Machine Intelligence:: Deep Learning Week

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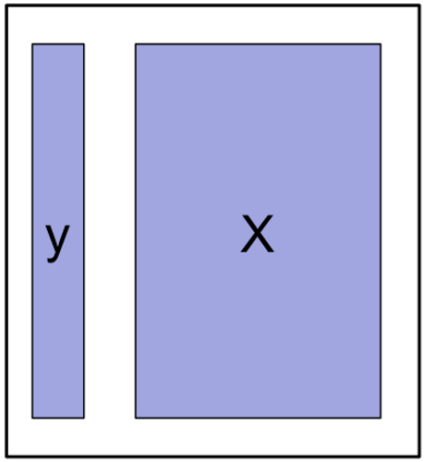
Most of the slides were developed by Oliver Dürr & Beate Sick

Outline of the DL Module (tentative)

The course is split in 8 sessions, each 4 lectures long. Topics might be adapted during the course

Day	Date	Time	Topic
1	15.04.2025	09:00-12:30	Introduction to Deep Learning & Keras, first NNs
-	21.04.2025	-	FRÜHLINGS-FERIEN
-	28.04.2025	-	FRÜHLINGS-FERIEN
2	06.05.2025	09:00-12:30	Loss, Optimization, Regression, Classification
3	13.05.2025	09:00-12:30	Computer vision, CNN-archictecture
4	20.05.2025	09:00-12:30	DL in practice, pretrained (foundation) models
5	27.05.2025	09:00-12:30	Model evaluation, baselines, xAI, troubleshooting
6	03.06.2025	09:00-12:30	Generative Models, Transformer-architecture
7	10.06.2025	09:00-12:30	Vision Transformer
8	17.06.2025	09:00-12:30	Projects, deep Ensembling

Supervised DL for Classification or Regression tasks



Supervised Learning

- Typical supervised DL task: predict y given x
  - **Classification**
    - Point prediction: Predict a class label
    - Probabilistic prediction: predict a discrete probability distribution over the class labels
    - First, we focus on probabilistic binary classification where $Y \in \{0,1\}$
  - Regression
    - Point prediction: Predict a number
    - Probabilistic prediction: predict a continuous distributions

Probabilistic vs deterministic models

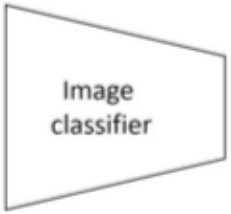
Likelihood L_i of the observed outcome y_i under the predicted conditional outcome distribution $P(Y|x_i)$

Deterministic

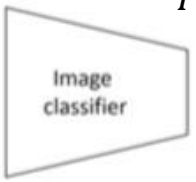
Probabilistic

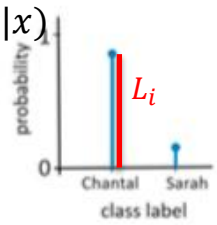
"Classification"

Chantal



Chantal

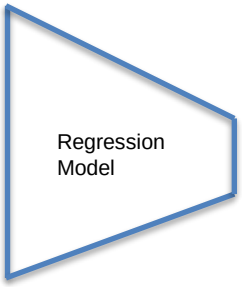




(x_i, y_i)=(Bild,Chantal)

y

"Regression"



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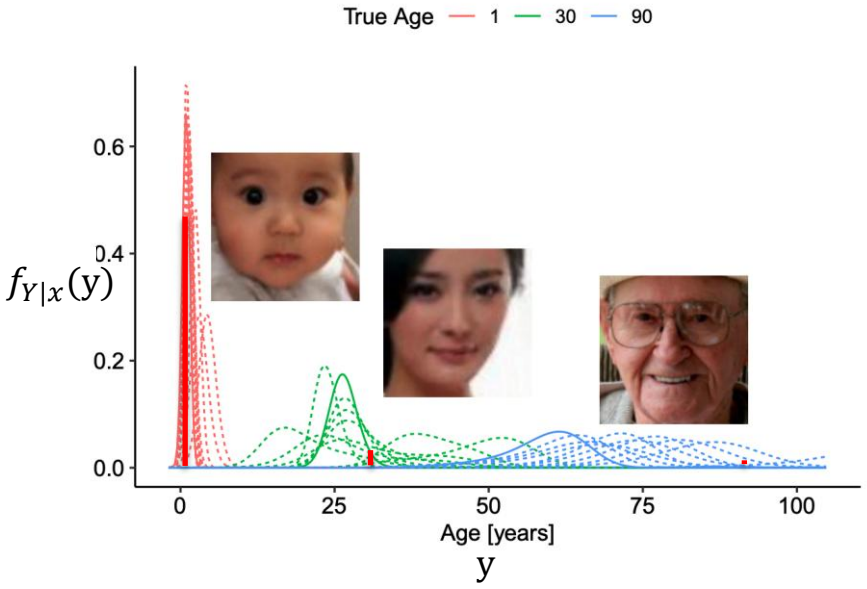
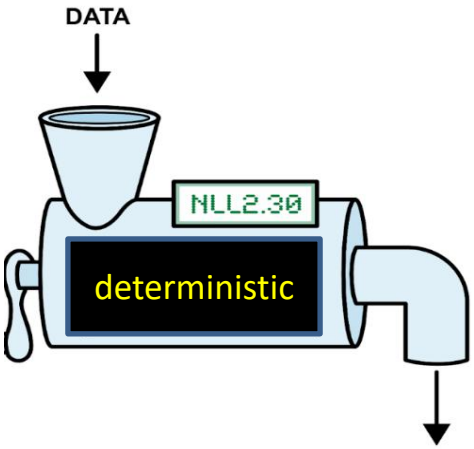
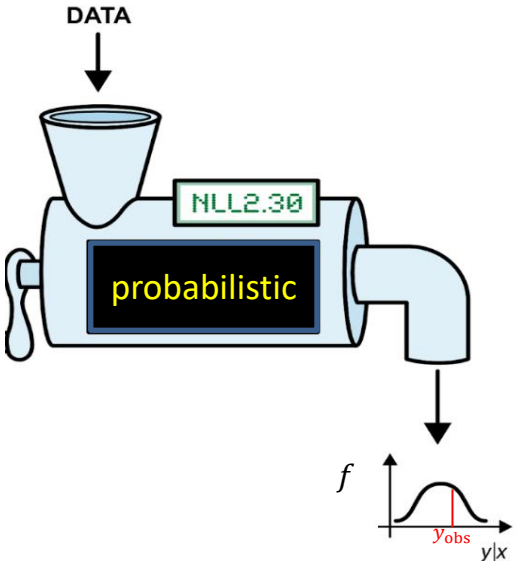


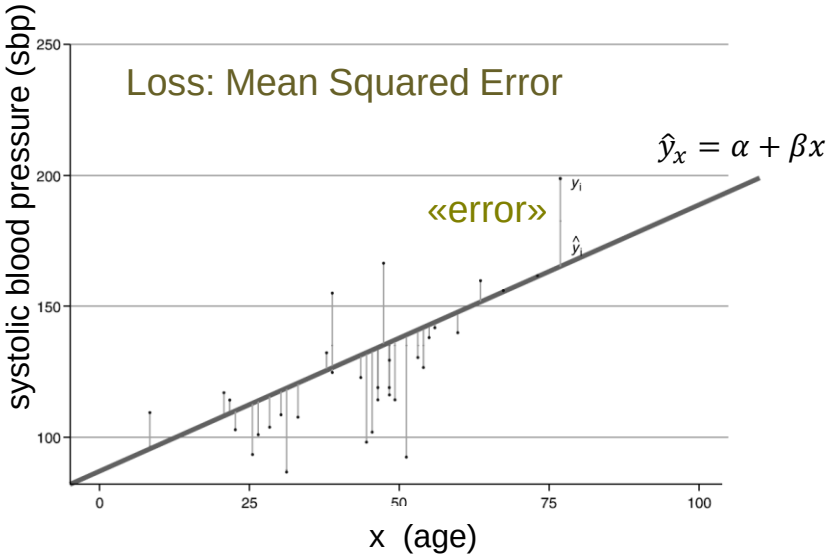
Conditional probability distribution $P(y|x)$ for continuous y aka $f_{Y|x}(y)$

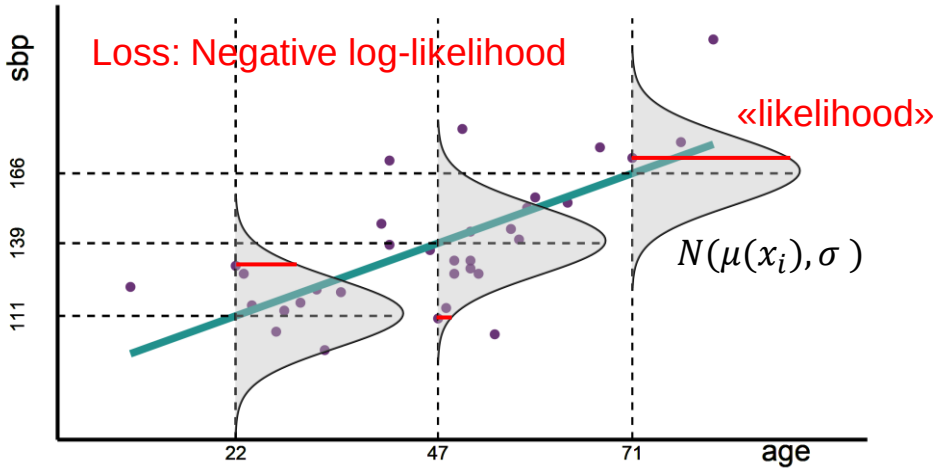
Non-probabilistic versus probabilistic regression DL models



$\hat{y} = 117$



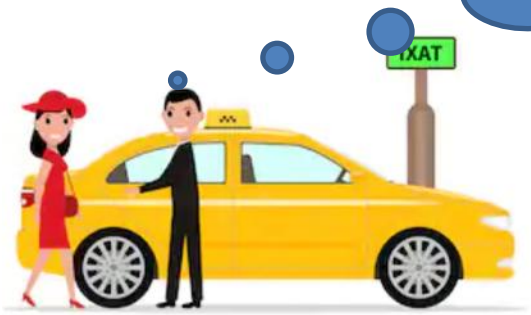


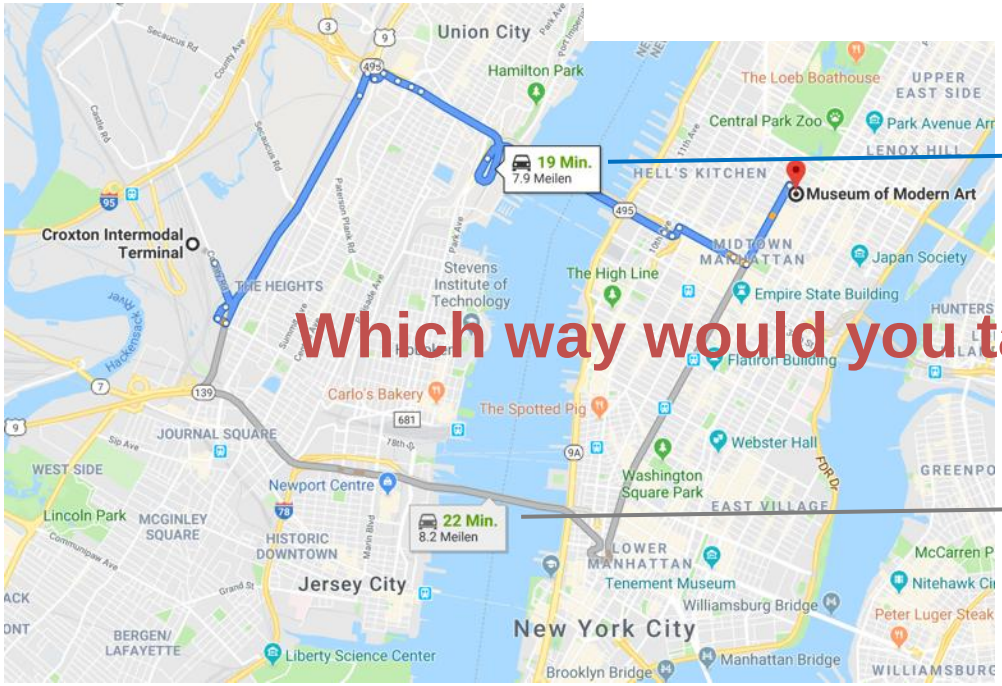


Probabilistic models in everyday tasks

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

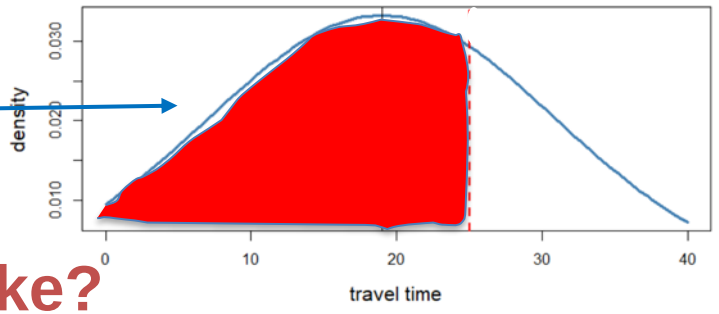
Let's use my probabilistic travel time gadget!



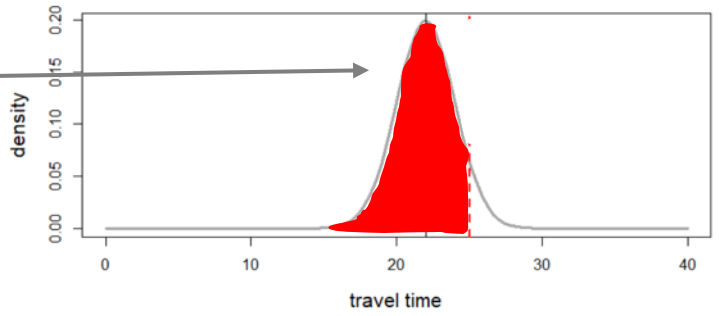


Which way would you take?

Chance to get tip: 69%



Chance to get tip: 93%

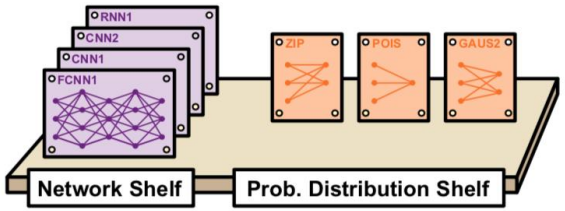


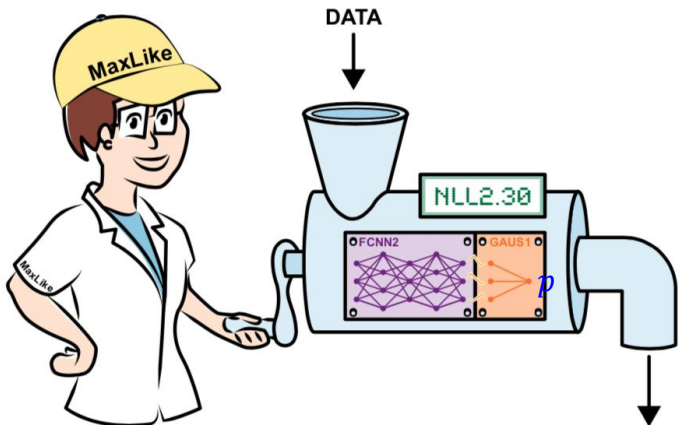
Guiding Theme of the course

- We treat DL as probabilistic models to model a conditional outcome distribution $P(y|x)$
- The models are fitted to training data with maximum likelihood (or Bayes)

Input X determines choice of the NN architectures:

- Tabular data → fcNN, tabPFN
- Images → CNN, viT
- Text → LLMs

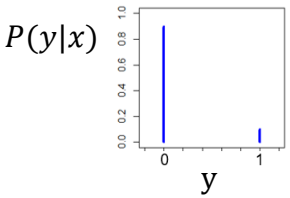




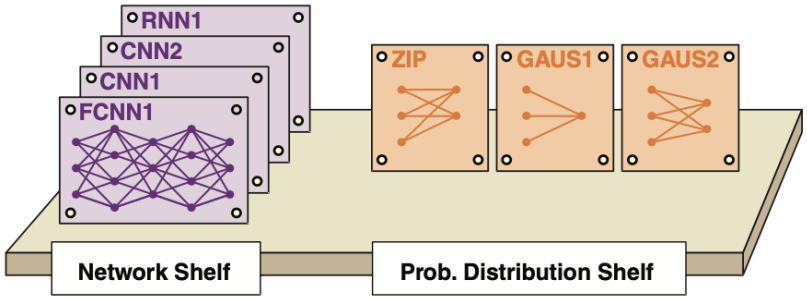
Family of outcome distribution, parameters are controlled by NN:

- Bernoulli (y: binary)
- Multi-Nomial (y: classes)
- Poisson (y: count)
- Negative Binomial (y: count)
- Gaussian (y: real number)
- Weibull (y: real number)
- …

(Y|x)~Ber($p(Y = 1|x)$)

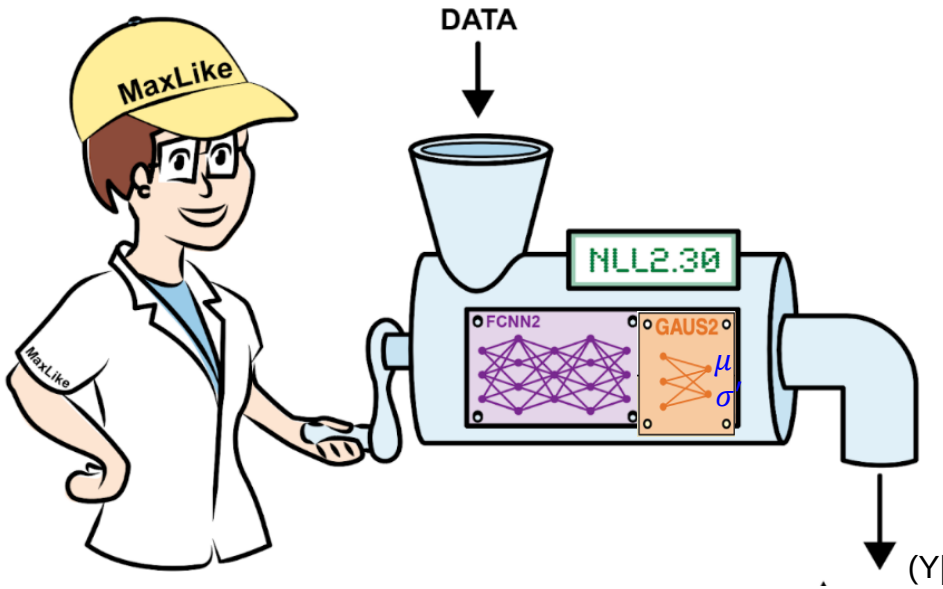


Probabilistic Deep Learning



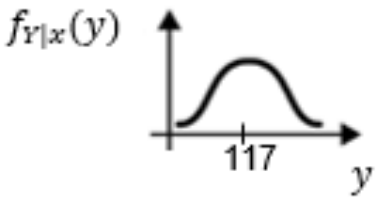
Family of outcome distribution

- Gaussian
- Bernoulli
- Poisson
- …



In classical probabilistic deep learning deep NNs are used to control the parameters of a pre-defined conditional outcome distribution.

$(Y|x) \sim N(\mu(x), \sigma(x)^2)$



O. Dürr, B. Sick, E. Murina. Probabilistic deep learning: With python, keras and tensorflow probability. Manning Book (2020)

How to design a NN to do Logistic Regression?

Note: this is a special case of binary classification

Recall logistic regression from statistics

$Y \in \{0,1\}$

$(\mathrm{Y}|\mathrm{X}_i) \sim \mathrm{Ber}(p_{x_i})$

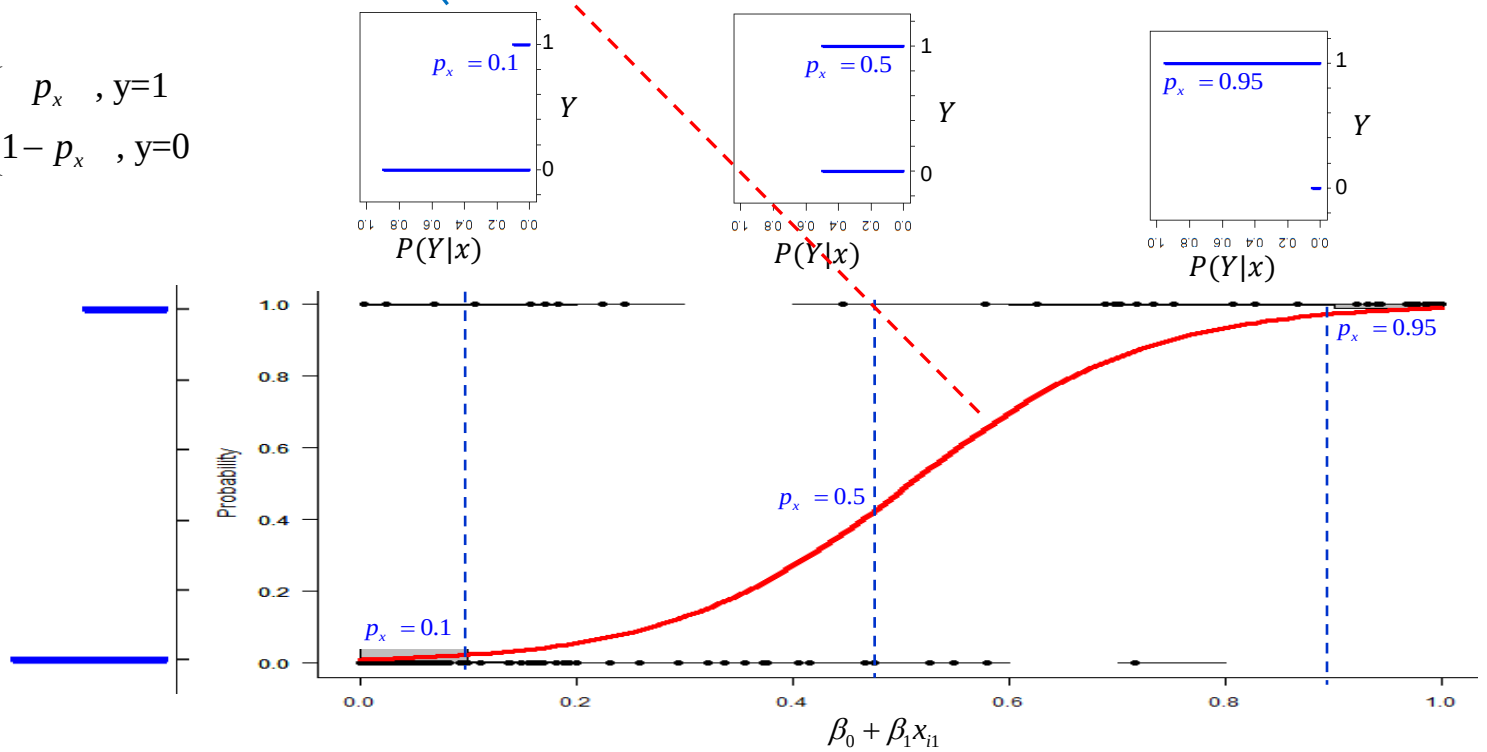
$$\log\left(\frac{p_{x_i}}{1-p_{x_i}}\right) = \beta_0 + \beta_1 x_{i1}$$

$$\mathrm{P}(Y = 1|x_i) = p_{x_i} = \sigma(\beta_0 + \beta_1 x_{i1}) = \frac{1}{1+e^{-(\beta_0+\beta_1 x_{i1})}}$$

probabilistic prediction

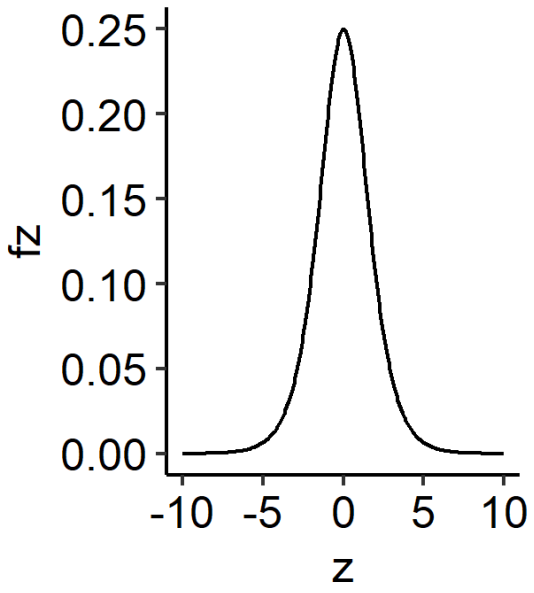
Logisic regression predicts a conditional Bernoulli $P(Y|x_i)$

$$P(\mathrm{Y} \mid \mathrm{X} = \mathrm{x}) = \begin{cases} p_x & , \mathrm{y}=1 \\ 1-p_x & , \mathrm{y}=0 \end{cases}$$



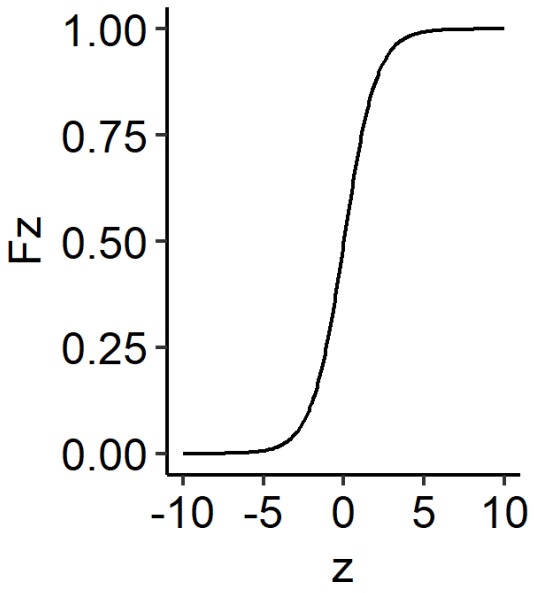
Recall the Standard Logistic Distribution

PDF (f_Z)



$$f_Z(z) = \frac{e^{-z}}{(1+e^{-z})^2}$$

CDF (F_Z)

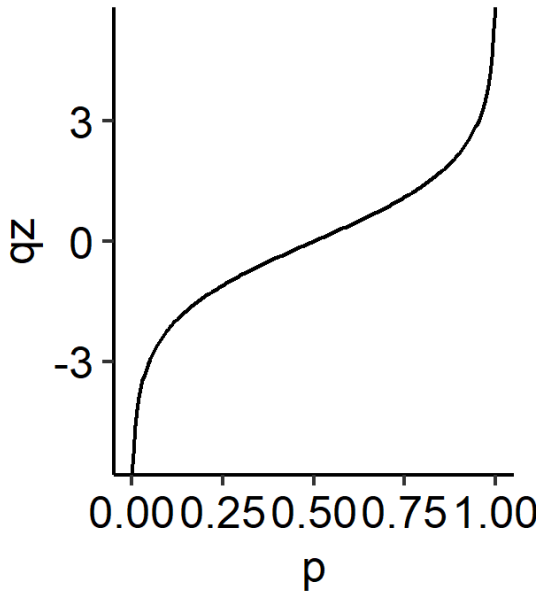


$$F_Z(z) = \frac{1}{1+e^{-z}}$$

$$F_Z(z) = \text{expit}(z)$$

aka “sigmoid”

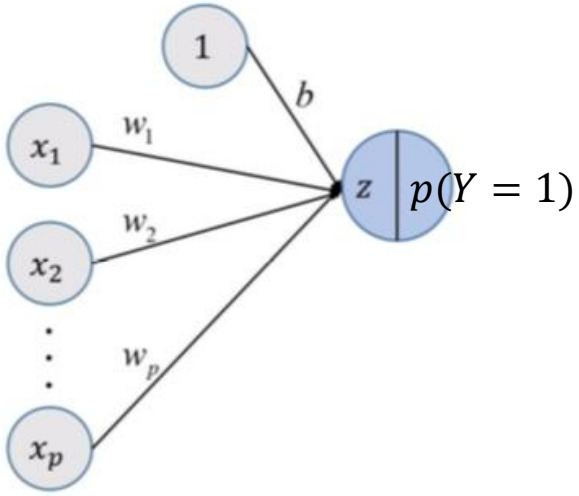
Quantiles function (F_Z^{-1})

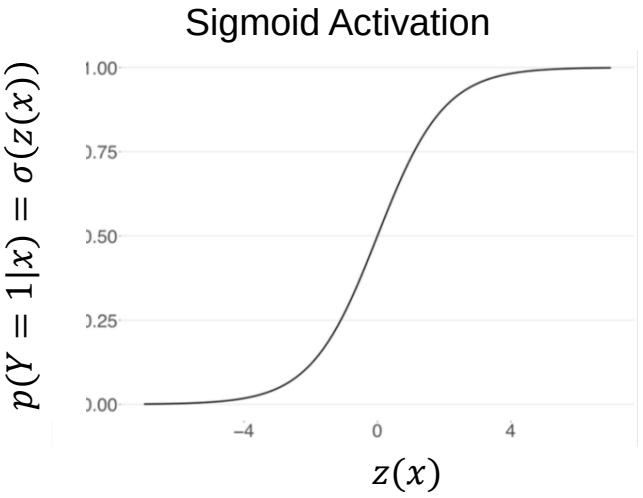


$$F_Z^{-1}(p) = \log\frac{p}{1-p}$$

$$F_Z^{-1}(p) = \log(\text{odds})$$
$$= \text{logit}(p)$$

Logistic regression as NN
Activation in the last layer: "sigmoid"



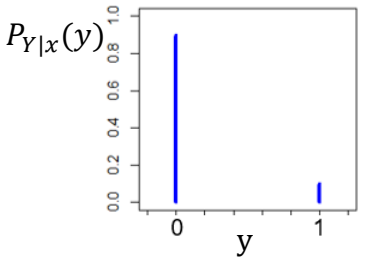


$$z(x) = b + x_1 \cdot w_1 + x_2 \cdot w_2 + \cdots x_p \cdot w_p$$

$$p(Y = 1|x) = \sigma(z) = \sigma\left(\beta_0 + \beta_1 x_{i1} + \cdots + \beta_{ip} x_{ip}\right) = \frac{1}{1 + e^{-(\beta_0 + \beta_1 x_{i1} + \cdots + \beta_{ip} x_{ip})}}$$

The output after the sigmoid activation:

$$P(y_i = 1|x_i) = \sigma\left(\beta_0 + \beta_1 x_{i1} + \cdots + \beta_{ip} x_{ip}\right)$$



→ A NN without hidden layers and
with one output node and a sigmoid-activation is a logistic regression model!

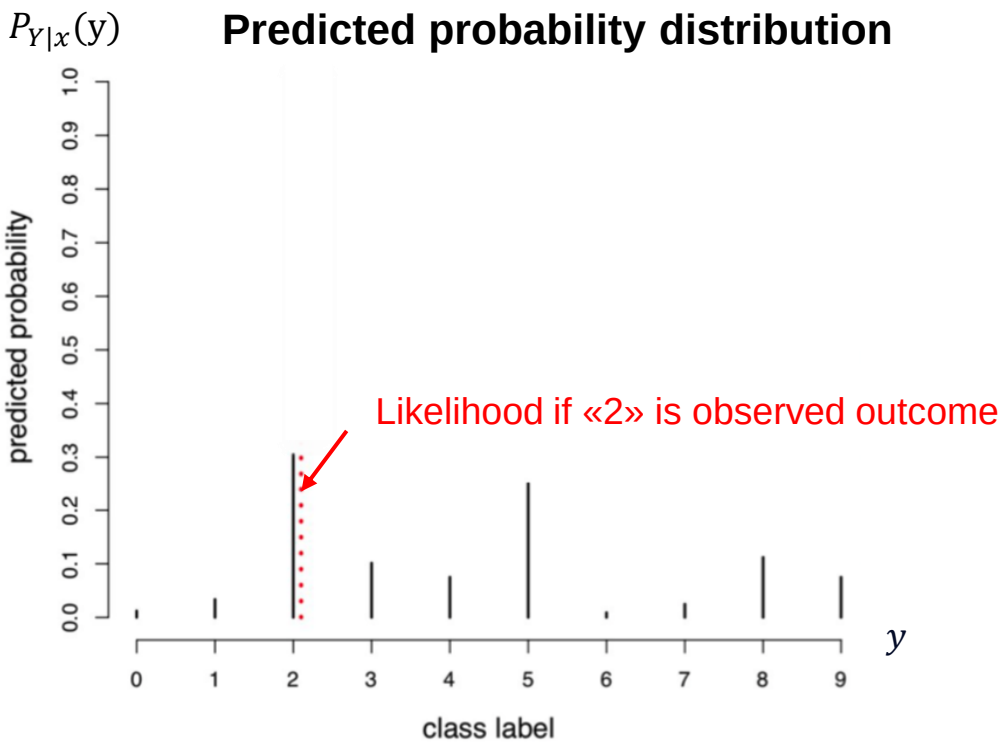
How to design a NN to do Multinomial Regression?

Note: this is a special case of multi-class classification

Multinomial regression is a special multi-class regression

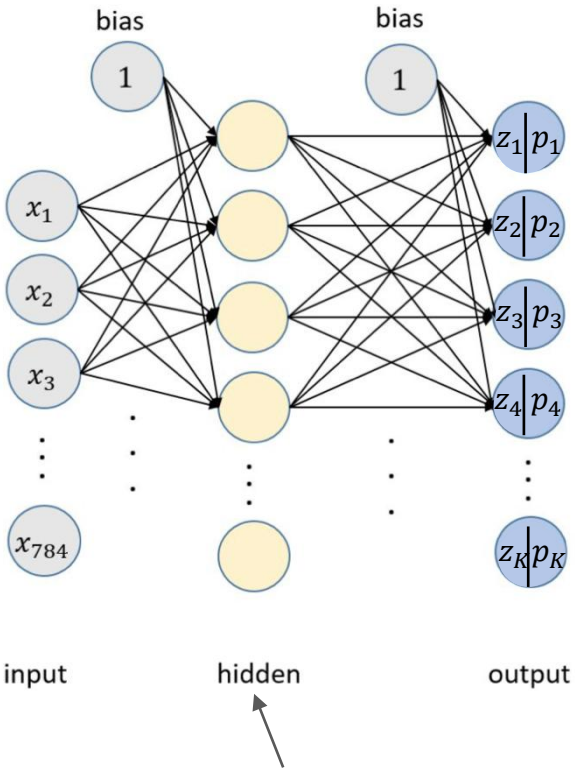
Multinomial regression is used when the outcome variable Y is categorial nominal and has more than two categories, $c_1, c_2, \dots, c_k$, that do not have an order.

$Y \in \{c1, c2, \dots, cK\}$, $P_{Y|x}(Y = c_k) = P(Y = \mathrm{c_k}|\mathrm{x}) = \mathrm{p_k(x)}$, $\sum_{k=1}^{K} p_k(x) = 1$



Remark: It Y is not nominal but ordinal, often a proportional odds model is fitted which does assume more than just $\sum_k p_k = 1$.

Multi-class regression as NN
Activation in the last layer: "softmax"



We'll talk about hidden layers soon

$p_0, p_1 \ldots p_9$ are probabilities for the classes c_1 to c_K.

Incoming to last layer z_i $i = 1 \cdots K$

$$p_i = \frac{e^{z_i}}{\sum_{j=0}^{K} e^{z_j}}$$

Makes outcome positive

Ensures that pi's sum up to one

This activation is called *softmax*

NN with "softmax" activation in last layer outputs the probabilities for the classes.

Which loss to use in probabilistic DL?

Negative Log Likelihood!

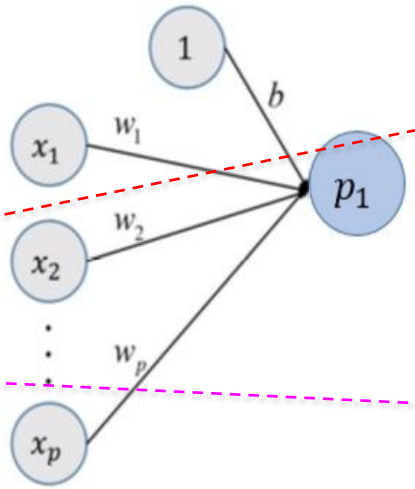
NLL-loss for binary classification

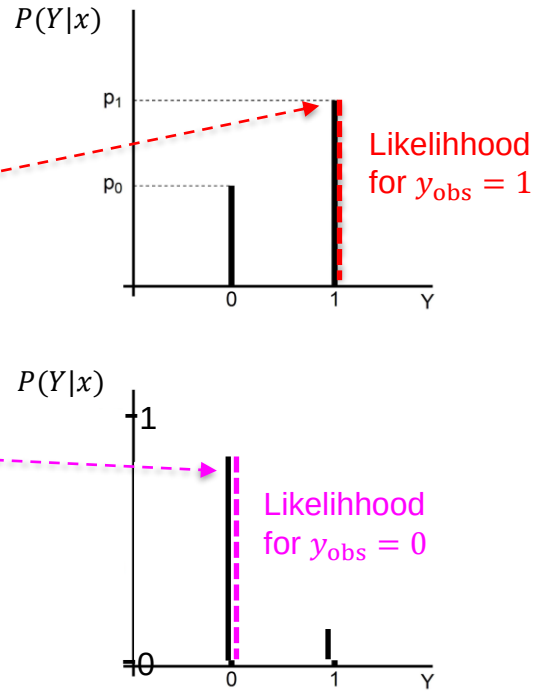
Maximum likelihood principle in logistic regression

probabilistic prediction

Training data set

x1	…	xp	y
0.4	…	-1.3	0
1.1	…	0.2	1
:	:	:	:
0.6	…	-0.9	0





Given (=conditioned on) the input featurs x of an observation i, a well trained NN

- should predict large $p_1 = P(Y = 1|x)$ if the observed class is $y_i = 1$
- should predict small p_1 hence large $p_0 = P(Y = 0|x)$ if observed is $y_i = 0$

→ The likelihood (for the observed outcome) or LogLikelihood should be large

$$\text{LogLikelihood} = \sum_{i=1}^{n} [y_i \log(p_{1i}) + (1 - y_i) \log(1 - p_{1i})]$$

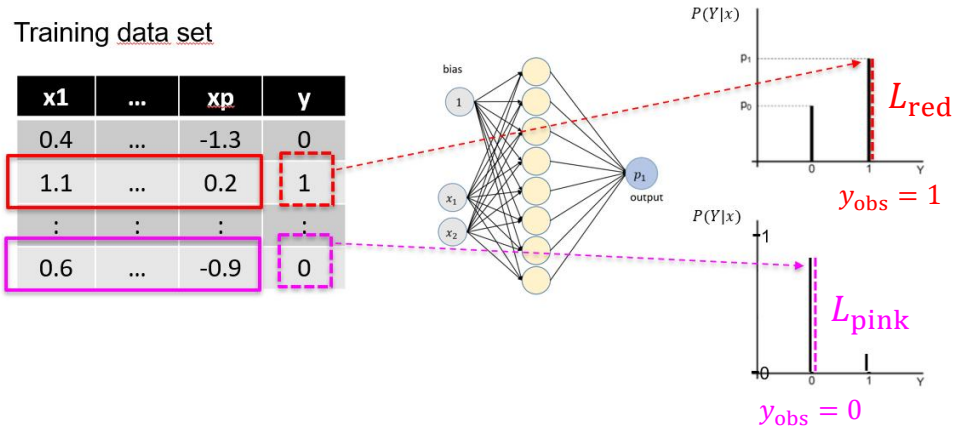
Notation trick in statistics – it selects correct log-probability since $y_i \in \{0,1\}$

Fitting a "logistic regression NN"

The Likelihood of an observation i is the likelihood (probability), that the predicted probability distribution $P(Y|x_i)$ assigns to the observed outcome y_i.

Note: the predicted $P(Y \mid x_i)$ and the corresponding likelihood for the observed y_i depends on the data-point (x_i, y_i) and the model parameter values

→ The higher the likelihood, the better is the model prediction $P(Y|x)$



L_{red} is likelihood of red observation with $y_{obs} = 1$

L_{pink} is likelihood of pink observation with $y_{obs} = 0$

Maximum likelihood principle:

Statistical models are fit to maximize the average LogLikelihood

$$L = \frac{1}{N}\sum L_i = \frac{1}{N}\sum [y_i \log(p_{1i}) + (1 - y_i)\log(1 - p_{1i})]$$

we often use the simplified notation average logLik : $\mathbf{L = \frac{1}{N}\sum log(p_i)}$

Predicted probability for the observed outcome y_{obs}

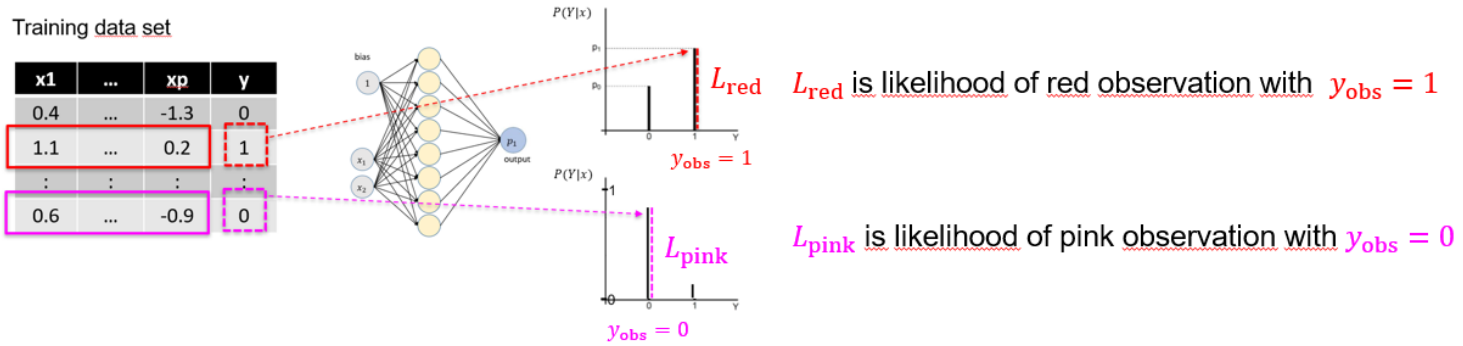
NLL Loss for probabilistic binary classification

In DL we aim to minimize a loss function $L(\text{data}, w)$ which depends on the weights

→ Instead of maximizing the average LogLikelihood

we minimize the averaged Negative LogLikelihood (NLL):

$$\textbf{loss} = \textbf{NLL} = -\frac{1}{N}\sum \log(L_i) = -\frac{1}{N}\sum \log(p_i)$$



The best possible value of the NLL contribution of an observation i is $-\log(\mathrm{L_i}) = -\log(1) = 0$

The worst possible value of the NLL contribution of an observation i $-\log(\mathrm{L_i}) = -\log(0) = \infty$

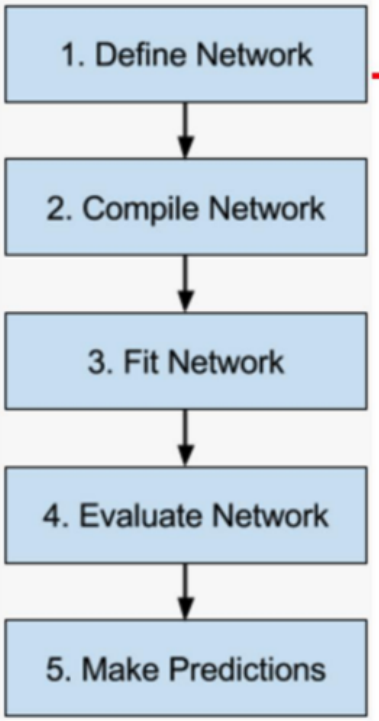
Note: In Keras the NLL for binary outcome is called 'binary_crossentropy',
if we do probabilistc binary classification with 1 output node with sigmoid activation.
If we would use 2 output nodes and softmax than the NLL is called 'categorical_crossentropy'

Define the network

Sequential API, layers output are the input for the next layer, Alternative Functional API

Keras

Hidden layer with 8 Neurons, Activation function: sigmoid




```
# Define fcNN
model = Sequential()
model.add(Dense(8,
                input_shape=(2,),
                 activation='sigmoid'))
model.add(Dense(1,
                 activation='sigmoid'))
```

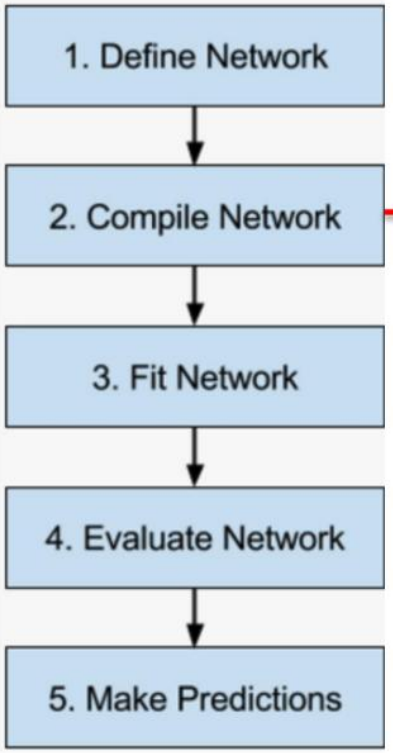
Last layer with one output neuron for binary classification

Input shape needs to be defined only at the beginning.

Alternative: `input_dim=2`, `Functional API` or `Sequential API`

Compile the network

Keras




```
model.compile(optimizer=SGD(learning_rate=0.01)
              loss='binary_crossentropy',
              metrics=['accuracy'])
```

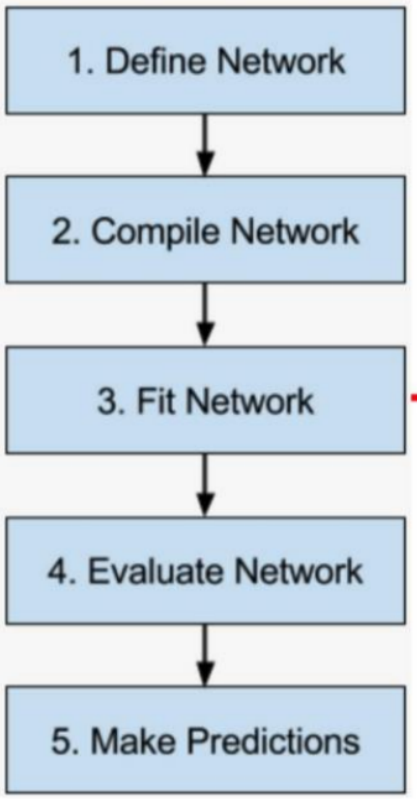
Which optimizer should be used?
Here Stochastic Gradient Descent

Loss Function to optimize
Here: Binary CE

Which metrics do we want to track,
Here: Accuracy

Fit the network

Keras



Data Tensor X for training

Label Tensor Y

Validation at
End of each epoch

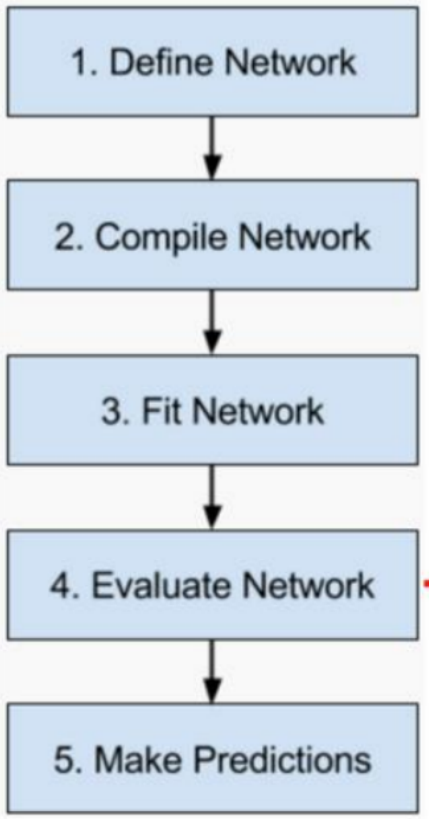
```
history = model.fit(X_train,
                    y_train,
                    validation_data=(X_val, y_val),
                    epochs=1000,
                    batch_size=10,
                    verbose=1)
```

How many time do we feed the whole dataset to the model

How many samples per batch, 1 batch = 1 iteration of weight updates

Should we see the whole output? If no verbose = 0

Evaluate the network



Unseen (to the model) Test Data X with labels Y

```
model.evaluate(X_test, y_test, verbose=0)
```

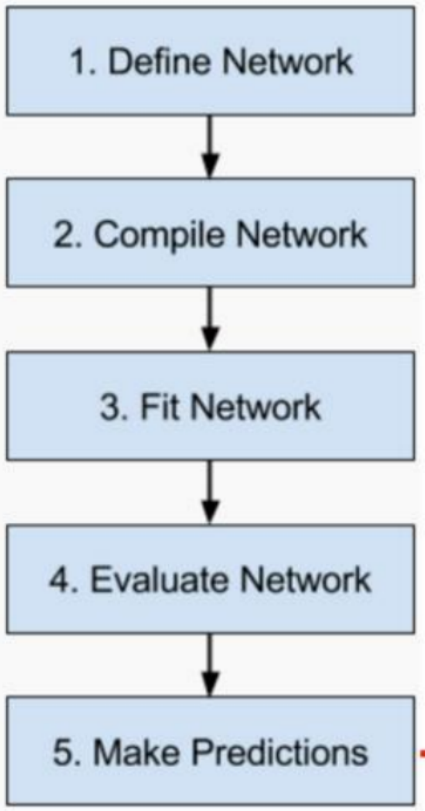
```
Test Loss: 0.33591118454933167, Test Accuracy: 0.8581818342208862
```

Remember from the .compile

```
loss='binary_crossentropy',
metrics=['accuracy'])
```

Make Predictions

Keras



predict with the model,
Weights are fixed now

First 10 rows
(observations) from
Testdata

All features, here: 2

```
model.predict(X_test[0:10,:])
```

```
1/1 [==============================] - 0s 148ms/step
array([[5.9251189e-01],
       [8.8978779e-01],
       [7.8563684e-01],
       [9.1934395e-01],
       [6.1078304e-01],
       [8.2838058e-01],
       [2.5862646e-01],
       [3.1314052e-05],
       [2.6938611e-01],
       [3.7005499e-02]], dtype=float32)
```

Each of the observations
Gets a probability to
Belong to class 1

Losses in Keras

keras.io/api/losses/

Developer guides

Code examples

Keras 3 API documentation

- Models API
- Layers API
- Callbacks API
- Ops API
- Optimizers
- Metrics
- **Losses**
  - Probabilistic losses
  - Regression losses
  - Hinge losses for "maximum-margin" classification
- Data loading
- Built-in small datasets
- Keras Applications
- Mixed precision
- Multi-device distribution
- RNG API
- Utilities

The purpose of loss functions is to compute the quantity that a model should seek to minimize during training.

Available losses

Note that all losses are available both via a class handle and via a function handle. The class handles enable you to pass configuration arguments to the constructor (e.g. `loss_fn = CategoricalCrossentropy(from_logits=True)`), and they perform reduction by default when used in a standalone way (see details below).

Probabilistic losses

- BinaryCrossentropy class
- BinaryFocalCrossentropy class
- CategoricalCrossentropy class
- CategoricalFocalCrossentropy class
- SparseCategoricalCrossentropy class
- Poisson class
- CTC class
- KLDivergence class
- binary_crossentropy function
- categorical_crossentropy function
- sparse_categorical_crossentropy function
- poisson function
- ctc function
- kl_divergence function

Regression losses

- MeanSquaredError class
- MeanAbsoluteError class
- MeanAbsolutePercentageError class
- MeanSquaredLogarithmicError class
- CosineSimilarity class

► Keras 3 API documentation / Losses / Probabilistic losses

Probabilistic losses

BinaryCrossentropy class [so

```
keras.losses.BinaryCrossentropy(
    from_logits=False,
    label_smoothing=0.0,
    axis=-1,
    reduction="sum_over_batch_size",
    name="binary_crossentropy",
    dtype=None,
)
```

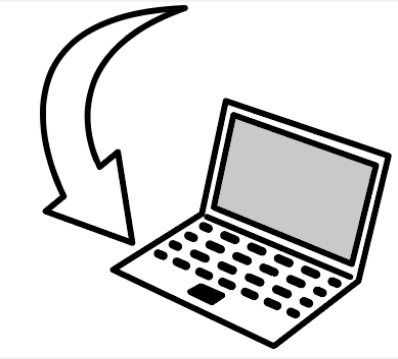
► Keras 3 API documentation / Losses / Regression losses

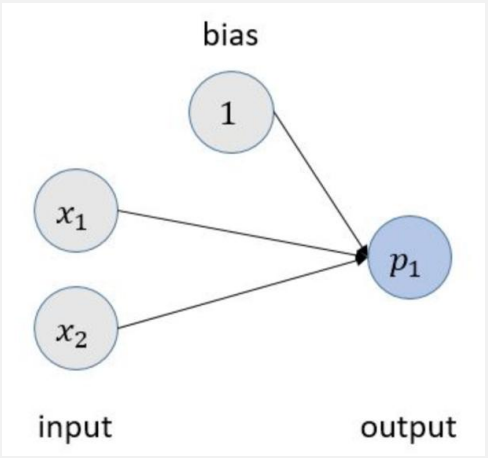
Regression losses

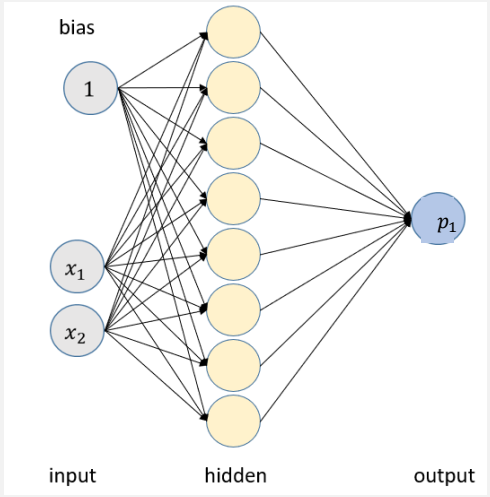
MeanSquaredError class [source]

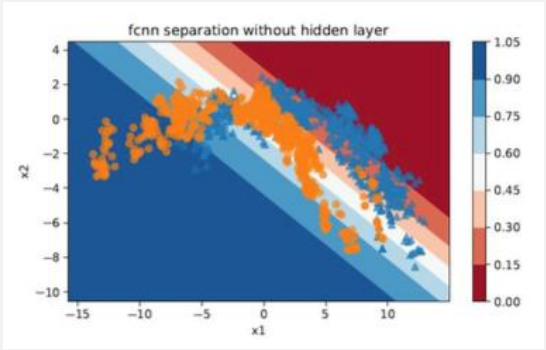
```
keras.losses.MeanSquaredError(
    reduction="sum_over_batch_size", name="mean_squared_error", dtype=None
)
```

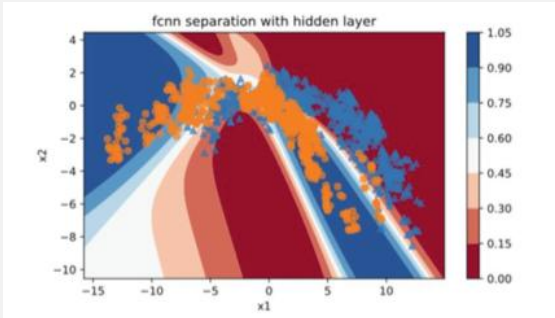
Exercise: Keras for banknote classification



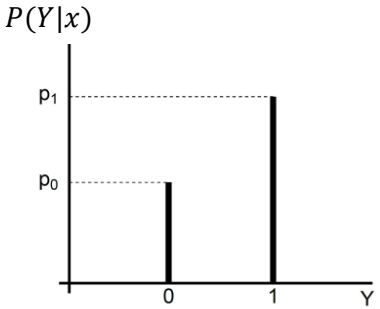








$$(Y|x) \sim \mathrm{Ber}\big(p(x)\big)$$
$$p(x) = P(Y = 1|x)$$



Open NB [02_fcnn_with_banknote_keras_torch.ipynb]
and use Keras to train a NN with and w/o hidden layer

How to use a NN to do Linear Regression?

Recall linear regression from statistics

$$(Y|X = x_i) \sim \mathrm{N}(\mu(x_i), \sigma^2)$$

$Y \in \mathbb{R}$,
$\mu_x \in \mathbb{R}$

point prediction

probabilistic prediction

$$y_i = \mu(x_i) + \varepsilon_i = \beta_0 + \beta_1 \cdot x_{i1} + \varepsilon_i$$
$$\hat{E}(Y_{X_i}) = \hat{\mu}_{x_i} = \hat{\beta}_0 + \hat{\beta}_1 \cdot x_{i1}$$
$$\mathrm{Var}(Y_{X_i}) = \mathrm{Var}(\varepsilon_i) = \sigma^2$$
$$\varepsilon_i \sim N(0, \sigma^2)$$

Variance is assumed to be constant

Probabilistic linear regression predicts for each input x_i a Gaussian conditional probability distribution for the output $P(Y|x_i)$ that assigns each possible value of Y a likelihood.

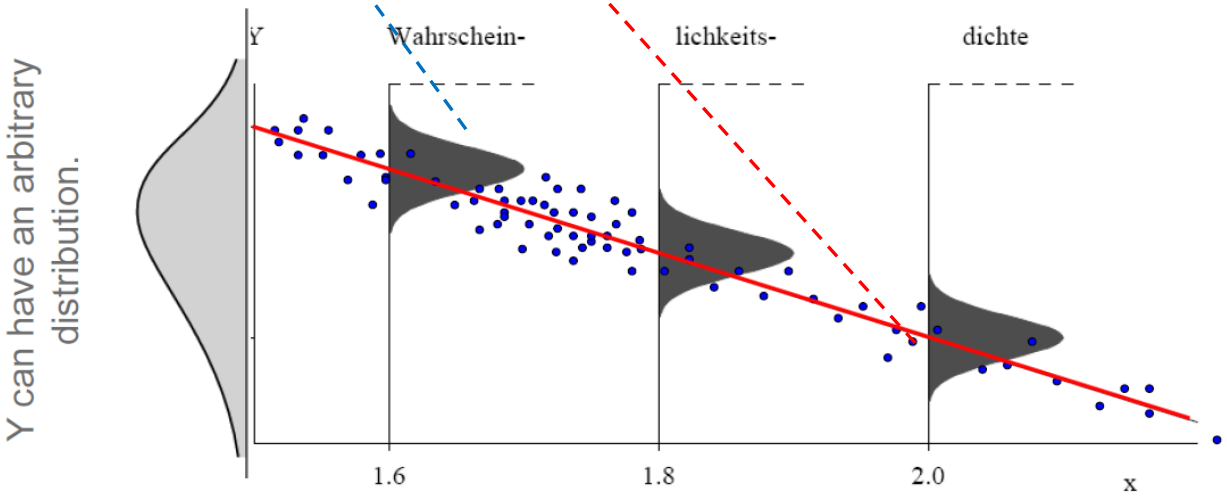
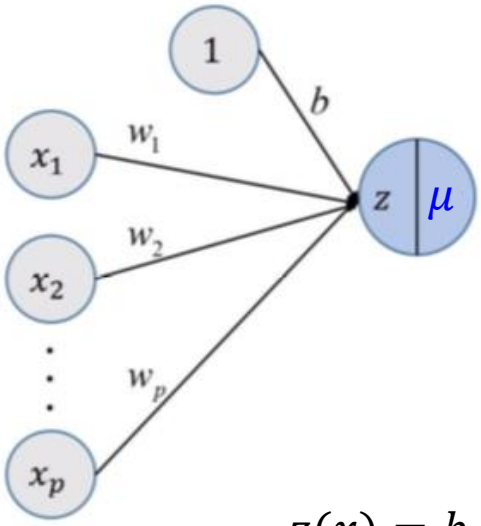
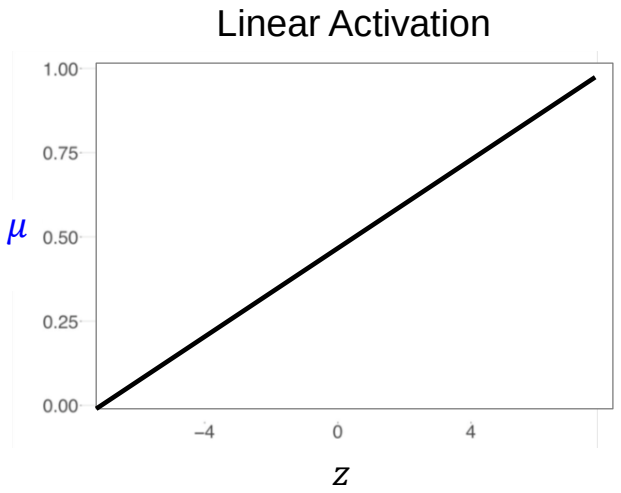


Image credits: Book of Werner Stahel: Angewandte Statistik

Linear Regression as NN
Activation in the last layer: "linear"

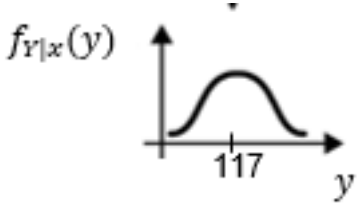




$$z(x) = b + x_1 \cdot w_1 + x_2 \cdot w_2 + \cdots x_p \cdot w_p$$

$$\mu(x) = z(x)$$

$$(Y|x) \sim N(\mu(x), \sigma^2)$$



The output after the linear activation can be interpreted as estimated expeced value of the Gauss $\mu(x) = E(Y|x)$

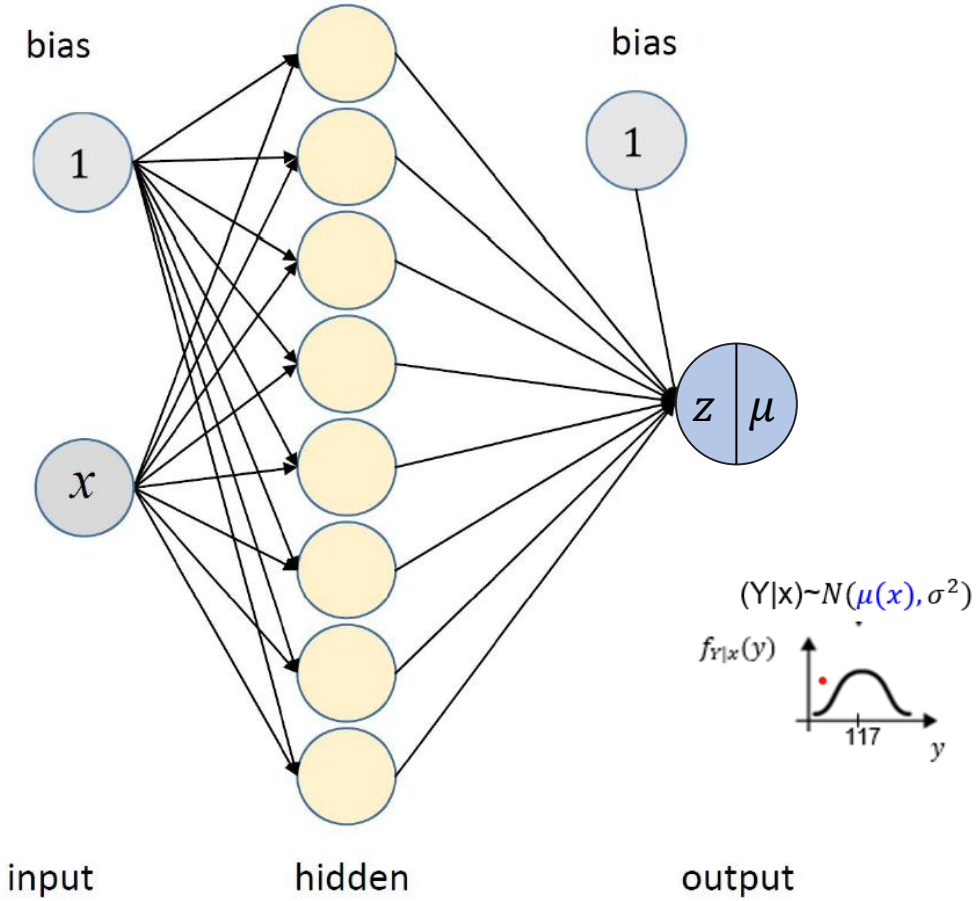
→ A fcNN without hidden layers and with one output node and a sigmoid-activation is a logistic regression model!

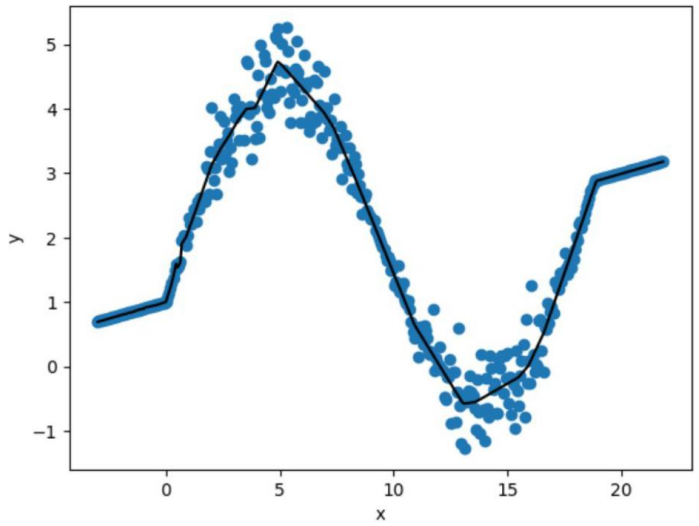
Remark: after fitting the linear predictor $\hat{\mu}(x)$ the constant variance is estimated from the residuals

How to use a NN to do Non-linear Regression?


WE NEED TO GO
DEEPER
memegene

Non-linear Regression as NN
Activation in hidden layer non-linear, in last layer linear



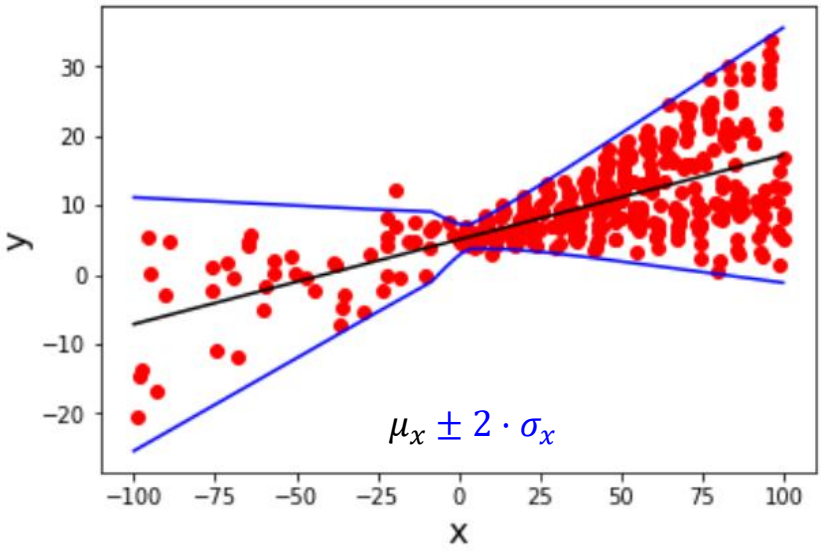


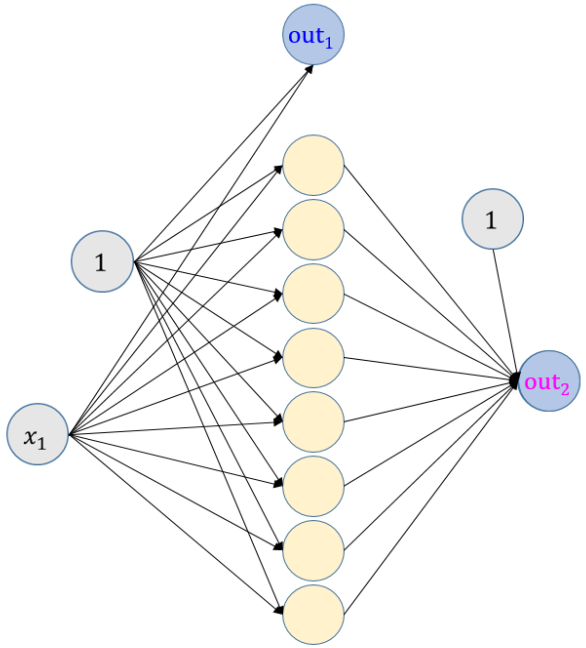
Here, the conditional outcome distribution is a Gaussian with a μ that depends non-linearly on x a variance σ^2 that is constant

Remark: It has been shown, that a NN with one (large)hidden layers can approximate any function, if the the hidden layer holds enough neurons.

NN for linear regression with not-constant variance

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

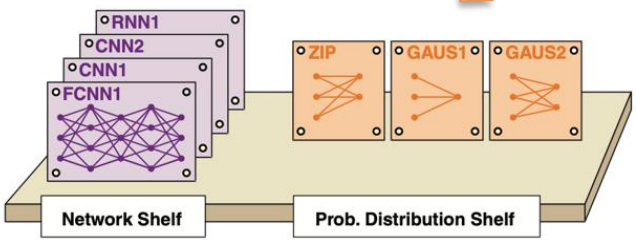


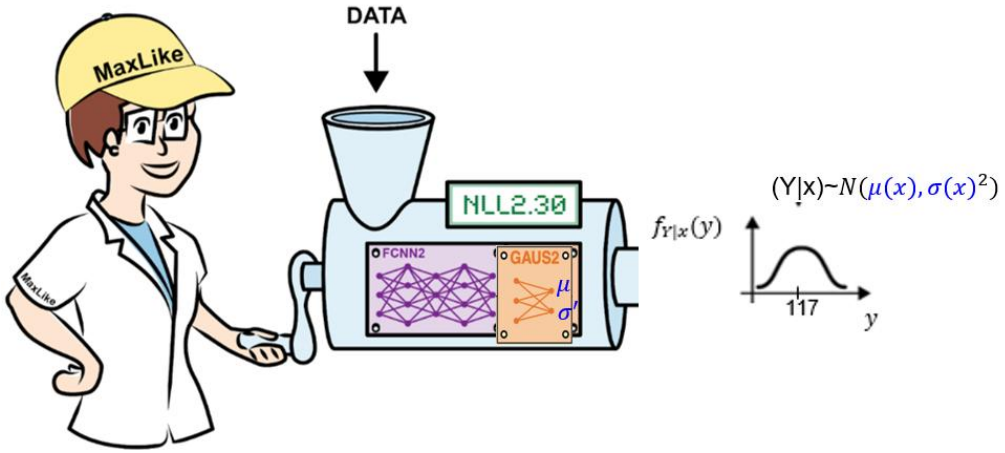


$$\mu_{x_i} = \text{out}_{1_i}$$

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

NLL is used as loss function which depends on outcome distribution



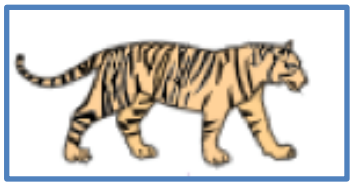


Training: Tune the weights to minimize the loss

Input $x^{(i)}$

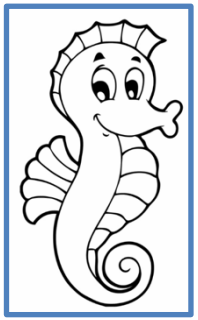
True class $y^{(i)}$

predicted class
(class with highest predicted probability)



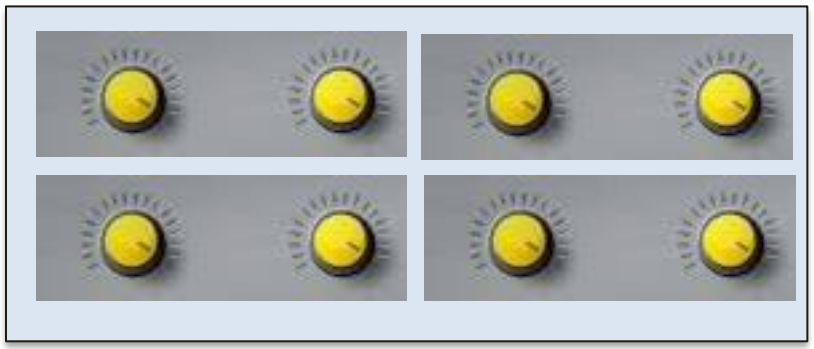
Tiger → Lion 👎

Tiger → Tiger 👍



Seehorse → Seehorse 👍

Neural network with many weights w



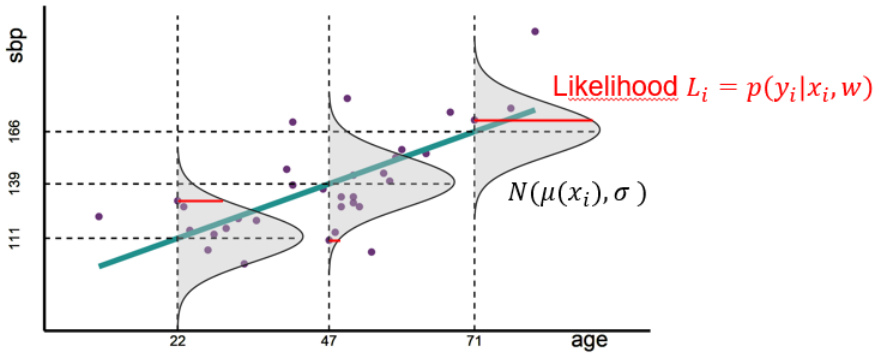
...

Trainingsprinciple:
Weights are tuned so a loss functions gets minimized.

$$\hat{w} = \underset{w}{\operatorname{argmin}}\ \operatorname{loss}\left(\left\{y^{(i)}, x^{(i)}\right\}, w\right)$$

NLL-loss for regression with constant variance

Recap: Maximum Likelihood (one of the most beautiful ideas in statistics)



Ronald Fisher in 1913
Also used before by Gauss, Laplace

Tune the parameters weights of the network such, that observed data (training data) is most likely under the predicted outcome distribution.

We assume iid training data → multiplication of likelihood over all data points:

$$\hat{w} = \underset{w}{\operatorname{argmax}} \prod_{i=1}^{N} L_i = \underset{w}{\operatorname{argmax}} \prod_{i=1}^{N} p(y_i|x_i, w)$$

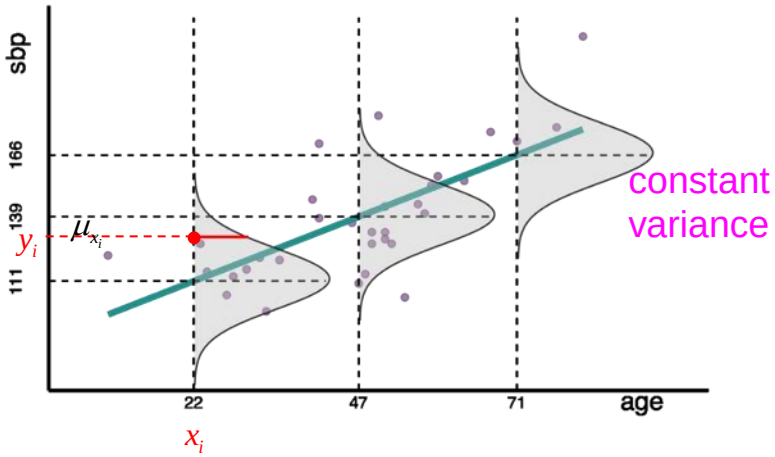
Practically: Use Negative Log-Likelihood NLL as loss and minimize NLL

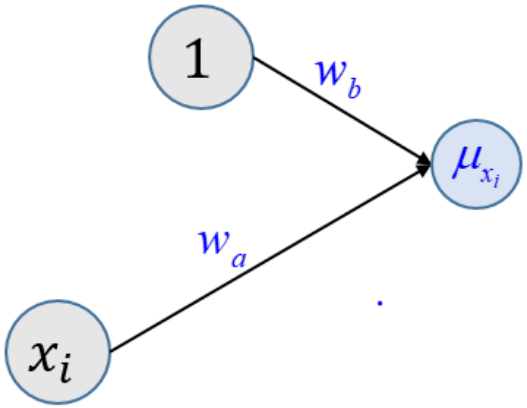
take log; minimize after multiplication with -1, note that NLL in DL is usually the mean-negative log-likelihodd

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

Fit "linear regression NN" via Maximum likelihood principle

$$Y_{X_i} \sim \mathrm{N}(\mu_{x_i} = w_a \cdot x_i + w_b \ , \sigma^2)$$





ML-principle:

$$\mathbf{w}_{\mathrm{ML}} = \underset{w}{\operatorname{argmax}} \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} \, \mathrm{e}^{-\frac{\left(y_i - \mu_{x_i}\right)^2}{2\sigma^2}}$$

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

Negative Log-Likelihood (NLL)

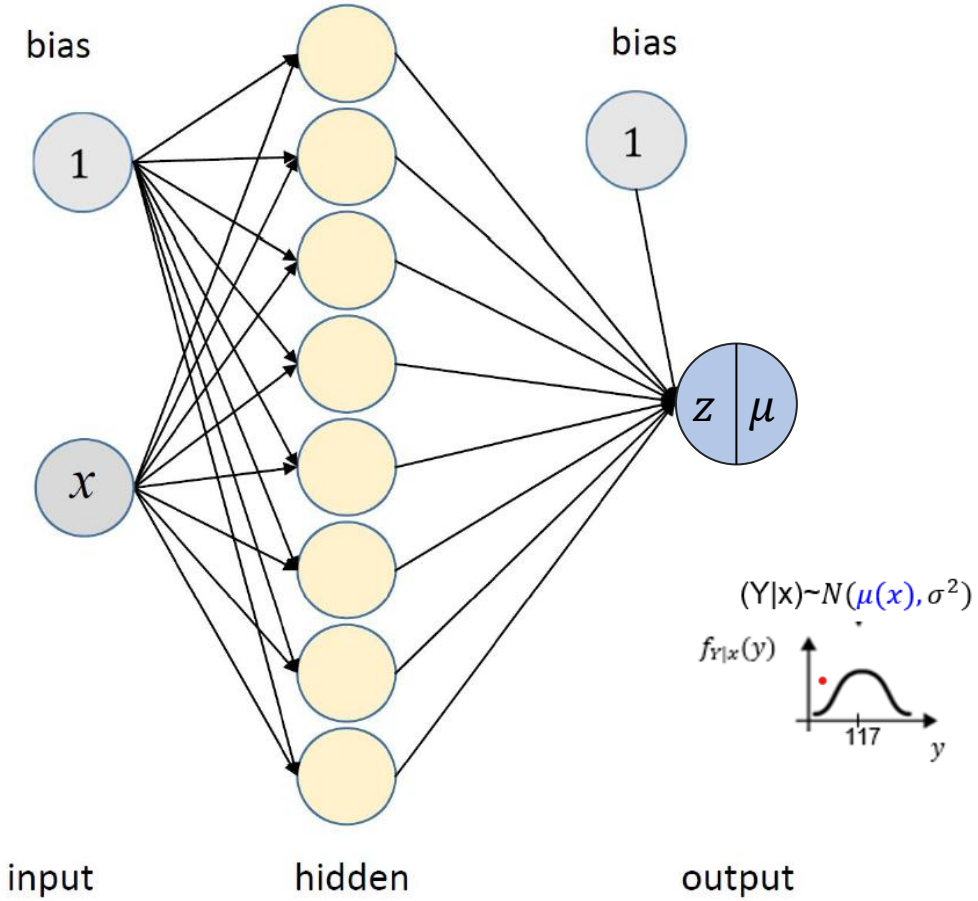
$$(\hat{w}_a, \hat{w}_b)_{\mathrm{ML}} = \underset{w_a, w_b}{\operatorname{argmin}} \frac{1}{n} \sum_{i=1}^{n} \left(y_i - (w_a \cdot x_i + w_b)\right)^2$$

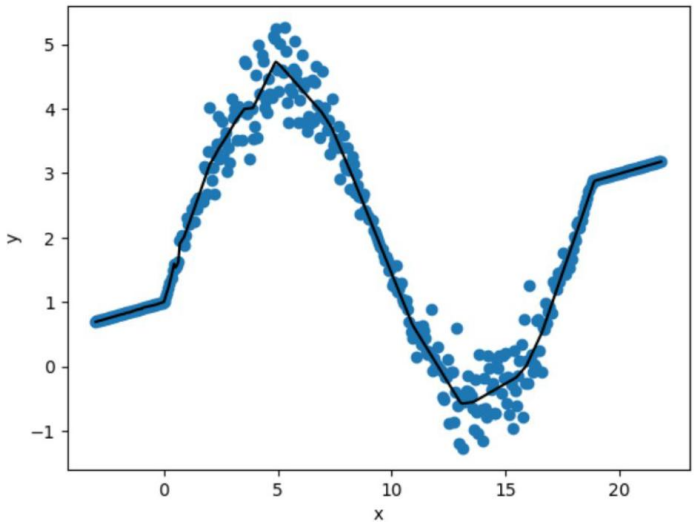
Minimize MSE loss

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

Minimizing NLL loss $\overset{\sigma \ const}{\Longrightarrow}$ Minimizing MSE loss

Non-linear Regression as NN
Activation in hidden layer non-linear, in last layer linear



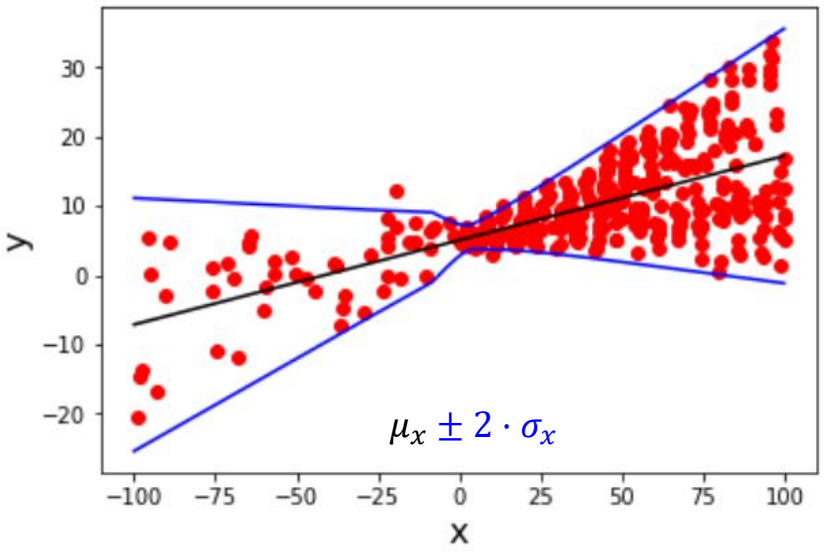


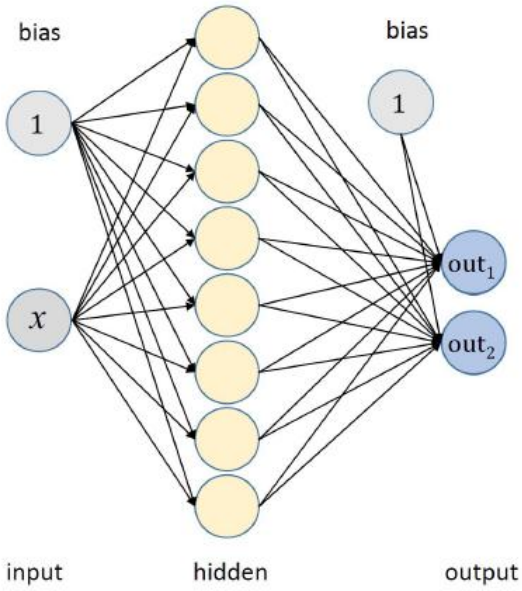
Here, the conditional outcome distribution is a Gaussian with a μ that depends non-linearly on x a variance σ^2 that is constant

Remark: It has been shown, that a NN with one hidden layers can approximate any function, if the the hidden layer holds enough neurons.

Linear regression with flexible non-constant variance

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





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

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

Minimize the mean negative log-likelihood (NLL) on train data:

$$NLL(w) = \frac{1}{n} \sum_{train-data} -log(p(y_i|x_i, w)$$

gradient descent with NLL loss

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

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

Define custom NLL loss for a probabilistic model

- Some keras losses correspond to NLL, e.g.
  - Linear Regression with constant variance
    - Mean Squared Error (keras.losses.mse)
  - Multiclass classification
    - Categorical_cross_entropy (keras.losses.categorical_crossentropy)

- For a given outcome distribution family, you can build your custom NLL loss even if keras does not provide it
  1. Define a model with as many outputs as the number of parameters of the outcome distribution family
  2. Link the outputs of the NN to the parameters of the outcome distribution
  3. Use negative log likelihood as loss function

See https://github.com/tensorchiefs/dlwbl_eth25/blob/master/notebooks/01_hello_prob_dl.ipynb

1. Define a model with as many outputs as the number of parameters of the distribution

```
# Define the model
inputs = Input(shape=(1,))
hidden = layers.Dense(10, activation="relu")(inputs)
# ... more hidden layers ...
outputs = layers.Dense(2)(hidden)  # <--- Outputs mean and log(sd)
model = Model(inputs=inputs, outputs=outputs)
```

[8] ✓ 0.0s Python

2. Link the outputs of the model to the parameters of the distribution

```
# Wrapper function to convert model output to a PyTorch Normal distribution
@staticmethod
def output_to_gaussian_distribution(output):
    mean = output[:, 0:1]   # Gets the first column while keeping dimensions (like output[, 1, drop=FALSE] in R)
    log_sd = output[:, 1:2] # Gets the second column while keeping dimensions
    scale = torch.exp(log_sd) # Inverse link function to ensure positive scale
    return Normal(loc=mean, scale=scale)
```

[7] ✓ 0.0s Python

3. Define NLL

```
# Custom Negative Log-Likelihood Loss
def negative_log_likelihood(y_true, output):
    dist = output_to_gaussian_distribution(output)
    return -dist.log_prob(torch.tensor(y_true)).mean()

# Compile the model
model.compile(optimizer="adam", loss=negative_log_likelihood)
```

[10] ✓ 0.0s Python

Exercise: Define a custom loss function

Notebook: 02_custom_loss.ipynb

https://github.com/tensorchiefs/dl_course_2025/blob/main/notebooks/02_custom_loss.ipynb

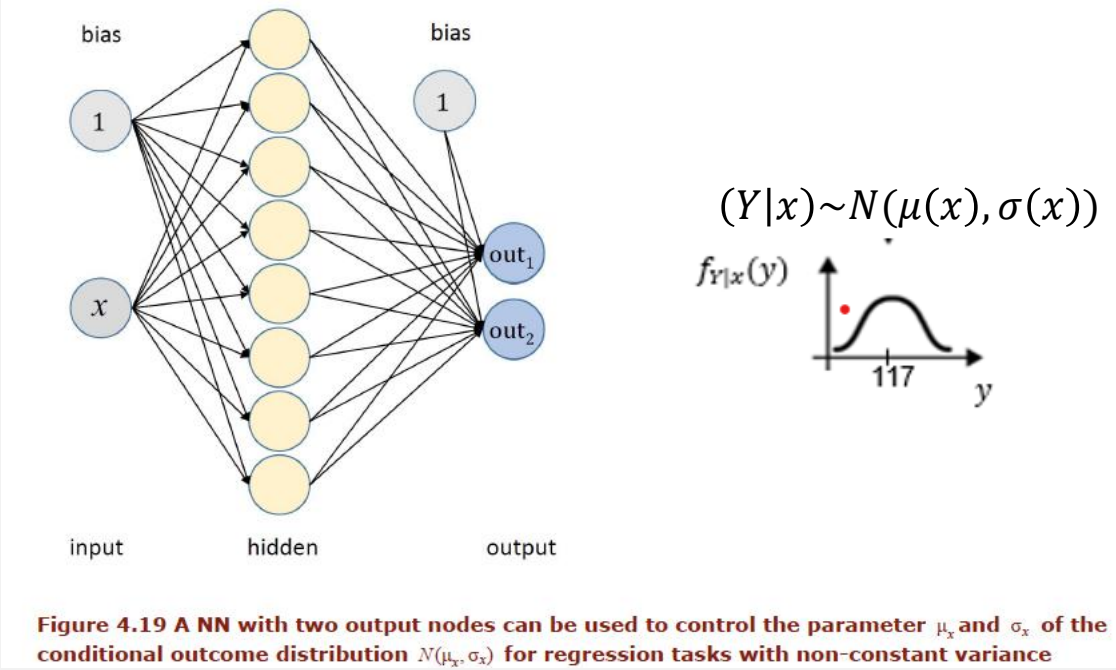
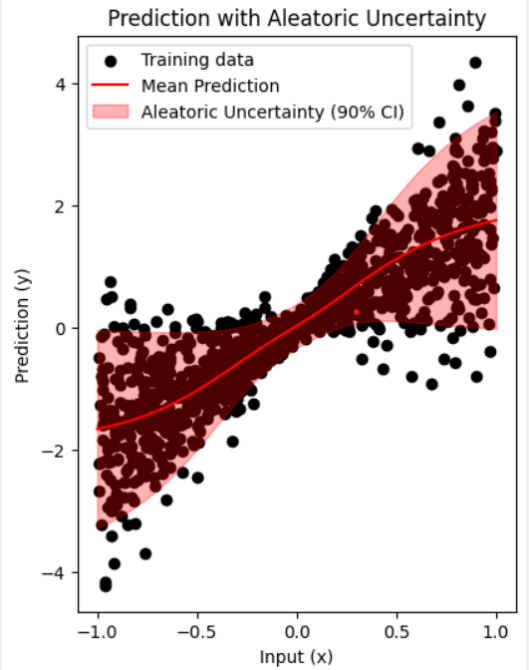


Figure 4.19 A NN with two output nodes can be used to control the parameter μ_x and σ_x of the conditional outcome distribution $N(\mu_x, \sigma_x)$ for regression tasks with non-constant variance



Summary

- If the outcome is continuous we say we do regression
- If the outcome is categorical we say we do classification
- Probabilistic models predict an outcome distribution that assigns for each possible outcome a probability/likelihood
- When using NNs to fit a probabilistic model we use the NLL as loss
- The NLL-contribution of one data point (x_i, y_i) is $-\log(L_i)$: the negative log of the likelihood L_i which is by the predicted outcome distribution assigned to the observed value y_i (see visualization).
- Hidden layers allow for
  - Non linear decision boundaries if the outcome is categorical
  - For non-linear regression modeling with flexible variance if the outcome is continuous
- For a binary classification task, we can use
  - a single neuron in the last layer with the sigmoid activation and the Keras 'binary_crossentropy'.
  - Two neurons in the last layer with the softmax activation and the Keras loss ''categorical_crossentropy'
- For a regression task where the outcome distribution is a Gaussian $N(\mu(x), \sigma(x))$, we can use a NN with two neurons in the last layer and a custom NLL loss using one NN-output to determine $\mu(x)$, and the other NN-output to determine $\sigma(x)$, needed to describe the predicted outcome distribution, under which the likelihood of the observation needs to be determined