Workshop 2: Regression and Neural Networks

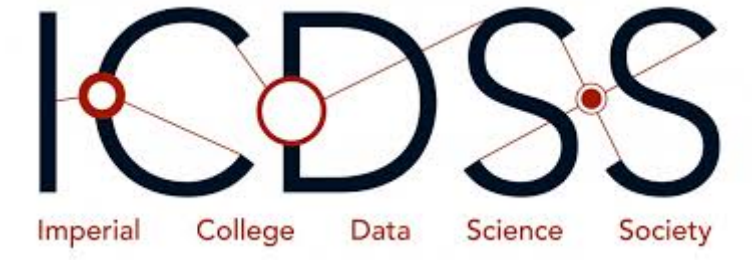
https://github.com/Imperial-College-Data-Science-Society/workshops
(https://github.com/Imperial-College-Data-Science-Society/workshops)

1. Introduction to Data Science
2. **Regression and Neural Networks**
3. Classifying Character and Organ Images
4. Demystifying Causality and Causal Inference
5. A Primer to Data Engineering
6. Natural Language Processing (NLP) by using Attention
7. Art and Music using GANs
8. Probabilistic Programming in Practice
9. Missing Data in Supervised Learning

Today

You can access the material via:

- Binder
- Local Jupyter Notebook with a suitable virtual environment and dependencies installed
- The PDF slides
- Following my slides on MS Teams



Projects

Thoughts?

References I used to prepare this session:

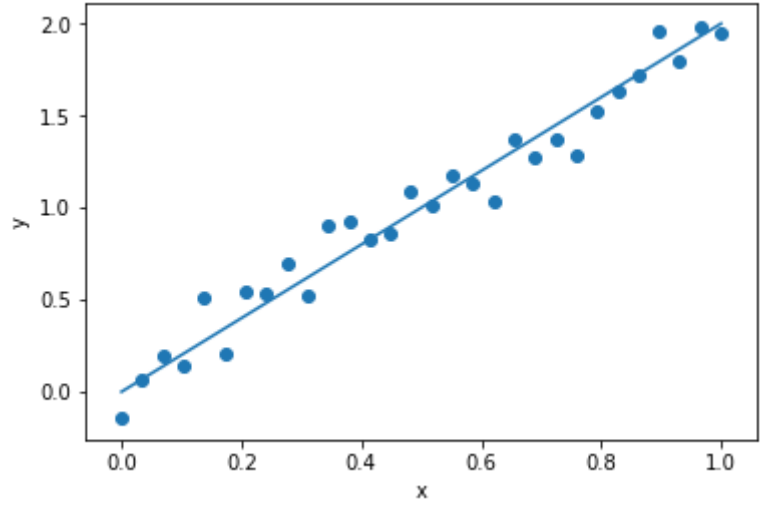
- Past ICDSS workshops
- Patrick Rebischini's notes: http://www.stats.ox.ac.uk/~rebeschi/teaching/AFoL/20/index.html (http://www.stats.ox.ac.uk/~rebeschi/teaching/AFoL/20/index.html)
- https://fleuret.org/ee559/ (https://fleuret.org/ee559/)
- https://en.wikipedia.org/wiki/Ordinary_least_squares (https://en.wikipedia.org/wiki/Ordinary_least_squares)
- https://www.astroml.org/book_figures/chapter9/fig_neural_network.html (https://www.astroml.org/book_figures/chapter9/fig_neural_network.html)
- https://github.com/pytorch/examples/blob/master/mnist/main.py (https://github.com/pytorch/examples/blob/master/mnist/main.py)
- Lakshminarayanan et al. (2016) http://papers.nips.cc/paper/5234-mondrian-forests-efficient-online-random-forests.pdf (http://papers.nips.cc/paper/5234-mondrian-forests-efficient-online-random-forests.pdf)
- Garnelo et al. (2018) https://arxiv.org/pdf/1807.01622.pdf (https://arxiv.org/pdf/1807.01622.pdf) Other recommended reading:
- Regression and Other Stories by Andrew Gelman, Jennifer Hill and Aki Vehtari
- Elements of Statistical Learning

Introduction

Suppose we have some $(x_1, y_1), \ldots, (x_{100}, y_{100})$ that is generated by $y = 2x + \text{noise}$.

In [1]:
```
import numpy as np
import matplotlib.pyplot as plt
x = np.linspace(0, 1, 30)
noise = 0.1*np.random.normal(size=30)
y = 2*x + noise
plt.scatter(x, y)
plt.plot(x, 2*x)
plt.xlabel("x")
plt.ylabel("y")
```

Out[1]:
```
Text(0, 0.5, 'y')
```



In practice, we don't know the underlying data-generating process, but rather we can pose **"hypotheses"** as to how the data is generated. For example in the above example:

- **Linear Models:** $y = x\beta + \sigma\mathcal{N}(0, 1)$ where β represents the gradient of the slope and σ is the amplitude of the noise.
- **Nonparametric models:** $y = f(x) + \sigma\mathcal{N}(0, 1)$ where f is some function in some hypothesis function space $\mathcal{H}$. E.g. $f(x) = x\beta$
    - Neural networks
    - Regression trees, random forests
    - Gaussian processes
- $y = \sum_{i=1}^{T} w_i \times f_i(x) + g(x)$ where w_i represent weights, $f_i \in \mathcal{H}$ and $g(x)$ represents the noise for value x.
- etc...

Once we have a hypothesis we can **estimate f** using many different tools!

Out of sample prediction

Given x_*, the prediction would be $f_*(x_*)$, where f_* is the estimated function of f.

But first, to formulate the hypothesis, we need to scrutinate the data via exploratory data analysis.

For the data above, clearly a linear model (straight line) plus some small Gaussian noise is sufficient. So the task is just to estimate β and σ so that the line **fits the dots well**.

General setting

In practice, we have to deal with data coming in different formats and possible generating processes. E.g. from the exponential family:

- **Count data**: $y_i \sim \text{Poisson}(f(x_i))$ or $y_i \sim \text{NegativeBinomial}(f(x_i))$
  - Football goals, disease infection counts
- **Binomial or Multinomial**: $y_i \sim \text{Binomial}(n, f(x_i))$, $y_i \sim \text{Multinomial}(f_1(x_i), \ldots, f_k(x_i))$ etc...
  - Coin toss outcomes, customer subscription outcome, classifying digits or characters
- **Gamma**: $y_i \sim \text{Gamma}(k, f(x_i))$
  - Rainfall

Gaussian noise regression

For illustration purposes, let's focus on regression in the setting $y = f(x) + \sigma\mathcal{N}(0, 1)$ for $f \in \mathcal{H}$ and $\sigma \geq 0$.

Foundations of Statistical Learning

Previously, I mentioned that we need to build a function that **fits the dots well**. There are 2 types of notions in statistical learning: **prediction** and **estimation**. We will use the following notation:

- n training points
- $X_1, \dots, X_n$ are *features* in a *feature space* $\mathcal{X}$. Could be a mixture of categorial or continuous features.
- $Y_1, \dots, Y_n$ are labels/response in a space $\mathcal{Y}$ (e.g. $\mathbb{R}$ or $\mathbb{R}^k$)
- **[For your interest:]** Some probability space $(\mathcal{X}, \mathcal{B}, \mathbb{P})$ where we can measure probabilities of events in the set $\mathcal{B}$. e.g. the set of all possible cointoss outcomes is a set $\mathcal{B}$
- **Hypothesis space** $\mathcal{H} \subset \mathcal{C} := \{f : f : \mathcal{X} \to \mathcal{Y}\}$: Restriction of the types of functions we want to use. e.g. for a type of neural network, the multilayer perceptron (MLP) with m layers, we have
  $\mathcal{H} := \{f : \mathcal{X} \to \mathcal{Y} : f(\cdot) = f(\cdot; \sigma_1, \dots, \sigma_m, W_1, \dots, W_m), \text{ where } \sigma_i, .$
  W_i are the activation functions and weights$\}$
- **Prediction Loss function** $\ell : \mathcal{H} \times \mathcal{X} \times \mathcal{Y} \to \mathbb{R}_+$: To define what **fits the dots well** means.

Prediction

We want to pick f such that it minimises the **expected or population risk** when a new independent datapoint (X, Y) comes in

$$f_* := \text{argmin}_{f \in \mathcal{C}} \mathbb{E}_{\mathbb{P}} \left[\ell(f, X, Y) \right] := \text{argmin}_{f \in \mathcal{C}} r(f)$$

We denote f_* is the **optimum**, which is unknown. We want to construct an approximation to f_* based on the n training points and the hypothesis $\mathcal{H}$ that controls the complexity of f. This approximation is close to

$$f_{**} := \text{argmin}_{f \in \mathcal{H}} \mathbb{E}_{\mathbb{P}} \left[\ell(f, X, Y) \right]$$

Define the **excess risk** as

$$r(f) - r(f_{**}) = [r(f) - r(f_*)] + [r(f_*) - r(f_{**})],$$

where $f \in \mathcal{H}$. **The goal of statistical learning for prediction is to minimise the excess risk** with respect to the sample size n and the space of functions $\mathcal{H}$. Note that the decomposition yields an approximation and estimation error.

Difficult to do in practice, so we need **empirical risk minimisation** via the observed training set $(X_i, Y_i)_{i=1}^n$ as a proxy for the expected/population risk:

$$R(f) := \frac{1}{n} \sum_{i=1}^{n} \ell(f, X_i, Y_i), \qquad f_*^R := \operatorname{argmin}_{f \in \mathcal{H}} R(f)$$

to minimise

$$r(f) - r(f_{**}).$$

Key takeaways and Bigger Picture:

- It is important to understand the tradeoff between optimisation and statistical errors.
- Optimisation is only 1 part of the inequality, and vice versa for statistical modelling errors.

More details in Rebischini's notes!

Estimation

We need:

- Some training set of size n generated by $f_* \in \mathcal{H}$
- Loss function $\ell : \mathcal{H} \times \mathcal{H} \to \mathbb{R}_+$

Return:

- An algorithm that returns an estimate of f_* that minimises and controls $\ell(f, f_*)$ based on the n training points and $\mathcal{H}$.

Back to Gaussian noise regression

There are lots of ways we can pose this problem. One way is to use

- $\ell(f, X, Y) = ||f(X) - y||_2^2$ - the **\ell_2 loss**
  $= (f(X) - y)^2$
- $\ell(f, X, Y) = |f(X) - y|$ - the **\ell_1 loss**
- This yields the **mean squared error (MSE)** $R(f) = \frac{1}{n} \sum_{i=1}^{n} (f(x_i) - y_i)^2$

In theory, these give

$$\ell_2 : f_{**}(x) = E[Y|X = x]$$

$$\ell_1 : f_{**}(x) = \text{Median}[Y|X = x]$$

Depending on the situation, we can either use approximate gradient-based methods (e.g. gradient descent), Monte Carlo methods or the analytical maximum likelihood estimation (MLE).

Linear regression

$$y = X\beta_0 + \sigma\mathcal{N}(0, 1)$$

$\beta_0 = (1, \beta_{0,1}, \dots, \beta_{0,d-1})^T$ - the 1 represents the intercept.

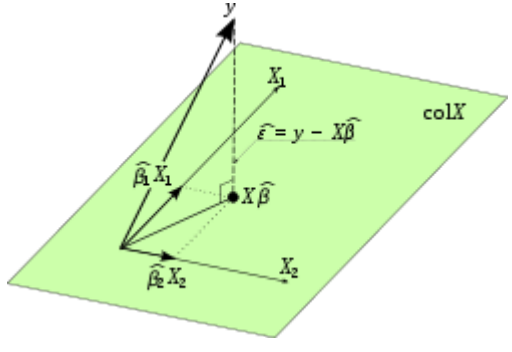
We also call this **ordinary least squares**:

- Assume that X is full rank

$$\hat{\beta} = \text{argmin}_\beta ||y - X\beta||_2^2 \iff X^T(y - X\beta) = 0 \iff \hat{\beta}$$
$$= X(X^TX)^{-1}X^Ty \sim \mathcal{N}(X\beta_0, \sigma^2 X(X^TX)^{-1}X^T)$$

Geometrically: $y - X\hat{\beta} \perp X\beta_0 \iff \hat{\beta}$ minimises $||y - X\beta||_2^2$

https://en.wikipedia.org/wiki/Ordinary_least_squares (https://en.wikipedia.org/wiki/Ordinary_least_squares):



Can also solve this via gradient descent:

- Remember excess risk <= approximationLoss + statisticalLoss

In [2]:
```
import statsmodels.api as sm

# fit the model
m = sm.OLS(y, sm.tools.add_constant(x))
res = m.fit()

print(res.summary(), "\n sigma~", np.sqrt(sum(res.resid**2) / (30 - 2)))
```

```
                            OLS Regression Results
==============================================================================
Dep. Variable:                      y   R-squared:                       0.962
Model:                            OLS   Adj. R-squared:                  0.960
Method:                 Least Squares   F-statistic:                     704.6
Date:                Sun, 18 Oct 2020   Prob (F-statistic):           2.16e-21
Time:                        17:39:37   Log-Likelihood:                 22.372
No. Observations:                  30   AIC:                            -40.74
Df Residuals:                      28   BIC:                            -37.94
Df Model:                           1
Covariance Type:            nonrobust
==============================================================================
                 coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------
const          0.0381      0.042      0.901      0.375      -0.049       0.125
x1             1.9292      0.073     26.543      0.000       1.780       2.078
==============================================================================
Omnibus:                        0.416   Durbin-Watson:                   2.299
Prob(Omnibus):                  0.812   Jarque-Bera (JB):                0.547
Skew:                           0.017   Prob(JB):                        0.761
Kurtosis:                       2.339   Cond. No.                         4.25
==============================================================================

Notes:
[1] Standard Errors assume that the covariance matrix of the errors is correct
ly specified.
 sigma~ 0.11881627238852428
```

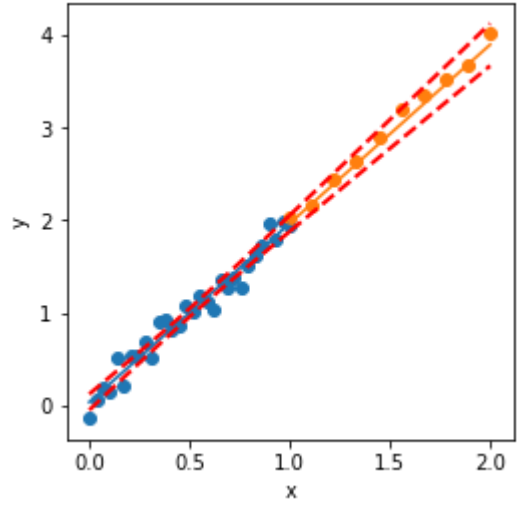
We can see that our algorithm manages to estimate the parameters of the models pretty well:

- $\hat{\beta} \approx 2$ with 95% confidence intervals [1.945, 2.091]
- $const \approx 0$ with 95% confidence intervals [-0.048, 0.036]
- $\hat{\sigma}^2 \approx 0.01$
- **95% confidence intervals** = if I sample the data infinitely many times and estimate infinitely many confidence intervals, I will expect that 95% of the time the confidence intervals will contain the true, unknown parameter value.

Given x_* as a test point, the prediction would be $\hat{y} = x_*^T \hat{\beta}$.

In [3]:
```
# Fit of the OLS estimator
x_test = np.linspace(1, 2, 10)
noise = 0.1*np.random.normal(size=10)
y_test = 2*x_test + noise
plt.figure(figsize=(4,4))
plt.scatter(x, y)
plt.plot(x, res.predict(sm.add_constant(x)))
pred_int_train = res.get_prediction(sm.add_constant(x)).conf_int()
plt.plot(x, pred_int_train[:,0], 'r--', lw=2); plt.plot(x, pred_int_train[:,1],
'r--', lw=2)

# the prediction intervals. Note that htey can be larger
plt.scatter(x_test, y_test)
plt.plot(x_test, res.predict(sm.add_constant(x_test)))
pred_int_test = res.get_prediction(sm.add_constant(x_test)).conf_int()
plt.plot(x_test, pred_int_test[:,0], 'r--', lw=2); plt.plot(x_test, pred_int_tes
t[:,1], 'r--', lw=2)
plt.xlabel("x"); plt.ylabel("y")
```

Out[3]:
```
Text(0, 0.5, 'y')
```



Other regression methods

- Regression trees: Classification and Regression Trees (CART)
- XGBoost: Tree-boosting algorithm widely used in production pipelines for firms like Amazon
- Random forest: Most popular tree-based algorithm
- Mondrian Forest: Nice statistical and online properties

Regression tree

A tree is a histogram or step function. $f(x) = \sum_{k=1}^{K} \beta_k I(x \in \Omega_k)$.

Example of a tree (Lakshminarayanan et al. (2016))

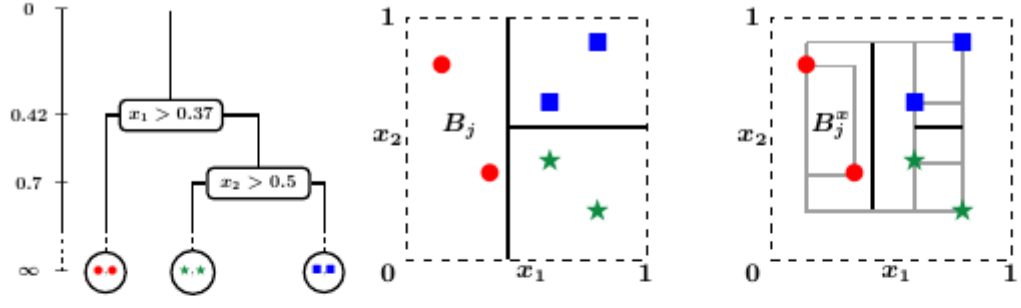
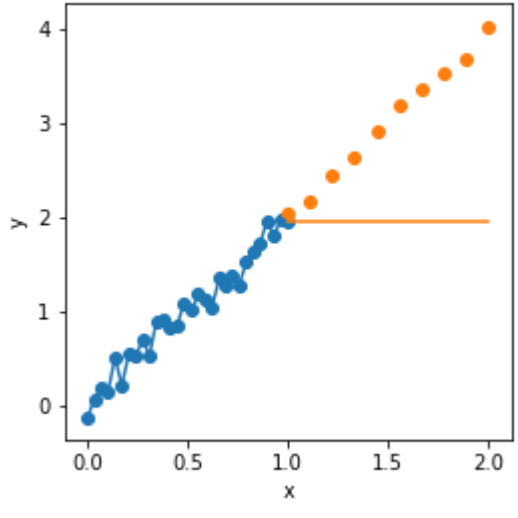


Figure 1: (left) A Mondrian tree over six *data points* in $[0, 1]^2$. Every node in the tree represents a split and is embedded in time (vertical axis). **(middle)** An ordinary decision tree partitions the whole space. **(right)** In a Mondrian tree, splits are committed only within the range of the data in each block (denoted by gray rectangles). Let $j = \mathsf{left}(\epsilon)$ be the left child of the root: then $B_j = (0, 0.37] \times (0, 1]$ is the block containing the red circles and $B_j^x \subseteq B_j$ is the smallest rectangle enclosing the two data points. (Adapted from [16], with permission.)

In [4]:
```
from sklearn.tree import DecisionTreeRegressor
# Fit regression model
m_tree = DecisionTreeRegressor(max_depth=5)
m_tree.fit(np.expand_dims(x, 1), y)
y_pred = m_tree.predict(np.expand_dims(x_test, 1))

plt.figure(figsize=(4,4))
plt.scatter(x, y)
plt.plot(x, m_tree.predict(np.expand_dims(x, 1)))

# the prediction intervals. Note that htey can be larger
plt.scatter(x_test, y_test)
plt.plot(x_test, y_pred)
plt.xlabel("x")
plt.ylabel("y")
```

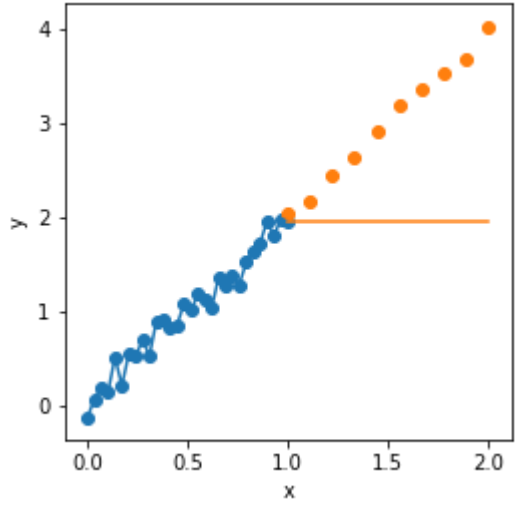
Out[4]:
```
Text(0, 0.5, 'y')
```



XGBoost

In [5]:
```
import xgboost as xgb

num_round = 10
m_xgb = xgb.XGBRegressor(objective ='reg:squarederror', n_estimators=1000)
m_xgb.fit(np.expand_dims(x, 1), y)

plt.figure(figsize=(4,4))
plt.scatter(x, y)
plt.plot(x, m_xgb.predict(np.expand_dims(x, 1)))

# the prediction intervals. Note that htey can be larger
plt.scatter(x_test, y_test)
plt.plot(x_test, m_xgb.predict(np.expand_dims(x_test, 1)))
plt.xlabel("x")
plt.ylabel("y")
```

Out[5]:
```
Text(0, 0.5, 'y')
```



Random Forest

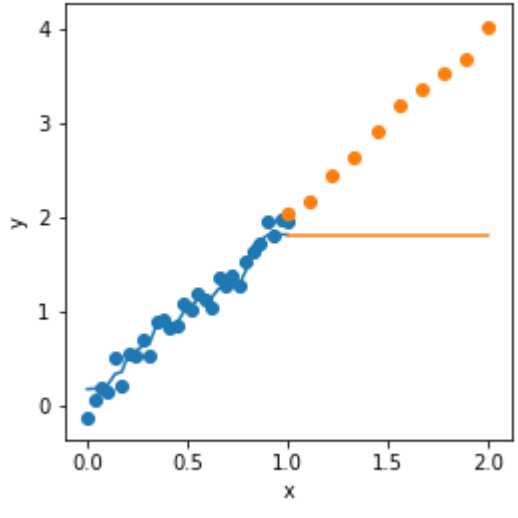
This essentially uses bagging:

$$\hat{f}(x) = \frac{1}{T} \sum_{t=1}^{T} \hat{f}_t(x)$$

, where $\hat{f}_t$ are trained regression trees from randomly sampled (with replacement) sets $\{(x_j, y_j)_j\}_t$ using random feature subsets.

In [6]:
```
from sklearn.ensemble import RandomForestRegressor
from sklearn.datasets import make_regression
m_rf = RandomForestRegressor(max_depth=2, random_state=0)
m_rf.fit(np.expand_dims(x, 1), y)
m_rf.predict(np.expand_dims(x_test, 1))

plt.figure(figsize=(4,4))
plt.scatter(x, y)
plt.plot(x, m_rf.predict(np.expand_dims(x, 1)))

# the prediction intervals. Note that htey can be larger
plt.scatter(x_test, y_test)
plt.plot(x_test,m_rf.predict(np.expand_dims(x_test, 1)))
plt.xlabel("x")
plt.ylabel("y")
```

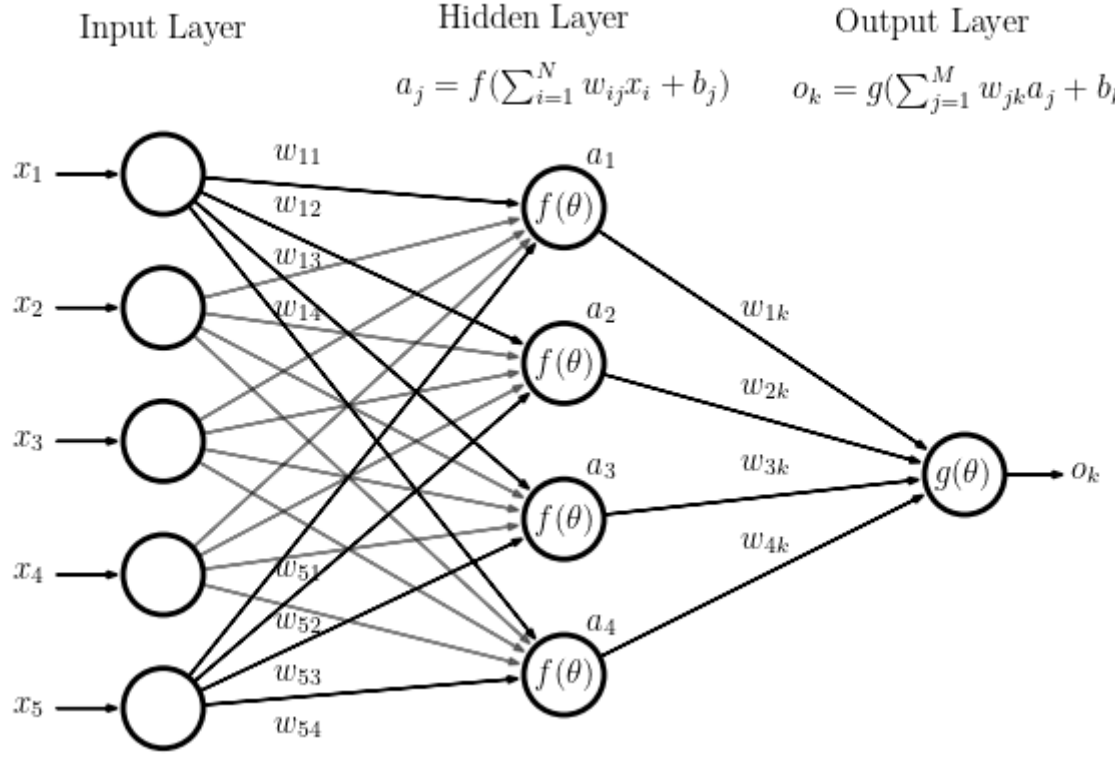
Out[6]:
```
Text(0, 0.5, 'y')
```



Neural Networks

Neural networks are essentially parametric functions that are composed of **layers of neurons**.

https://www.astroml.org/book_figures/chapter9/fig_neural_network.html (https://www.astroml.org/book_figures/chapter9/fig_neural_network.html)



- Multilayer Perceptron (MLP): $f(x) = f_n \circ \cdots f_1(x)$ with $f_j = W_j x + b_j$ with weights W_j and biases b_j.
- Can also have other useful layers like max-pooling, batch normalisation, attention and convolution (feature extraction).
- Parameter optimisation via gradient-based methods such as stochastic gradient descent. Using the backpropagation trick, can allow for efficient optimisation. Optimisation speed can be enhanced using multiple GPU or TPU memory.

Key applications:

- Image processing: classification, denoising, inpainting, generation
- Function approximations for complex models and algorithms
- Time series, recommendation engines

Key issues:

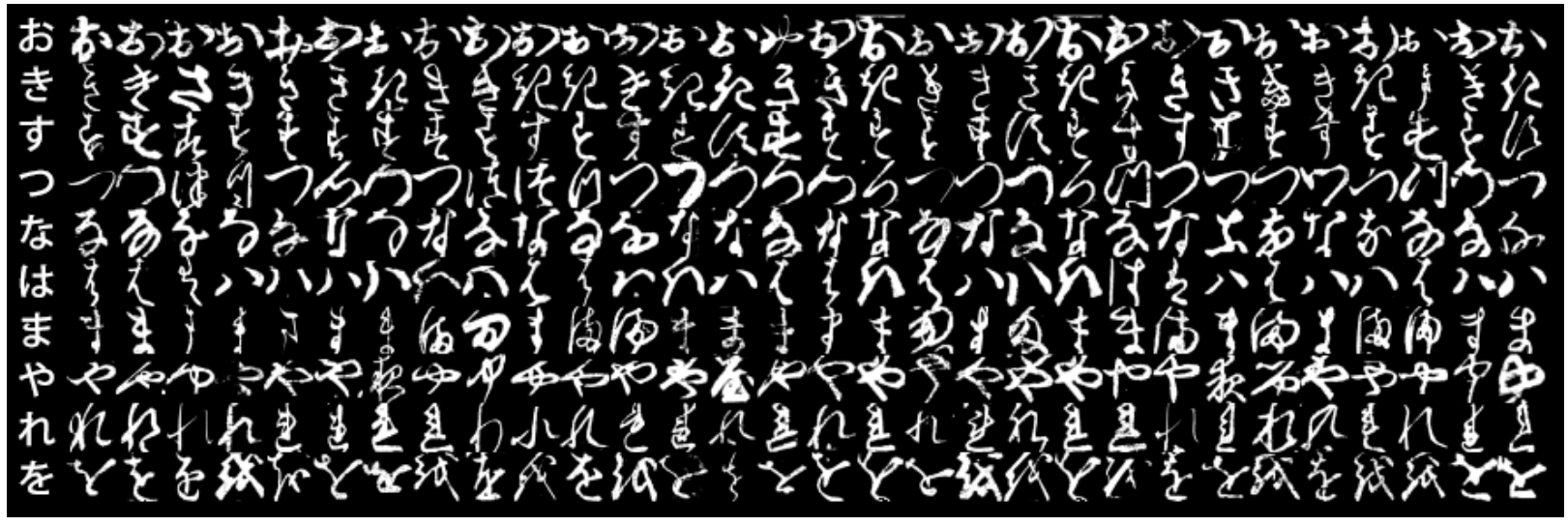
- Overparameterisation: regularisation and sparsity
- Feature engineering
- Vanishing gradient: batch normalisation and dropout

Image Classification

In [7]:

```
# https://github.com/pytorch/examples/blob/master/mnist/main.py
# Code is in the folder in the main.py script
# Don't run it during the session - might take a while!
# %run main.py

# we will use pretrained models from torchvision
import torch
from torchvision import datasets, transforms
transform=transforms.Compose([
    transforms.ToTensor(),
    transforms.Normalize((0.1307,), (0.3081,))
])

# https://github.com/rois-codh/kmnist
# We will use the Kuzushiji-MNIST dataset
dataset2 = datasets.KMNIST('../data', train=False,
                    transform=transform, download=True)
test_loader = torch.utils.data.DataLoader(dataset2, batch_size=16)
for img_batch, label_batch in test_loader:
    print(img_batch.shape, label_batch)
    break
```

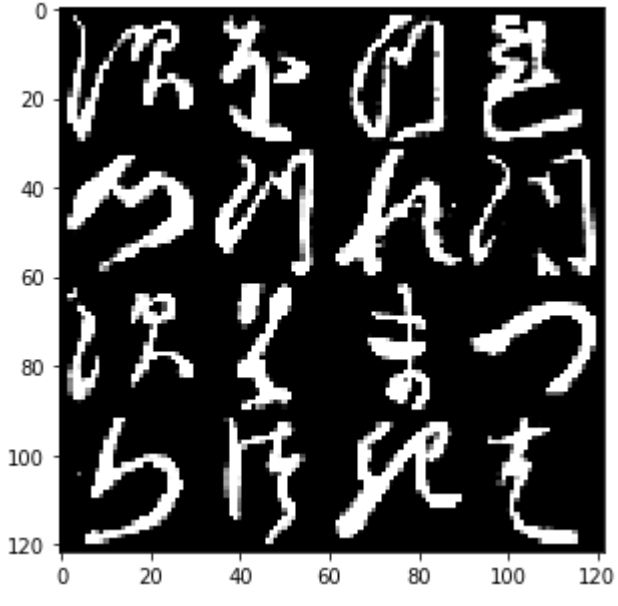
```
torch.Size([16, 1, 28, 28]) tensor([2, 9, 3, 8, 3, 3, 8, 3, 2, 5, 6, 3, 3, 3,
1, 5])
```



In [8]:
```
from torchvision.utils import make_grid

# Read images into torch.Tensor
all_imgs = img_batch
# Visualize sample on a grid
img_grid = make_grid(all_imgs, nrow=4)
plt.figure(figsize=(5,5))
plt.imshow(img_grid.permute(1, 2, 0).numpy())
```

```
Clipping input data to the valid range for imshow with RGB data ([0..1] for fl
oats or [0..255] for integers).
```

Out[8]:
```
<matplotlib.image.AxesImage at 0x7fb989f912e8>
```



In [9]:
```
from main import Net
model = Net()
# load some model I pretrained on GPU memory into CPU memory
model.load_state_dict(torch.load("kmnist_cnn.pt", map_location=torch.device('cpu')))
model.eval()
model(img_batch).argmax(dim=1, keepdim=True), label_batch
```

Out[9]:
```
(tensor([[3],
         [9],
         [3],
         [8],
         [3],
         [3],
         [8],
         [3],
         [2],
         [5],
         [6],
         [3],
         [3],
         [3],
         [1],
         [5]]),
 tensor([2, 9, 3, 8, 3, 3, 8, 3, 2, 5, 6, 3, 3, 3, 1, 5]))
```

Image Inpainting

https://arxiv.org/pdf/1807.01622.pdf (https://arxiv.org/pdf/1807.01622.pdf)

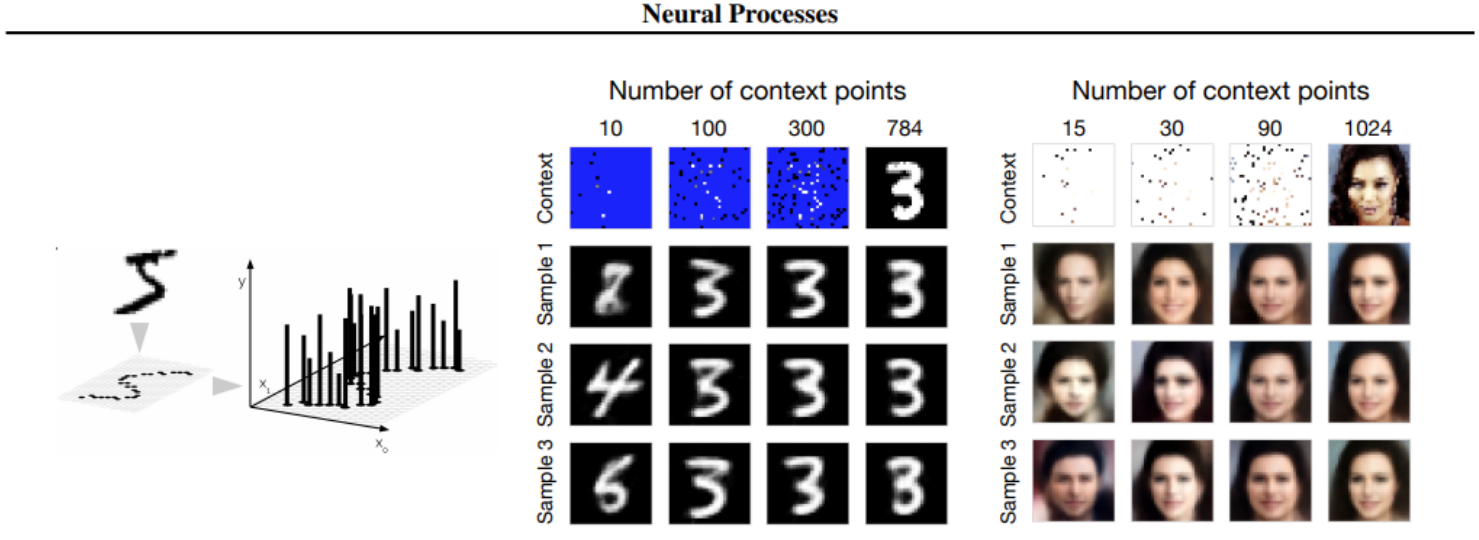


Figure 4. **Pixel-wise regression on MNIST and CelebA** The diagram on the left visualises how pixel-wise image completion can be framed as a 2-D regression task where f(pixel coordinates) = pixel brightness. The figures to the right of the diagram show the results on image completion for MNIST and CelebA. The images on the top correspond to the context points provided to the model. For better clarity the unobserved pixels have been coloured blue for the MNIST images and white for CelebA. Each of the rows corresponds to a different sample given the context points. As the number of context points increases the predicted pixels get closer to the underlying ones and the variance across samples decreases.

High-dimensional regression

Overview:

- Classical statistics: $d < \infty, n \to \infty$
- Non-asymptotic: $d < \infty, n < \infty$
- Non-parametric: $d \to \infty, n < \infty$
- Asymptotic: $d \to \infty, n \to \infty$

In the realm of high-dimensional statistics, we usually have $d > n$ or e.g. $d = \mathcal{O}(n^\alpha)$, where d is the number of features and n is the number of data points.

This happens when you have lots of features and the actual data generating features are **sparse**, i.e. d is large but a small d_0 is used or are important for the regression. Therefore the usual linear regression assumption that $\boldsymbol{X}$ **is full rank** will not hold. We can, however, introduce regularisation and use the Least-angle regression (LARS; Efron, Hastie, Johnstone and Tibshirani (2004)) algorithm to fit our model. The Lasso

$$\text{minimise } ||y - X\beta||_2^2, \quad \text{subject to } \sum_{j=1}^{d} |\beta_j| \leq t$$

We now work with a diabetes dataset:

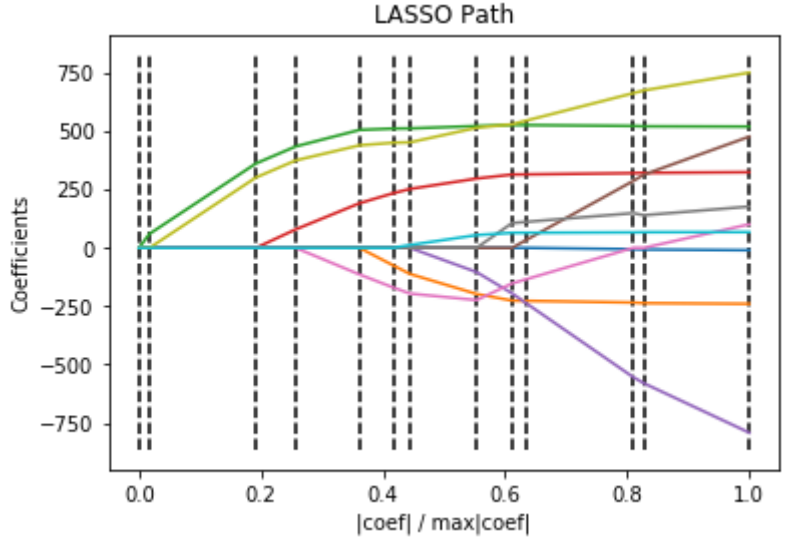
Suppose we have a large number of features. We want to **select** the ones that can represent the sparsity.

In [2]:
```
import numpy as np
import matplotlib.pyplot as plt

from sklearn import linear_model
from sklearn import datasets

X, y = datasets.load_diabetes(return_X_y=True)

print("Computing regularization path using the LARS ...")
_, _, coefs = linear_model.lars_path(X, y, method='lasso', verbose=True)

xx = np.sum(np.abs(coefs.T), axis=1)
xx /= xx[-1]
```

```
Computing regularization path using the LARS ...
.
```

In [11]:

```
plt.plot(xx, coefs.T)
ymin, ymax = plt.ylim()
plt.vlines(xx, ymin, ymax, linestyle='dashed')
plt.xlabel('|coef| / max|coef|')
plt.ylabel('Coefficients')
plt.title('LASSO Path')
plt.axis('tight')
plt.show()
```



Importance Notice!

We are proposal a constitution change so that we can better deliver quality events to you! Please do participate in our upcoming general meeting (even just coming for a vote will be very helpful!).

Some of the changes:

- Introduction of more official committee roles
- Update of the manifesto e.g. societal goals, motto - we were only founded 3 years ago!

More details to come!

Thank you for your attention!

https://github.com/Imperial-College-Data-Science-Society/workshops (https://github.com/Imperial-College-Data-Science-Society/workshops)

1. Introduction to Data Science
2. **Regression and Neural Networks**
3. Classifying Character and Organ Images
4. Demystifying Causality and Causal Inference
5. A Primer to Data Engineering
6. Natural Language Processing (NLP) by using Attention
7. Art and Music using GANs
8. Probabilistic Programming in Practice
9. Missing Data in Supervised Learning