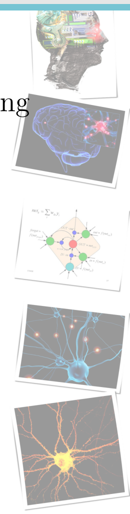

A quick introduction to machine learning
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University of Essex
MiSoC

June 22, 2022

Welcome/course contents

- What will this course cover?
  - Day 1: An intro to machine learning (ML)
  - Day 1: ML labs
  - Day 2: An intro to causal inference
  - Day 2: ML and causal inference labs
- Textbooks?
  - Mitchell, T. M. (1997). Machine learning.[1]
  - Bishop, C. M. (2006). Pattern recognition and machine learning. springer.[2]
  - Wasserman, L. (2013). All of statistics: a concise course in statistical inference. Springer Science & Business Media.[3]

[1] http://www.cs.cmu.edu/~tom/mlbook.html
[2] https://www.microsoft.com/en-us/research/publication/pattern-recognition-machine-learning/
[3] http://www.stat.cmu.edu/~larry/all-of-statistics/index.html

Better science through data

Hey, Tony, Stewart Tansley, and Kristin M. Tolle. "Jim Gray on eScience: a transformed scientific method." (2009).[4]

- Thousand years ago: empirical branch
  - You observed stuff and you wrote down about it
- Last few hundred years: theoretical branch
  - Equations of gravity, equations of electromagnetism
- Last few decades: computational branch
  - Modelling at the micro level, observing at the macro level
- Today: data exploration
  - Let machines create models using vast amounts of data

[4] http://languagelog.ldc.upenn.edu/myl/JimGrayOnE-Science.pdf

Better business through data

- There was a report by Mckinsey

Manyika, J., Chui, M., Brown, B., Bughin, J., Dobbs, R., Roxburgh, C., & Hung Byers, A. (2011). Big data: The next frontier for innovation, competition, and productivity. McKinsey Global Institute.[5]

- Urges everyone to monetise "Big Data"
- Use the data provided within your organisation to gain insights
- Has some numbers as to how much this is worth
- Proposes a number of methods, most of them associated with machine learning and databases

[5] http://www.mckinsey.com/business-functions/digital-mckinsey/our-insights/big-data-the-next-frontier-for-innovation

Why is it popular now?

- **Algorithms + data + tools**
- Breiman, L. (2001). Statistical modeling: The two cultures (with comments and a rejoinder by the author). Statistical science, 16(3), 199-231.[6]
- Anderson, P. W. (1972). More is different. Science, 177(4047), 393-396.[7]
- Pedregosa, et.al. (2011). Scikit-learn: Machine learning in Python. the Journal of machine Learning research, 12, 2825-2830.[8]

[6] http://projecteuclid.org/download/pdf_1/euclid.ss/1009213726%20
[7] https://www.tkm.kit.edu/downloads/TKM1_2011_more_is_different_PWA.pdf
[8] https://www.jmlr.org/papers/volume12/pedregosa11a/pedregosa11a.pdf

So this course covers tools

- ML theory
  - *Supervised learning Regression Classification*
  - Understanding basic modelling
  - Confirming your model is sane
  - Tuning your model
  - **All within a very applied setting**
- Tools
  - Numpy
  - Scikit-learn

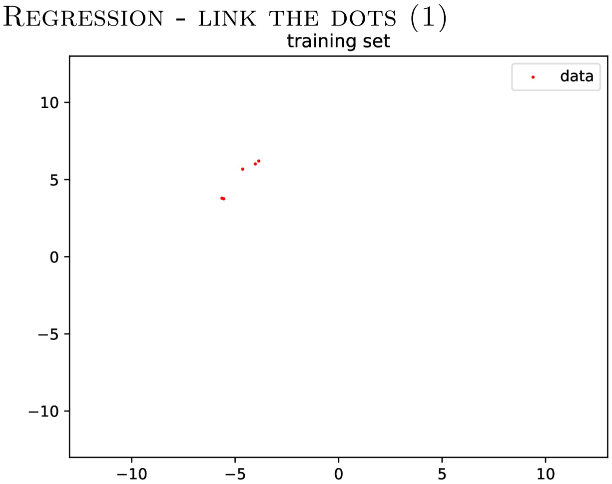
What is supervised learning?

- Imagine someone gives you a group of smokers
  - And asks the question – what is their life expectancy?
- **Completely made up imaginary data**

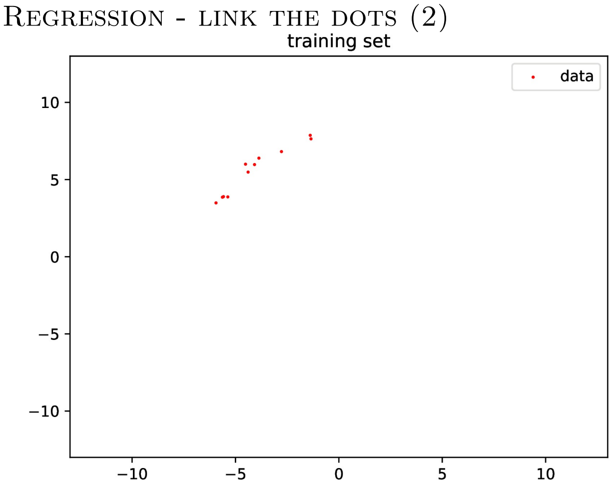
Some abstraction

- We are given inputs $x_0, x_1 ... x_n$ and we are looking to predict y
- Let's plot!

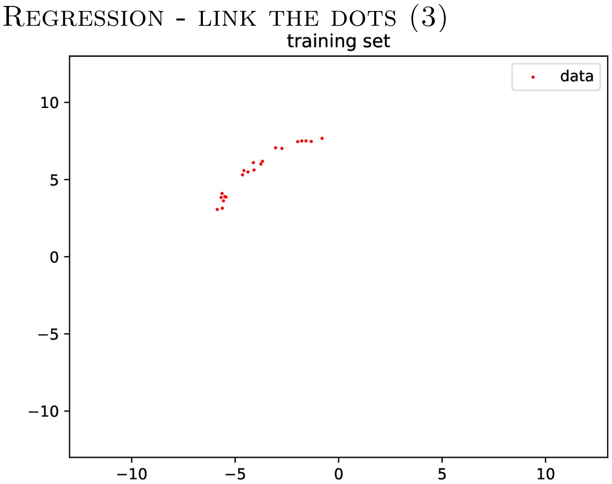
Regression - link the dots (1)



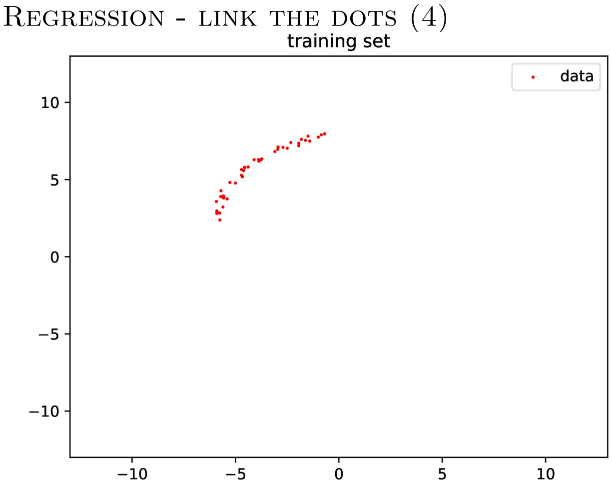
Regression - link the dots (2)



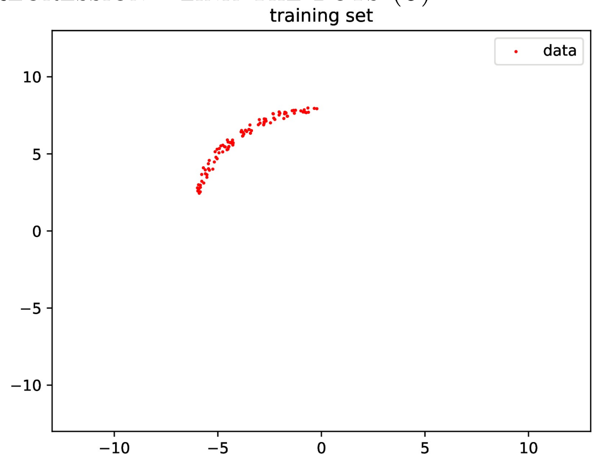
Regression - link the dots (3)



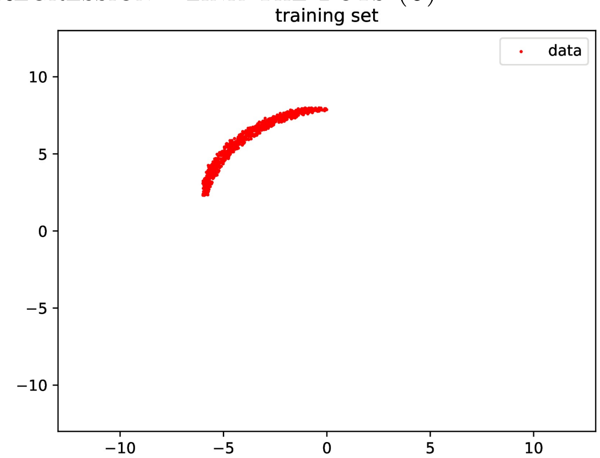
Regression - link the dots (4)



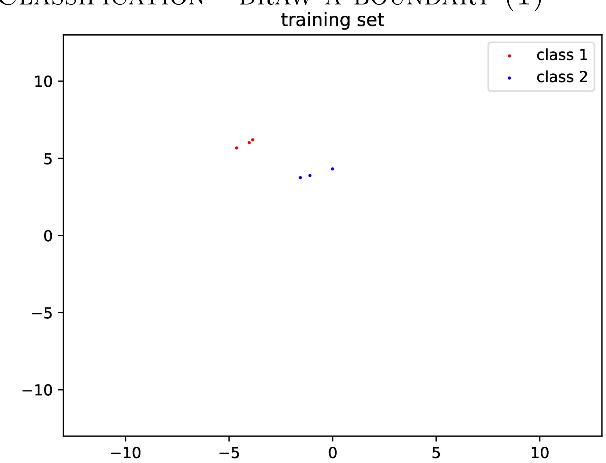
Regression - link the dots (5)



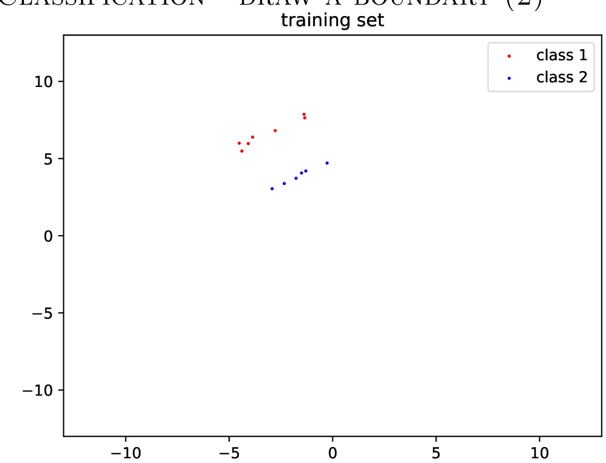
Regression - link the dots (6)



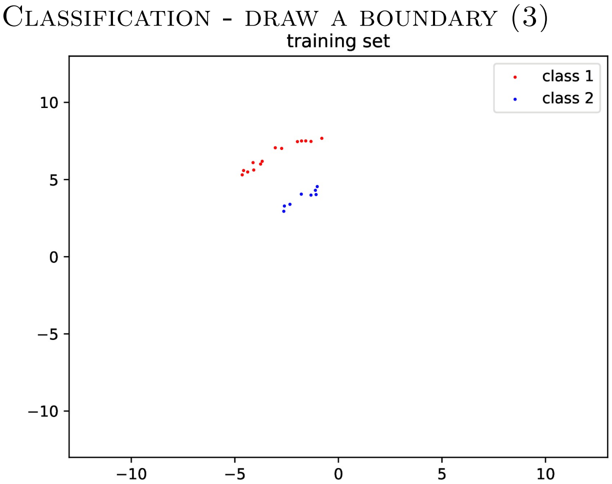
Classification - draw a boundary (1)



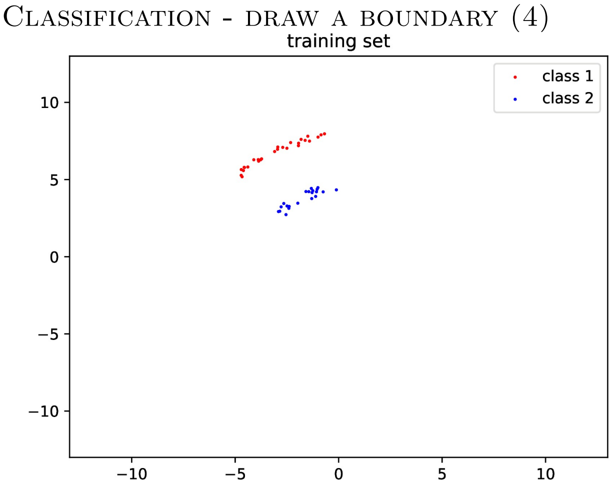
Classification - draw a boundary (2)



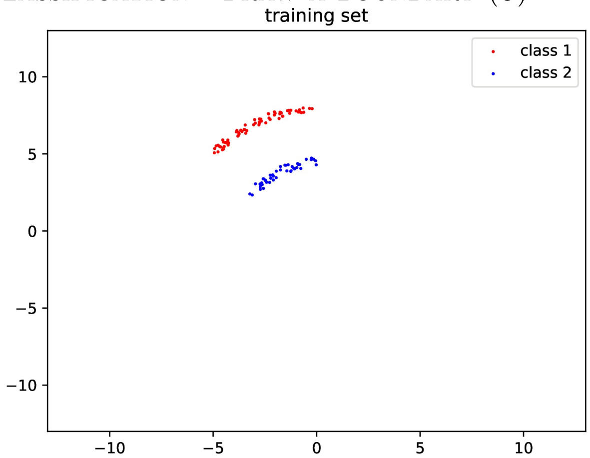
Classification - draw a boundary (3)



Classification - draw a boundary (4)



Classification - draw a boundary (5)



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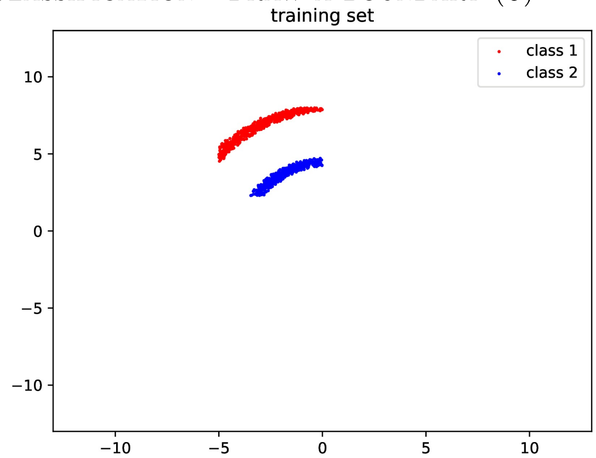
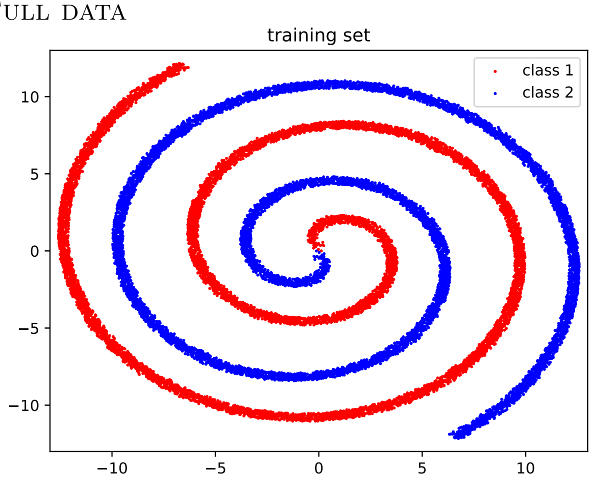


Full data



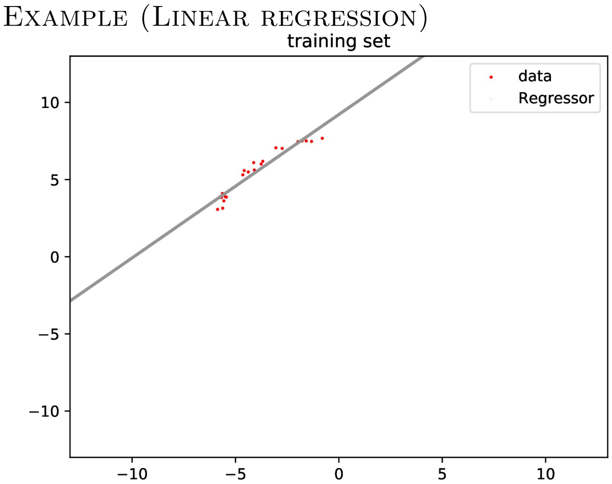
Intuition

- That's it - we are given data, and we need to come up with an algorithm to join it up – but in high dimensions
  - Can can be binary, categorical, real-valued
- How well well a function joins the data is called the "loss"
- Very low loss is not good, it might not generalise that well to unseen data points – you can learn to memorise data instances

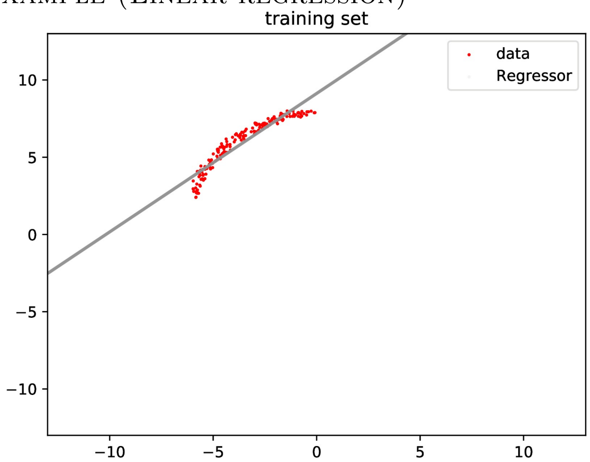
Linear regression

- Linear and logistic regression
  - Logistic regression does classification
- You just assume everything is a line

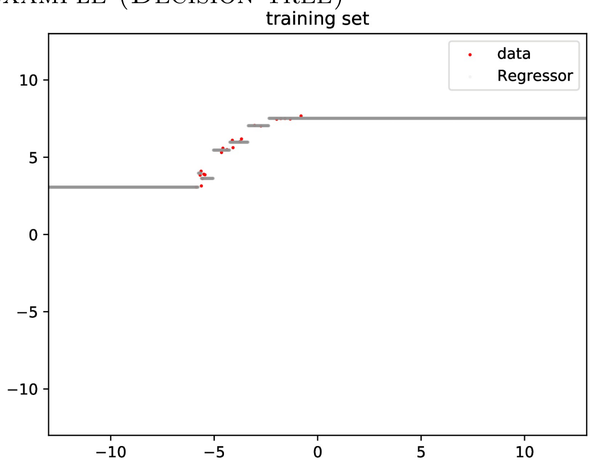
Example (Linear regression)



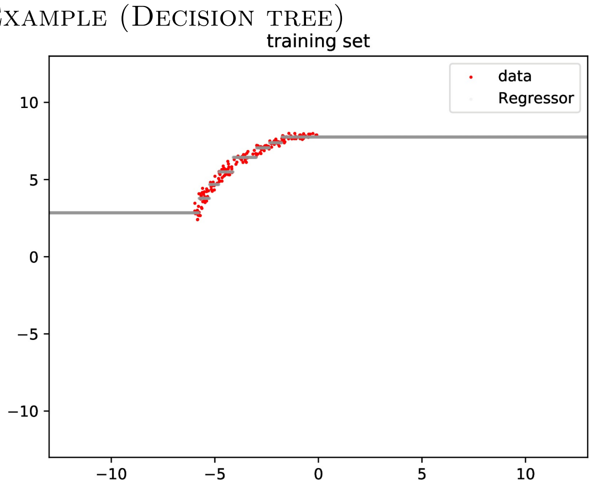
Example (Linear regression)



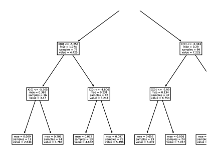
Example (Decision tree)



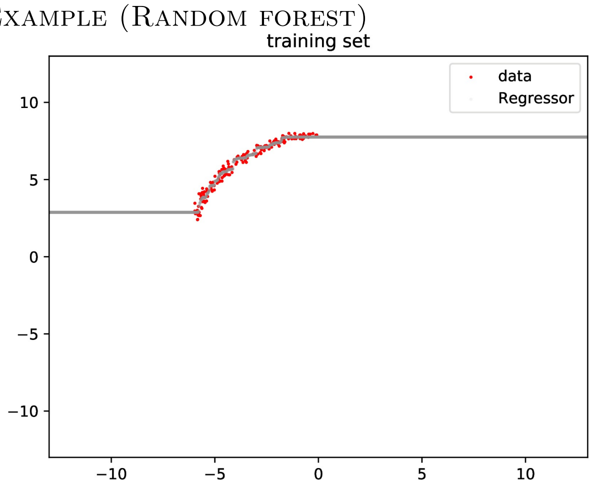
Example (Decision tree)



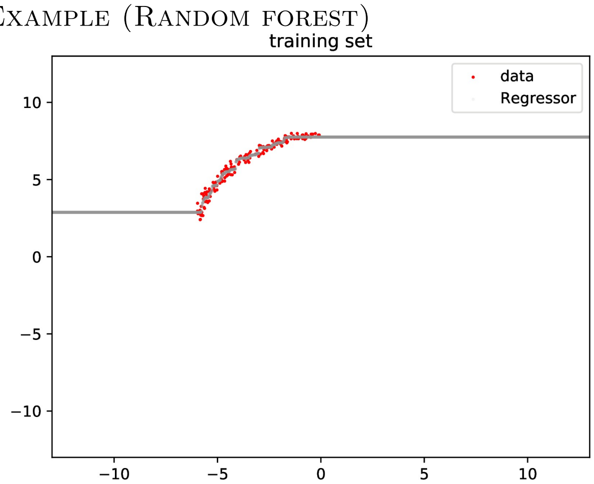
Example (Decision tree — internal)



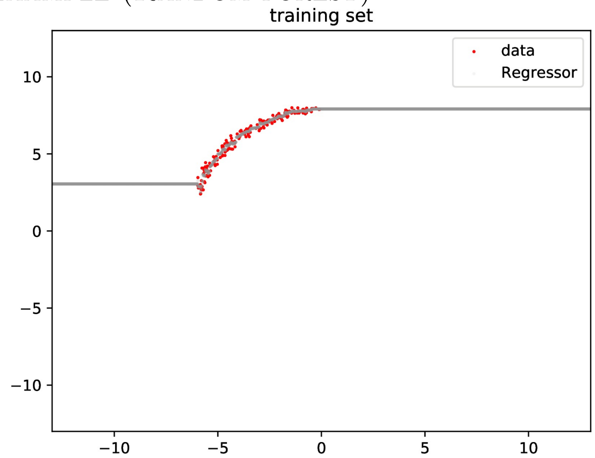
Example (Random forest)



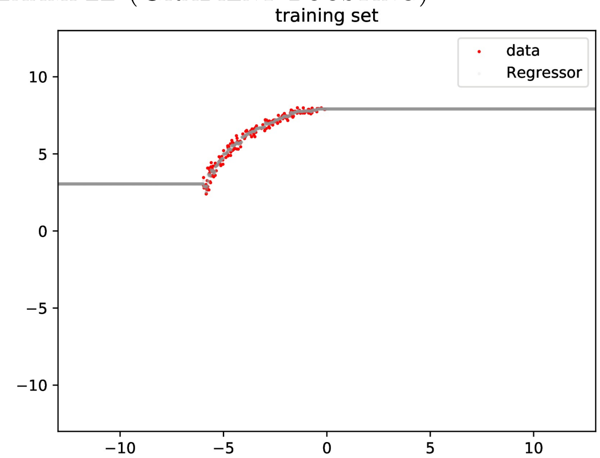
Example (Random forest)



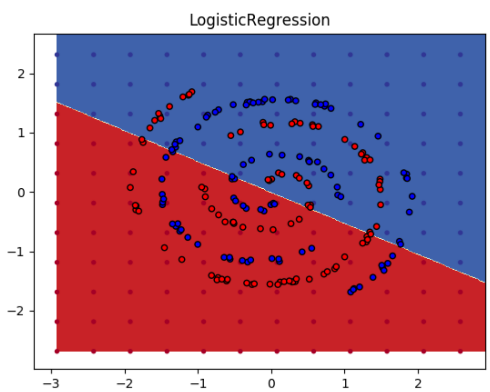
Example (Random forest)



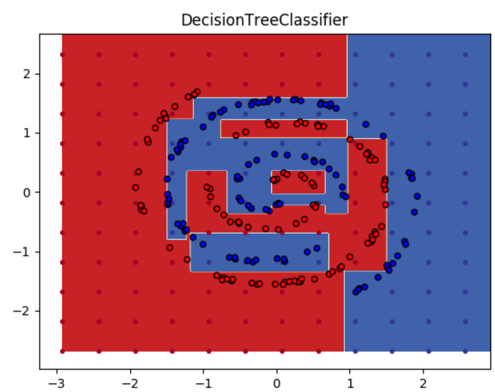
Example (Gradient boosting)



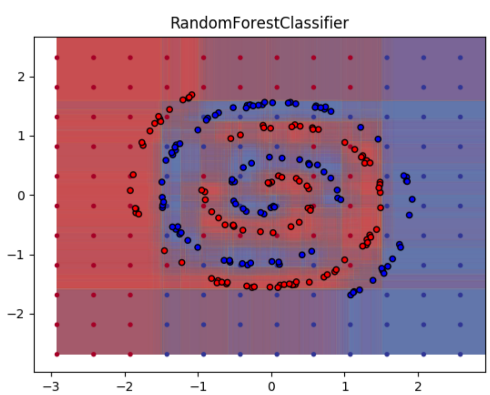
Classification (Logistic regression)



Classification (Decision trees)



Classification (Random forests)



Data dimensionality

- Until now we have seen input data of 1 (for regression) or two (for classification) dimensions
- How about higher dimensional data?
  - Some times data can have millions of features
- Let's examine more high dimensional dataset
- Visualisation becomes harder

Diabetes data

Efron, B., Hastie, T., Johnstone, I., & Tibshirani, R. (2004). Least angle regression. Annals of statistics, 32(2), 407-499.[9]

Feature	Description
X_0	age in years
X_1	sex
X_2	bmi body mass index
X_3	bp average blood pressure
X_4	s1 tc, total serum cholesterol
X_5	s2 ldl, low-density lipoproteins
X_6	s3 hdl, high-density lipoproteins
X_7	s4 tch, total cholesterol / HDL
X_8	s5 ltg, possibly log of serum triglycerides level
X_9	s6 glu, blood sugar level
y	disease progression one year after baseline

[9] https://scikit-learn.org/stable/datasets/toy_dataset.html#diabetes-dataset

Quality assessment

- In lower dimensions, the visualisations we did provided some insights to the quality of our methods
  - This is impossible in higher dimensions
- We need to measure some kind of metric that denotes quality of fit

Metrics

- For regression,
  - Mean Squared Error
  - Mean Absolute Error
- For classification
  - Accuracy
  - Mean Squared Error
  - Cross-entropy loss
  - AUC
- Each one has different benefits, e.g. absolute errors tend to be more robust to outliers

Accuracy

- Each row is now assigned to a class of $y_i \in 0..20$
- Accuracy is the obvious one
  - $accuracy = \frac{1}{N}\sum_{i=0}^{N-1} y_i = \hat{f}(x)$
  - The higher the accuracy the better
- What if the dataset is unbalanced - how informative is accuracy then?
- There are multiple metric functions
  - Use the one appropriate for your problem

Mean Squared Error (MSE)

- Reality is $f(x)$
- Our model is $\hat{f}(x)$ (e.g. a decision tree)
- Sample from the model are $\{y_0 ... y_N\}$
  - $MSE = \frac{1}{N}\sum_{i=1}^{N}\left(y_i - \hat{f}(x_i)\right)^2$
- For every possible sample
  - $E\left[\left(y - \hat{f}(x)\right)^2\right]$

Train/validation/test split

- Basic idea: split your data into three portions
- 1. train, you used that to train your classifier/regressor
- 2. validation, you use that to assess the quality of your method, retraining as you see fit
- 3. test, you report results on this
- Common split is 60%/20%/20%

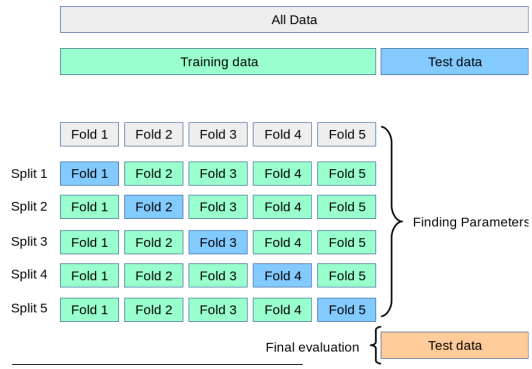
Cross validation

- How about we split our data into multiple validation sets and find the mean?
- Colliqualyy goes by names like 5-fold CV, 10-fold CV
-

Introduction | Classic algorithms for joining those dots | Higher dimensions | Testin' | Tuning

Pictorial depiction of 5-fold CV

Copied from SKlearns website[10]



[10] https://scikit-learn.org/stable/_images/grid_search_cross_validation.png

Introduction | Classic algorithms for joining those dots | Higher dimensions | Testin' | Tuning

Hyperparameters

- How many trees?
- Tree depth?
- l2 regularisation?