Machine Learning 1.03: Random Forests

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This lecture

- Last lecture:
  - Decision trees
    Input = real
    Output = categorical (integer)

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This lecture

- Last lecture:
  - Decision trees
    Input = real
    Output = categorical (integer)
- This lecture:
  - Decision trees
    Input = real, categorical, directional
    Output = real, categorical, directional
  - Multiple outputs
  - Missing data
  - Bagging
  - **Random forests**
- Goal: One good algorithm for most supervised problems!

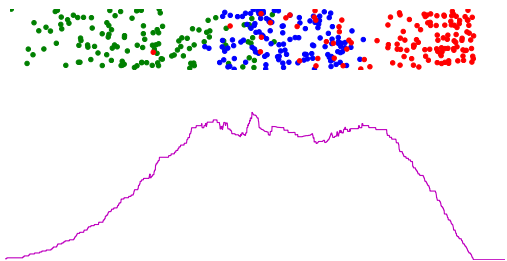
Inputs

Real input

(from last time)

- Find the greatest info gain (or Gini impurity) across all axes

  (1 axis shown, vertical offset for visualisation only)



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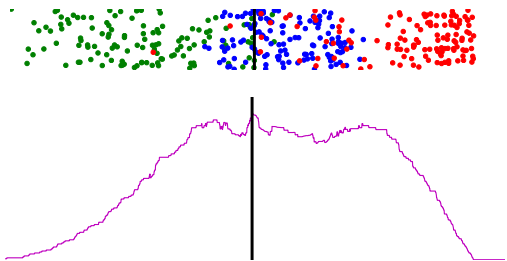

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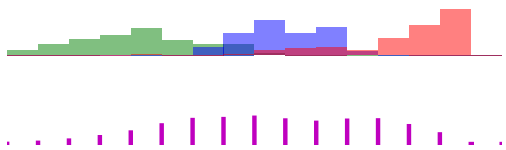
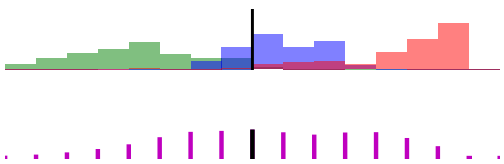
Quantised real input

- Continuous data may be collected **quantised**,
- e.g. When asking "What is your age?"
  ask which of 12–17, 18–24 etc. it falls into rather than a specific value



Quantised real input

- Continuous data may be collected **quantised**,
- e.g. When asking "What is your age?"
  ask which of 12–17, 18–24 etc. it falls into rather than a specific value
- Still split – just have to do it between bins
  (Information gain shown as spikes as only defined at bin transitions)



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Categorical input

- Similar to quantised (histogram of classes)...
  ...but unordered
- e.g. "What is your favourite cheese?"
- Spliting no longer makes sense!

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  - Try every assignment of class to the left/right side and choose best
    (with one class always going left to account for symmetry)
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Categorical input

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- Two choices:
  - Try every assignment of class to the left/right side and choose best
    (with one class always going left to account for symmetry)
  - One class goes down left branch, rest go right

- No difference for 2 or 3 classes!
- One left, rest right is preferred if more:
  - Fixed storage requirement/simpler code
  - Number of combinations grows linearly
    ($\mathcal{O}(n)$, not $\mathcal{O}(2^{n-1})$ where n is the numbers of classes)

Directional input

- Direction = Real number(s) that wrap around (modular arithmetic)
- Examples:
  - Angles
  - Time of day, day of week, month of year...
  - Octaves (music)

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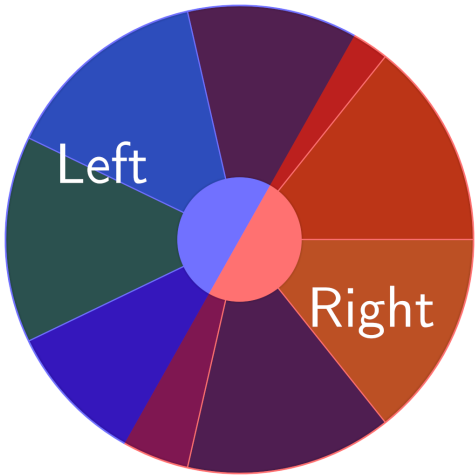
Directional input

- Direction = Real number(s) that wrap around (modular arithmetic)
- Examples:
  - Angles
  - Time of day, day of week, month of year...
  - Octaves (music)

- Single split makes no sense...
  ...chop in half instead!

- Use unit length vectors instead of angles,
  $\theta \to [\cos(\theta), \sin(\theta)]^T$
  Dot product feature with "left angle" and send left if positive



Outputs

Regression

- Classification:
  - Split to minimise Gini impurity or maximise information gain
  - Leaf gives answer as most common class to reach it

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Regression

- Classification:
  - Split to minimise Gini impurity or maximise information gain
  - Leaf gives answer as most common class to reach it
- Regression:
  - Split to minimise variance or maximise information gain
  - Leaf gives answer as mean value to reach it
    (median/medoid only rarely confers an advantage)
- Otherwise identical!

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Variance reduction

- Variance of output measures how consistent a node is...
  ...so choose splits that minimise it

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- Variance of left node:

$$\sigma_l^2 = \mathbb{E}\left[(f(x) - \mathbb{E}\left[f(x)\right])^2\right]$$

similarly for right, σ_r^2 (expectations estimated using data that reaches node)

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- Minimise weighted combination:

$$L(\texttt{split}) = \frac{n_l}{n}\sigma_l^2 + \frac{n_r}{n}\sigma_r^2$$

n = total exemplar count
n_l = exemplars traveling down left branch
n_r = exemplars traveling down right branch

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Information gain

- Not used very often – variance reduction both good and faster
- Including to show generalisation

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Information gain

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- Fit Gaussian to output variable, entropy is

$$\frac{1}{2}\log\left(2\pi e\sigma^2\right)$$

- Hence information gain of a split:

$$I(\texttt{split}) = \frac{1}{2}\log\left(2\pi e\sigma_p^2\right) - \frac{n_l}{2n}\log\left(2\pi e\sigma_l^2\right) - \frac{n_r}{2n}\log\left(2\pi e\sigma_r^2\right)$$

(reusing variables from previous slide, $+p$ subscript for parent)

Directional output

- Regression with different rules
- Example of unusual data type[1]

- Represent angles with unit length vectors, $\{\hat{x}_1, \hat{x}_2, \ldots, \hat{x}_n\}$, $\hat{x}_i = [\cos\theta_i, \sin\theta_i]^T$
- "Mean" angle $= \frac{\sum \hat{x}}{|\sum \hat{x}|}$
  (use for leaf nodes)

- Residual, $r = \frac{|\sum \hat{x}|}{n}$
- Variance $= 1 - r$
  (use to select splits with variance reduction)

[1] This is assuming the data is distributed with the von-Mises distribution

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Multiple outputs I

- Predicting multiple outputs from a single tree
- Information gain $\rightarrow$ bits are added (assuming independent)
- e.g. 3D positions can use the entropy of a multivariate Gaussian
- Everything else requires some kind of hack!

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Multiple outputs I

- Predicting multiple outputs from a single tree
- Information gain $\rightarrow$ bits are added (assuming independent)
- e.g. 3D positions can use the entropy of a multivariate Gaussian
- Everything else requires some kind of hack!
- Could train n models instead. How to decide?
  (one per output)
  - Outputs uncorrelated: Separate models
  - $\vdots$
  - Outputs correlated: One model
- This means you never actually add bits!

Missing data

- Some exemplars have incomplete feature vectors
- Usually fill in, e.g. with mean, mode, another ML model

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Missing data

- Some exemplars have incomplete feature vectors
- Usually fill in, e.g. with mean, mode, another ML model

- Decision tree:
  - Fill in (meh)
  - Go down both branches! (missing data rare)
  - Randomly go down one branch (missing data common)

Random Forests

Ensemble learning I

- Random forest = decision trees + ensemble learning

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Ensemble learning I

- Random forest = decision trees + ensemble learning
- Ensemble learning = combining multiple estimators
  - Different models (e.g. linear regression, decision tree, SVM, neural network)

    or
  - Same model, randomised training so each is different

  (using estimator to distinguish from model)

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  - Different models (e.g. linear regression, decision tree, SVM, neural network)
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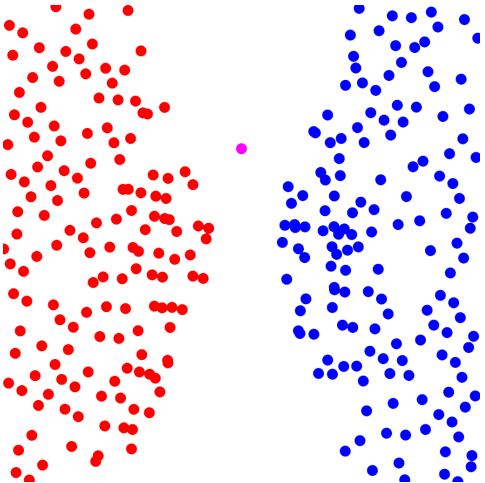
  (using estimator to distinguish from model)
- Random forest:
  - Many decision trees (hence name)
  - Randomised training using **bagging**,
    a specific ensemble learning technique

Ensemble learning II

- Which class (red or blue) should the magneta dot be?



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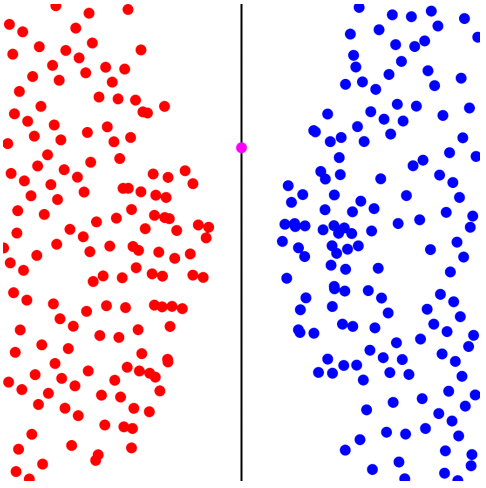

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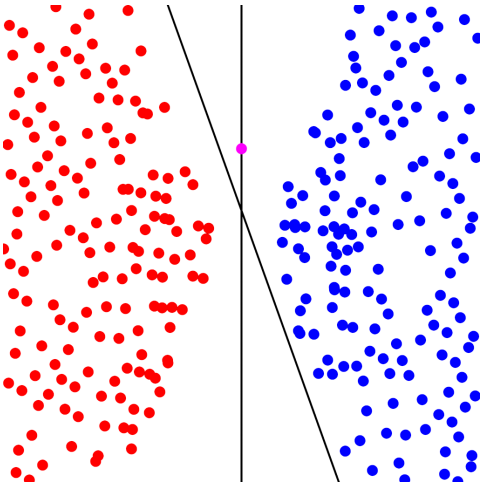

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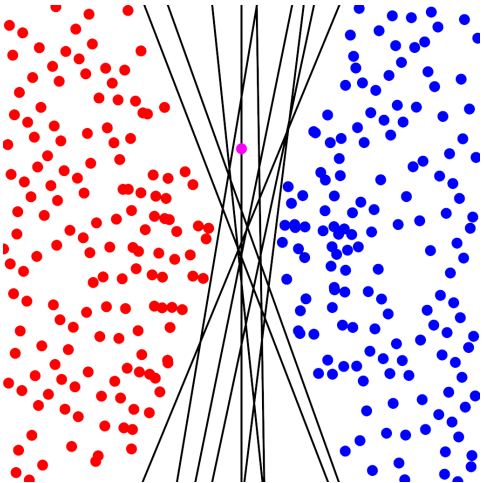

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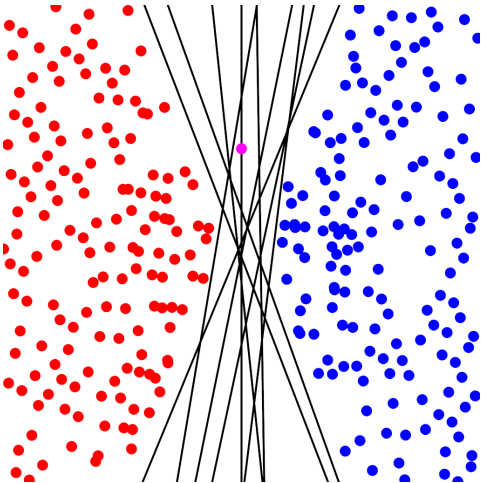
  - Insufficient data
  - Noisy data
  - **Model not complex enough**
    (curved boundaries can also separate this data!)



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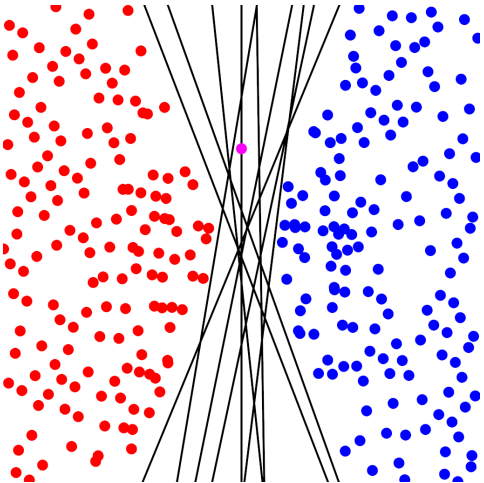
- An ensemble generates many estimators...
  ...and hence captures the ambiguity

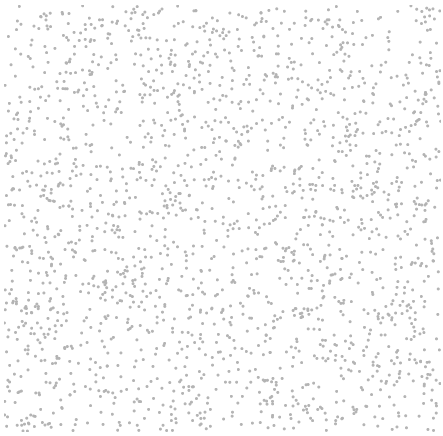


Ensemble learning III

- Ensembles need **diversity**, which is not well defined!
- Estimators should make different mistakes, i.e. if they all make the same mistake the ensemble will repeat it
- Increasing estimator diversity at the expense of their individual performance often makes the ensemble better! (up to a limit)

An aside: Accuracy of an estimate

- Estimate a statistic of a population
  e.g. mean love of cheese within UK



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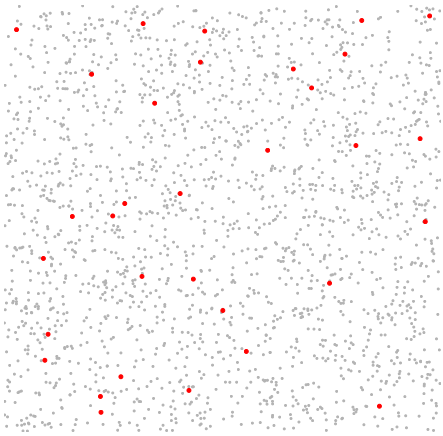

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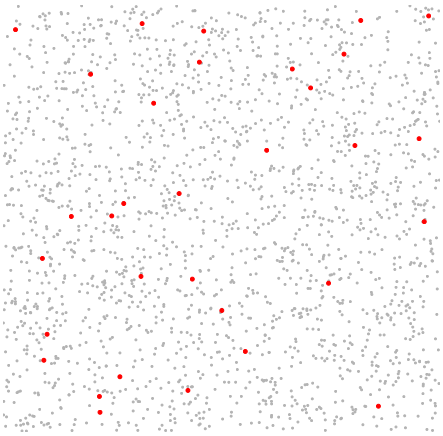

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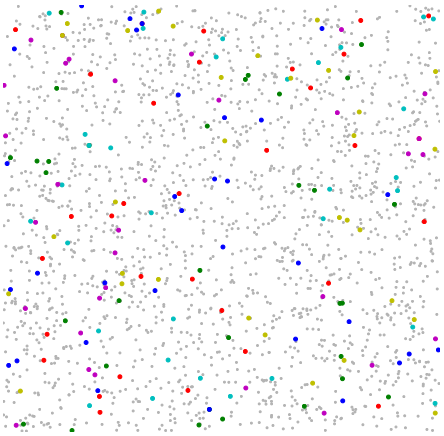
- How accurate is this estimate?
- Estimate as standard deviation of many repetitions of the experiment...
  - $\mu = \{0.868, 0.870, 0.885, 0.904, 0.891, 0.893\}$
  - $\mu^* = 0.885$, $\sigma^* = 0.013$

  (Numbers simulated/made up; true $\mu = 0.883$)



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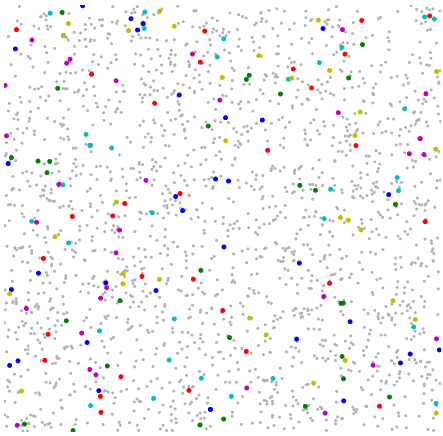
- Hardly practical!
  (asked 192 people – prefer to add to original experiment)



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Bootstrapping

- Instead of collecting more data...
  ...fake it from available data

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Bootstrapping

- Instead of collecting more data...
  ...fake it from available data
- Given data set of size n:
  Create new data set by drawing, with replacement, n times
  (will be repetitions)
- Can calculate statistic on each new data set, and estimate accuracy as variance
  (or any other measure, e.g. a confidence interval)

Bagging

- An ensemble technique!
- Short for "Bootstrap AGGregatING"
- Bagging = Bootstrapping applied to estimator output
  (via optimised parameters)

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- Algorithm:
  1. Select S, size of ensemble
  2. Create S bootstrap draws of original data set
  3. Train estimator on each
  4. Combine outputs of all estimators for each query

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Random subspace method

- Another ensemble technique!
- Bootstrap applied to features
  i.e. fit each estimator with a random subset of features
- For decision tree: New bootstrap for each split.
- Remove the duplicates (makes no difference, saves computation)

Random forests

- Random forest = decision trees + bagging + random subspace method
- Algorithm:
  1. Select S, number of trees (more is better, up to a limit).
  2. Create S bootstrap draws of original data set.
  3. Train decision tree on each, with random subspace method
  4. Combine outputs of all trees for each query.

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Combine output?

- Classification:
  - The decision trees vote – ensemble outputs winner.
- Regression:
  - Take the mean/median of all of the estimates.

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Combine output?

- Classification:
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- Regression:
  - Take the mean/median of all of the estimates.
- Can generate probabilities!
  - Classification: Create histogram
  - Regression: Fit Gaussian distribution

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A tweak

- Random subspace method selects around 63% of features
- Can typically get away with much, much less (faster and performs better!)

- Instead: Select $\left\lceil \sqrt{f} \right\rceil$, where f is the number of features
- Above good default; can optimise as hyperparameter

Examples

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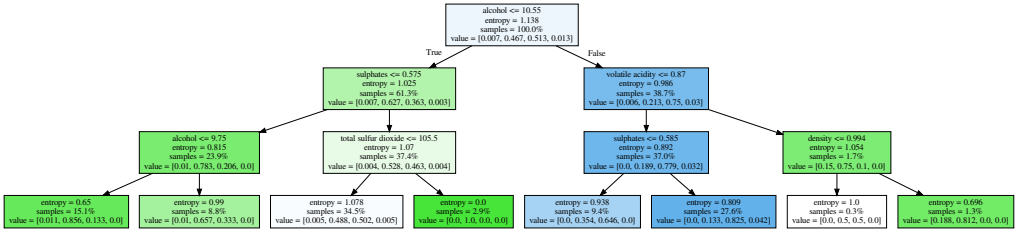
Red wine I

- 1599 exemplars, split: 1199 train, 400 test.
- Input: 11 measurable features:
  - fixed acidity
  - volatile acidity
  - citric acid
  - residual sugar
  - chlorides
  - free sulfur dioxide
  - total sulfur dioxide
  - density
  - pH
  - sulphates
  - alcohol
- Output: 1–10 human rating

  (reduced to 1–5 here, to fit on screen)
- Can be used for classification or regression!

Red wine II

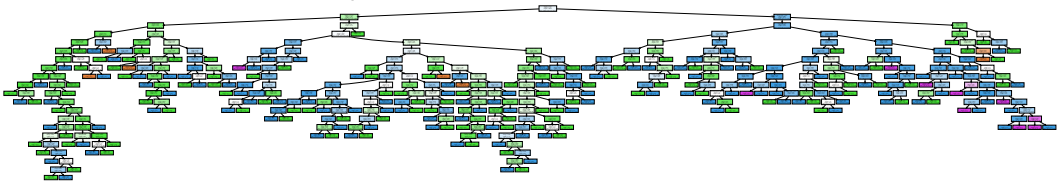
Classification tree, max depth 3:



Accuracy = 69% Explainable?

Red wine III

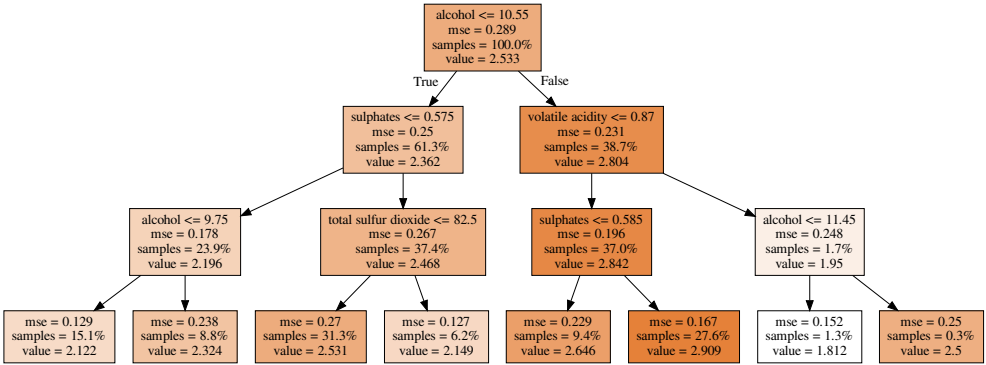
Classification tree, unlimited depth:



Accuracy = 71% Explainable?

Red wine IV

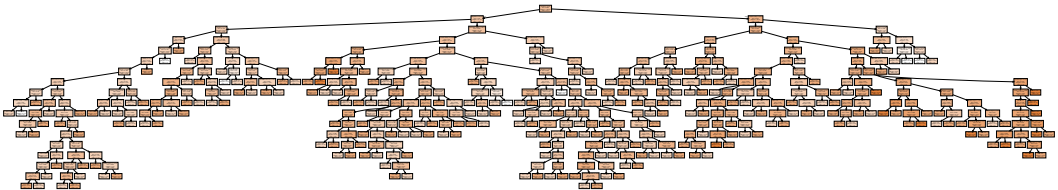
Regression tree, max depth 3:



Mean error = 0.36

Red wine V

Regression tree, unlimited depth:



Mean error = 0.33

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Red wine VI

- Random forests with 32 trees
- Classification: Accuracy = 79% (better than 71%)
- Regression: Mean error = 0.30 (better than 0.33)
- Basically impossible to visualise/understand!

Kinect I

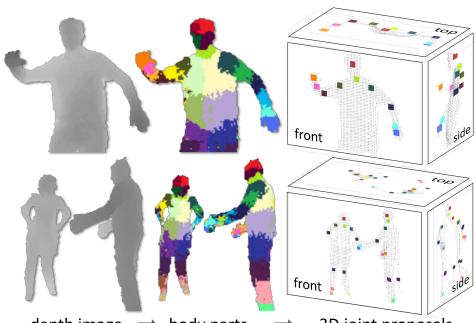
- A depth sensor for gaming
- Tracks you as you move

- Uses random forests!
  (original version at least)

Kinect II

- Steps:
  1. Depth using structured light (infrared)
  2. Label body parts
  3. Fit skeleton

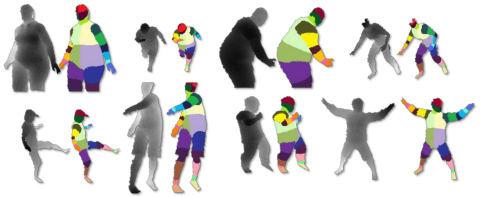
- Body part labelling:
  Classification forest run on every input pixel



Kinect III

- Early example of **simulating** training data
  (now used extensively with deep learning)
- Collected:
  - 15 full body scans, labelled with body parts
  - 100K body poses from motion capture
- Used to generate one million random Kinect inputs. . .
  . . . with ground truth labels
  (also randomised Kinect placement)
  (took 24 hours using 1000 node cluster)
- Used real data for testing (8808 images)

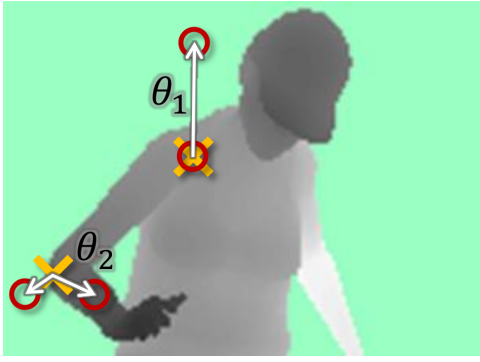
Synthetic data for training:



Real data for testing:

Kinect III

- Random forest:
  - 3 trees
  - 20 deep
  - 300K images per tree, each providing 2000 pixels
  - Images unique for each tree – not bagging
  - Considered 2000 features per split, each with 50 split points



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  - 3 trees
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  - 300K images per tree, each providing 2000 pixels
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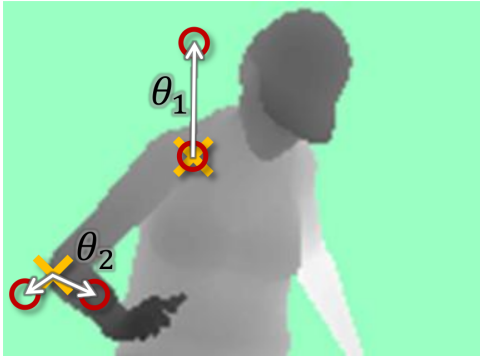
- Features:
  - Depth differences between pixels
  - Two randomly generated offsets to make comparison between
  - This is done on the fly – implicit feature vector length is millions!



Summary

- "Upgraded" decision trees to
  - Handle typical inputs
  - Handle typical outputs
  - Random forests! (still one of the best)
  - Output probabilities
- Notes:
  - One of the fastest algortihms
  - Many variants, e.g. gradient boosting
- Next lecture:
  Making sure a ML system is working!

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Further reading

- The Kinect paper:
  "Real-Time Human Pose Recognition in Parts from Single Depth Images"
  by **Shotton, Fitzgibbon, Cook, Sharp and Finocchio**
  `https://www.microsoft.com/en-us/research/wp-content/uploads/2016/02/BodyPartRecognition.pdf`

- For more kinds of random forest:
  "Decision Forests for Classification, Regression, Density Estimation, Manifold Learning and Semi-Supervised Learning" by **Criminisi, Shotton and Konukoglu**
  `http://research.microsoft.com/apps/pubs/default.aspx?id=155552`

- For more on ensemble methods:
  "Diversity creation methods: a survey and categorisation"
  by **Brown, Wyatt, Harris and Yao**
  `http://citeseerx.ist.psu.edu/viewdoc/download?doi=10.1.1.421.349&rep=rep1&type=pdf`

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Kinect image from Wikipedia, in public domain, `https://en.wikipedia.org/wiki/Kinect#/media/File:Xbox-360-Kinect-Standalone.png`

Kinect algorithm images from "Real-Time Human Pose Recognition in Parts from Single Depth Images"; see previous slide, fair use.

Wine data set from `https://archive.ics.uci.edu/ml/datasets/wine+quality`