

# Statistical Learning

## Lecture 12a - Neural Networks - Deep Learning

ANU - RSFAS

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# Deep Learning

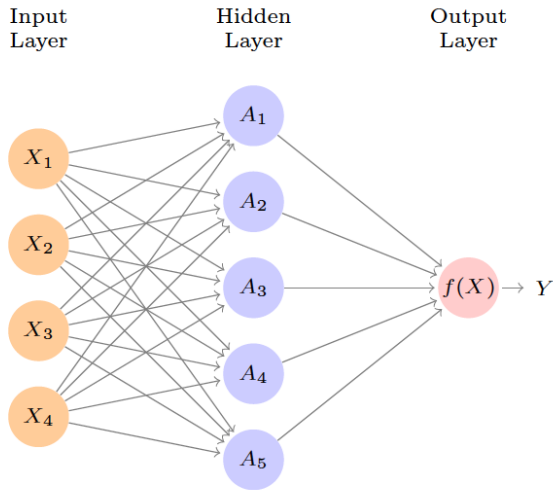
- Neural networks became popular in the 1980s. Lots of successes and hype.
- Then along came SVMs, Random Forests and Boosting in the 1990s, and Neural Networks took a back seat.
- Re-emerged around 2010 as Deep Learning. By 2020s very dominant and successful. Part of success due to vast improvements in computing power, larger training sets, and software: Tensor flow (Google) and PyTorch (Facebook).

# Deep Learning

- Much of the credit goes to three pioneers (computer scientists) and their students: Yann LeCun, Geoffrey Hinton and Yoshua Bengio, who received the 2019 ACM Turing Award for their work in Neural Networks.



# Nueral Networks - Single Layer

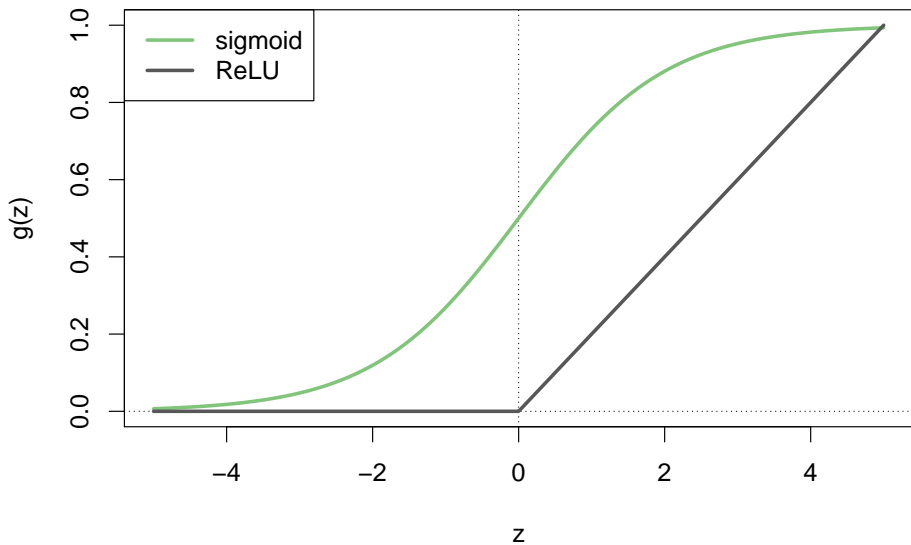


# Nueral Networks - Single Layer

$$\begin{aligned}f(X) &= \beta_0 + \sum_{i=1}^K \beta_k h_k(X) \\&= \beta_0 + \sum_{i=1}^K \beta_k g(w_{k0} + \sum_{j=1}^p w_{kj} X_j) \\&= \beta_0 + \sum_{i=1}^K \beta_k A_k\end{aligned}$$

- $g(\cdot)$  is non-linear **activation function** - specified in advance
- Each  $A_k$  is a different transformation  $h_k(X)$  of the original features (covariates) - similar in flavor to the basis functions in Chapter 7 for non-linear fits.

- $A_k$  are called the **activations** in the **hidden layer**.
- $g(z)$  is called the activation function. Popular are the **sigmoid** and **rectified linear**
- Activation functions in hidden layers are typically nonlinear, otherwise the model collapses to a linear model.
- So the activations are like derived features – nonlinear transformations of linear combinations of the features.
- Moreover, having a nonlinear activation function allows the model to capture complex nonlinearities and interaction effects.



- Consider a simple example:

$$X = (X_1, X_2), \quad K = 2, \quad p = 2, \quad g(z) = z^2$$

$$\begin{aligned} \beta_0 &= 0, & \beta_1 &= \frac{1}{4}, & \beta_2 &= -\frac{1}{4} \\ w_{10} &= 0, & w_{11} &= 1, & w_{12} &= 1 \\ w_{20} &= 0, & w_{21} &= 1, & w_{22} &= -1 \end{aligned}$$

- So we have:

$$\begin{aligned} h_1(X) &= (0 + X_1 + X_2)^2 \\ h_2(X) &= (0 + X_1 - X_2)^2 \end{aligned}$$

$$\begin{aligned} f(X) &= 0 + \frac{1}{4} ((0 + X_1 + X_2)^2) - \frac{1}{4} ((0 + X_1 - X_2)^2) \\ &= \frac{1}{4} ((X_1 + X_2)^2 - (X_1 - X_2)^2) \\ &= X_1 X_2 \end{aligned}$$



# Fitting

- Fitting a neural network requires estimating the unknown parameters.
- For a quantitative response this is typically done via least-squares:

$$\sum_{i=1}^n (y_i - f(x_i))^2$$

- Let's revisit the Baseball Salary data
- This is a regression problem, where the goal is to predict the Salary of a baseball player in 1987 using his performance statistics from 1986.
- After removing players with missing responses, we are left with 263 players and 19 variables.
- We randomly split the data into a training set of 176 players (two thirds), and a test set of 87 players (one third).

```
library(ISLR2); data("Hitters"); summary(Hitters[,1:8])
```

##	AtBat	Hits	HmRun	Runs
##	Min. : 16.0	Min. : 1	Min. : 0.00	Min. : 0.00
##	1st Qu.:255.2	1st Qu.: 64	1st Qu.: 4.00	1st Qu.: 30.25
##	Median :379.5	Median : 96	Median : 8.00	Median : 48.00
##	Mean :380.9	Mean :101	Mean :10.77	Mean : 50.91
##	3rd Qu.:512.0	3rd Qu.:137	3rd Qu.:16.00	3rd Qu.: 69.00
##	Max. :687.0	Max. :238	Max. :40.00	Max. :130.00
##	RBI	Walks	Years	CatBat
##	Min. : 0.00	Min. : 0.00	Min. : 1.000	Min. : 19.0
##	1st Qu.: 28.00	1st Qu.: 22.00	1st Qu.: 4.000	1st Qu.: 816.8
##	Median : 44.00	Median : 35.00	Median : 6.000	Median : 1928.0
##	Mean : 48.03	Mean : 38.74	Mean : 7.444	Mean : 2648.7
##	3rd Qu.: 64.75	3rd Qu.: 53.00	3rd Qu.:11.000	3rd Qu.: 3924.2
##	Max. :121.00	Max. :105.00	Max. :24.000	Max. :14053.0

```
summary(Hitters[, -c(1:8)])
```

```
##           CHits           CHmRun           CRuns           CRBI
## Min.      : 4.0    Min.      : 0.00    Min.      : 1.0    Min.      : 0.00
## 1st Qu.: 209.0    1st Qu.: 14.00    1st Qu.: 100.2    1st Qu.: 88.75
## Median : 508.0    Median : 37.50    Median : 247.0    Median : 220.50
## Mean     : 717.6    Mean     : 69.49    Mean     : 358.8    Mean     : 330.12
## 3rd Qu.: 1059.2    3rd Qu.: 90.00    3rd Qu.: 526.2    3rd Qu.: 426.25
## Max.     : 4256.0    Max.     : 548.00    Max.     : 2165.0    Max.     : 1659.00
##
##           CWalks           League Division           PutOuts           Assists
## Min.      : 0.00    A:175    E:157    Min.      : 0.0    Min.      : 0.0
## 1st Qu.: 67.25    N:147    W:165    1st Qu.: 109.2    1st Qu.: 7.0
## Median : 170.50                                Median : 212.0    Median : 39.5
## Mean     : 260.24                                Mean     : 288.9    Mean     : 106.9
## 3rd Qu.: 339.25                                3rd Qu.: 325.0    3rd Qu.: 166.0
## Max.     : 1566.00                                Max.     : 1378.0    Max.     : 492.0
##
##           Errors           Salary           NewLeague
## Min.      : 0.00    Min.      : 67.5    A:176
## 1st Qu.: 3.00    1st Qu.: 190.0    N:146
## Median : 6.00    Median : 425.0
## Mean     : 8.04    Mean     : 535.9
## 3rd Qu.: 11.00    3rd Qu.: 750.0
## Max.     : 32.00    Max.     : 2460.0
##
##           NA's           :59
```

```
hit.na <- na.omit(Hitters)
n <- nrow(hit.na)
set.seed(100)
ntest <- trunc(n / 3)
testid <- sample(1:n, ntest)
```

```
lfit <- lm(Salary ~ ., data = hit.na[-testid, ])  
lpred <- predict(lfit, hit.na[testid, ])  
with(hit.na[testid, ], mean(abs(lpred - Salary)))
```

```
## [1] 234.7266
```

```
library(faraway)
summary(lfit)
```

```
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept) 227.612145 114.776318  1.9831 0.049112
## AtBat      -2.108462    0.792265 -2.6613 0.008598
## Hits       7.368520    3.011349  2.4469 0.015519
## HmRun       5.625222    8.024779  0.7010 0.484359
## Runs      -3.015865    4.002006 -0.7536 0.452232
## RBI        0.386283    3.562024  0.1084 0.913782
## Walks      4.574976    2.497751  1.8316 0.068913
## Years     -2.044161   16.833435 -0.1214 0.903503
## CAtBat     -0.426314    0.183867 -2.3186 0.021715
## CHits      1.345224    0.881618  1.5259 0.129070
## CHmRun     2.224998    2.066412  1.0767 0.283257
## CRuns      1.047251    0.968980  1.0808 0.281464
## CRBI      -0.106637    0.940625 -0.1134 0.909885
## CWalks     -0.640045    0.434949 -1.4715 0.143159
## LeagueN    74.793873   96.043111  0.7788 0.437305
## DivisionW  -91.669238   53.891965 -1.7010 0.090939
## PutOuts     0.398458    0.103197  3.8611 0.000165
## Assists     0.302098    0.282269  1.0702 0.286161
## Errors      0.091908    5.456629  0.0168 0.986583
## NewLeagueN -69.305248   95.146238 -0.7284 0.467456
##
## n = 176, p = 20, Residual SE = 326.96086, R-Squared = 0.59
```

- Let's try with Lasso:

```
x <- scale(model.matrix(Salary ~ . - 1, data = hit.na))  
y <- hit.na$Salary
```

```
library(glmnet)
```

```
## Loading required package: Matrix
```

```
## Loaded glmnet 4.1-4
```

```
cvfit <- cv.glmnet(x[-testid, ], y[-testid],  
  type.measure = "mse", alpha=1)  
cpred <- predict(cvfit, x[testid, ], s = "lambda.min")  
mean(abs(y[testid] - cpred))
```

```
## [1] 231.1828
```



- Let's try the neural network package described in *Extending the Linear Model with R* by Julian Faraway - Chapter 17.

```
library(nnet)
nnmod1 <- nnet(Salary ~ ., size=2, linout=T,
               data = hit.na[-testid, ])

## # weights:  43
## initial  value 95252155.873999
## final    value 40289843.115943
## converged

nn.pred <- predict(nnmod1, newdata =
                   hit.na[testid, ])
with(hit.na[testid, ], mean(abs(nn.pred - Salary)))

## [1] 309.6678
```

```
bestrss <- nnmdl$value
for(i in 1:100){nnmdl <- nnet(Salary ~ ., size=2, linout=T,
                             data = hit.na[-testid, ], trace=F)

if(nnmdl$value < bestrss){
  bestnn <- nnmdl
  bestrss <- nnmdl$value
}}
bestnn$value
```

```
## [1] 20470074
```

```
nn.pred <- predict(bestnn, newdata =  
                      hit.na[testid, ])  
with(hit.na[testid, ], mean(abs(nn.pred - Salary)))
```

```
## [1] 235.2443
```

```
summary(bestnn)
```

```
## a 19-2-1 network with 43 weights
## options were - linear output units
##   b->h1   i1->h1   i2->h1   i3->h1   i4->h1   i5->h1   i6->h1   i7->h1   i8->h1
##  -4.55 -282.82   13.68  187.88  401.48  627.12  -92.01  -51.13 -191.79
## i10->h1 i11->h1 i12->h1 i13->h1 i14->h1 i15->h1 i16->h1 i17->h1 i18->h1
## 294.39  752.03  346.29 -462.19 -55.52 -50.08   20.09   22.71   82.65
##   b->h2   i1->h2   i2->h2   i3->h2   i4->h2   i5->h2   i6->h2   i7->h2   i8->h2
##   0.46   -2.10   -0.36   -0.12    0.38   -0.03    0.25    0.56    0.98
## i10->h2 i11->h2 i12->h2 i13->h2 i14->h2 i15->h2 i16->h2 i17->h2 i18->h2
## -0.58    0.75   -0.70   -0.04    0.31   -0.54   -0.26    0.94   -0.30
##   b->o    h1->o    h2->o
## 114.61  554.34  354.46
```

- $i_1 \rightarrow h_1$  is the link between the input variable and the first hidden neuron.
- $b$  refers to the 'bias' (intercept for statisticians) and takes a constant value of 1.

```
head(nn.pred)
```

```
##           [,1]  
## -Ron Kittle    469.0637  
## -Jose Cruz     1023.4016  
## -Rance Mulliniks 469.0637  
## -Andres Galarraga 114.6055  
## -Glenn Wilson   469.0637  
## -Argenis Salazar 469.0637
```

Decay:  $SSE + \lambda \sum_{i=1}^2 w_i^2$

```
nnmod2 <- nnet(Salary ~ ., size=25, linout=T,  
               data = hit.na[-testid, ], decay=0.2)
```

```
## # weights: 526  
## initial value 95327483.811962  
## iter 10 value 34072982.723676  
## iter 20 value 27859249.155203  
## iter 30 value 27524115.043616  
## iter 40 value 27483287.685563  
## iter 50 value 26490703.037836  
## iter 60 value 26189411.862088  
## iter 70 value 23035989.425496  
## iter 80 value 22827226.520125  
## iter 90 value 22758719.218448  
## iter 100 value 22705847.303065  
## final value 22705847.303065  
## stopped after 100 iterations
```

```
head(nn.pred)
```

```
##           [,1]  
## -Ron Kittle    766.4460  
## -Jose Cruz     766.4460  
## -Rance Mulliniks 529.2157  
## -Andres Galarraga 650.5051  
## -Glenn Wilson   766.4460  
## -Argenis Salazar 688.8484
```

```
library(torch)
library(luz) # high-level interface for torch
library(torchvision) # for datasets and image transformation
library(torchdatasets) # for datasets we are going to use
library(zeallot)
torch_manual_seed(13)
```

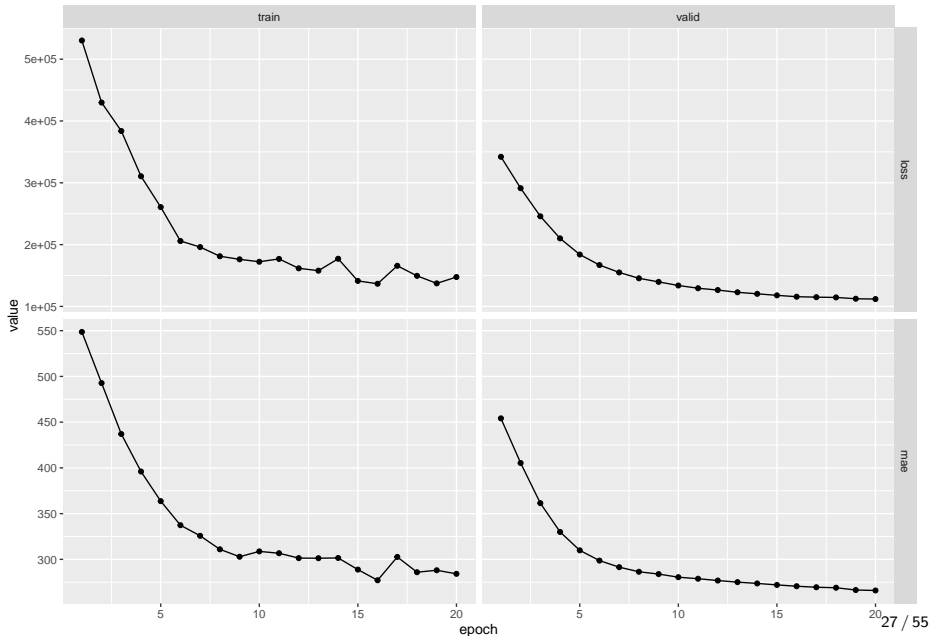
```
modnn <- nn_module(
  initialize = function(input_size) {
    self$hidden <- nn_linear(input_size, 50)
    self$activation <- nn_relu()
    self$dropout <- nn_dropout(0.4)
    self$output <- nn_linear(50, 1)
  },
  forward = function(x) {
    x %>%
      self$hidden() %>%
      self$activation() %>%
      self$dropout() %>%
      self$output()
  }
)
```



```
modnn <- modnn %>%  
  setup(  
    loss = nn_mse_loss(),  
    optimizer = optim_rmsprop,  
    metrics = list(luz_metric_mae())  
  ) %>%  
  set_hparams(input_size = ncol(x))
```

```
fitted <- modnn %>%  
  fit(  
    data = list(x[-testid, ],  
                matrix(y[-testid], ncol = 1)),  
    valid_data = list(x[testid, ],  
                      matrix(y[testid], ncol = 1)),  
    epochs = 20  
  )
```

## plot(fitted)



```
npred <- predict(fitted, x[testid, ])  
mean(abs(y[testid] - npred))
```

```
## torch_tensor  
## 355.594  
## [ CPUFloatType{} ]
```

## Some 'Results' - discussed in the textbook

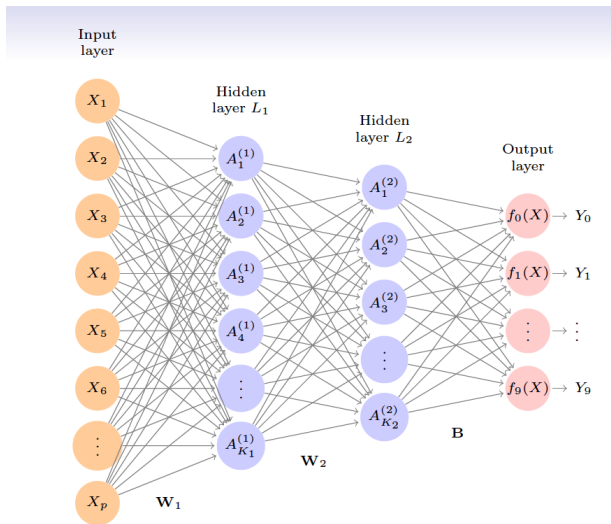
- A linear model was used to fit the training data, and make predictions on the test data. The model has 20 parameters.
- The same linear model was fit with lasso regularization. The tuning parameter was selected by 10-fold cross-validation on the training data. It selected a model with 12 variables having nonzero coefficients.
- A neural network with one hidden layer consisting of 64 ReLU units was fit to the data. This model has 1,409 parameters. **A lot of tweaking involved.**

Model	# Parameters	Mean Abs. Error	Test Set $R^2$
Linear Regression	20	254.7	0.56
Lasso	12	252.3	0.51
Neural Network	1409	257.4	0.54

	Coefficient	Std. error	t-statistic	p-value
Intercept	-226.67	86.26	-2.63	0.0103
Hits	3.06	1.02	3.00	0.0036
Walks	0.181	2.04	0.09	0.9294
CRuns	0.859	0.12	7.09	< 0.0001
PutOuts	0.465	0.13	3.60	0.0005

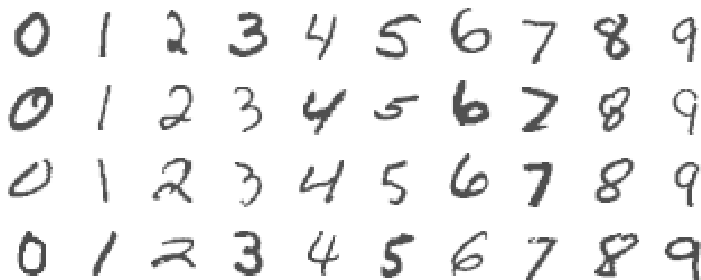
**TABLE 10.3.** *Least squares coefficient estimates associated with the regression of **Salary** on four variables chosen by lasso on the **Hitters** data set. This model achieved the best performance on the test data, with a mean absolute error of 224.8. The results reported here were obtained from a regression on the test data, which was not used in fitting the lasso model.*

# Multi-Hidden Layers





## Example: MNIST Digits



- Handwritten digits: 28 x 28 grayscale images
- 60K train and 10K test images
- Features (covariates) are the 784 pixel grayscale values  $\in (0; 255)$
- Labels (response) are the digit class 0-9

## Example: MNIST Digits

- Goal: build a classifier to predict the image class.
- The authors built a two-layer network with 256 units at first layer and 128 units at second layer.
- 10 units at output layer
- Along with intercepts (called biases) there are 235,146 parameters (referred to as weights)

## Details of Output Layer

- Let  $Z_m = \beta_{0m} + \sum_{\ell=1}^{K_2} \beta_{m\ell} A_{\ell}^{(2)}$ ,  $m = 0, 1, 2, \dots, 9$  be the 10 linear combinations of the activations at the second level.
- The output activation function encodes the **softmax** function (similar to multinomial logistic regression):

$$f_m(X) = P(Y = m|X) = \frac{\exp(Z_m)}{\sum_{\ell=0}^9 \exp(Z_{\ell})}$$

- The model is by minimizing the negative multinomial log-likelihood (or cross-entropy):

$$-\sum_{i=1}^n \sum_{m=0}^9 y_{im} \log(f_m(x_i))$$

- $y_{im}$  is 1 if true class for observation  $i$  is  $m$ , else 0 – i.e. **one-hot encoded** (levels of a factor - dummy variables).

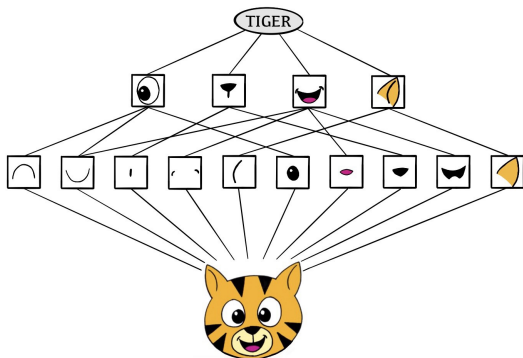
# Results

Method	Test Error
Neural Network + Ridge Regularization	2.3%
Neural Network + Dropout Regularization	1.8%
Multinomial Logistic Regression	7.2%
Linear Discriminant Analysis	12.7%

- Early success for neural networks in the 1990s.
- With so many parameters, regularization is essential.
- Very overworked problem – best reported rates are  $< 0.5\%$ !
- Human error rate is reported to be around  $0.2\%$ , or 20 of the 10K test images.



# How CNNs Work



- The CNN builds up an image in a hierarchical fashion.
- Edges and shapes are recognized and pieced together to form more complex shapes, eventually assembling the target image.
- This hierarchical construction is achieved using **convolution** and **pooling** layers.

# Convolution Filter

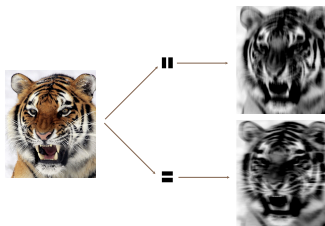
$$\text{Input Image} = \begin{bmatrix} a & b & c \\ d & e & f \\ g & h & i \\ j & k & l \end{bmatrix} \quad \text{Convolution Filter} = \begin{bmatrix} \alpha & \beta \\ \gamma & \delta \end{bmatrix}.$$

$$\text{Convolved Image} = \begin{bmatrix} a\alpha + b\beta + d\gamma + e\delta & b\alpha + c\beta + e\gamma + f\delta \\ d\alpha + e\beta + g\gamma + h\delta & e\alpha + f\beta + h\gamma + i\delta \\ g\alpha + h\beta + j\gamma + k\delta & h\alpha + i\beta + k\gamma + l\delta \end{bmatrix}$$

- The filter is itself an image, and represents a small shape, edge etc.
- We slide it around the input image, scoring for matches.
- The scoring is done via dot-products.
- If the subimage of the input image is similar to the filter, the score is high, otherwise low.



# Convolution Example



- The idea of convolution with a filter is to find common patterns that occur in different parts of the image.
- The two filters shown here highlight vertical and horizontal stripes.
- The result of the convolution is a new feature map.
- Since images have three color channels, the filter does as well: one filter per channel, and dot-products are summed.
- The weights in the filters are **learned** by the network.

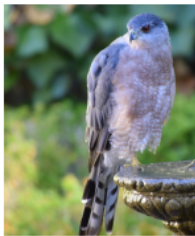
# Pooling

$$\text{Max pool} \begin{bmatrix} 1 & 2 & 5 & 3 \\ 3 & 0 & 1 & 2 \\ 2 & 1 & 3 & 4 \\ 1 & 1 & 2 & 0 \end{bmatrix} \rightarrow \begin{bmatrix} 3 & 5 \\ 2 & 4 \end{bmatrix}$$

- Each non-overlapping  $2 \times 2$  block is replaced by its maximum.
- This sharpens the feature identification.
- Allows for locational invariance.
- Reduces the dimension by a factor of 4 – i.e. factor of 2 in each dimension.

- Many convolve + pool layers.
- Filters are typically small, e.g. each channel  $3 \times 3$ .
- Each filter creates a new channel in convolution layer.
- As pooling reduces size, the number of filters/channels is typically increased.
- Number of layers can be very large. E.g. *resnet50* trained on *imagenet* 1000-class image data base has 50 layers!
- There are many tuning parameters to be selected in constructing such a network, apart from the number, nature, and sizes of each layer.

# Using Pretrained CNN Models



```
img_dir <- "book_images"
image_names <- list.files(img_dir)
num_images <- length(image_names)
x <- torch_empty(num_images, 3, 224, 224)
for (i in 1:num_images) {
  img_path <- file.path(img_dir, image_names[i])
  img <- img_path %>%
    base_loader() %>%
    transform_to_tensor() %>%
    transform_resize(c(224, 224)) %>%
    # normalize with imagenet mean and stds.
    transform_normalize(
      mean = c(0.485, 0.456, 0.406),
      std = c(0.229, 0.224, 0.225)
    )
  x[i,,, ] <- img
}
```

- We then load the trained network. The model has 18 layers, with a fair bit of complexity.

```
model <- torchvision::model_resnet18(pretrained = TRUE)
model$eval() # put the model in evaluation mode
```

- Finally, we classify our six images, and return the top three class choices in terms of predicted probability for each.

```
preds <- model(x)

mapping <- jsonlite::read_json("https://s3.amazonaws.com/deep-learning-models/image-classification/v1/tf/models/imagenet1000_synonyms/imagenet1000_synonyms.json")
sapply(function(x) x[[2]])

top3 <- torch_topk(preds, dim = 2, k = 3)

top3_prob <- top3[[1]] %>%
  nnf_softmax(dim = 2) %>%
  torch_unbind() %>%
  lapply(as.numeric)

top3_class <- top3[[2]] %>%
  torch_unbind() %>%
  lapply(function(x) mapping[as.integer(x)])

result <- purrr::map2(top3_prob, top3_class, function(pr, cl) {
  names(pr) <- cl
  pr
})
names(result) <- image_names
print(result)
```

```

## $flamingo.jpg
##      flamingo      spoonbill white_stork
## 0.978211880 0.017045746 0.004742352
##
## $hawk_cropped.jpeg
##      kite      jay      magpie
## 0.6157817 0.2311856 0.1530327
##
## $hawk.jpg
##      eel      agama common_newt
## 0.5391129 0.2527186 0.2081685
##
## $huey.jpg
##      Lhasa Tibetan_terrier      Shih-Tzu
## 0.79760402      0.12013000      0.08226602
##
## $kitty.jpg
##      Saint_Bernard      guinea_pig Bernese_mountain_dog
##      0.3946652      0.3427011      0.2626338
##
## $weaver.jpg
## hummingbird      lorikeet      bee_eater
## 0.3633279 0.3577298 0.2789424

```



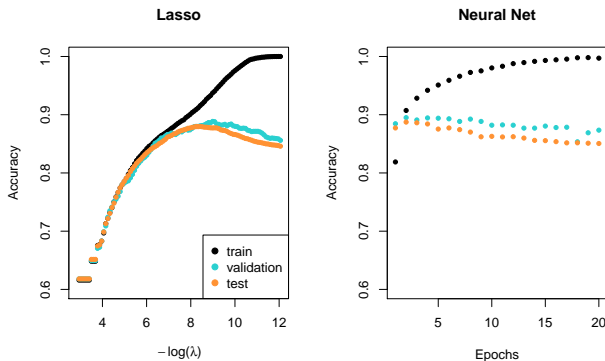
# Document Classification: IMDB Movie Reviews

- The **IMDB** corpus consists of user-supplied movie ratings for a large collection of movies. Each has been labeled for sentiment as **positive** or **negative**.
- Labeled training and test sets, each consisting of 25,000 reviews, and each balanced with regard to sentiment.
- We wish to build a classifier to predict the sentiment of a review.

# Featurization (Derived Covariates): Bag-of-Words

- Documents have different lengths, and consist of sequences of words.
- How do we create features  $X$  to characterize a document?
- From a dictionary, identify the 10K most frequently occurring words.
- Create a binary vector of length  $p = 10K$  for each document, and score a 1 in every position that the corresponding word occurred.
- With  $n$  documents, we now have a  $n \times p$  sparse feature matrix  $X$ .
- We compare a lasso logistic regression model to a two-hidden-layer neural network on the next slide. (No convolutions here!)
- *Bag-of-words* are **unigrams**. We can instead use **bigrams** (occurrences of adjacent word pairs), and in general **m-grams**.

# Results



- Simpler lasso logistic regression model works as well as neural network in this case.
- **glmnet** was used to fit the lasso model, and is very effective because it can exploit sparsity in the  $X$  matrix.

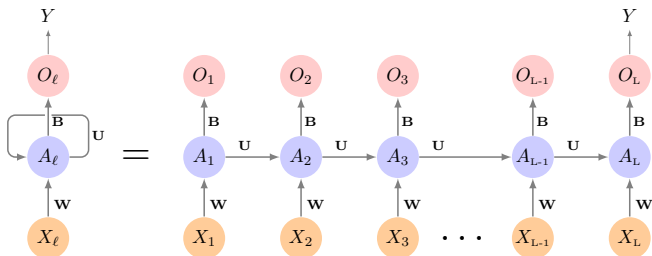
# Recurrent Neural Networks

Often data arise as sequences:

- Documents are sequences of words, and their relative positions have meaning.
- Time-series such as weather data or financial indices.
- Recorded speech or music.
- Handwriting, such as doctor's notes.

RNNs build models that take into account this sequential nature of the data, and build a memory of the past.

# Recurrent Neural Networks



- For the IMBD data - each document represented as a series of  $L$  words ( $X_\ell$ ) represents a word
- An application of this applied to IMBD data described in the textbook only achieved a achieved 76% accuracy.
- The lasso performed still better – however expanded versions of RNNs have now performed better.

# When to Use Deep Learning

- CNNs have had enormous successes in image classification and modeling, and are starting to be used in medical diagnosis. Examples include digital mammography, ophthalmology, MRI scans, and digital X-rays.
- RNNs have had big wins in speech modeling, language translation, and forecasting.

Should we always use deep learning models?

- Often the big successes occur when the **signal-to-noise ratio** is high – e.g. image recognition and language translation. Datasets are large, and overfitting is not a big problem.
- For noisier data, simpler models can often work better.

# Final Graph of the Course

