# Weak teachers: Assisted specification of discrete choice models using ensemble learning



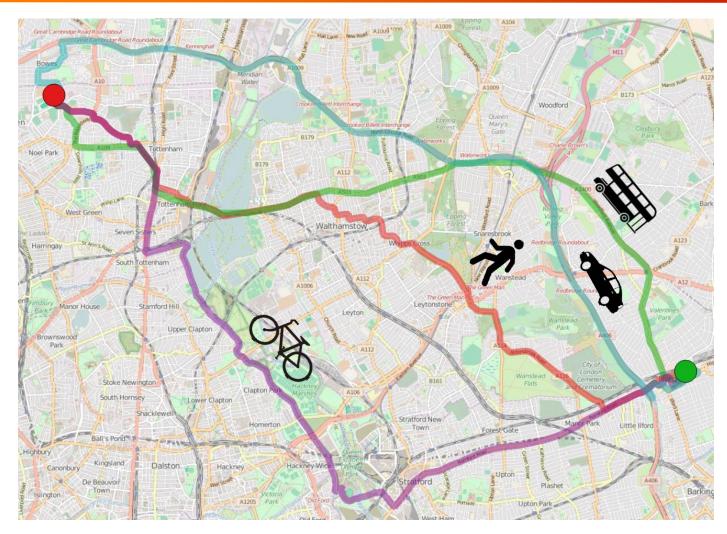
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## Mode choice







## Two approaches

- 1. Discrete Choice Models (DCMs)
  - Aim to describe behaviour of population
    - Emphasis on model structure
    - Less focus on model validation
- 2. Machine Learning (ML) classifiers
  - Aim to predict unknown class for a feature vector
    - Emphasis on model validation
    - Less focus on model structure





#### **DCMs**

- Highly interpretable
- Can check for consistency with behavioural theory
- Need to manually specify utility functions





## ML

- No need for manual specification
- Can automatically model non-linear interactions

- Model can not be easily interpreted
- Better predictive ability than DCMs?





#### Motivation

How to assist with specification of DCM utility functions...

...in order to reduce complexity of manual search...

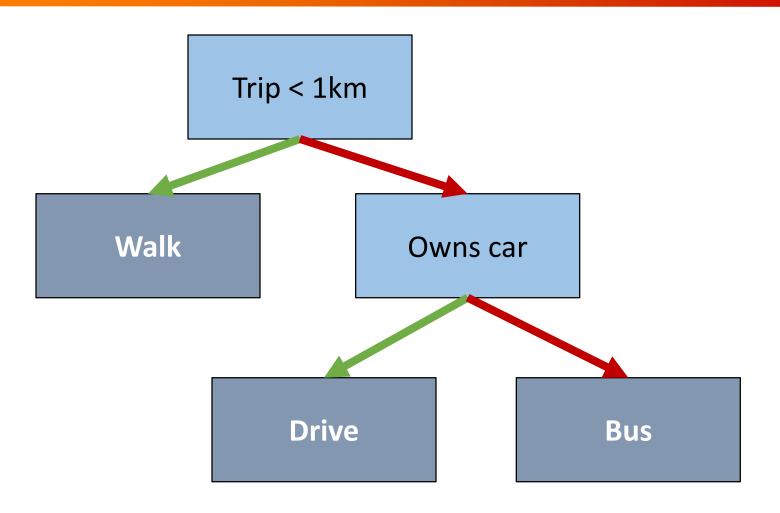
...and improve performance of resulting classifiers?

(Use ensembles of Decision trees as weak teachers!)





## Decision trees (DTs)







#### DTs

Recursive hierarchical structure of binary splits

- To calculate split at a node:
  - For each feature:
    - Sort the data at a node over each feature
    - Calculate the gain in entropy for every possible split point
  - Identify split with the highest gain (across all features)
  - Repeat for new sub-nodes
- Sub-nodes model interaction of input features





#### DTs

 Splits are not sensitive to scaling/any monotonic transformations of features

Information gain is known for each split





## Ensemble learning

- Individual DTs have very high variance
  - Perform poorly in non-trivial cases
- Can be used as weak learners in ensembles of multiple DTs – exploiting wisdom of crowds
- By averaging effects of binary splits over DTs, complex non-linear relationships can be modelled
- Loss of interpretability compared to individual DT





## **Gradient boosting**

Fit a DT to all available data

 Subtract the predictions of the DT (multiplied by learning rate) from the data

Repeat until stopping criteria is met





## Extreme gradient boosting

 Each DT in ensemble is a regression tree predicting continuous value

- Passed through *softmax* (logistic) function to generate class probabilities
  - Each tree directly predicts choice probabilities





#### DTs as weak teachers

 Feature importances – sum gain over all splits for each features

• Feature interactions — sum gain for each hierarchical combination of n features

 Non-linear interactions of input features investigate distribution of split values over all splits for each feature





## Assisted specification approach

- 1. Optimise the hyper-parameters of GBDT model on (training) dataset
- 2. Train optimised GBDT model on the same dataset
- Investigate structure of GDBT model, using it to inform utility specifications for DCM
- 4. Estimate assisted specification DCM
- 5. Simplify DCM by combining parameters where necessary





## Methodology

- 3 years of London mode choice data
  - 2012/13-2013/14 train
  - 2014/15 test

100 iterations of bootstrapping to estimate model performance





#### **Models**

- Two baseline DCMs:
  - Dummy MNL (MS-MNL)
  - ML Logistic Regression (LR)
- Four ML algorithms:
  - Gradient Boosting Decision Trees (GBDT)
  - Artificial Neural Network (ANN)
  - Random Forest (RF)
  - Extremely randomised Trees (ET)





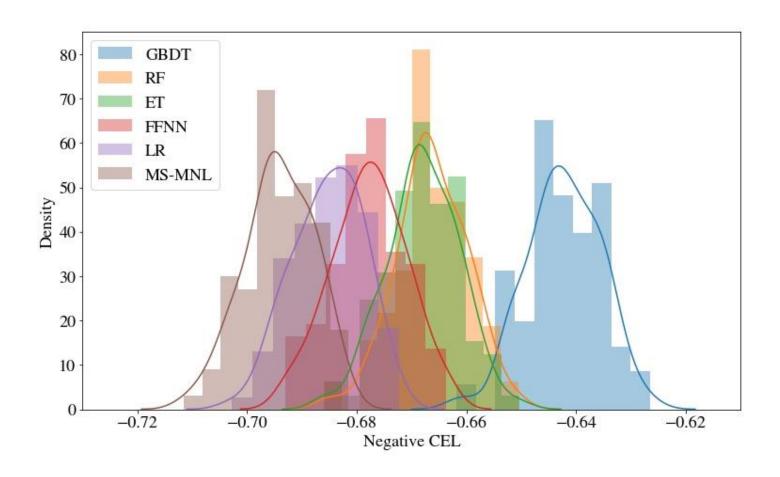
## Dummy MNL

- Estimate MNL model with all features
  - Attributes included for appropriate mode (e.g. driving duration in driving utility only)
  - No feature interactions
  - All socio-economic variables included as dummy-variables
  - A-priori bins used for age (child <18, adult 18-64, pensioner 65+) and departure time (AM peak, inter-peak, PM peak, overnight)
- Combine parameters where necessary, so that all parameters are significant
- Check parameter signs are consistent with expected values





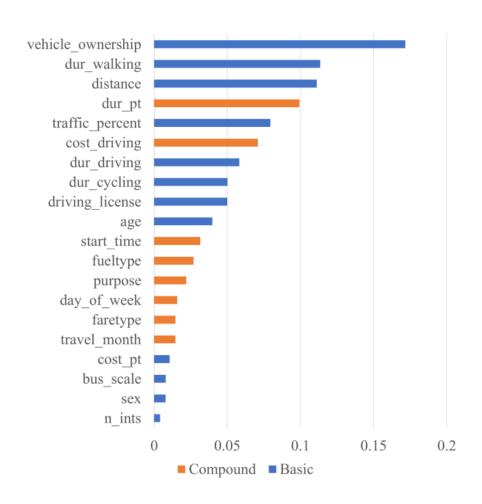
## Results – benchmark models







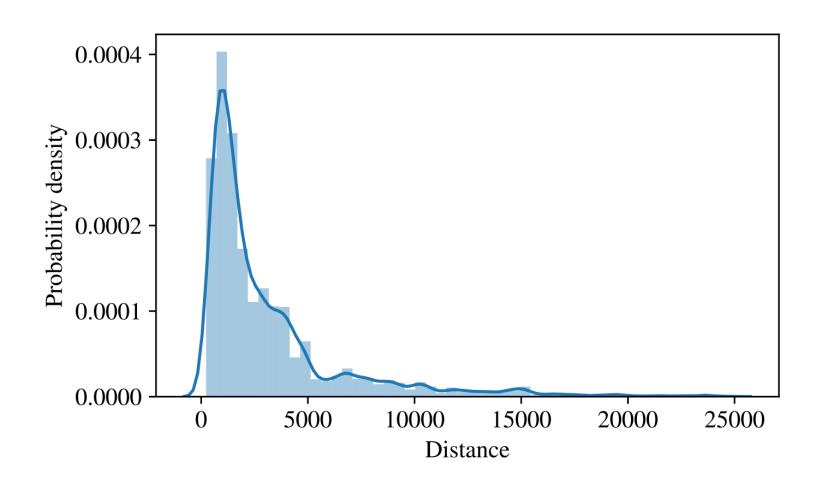
## Feature importances







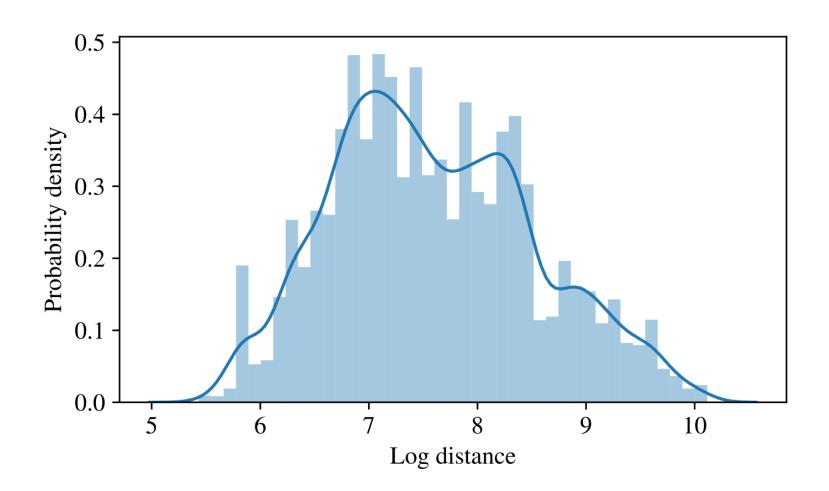
## Distance split distribution







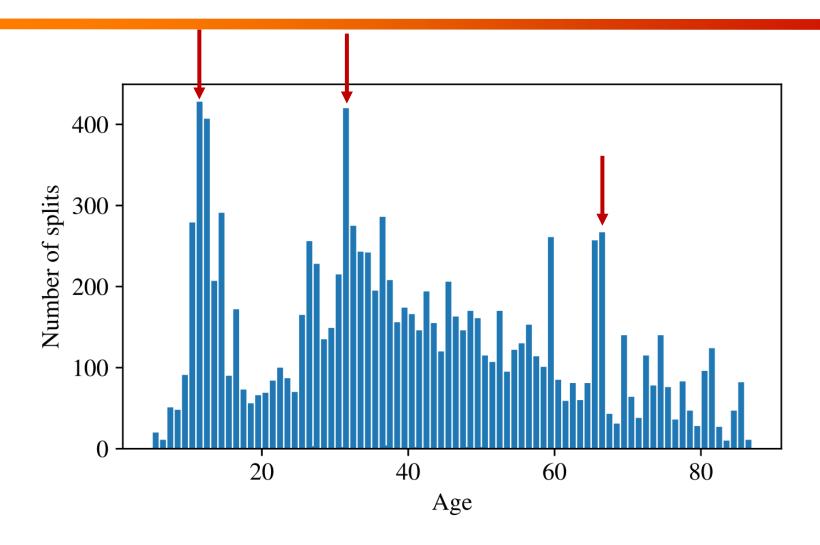
# Log-distance







# Age split distribution







#### Feature interactions

- Of 10 most important second order feature interactions, 6 include car ownership
- Most import second order is car-ownership with driving license ownership
- Most important third order feature interaction with 2 socio-economic variables contains both carownership and driving license ownership
- Car ownership and driving license therefore fully interacted with variables in model (6 parameters for each variable before simplification)





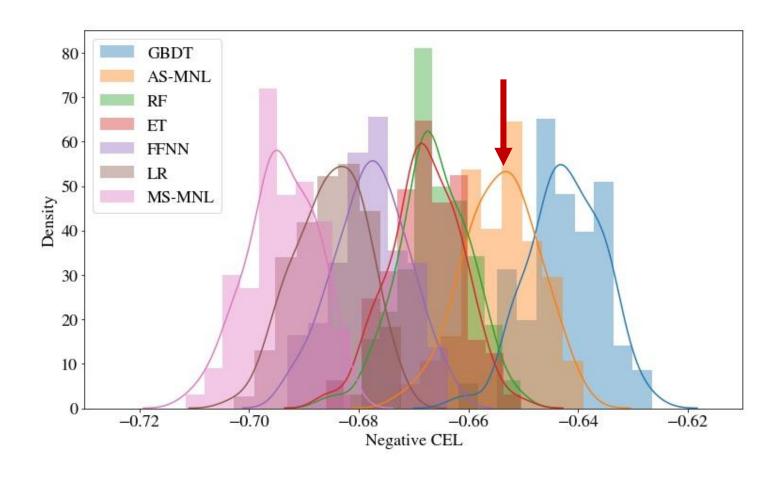
### Final AS-MNL model

- 100 parameters
  - All significant
  - All but fuel-cost parameter for no-car ownership driving license holders have expected signs





### **AS-MNL** results







#### Conclusions

 Gap between ML and DCM for this problem is smaller than suggested by previous research

 AS-MNL achieves better performance than all but best ML model (GBDT)

 AS-MNL maintains interpretable linear utility specification with significant parameters





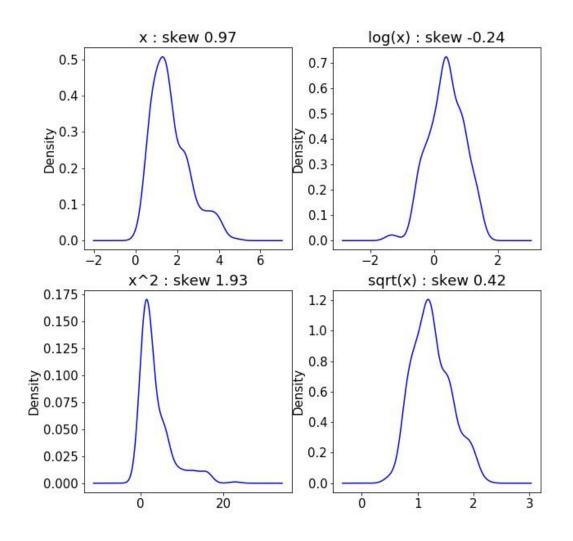
#### Further work

- Formalise framework into assisted specification report
  - User specifies alternative-specific and socio-economic variables
  - User specifies complexity/number of parameters in the model
  - Report generated suggesting which non-linear transformations/feature interactions/splines etc to include in the model
  - User can investigate suggestions using traditional model specification, retaining control over process





## Parking cost for car ownership







## Thank you

Hillel, Tim, Mohammed Z E B Elshafie, and Ying Jin (2018). "Recreating Passenger Mode Choice-Sets for Transport Simulation: A Case Study of London, UK". In: *Proceedings of the Institution of Civil Engineers - Smart Infrastructure and Construction* 171.1, pp. 29–42.

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