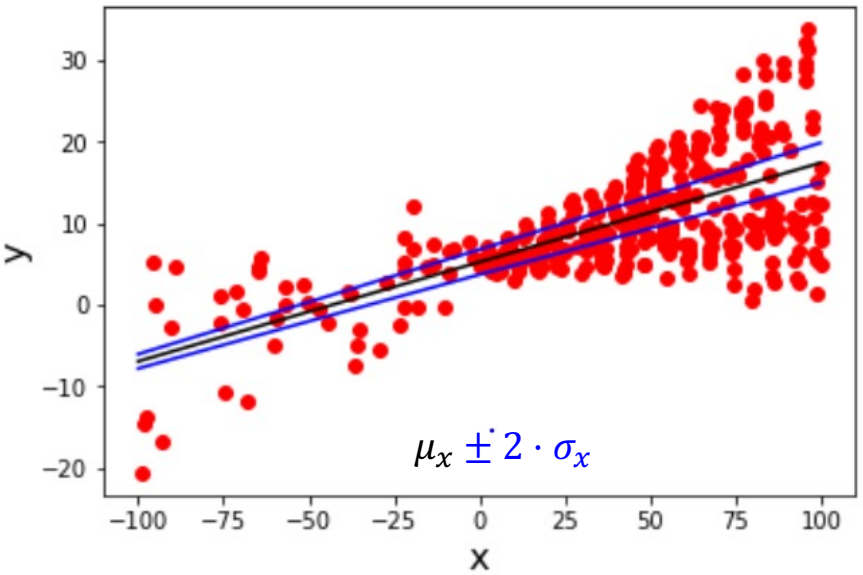
For lin regregession with constant variance, minimizing the NLL is equivalent to minimizing the MSE

SGD

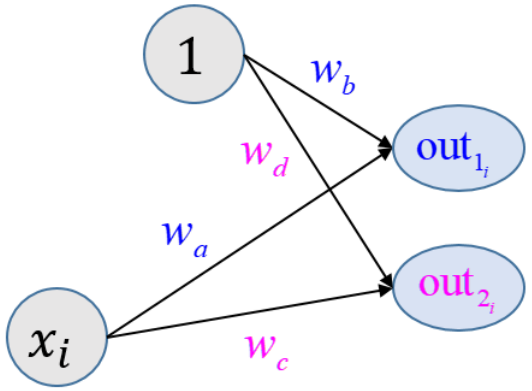
$\hat{a}$ $\hat{b}$

Fit a probabilistic regression with non-constant variance

$$(Y|X_i) \sim N(\mu_{x_i}, \sigma_x^2)$$



$$Y_{X_i} \sim N(\mu_{x_i}, \sigma_x^2)$$

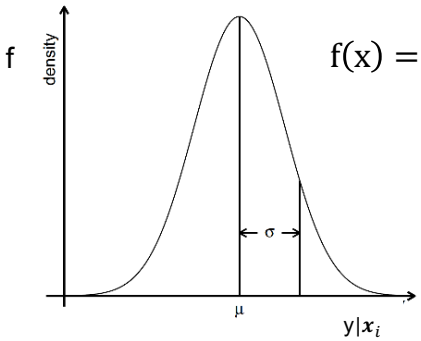


$$\mu_{x_i} = out_{1_i}$$

$$\sigma_{x_i} = e^{out_{2_i}}$$

$$\hat{w} = \underset{w}{\operatorname{argmin}} \sum_{i=1}^{n} -\log\left(\frac{1}{\sqrt{2\pi\sigma_{x_i}^2}}\right) + \frac{(y_i - \mu_{x_i})^2}{2\sigma_{x_i}^2}$$

Gaussian CPD



$$f(x) = \frac{1}{\sqrt{2\pi\sigma_{x_i}^2}} \cdot e^{-\frac{(y_i-\mu_{x_i})^2}{2\sigma_{x_i}^2}}$$

SGD

$\hat{w}_a$ $\hat{w}_b$

$\hat{w}_c$ $\hat{w}_d$

Modelling the standard deviation (positive values)

- The variance or standard deviation are both non-negative $\sigma_{x_i} \geq 0$.
- Neural networks output is not constrained.
- Two common approaches to fix this (exp or softplus)

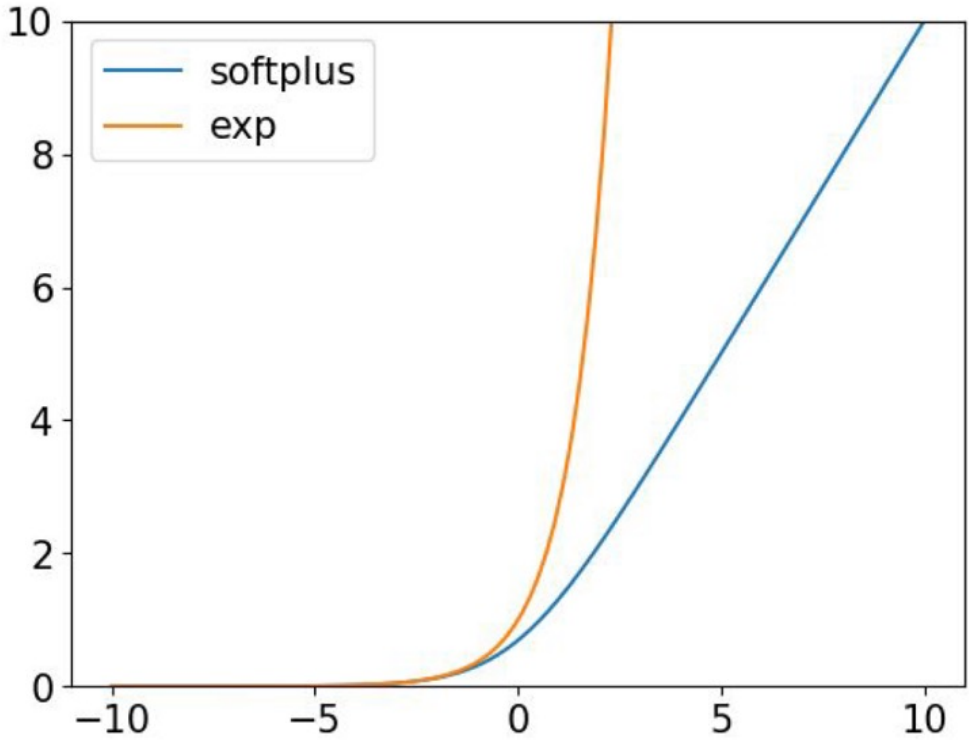
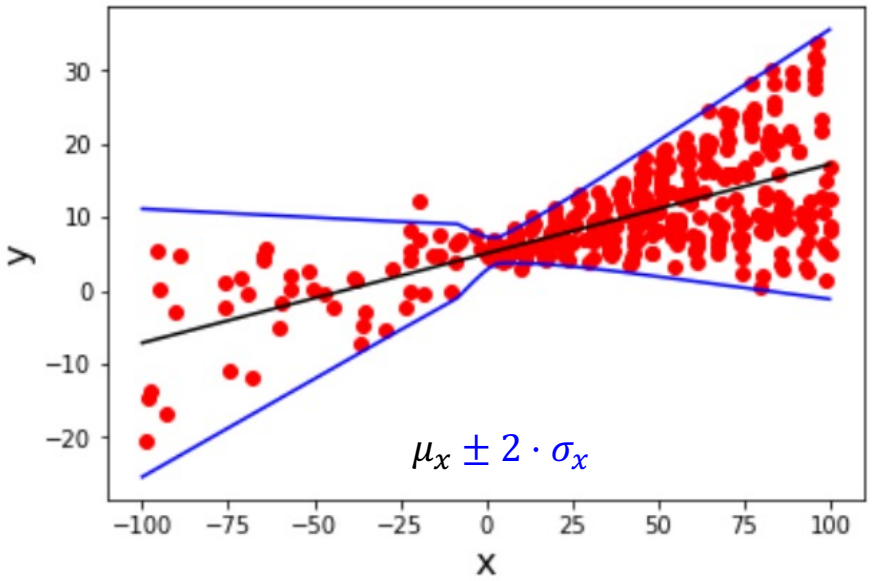
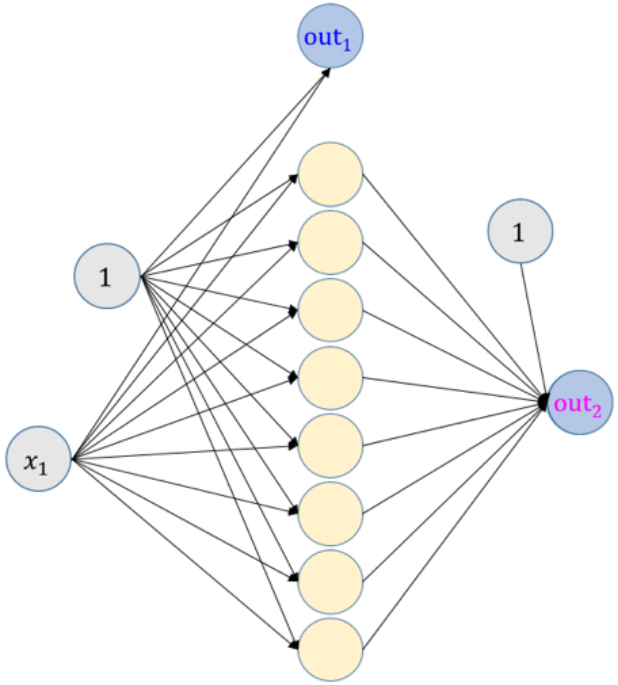


Figure 5.sp: The softplus function compared with the exponential function. Both functions map arbitrary values to positive values.

Fit a probabilistic regression with flexible non-constant variance

$$(Y|X_i) \sim N(\mu_{x_i}, \sigma_x^2)$$





$$\mu_{x_i} = \text{out}_{1_i}$$

$$\sigma_{x_i} = e^{\text{out}_{2_i}}$$

Minimize the negative log-likelihood (NLL):

$$\hat{\mathbf{w}}_{\text{ML}} = \underset{w}{\text{argmin}} \sum_{i=1}^{n} -\log\left(\frac{1}{\sqrt{2\pi\sigma^2}} - \frac{(y_i - \mu_{x_i})^2}{2\sigma_{x_i}^2}\right)$$

SGD

$$\hat{w}_1, \ \hat{w}_{.2}, \ \ldots, \ \hat{w}_{.27}$$

Note: we do not need to know the "ground truth for σ_x" – the likelihood does the job!

How to evaluate a probabilistic prediction model?

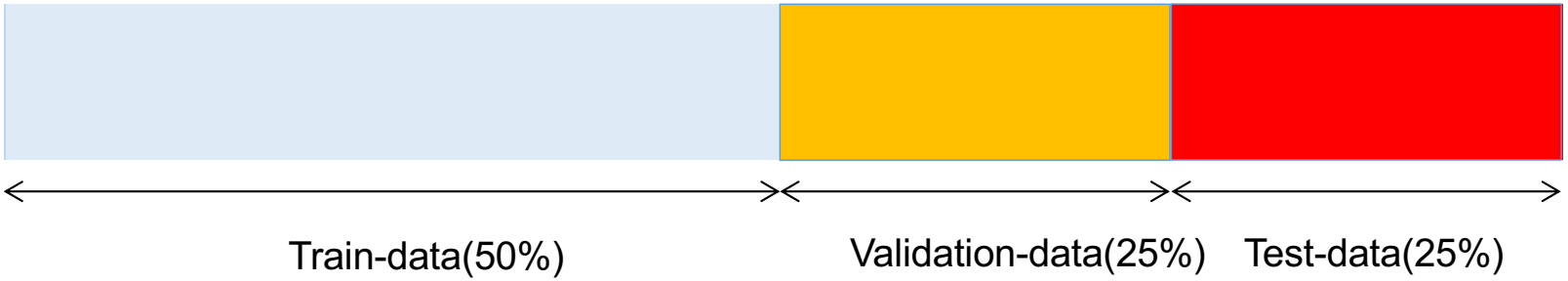
Aim

- For fitting / training there is the NLL (a.k.a. categorical x entropie)
- How to evaluate…

Check prediction quality on NEW data

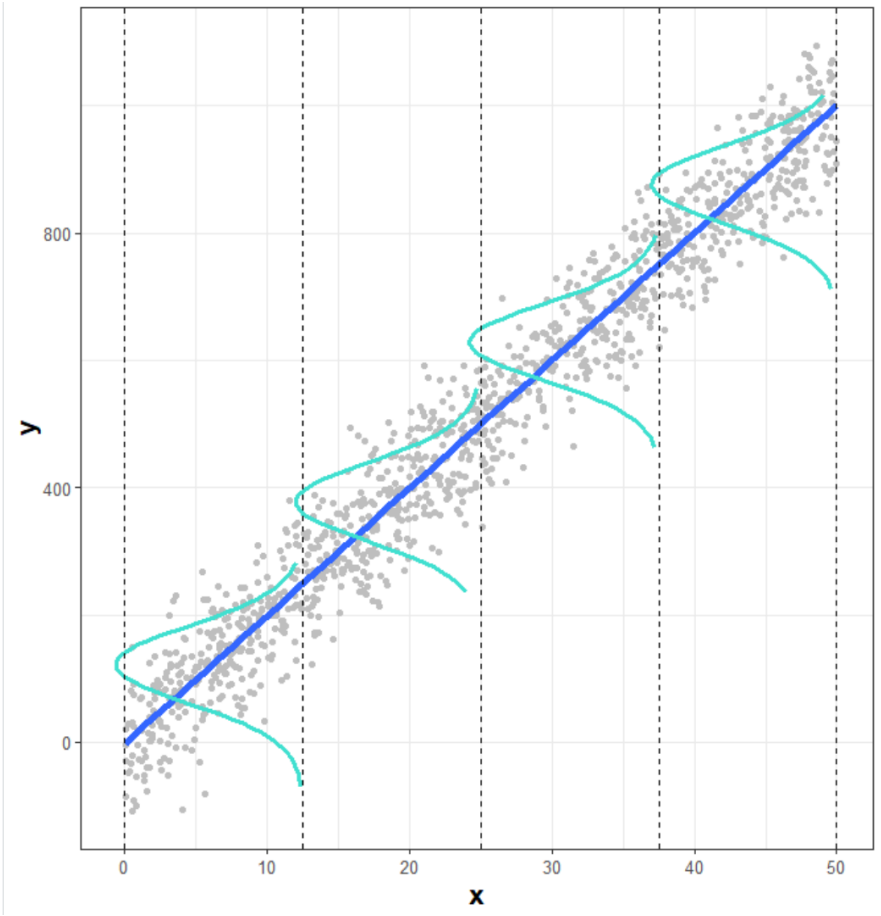
Nils Bohr, physics Nobel price 1922

Common data split:

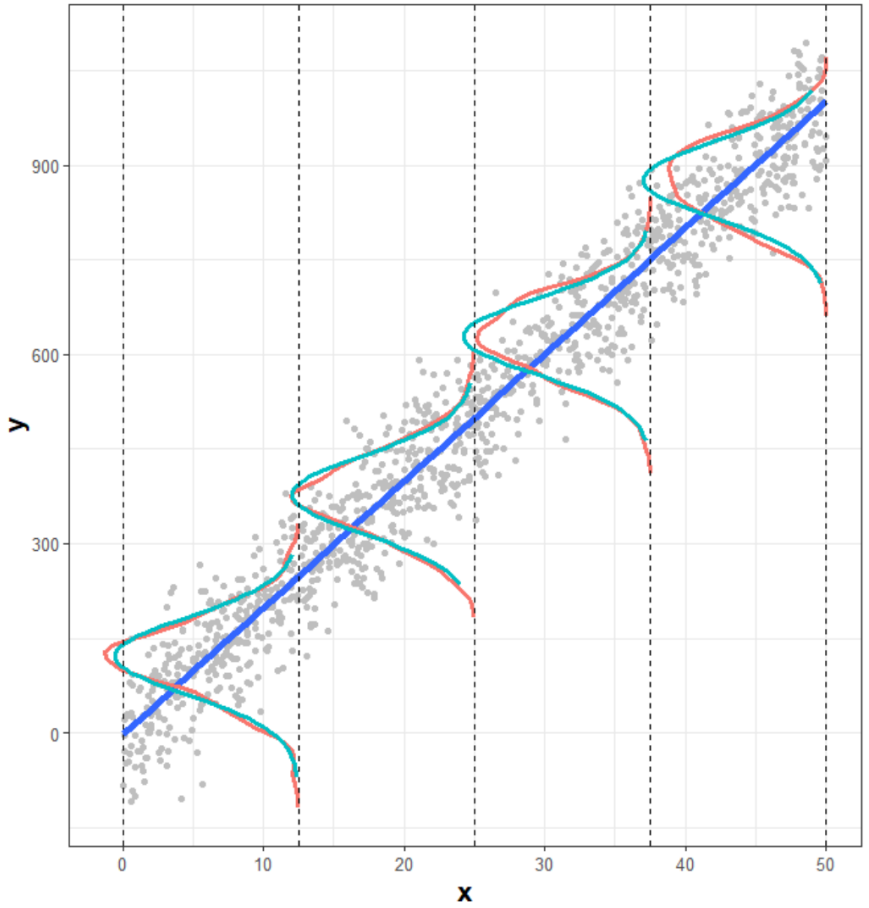


Visually: Do predicted and observed outcome distribution match?

Validation data along with predicted outcome distribution (Gauss with const σ)

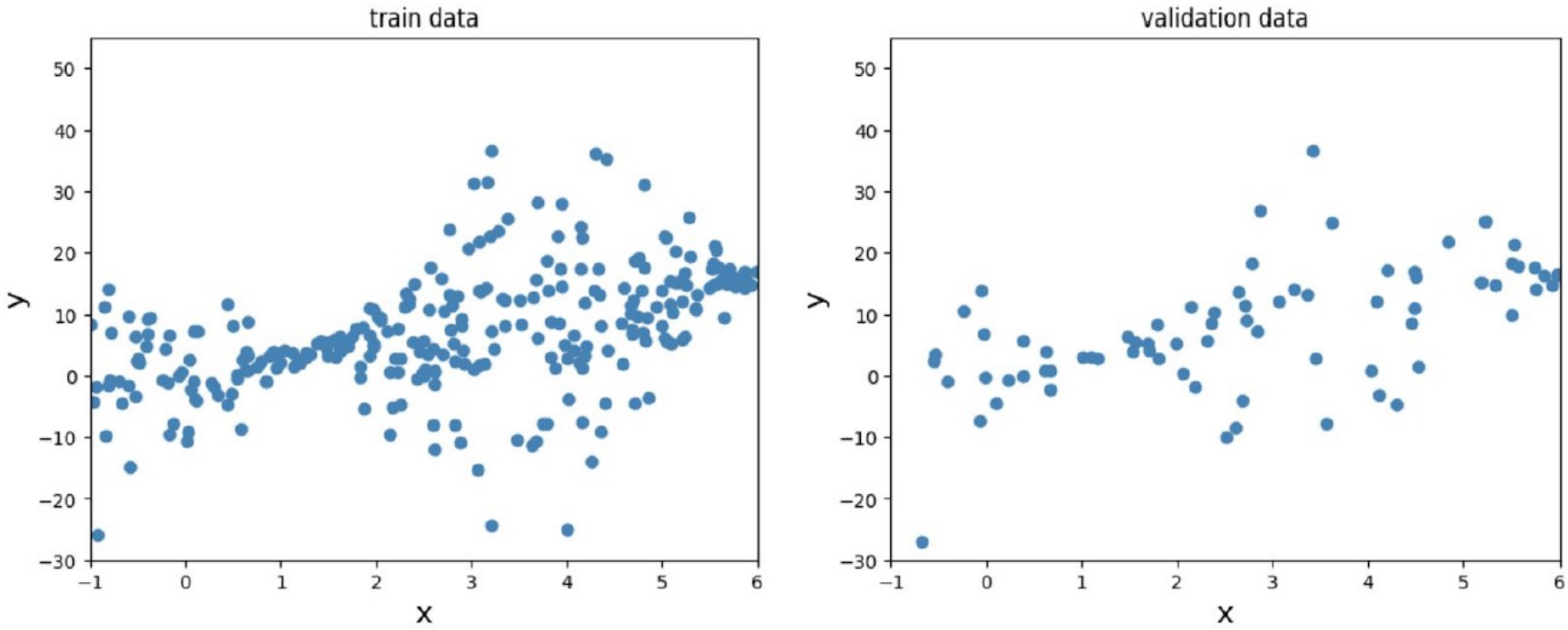


Validation data along with predicted and observed outcome distribution



A large validation data set is needed to ensure underlying assumption:
observed distribution = data generating distribution

Example: Simulated data for linear regression models

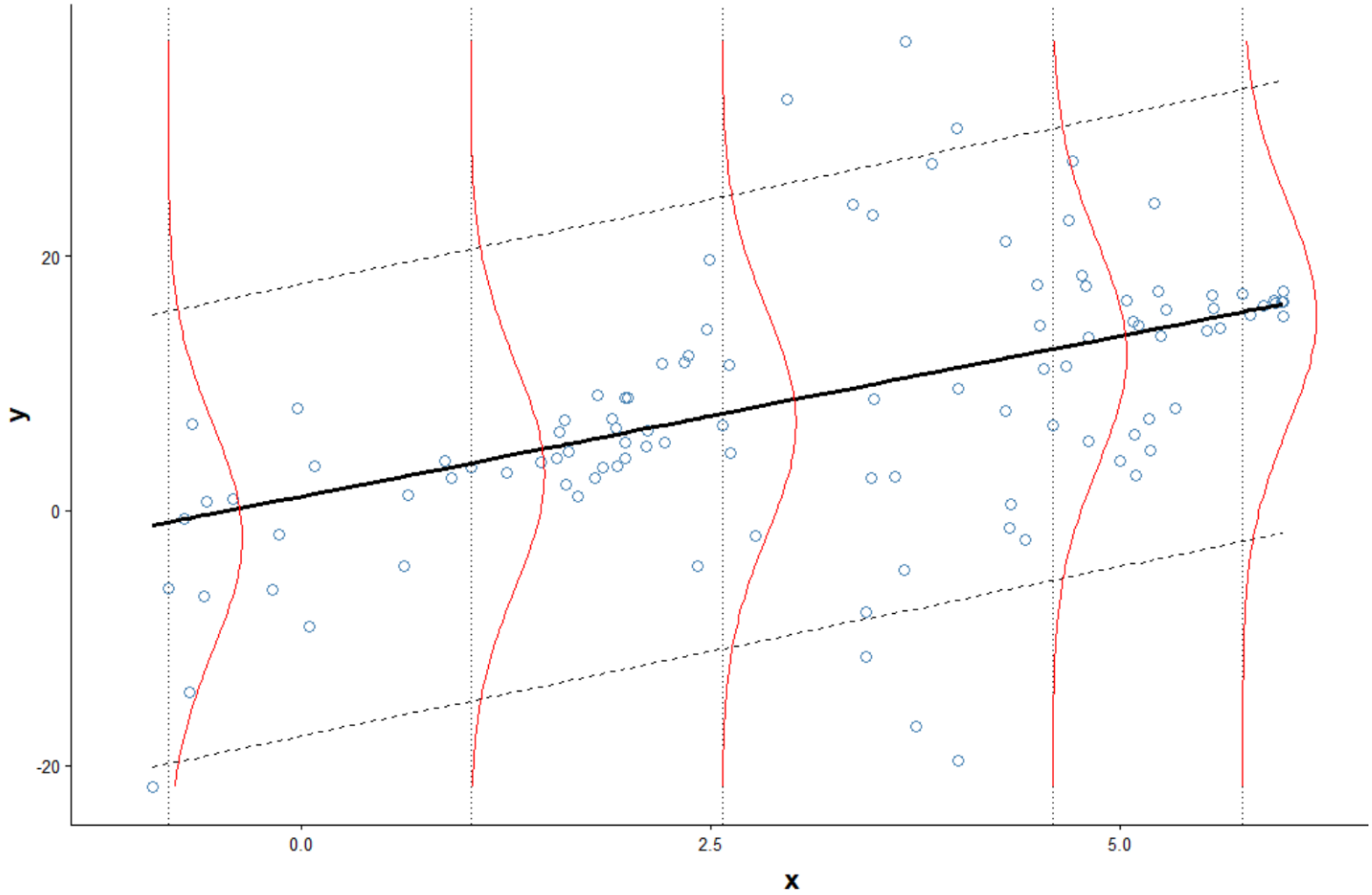


Model_1 (linear regression with constant variance): $(y \mid x) \sim N(\mu_x, \sigma^2)$

Model_2 (linear regression with flexible variance): $(y \mid x) \sim N(\mu_x, \sigma_x^2)$

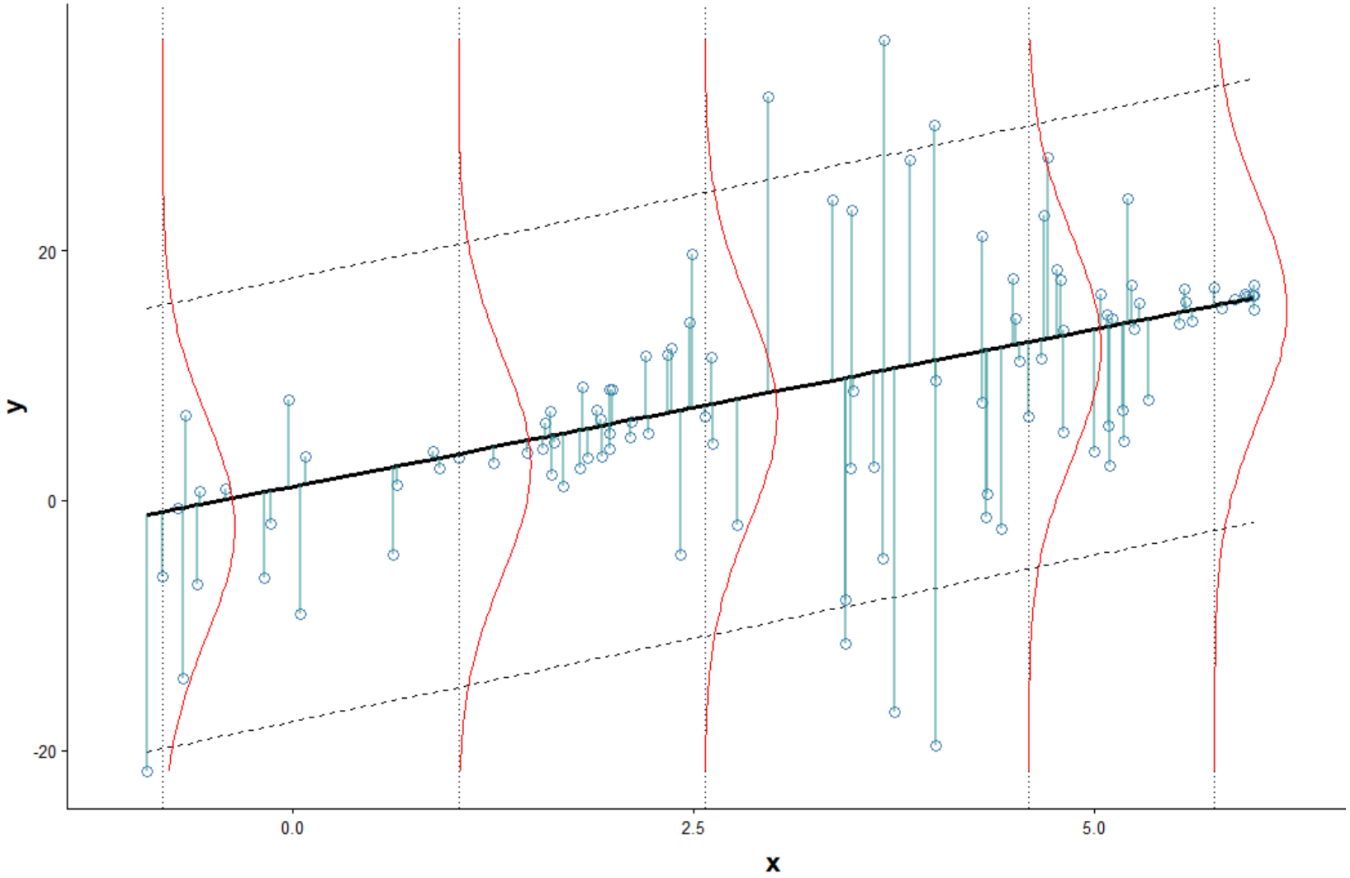
Predicted outcome distribution from model_1 (constant σ)

Validation data



Root mean square error (RMSE) or mean absolute error (MAE)

Validation data



$$\text{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{\mu}_{x_i})^2}$$

$$\text{MAE} = \frac{1}{n}\sum_{i=1}^{n}\left|y_i - \hat{\mu}_{x_i}\right|$$

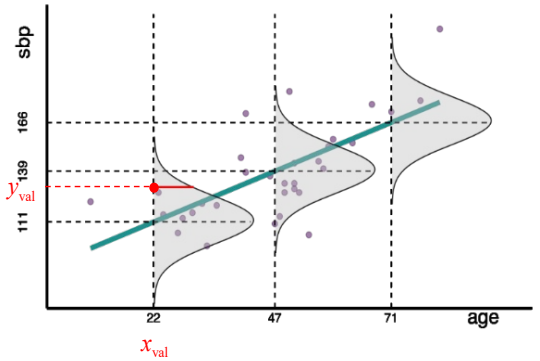
RMSE and MAE alone do not capture performance for probabilistic models!

Both only depend on the mean (μ) of the CPD, but not on it's shape or spread (σ) and are not appropriate to evaluate the quality of the predicted distribution of a probabilistic model.

Use the NLL to score a probabilistic prediction model

A score *S* takes the CPD and *one test instance* and yields a real number
(the smaller the score the better is the predicted CPD)

$$S_{\mathrm{NLL}}\left(p(y \mid x_{val}), y_{val}\right) = -\log\left(p(y_{val} \mid x_{val})\right)$$



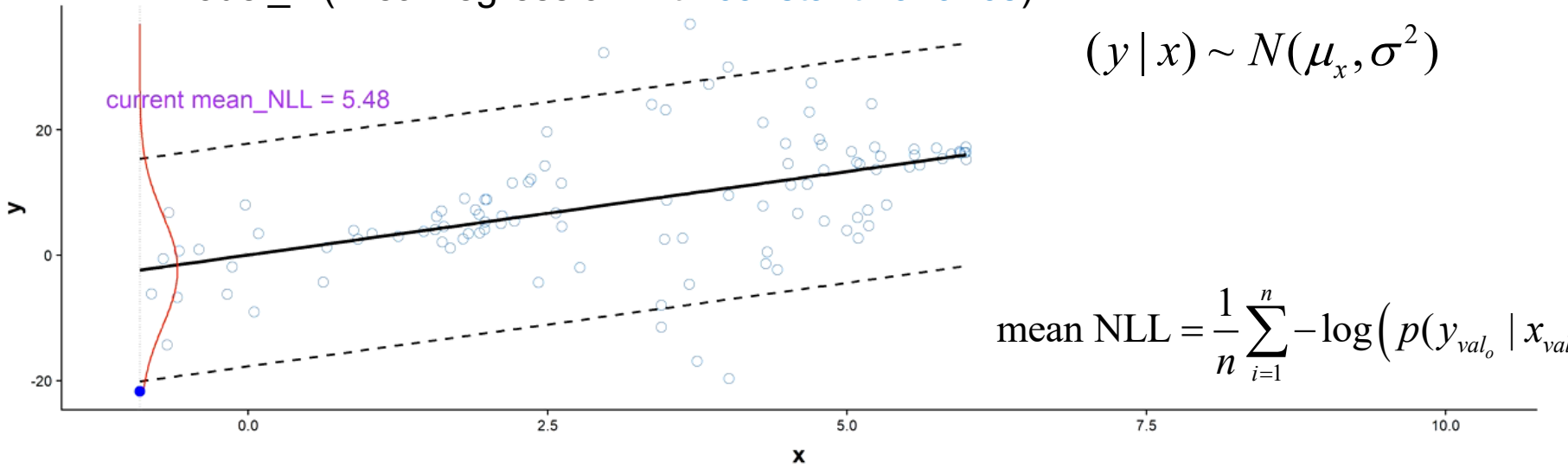
Definition of the term “strictly proper”: A strictly proper score is then and only then minimal, when the predicted CPD matches the true CPD.

It is provable that the negative log-likelihood (NLL, aka log-score) is the only smooth, proper and local score for continuous variables

(Bernardo, J. M., 1979: Expected information as expected utility. *Ann. Stat.,* **7,** 686–690)

Use validation NLL to compare probabilistic models

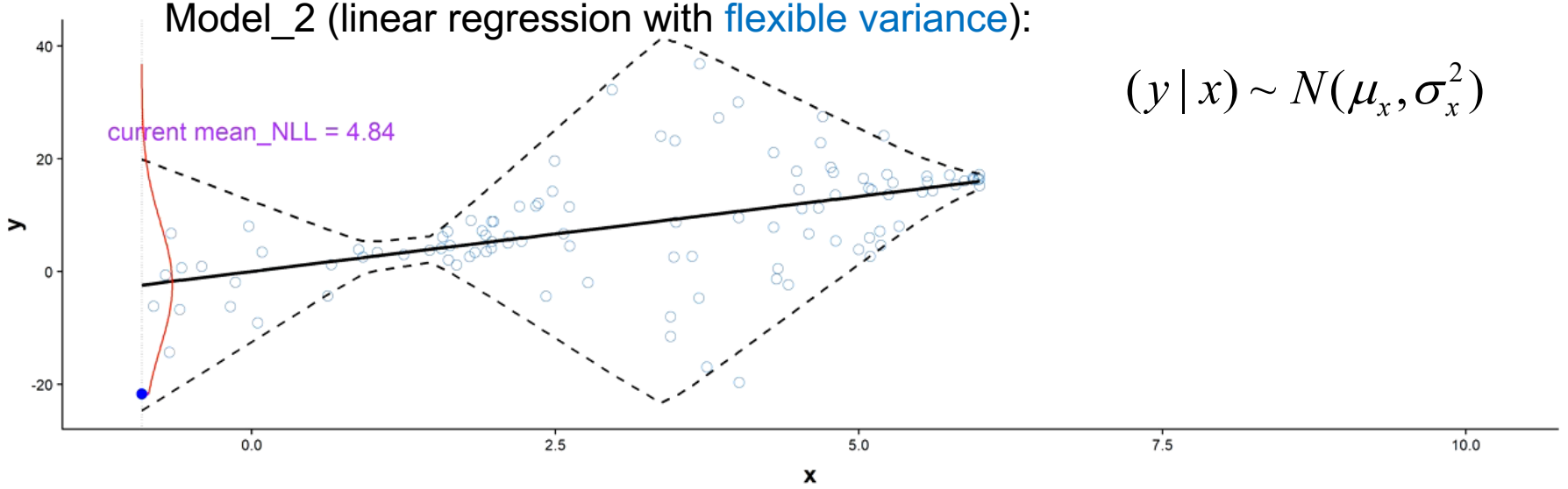
Model_1 (linear regression with constant variance):



$$(y \mid x) \sim N(\mu_x, \sigma^2)$$

$$\text{mean NLL} = \frac{1}{n}\sum_{i=1}^{n} -\log\left(p(y_{val_o} \mid x_{val_i})\right)$$

Model_2 (linear regression with flexible variance):



$$(y \mid x) \sim N(\mu_x, \sigma_x^2)$$

Tensorchief's youtu.be channel

NLL as general cure-all in probabilistic modeling

Training of probabilistic models

- Maximize likelihood ↔ minimize negative log-likelihood (NLL)

Evaluation / model comparison:

- The log-score (NLL) is strictly proper score for regression*.
- The log-score (NLL) is also strictly proper for classification** models.

=> To evaluate or compare probabilistic models: use the validation NLL!

The NLL, one score to rule them all!

* For regression you could also use the non-local but strictly proper CPRS
**For classification you could also use the strictly proper Brier score

Two practical ways of modeling and fitting CPD

Approach 1 (using standard Keras):

- Use the nodes in the last layer of a NN to control the parameters of a CPD (e.g. μ and σ in case of a Gaussian)
- Use the CPD the determine the likelihood for each observation and compute the NLL over all training observations, which serves as loss.
- Keras has build in loss functions (https://keras.io/losses/) for the following CPDs:
  - Discrete outcomes
    - Bernoulli CPD: loss='binary_crossentropy '
    - Categorical CPD: loss='categorical_crossentropy '
    - Poisson CPD: loss='poisson'
  - Continuous outcomes
    - Gaussians CPD (with fixed σ): loss='mean_squared_error'

Approach 2 (using tensorFlow robability):

- use CPDs and corresponding loss functions from TFP

TensorFlow Probability

TFP: Working with probability distributions

```
import tensorflow_probability as tfp
tfd = tfp.distributions
d = tfd.Normal(loc=[3], scale=1.5)
x = d.sample(2)
px = d.prob(x)
print(x)
print(px)
```

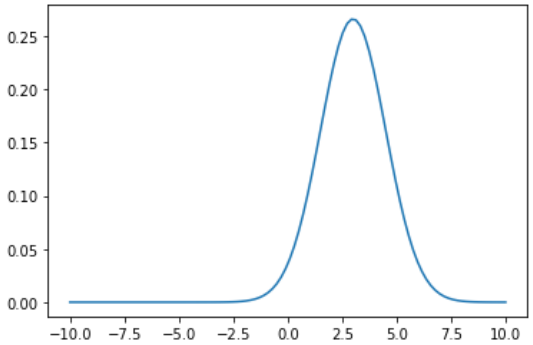
Creates a 1D Normal distribution with a mean of 3 and a standard deviation of 1.5

Samples two realizations from the Normal distribution

Computes the likelihood for each of the two sampled values in the defined Normal distribution

```
tf.Tensor( [[2.3158536][5.8714476]],
shape=(2, 1), dtype=float32)

tf.Tensor( [[0.23968826][0.04256715]],
shape=(2, 1), dtype=float32)
```

```
x = np.linspace(-10,10,100)
plt.plot(x, d.prob(x))
plt.show()
```



https://towardsdatascience.com/introduction-to-tensorflow-probability-6d5871586c0e

TensorFlow Distributions [Do Demo]

TensorFlow Probability (TFP) is nice add-on to Keras:

Methods for Tensorflow distributions	Description	Numerical result when calling the method on `dist = tfd.Normal(loc=1.0, scale=0.1)`

`sample(n)`	Samples *n* numbers from the distribution.	`dist.sample(3).numpy()`
		
		`array([1.0985107, 1.0344477, 0.9714464], dtype=float32)`
		
		Note that these are random numbers

`prob(value)`	Returns the likelihood (probability density in the case of models for continuous outcomes) or probability (in the case of models for discrete outcomes) for the values (tensor)	`dist.prob((0,1,2)).numpy()`
		
		`array([7.694609e-22, 3.989423e+00, 7.694609e-22], dtype=float32)`

`log_prob(value)`	Returns the log-likelihood or log-probability for the values (tensor)	`dist.log_prob((0,1,2)).numpy()`
		
		`array([-48.616352 ,   1.3836466, -48.616352 ], dtype=float32)`

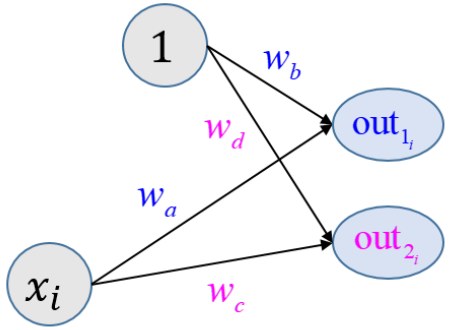
`cdf(value)`	Returns the cumulative distribution function (CDF) that this is a sum or the integral, up to the given values (tensor)	`dist.cdf((0,1,2)).numpy()`
		
		`array([7.619854e-24, 5.000000e-01, 1.000000e+00], dtype=float32)`

`mean()`	Returns the mean of the distribution	`dist.mean().numpy()`
		
		`1.0`

`stddev()`	Returns the standard deviation of the distribution	`dist.stddev().numpy()`
		
		`0.1`

TFP Lambda Layer for outputting a TFP distribution

- Lambda Layer connects the output of the network with the distribution



The Lambda Layer

In [74]:
```
from tensorflow.keras.layers import Input
from tensorflow.keras.layers import Dense
from tensorflow.keras.models import Model
from tensorflow.keras.optimizers import Adam

def my_dist(params):
  return tfd.Normal(
      loc=params[:,0:1], #First for location
      scale=1e-3 + tf.math.softplus(0.05 * params[:,1:2])
  )

inputs = Input(shape=(1,))
h1  = Dense(10)(inputs)
# Here could be large network
params = Dense(2)(h1) #We have to parameters
dist = tfp.layers.DistributionLambda(my_dist)(params) #Connecting Network
model = Model(inputs=inputs, outputs=dist)
model.summary()
```

https://github.com/tensorchiefs/dl_course_2022/blob/master/notebooks/12_TensorFlowDistributions_Demo.ipynb

Get the loss and predicted CPD from the TFP distribution

```
[ ]  1 def NLL(y, distr):
     2   return -distr.log_prob(y) #Just NLL, works for all distributions
     3
     4 model.compile(Adam(), loss=NLL) #F
```

```
  1 model = Model(inputs=inputs, outputs=dist)
  2 x = np.asarray([[1],[2.3]], dtype='float32')
  3 x.shape
  4 cpd = model(x) # Returns a CPD for the x
```

```
[ ]  1 cpd.mean() #The expectations at the positions
```

```
<tf.Tensor: shape=(2, 1), dtype=float32, numpy=
array([[-0.24419746],
       [-0.5616542 ]], dtype=float32)>
```

```
[ ]  1 cpd.stddev() #The spread at the positions
```

```
<tf.Tensor: shape=(2, 1), dtype=float32, numpy=
array([[0.71965677],
       [0.75376725]], dtype=float32)>
```

TensorFlow Distributions [Do Demo]

TensorFlow Probability (TFP) is nice add-on to Keras:

Demo 12_TensorFlowDistributions_Demo.ipynb

Model the CPD

Machen Sie Aufgabe 13_linreg_with_tfp

Modeling count data:

M2: Poisson regression

The camper example

N=250 groups visiting a national park

Y=count: number of fishes cought

X1=persons: number of persons in group

X2=child: number of children in the group

X3=bait: indicates of life bait was used

X4=camper: indicates if camper is brought

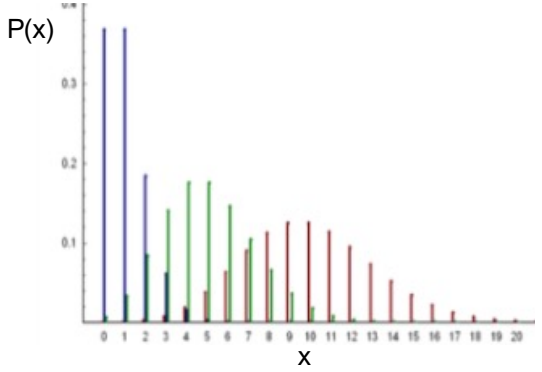
Data: https://stats.idre.ucla.edu/r/dae/zip

Recall the classical Poisson model for count data

X: number of incidences **per time unit**

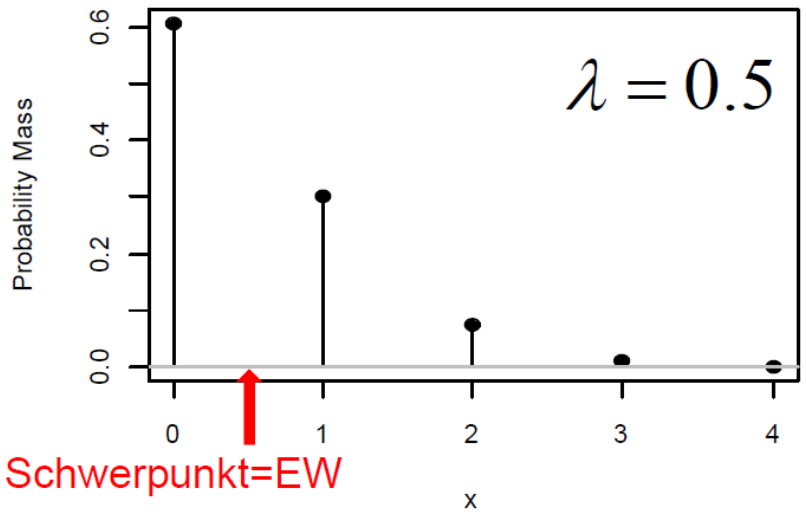
The Poisson model is appropriate to model **counts X per unit**, assuming that
1) the unknown incidence rate λ (per time unit) is constant and
2) the incidences occur independently

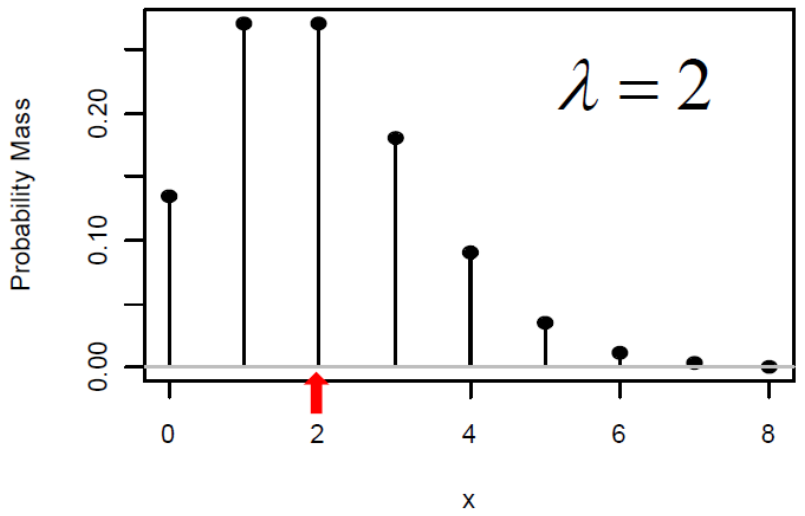
$$P(X = x) = \frac{\lambda^x}{x!} e^{-\lambda} \quad , \qquad x = 0, 1, 2, \ldots$$

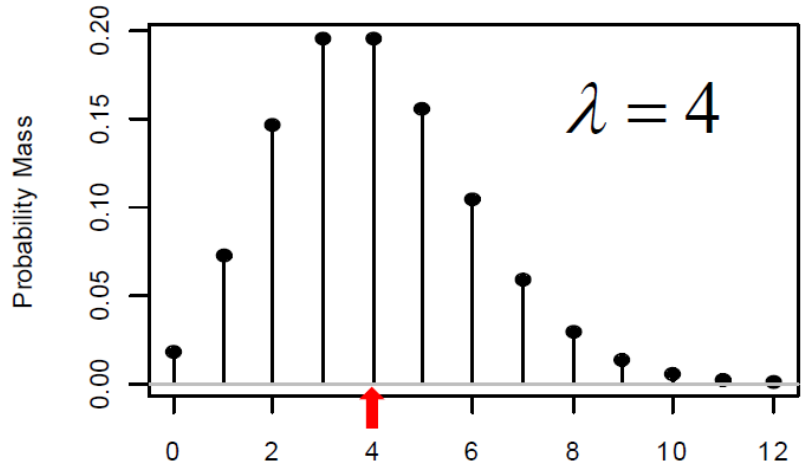


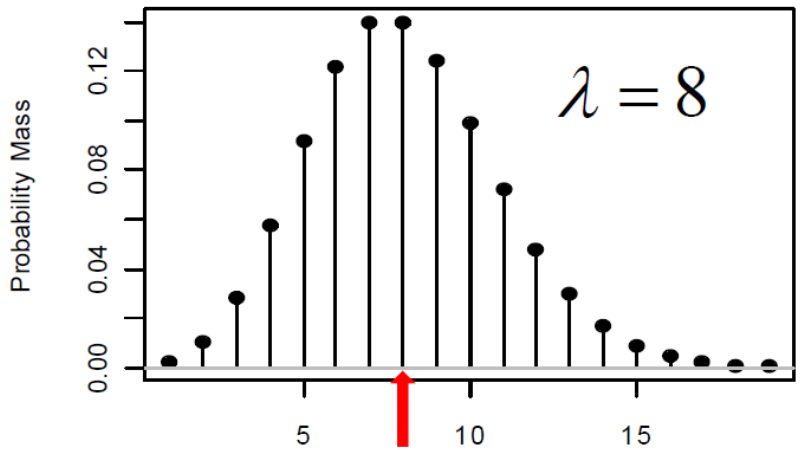
$E(X) = Var(X) = \lambda$: expected number of counts per time unit

The shape and mean of the Poisson distribution depends on λ









The Poisson distribution in tfp

```
dist = tfd.poisson.Poisson(rate = 2) #A

vals = np.linspace(0,10,11) #B

p = dist.prob(vals) #C
```

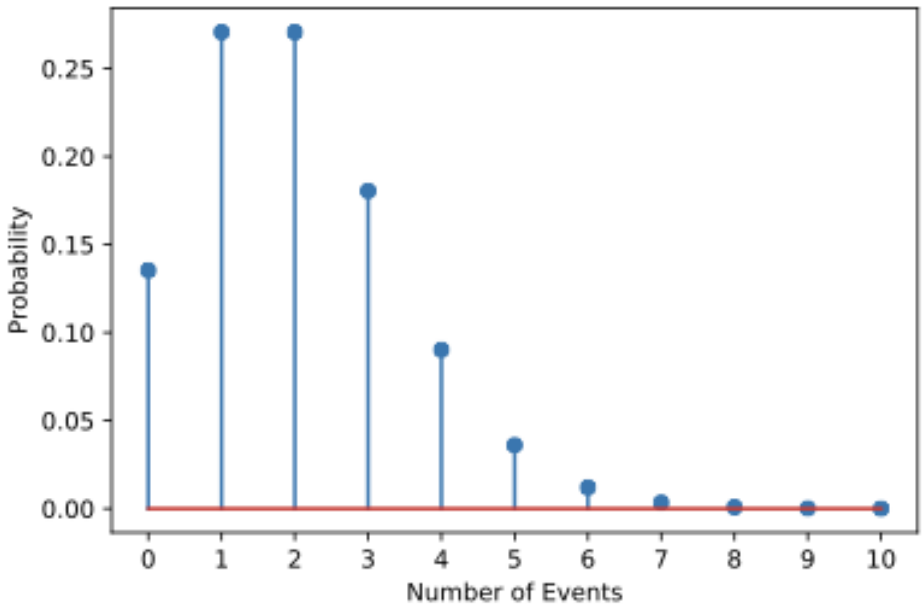


Figure 5.13 Poisson distribution for the case that there are, on average, two events per unit

Poisson regression for count data

Goal: Predict a Poisson CPD for (Y|X=x) which depends on predictor values

CPD: $Y_{X_i} = (\mathrm{Y}|\mathrm{X}_i) \sim \mathrm{Pois}(\lambda_{x_i})$

We only need to model λ_x to fix the Poisson CPD!

Model:

$$\log(\lambda_i) = \underbrace{\beta_0 + \beta_1 x_{i1} + \ldots + \beta_p x_{ip}}_{\text{Linear predictor } \eta_i}$$

link-function: ensures positive λ after back-transformation

CPD encoded by Poisson regression

$$\text{CPD:}\quad Y_{X_i} = (\mathrm{Y}|\mathrm{X}_i) \sim \mathrm{Pois}(\lambda_{x_i})$$

$$\mathrm{Y}_x \in \bullet_0 \quad , \quad \lambda_x \in \sim$$

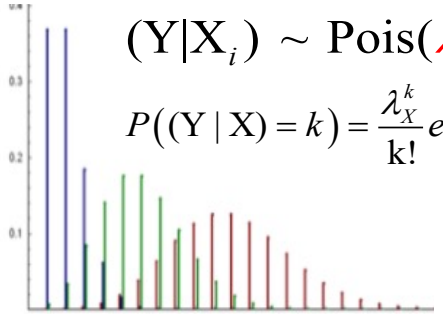
$$\log\left(E(\mathrm{Y}_{x_i})\right) = \log(\lambda_{x_i}) = \beta_0 + \beta_1 x_{i1}$$

$$E(Y_{x_i}) = \mathrm{Var}(Y_{x_i}) = \lambda_{x_i} = e^{\beta_0 + \beta_1 x_{i1}}$$

The predicted value of the Poisson regression gives the only one parameter of the CPD: λ_x that depends on the predictor values. We have no error term in the regression formula since the uncertainty of the outcome (counts) is given by the probabilistic Poisson model Pois(λ_x)

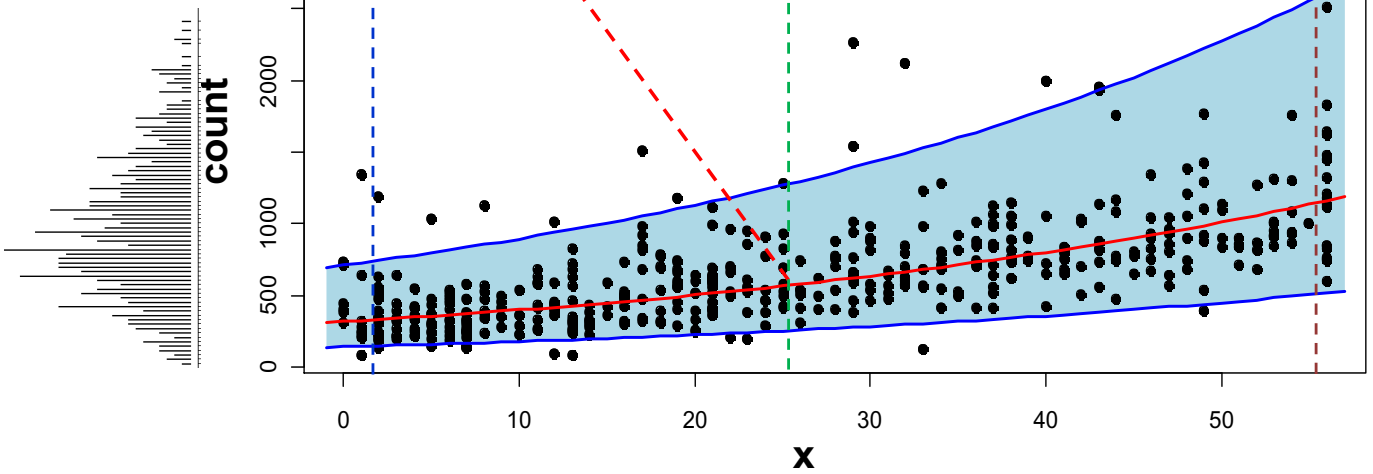
$$(\mathrm{Y}|\mathrm{X}_i) \sim \mathrm{Pois}(\lambda_{x_i})$$

$$P\left((\mathrm{Y} \mid \mathrm{X}) = k\right) = \frac{\lambda_X^k}{\mathrm{k!}} e^{-\lambda_X} \quad , \quad k = 0,1,2,\ldots$$



$$\mathrm{Y} \sim \mathrm{V}^{discrete}_{arbirary}$$

$$(\mathrm{Y}|\mathrm{X}_i) \sim \mathrm{Pois}(\lambda_{x_i})$$



Model 2: Poisson regression via NNs in keras

We use a NN without hidden layer to control the rate λ.

```
inputs = Input(shape=(X_train.shape[1],))
rate = Dense(1,
             activation=tf.exp)(inputs) #A
p_y = tfp.layers.DistributionLambda(tfd.Poisson)(rate)

model_p = Model(inputs=inputs, outputs=p_y) #C
```

Using the exp-activation ensures that the rate λ is a positive number

Glueing the NN and the output layer together. Note that output p_y is a tf.distribution

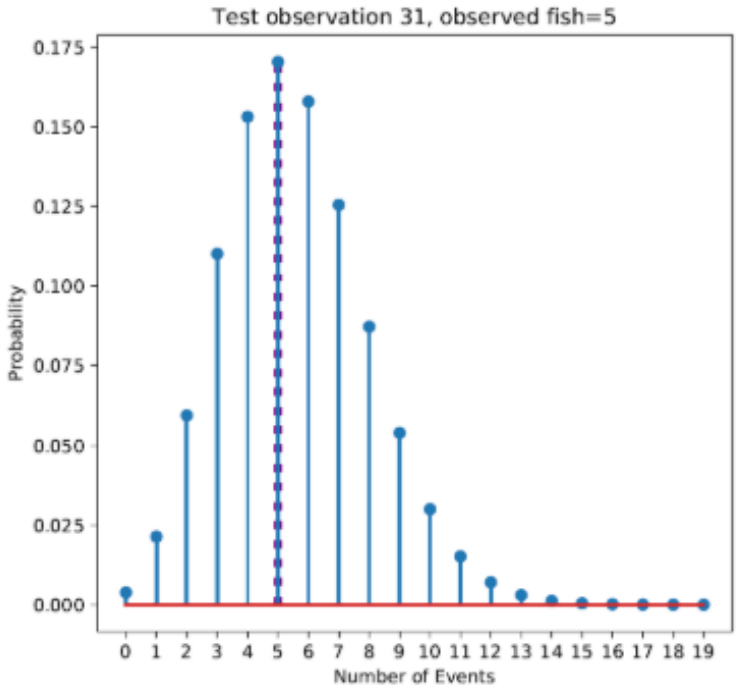
```
def NLL(y_true, y_hat): #D
  return -y_hat.log_prob(y_true)

model_p.compile(Adam(learning_rate=0.01), loss=NLL)
model_p.summary()
```

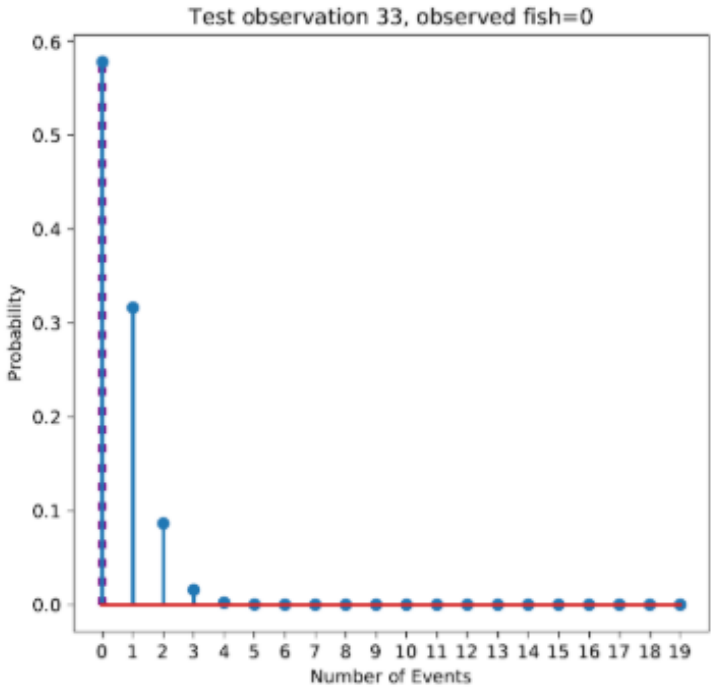
The second argument is the output of the model and thus a TFP distribution. It's as simple as calling log_prob to calculate the log probability of the observation that's needed to calculate the NLL

Model 2: Poisson regression, get test NLL from Gaussian CPD

Predict CPD for outcome in test data:

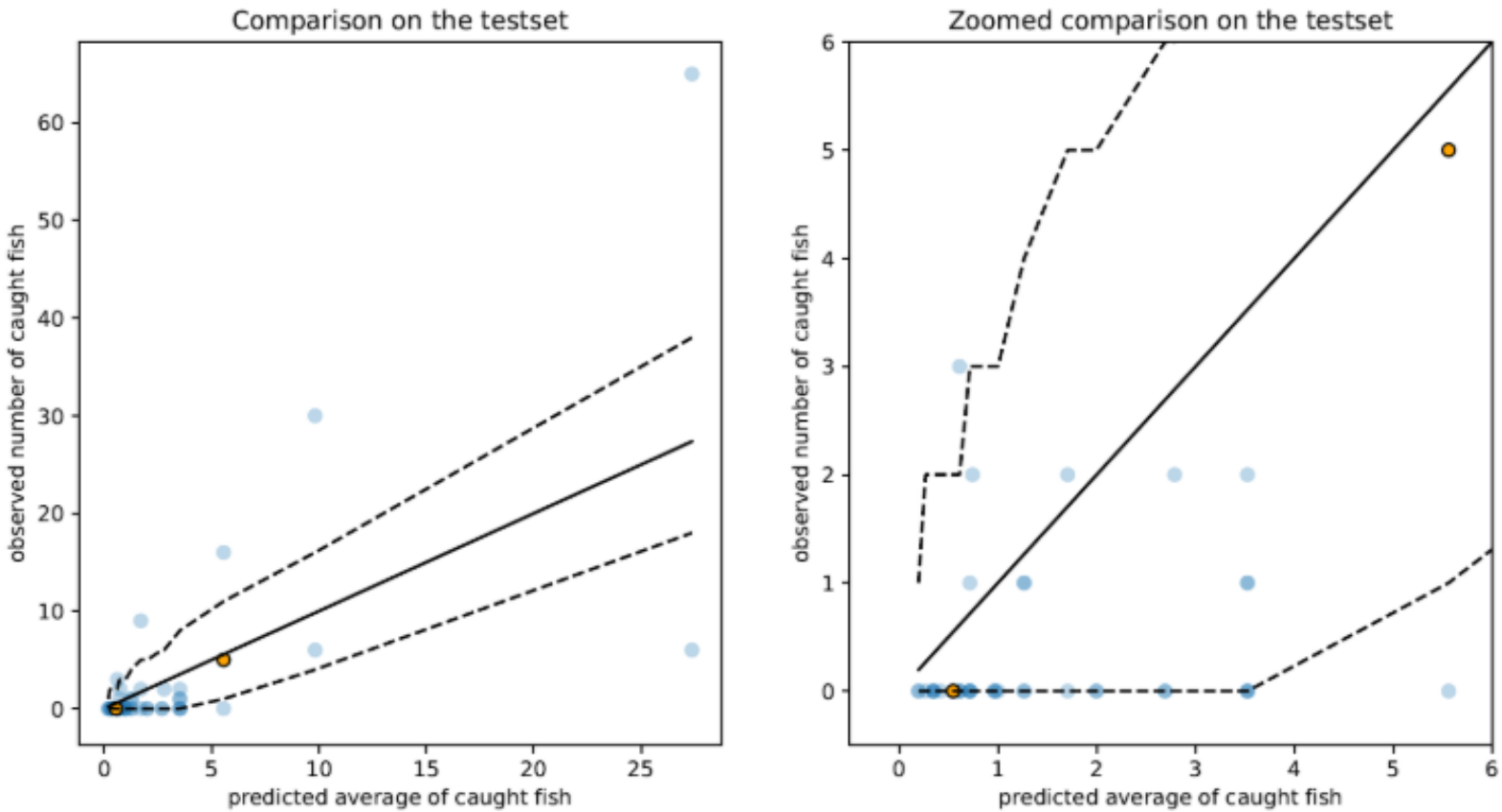
Group 31 used livebait, had a camper and were 4 persons with one child. Y=5 fish.
Group 33 used livebait, didn't have a camper and were 4 persons with two childern. Y=0 fish.





What is the likelihood of the observed outcome in test obs 31 and 33?

Model 2: Poisson regression, visualize the CPDs by quantiles



The mean of the CPD is depicted by the solid lines.
The dashed lines represent the 0.025 and 0.975 quantiles,
yielding the borders of a 95% prediction interval.

Note that different combinations of predictor values can yield the same parameters of the CPD.

Ufzgi

14_poisreg_with_tfp.ipynb

https://github.com/tensorchiefs/dl_course_2022/blob/master/notebooks/14_poisreg_with_tfp.ipynb

Summary

- A probabilistic model predicts for each input a whole conditional probability distribution (CPD).
- The predicted CPD assigns for each possible outcome *y*, a probability with which it's expected.
- The negative log-likelihood (NLL) measures how well the CPD matches the actual distribution of the outcomes (lower is better).
- The NLL is used as a loss function when training a probabilistic model.
- The NLL on new data is used to measure, and to compare, the prediction performance of different probabilistic models.
- Using a proper choice for the CPD enhances the performance of your models.
- For continuous data, a common first choice is a Normal distribution
- For count data, common choices for distribution are Poisson, Negative-Binomial, or Zero-inflated Poisson (ZIP).