“Science … resolves the whole into parts, the organism into organs, the obscure into the known. … Science gives us knowledge, but only philosophy can give us wisdom … [to] synthesize knowledge to resolve the obscure into the known.”

After the Philosopher Durant.

Graham Williams, Australian Taxation Office

Last Updated 7 October 2014
Ensembles for the Data Scientist

We present an overview of the use of ensembles in Data Mining, particularly in the context of so-called “Big Data”. Starting from the beginning we review how we stumbled on the concept of multiple models, found it useful, and developed it into boosted decision stumps, random forests, and ensembles of nuggets.

Introducing the Concepts of

• Ensembles

• Big Data

• Ensembles for Big Data in R in the ATO
Original brush with ensembles came during PhD research at the ANU in 1987. Implemented a decision tree builder and used it to predict the likelihood of a parcel of land in Australia being suitable for grazing cattle. It used a rather small dataset, allowing calculations to be confirmed by hand – and demonstrating “random” choices for selecting variables.

Setting the Scene – 1987 – Do Ensembles Make Sense?

The ensemble concept was presented at the first Australian AI Conference in Sydney in November 1987, with Ross Quinlan as the session chair. As recounted in a chapter in Journeys to Data Mining, the idea of not going with the best single model, but combining multiple models was challenged – it is now the approach of choice for many data scientists.

- Concept presented at the first Australian AI Conference in 1987
- Multiple Inductive Learning
- “Why would you build more than one model?” - J. R. Quinlan.

Another chapter as recommended reading on the history of Data Mining is Gregory Piatetski-Shapiro's The Journey of Knowledge Discovery.

Ensembles combine the results from multiple models into a single decision. Over the years ensembles have been demonstrated to produce “better” models than a single model. We might ask the question “Which of several models is actually the best model?” The answer often depends on context. Compare it to a panel of experts.

Why not build all of the very similarly good decision trees, and combine them into a single ensemble model?

- Adaptive Boosting
- Bootstrap Aggregation
- Random Forests
- Bucket of Models

By combining multiple models, we can improve accuracy, reduce bias and variance, and provide an overall robust model when applied to new data.
Another development from the 1990's is the concept of evolutionary hot spots discovery, working with Professors Zhexue Huang and Xin Yao, applied to health care data. Cluster a large population of M entities into N (<<M) clusters. Describe each cluster by a decision tree, convert to rules, and each rule is then a hot spot measured for interestingness – evolve.

Cluster → Decision Tree → Interestingness

Evolutionary Optimisation

Identify Doctor Shoppers and Over-Prescribers
A new ensemble approach has been developed to analyse big data using ensembles and hot spots analysis – nugget discovery. This experimental approach is being developed through a project which aims to identify compliance issues with Activity Statement refunds.

Annual ATO budget is $3 billion to collect $300 billion revenue for Government

2 million businesses

20 million lodgments

2 million refunds totalling $20 billion

Poor targeting leads to significantly “higher touch” than required.

Yes

No

GST Collected each year is approximately $50 billion

$m billion protected

$n billion refunds

$m << n

Analytics

All figures are unofficial approximate/estimates – see, e.g.,

Global Models versus Local Models

Traditional approaches fail for big data as they often attempt to build one model over the whole population. The approach here is to automatically identify previously unknown behavioural groups, and micro model within the groups. An ensemble of local models predict the risk (+ve/-ve) of an entity, which is then aggregated for an overall risk.

• Local populations with markedly different behaviours and properties to those of the global population are key to developing models in the big data world.

• Our approach here is to develop a massive ensemble of local models that can be aggregated to better reason over the global population.

Acknowledgement ATO Data Scientists: Dr Frank Lu, Dr Lifang Gu, Dr Nandita Sharma, Nicole Wade
The overall algorithm combines **weighted subspace cluster analysis** to identify behaviourally coherent groups, **decision tree induction** to build business interpretable rules, and **evolutionary algorithms** to identify the best risk scorers. An agile approach is used to deliver regular expert feedback into the modelling process.

Training dataset: 2013, 2 million refunds, 1,000 features
We might “discover” in a data-driven algorithm 20,000 nuggets covering the 2 million credit Business Activity Statement lodgements over one year. We now need to measure how “interesting” each nugget is. A simple approach is to define a collection of attributes for each nugget, and combine them to measure the nugget.

**Population Attributes**
- Percentage of GST
- Percentage of BAS
- ...

**Demographics Attributes**
- Percentage Gov
- Percentage Large
- ...

**Training Attributes**
- Percentage known fraud
- Percentage known productive cases
- Percentage known revenue protected
- ...

**Z-score**
Standardise the range of different characteristics.

**Shift**
Shift the values by the addition on the value on nugget of whole population.

**Scale**
To normalise the values to 0 to 1 or -1 to 1

**Weighting**
To make the effective nuggets contribute more and reduce the influence of noisy nuggets
Risk Scorers – The Genetic Code for Evolutionary Process

Each possible risk scorer is a formula in the language of the measures, transforms, and weights, over the nuggets. There is an infinite number of possible risk scorers for any population of nuggets – and we need to identify good risk scorers across this infinite search space. Heuristic search is required, and evolutionary optimisation is a candidate.

\[ r(b) = \sum_{i=1}^{n_c} a_i \times \sum_{j \in ng[b]} w_{ij} \times v_{ij} \]

- \( a_i \) = weight for attribute \( i \)
- \( n_c \) = number of characteristics
- \( ng[b] \) = nuggets that match BAS b
- \( w_{ij} \) = weight for attribute \( i \) in nugget \( j \)
- \( v_{ij} \) = transformed value of \( a_i \) in \( ng_j \)

We need to discover the attribute weights, nugget weights and aggregation function.
Risk Scorers – Evolutionary Optimisation

Evolutionary optimisation is a biologically inspired computational algorithm developed by artificial intelligence researchers. Given a population of genetic material, randomly mutate and cross pollinate the genes, under the guidance of a measure of fitness – Our measure here is based also on feedback of a team of professional auditors.

Define an individual – the representation of a risk scorer

Initialise a population of individuals

Evaluate fitness

Apply variation operators to population

Select individuals for new population

Evaluate fitness of new individuals

Terminate evolution?

Optimised Risk Scorer

- needs diversity
- tries to maintain diversity
- tends to choose fitter individuals
- human experts evaluate, feedback is used to improve optimiser
- compute in parallel for efficiency
- compute in parallel for efficiency

no

yes
The ATO introduced the use of open source tools for data mining over 10 years with the set up of Corporate Analytics. We recognise that we need toolkits with a variety and different tools, changing regularly, open and closed source. As Gartner noted, it is no surprise that the latest technology for data science is coming through the open source route.

- Network of Ubuntu servers: 32 parallel threads, 750GB RAM
- Running open source from the ground up – GNU/Linux OS
- Powerful suite of well established open source Unix tools
  - C, awk, sed, wc, diff, meld, tr, cvs, latex, perl, python, R
  - Concept of many specialised tools working together through a standard interface referred to as “pipes”.
  - Pipes now a powerful new concept in R.

- Scaling out rather than scaling up – add new computers to the grid, not necessarily larger computers – R, Spark, Python, ...
… and then there were 7 billion models

The November edition of the IEEE Computational Intelligence Magazine contains an article where I discuss turning ensemble concepts into the extreme, reflecting on the need for the pendulum to swing back toward protecting privacy, and the resulting focus on massively ensembled models, each “model” modelling an individual.

Big Data Opportunities and Challenges – Extreme Data Distribution: Privacy and Ownership.
Open Source R as Credible Software

We continue to be discouraged by the fear, uncertainty and doubt that is offered by many vendors who have a natural concern about loss of business. Instead we need a variety of tools that will make up the most effective toolkits for Data Scientists including the state-of-the-art that only open source can deliver, as identified by Gartner 2014.

Dept Immigration: Data Scientists deliver sophisticated risk models to protect Australia's borders. Gavin McCairns says “the department bought $15 million worth of software---but it's gathering dust.”

SAS responded: “… R in a production system, it can be scary …”

Every Australian Tax Return lodged today is risk scored by at least one model developed using open source software (often an R-based model).
Key Messages – Ensembles

The state-of-the-art Analytic Model developed here introduces a new approach to big data analytics. The technology takes us beyond traditional algorithms and prepares us for delivering new capabilities to support the ATO move to providing better interactions with Tax Payers. New ideas undergoing research and refinement to discover the unknowns.

Why have only one model when you can have a population of 20,000 models?

Data Scientists synthesise data into information, information into knowledge, and knowledge into wisdom, to resolve the obscure into the known.

An ensemble of many models (20,000 or even many more?) delivers the expertise on local understanding to global applicability.
Now's a great time to grab some snacks and drinks and meet some of our data science colleagues – networking...
I'll also be presenting a broader talk on data science and ensembles at IAPA on Thursday 16th October – next week.
Join us for the next Canberra R User Group and Data Science meeting, first Tuesday in November.

Keep an eye on http://innovationspace.net.au