Introduction to machine learning and neural networks

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Introduction and overview

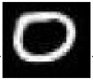
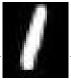
Problem 1: avoiding overfitting in regression

Problem 2: classifying images of digits

Problem 3: predicting earth system model parameters

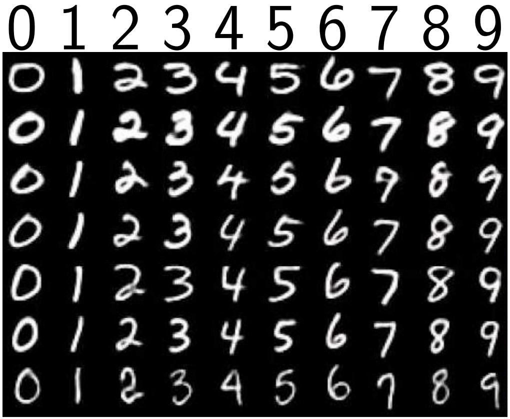
Machine learning intro: image classification example

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

- Inputs/features x can be easily computed using traditional algorithms, e.g. matrix of pixel intensities in an image.
- Outputs/labels y are what we want to predict, easy to get by asking a human, but hard to compute using traditional algorithms, e.g. image class.
- 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

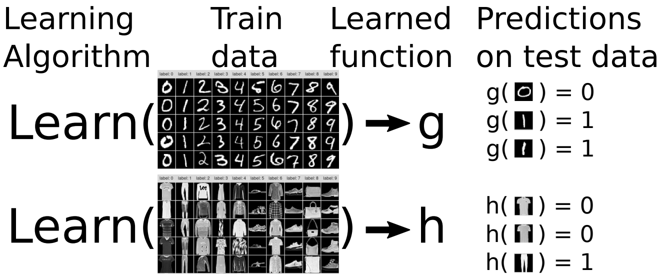
I give you a training data set with paired inputs/outputs, e.g.



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 $y \in \{0, 1, \ldots, 9\}$ 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 types of problems, which different 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 explain three learning problems:

- Regression with a single input, to demonstrate how to avoid overfitting.
- Classification of digit images, to demonstrate how to compare machine learning algorithms in terms of test/prediction accuracy.
- Regression for predicting earth system model parameters, as a relevant application.

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Problem 1: avoiding overfitting in regression

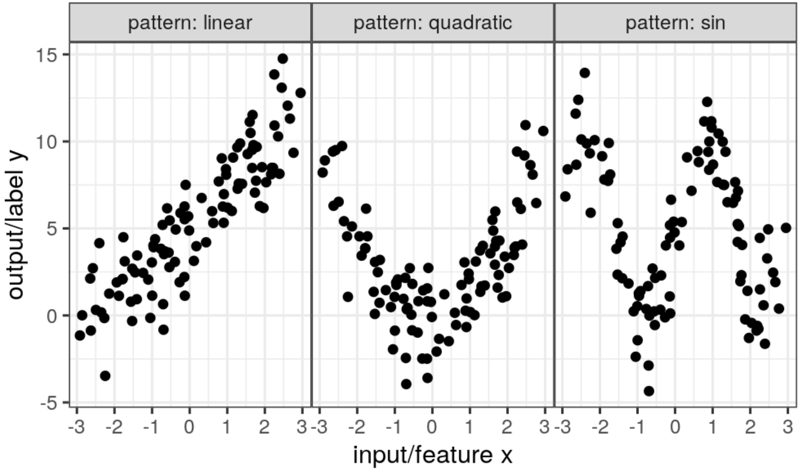
Problem 2: classifying images of digits

Problem 3: predicting earth system model parameters

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.
- Any machine learning algorithm is prone to overfit, which means providing better predictions on the train/subtrain set than on a held-out validation/test set. (BAD)
- To learn a model which does NOT overfit (GOOD), you need to first divide your train set into subtrain/validation sets.
- Code for figures in this section: `https://github.com/tdhock/2020-yiqi-summer-school/blob/master/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 $f(x) \in \mathbb{R}$.

Neural network prediction function

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

With $L-1$ hidden layers, we have for all $l \in \{1, \dots, L\}$:

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

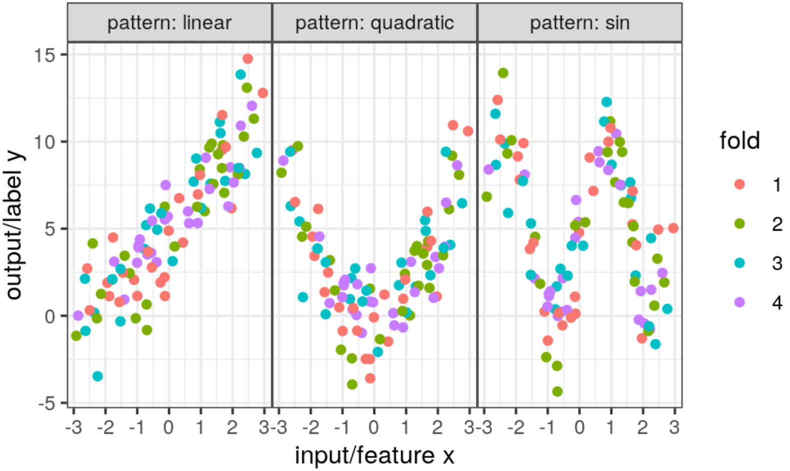
The hyper-parameters which must be fixed prior to learning:

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

The weight matrices $\mathbf{W}_l$ are learned using gradient descent.

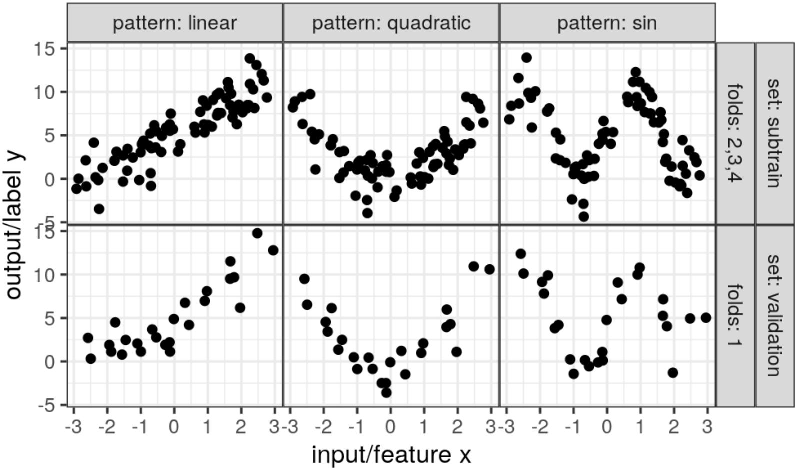
- In each **iteration** of gradient descent, the weights are updated in order to get better predictions on subtrain data.
- An **epoch** computes gradients on all subtrain data; there can be from 1 to N(subtrain size) iterations per epoch.

Illustration of 4-fold cross-validation



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

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.

CSV data tables for machine learning

- One row for each observation.
- One column for the output/label/y (in regression the label is a real number, in classification the label is a class/category).
- The other columns should be inputs/features/X that will be used to predict the corresponding output/label/y.

Example: `https://raw.githubusercontent.com/tdhock/2020-yiqi-summer-school/master/data_linear.csv`

```
              x           y
1: -1.40694802  0.933196336
2: -0.76725660  3.832773444
3:  0.43712018  4.202983135
4:  2.44924674 13.089055084
...
```

Result of reading CSV data into R

Result is:

```
> sim.data
     pattern          x          y fold
  1:  linear -1.4069480  0.9331963    4
  2:  linear -0.7672566  3.8327734    3
  3:  linear  0.4371202  4.2029831    1
  4:  linear  2.4492467 13.0890551    2
  5:  linear -1.7899084  2.0791987    3
 ---
296:     sin  1.7838530  4.0502991    1
297:     sin -0.2683533 -0.1097264    1
298:     sin -0.5394955 -0.5539398    1
299:     sin  1.8652215 -0.2262517    4
300:     sin  0.6295997  8.8124249    4
```

Assign each observation to subtrain/validation set

```
validation.fold <- 1
sim.data[, set := ifelse(
  fold==validation.fold, "validation", "subtrain")]
> sim.data
     pattern          x          y fold        set
  1:  linear -1.4069480  0.9331963    4   subtrain
  2:  linear -0.7672566  3.8327734    3   subtrain
  3:  linear  0.4371202  4.2029831    1 validation
  4:  linear  2.4492467 13.0890551    2   subtrain
  5:  linear -1.7899084  2.0791987    3   subtrain
 ---
296:     sin  1.7838530  4.0502991    1 validation
297:     sin -0.2683533 -0.1097264    1 validation
298:     sin -0.5394955 -0.5539398    1 validation
299:     sin  1.8652215 -0.2262517    4   subtrain
300:     sin  0.6295997  8.8124249    4   subtrain
```

Neural network with one hidden layer, 20 hidden units

Use for loops to fit different neural network models for each data set and number of iterations.

```
maxit.values <- 10^seq(0, 4)
pattern.values <- c("linear", "quadratic", "sin")
for(i in maxit.values)for(p in pattern.values){
  pattern.data <- sim.data[pattern==p]
  fit <- nnet::nnet(
    y ~ x,
    pattern.data[set=="subtrain"],
    size=20,     #hidden units
    linout=TRUE, #for regression
    maxit=i)     #max number of iterations
...
```

Neural network prediction function

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

For the nnet code, we have:

$$\begin{aligned} f_1(t) &= A_1(\mathbf{W}_1^\intercal t), \\ f_2(t) &= A_2(\mathbf{W}_2^\intercal t), \\ f(x) &= f_2[f_1(x)] = A_2[\mathbf{W}_2^\intercal A_1(\mathbf{W}_1^\intercal x)]. \end{aligned}$$

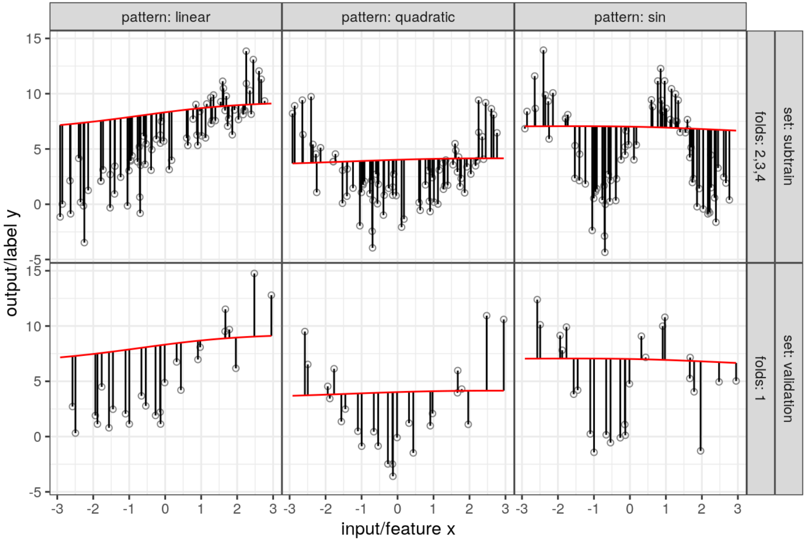
The hyper-parameters are fixed prior to learning:

- Number of layers $L = 2$.
- Activation functions A_1=sigmoid, A_2=identity.
- Number of units in the hidden layer $u_1 = 20$.
- No sparsity in the weight matrices (fully connected).

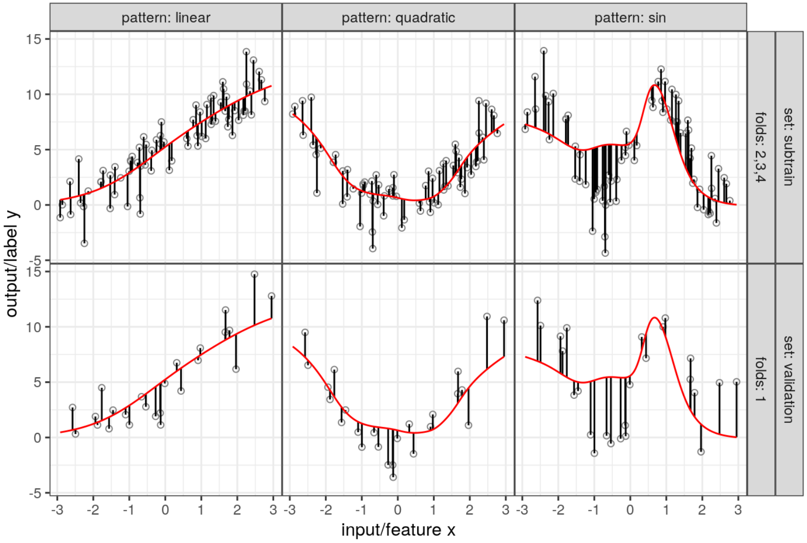
The weight matrices $\mathbf{W}_1, \mathbf{W}_2$ are learned using gradient descent.

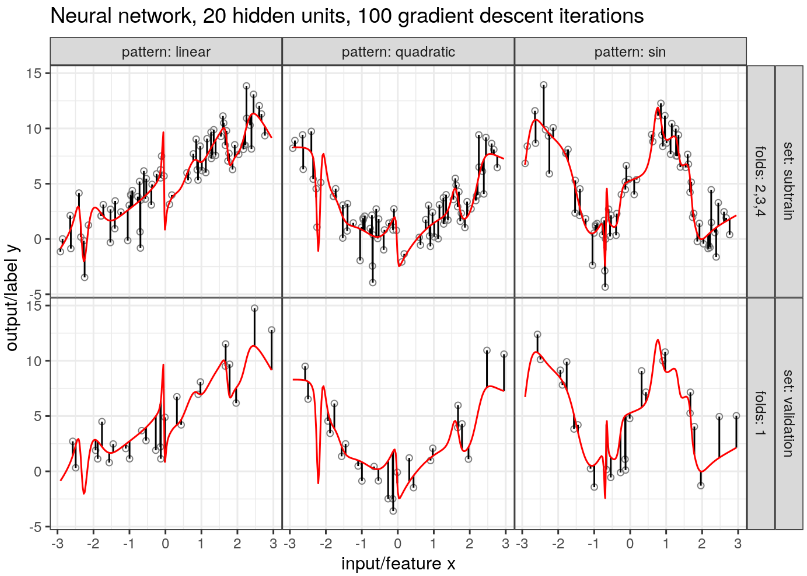
- "Full gradient" method is used, so in each **epoch** there is 1 iteration/update to the weights that is based on the gradient summed over all subtrain data.

Neural network, 20 hidden units, 1 gradient descent iterations



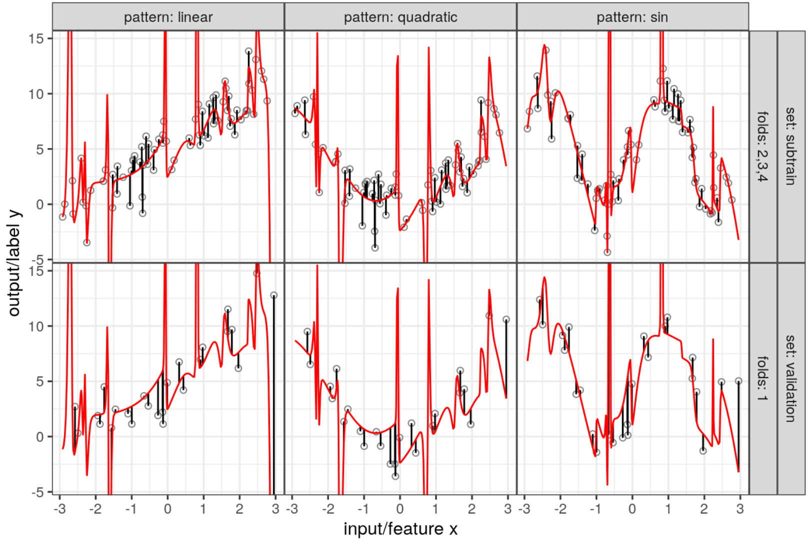
Neural network, 20 hidden units, 10 gradient descent iterations

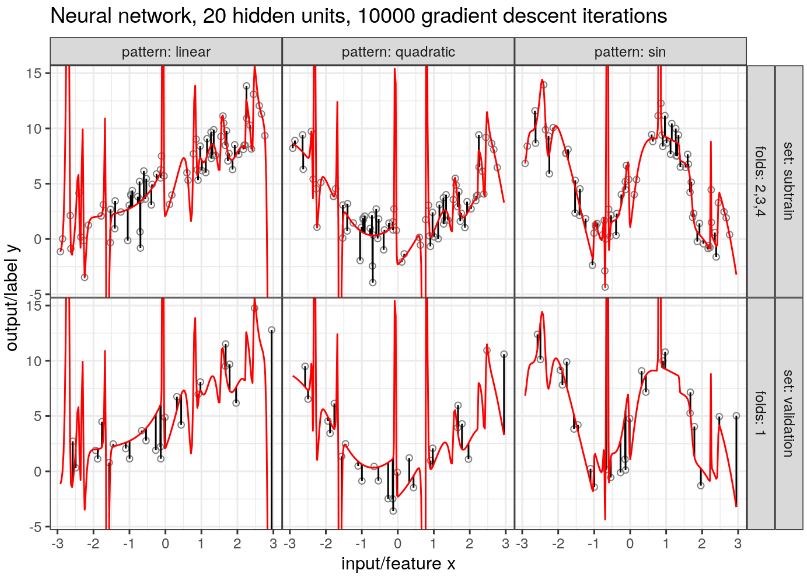


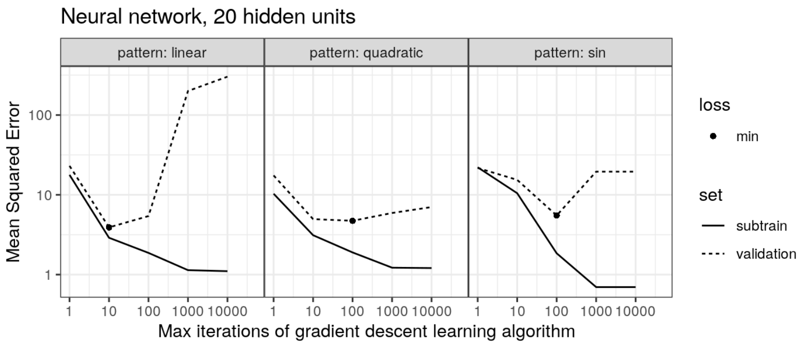


Neural network, 20 hidden units, 100 gradient descent iterations
pattern: linear
pattern: quadratic
pattern: sin
folds: 2,3,4
set: subtrain
folds: 1
set: validation
output/label y
input/feature x
15
10
5
0
-5
-3
-2
-1
0
1
2
3

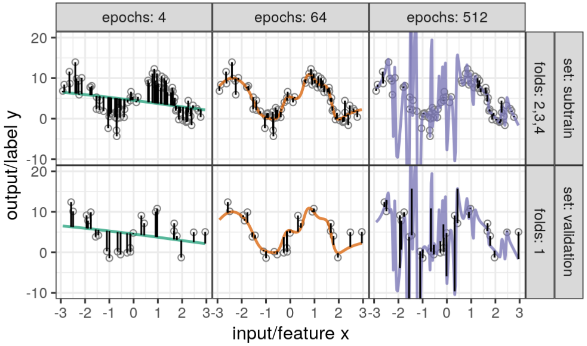
Neural network, 20 hidden units, 1000 gradient descent iterations



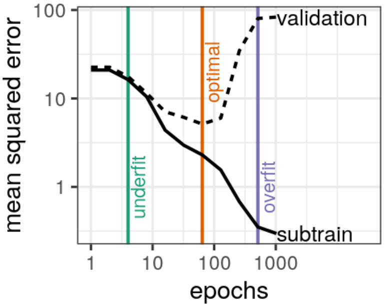

Neural network, 20 hidden units, 10000 gradient descent iterations
pattern: linear
pattern: quadratic
pattern: sin
folds: 2,3,4
set: subtrain
folds: 1
set: validation
output/label y
input/feature x
15
10
5
0
-5
-3
-2
-1
0
1
2
3



Neural network, 20 hidden units
pattern: linear
pattern: quadratic
pattern: sin
Mean Squared Error
100
10
1
1
10
100
1000
10000
Max iterations of gradient descent learning algorithm
loss
min
set
subtrain
validation



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



mean squared error
epochs
100
10
1
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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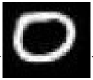
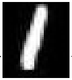
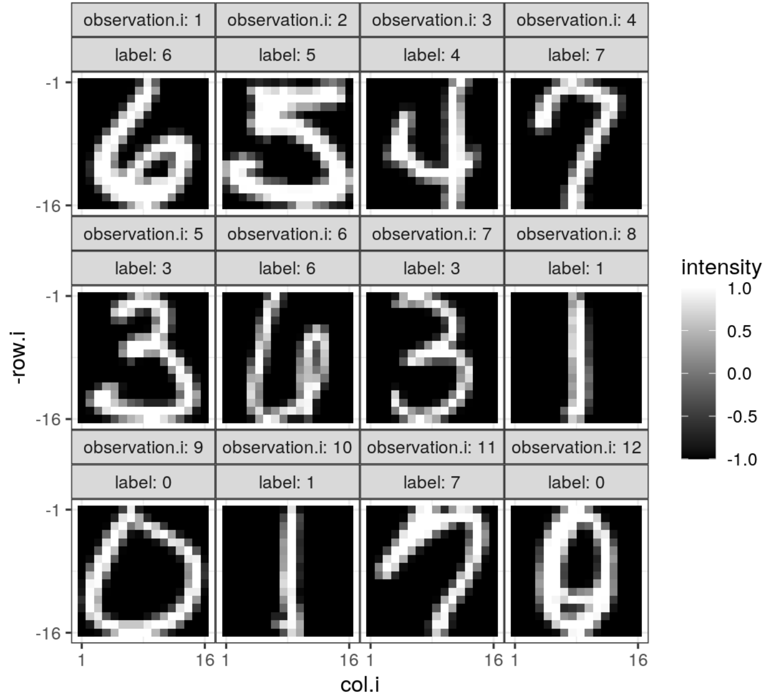
Image classification

- 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/2020-yiqi-summer-school/blob/master/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
-row.i
-1
-16
col.i
1
16
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
...
```

Conversion to array for input to 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/`

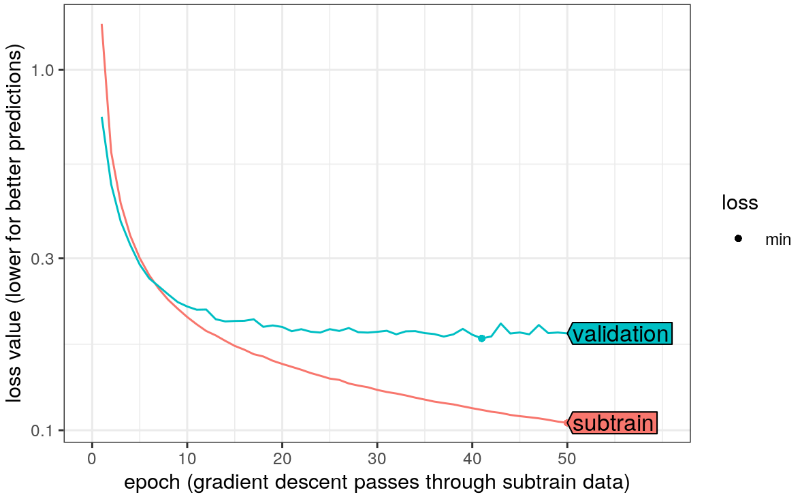
Keras model fitting

```
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).

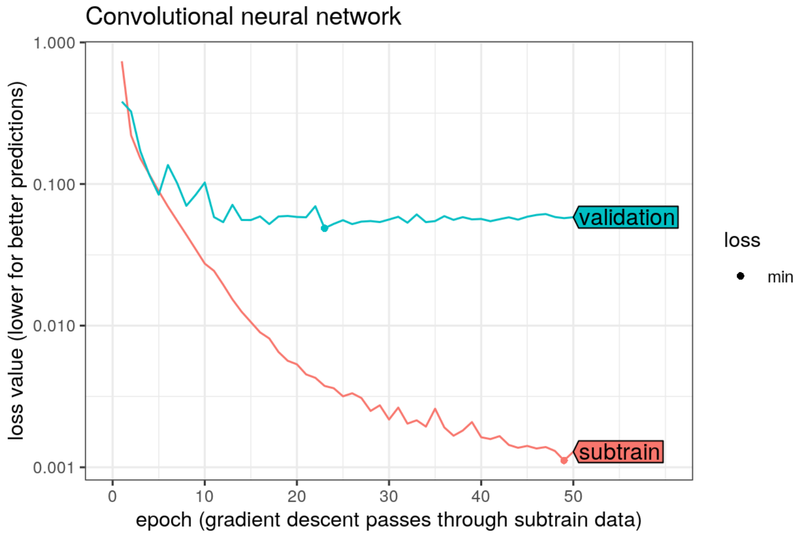
Linear model



Sparse (convolutional) model R code

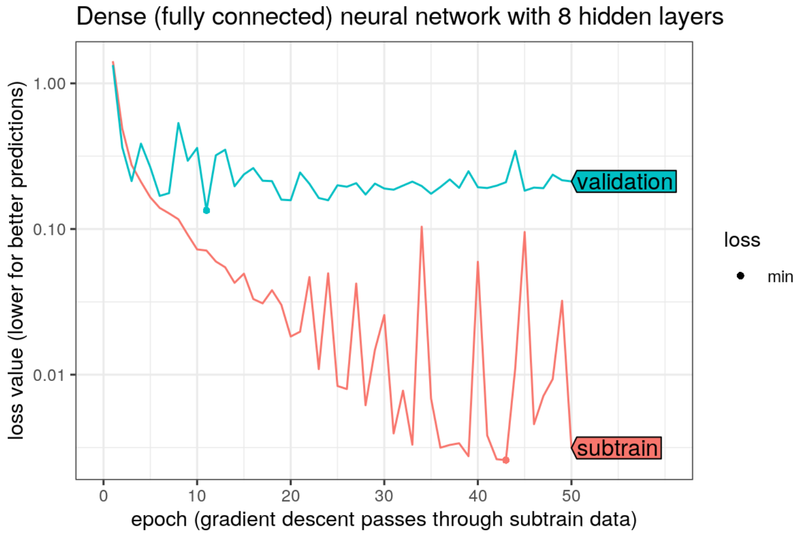
```
library(keras)
conv.model <- keras_model_sequential() %>%
  layer_conv_2d(
    input_shape = dim(zip.X.array)[-1],
    filters = 20,
    kernel_size = c(3,3),
    activation = 'relu') %>%
  layer_max_pooling_2d(pool_size = c(2, 2)) %>%
  layer_flatten() %>%
  layer_dense(units = 100, activation =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

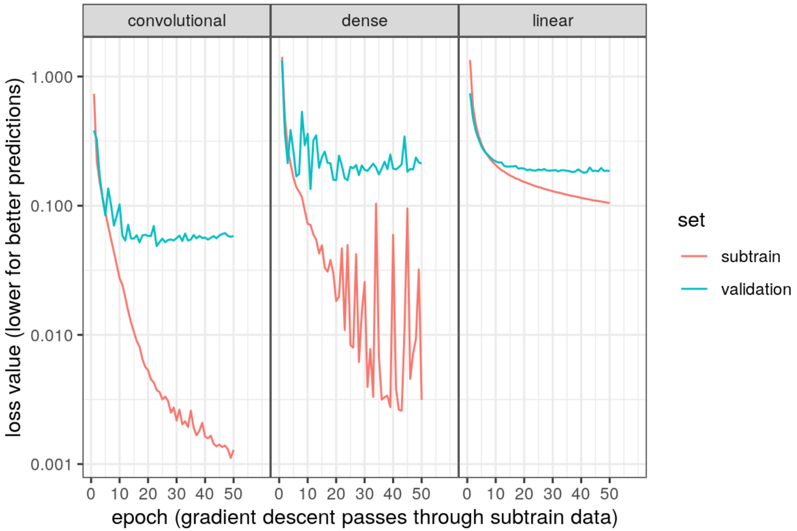
- Sparse: few inputs are used to predict each unit in `layer_conv_2d`.
- Exploits structure of image data to make learning easier/faster.


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

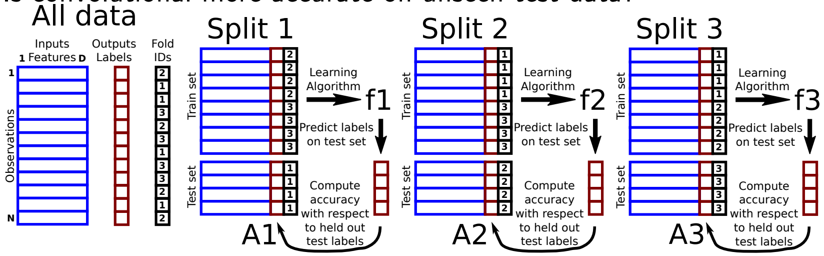
```
library(keras)
dense.model <- keras_model_sequential() %>%
  layer_flatten(
    input_shape = dim(zip.X.array)[-1]) %>%
  layer_dense(units = 100, activation = 'relu') %>%
  layer_dense(units = 100, activation = 'relu') %>%
  layer_dense(units = 100, activation = 'relu') %>%
  layer_dense(units = 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
loss value (lower for better predictions)
1.000
0.100
0.010
0.001
0
10
20
30
40
50
epoch (gradient descent passes through subtrain data)
set
subtrain
validation

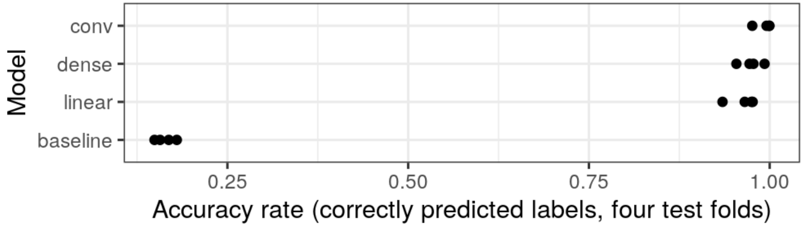
K-fold cross-validation for model evaluation

Is convolutional more accurate on unseen test data?



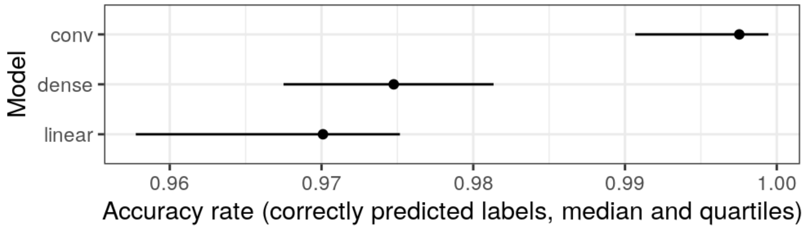
- Randomly assign a fold ID from 1 to K to each observation.
- Hold out the observations with the Split ID as test set.
- Use the other observations as the train set.
- Run learning algorithm on train set (including hyper-parmeter selection), outputs learned function (f1-f3).
- Finally compute and plot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

Accuracy rates for each test fold



- Always a good idea to compare with the trivial baseline model which always predicts the most frequent class in the train set. (ignoring all inputs/features)
- Here we see that the 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/2020-yiqi-summer-school/blob/master/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

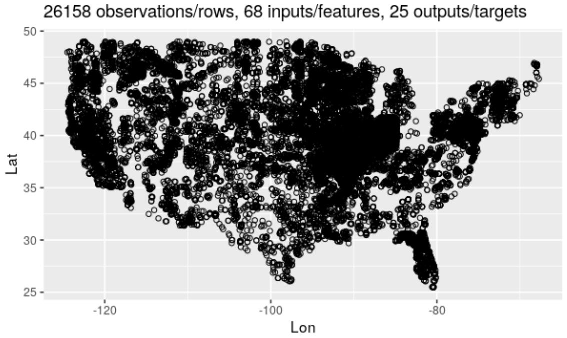
Problem 1: avoiding overfitting in regression

Problem 2: classifying images of digits

Problem 3: predicting earth system model parameters

Problem setting

Data from: F. Tao, Z. Zhou, Y. Huang, Q. Li, X. Lu, S. Ma, X. Huang, Y. Liang, G. Hugelius, L. Jiang, R. Doughty, Z. Ren, and Y. Luo. Deep learning optimizes data-driven representation of soil organic carbon in earth system model over the conterminous United States. Frontiers in Big Data, 3:17, 2020.


26158 observations/rows, 68 inputs/features, 25 outputs/targets
Lat
50
45
40
35
30
25
-120
-100
-80
Lon

Soil vertical profile data gathered at shown sites, and used to fit an earth system model.

Inputs

Each site (row) has the following environmental features (columns):

```
        Lat       Lon Climate Soil_Type Veg_Cover ...
1: 47.24611 -111.0525       2        11        10
2: 47.68296 -111.2014       2        11        10
3: 45.35806 -116.8119       3        11        10
4: 46.73885 -102.7589       4        11        12
5: 47.65490 -111.5828       2        11        10
6: 48.49139 -109.8028       2        11        10
...
```

Outputs

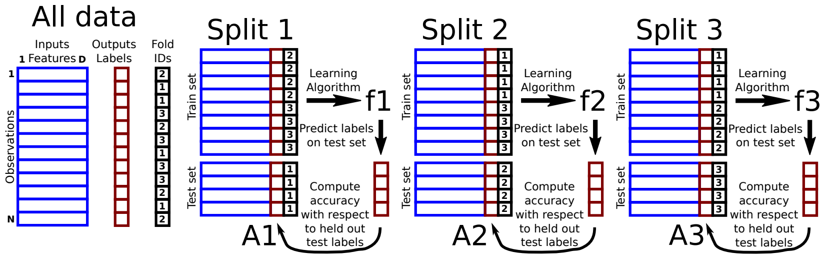
We have fit an earth system model, which has the following parameters (columns) at each site (rows):

```
          cryo    maxpsi     tau4s3     fs2s3
[1,] 0.5559403 0.4472416 0.04058302 0.4105497
[2,] 0.4982079 0.5201390 0.19487388 0.3721377
[3,] 0.4878875 0.4155263 0.30624590 0.4009429
[4,] 0.4976373 0.4327989 0.25603125 0.1208804
[5,] 0.4469068 0.4972995 0.41847923 0.1809647
[6,] 0.4836617 0.4874783 0.17804971 0.2925210
...
```

Problem statement

To what extent can we predict the earth system model parameters at a new site, assuming we have the environmental features / inputs available?

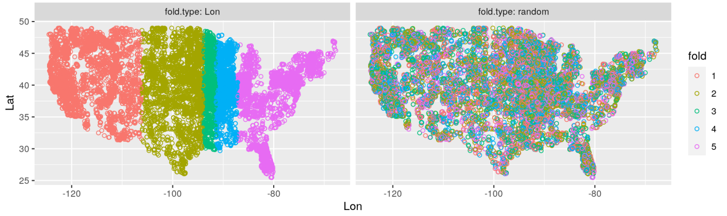
- Cross-validation splits data into train and test sets.
- Neural network learning algorithm run on train set.
- Predictions and accuracy/loss computed on test set.

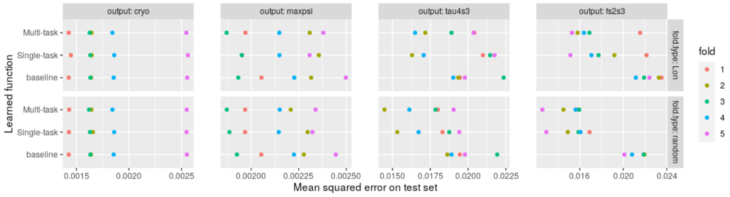


Neural network architecture taken from paper

```
keras_model_sequential() %>%
  layer_dense(
    units = 256, activation = 'relu',
    input_shape = ncol(keep.mat.list[["input"]])) %>%
  layer_dropout(0.3) %>%
  layer_dense(units = 512, activation = 'relu') %>%
  layer_dropout(0.5) %>%
  layer_dense(units = 512, activation = 'relu') %>%
  layer_dropout(0.5) %>%
  layer_dense(units = 256, activation = 'relu') %>%
  layer_dropout(0.3) %>%
  layer_dense(units = 1 OR 25) %>%
  compile(
    loss = loss_mean_squared_error,
    optimizer = optimizer_adadelta()
  )
```

Neural networks often more accurate than baseline





Multi-task:	single neural network which predicts all 25 outputs.
Single-task:	25 neural networks, each trained seperately to predict a single output.
baseline:	always predict the mean of the labels/outputs in the train set (ignores inputs/features).