Introduction to machine learning and neural networks, with an application to earth system modeling

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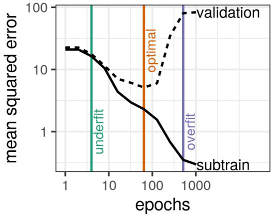
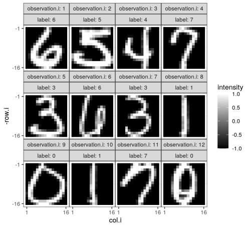
Introduction and overview

Example 1: avoiding overfitting in regression, overview of concepts



Example 2: classifying images of digits, coding demos

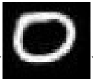
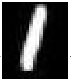


Summary and quiz questions

Machine learning intro: image classification example

ML is all about learning predictive functions $f(x) \approx y$, where

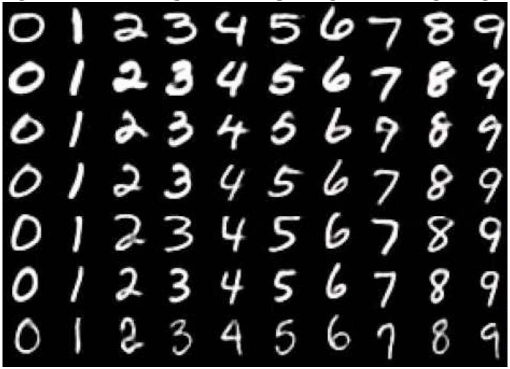
- Inputs/features x can be easily computed using traditional algorithms. For example, matrix of pixel intensities in an image.
- Outputs/labels y are what we want to predict, typically more difficult/costly to measure than inputs. For example, to get an image class label, you may have to ask a human.
- Input x = image of digit, output $y \in \{0, 1, \dots, 9\}$,
  – this is a classification problem with 10 classes.

  $f($$) = 0$, $f($$) = 1$
- Traditional/unsupervised algorithm: I give you a pixel intensity matrix $x \in \mathbb{R}^{28\times 28}$, you code a function f that returns one of the 10 possible digits. Q: how to do that?

Supervised machine learning algorithms

I give you a training data set with paired inputs/outputs, e.g.

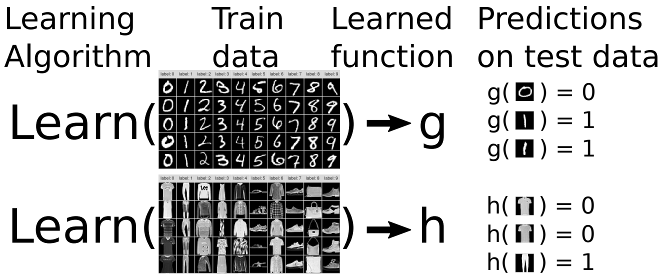
0 1 2 3 4 5 6 7 8 9



Your job is to code an algorithm, LEARN, that infers a function f from the training data. (you don't code f)

Source: github.com/cazala/mnist

Advantages of supervised machine learning



- Input $x \in \mathbb{R}^{28 \times 28}$, output $y \in \{0, 1, \dots, 9\}$ types the same!
- Can use same learning algorithm regardless of pattern.
- Pattern encoded in the labels (not the algorithm).
- Useful if there are many un-labeled data, but few labeled data (or getting labels is long/costly).
- State-of-the-art accuracy (if there is enough training data).

Sources: github.com/cazala/mnist, github.com/zalandoresearch/fashion-mnist

Overview of tutorial

In this tutorial we will discuss two kinds of problems, which differ by the type of the output/label/y variable we want to predict.

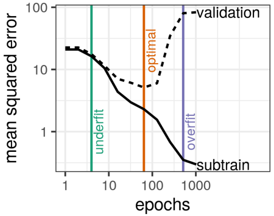
- Regression, y is a real number.
- Classification, y is an integer representing a category.

The rest of the tutorial will focus on three examples:

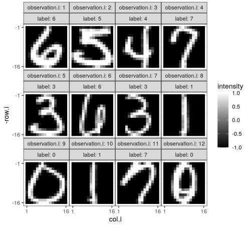
1. Regression with a single input, to demonstrate how to avoid overfitting.
2. Classification of digit images, to demonstrate how to compare machine learning algorithms in terms of test/prediction accuracy.

Introduction and overview

Example 1: avoiding overfitting in regression, overview of concepts



Example 2: classifying images of digits, coding demos

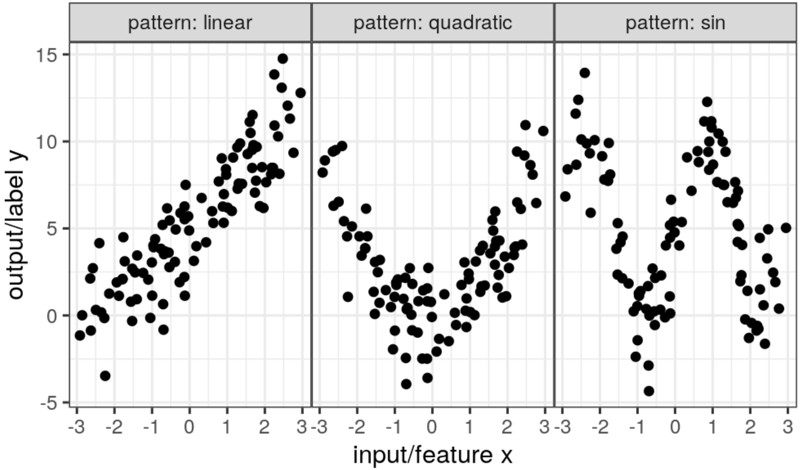


Summary and quiz questions

Goal of this section: demonstrate how to avoid overfitting

- The goal of supervised machine learning is to get accurate predictions on new/unseen/held-out test data.
- The data used during learning are caled the train set.
- Any machine learning algorithm is prone to overfit, which means providing better predictions on the train set than on a held-out validation/test set. (BAD)
- To learn a model which does NOT overfit (GOOD), you need to divide your train set into subtrain/validation sets (subtrain used as input to gradient descent algorithm, validation set used to control number of iterations of gradient descent).
- Code for figures in this section: `https://github.com/tdhock/2023-res-baz-az/blob/main/figure-overfitting.R`

Three different data sets/patterns



- We illustrate this using a single input/feature $x \in \mathbb{R}$.
- We use a regression problem with outputs $y \in \mathbb{R}$.
- Goal is to learn a function $f(x) \in \mathbb{R}$.

K-fold cross-validation for splitting data

- One way to split is via K-fold cross-validation.
- Each row is assigned a fold ID number from 1 to K.
- For each for ID, those data are held out, and other data are kept.
- Popular relative to other splitting methods because of simplicity and fairness (each row is held out one time).

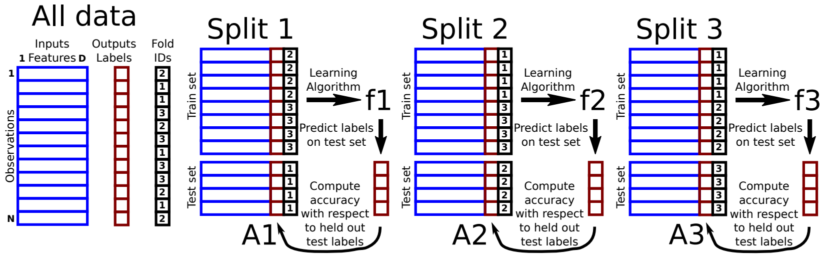
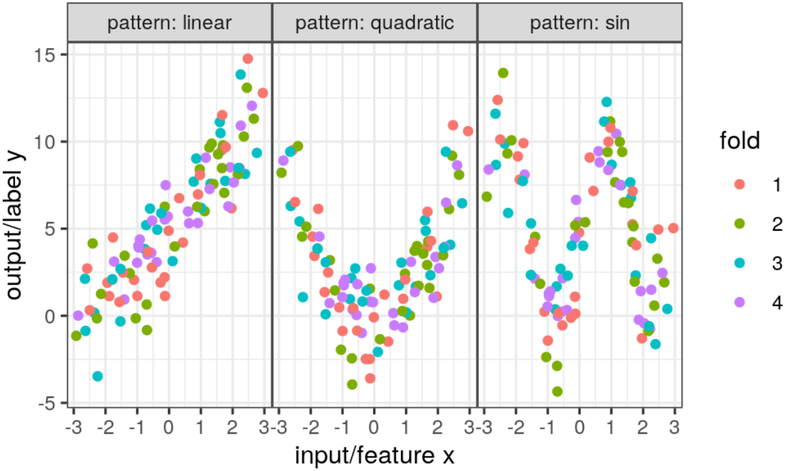


Illustration of 4-fold cross-validation

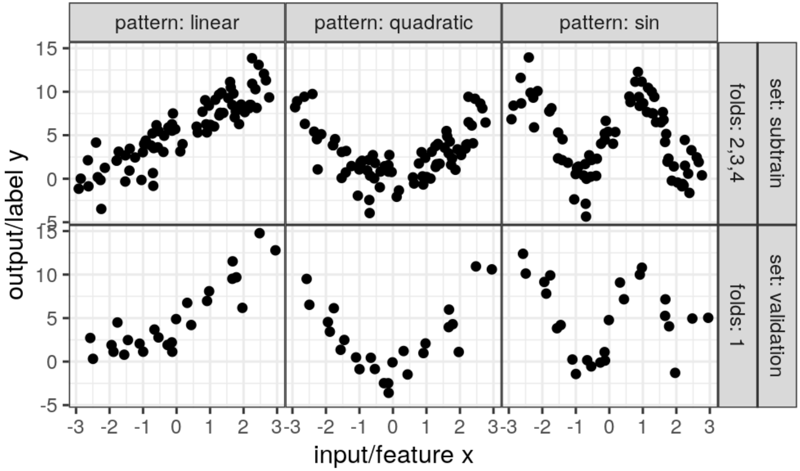


Randomly assign each observation a fold ID from 1 to 4.

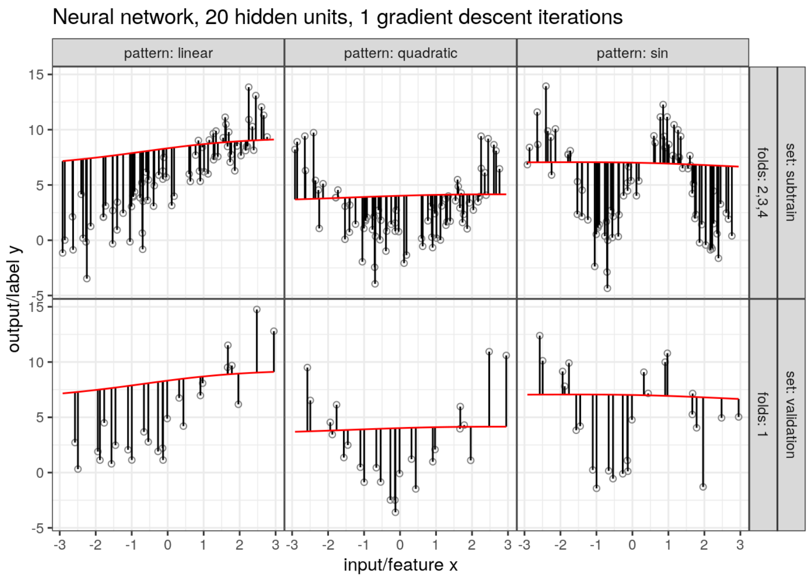
Neural network learning algorithm

- We will fit a neural network to these data.
- The neural network learns how to predict the outputs from the inputs.
- The learning algorithm is gradient descent, which iteratively minimizes the loss of the predictions with respect to the labels in the subtrain set.
- We also compute the loss on the validation set, so we can select the number of gradient descent iterations that gives the best predictions on new data (avoiding overfitting).

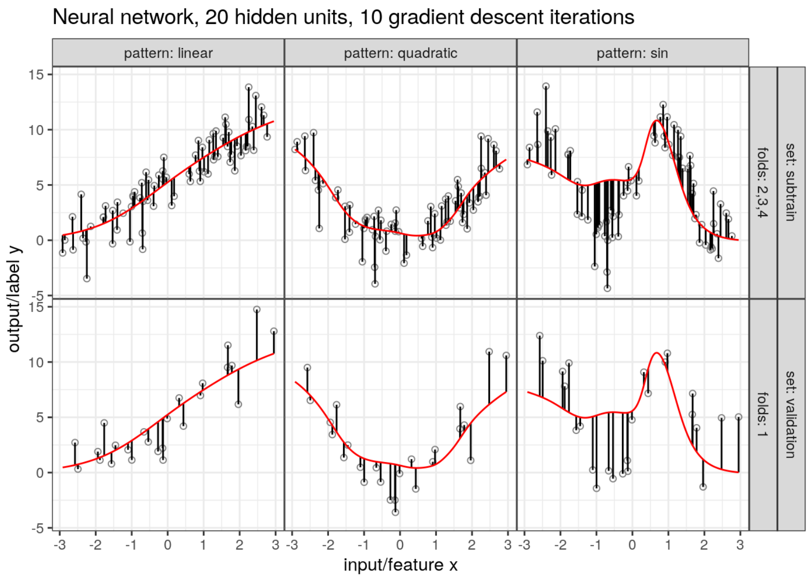
Illustration of subtrain/validation split



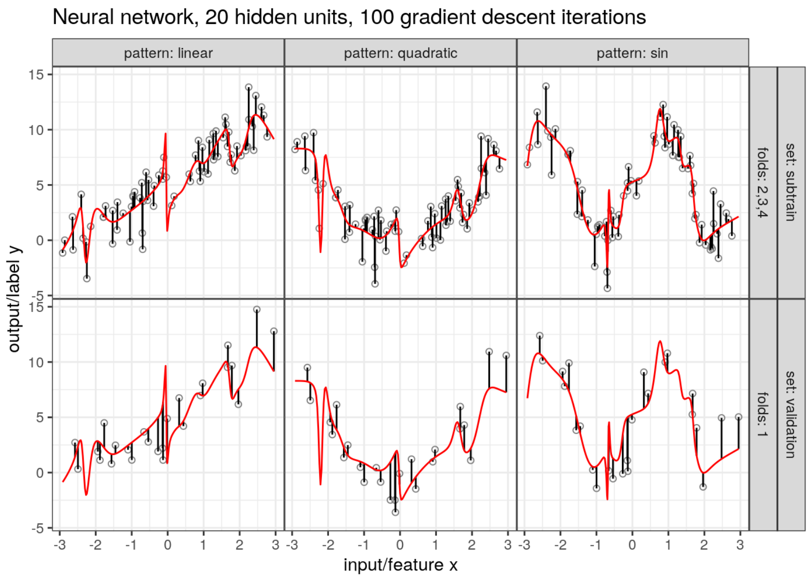
- For validation fold 1, all observations with that fold ID are considered the validation set.
- All other observations are considered the subtrain set.



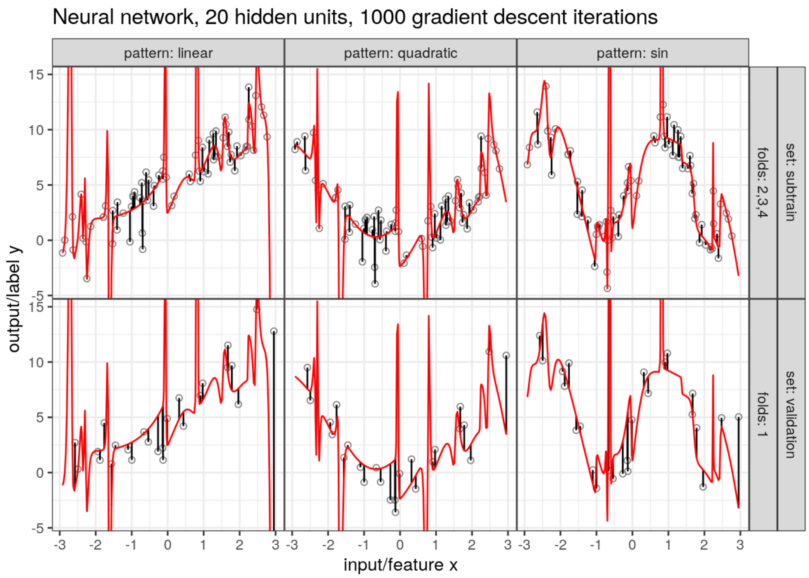
Data=grey dots, predictions=red curve, loss=black vertical line segments



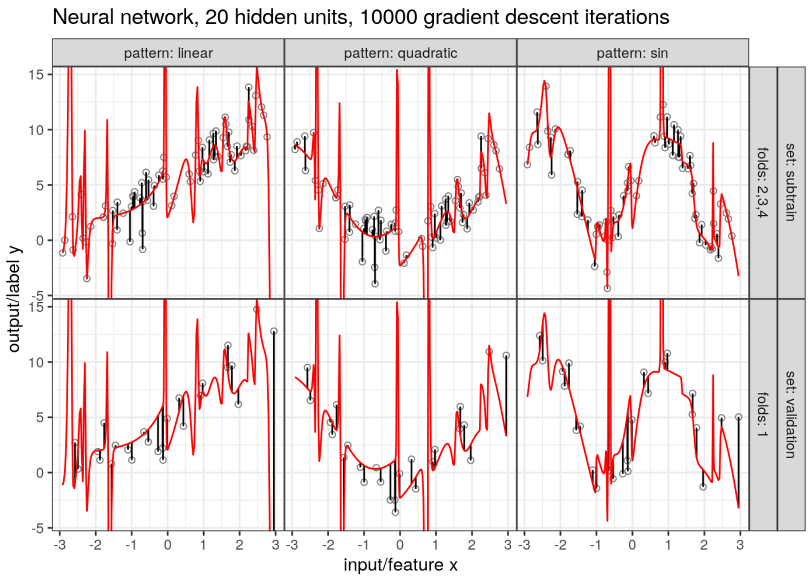
Data=grey dots, predictions=red curve, loss=black vertical line segments



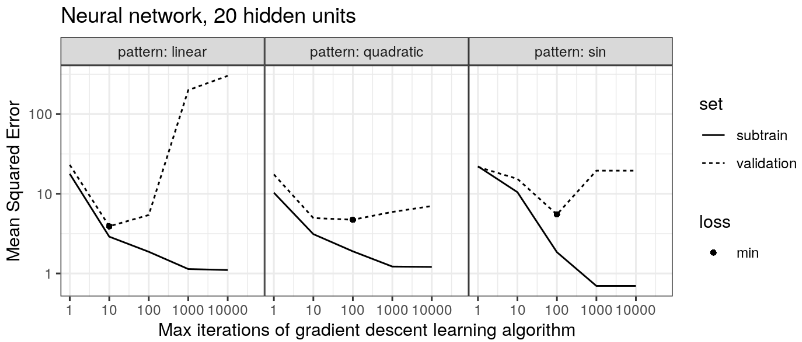
Data=grey dots, predictions=red curve, loss=black vertical line segments



Data=grey dots, predictions=red curve, loss=black vertical line segments



Data=grey dots, predictions=red curve, loss=black vertical line segments



Data=grey dots, predictions=red curve, loss=black vertical line segments

Neural network prediction function

For an input feature vector $\mathbf{x} \in \mathbb{R}^{u_1}$, the prediction function for a neural network with L layers (functions to learn) is:

$$f(\mathbf{x}) = f_L[\cdots f_1[\mathbf{x}]]. \tag{1}$$

We have for all $l \in \{1, \ldots, L\}$:

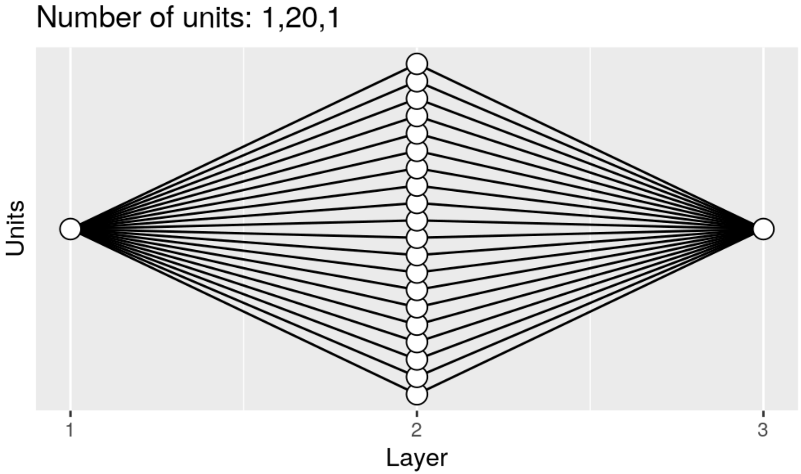
$$f_l(t) = A_l(\mathbf{W}_l^\intercal t), \tag{2}$$

The hyper-parameters which must be fixed prior to learning:

- Number of functions to learn L.
- Activation functions A_l (classically sigmoid, typically ReLU).
- Number of hidden units per layer $(u_1, \ldots, u_{L-1})$.
- Sparsity pattern in the weight matrices $\mathbf{W}_l \in \mathbb{R}^{u_l \times u_{l-1}}$.

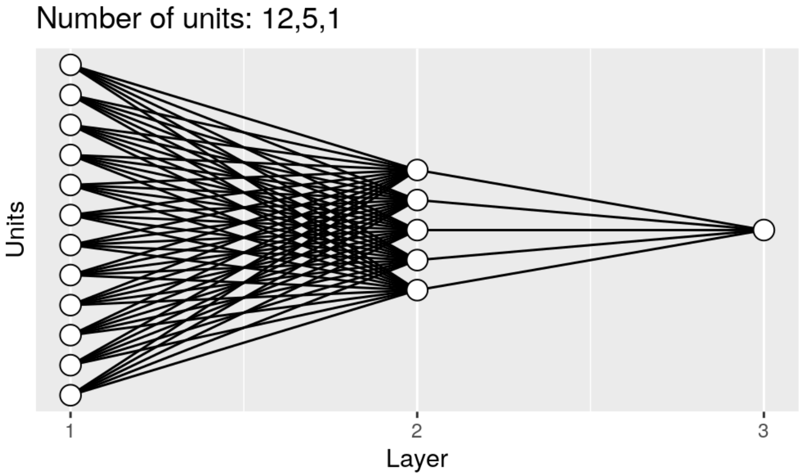
Network for 1 input, 1 output, 1 hidden layer

Neural network diagrams show how each unit (node) is computed by applying the weights (edges) to the values of the units at the previous layer.



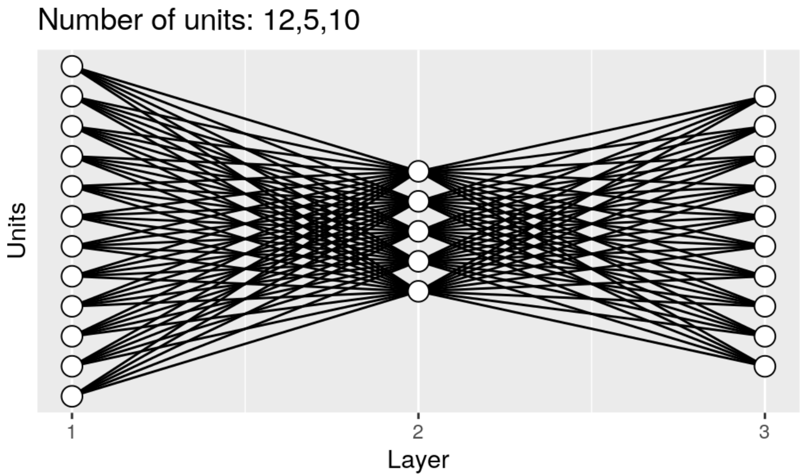
Network for 12 inputs, 1 output, 1 hidden layer

Neural network diagrams show how each unit (node) is computed by applying the weights (edges) to the values of the units at the previous layer.



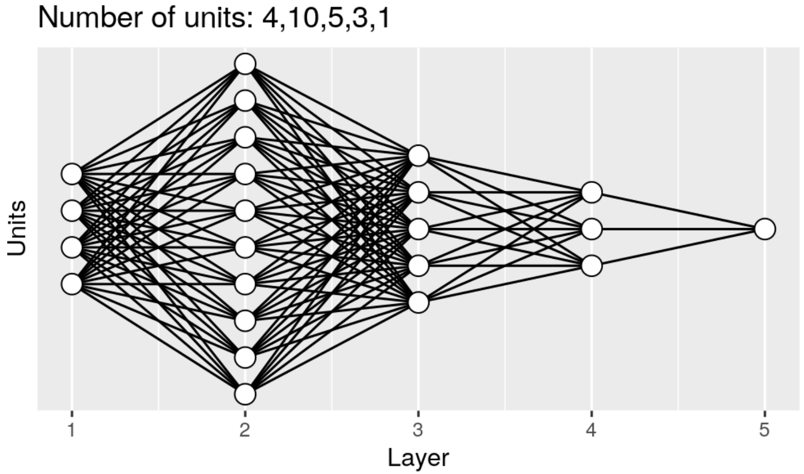
Network for 12 inputs, 10 outputs, 1 hidden layer

Neural network diagrams show how each unit (node) is computed by applying the weights (edges) to the values of the units at the previous layer.

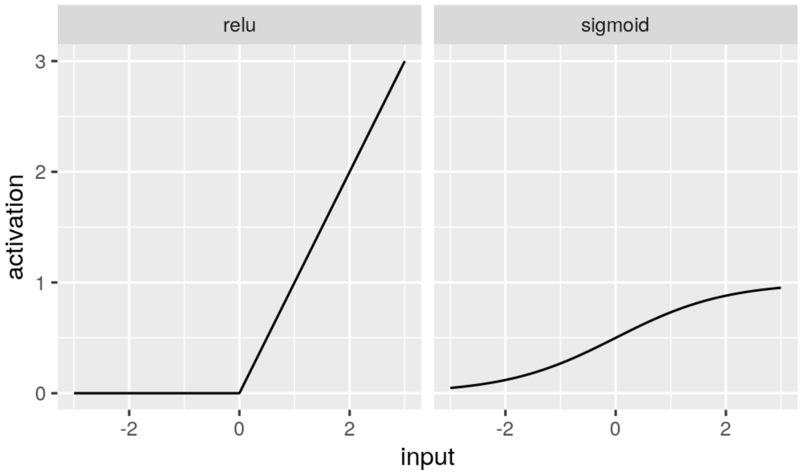


Network for 4 inputs, 1 output, 3 hidden layers

Neural network diagrams show how each unit (node) is computed by applying the weights (edges) to the values of the units at the previous layer.



Non-linear activation functions A_l



Each layer except the last should have a activation function A_l which is not linear (last layer activation should be identity/linear).

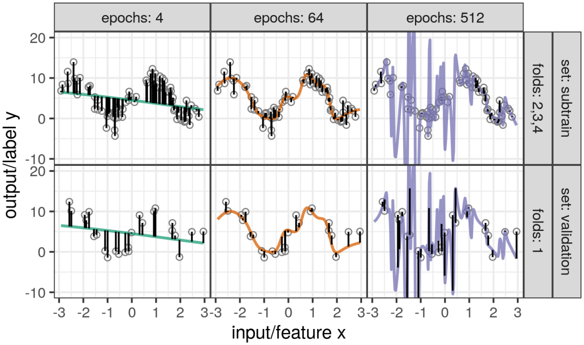
Gradient Descent Learning

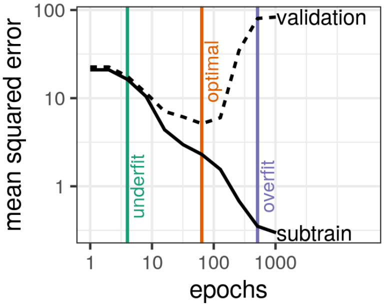
The neural network prediction function $f(\mathbf{x}) = f_L[\cdots f_1[\mathbf{x}]]$ has $l \in \{1, \dots, L\}$ component functions to learn:

$$f_l(t) = A_l(\mathbf{W}_l^\intercal t), \tag{3}$$

The weight matrices $\mathbf{W}_l \in \mathbb{R}^{u_l \times u_{l-1}}$ are learned using gradient descent.

- A loss function $\mathcal{L}[f(\mathbf{x}), y]$ computes how bad are predictions with respect to labels y (ex: mean squared error for regression, cross entropy loss for classificationc).
- In each **iteration** of gradient descent, the weights are updated in order to get better predictions on subtrain data.
- An **epoch** computes gradients on all subtrain data; there can be from 1 to N(subtrain size) iterations per epoch.


epochs: 4
epochs: 64
epochs: 512
set: subtrain
folds: 2,3,4
set: validation
folds: 1
output/label y
input/feature x
20
10
0
-10
-3
-2
-1
0
1
2
3


mean squared error
epochs
100
10
1
1
10
100
1000
validation
subtrain
underfit
optimal
overfit

Summary of how to avoid overfitting

- Happens when subtrain error/loss decreases but validation error increases (as a function of some hyper-parameter)
- Here the hyper-parameter is the number of iterations of gradient descent, and overfitting starts after a certain number of iterations.
- To maximize prediction accuracy you need to choose a hyper-parameter with minimal validation error/loss.
- This optimal hyper-parameter will depend on the data set.
- To get optimal prediction accuracy in any machine learning analysis, you always need to do this, because you never know the best hyper-parameters in advance.

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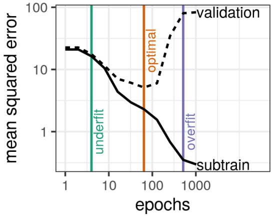
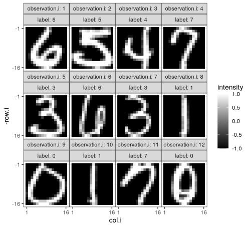
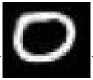
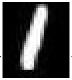


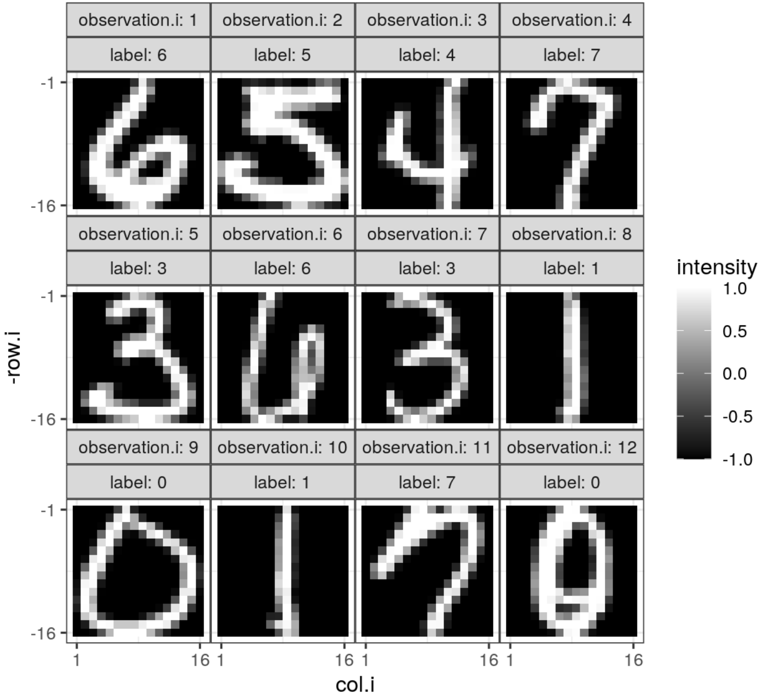
Example 2: classifying images of digits, coding demos



Summary and quiz questions

Image classification

- One of the most popular/successful applications of machine learning.
- Input: image file $x \in \mathbb{R}^{h \times w \times c}$ where h is the height in pixels, w is the width, c is the number of channels, e.g. RGB image $c = 3$ channels.
- In this tutorial we use images with $h = w = 16$ pixels and $c = 1$ channel (grayscale, smaller values are darker).
- Output: class/category y (from a finite set).
- In this tutorial there are ten image classes $y \in \{0, 1, \dots, 9\}$, one for each digit.
- Want to learn f such that $f($$) = 0$, $f($$) = 1$, etc.
- Code for figures in this section: `https://github.com/tdhock/2023-res-baz-az/blob/main/figure-validation-loss.R`



observation.i: 1
label: 6
observation.i: 2
label: 5
observation.i: 3
label: 4
observation.i: 4
label: 7
observation.i: 5
label: 3
observation.i: 6
label: 6
observation.i: 7
label: 3
observation.i: 8
label: 1
observation.i: 9
label: 0
observation.i: 10
label: 1
observation.i: 11
label: 7
observation.i: 12
label: 0
-1
-16
-row.i
1
16
col.i
intensity
1.0
0.5
0.0
-0.5
-1.0

Representation of digits in CSV

- Each image/observation is one row.
- First column is output/label/class to predict.
- Other 256 columns are inputs/features (pixel intensity values).

Data from

`https://web.stanford.edu/~hastie/ElemStatLearn/datasets/zip.train.gz`

```
 1:   6 -1 -1   ... -1.000 -1.000   -1
 2:   5 -1 -1   ... -0.671 -0.828   -1
 3:   4 -1 -1   ... -1.000 -1.000   -1
 4:   7 -1 -1   ... -1.000 -1.000   -1
 5:   3 -1 -1   ... -0.883 -1.000   -1
 6:   6 -1 -1   ... -1.000 -1.000   -1
...
```

Converting label column to matrix for neural network

This is a “one hot” encoding of the class labels.

```
zip.dt <- data.table::fread("zip.gz")
zip.y.mat <- keras::to_categorical(zip.dt$V1)
```

```
      0 1 2 3 4 5 6 7 8 9
 [1,] 0 0 0 0 0 0 1 0 0 0
 [2,] 0 0 0 0 0 1 0 0 0 0
 [3,] 0 0 0 0 1 0 0 0 0 0
 [4,] 0 0 0 0 0 0 0 1 0 0
 [5,] 0 0 0 1 0 0 0 0 0 0
 [6,] 0 0 0 0 0 0 1 0 0 0
...
```

Converting inputs to tensor (multi-dim array) for neural network

Use array function with all columns except first as data.

```
zip.size <- 16
zip.X.array <- array(
  data = unlist(zip.dt[1:nrow(zip.dt),-1]),
  dim = c(nrow(zip.dt), zip.size, zip.size, 1))
```

Need to specify dimensions of array:

- Observations: same as the number of rows in the CSV table.
- Pixels wide: 16.
- Pixels high: 16.
- Channels: 1 (greyscale image).

Linear model R code

```
library(keras)
linear.model <- keras::keras_model_sequential() %>%
  keras::layer_flatten(
    input_shape = c(16, 16, 1)) %>%
  keras::layer_dense(
    units = 10,
    activation = 'softmax')
```

- First layer must specify shape of inputs (here 16x16x1).
- `layer_flatten` converts any shape to a single dimension of units (here 256).
- `layer_dense` uses all units in the previous layer to predict each unit in the layer.
- `units=10` because there are ten possible classes for an output.
- `activation='softmax'` is required for the last/output layer in multi-class classification problems.

Keras model compilation

```
linear.model %>% keras::compile(
  loss = keras::loss_categorical_crossentropy,
  optimizer = keras::optimizer_adadelta(),
  metrics = c('accuracy')
)
```

In `compile` you can specify

- a `loss` function, which is directly optimized/minimized in each iteration of the gradient descent learning algorithm. https://keras.io/api/losses/
- an `optimizer`, which is the version of gradient descent learning algorithm to use. https://keras.io/api/optimizers/
- an evaluation `metric` to monitor, not directly optimized via gradient descent, but usually more relevant/interpretable for the application (e.g. accuracy is the proportion of correctly predicted labels). https://keras.io/api/metrics/

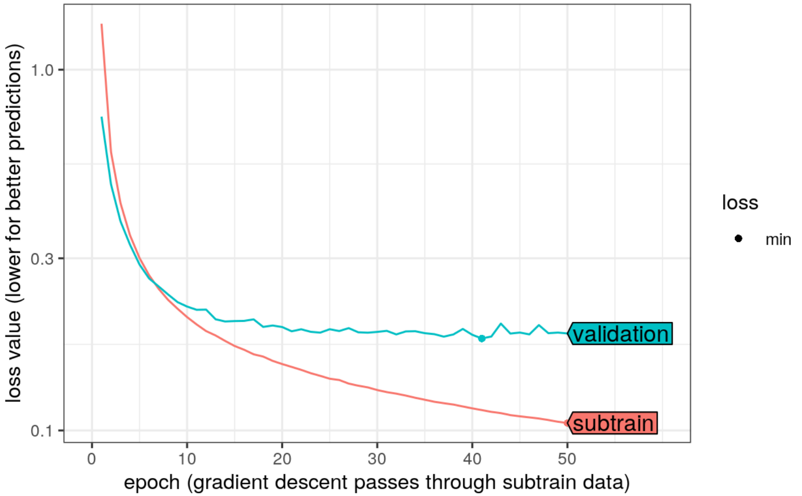
Keras model fitting

```
linear.model %>% keras::fit(
  zip.X.array, zip.y.mat,
  epochs = 50,
  validation_split = 0.2
)
```

In `fit` you can specify

- Train data inputs `zip.X.array` and outputs `zip.y.mat` (required).
- Number of full passes of gradient descent through the subtrain data (`epochs`). In each epoch the gradient with respect to each subtrain observation is computed once.
- `validation_split=0.2` which means to use 80% subtrain (used for gradient descent parameter updates), 20% validation (used for hyper-parameter selection).

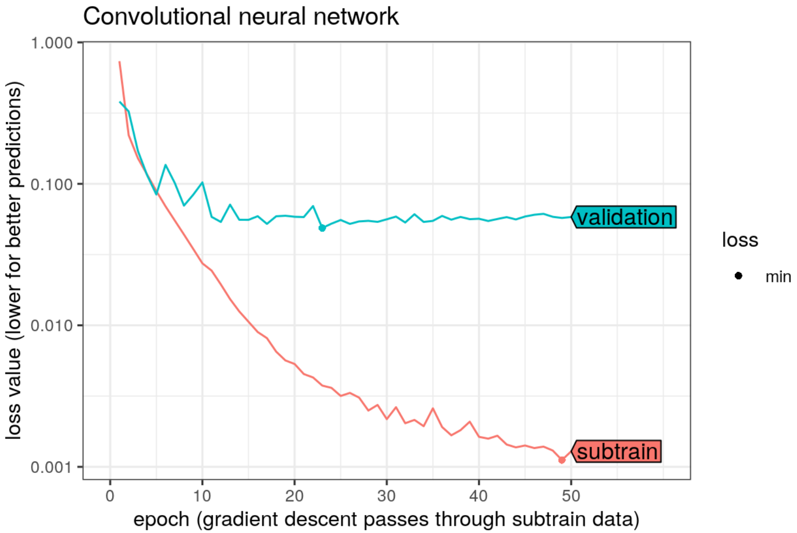
Linear model



Sparse (convolutional) model R code

```
library(keras)
conv.model <- keras_model_sequential() %>%
  layer_conv_2d(
    input_shape = dim(zip.X.array)[-1],
    filters = 20,
    kernel_size = c(3,3),
    activation = 'relu') %>%
  layer_max_pooling_2d(pool_size = c(2, 2)) %>%
  layer_flatten() %>%
  layer_dense(units = 100, activation = 'relu') %>%
  layer_dense(
    units = ncol(zip.y.mat),
    activation = 'softmax')
```

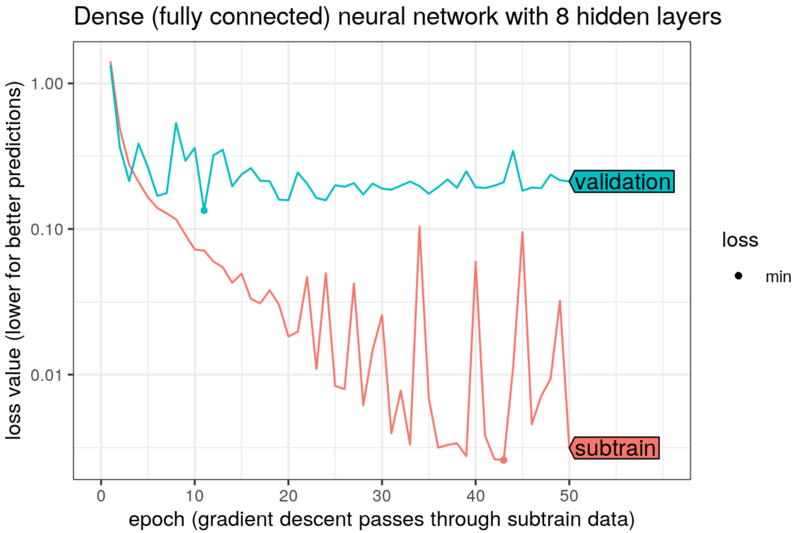
- Sparse: few inputs are used to predict each unit in `layer_conv_2d`.
- Exploits structure of image data to make learning easier/faster.

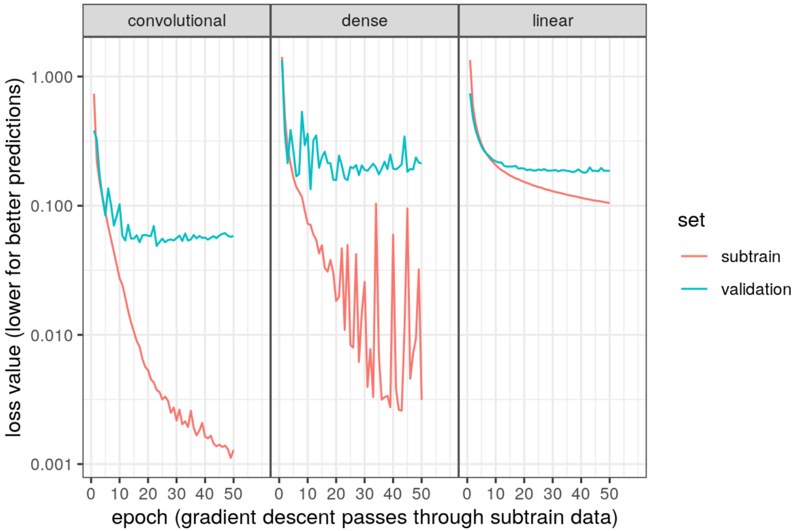


Convolutional neural network
1.000
0.100
0.010
0.001
loss value (lower for better predictions)
0
10
20
30
40
50
epoch (gradient descent passes through subtrain data)
validation
subtrain
loss
● min

Dense (fully connected) neural network R code

```
library(keras)
dense.model <- keras_model_sequential() %>%
  layer_flatten(
    input_shape = dim(zip.X.array)[-1]) %>%
  layer_dense(units = 100, activation = 'relu') %>%
  layer_dense(units = 100, activation = 'relu') %>%
  layer_dense(units = 100, activation = 'relu') %>%
  layer_dense(units = 100, activation = 'relu') %>%
  layer_dense(units = 100, activation = 'relu') %>%
  layer_dense(units = 100, activation = 'relu') %>%
  layer_dense(units = 100, activation = 'relu') %>%
  layer_dense(units = 100, activation = 'relu') %>%
  layer_dense(
    units = ncol(zip.y.mat),
    activation = 'softmax')
```

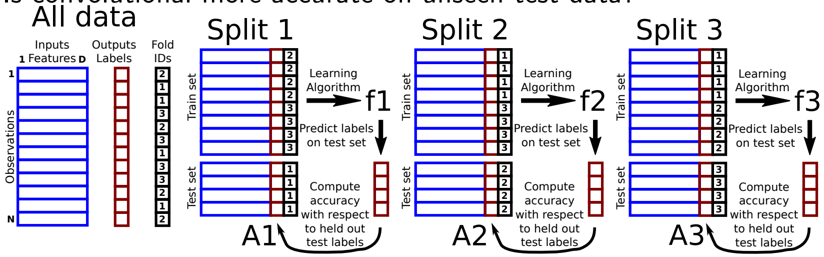

Dense (fully connected) neural network with 8 hidden layers
loss value (lower for better predictions)
1.00
0.10
0.01
0
10
20
30
40
50
epoch (gradient descent passes through subtrain data)
validation
subtrain
loss
● min



convolutional
dense
linear
1.000
0.100
0.010
0.001
loss value (lower for better predictions)
0
10
20
30
40
50
epoch (gradient descent passes through subtrain data)
set
subtrain
validation

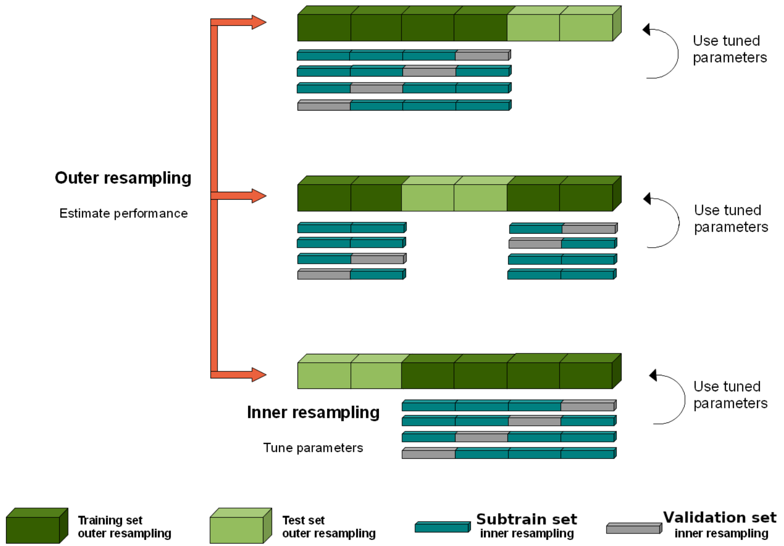
K-fold cross-validation for model evaluation

Is convolutional more accurate on unseen test data?



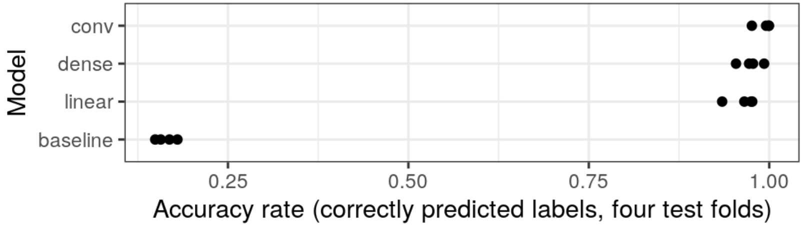
- Randomly assign a fold ID from 1 to K to each observation.
- Hold out the observations with the Split ID as test set.
- Use the other observations as the train set.
- Run learning algorithm on train set (including hyper-parmeter selection), outputs learned function (f1-f3).
- Finally compute and plot the prediction accuracy (A1-A3) with respect to the held-out test set.

Two kinds of cross-validation must be used



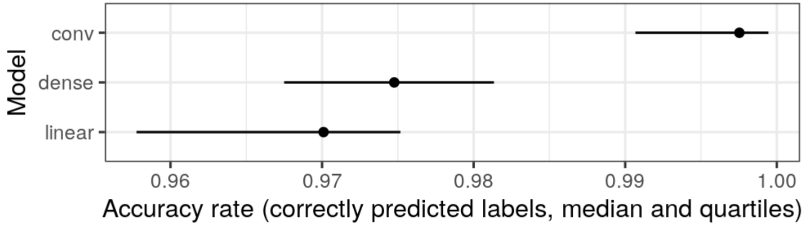
Source: `https://mlr.mlr-org.com/articles/tutorial/nested_resampling.html`

Accuracy rates for each test fold



- Always a good idea to compare with the trivial/featureless baseline model which always predicts the most frequent class in the train set. (ignoring all inputs/features)
- Here we see that the featureless baseline is much less accurate than the three learned models, which are clearly learning something non-trivial.
- Code for test accuracy figures: `https://github.com/tdhock/2023-res-baz-az/blob/main/figure-test-accuracy.R`

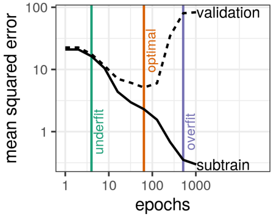
Zoom to learned models



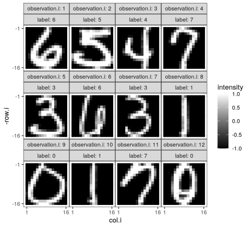
- Dense neural network slightly more accurate than linear model, convolutional significantly more accurate than others.
- Conclusion: convolutional neural network should be preferred for most accurate predictions in these data.
- Maybe not the same conclusion in other data sets, with the same models. (always need to do cross-validation experiments to see which model is best in any given data set)
- Maybe other models/algorithms would be even more accurate in these data. (more/less layers, more/less units, completely different algorithm such as random forests, boosting, etc)

Introduction and overview

Example 1: avoiding overfitting in regression, overview of concepts



Example 2: classifying images of digits, coding demos



Summary and quiz questions

Summary

Thanks for participating! We have studied

- Three examples of machine learning problems.
- Two kinds of problems, regression y=real number, classification y=integer category.
- Splitting a data set into train/test/subtrain/validation sets for learning hyper-parameters and evaluating prediction accuracy.
- Overfitting and how to avoid it by choosing hyper-parameters based on a validation set.
- Comparing prediction accuracy of learning algorithms with each other and to a featureless baseline.

Quiz questions

- When using a design matrix to represent machine learning inputs, what does each row and column represent?
- When splitting data into train/test sets, what is the purpose of each set? When splitting a train set into subtrain/validation sets, what is the purpose of each set?
- In order to determine if any non-trivial predictive relationship between inputs and output has been learned, a comparison with a featureless baseline that ignores the inputs must be used. How do you compute the baseline predictions, for regression and classification problems?
- How can you tell if machine learning model predictions are underfitting or overfitting?
- Many learning algorithms require input of the number of iterations or epochs. For example in R the `nnet` function has the `maxit` argument and the keras::fit function has the `epochs` argument. How should this parameter be chosen?