Module 11: Neural Networks

TMA4268 Statistical Learning V2020

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Acknowledgements

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Learning material for this module

Todo

See also *References and further reading* (last slide), for further reading material.

What will you learn?

- Translating from statistical to neural networks language
  - linear regression
  - logistic regression
  - multiclass (multinomial) regression
- Feedforward networks
- Neural network parts: model – method – algorithm – recent developents
- Deep learning
  - the timeline
  - Keras

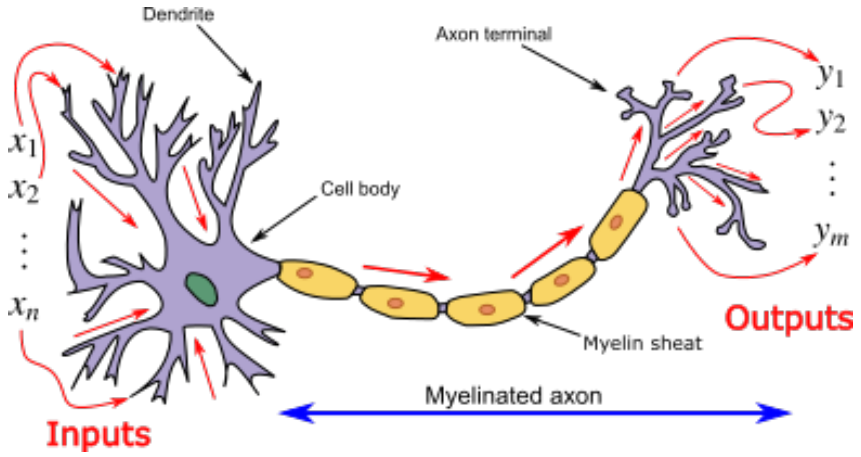
Introduction

- Neural networks (NN) were first introduced in the 1990's.
- Shift from statistics to computer science and machine learning, as they are highly parameterized
- Statisticians were skeptical: "It's just a nonlinear model".
- After the first hype, NNs were pushed aside by boosting and support vector machines.
- Revival since 2010: The emergence of *Deep learning* as a consequence of improved computer resources, some innovations, and applications to image and video classification, and speech and text processing

Why a module on neural networks?

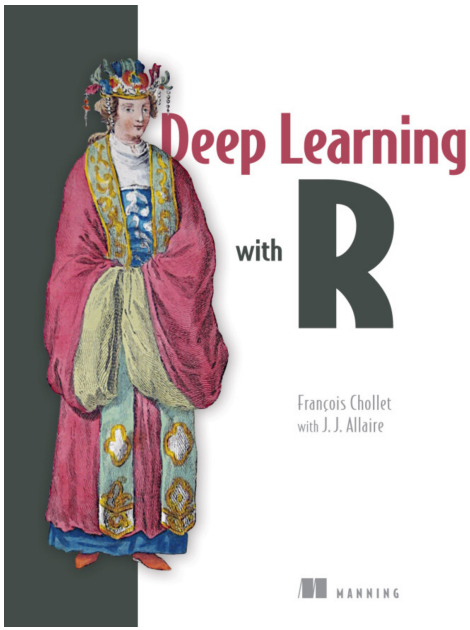
- Every day you read about the success of AI, machine learning – and in particular *deep learning*.
- In the last five years the field of deep learning has gone from low level performance to excellent performance – particularly in image recognition and speech transcription.
- Deep learning is based on a layered artificial neural network structure.

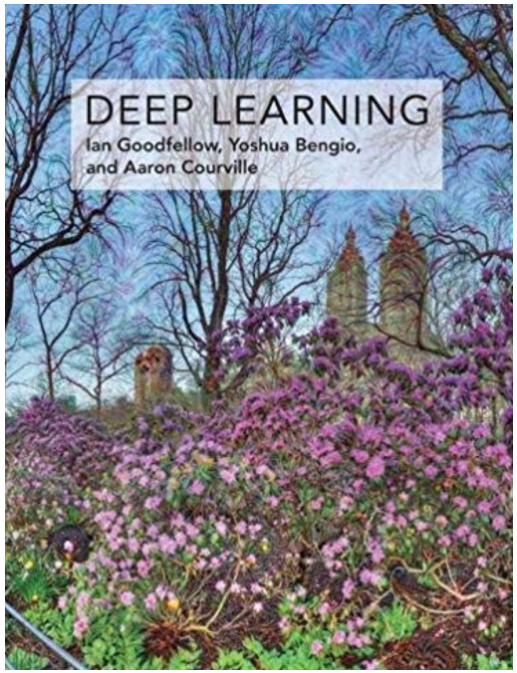
So we first need to understand: what is a *neural network*?



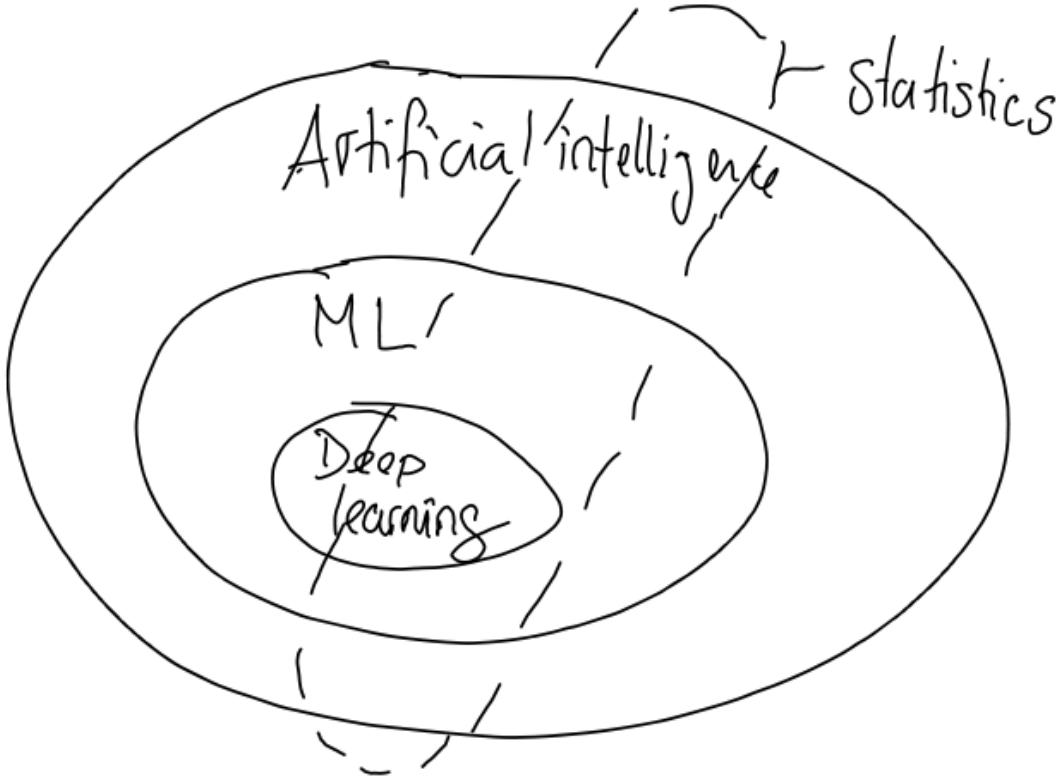
Neuron and myelinated axon, with signal flow from inputs at dendrites to outputs at axon terminals. Image credits: By Egm4313.s12 (Prof. Loc Vu-Quoc) https://commons.wikimedia.org/w/index.php?curid=72816083

- There are several (self-study) learning resources (some listed under 'further references') that the student my turn to for further knowledge into deep learning, but this presentation is heavily based on Chollet and Allaire (2018), with added formulas and theory.
- There is a new IT3030 deep learning course at NTNU.





AI, machine learning and statistics



- Artificial intelligence (AI) dates back to the 1950s, and can be seen as *the effort to automate intellectual tasks normally performed by humans* (page 4, Chollet and Allaire (2018)).

- AI was first based on hardcoded rules (like in chess programs), but turned out to be intractable for solving more complex, fuzzy problems.

- With the field of *machine learning* the shift is that a system is *trained* rather than explicitly programmed.

Machine learning

- Machine learning is related to mathematical statistics, but differs in many ways.
- ML deals with much larger and more complex data sets than what is usually done in statistics.
- The focus in ML is oriented towards *engineering*, and ideas are proven *empirically* rather than theoretically (which is the case in mathematical statistics).

According to Chollet and Allaire (2018) (page 19):

> *Machine learning isn't mathematics or physics, where major advancements can be done with a pen and a piece of paper. It's an engineering science.*

From statistics to artificial neural networks

Recapitulate from Module 3 with the bodyfat dataset that contained the following variables.

- `bodyfat`: % of body fat.
- `age`: age of the person.
- `weight`: body weighth.
- `height`: body height.
- `neck`: neck thickness.
- `bmi`: bmi.
- `abdomen`: circumference of abdomen.
- `hip`: circumference of hip.

We will now look at modelling the `bodyfat` as response and using all other variables as covariates - this will give us

- one numerical output (response), and
- seven covariates
- one intercept

Let n be the number of observations in the training set, here $n = 243$.

Multiple linear regression model

(from Module 3)

We assume

$$Y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_p x_{ip} + \varepsilon_i = x_i^T \beta + \varepsilon_i \ ,$$

for $i = 1, \ldots, n$, where x_{ij} is the value jth predictor for the ith datapoint, and $\beta^\top = (\beta_0, \beta_1, \ldots, \beta_p)$ the regression coeffficients.

We used the compact matrix notation for all observations $i = 1, \ldots, n$ together:

$$Y = X\beta + \varepsilon \ .$$

Assumptions:

1. $\mathrm{E}(\varepsilon) = 0$.
2. $\mathrm{Cov}(\varepsilon) = \mathrm{E}(\varepsilon\varepsilon^T) = \sigma^2 I$.
3. The design matrix has full rank, $\mathrm{rank}(X) = p + 1$. (We assume $n >> (p + 1)$.)

The classical *normal* linear regression model is obtained if additionally

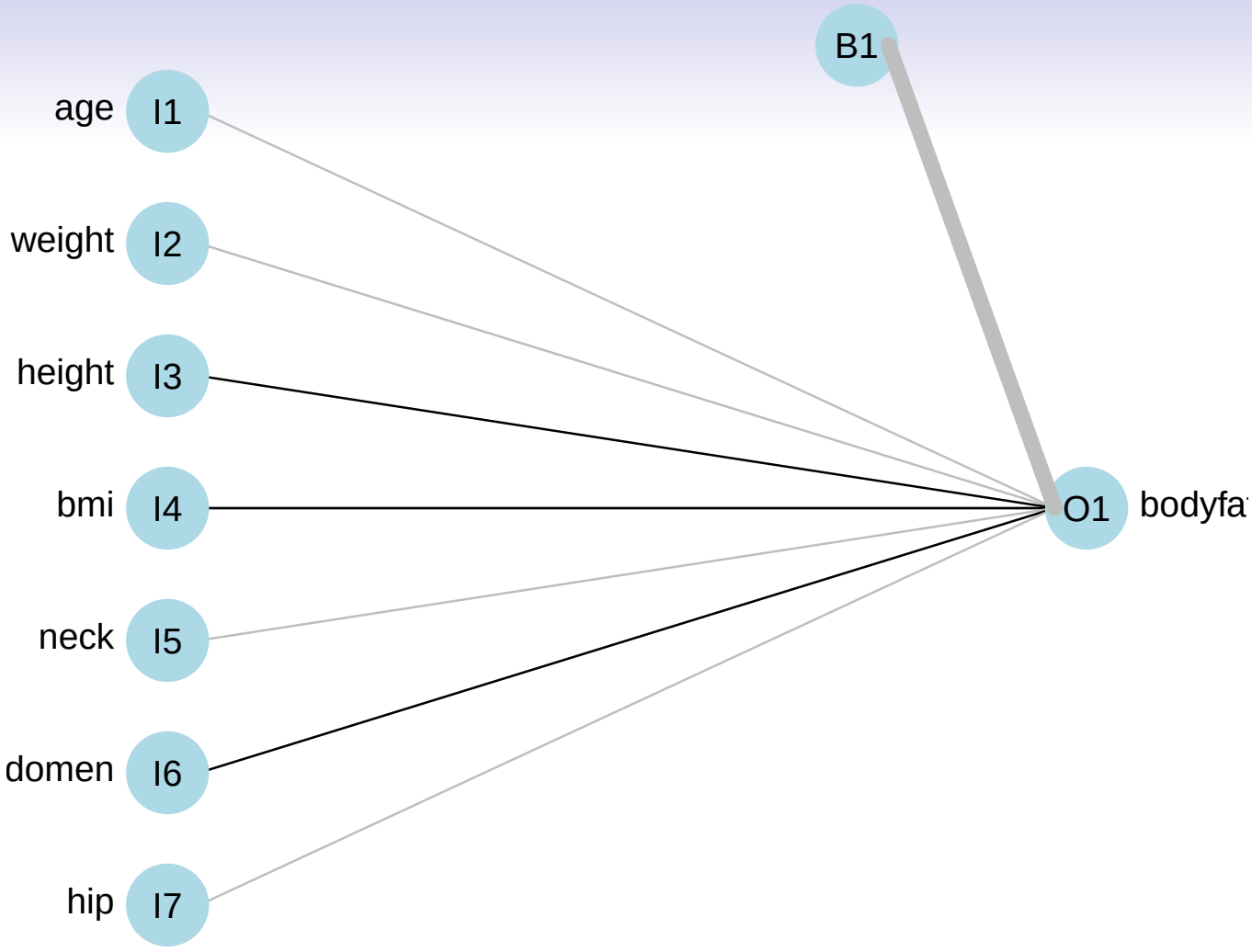
4. $\varepsilon \sim N_n(0, \sigma^2 I)$ holds. Here N_n denotes the n-dimensional multivarate normal distribution.

From statistical model to network architecture

How can our statistical model be represented as a network?

We need *new concepts*:

- Covariates $\rightarrow$ *input nodes* in an *input layer*.
- The intercept $\rightarrow$ *bias* node.
- The response $\rightarrow$ *output node* in an *output layer*.
- The regression coefficients $\rightarrow$ *weights* (often written on the arrows from the inputs to the output layer).



- All lines going into the output node signifies that we multiply the covariate values in the input nodes with the weights (regression coefficients), and then sum.
- This sum can be sent through a socalled *activition function* (here just the identity function).

- *Regression notation:*

$$Y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_p x_{ip} + \varepsilon_i \ .$$

- *Neural network notation:*

$$y_1(x_i) = \phi_o(w_0 + w_1 x_{i1} + \cdots + w_p x_{ip}) \ ,$$

where $\phi_o(x) = x$ (identity function).

- We do not say anything of what is random and fixed, and do not make any assumption distribution of a random variable.
- In the statistics world we would have written $\hat{y}_1(x_i)$ to specify that we are estimating a predicted value of the response for the given covariate value. To be able to distinguish this predicted response from the observed response we use the notation:

$$\hat{y}_1(x_i) = \phi_o(w_0 + w_1 x_{i1} + \cdots + w_p x_{ip})$$

The only difference to our MLR model is then that we would have called the ws $\hat{\beta}$s instead.

Statistical parameter estimation

- In multiple linear regression, the parameters β are estimated with maximum likelihood and least squares (equivalent under Normal assumption).

- **Remember**: The estimator $\hat{\beta}$ is found by minimizing the RSS for a multiple linear regression model:

$$\begin{aligned} \text{RSS} &= \sum_{i=1}^{n}(y_i - \hat{y}_i)^2 = \sum_{i=1}^{n}(y_i - \hat{\beta}_0 - \hat{\beta}_1 x_{i1} - \hat{\beta}_2 x_{i2} - ... - \hat{\beta}_p x_{ip})^2 \\ &= \sum_{i=1}^{n}(y_i - x_i^T\beta)^2 = (Y - X\hat{\beta})^T(Y - X\hat{\beta}) \ . \end{aligned}$$

  Solution:

$$\hat{\beta} = (X^T X)^{-1} X^T Y \ .$$

Neural networks: loss function and gradient descent

We now translate what we did for the regression setup into the neural networks world:

1. Replace the parameters β with *network weights* w.
2. Replace the RSS in our *training data set* with the following *loss function* (*mean squared error*)

$$J(w) = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_1(x_i))^2 \ ,$$

where $J(w)$ indicates that the unknown parameters are the weights w.

3. Replace *minimizing* the loss function (RSS) via
   - calculate the derivative of the loss function with respect to each of our parameters
   - solve the $(p+1)$ linear equations.

   $\rightarrow$ *more general minization procedures* that work also when the loss function does not have a closed form.

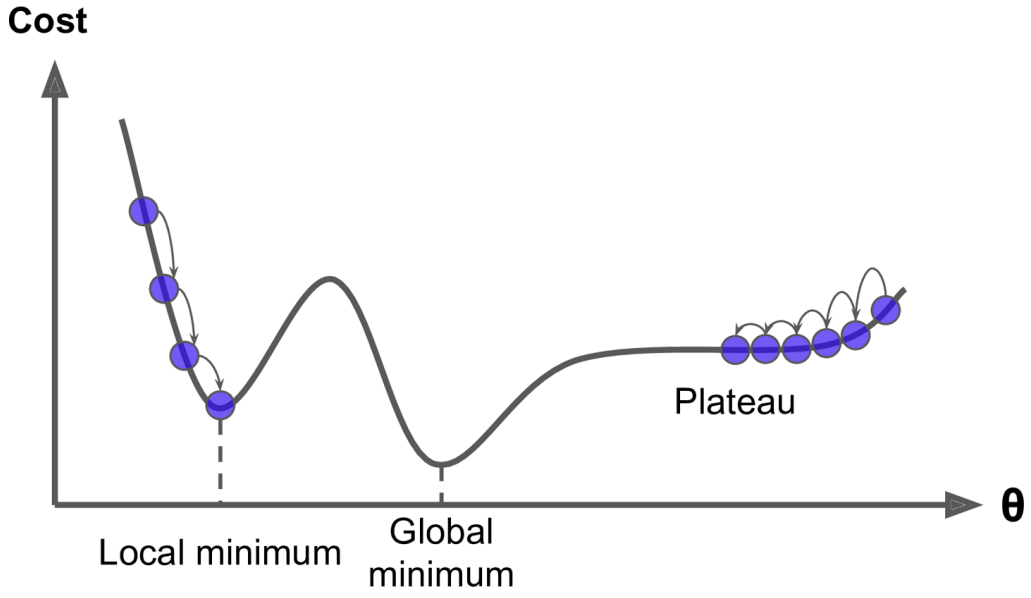
Finding optimal weights: Algorithm

1. Let $t = 0$ and denote the given initial values for the weights $w^{(t)}$,
2. Until convergence, repeat
   a) Calculate the predictions $\hat{y}_1(x_i)$
   b) calculate the loss function $J(w^{(t)})$,
   c) find the gradient (direction) in the $(p+1)$-dimensional space of the weights, and evaluate this at the current weight values $\nabla J(w^{(0)}) = \frac{\partial J}{\partial w}(w^{(0)})$
   d) go with a given step length (learning rate) λ in the direction of the negative of the gradient of the loss function to get

$$w^{(t+1)} = w^{(t)} - \lambda \nabla J(w^{(t)})$$

   e) Set $t = t + 1$, go to a) and continue to e) several times until you arrive at a (local) optimum
3. The final values of the weights in that $(p+1)$ dimensional space are our parameter estimates and your network is *trained*.

Gradient descent and local minima



(https://github.com/SoojungHong/MachineLearning/wiki/Gradient-Descent)

Other figures that give good illustration of the optimization problem in Chollet and Allaire (2018):

- 2.11: SGD down a 1D loess curve
- 2.12: Gradient descent down a 2D loss surface
- 2.13: local and global minimum

Backpropagation

- In neural networks the gradient part of the gradient descent algorithm is implemented efficiently in an algorithm called *backpropagation* (see later).

Here we compare

- the MLR solution with `lm`
- the neural network solution with `nnet` [1]

[1] Uses an improved gradient descent with Hessian information and the BFGS-algorithm. BFGS is a quasi-Newton method (also known as a variable metric algorithm), specifically that published simultaneously in 1970 by Broyden, Fletcher, Goldfarb and Shanno. This uses function values and gradients to build up a picture of the surface to be optimized.

Continuous outcome

Linear regression vs. neural networks: an example.

```
fit = lm(bodyfat ~ age + weight + height + bmi + neck + abdomen + hip,
    data = d.bodyfat)
fitnnet = nnet(bodyfat ~ age + weight + height + bmi + neck + abdomen +
    hip, data = d.bodyfat, linout = TRUE, size = 0, skip = TRUE, maxit = 1000,
    entropy = FALSE)
```

```
## # weights:  8
## initial  value 1730433.495727
## iter  10 value 4471.516449
## final  value 4415.453729
## converged
```

```
cbind(fitnnet$wts, fit$coefficients)
```

```
##                       [,1]          [,2]
## (Intercept) -9.748931e+01 -9.748903e+01
## age         -9.607523e-04 -9.607669e-04
## weight      -6.292838e-01 -6.292820e-01
## height       3.974902e-01  3.974884e-01
## bmi          1.785338e+00  1.785330e+00
## neck        -4.945734e-01 -4.945725e-01
## abdomen      8.945187e-01  8.945189e-01
## hip         -1.255554e-01 -1.255549e-01
```

Binary outcome: Diabetes

Aim is to predict if a person has diabetes[2]. The data stem from a population of women of Pima Indian heritage in the US, available in the R `MASS` package. The following information is available for each woman:

- `diabetes`: `0`= not present, `1`= present
- `npreg`: number of pregnancies
- `glu`: plasma glucose concentration in an oral glucose tolerance test
- `bp`: diastolic blood pressure (mmHg)
- `skin`: triceps skin fold thickness (mm)
- `bmi`: body mass index (weight in kg/(height in m)^2)
- `ped`: diabetes pedigree function.
- `age`: age in years

[2]Logistic regression is the "hello world" of machine learning.

The statistical model: Logistic regression

- $i = 1, \ldots, n$ observations in the training set. We will use r (instead of p) to be the number of covariates, to avoid confusion with the probability p.

- The binary reponse $Y_i \in \{1, 0\}$ with

$$\mathrm{P}(Y_i = 1) = p_i$$

and

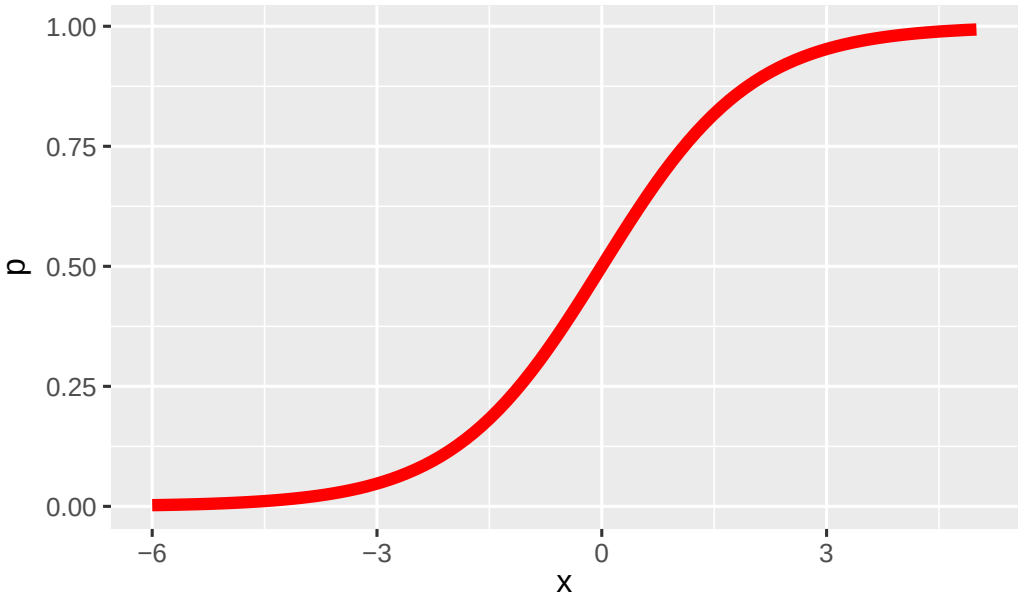
$$\log\left(\frac{p_i}{1 - p_i}\right) = \beta^\top x_i \ ,$$

where $\log(\frac{x}{1-x})$ is the *logistic function* .

- Therefore

$$p_i = \frac{\exp(\beta^\top x_i)}{1 + \exp(\beta^\top x_i)} = \frac{1}{1 + \exp(-\beta^\top x_i)} \ .$$

- This function is S-shaped, and ranges between 0 and 1 (so the p_i is between 0 and 1).



Parameter estimation in the statistical model

(Maximum likelihood)

- Given n independent pairs of covariates and responses $\{x_i, y_i\}$, the log-likelihood function of a logistic regression model can be written as:

$$\ln(L(\beta)) = l(\beta) = \sum_{i=1}^{n} \Big(y_i \ln p_i + (1 - y_i) \ln(1 - p_i) \Big) \ .$$

- Maximiation: set the $r + 1$ partial derivatives (to form the gradient) to 0.
- No closed form solution, thus we use a *gradient-based method* (the Newton-Raphson or Fisher scoring algorithm to find $\hat{\beta}$ and $SD(\hat{\beta})$:

$$\beta^{(t+1)} = \beta^{(t)} + F(\beta^{(t)})^{-1} s(\beta^{(t)}) \ ,$$

where the gradient of the log-likelihood $s(\beta) = \frac{\partial l}{\partial \beta}$ is called the score vector, and here the new quantity $F(\beta^{(t)})^{-1}$ is called the inverse *expected Fisher information matrix.*

The neural network model: architecture and activation function

- Remember: in the neural network (NN) version of *linear regression*, we had:

$$y_1(x_i) = w_0 + w_1 x_{i1} + \cdots + w_r x_{ir} \ ,$$

with activation function $\phi_o(x) = x$.

- In the NN version of *logistic regression* we instead have the *sigmoid activation function* $\phi_o(x) = \frac{1}{1+\exp(-x)}$, often denoted as $\sigma(x)$. Again, we prefer to use $\hat{y}_1(x_i)$ and get:

$$\hat{y}_1(x_i) = \frac{1}{1 + \exp(-(w_0 + w_1 x_{i1} + \cdots + w_r x_{ir}))} \in (0, 1) \ .$$

Neural networks: loss function and gradient descent

- For NNs we use *binomial cross-entropy loss*

$$J(w) = -\frac{1}{n}\sum_{i=1}^{n}(y_i \ln(\hat{y}_1(x_i)) + (1-y_i)\ln(1-\hat{y}_1(x_i)) \ ,$$

  which is a scaled version of the negative of the binomial loglikelihood!

- Optimization is done also with gradient descent, but we need the chain rule (due to the activation function) to get the partial derivatives for the gradient direction.

- Same backpropagation algorithm is again applicable, using the activation and loss functions given here.

Parameter estimation vs. network weights

```
fitlogist = glm(diabetes ~ npreg + glu + bp + skin + bmi + ped + age,
    data = train, family = binomial(link = "logit"))
summary(fitlogist)
```

```
##
## Call:
## glm(formula = diabetes ~ npreg + glu + bp + skin + bmi + ped +
##     age, family = binomial(link = "logit"), data = train)
##
## Deviance Residuals:
##     Min       1Q   Median       3Q      Max
## -1.9830  -0.6773  -0.3681   0.6439   2.3154
##
## Coefficients:
##              Estimate Std. Error z value Pr(>|z|)
## (Intercept) -9.773062   1.770386  -5.520 3.38e-08 ***
## npreg        0.103183   0.064694   1.595  0.11073
## glu          0.032117   0.006787   4.732 2.22e-06 ***
## bp          -0.004768   0.018541  -0.257  0.79707
## skin        -0.001917   0.022500  -0.085  0.93211
## bmi          0.083624   0.042827   1.953  0.05087 .
## ped          1.820410   0.665514   2.735  0.00623 **
## age          0.041184   0.022091   1.864  0.06228 .
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
##     Null deviance: 256.41  on 199  degrees of freedom
## Residual deviance: 178.39  on 192  degrees of freedom
```

```r
set.seed(787879)
library(nnet)
fitnnet = nnet(diabetes ~ npreg + glu + bp + skin + bmi + ped + age,
    data = train, linout = FALSE, size = 0, skip = TRUE, maxit = 1000,
    entropy = TRUE, Wts = fitlogist$coefficients + rnorm(8, 0, 0.1))
```

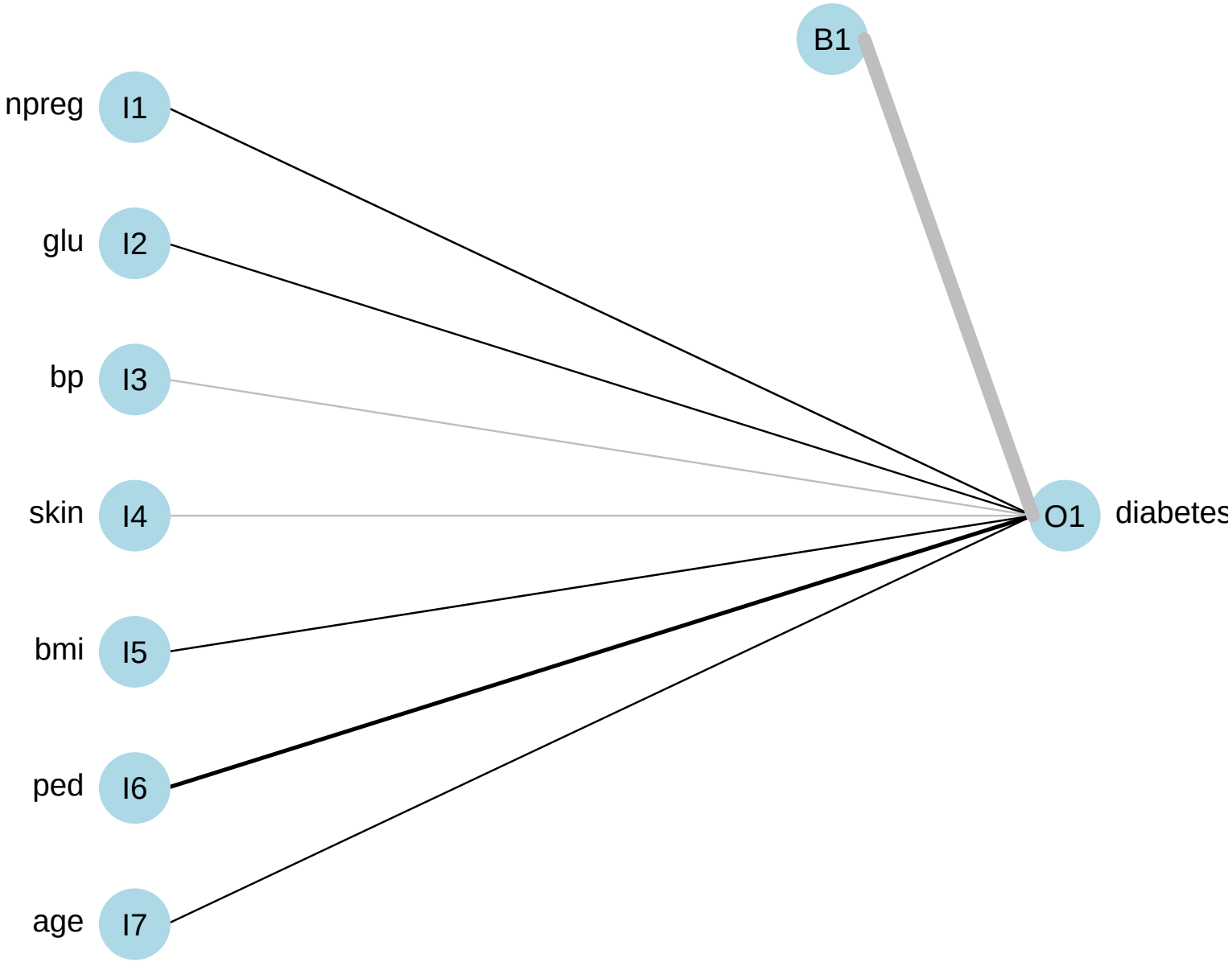
```
## # weights:  8
## initial  value 213.575955
## iter  10 value 89.511044
## final  value 89.195333
## converged
```

```r
# entropy=TRUE because default is least squares
cbind(fitnnet$wts, fitlogist$coefficients)
```

```
##                      [,1]         [,2]
## (Intercept) -9.773046277 -9.773061533
## npreg        0.103183171  0.103183427
## glu          0.032116832  0.032116823
## bp          -0.004767678 -0.004767542
## skin        -0.001917105 -0.001916632
## bmi          0.083624151  0.083623912
## ped          1.820397792  1.820410367
## age          0.041183744  0.041183529
```

By setting `entropy=TRUE` we minimize the cross-entropy loss.

```
plotnet(fitnnet)
```



But, there may also exist local minima.

```
set.seed(123)
fitnnet = nnet(diabetes ~ npreg + glu + bp + skin + bmi + ped + age,
    data = train, linout = FALSE, size = 0, skip = TRUE, maxit = 10000,
    entropy = TRUE, Wts = fitlogist$coefficients + rnorm(8, 0, 1))
```

```
## # weights:  8
## initial  value 24315.298582
## final  value 12526.062906
## converged
```

```
cbind(fitnnet$wts, fitlogist$coefficients)
```

```
##                     [,1]         [,2]
## (Intercept)   -36.733537 -9.773061533
## npreg         -77.126994  0.103183427
## glu         -2984.409175  0.032116823
## bp          -1835.934259 -0.004767542
## skin         -718.072629 -0.001916632
## bmi          -818.561311  0.083623912
## ped            -8.687473  1.820410367
## age          -773.023878  0.041183529
```

Why can NN and logistic regression lead to such different results?

Multiclass regression

Which type of iris species?

The `iris` flower data set was introduced by the British statistician and biologist Ronald Fisher in 1936.

- **Three plant species**: {setosa, virginica, versicolor}.
- **Four features**: `Sepal.Length`, `Sepal.Width`, `Petal.Length` and `Petal.Width`.

The aim is to predict the species of an iris plant.

The statistical model

We only briefly mentioned multiclass regression in module 4.

- Assume we have independent observation pairs (x_i, Y_i), where the covariate vector x_i consists of the same measurements for each response category.

- Each observation can only belong to one response class, $Y_i \in \{1, \ldots, C\}$.

- *Dummy variable coding* of the response in a C-dimensional vector: $y_i = (0, 0, \ldots, 0, 1, 0, \ldots, 0)$ with a value of 1 in the c^{th} element of y_i if the class is c.

- Probabilities that the response is category c for subject i

$$p_{ic} = P(Y_i = c) \ ,$$

where $\sum_{c=1}^{C} p_{ic} = 1$. In statistics we do not model p_{i1}, because $p_{i1} = 1 - \sum_{c=2}^{C} p_{ic}$, and $\beta_1 = 0$.

- Generalization of the logistic regression model:

$$p_{ic} = P(Y_i = c) = \frac{\exp(x_i^T \beta_c)}{1 + \sum_{s=2}^{C} \exp(x_i^T \beta_s)}$$

- Classification to the class with the highest probability, $\underset{c}{\text{argmax}}(p_{ic})$.

Parameter estimation in the statistical model

- The likelihood of the multinomial regression model can be written as

$$\ln(L(\beta) \propto \sum_{i=1}^{n} \sum_{c=1}^{C} y_{ic} \ln(p_{ic}) \ ,$$

  where $p_{iC} = 1 - p_{i1} - p_{i2} - \cdots - p_{i,C-1}$, and the regression parameters enter via the p_{ic}s.

- Parameter estimation is done in the same way as for the logistic regression, with the Fisher scoring algorithm (with score vector and Fisher information matrix).

- However (and this might be confusing), an efficient function in R also relies on neural networks for optimization (see below).

Neural network architecture and activation function

- Builds an output layer with C nodes and corresponding 0/1 targets (responses) using the dummy variable coding of the responses, called *one-hot coding*.

- The activation function for the ouput layer is called *softmax*. For each class $c = 1, \ldots, C$ it is given as

$$\hat{y}_c(x_i) = \frac{\exp(x_i^T w_c)}{\sum_{s=1}^{C} \exp(x_i^T w_s)} \ ,$$

  where each w_s is a $r + 1$ dimensional vector of weights.
- Note: there is some redundancy here, since $\sum_{c=1}^{C} \hat{y}_c(x_i) = 1$, so we could have had $C - 1$ output nodes, but this is not done.

- The focus of neural networks is not to interpret the weights, and there is no need to assume full rank of a matrix with output nodes.

Q: How many parameters are we estimating?

Neural networks: loss function and gradient descent

- For parameter estimation we looked at maximizing the log-likelihood of the statistical model. For neural networks the negative of the multinomial loglikelihood is a scaled version of the *categorical cross-entropy loss*

$$J(w) = -\frac{1}{n}\sum_{i=1}^{n}\frac{1}{C}\sum_{c=1}^{C}(y_{ic}\ln(\hat{y}_c(x_i)) \ .$$

- The optimization is done using gradient descent, with minor changes from what was done for the logistic regression due to the added sum and the small change in the activation function.

Fitting multinomial regression vs a neural network

First select a training sample

```
library(nnet)
set.seed(123)
train = sample(1:150, 50)
iris_train = ird[train, ]
iris_test = ird[-train, ]
```

Then fit the `nnet()` (by default using the softmax activation function)

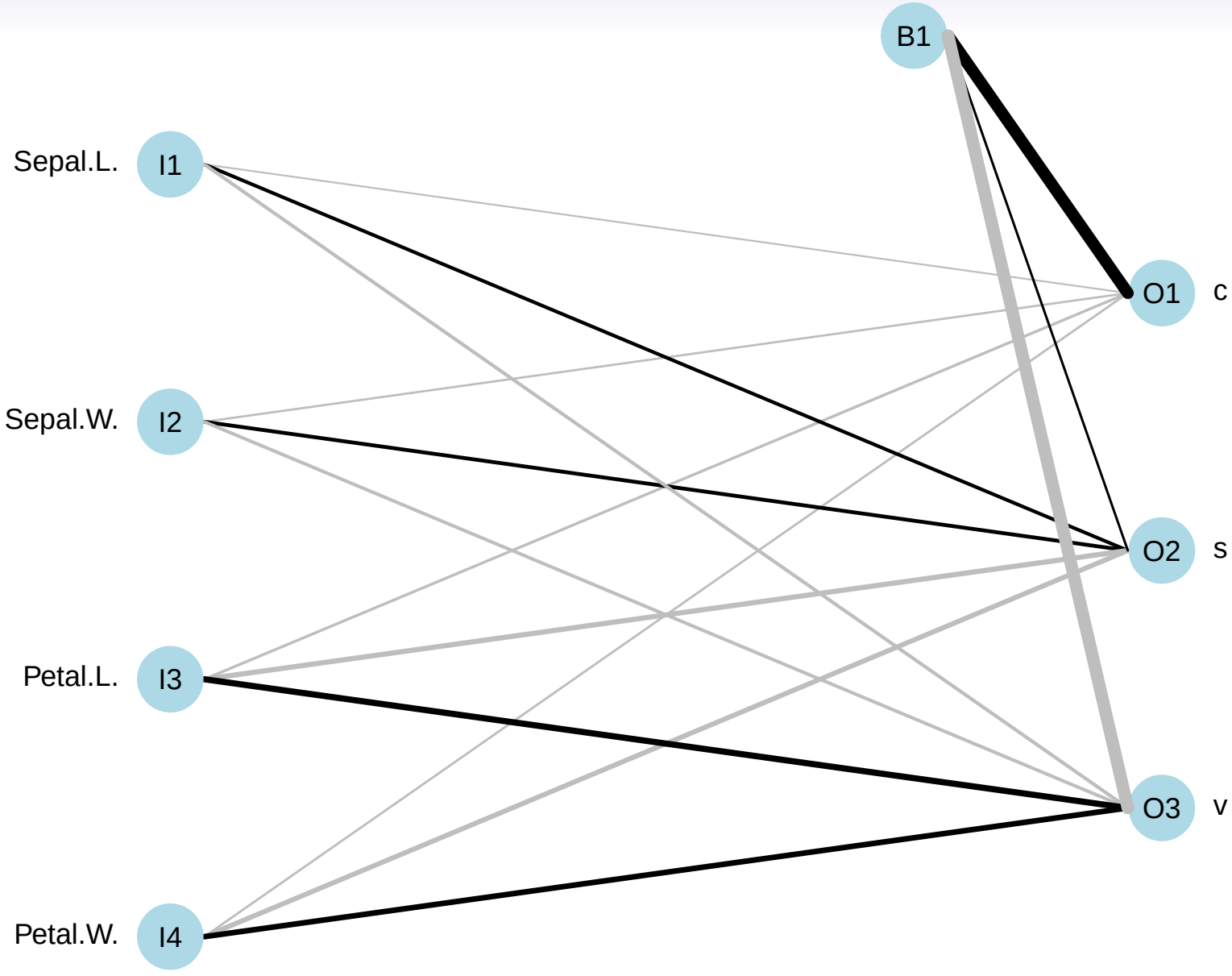
```
set.seed(123)
iris.nnet <- nnet(species ~ ., data = ird, subset = train, size = 0,
    skip = TRUE, rang = 0.1, maxit = 200)
```

```
## # weights:  15
## initial  value 56.732848
## iter  10 value 2.748260
## iter  20 value 0.012982
## final  value 0.000093
## converged
```

- How many weights have been estimated?
- What does the graph look like?

```
summary(iris.nnet)
```

```
## a 4-0-3 network with 15 weights
## options were - skip-layer connections  softmax modelling
##   b->o1  i1->o1  i2->o1  i3->o1  i4->o1
##  113.44   -0.36   -4.82  -11.51   -6.65
##   b->o2  i1->o2  i2->o2  i3->o2  i4->o2
##    7.56   20.19   23.17  -38.05  -36.15
##   b->o3  i1->o3  i2->o3  i3->o3  i4->o3
## -121.04  -19.78  -18.26   49.66   42.79
```


B1
Sepal.L.
I1
Sepal.W.
I2
Petal.L.
I3
Petal.W.
I4
O1
c
O2
s
O3
v

Fitting the multinomial regression. This is also done with nnet, but using a wrapper `multinom` (this has it's own settings, so results are not necessarily the same as above).

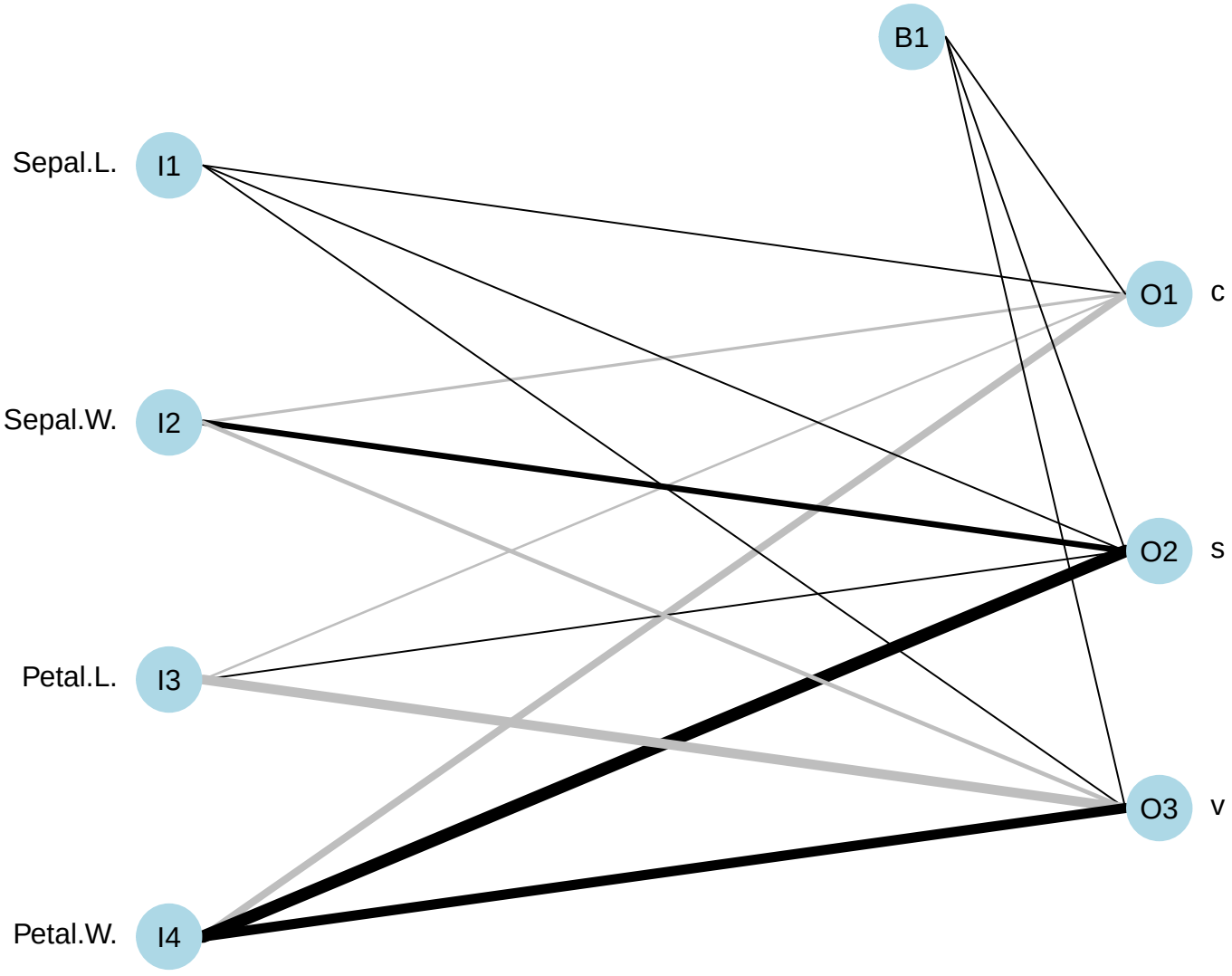
```
library(caret)
fit = multinom(species ~ -1 + ., family = multinomial, data = iris_train)
```

```
## # weights:  15 (8 variable)
## initial  value 54.930614
## iter  10 value 4.353139
## iter  20 value 0.139411
## iter  30 value 0.065218
## iter  40 value 0.056419
## iter  50 value 0.045548
## iter  60 value 0.020867
## iter  70 value 0.016116
## iter  80 value 0.012952
## iter  90 value 0.012787
## iter 100 value 0.009090
## final  value 0.009090
## stopped after 100 iterations
```

```
coef(fit)
```

```
##    Sepal.L.  Sepal.W.  Petal.L.  Petal.W.
## s  -5.91976  21.30247 -12.52073 -2.774511
## v -39.93182 -28.07162  53.73326 41.264390
```

Problem: `multinom()` seems to fit an intercept *plus* an offset node (B), thus we have to remove the intercept manually (by saying `-1` in the above formula).



The performance of multinomial regression vs nnet

```
testclass = predict(fit, new = iris_test)
confusionMatrix(data = testclass, reference = iris_test$species)$table
```

```
##           Reference
## Prediction  c  s  v
##          c 28  0  0
##          s  0 36  0
##          v  4  0 32
```

```
table(predict(iris.nnet, iris_test, type = "class"), iris_test$species)
```

```
##
##      c  s  v
##   c 31  0  7
##   s  0 36  0
##   v  1  0 25
```

For more on multinomial regression with R, check here.

Summing up

1. *Multiple linear regression*
   - NN with one input layer and one node in the output layer,
   - linear activation function,
   - mean squared loss.

2. *Logistic regression* (2 classes)
   - NN with one input layer and one node in the output layer,
   - sigmoid activation function,
   - and binary cross-entropy loss.

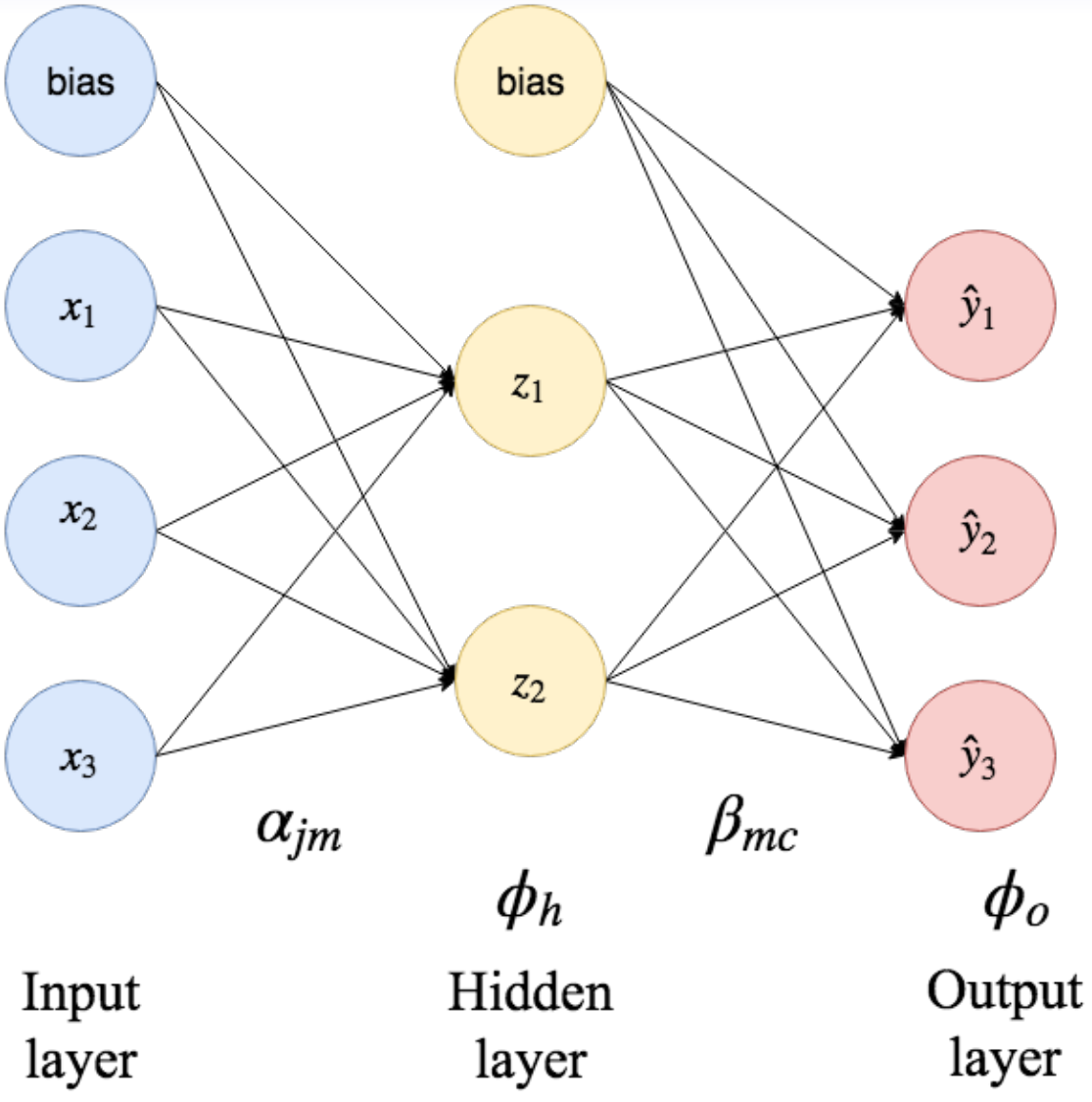
3. *Multinomial regression* ($C > 2$ classes)
   - NN with one input layer and C nodes in the output layer,
   - softmax activation function,
   - categorical cross-entropy loss.

But:

- These are only linear models (linear boundaries).
- Parameters (weights) found using gradient descent algorithms where the learning rate (step length) must be set.

Feedforward networks

- Connections are only forward in the network, but no feedback connections that sends the output of the model back into the network.
- Examples: Linear, logistic and multinomial regression with without any *hidden layers* (between the input and output layers).
- We may have no hidden layer, one (to be studied next), or many.
- Adding *hidden layers* with *non-linear activation functions* between the input and output layer will make nonlinear statistical models.
- The number of hidden layers is called the *depth* of the network, and the number of nodes in a layer is called the *width* of the layer.


bias
bias
x_1
x_2
x_3
z_1
z_2
$\hat{y}_1$
$\hat{y}_2$
$\hat{y}_3$
α_{jm}
β_{mc}
ϕ_h
ϕ_o
Input layer
Hidden layer
Output layer

The single hidden layer feedforward network

The nodes are also called *neurons*.

Notation

1. Inputs (input layer nodes), $j = 1, \ldots p$: $x_1, x_2, \ldots, x_p$, or as a vector x.
2. The nodes in the hidden layer, $m = 1, \ldots, M$: $z_1, z_2, \ldots, z_m$, or as vector z, and the hidden layer activation function ϕ_h.

$$z_m(x) = \phi_h(\alpha_{0m} + \sum_{j=1}^{p} \alpha_{jm} x_j)$$

where α_{jm} is the weight[3] from input j to hidden node m, and α_{0m} is the bias term for the mth hidden node. The hidden nodes can be thought of as *latent variables*.

[3] We stick with greek letters α and β for parameters, but call them weights.

3. The node(s) in the output layer, $c = 1, \ldots C$: $y_1, y_2, \ldots, y_C$, or as vector y, and output layer activation function ϕ_o.

$$\hat{y}_c(x) = \phi_o(\beta_{0c} + \sum_{m=1}^{M} \beta_{mc} z_m(x))$$

where β_{mc} is from hidden neuron m to ouput node c, and β_{0c} is the bias term for the cth output node.

4. Taken together

$$\hat{y}_c(x) = \phi_o(\beta_{0c} + \sum_{m=1}^{M} \beta_{mc} z_m) = \phi_o(\beta_{0c} + \sum_{m=1}^{M} \beta_{mc} \phi_h(\alpha_{0m} + \sum_{j=1}^{p} \alpha_{jm} x_j))$$

Hands on:

- Identify p, M, C in the network figure above, and relate that to the $y_c(x)$ equation.
- How many parameters need to be estimated for this network?
- What determines the values of p and C?
- How is M determined?

Special case: linear activation function for the hidden layer

If we assume that $\phi_h(z) = z$ (linear or identity activiation):

$$\hat{y}_c(x) = \phi_o(\beta_{0c} + \sum_{m=1}^{M} \beta_{mc}(\alpha_{0m} + \sum_{j=1}^{p} \alpha_{jm} x_j))$$

Q: Does this look like something you have seen before?
A:

Universal approximation property

- Think of the goal of a feedforward network to approximate some function f, mapping our input vector x to an output value y.

- What type of mathematical function can a feedforward neural network with one hidden layer and linear output activation represent?

The *universal approximation theorem*[4] says that a feedforward network with

- a *linear output layer*
- at least one hidden layer with a "squashing" activation function and "enough" hidden units

can approximate any (Borel measurable) function from one finite-dimensional space (our input layer) to another (our output layer) with any desired non-zero amount of error.

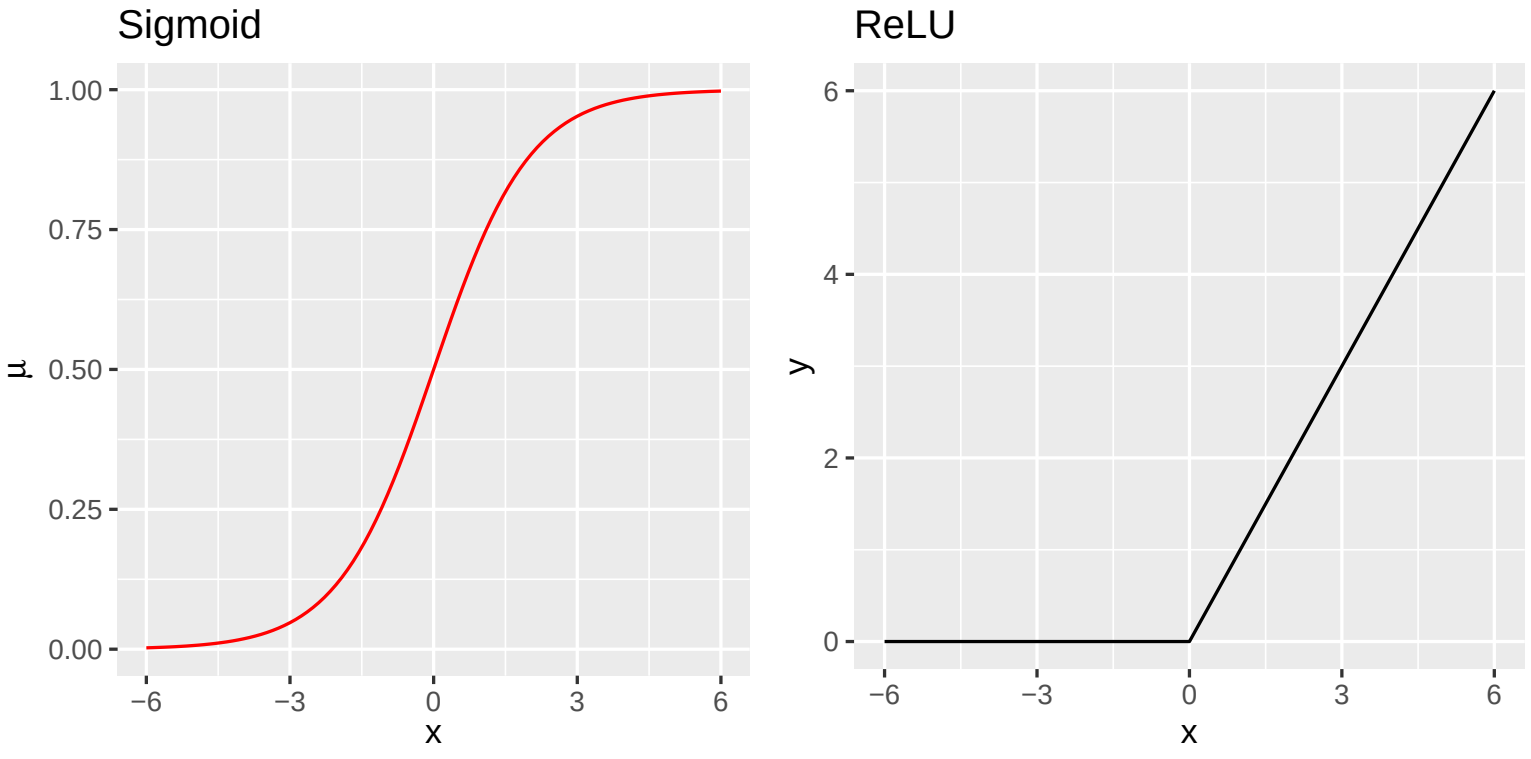
---

[4] Goodfellow et al 2016, p.198, https://www.deeplearningbook.org

The universal approximation theorem holds for

- The **sigmoid** $\phi(a) = 1/(1 + \exp(-a))$ (logistic) activation functions.
- The **rectified linear unit (ReLU)** $\phi_h(a) = \max(0, a)$ activation functions

in the hidden layer.



- The ReLU activiation function has replaced the sigmoid function as default in the hidden layer(s) of a feedforward network.

- Even though a large feedforward network with one hidden layer may be able to represent a desired function, we may not be able to estimate the parameters of the function:
  - we may choose a too many or too few nodes in the hidden layer.
  - our optimization routine may fail.
  - we may overfit/underfit the training data.

- Alternative: networks with more than one hidden layer, but fewer total number of nodes but more layers. A network with *many hidden layers* is called a *deep network*.

The `nnet` R package

- For simplicity (since we only have one week to work with this module), we will use the `nnet` R package by Brian Ripley instead of the currently very popular `keras` package for deep learning (the `keras` package will be presented for completeness).
- `nnet` fits *one hidden layer* with *sigmoid activiation function*. The implementation is not gradient descent, but instead BFGS using `optim`.
- Type `?nnet()` into your R-console to see the arguments of `nnet()`.
- If the response in formula is a factor, an appropriate classification network is constructed; this has one output and entropy fit if the number of levels is two, and a number of outputs equal to the number of classes and a softmax output stage for more levels.

Examples

Boston house prices

Objective: To predict the median price of owner-occupied homes in a given Boston suburb in the mid-1970s using 10 input variables. This data set is both available in the `MASS` and `keras` R package.

Preparing the data

- Only 506, split between 404 training samples and 102 test samples (this split already done in the `keras` library)
- Each feature in the input data (for example, the crime rate) has a different scale, some values are proportions, which take values between 0 and 1; others take values between 1 and 12, others between 0 and 100, and so on.

```
library(keras)
dataset <- dataset_boston_housing()
c(c(train_data, train_targets), c(test_data, test_targets)) %<-% dataset
str(train_targets)
```

```
##  num [1:404(1d)] 15.2 42.3 50 21.1 17.7 18.5 11.3 15.6 15.6 14.4 ...
```

```
head(train_data)
```

```
##         [,1] [,2]  [,3] [,4]  [,5]  [,6]  [,7]   [,8] [,9] [,10] [,11]
## [1,] 1.23247  0.0  8.14    0 0.538 6.142  91.7 3.9769    4   307  21.0
## [2,] 0.02177 82.5  2.03    0 0.415 7.610  15.7 6.2700    2   348  14.7
## [3,] 4.89822  0.0 18.10    0 0.631 4.970 100.0 1.3325   24   666  20.2
## [4,] 0.03961  0.0  5.19    0 0.515 6.037  34.5 5.9853    5   224  20.2
## [5,] 3.69311  0.0 18.10    0 0.713 6.376  88.4 2.5671   24   666  20.2
## [6,] 0.28392  0.0  7.38    0 0.493 5.708  74.3 4.7211    5   287  19.6
##       [,12] [,13]
## [1,] 396.90 18.72
## [2,] 395.38  3.11
## [3,] 375.52  3.26
## [4,] 396.90  8.01
## [5,] 391.43 14.65
## [6,] 391.13 11.74
```

The column names are missing (could get them by using the Boston dataset loaded from the MASS library).

- To make the optimization easier with gradient based methods do feature-wise normalization.

```
org_train = train_data
mean <- apply(train_data, 2, mean)
std <- apply(train_data, 2, sd)
train_data <- scale(train_data, center = mean, scale = std)
test_data <- scale(test_data, center = mean, scale = std)
```

- **Note**: the quantities used for normalizing the test data are computed using the training data. You should never use in your workflow any quantity computed on the test data, even for something as simple as data normalization. This also means that we need to do this standardization again (from scratch) if we need to do cross-validation.

Just checking out one hidden layer with 5 units to get going.

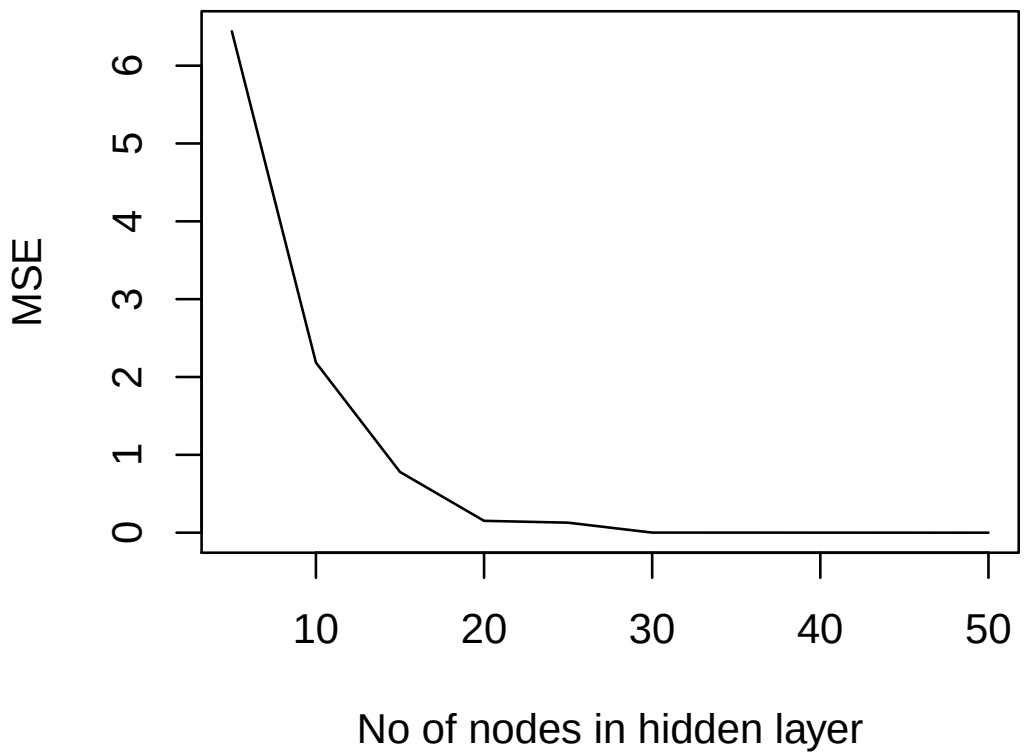
```
library(nnet)
fit5 <- nnet(train_targets ~ ., data = train_data, size = 5, linout = TRUE,
    maxit = 1000)
```

```
## # weights:  76
## initial  value 222875.445564
## iter  10 value 9625.869446
## iter  20 value 7008.319688
## iter  30 value 5889.493080
## iter  40 value 4914.814874
## iter  50 value 4116.546650
## iter  60 value 3860.485941
## iter  70 value 3705.511019
## iter  80 value 3660.347303
## iter  90 value 3616.529740
## iter 100 value 3566.523287
## iter 110 value 3549.835275
## iter 120 value 3519.659951
## iter 130 value 3450.648101
## iter 140 value 3359.604509
## iter 150 value 3313.298120
## iter 160 value 3281.887294
## iter 170 value 3256.471450
## iter 180 value 3239.303308
## iter 190 value 3205.304637
## iter 200 value 3180.026739
## iter 210 value 3166.982443
## iter 220 value 3165.194791
## iter 230 value 3164.924614
## iter 240 value 3164.431322
```

How to find best number of hidden nodes?

→ Cross-validation! (Time-consumring, so only results shown below.)

```
grid = c(5, 10, 15, 20, 25, 30, 50)
```



The best model here was the model with 50 nodes, the largest model we tried. Fitting that model on the full training set and testing on the test set:

```
library(nnet)
fit50 <- nnet(train_targets ~ ., data = train_data, size = 50, linout = TRUE,
    maxit = 5000, trace = F)
# head(summary(fit50))
pred = predict(fit50, newdata = test_data, type = "raw")
sqrt(mean((pred[, 1] - test_targets)^2))
```

```
## [1] 5.090128
```

```
mae = mean(abs(pred[, 1] - test_targets))
mae
```

```
## [1] 3.535428
```

- See here: https://www.math.ntnu.no/emner/TMA4268/2018v/11NN/11-neural_networks_boston_housing.html for running two hidden layers of 64 nodes each with `keras`. (This gave a mean absolute error on the test set of 2.68 after early stopping.)

Neural network parts

We now focus on the different elements of neural networks.

1) Output layer activation
2) Hidden layer activation
3) Network architecture
4) Loss function
5) Optimizers

1) Output layer activation

These choices have been guided by solutions in statistics (multiple linear regression, logistic regression, multiclass regression)

- Linear: for regression problems
- Sigmoid: for two-class classification problems
- Softmax: for more than two classes classification problems

Remark: it is important that the output activation is matched with an appropriate loss function.

2) Hidden layer activation

(See chapter 6.3 in Goodfellow, Bengio, and Courville (2016))

- ReLU ($\phi_h(a) = \max(0, a)$) is standard choice for deep networks (many hidden layers and many nodes) today.
- Sigmoid ($\phi_h(a) = \sigma(a) = 1/(1 + \exp(-a))$) or hyperbolic tangent ($\phi_h(a) = \tanh(z)$).
- Radial basis functions: as we looked at in Module 9.
- Softplus: $\phi_h(a) = \ln(1 + \exp(a))$
- Hard tanh: $\phi_h(a) = \max(-1, \min(1, a))$

Among all the possibilities, ReLU is nowadays the most popular one. Why?

- The function is piecewise linear, but *in total non-linear*.
- Replacing sigmoid with ReLU is reported to be one of the major changes that have improved the performance of the feedforward networks[5].
- Easy to use with gradient descent – even though the function is not differentiable at 0. As we will touch upon later, we don't expect to train a network until the gradient is 0. The derivative from the left at 0 is 0, and the derivative from the right is 1[6].

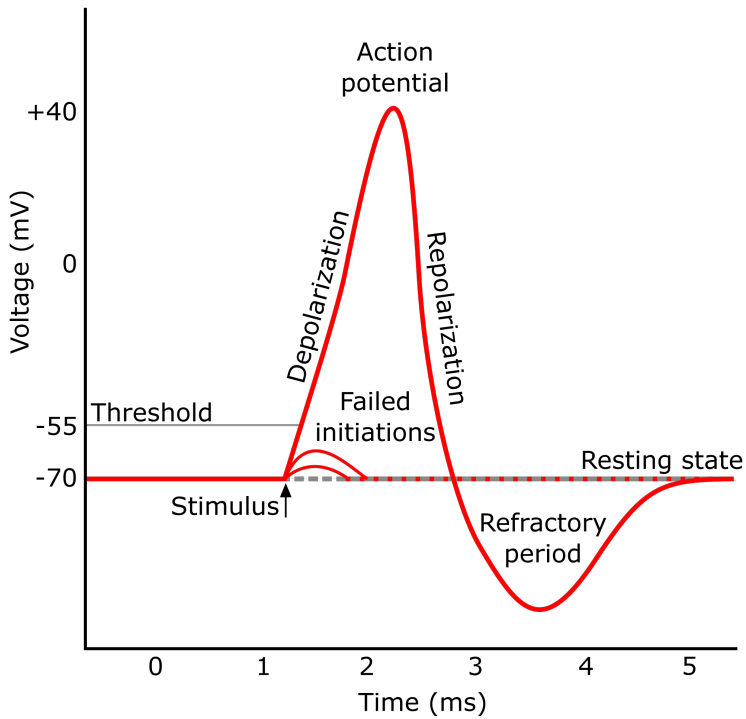
[5] Goodfellow et al, page 226

[6] See Goodfellow et al, p.192 for a discussion on this topic.

ReLU can also be motivated from biology.

- For some inputs a biological neuron can be completely inactive
- For some inputs a biological neuron output can be proportional to the input
- But, most of the time a biological neuron is inactive.

According to Goodfellow, Bengio, and Courville (2016), page 191, hidden unit design is an *active area of research.*



https://commons.wikimedia.org/wiki/File:Action_potential.svg

Q: Why can we not just use linar activation function in all hidden layers?

A:

3) Network architecture

Network architecture contains three components:

- *Width*: How many nodes are in each layer of the network?
- *Depth*: How deep is the network (how many hidden layers)?
- *Connectivity*: How are the nodes connected to each other?

This depends on the problem, and here experience is important.

- We will only consider *feedforward networks*, where all nodes in one layer are connected to all the nodes in the next layer. The layers are then *fully connected* and *dense*.

However, the recent practice, see e.g. Chollet and Allaire (2018), Section 4.5.6 and Goodfellow, Bengio, and Courville (2016), page 229, is to

- choose a too large network (too many nodes and/or too many layers) so that if trained until convergence (optimum) then the this would result in overfitting, and
- then use other means to avoid this (various variants of regularization and hyperparameter optimization).

This simplifies the choice of network architecture to *choose a large enough network*.

4) Loss function ("Method")

- The choice of loss function is closely related to the output layer activation function.
- To sum up, the popular problem types, output activation and loss functions are:

Problem	Output activation	Loss function
Regression	`linear`	`mse`
Classification (C=2)	`sigmoid`	`binary_crossentropy`
Classification (C>2)	`softmax`	`categorical_crossentropy`

Due to how estimation is done (see below), the loss functions chosen "need" to be:

- differentiable
- possible to compute for each single training data point (or a mini-batch – to be explained soon)

Note:

- 1980-1990s: the mean squared error was the prominent loss function also for classification problems, but this has subsequently changed.
- We have not explicitly assumed anything about any probability distribution of the responses (not even assumed that the responses are random variables). However, we know which statistical model assumptions would give the loss functions as related to the negative of the loglikelihood.

5) Optimizors

Let the unknown parameters be denoted θ (what we have previously denotes as αs and βs), and the loss function to be minimized $J(\theta)$.

- Gradient descent
- Mini-batch stochastic gradient descent (SGD)
- Backpropagation

Gradient descent

Remember:
Given the gradient $\nabla J(\theta^{(t)})$[7] of the loss function evaluated at the current estimate $\theta^{(t)}$, then the algorithm estimates the parameter at the next step as:

$$\theta^{(t+1)} = \theta^{(t)} - \lambda \nabla_\theta J(\theta^{(t)}) \ ,$$

where λ is the *learning rate* (usually a small value). In `keras` the default learning rate is 0.01.

Q: Why are we moving in the direction of the negative of the gradient? Why not the positive?

[7] Remember that the gradient is the vector of partical derivative of the loss function with respect to each of the parameter in the network.

Mini-batch stochastic gradient descent (SGD)

The loss function is computed as a mean over all training examples.

$$J(\theta) = \frac{1}{n} \sum_{i=1}^{n} J(x_i, y_i)$$

This means that the gradient will also be a mean over the gradient contribution from each training example.

$$\nabla_\theta J(\theta) = \frac{1}{n} \sum_{i=1}^{n} \nabla_\theta J(x_i, y_i)$$

To build a network that generalizes well, it is important to have many training examples, but that would make us spend a lot of time and computer resources at calculating each gradient descent step.

We observe that we may see the gradient as an average over many individual gradients, and think of this as an estimator for an expectation. This expectation can we (also) approximate by the average gradient over just a *mini-batch* (random sample) of the observations.

The idea here is that the optimizer will converge much faster if they can rapidly compute approximate estimates of the gradient, instead of slowly computing the exact gradient (using all training data).

In addition with multicore systems, mini-batches may be processed in parallell and the batch size is often a power of 2 (32 or 256).

It also turns out that small batches also serves as a regularization effect maybe due to the variability they bring to the optimization process.

This means that for (mini-batch) stochastic gradient descent we do as follows:

1. Divide all the training samples randomly into mini-batches.
2. For each mini-batch: Make predictions of the reponses in the mini-batch in a *forward pass*.
3. Compute the loss for the training data in this batch.
4. Compute the gradient of the loss with regard to the model's parameters (*backward pass*) based on the training data in the batch. $\nabla^*_\theta J(\theta^{(t)})$
5. Update all weighs, but just using the average gradient from the mini-batch $\theta^{(t+1)} = \theta^{(t)} - \lambda \nabla^*_\theta J(\theta^{(t)})$
6. Repeat 2-5 until convergence. (Could have gone back to 1, but often not done.)

- The algorithm defined above is called mini-batch SGD. The Stochastic part comes from the fact that we are randomly sampling batches from the training data.
- Stochastic gradient descent (SGD) for size equals to 1.
- Mini-batch SGD is a compromise between SGD (one sample per iteration) and full gradient descent (full dataset per iteration)

Backpropagation algorithm

Computing the analytical expression for the gradient ∇J is not difficult, but the numerical evaluation may be expensive. The Backpropagation algorithm is an simple and inexpensive way to calculate the gradient.

The chain rue is used to compute derivatives of functions of other functions where the derivatives are known, this is done efficiently with backpropagation.

Backpropagation starts with the value of the loss function and works backward from the top layers to the bottom layers, applying the chain rule to compute the contribution that each parameter have in the loss value.

More information:

- Mathematical details in Goodfellow, Bengio, and Courville (2016) Section 6.5 (pages 204-238),
- 3Blue1Brown: video overview: https://www.youtube.com/watch?v=Ilg3gGewQ5U and chain rule maths https://www.youtube.com/watch?v=tIeHLnjs5U8

Variations of SDG — with adaptive learning rates

General concept:

- momentum term: previous gradients are allowed to contribute.

Named variants: In `keras` the "default optimizer" is RMSprop.

- AdaGrad: individually adapt the learning rates of all model parameters by scaling them inversely proportional to the square root of the sum of all their historical squared values. (Nice properties for convex problems, but with non-linear hidden activation function we do not have a convex problem.)
- RMSprop: modification to AdaGrad in non-convex setting. Scales with exponentially weighted moving average instead of all historical squared gradient values.

Further reading on optimizers

- Keras documentation for Optimizers
- An overview of gradient descent optimization algorithms
- Overview of mini-batch gradient descent
- Andrew Ng explains about RMSprop in Coursera course: Improving Deep Neural Networks: Hyperparameter tuning, Regularization and Optimization

Regularization

Goodfellow, Bengio, and Courville (2016), Chapter 7, define regularization as *any modification we make to a learning algorithm that is intended to reduce its generalization error but not its training error.*

We looked at regularization in Module 6, where our aim was to trade *increased bias* for *reduced variance*. Another way of looking at this is we need not focus entirely on finding the model of "correct size", but instead find a large model that has been regularized properly.

In Module 6 we looked in particular at adding a penalty to the loss function. The penalties we looked at were of type absolute value of parameter (L_1, lasso, where we looked at this as model selection) and square value of parameter (L_2, ridge regression). This can also done for neural networks.

In neural networks, *weight decay* is the expression for adding a L_2-penalty to the loss function, and is available in the `nnet` R package.

Other versions of regularization are *dataset augmentation* and *label smoothing*:

- Dataset augmentation means adding fake data to the dataset, in order that the trained model will generalize better. For some learning task it is straightforward to create the new fake data — for image data this can be done by rotating and scaling the images.
- Label smoothing is motivated by the fact that the training data may contain errors in the reponses recorded, and replaced the one-hot coding for C classes with $\epsilon/(C-1)$ and $1-\epsilon$ for some small ϵ.

Early stopping

(Based on Goodfellow, Bengio, and Courville (2016), Section 7.8)
The most commonly used for of regularization is *early stopping*.
If we have chosen a sufficiently large model with the capacity to overfit the training data, we would observe that the training error decreases steadily during training, but the error on the validation set at some point begins to increase.
If we stop the learning early and return the parameters giving the test performance on the validation set, this model would hopefully be a better model than if we trained the model until convergence — and this model will then also give a better test set error.

It is possible to think of the number of *training steps* as a hyperparameter. This hyperparameter can easily be set, and the cost is just that we need to monitor the performance on the validation set during training. Alternatively, cross-validation can be used.

One strategy is to first find the optimal stopping time for the training based on the valiation set (or with cross-validation with small data sets), and then retrain the full training set (including the validation part) and stop at the selected stopping time.

Why is early stopping a regularization technique? By early stopping the optimization procedure has only seen a relatively small part of the parameter space in the neighbourhood of the intitial parameter value. See Goodfellow, Bengio, and Courville (2016), page 250 for a relationship with L_2 regularization.

Hyperparameter optimization

How to avoid overfitting:

- reduce network size,
- collect more observations,
- regularization (including early stopping and drop-out)

The network architacture, the number of batches to run before terminating the optimzation, the drop-out rate, are all examples of hyperparameters that need to be chosen in a sensible way before fitting the final model.

It is important that the hyperparameters are chosen on a validation set or by cross-validation.

However, a "popular" term is *validation-set overfitting* and refers to using the validation set to decide many hyperparameters, so many that you may effectively overfit the validation set.

In statistics we use design of experiments to explore these hyperparameters, and just using marginal grids (one hyperparameter at a time) is common in machine learning.

Example on DOE:hyperparameter optimization with boosting (which of cause also can be used for neural networks). Article: Design of experiments and response surface methodology to tune machine learning hyperparameters, with a random forest case-study (2018), Gustavo A. Lujan-Moreno, Phillip R. Howard, Omar G. Rojas, Douglas Montgomery, Expert Systems with Applications, Volume 109, https://doi.org/10.1016/j.eswa.2018.05.024

Dropout

(Based on Goodfellow, Bengio, and Courville (2016), Section 7.12, and Chollet and Allaire (2018) 4.4.3)
Dropout was developed by Geoff Hinton and his students.

- During training: randomly *dropout* (set to zero) outputs in a layer. Drop-out rates may be chosen between 0.2 and 0.5.
- During test: not dropout, but scale done the layer output values by a factor equal to the drop-out rate (since now more units are active than we had during training)

Alternatively, the drop-out and scaling (now upscaling) can be done during training.

One way to look at dropout is on the lines of what we did in Module 8 when we used bootstrapping to produced many data sets and then fitted a model to each of them and then took the average (bagging). But randomly dropping out outputs in a layer, this can be looked as mimicking bagging — in an efficient way.

See Goodfellow, Bengio, and Courville (2016), Section 7.12 for more insight into the mathematics behind drop-out.

https://www.reddit.com/r/MachineLearning/comments/4w6tsv/ama_we_are_the_google_brain_team_wed_love_to/

The following is a direct quotation.

figplucker: **How was 'Dropout' conceived? Was there an 'aha' moment?**

geoffhinton (2 years ago)

There were actually three aha moments. One was in about 2004 when Radford Neal suggested to me that the brain might be big because it was learning a large ensemble of models. I thought this would be a very inefficient use of hardware since the same features would need to be invented separately by different models. Then I realized that the "models" could just be the subset of active neurons. This would allow combinatorially many models and might explain why randomness in spiking was helpful.

Soon after that I went to my bank. The tellers kept changing and I asked one of them why. He said he didn't know but they got moved around a lot. I figured it must be because it would require cooperation between employees to successfully defraud the bank. **This made me realize that randomly removing a different**

Metrics

Provides different forms to measure how well the predictions are compared with the true values.

- `accuracy`: Percentage of correct classifications
- `mae`: Mean absolute error.

These metrics can be monitored during training (on validation set) or in the end on the test set, and can be the basis for the choice when to top training.

Deep learning

Timeline

(based on Chollet and Allaire (2018))

Neural networks were investigated in "toy form" in the 1950s. The first big step was taken in the 1980s when the backpropagation algorithm were developed (rediscovered) to perform gradient descent in an efficient way.

In 1989 (Bell Labs, Yann LeCun) used convolutional neural networks to classifying handwritten digits, and *LeNet* was used in the US Postal Service for reading ZIP codes in the 1990s.

Not so much seen (?) activity in the neural network field in the 2000s.

In 2011 neural networks with many layers (and trained with GPUs) were performing well on image classification tasks. The *ImageNet* classification challenge (classify high resolution colour images into 1k different categories after training on 1.4M images) was won by solutions with deep convolutional neural networks (convnets). In 2011 the accuracy was 74.3%, in 2012 83.6% and in 2015 96.4%.

From 2012, convnets is the general solution for computer vision tasks. Other application areas are natural language processing.

Deep?

Deep learning does not mean a deeper understanding, but refers to sucessive layers of representations - where the number of layers gives the *depth* of the model. Often tens to hundreds of layers are used. Deep neural networks are not seen as models of the brain, and are not related to neurobiology.

A deep network can be seen as many stages of *information-destillation* (Chollet and Allaire (2018), page 9), where each stage performes a simple data transformation. These transformations are not curated by the data analyst, but is estimated in the network.

In statistics we first select a set of inputs, then look at how these inputs should be transformed (projections in simple form or high-dimensional and nonlinear forms), before we apply some statistical methods. This transformation step can be called *feature engineering* and has been automated in deep learning.

Deep Learning is an algorithm which has no theoretical limitations of what it can learn; the more data you give and the more computational time you provide, the better it is.

Geoffrey Hinton (Google)

In addition, this built-in feature engineering of the deep network is not performed in a greedy fashion, but *jointly* with estimating/learning the full model.

The success of deep learning is dependent upon the breakthroughts in hardware development, expecially with faster CPUs and massively parallell graphical processing units (GPUs). Tensor processing units (TPUs) is the next step.

Achievements of deep learning includes high quality (near-human to super human) image classification, speech recognition, handwriting transcription, machine translation, digital assistants, autonomous driving, advertise targeting, web searches, playing Go and chess.

The R keras package

Earlier good programming skills in C++ was essential to work in deep learning. In addition also skills on programming for GPUs were needed (e.g NVIDIA CUDA programming interface). With the launch of the Keras library now users may only need basic skills in Python or R.

Keras can be seen as a way to use LEGO bricks in deep learning. To quote the web-page:

Keras is a high-level neural networks API, written in Python and capable of running on top of TensorFlow, CNTK, or Theano. It was developed with a focus on enabling fast experimentation. Being able to go from idea to result with the least possible delay is key to doing good research.

Tensorflow is a *symbolic-tensor manipulation* framework that also can perform autodifferentiation.

A tensor is defined by its number of axis (below), shape (dimension) and data type (double, integer, character)

- 0D tensor is a scalar
- 1D tensor is a vector
- 2D tensor is a matrix - and the two *axis* of the tensor is the rows and columns
- 3D tensor generalization of a matrix, and may be used for time series data
- 4D tensors may be used for images (samples, height, width, channels), and
- 5D tensors may be used for video (as 4D, plus frames).

Tensor operations (reshaping, dot product) are performed in TensorFlow.

The use of Tensorflow in R Keras is referred to as "using Tensorflow as a backend engine". Tensorflow is the default backend.

More information on the R solution: https://keras.rstudio.com/

Cheat-sheet for R Keras:
https://github.com/rstudio/cheatsheets/raw/master/keras.pdf

Simple data analysis workflow

1. Select training and test data
2. Define the model(s): layers, nodes in layers, activation function
3. Configure the learning process by choosing a loss function, an optimizer, and some metrics to monitor. If needed decide on an evaluation protocol (validation set, cross-validation, iterated cross-validation)
4. Perform any needed preprocessing of data to fit the choices in 2 and 3
5. Fit the model to the data
6. Make preditions for test data or use the model

Chollet and Allaire (2018) Section 4.5 has the following recommentations for step 3+5:

- Develop a first model that performs better than a basic baseline (maybe the basic baseline could be standard statistics solutions)
- Develop a model that overfits the data
- Regularize and tune hyperparameters

Here is a tutorial:
https://keras.rstudio.com/articles/tutorial_overfit_underfit.html

MNIST dataset

This is a larger image version of the handwritten digits data set (a different version, ZIP-codes is found under Recommended exercises). This data analysis is based on https://www.math.ntnu.no/emner/TMA4268/2018v/11NN/8-neural_networks_mnist.html and the `R keras` cheat sheet. An advanced version using convolutional neural nets is found here: https://www.math.ntnu.no/emner/TMA4268/2018v/11NN/12-neural_networks_convolution_mnist.html

Objective: classify the digit contained in an image (128×128 greyscale). Problem type: Multiclass classification based on image data.

Labels for the training data:

```
## train_labels
##    0    1    2    3    4    5    6    7    8    9
## 5923 6742 5958 6131 5842 5421 5918 6265 5851 5949
```

1. Training and test data

60 000 images for training and 10 000 images for testing.

```
# Training data
train_images <- mnist$train$x
train_labels <- mnist$train$y

# Test data
test_images <- mnist$test$x
test_labels <- mnist$test$y
org_testlabels <- test_labels
```

The `train_images` is a tensor (generalization of a matrix) with 3 axis, `(samples, height, width)`.

2. Defining the model

In this case we are using a `layer_dense` (fully connected) which expects an input tensor of rank equal to two `(sample, features)` where each `sample` should contain `28*28=784` pixels. Adding a bias term (intercept) is default for `layer_dense`.

```
network <- keras_model_sequential() %>% layer_dense(units = 512, activation = "relu",
    input_shape = c(28 * 28)) %>% layer_dense(units = 10, activation = "softmax")
summary(network)
```

```
## Model: "sequential"
## _________________________________________________________________________
## Layer (type)                         Output Shape                     Param #
## =========================================================================
## dense (Dense)                        (None, 512)                      401920
## _________________________________________________________________________
## dense_1 (Dense)                      (None, 10)                       5130
## =========================================================================
## Total params: 407,050
## Trainable params: 407,050
## Non-trainable params: 0
## _________________________________________________________________________
```

As activation function we use `relu` for the hidden layer, and `softmax` for the output layer - since we have 10 classes (where one is correct each time). We could have included more layers in our model - and then maybe used early stopping if our model was chosen too big.

3. Configure the learning process

We next need to choose the loss function we will use, which is cross-entropy, and then the version of the optimizer. Here htis is RMSprop. Finally, which measure - metrics - do we want to monitor in our training phase? Here we choose accuracy (=percentage correctly classified).

```
network %>% compile(optimizer = "rmsprop", loss = "categorical_crossentropy",
    metrics = c("accuracy"))
```

4. Preprocessing to match with model inputs and outputs

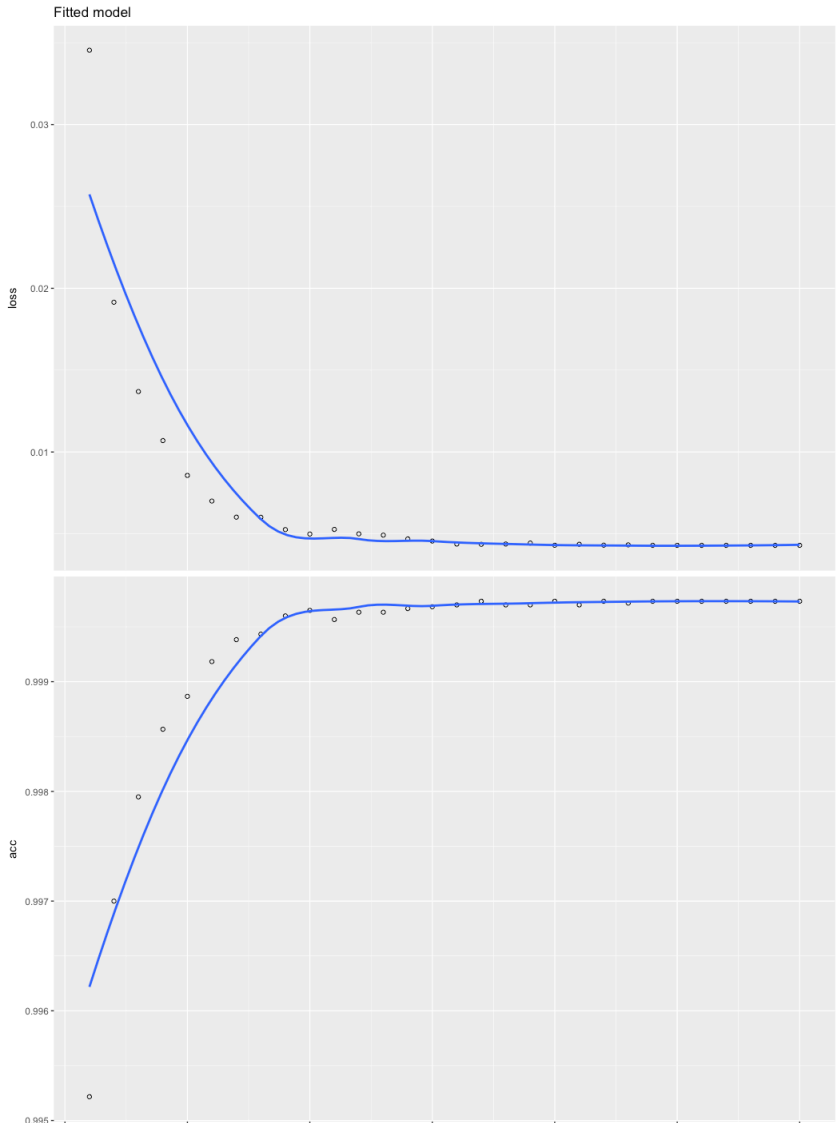
The training data is scored in an array of dimension (60000, 28, 28) of type integer with values in the [0, 255] interval. The data must be reshaped into the shape the network expects (28*28). In addition the grey scale values are scales to be in the [0, 1] interval.
Also, the response must be transformed from 0-10 to a vector of 0s and 1s (dummy variable coding) aka one-hot-coding.

```
train_images <- array_reshape(train_images, c(60000, 28 * 28))
train_images <- train_images/255
train_labels <- to_categorical(train_labels)

test_images <- array_reshape(test_images, c(10000, 28 * 28))
test_images <- test_images/255
test_labels <- to_categorical(test_labels)
```

###5. Fit the model

```
fitted<-network %>% fit(train_images, train_labels,
 epochs = 30, batch_size = 128)
library(ggplot2)
plot(fitted)+ggtitle("Fitted model")
```



###6. Evaluation and prediction

```
network %>% evaluate(test_images, test_labels)
testres = network %>% predict_classes(test_images)
# $loss [1] 0.1194063 $acc [1] 0.9827
confusionMatrix(factor(testres), factor(org_testlabels))
```

```
Confusion Matrix and Statistics

          Reference
Prediction    0    1    2    3    4    5    6    7    8    9
         0  971    0    3    0    1    2    5    1    1    1
         1    1 1128    2    0    0    0    2    2    2    3
         2    1    1 1009    3    3    0    2    7    2    0
         3    0    1    2  997    0   11    1    3    4    3
         4    1    0    2    0  969    1    4    2    3    7
         5    0    1    0    1    0  871    3    0    1    4
         6    3    2    2    0    3    4  940    0    1    0
         7    1    1    4    2    1    0    0 1002    2    3
         8    2    1    7    0    0    2    1    4  953    1
         9    0    0    1    7    5    1    0    7    5  987

Overall Statistics

               Accuracy : 0.9827
                 95% CI : (0.9799, 0.9852)
    No Information Rate : 0.1135
    P-Value [Acc > NIR] : < 2.2e-16

                  Kappa : 0.9808
 Mcnemar's Test P-Value : NA
```

Kaggle

Kaggle has hosted machine-learning competitions since 2010, and by looking at solutions to competitions it is possible to get an overview of what works. In 2016-2017 gradient boosting methods won the competitions with structured data ("shallow" learning problems), while deeplearning won perceptual problems (as image classification), Chollet and Allaire (2018) (page 18). Kaggle has helped (and is helping) the rise in deep learning.

Other analyses

Boston housing price

taken from Chollet and Allaire (2018):
https://www.math.ntnu.no/emner/TMA4268/2018v/11NN/11-neural_networks_boston_housing.html

Movie data base

https://www.math.ntnu.no/emner/TMA4268/2018v/11NN/9-neural_networks_imdb.html

Reuters data

https://www.math.ntnu.no/emner/TMA4268/2018v/11NN/10-neural_networks_reuters.html

Summing up

- Feedforward network architecture: mathematical formula - layers of multivariate transformed (`relu`, `linear`, `sigmoid`) inner products - sequentially connected.
- What is the number of parameters that need to be estimated? Intercept term (for each layer) is possible and is referred to as "bias term".
- Loss function to minimize (on output layer): regression (mean squared), classification binary (binary crossentropy), classification multiple classes (categorical crossentropy) — and remember to connect to the correct choice of output activiation function: mean squared loss goes with linear activiation, binary crossentropy with sigmoid, categorical crossentropy with softmax.
- How to minimize the loss function: gradient based (chain rule) back-propagation - many variants.
- Technicalities: `nnet` in R
- Optional: `keras` in R. Use of tensors. Piping sequential layers, piping to estimation and then to evaluation (metrics).

Not covered

(The first two topics are covered in Chollet and Allaire (2018))
Recurrent networks: extending the feedforward network to also have feedback connections. This is a popular type of network to analyse time series data and natural language applications.
Convolutional networks: some layers in a sequential network contain operations specially suitable for grid-like topology (images). Convolution is used in place of general layer (where we do matrix multiplication) in at least one layer. A popular operation is *pooling*.
Explanable AI (XAI): how to use methods on the network or the predictions of the network to figure out the underlying reasoning of the network. Popular methods are called LIME (local linear regression), Shaply (concept from game theory). The `DALEX` R package contains different socalled *explainers*
https://arxiv.org/abs/1806.08915.

References and further reading

- https://youtu.be/aircAruvnKk from 3BLUE1BROWN - 4 videos - using the MNIST-data set as the running example
- Look at how the hidden layer behave: https://playground.tensorflow.org
- Friedman, Hastie, and Tibshirani (2001),Chapter 11: Neural Networks
- Efron and Hastie (2016), Chapter 18: Neural Networks and Deep Learning
- Chollet and Allaire (2018)
- Goodfellow, Bengio, and Courville (2016) (to be used in IT3030) https://www.deeplearningbook.org/
- Explaining backpropagation http://neuralnetworksanddeeplearning.com/chap2.html
- Slides from MA8701 (Thiago Martins) https://www.math.ntnu.no/emner/MA8701/2019v/DeepLearning/

Acknowledgements

Chollet, François, and J. J. Allaire. 2018. *Deep Learning with R.* Manning Press.
https://www.manning.com/books/deep-learning-with-r.

Efron, Bradley, and Trevor Hastie. 2016. *Computer Age Statistical Inference - Algorithms, Evidence, and Data Science.* Cambridge University Press.

Friedman, Jerome, Trevor Hastie, and Robert Tibshirani. 2001. *The Elements of Statistical Learning.* Vol. 1. Springer series in statistics New York.

Goodfellow, Ian, Yoshua Bengio, and Aaron Courville. 2016. *Deep Learning.* MIT Press.