Granger-causal Attentive Mixtures of Experts: Learning Important Features with Neural Networks

Author(s):
Schwab, Patrick; Miladinovic, Djordje; Karlen, Walter

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Granger-causal Attentive Mixtures of Experts

Patrick Schwab \(^1\)  Walter Karlen \(^1\)

Abstract

Several methods have recently been proposed to detect salient input features for outputs of neural networks. Those methods offer a qualitative glimpse at feature importance, but they fall short of providing quantifiable attributions that can be compared across decisions and measures of the expected quality of their explanations. To address these shortcomings, we present an attentive mixture of experts (AME) that couples attentive gating with a Granger-causal objective to jointly produce accurate predictions as well as measures of feature importance. We demonstrate the utility of AMEs by determining factors driving demand for medical prescriptions, comparing predictive features for Parkinson’s disease and pinpointing discriminatory genes across cancer types.

1. Introduction

Neural networks are often criticised for being black-box models. Researchers have attempted to address this criticism by developing tools that provide visualisations and qualitative explanations of the inner workings of neural networks (Bachrens et al., 2010; Simonyan et al., 2014; Zeiler & Fergus, 2014; Xu et al., 2015; Shrikumar et al., 2017; Zhang et al., 2017; Montavon et al., 2017; Koh & Liang, 2017). However, comparatively little progress has been made towards providing quantifiable measures of relative feature importance and their expected accuracy.

Quantifiable measures are desirable for the many machine-learning use cases in which both predictive performance and interpretability are of paramount importance (Kindermans et al., 2017; Smilkov et al., 2017; Doshi-Velez & Kim, 2017). Such measures facilitate communicating, adjusting and arguing for the decisions of machine-learning models (Riemer et al., 2016). They enable us to tell when algorithmic decisions might be biased or discriminating (Hardt et al., 2016) and uncover the basis of decisions when there are legal or ethical circumstances that call for explanations (Goodman & Flaxman, 2016). Moreover, information about the source of a decision is especially important when a wrong decision could potentially have severe consequences (Choi et al., 2016), when a model’s decisions are merely hints that suggest more thorough follow-up assessments (Schwab et al., 2017), and when a model discovers patterns that could advance the scientific understanding of the underlying phenomena (Shrikumar et al., 2017).

Estimating the relative contribution of input features towards individual outputs of a deep neural network is hard because the input features undergo multiple hierarchical, interdependent and non-linear transformations as they pass through the network (Montavon et al., 2017). We propose a new approach to importance attribution that optimises jointly for predictive performance and accurate attribution of feature importance in an end-to-end trained neural network. Our approach builds on the intuitive idea of distributing the feature groups of interest among experts in a mixture of experts model that uses attentive gating to assign weights to individual experts. By optimising the attentive gating networks with a Granger-causal objective, we ensure that the weights given to individual experts correlate strongly and measurably with their ability to contribute to the decision at hand. We demonstrate that our approach is able to combine the strength of neural networks as scalable feature extractors with the ability to quantitatively measure feature importance - enabling new use cases for neural networks in knowledge discovery from observational data and allowing measurably accurate attribution in existing ones.
Contributions. We subdivide this work along the following distinct contributions:

(i) We delineate an end-to-end trained attentive mixture of experts (AME) model that uses attentive gates to orchestrate the outputs of multiple heterogeneous expert networks.

(ii) We introduce a Granger-causal objective that ensures that the attention weights assigned by the attentive gates in AMEs correlate with the respective expert’s ability to contribute to an individual decision.

(iii) We demonstrate the utility of AMEs in a variety of settings by determining factors driving demand for medical prescriptions, comparing predictive features for Parkinson’s disease and pinpointing discriminatory genes across multiple types of cancer.

2. Related Work

There are two main categories of approaches towards attribution in neural networks:

Perturbation-based Approaches. In perturbation-based approaches, the sensitivity of individual inputs and neurons in a neural network are explained by modelling the impact of local perturbations (Ribeiro et al., 2016; Adler et al., 2016).

Gradient-based Sensitivity Analysis. Gradient-based approaches are based on the idea of following the gradient from output nodes to the input nodes to obtain the features that the output was most sensitive to (Baehrens et al., 2010; Simonyan et al., 2014). Several improvements to this technique have since been proposed (Zeiler & Fergus, 2014; Selvaraju et al., 2016; Smilkov et al., 2017; Sundararajan et al., 2017).

Both perturbation-based and gradient-based approaches share the same limitations: They neither provide measures of relative feature importance for all input features whose magnitude can be meaningfully compared across decisions, nor an expected accuracy for their explanations - limiting their use to qualitative analyses on singular decisions.

Orthogonal to the above-mentioned categories are approaches that provide attribution by pointing out the influential training data for a given decision (Koh & Liang, 2017). Similarly, AMEs are outside any of the above-mentioned categories, as they optimise jointly for predictive performance and accurate attribution in a single end-to-end trained model for each individual decision.

Mixtures of Experts. Conceptually, AMEs can be compared to hierarchical mixtures of experts (HME) with gating networks (Jacobs et al., 1991; Jordan & Jacobs, 1994). In HMEs, (Jacobs et al., 1991) trained a gating network that, based on the respective input sample, stochastically activates exactly one out of many specialised expert networks. The goal of their approach is to achieve decoupled, competing experts that decompose a given learning problem into subtasks that are ideally easier to solve. More recently, (Shazeer et al., 2017) proposed an end-to-end optimised mixture of experts layer that lowers computational cost in machine translation through conditional computation. The aforementioned mixture models use gating to increase either computational or predictive performance and require that each expert receives input of the same structure, thus making them unsuitable for heterogeneous inputs. Gating itself has been used in neural networks for a long time. For example, gating is used to enable learning long-term dependencies in Long Short-Term Memory layers (Hochreiter & Schmidhuber, 1997) and to facilitate training of deep neural architectures (Srivastava et al., 2015).

Attentive Models. Attentive models have been used in various domains to improve both interpretability (Xu et al., 2015; Schwab et al., 2017; Zhang et al., 2017; Riemer et al., 2016) and performance (Bahdanau et al., 2015; Yang et al., 2016). In computer vision, related works used attention in convolutional neural networks that selectively focus on input data (Ba et al., 2014) and internal convolutional filters (Stollenga et al., 2014). However, fundamentally, naïve soft attention mechanisms do not provide any incentive for a neural network to yield attention factors that correlate with feature importance. Soft attention mechanisms may therefore interact with other components of neural networks in opaque ways (Sundararajan et al., 2017). Furthermore, it is not possible to measure the expected quality of explanations provided by naïve soft attention mechanisms.

We therefore follow a new approach to attribution in deep neural networks that models and optimises explicitly for predictive performance as well as attribution accuracy. This approach has two key advantages over existing ones: It provides (i) a measure of the expected quality of the network’s attributions and has (ii) the ability to compare the relative magnitude of attributions across individual decisions - enabling the quantitative analysis of model errors and biases, and the identification of novel patterns over multiple independent decisions in observational data.

3. Attentive Mixtures of Experts

AMEs consist of \( n \) experts \( E_i \) and their corresponding attentive gating networks \( G_i \) with \( i \in [1, n] \). At prediction time, the attentive gating networks output an attention factor \( a_i \) for each expert to control its respective contribution \( y_i \) to the AMEs final prediction \( y \). All of the experts and the attentive gating network are neural networks with their own parameters and architectures. AMEs do not impose any restrictions on the expert networks other than that they need to expose their topmost feature representation \( h_i \) and
their local prediction \( y_i \) for a given input subset \( x_i \). As input to the gating networks, the hidden states \( h_i \) and local predictions \( y_i \) of each expert are concatenated to form the combined hidden state \( h_c \) of the whole AME. An important property to note is that AMEs do not require that every expert makes its predictions based on the same subset of the input data \( x \). Each expert may therefore operate on its own distinct subset \( x_i \) of the input data. In our experiments, we make use of this property to be able to quantify the impact of different feature groups \( x_i \) of the input data on the AME’s decisions. Figure 1 shows a conceptual overview of an AME’s components and their interactions.

We denote \( E_i(x_i) \) as the output \( y_i \) of the \( i \)th expert for the given subset of the input data \( x_i \). \( G_i(h_c) \) represents the output \( a_i \) of the \( i \)th attentive gating network \( G_i \) with respect to the combined hidden state \( h_c \) of the AME. The output \( y \) of an AME is then given by:

\[
y = \sum_{i=1}^{n} G_i(h_c)E_i(x_i)
\]  

(1)

AMEs use the attentive gating networks to control the contributions of the expert outputs \( E_i(x_i) \) (Figure 2). The output \( G_i(h_c) \) of the attentive gating network is the attention factor \( a_i \) for the \( i \)th expert. The attention factors dynamically modulate the contribution of each expert to the final prediction based on the current combined hidden state \( h_c \) of the AME. We calculate the attention factors \( a_i \) using:

\[
a_i = \frac{\exp(u_i^T u_{E_i})}{\sum_{j=1}^{n} \exp(u_j^T u_{E_j})}
\]  

(2)

where

\[
u_i = \text{activation}(W_i h_c + b_i)
\]  

(3)

corresponds to a single-hidden-layer multi-layer perceptron (MLP) with an activation function, a weight matrix \( W_i \) and bias \( b_i \) that yields \( u_i \) as a hidden representation of \( h_c \) (Yang et al., 2016). In equation (2), we calculate the attention factors \( a_i \) for each expert by computing a softmax over the dot-product similarity of \( u_i \) to the \( i \)th expert’s context vector \( u_{E_i} \). \( u_{E_i} \) corresponds to a hidden representation of the most informative combined hidden state \( h_c \) for expert \( E_i \) (Yang et al., 2016). We jointly optimise \( W_i, b_i \) and \( u_{E_i} \) with the other parameters during training. By comparing the current hidden representation \( u_i \) of \( h_i \) to the most informative hidden representation \( u_{E_i} \) for the \( i \)th expert, the attentive gating network learns to activate experts for those hidden states \( h_e \) in which they can most contribute to the final prediction \( y \) of the AME. Due to the use of an individual attention mechanism for each expert, the soft attention mechanism described by equations (3) and (2) differs significantly to that used in related works. Related works typically train a shared most informative state over a common hidden representation, i.e. (Yang et al., 2016), rather than an individual most informative state for each branch.

Conceptually, the formulation of equation (1) is reminiscent to that of gradient boosting (Friedman, 2002), where new estimators are iteratively added to reduce the residual error of the previous estimators, and to that of generalised additive models (Hastie & Tibshirani, 1990). Aside from lending themselves to end-to-end optimisation, we note that key characteristics of AMEs are the rich introspective ability, given both to the gating network as well as to human observers through the attention mechanism, and the ability of the attentive gating network to dynamically activate experts depending on the combined hidden state of the whole AME rather than just their inputs.

4. A Granger-causal Objective for Attentive Mixtures of Experts

In line with reports of related works that rely on gating networks (Bengio et al., 2015; Shazeer et al., 2017), we find that early on during training with mini-batch stochastic gradient descent our proposed attentive gating mechanism commonly collapses to either consistently assign an attention weight \( a_i = 1 \) to a single expert and 0 to all others, or to assign the same amount of attention \( a_i = \frac{1}{n} \) to all experts. Once the AME is stuck one of these local minima, it is unlikely to recover. The fundamental problem is that a naively-trained AME has no incentive to learn feature representations that yield accurate attributions. To combat this undesired tendency towards attributions that do not correspond to the experts’ respective ability to contribute, we introduce a secondary Granger-causal objective function \( \mathcal{L}_{\text{Granger}} \). Granger-causality follows the Humean definition of causality that declares a causal relationship \( X \rightarrow Y \) between random variables \( X \) and \( Y \) if we are better able to predict \( Y \) using all available information than if the information apart from \( X \) had been
used (Granger, 1969). In spite of its name, in empirical settings, Granger-causality is more akin to correlation than causation and we therefore strongly caution the reader to not mistake Granger-causality for the standard definition of causality (Pearl et al., 2009). Nonetheless, the theory of Granger-causality allows us to naturally define a simple and efficient loss function that ensures that the relative magnitudes of attention factors $a_i$ correlate with their respective expert’s ability to contribute to the AME’s final output $y$. Given a set of heterogenous input data $X$, we denote $\varepsilon_{X,i}$ as the AME’s prediction error without including any information from the $i$th expert and $\varepsilon_X$ as the AME’s prediction error when considering all available information (Figure 3). We then define the degree $\Delta \varepsilon_i$ to which the $i$th expert is able to contribute to the final output $y$ as the decrease in error associated with adding that expert’s information to the set of available information sources:

$$\Delta \varepsilon_{X,i} = \varepsilon_{X\setminus\{i\}} - \varepsilon_X$$  \hspace{1cm} (4)$$

We note that using $\Delta \varepsilon_{X,i}$ to define the degree of attribution intuitively resolves even cases where combinations of features enable improvements in the AME’s prediction error - both experts would be attributed equally for the decrease. Using $\Delta \varepsilon_i$, we define the desired attribution $\omega_i$ corresponding to the $i$th experts’ attention weights $a_i$, for a given input $X$ as:

$$\omega_i(X) = \frac{\Delta \varepsilon_{X,i}}{\sum_{j=1}^{n} \Delta \varepsilon_{X,j}}$$  \hspace{1cm} (5)$$

Where equation (5) normalises the attributions across all experts to ensure that they are on the same scale within and across decisions. We then arrive at the Granger-causal objective function $L_{\text{Granger}}$ by computing the mean Kullback-Leibler divergence KL over $n$ samples between the target distribution $\Omega$, with $\Omega(i) = \omega_i$, and the actual distribution $A$, with $A(i) = a_i$, of attention values:

$$L_{\text{Granger}} = \frac{1}{n} \sum_X \text{KL}(\Omega, A)$$  \hspace{1cm} (6)$$

Because the Granger-causal loss measures the probabilistic distance of the actual attributions to the desired Granger-causal attributions, it is valid to use it as a proxy for the expected quality of explanations. A Granger-causal loss of 0 indicates a perfect match with the Granger-causal attributions and satisfies both axioms outlined by (Sundararajan et al., 2017). We can therefore apply the familiar framework of cross-validation and held-out test data to estimate the expected accuracy of the attributions provided by the attention factors $a_i$. Finally, the total loss $L$ of the AME is the sum of the main loss, which may be arbitrarily chosen depending on the dataset at hand, and the Granger-causal loss:

$$L = L_{\text{main}} + L_{\text{Granger}}$$  \hspace{1cm} (7)$$

If desired, it is possible to express an a-priori preference for more accurate explanations over accurate predictions (or vice-versa) by weighting the components of $L$ accordingly. In terms of implementation, we estimate both $\varepsilon_X$ and $\varepsilon_{X\setminus\{i\}}$ using the ground truth labels $y_{\text{true}}$, the main loss $L_{\text{main}}$, and single-layer auxiliary models $f_{\text{aux}}$ and $f_{\text{aux},i}$ that receive as input the combined hidden state $h_c$ of the AME and the combined hidden state minus the hidden state and local prediction of the $i$th expert $h_{c\setminus\{h_i,y_i\}}$, respectively. Because $f_{\text{aux}}$ can be reused across experts, the error estimation requires only one additional auxiliary output per expert. We additionally clip $\Delta \varepsilon_{X,i}$ to be positive to not consider cases where $\varepsilon_X > \varepsilon_{X\setminus\{i\}}$, which might happen due to different degrees of intermittent convergence in the auxiliary outputs. Furthermore, we note that it is important to prevent gradient flow towards $\Delta \varepsilon_{X,i}$, e.g. using TensorFlow’s tf.stop_gradient, to prevent the network from optimising the error to match its desired attention values rather than the other way around.

Theoretically, training to provide attributions and predictions at the same time should have no adverse impact on the predictive performance of a neural network, as both objectives share a common feature space, i.e. being able to accurately attribute is helpful for producing predictions and vice-versa. In essence, AMEs make the attribution that is implicitly performed by a neural network explicit.

### 5. Experiments

In order to demonstrate the utility of AMEs, we performed experiments on a variety of tasks with distinctly different characteristics. Our experiments include settings with high numbers of samples, high numbers of features, high correlations between features and heterogenous input data. Specifically, we use AMEs to (i) determine the drivers of medical prescription demand at scale, (ii) compare predictive features for monitoring Parkinson’s disease, and (iii) pinpoint discriminatory genes across multiple types of cancers. The aim of our experiments is to showcase the breadth of tasks that neural networks as scalable, non-linear feature extractors can be used for when equipped with the ability to quantitatively measure feature importance across decisions. In addition, we wish to evaluate to what degree attentive gating decisions correlate with an expert’s ability to contribute and whether providing attributions has an adverse
effect on predictive performance. The source code for our experiments is available at https://github.com/d909b/attentive_mixtures_of_experts.

5.1. Drivers of Medical Prescription Demand

Accurate demand forecasts for medical prescriptions play an important role in preventing stock outages and keeping the cost of supply operations in check. However, demand forecasting for prescriptions is an extremely challenging task due to the large set of prescribed items with poorly understood characteristics and influence factors. To gain a deeper understanding of what factors drive demand for individual prescription items, we trained an AME model to predict the next month’s demand (in terms of revenue) for individual prescription items at the level of practices. The inspection of the assigned attention factors in the AME enables us to analyse which factors are most predictive for specific prescription items. This regression setting is challenging due to the highly heterogenous input data on different time scales and the need to scale to tens of millions of available training samples.

5.1.1. Dataset

We collected multiple heterogenous data streams covering the whole country of England, United Kingdom (UK) during the time frame from January 2011 to December 2012 (24 months). We used data streams corresponding to six feature groups. Each data stream listed below is represented as an expert in our AME model (Figure 4).

Demand History. As the primary data stream, we used the monthly data on all revenues generated by reimbursed prescription items in 9,455 general practices (GPs) in England, UK as released by the British National Health Service (NHS). To ensure a full history of the past demand for prescriptions, we removed those practices from the dataset that remained closed at any point during the prediction time frame. To remove the noise introduced by different prescription formulations and packagings, we aggregated all prescription items into their prescription item class as defined by their pharmaceutical code in the British National Formulary (BNF) reported by the NHS.

For context, we added the monthly total revenue, the region the current practice belongs to and the practice’s distance to that region’s centre as additional input features. We used the territory level 3 (TL3) regions as defined by (OECD, 2017) to geographically subdivide England into 145 regions.

Online Search Interest. We used Google Trends to retrieve the relative monthly online search interest for our time frame and regional code (GB-EN). In total, we queried online search interest for 109,779 medical terms from the comprehensive medical subject headings (MeSH) ontology (Lipscomb, 2000). As many of the medical terms in the MeSH ontology are not common in vernacular, ultimately only 9,225 (8.40%) out of the 109,779 medical terms had a search activity that was significant enough to return a result on Google Trends. We applied a principal component analysis (PCA) transform that explains more than 98% of the variance in the search interest data and reduces the feature vector to just 23 dimensions.

Regional Weather. Weather impacts consumption across a wide variety of industries (Lazo et al., 2011). We therefore added monthly weather data, including rainfall, days of air frost, hours of sunshine and average temperature data, from 23 UK Met Office stations to our dataset.

Regional Demographic, Economic and Labor Data. Regional demographic, economic and labor data in proximity to a practice could affect future prescription demand, as groups with different population-level profiles potentially require different types of care in different amounts. To further analyse the predictive potential of population-level factors, we added 45 yearly indicators on the demographic profile, 27 yearly indicators on the economic profile and 15 yearly indicators of the labor profile of each TL3 region from (OECD, 2017) to our dataset. We represented each of the three population-level feature groups as a distinct expert in our AME model. Analogous to the online search interest data, we applied PCA transforms that explain over 99% of the variance in the three feature groups.

Figure 4. An illustration of the process of converting an existing neural network (NN) of any architecture into an AME with experts $E_i$ operating on predefined feature subsets $x_i$. Because each expert is limited to make their local prediction based only on their subset of the data, the post-hoc analysis of the attention factors output by the attentive gating networks $G_i$ (red) enables us to quantify the contribution of individual experts on the output $y$. 

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1https://data.gov.uk/dataset/prescribing-by-gp-practice-presentation-level; accessed 20th January 2018

3https://trends.google.com/; accessed 20th January 2018

4http://www.metoffice.gov.uk/public/weather/climate-historic/; accessed 20th January 2018
5.1.2. Evaluation Setup

As baselines, we trained autoregressive integrated moving average (ARIMA) models, recurrent neural networks (RNN) and feedforward neural networks (FNN). The architectures of the RNN and FNN models were derived from the trained AME model (Figure 4). The main difference between the evaluated FNN and the RNN is that the former receives the input data collapsed over time rather than sequentially. Univariate ARIMA models are commonly used for forecasting in practice (Riemer et al., 2016) and, in this comparison, served as a baseline that does not make use of any information apart from the revenue history.

Preprocessing. Prior to fitting the models, we standardised the prescription revenue history data for each time series to the range [0, 1]. We preserved the minimum and maximum time series value as separate input features. We additionally normalised all numeric features, except the prescription revenue data, to have a mean value of 0 and a standard deviation of 1 using the data in the training set. All compared models benefited from the same preprocessing.

Hyperparameters. To ensure a fair comparison, we took a systematic approach towards hyperparameter search. For all models based on neural networks, we performed a hyperparameter search with hyperparameters chosen at random from predefined ranges over 35 runs. For our performance comparison, we selected those models from the hyperparameter search that achieved the best performance on the validation data. We used batch normalisation (Ioffe & Szegedy, 2015) and dropout in all the neural network models. Methodologically, we optimised the neural networks' mean squared error with early stopping on the validation set. For ARIMA, we used the iterative parameter selection algorithm from (Hyndman et al., 2007).

Dataset Split. We applied a random split by general practice to separate the available data into a training (60%), validation (20%) and test set (20%). We report the main properties of the different folds in Table 1.

Metrics. We compared the predictive accuracy of the different models by computing their symmetric mean absolute percentage error (SMAPE) (Flores, 1986) and rate of anomalous events (in %) on the held-out test set. We report the average ± standard deviation of CPU hours required for training and evaluation across the 35 runs. Table 2 shows the comparison of the symmetric mean absolute percentage error (SMAPE) and the rate of anomalous events (in %) on the held out test set of 1,891 practices (= 9.07 million time series). We also report the average ± standard deviation of CPU hours required for training and evaluation across the 35 runs.

<table>
<thead>
<tr>
<th>Method</th>
<th>SMAPE (%)</th>
<th>Anomaly (%)</th>
<th>CPU (hr)</th>
</tr>
</thead>
<tbody>
<tr>
<td>ARIMA</td>
<td>34.98</td>
<td>34.83</td>
<td>527.96</td>
</tr>
<tr>
<td>RNN</td>
<td>32.79</td>
<td>34.59</td>
<td>2.92 ± 1.08</td>
</tr>
<tr>
<td>FNN</td>
<td>32.87</td>
<td>34.83</td>
<td>0.25 ± 0.07</td>
</tr>
<tr>
<td>AME</td>
<td>32.84</td>
<td>34.83</td>
<td>2.28 ± 0.71</td>
</tr>
</tbody>
</table>

5.1.3. Results and Discussion

Performance. Our results showed that the extra information collected from various sources indeed improved the prediction performance over the univariate ARIMA baseline - especially for anomalous events (Table 2). This finding suggests that healthcare providers and suppliers should consider incorporating more open data sources into their forecasting models in order to reduce supply costs and to better manage the risk of out-of-stock events. In addition, we found that (i) providing attributions did not have an adverse impact on performance when comparing the AME and the corresponding FNN model and that (ii) the time to train AME models was comparable to that of RNNs.

Attribution. To map out the factors driving demand for prescription items, we plotted the mean contribution percentage \( MCP_i = \frac{\text{mean}(|a_i y_j|)}{\sum_{i=1}^{n} |a_i y_j|} \) and the average amount of attention given to experts for specific prescription items. Our results showed that there are significant differences in sensitivity profiles across the different prescription items (Figure 5). To determine the degree to which unmodulated \( y_i \) and modulated expert predictions \( a_i y_i \) correlate with the ground truth demand \( y_{true} \), we performed hypothesis tests using Kendall’s \( \tau \) (Kendall, 1945). We tested for correlation for each of the prescription items on the held-out test set. We applied the Benjamini-Hochberg-Yekutieli procedure (Benjamini & Yekutieli, 2001) at \( \alpha = 0.05 \) to control the false discovery rate due to multiple testing. The large differences - with the exception of the de-
Granger-causal Attentive Mixtures of Experts

(a) Demand History

(b) Online Search Interest

(c) Regional Weather

(d) Regional Demographic Data

(e) Regional Economic Data

(f) Regional Labor Data

Figure 5. The influence of experts specialised on demand history (a, red), online search interest (b, orange), regional weather (c, blue), regional demographic data (d, purple), regional economic data (e, brown) and regional labor data (f, grey) on the predictions $y$ made by the AME for each of the 1,368 prescription item classes (dots) in our held-out test set. For each item, we report the average attention (x-axis, in %) and the mean contribution percentage (MCP, y-axis) attributed to each expert. The dashed lines indicate the mean average attention and MCP over all prescription item classes. Symbols (star, square, circle, triangle) point out positions of a selected set of well-known prescription items that have significant correlations (Kendall’s $\tau$) to the ground truth demand $y_{true}$ in the respective experts.

5.2. Predictive Features for Parkinson’s Disease

Parkinson’s disease (PD) is a slowly progressing neurodegenerative disease for which there currently exists no cure. However, once diagnosed, the symptoms of PD can be managed effectively using surgical or pharmacological interventions. An early diagnosis can therefore significantly improve the quality of life of patients (Little et al., 2009). Because PD manifests itself through speech impairments, microphones could be used for this task (Little et al., 2009). We train an AME to classify a set of audio features as to whether they were produced by a person with or without PD. Analysing the attention weights assigned by the AME enables us to compare the suitability of various features for this task. In this setting, our goal was to evaluate the behavior of AMEs in the presence of highly correlated inputs.

Dataset. We used the Oxford Parkinson’s tele-monitoring dataset (Little et al., 2009) consisting of 195 sustained vowel phonations from 31 study participants (23 diagnosed with PD). (Little et al., 2009) reported 22 highly correlated features and determined several subsets of features that achieve similar performances on this dataset. For comparison, we use the results of (Little et al., 2009) as a baseline. We applied a stratified random split to separate the available data into 117 samples for training (60%), 39 samples for validation (20%) and 39 for testing (20%).

Hyperparameters. For each of the 22 features, we used a MLP with a single hidden layer with batch normalisation, 20% dropout rate and 16 neurons as expert networks in the AME. We trained the AME with a learning rate of 0.0003 and 25 epochs of early stopping patience on the validation set. We chose the hyperparameters based on a grid search against the validation set.

5.2.1. Results and Discussion

Performance. Our AME achieves a classification error of 7.69% on the test set, which is well within the best classification error interval of 9.4 ± 4.1% reported by (Little et al., 2009) using bootstrap resampling.

Attribution. We found an almost uniform distribution of attention factors of $3.39 \pm 0.22\%$ across all 22 features on the held-out test set ($L_{Granger} = 0.43$). The uniform distribution of attention factors indicates that many of the 22 features are redundant. Indeed, (Little et al., 2009) reported that a subset of just 4 of these features suffices to reach the performance of all available features. The AME therefore correctly identified that those features are largely equivalent in importance. However, because the differences between feature importances were within the range of the estimation error of attributions, it was not possible to determine the best subset of features from the attention factors. We hypothesise that a larger training set might raise the attribution accuracy to a level that enables distinguishing between highly correlated features.
5.3. Discriminatory Genes Across Cancer Types

With the widespread adoption of next generation sequencing, there now exists a wealth of genomic data from which we could infer genes that are predictive of specific phenotypes. Knowledge of the genomic factors related to phenotypes can help guide the development of treatments, as well as increase the understanding of the biological processes involved in complex diseases. To pinpoint the genes that differentiate between different types of cancer, we trained an AME model to classify gene expression data as being either breast invasive carcinoma (BRCA), kidney renal clear cell carcinoma (KIRC), colon adenocarcinoma (COAD), lung adenocarcinoma (LUAD) and prostate adenocarcinoma (PRAD). This setting is characterised by a large number of input genes out of which few are relevant.

Dataset. We used a subset of the data from The Cancer Genomic Atlas (TCGA) pan-cancer RNAseq dataset (Weinstein et al., 2013), which includes gene expression data from multiple cancer types in 800 individuals. To keep visualisations succinct, we used a subset of 100 genes as input data. We applied a stratified random split to separate the available data into 480 samples for training (60%), 160 samples for validation (20%) and 161 for testing (20%).

Hyperparameters. For each of the 100 genes, we used a MLP with a single hidden layer with batch normalisation and a single neuron as expert networks. We trained the AME with a learning rate of 0.001 and 12 epochs of early stopping patience on the validation set. We chose the hyperparameters based on a grid search against the validation set. We weighted the main and the Granger-causal loss of the AME with a 4:1 ratio. We additionally trained a FNN baseline with matching hyperparameters (100 neurons) and architecture. We trained each model on 35 random initialisations with the same hyperparameters.

5.3.1. Results and Discussion

Performance. Across the 35 runs, the best AME and FNN models both achieved classification errors of 0.62% on the test set - reinforcing our hypothesis that providing explicit attributions in neural networks has no adverse impact on performance.

Attribution. When inspecting the AMEs assigned attributions, we found that the AME based its decisions primarily on a small number of highly predictive genes for the different types of cancer (Figure 6). For 7 out of the 10 genes with the highest average attributions, we found prior works that report the same links between respective cancer type and gene locus as identified by the AME (see supplementary material).

6. Limitations

Expert Convergence. It is possible that an expert does not get weighted correspondingly to its feature group’s ability to contribute because it is either over- or underfit. Similarly, the expert network may simply not have enough capacity, not the best architecture, or right choice of hyperparameters to accurately represent the value of its underlying feature group. However, one can monitor the performance and convergence of experts through their local predictions $y_i$.

Confounding. A Granger-causal association does not imply causation because confounders could have influenced the attribution. Verifying causality from observational data is impossible for this very reason (Pearl et al., 2009). Nonetheless, as demonstrated by our experiments, AME’s ability to quantify predictive associations between inputs and outputs across decisions can provide valuable explanations and help generate insights from observational data.

7. Conclusion

We present a novel approach towards attribution in neural networks that is built on the intuitive idea of distributing the feature groups of interest among experts in a mixture of experts model that uses attentive gating to assign weights to individual experts. We show that the assigned attributions contain valuable information and that providing such attributions does not adversely impact predictive performance. Our approach enables new and exciting use cases for neural networks in knowledge discovery from observational data by providing measurably accurate attributions that can be compared across decisions.
Acknowledgments

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References


Granger-causal Attentive Mixtures of Experts


1. Source Code and Full List of Outputs
The source code for all experiments is available online at
https://github.com/d909b/attentive_mixtures_of_experts. A full list of expert mean contribution
percentages (MCPs), average attention factors $a_i$ and their respective effect sizes (Kendall’s $\tau$) and significances ($p$-values)
for the medical prescription demand forecasting experiment are also available at the same address.

2. Appendix: Medical Prescription Demand Experiment
Choice of Time Frame. We chose the evaluated time frame because overlapping and continuous historical data was
available from all listed data sources.
Closed Practices. For our purposes, we define closed practices as those practices that have had no revenue for more than
3 continuous months throughout the 24 month timeframe that we analysed.
MeSH Term Selection. We extracted all MeSH terms from the categories 'Diseases' (C), 'Drugs and Chemicals' (D) and
'Mental Disorders' (F03).

3. Appendix: Gene Expression Experiment
For 7 out of the 10 most predictive genes (by average attention assigned over all samples), we found prior reports that
suggest a link between those genes and the specific types of cancers they were most predictive for (by average attention
over the cancer type subsets):
- ABCC8 and breast carcinoma (BRCA) (Lehman et al., 2008; Soucek et al., 2015; Kim et al., 2017)
- ABCC5 and clear cell carcinoma (KIRC) (Eggen et al., 2012; Ween et al., 2015)
- HMG1L1 (also known as CTCF) and colon adenocarcinoma (COAD) (Giannakis et al., 2016)
- ABCA2 and COAD (Mack et al., 2007; 2008)
- ABCC10 and lung adenocarcinoma (LUAD) (Wangari-Talbot & Hopper-Borge, 2013)
- ABCC2 and ABCC3 for prostate adenocarcinoma (PRAD) (Karatas et al., 2016)

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1Institute of Robotics and Intelligent Systems, MHSL, D-HEST, ETH Zurich, Switzerland. Correspondence to: Patrick
Schwab <patrick.schwab@hest.ethz.ch>.
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Table S1. Full list of input features used in the multivariate models in the medical prescription demand forecasting experiment.

<table>
<thead>
<tr>
<th>Input Feature</th>
<th>Dimensionality</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a) Demand History</td>
<td></td>
</tr>
<tr>
<td>Monthly Prescription item revenue history</td>
<td>12 × 1</td>
</tr>
<tr>
<td>Min. and max. revenue</td>
<td>2</td>
</tr>
<tr>
<td>Monthly total revenues at practice</td>
<td>12 × 1</td>
</tr>
<tr>
<td>Month of forecast (one-hot)</td>
<td>12</td>
</tr>
<tr>
<td>TL3 Region (one-hot)</td>
<td>145</td>
</tr>
<tr>
<td>Prescription item type (embedding)</td>
<td>45</td>
</tr>
<tr>
<td>(b) Online Search Interest</td>
<td></td>
</tr>
<tr>
<td>Monthly online search interest in 9,225 search terms (PCA)</td>
<td>12 × 23</td>
</tr>
<tr>
<td>Prescription item type (embedding)</td>
<td>45</td>
</tr>
<tr>
<td>(c) Regional Weather</td>
<td></td>
</tr>
<tr>
<td>Monthly weather data</td>
<td>12 × 5</td>
</tr>
<tr>
<td>Distance to weather station</td>
<td>1</td>
</tr>
<tr>
<td>Prescription item type (embedding)</td>
<td>45</td>
</tr>
<tr>
<td>(d) Regional Demographic Data</td>
<td></td>
</tr>
<tr>
<td>Distance to TL3 region</td>
<td>1</td>
</tr>
<tr>
<td>Prescription Item type (embedding)</td>
<td>45</td>
</tr>
</tbody>
</table>

Note: All of the following features were aggregated into a single feature vector using a PCA transform.
Table S2. Full list of input features used in the multivariate models in the medical prescription demand forecasting experiment. (cont.)

<table>
<thead>
<tr>
<th>Input Feature</th>
<th>Dimensionality</th>
</tr>
</thead>
<tbody>
<tr>
<td>(e) Regional Economic Data</td>
<td></td>
</tr>
<tr>
<td>Distance to TL3 region</td>
<td>1</td>
</tr>
<tr>
<td>Prescription item type (embedding)</td>
<td>45</td>
</tr>
<tr>
<td>Note: All of the following features were aggregated into a single feature vector using a PCA transform.</td>
<td></td>
</tr>
<tr>
<td>Regional Gross Domestic Product (PDF), Pound Sterling</td>
<td>1</td>
</tr>
<tr>
<td>Disposable Household Income, Pound Sterling</td>
<td>1</td>
</tr>
<tr>
<td>Primary income of private Households, Pound Sterling</td>
<td>1</td>
</tr>
<tr>
<td>Regional employment, Number of people</td>
<td>1</td>
</tr>
<tr>
<td>Employment in information and communication, Number of people</td>
<td>1</td>
</tr>
<tr>
<td>Employment in financial and insurance, Number of people</td>
<td>1</td>
</tr>
<tr>
<td>Employment in real estate, Number of people</td>
<td>1</td>
</tr>
<tr>
<td>Employment in manufacturing, Number of people</td>
<td>1</td>
</tr>
<tr>
<td>Employment in construction, Number of people</td>
<td>1</td>
</tr>
<tr>
<td>Employment in agriculture, forestry and fishing, Number of people</td>
<td>1</td>
</tr>
<tr>
<td>Employment in distributive trade, repairs, transport, accommodation, food service, Number of people</td>
<td>1</td>
</tr>
<tr>
<td>Employment in professional, scientific, technical, administrative, support service, Number of people</td>
<td>1</td>
</tr>
<tr>
<td>Employment in public administration, compulsory secondary school, education, human health, Number of people</td>
<td>1</td>
</tr>
<tr>
<td>Employment in industry, including energy, Number of people</td>
<td>1</td>
</tr>
<tr>
<td>Employment in other services, Number of people</td>
<td>1</td>
</tr>
<tr>
<td>Regional Gross Value Added (GVA), Pound Sterling</td>
<td>1</td>
</tr>
<tr>
<td>GVA in information and communication, Pound Sterling</td>
<td>1</td>
</tr>
<tr>
<td>GVA in financial and insurance, Pound Sterling</td>
<td>1</td>
</tr>
<tr>
<td>GVA in real estate, Pound Sterling</td>
<td>1</td>
</tr>
<tr>
<td>GVA in manufacturing, Pound Sterling</td>
<td>1</td>
</tr>
<tr>
<td>GVA in construction, Pound Sterling</td>
<td>1</td>
</tr>
<tr>
<td>GVA in agriculture, Pound Sterling</td>
<td>1</td>
</tr>
<tr>
<td>GVA in distributive trade, repairs, transport, accommodation, food service, Pound Sterling</td>
<td>1</td>
</tr>
<tr>
<td>GVA in professional, scientific, technical, administrative, support service, Pound Sterling</td>
<td>1</td>
</tr>
<tr>
<td>GVA in public administration, compulsory secondary school, education, human health, Pound Sterling</td>
<td>1</td>
</tr>
<tr>
<td>GVA in industry, including energy, Pound Sterling</td>
<td>1</td>
</tr>
<tr>
<td>GVA in other services, Pound Sterling</td>
<td>1</td>
</tr>
<tr>
<td>(f) Regional Labor Data</td>
<td></td>
</tr>
<tr>
<td>Distance to TL3 region</td>
<td>1</td>
</tr>
<tr>
<td>Prescription item type (embedding)</td>
<td>45</td>
</tr>
<tr>
<td>Note: All of the following features were aggregated into a single feature vector using a PCA transform.</td>
<td></td>
</tr>
<tr>
<td>Unemployed, Number of people</td>
<td>1</td>
</tr>
<tr>
<td>Unemployment rate, % unemployed over labour force age 15+</td>
<td>1</td>
</tr>
<tr>
<td>Unemployment rate, age 15+, Growth index</td>
<td>1</td>
</tr>
<tr>
<td>Unemployment rate, age 15+, Growth index (2007=100)</td>
<td>1</td>
</tr>
<tr>
<td>Working age population, age 15-64, Number of people</td>
<td>1</td>
</tr>
<tr>
<td>Working age population, age 15+, Number of people</td>
<td>1</td>
</tr>
<tr>
<td>Labor force, age 15+, Number of people</td>
<td>1</td>
</tr>
<tr>
<td>Participation rate, age 15+, % labour force age 15+ over population age 15+</td>
<td>1</td>
</tr>
<tr>
<td>Participation rate, age 15+, % labour force age 15+ over population age 15+, Growth rate (2001=100)</td>
<td>1</td>
</tr>
<tr>
<td>Participation rate, age 15+, % labour force age 15+ over population age 15+, Growth rate (2007=100)</td>
<td>1</td>
</tr>
<tr>
<td>Employment in age band 15 - max. years, Number of people</td>
<td>1</td>
</tr>
<tr>
<td>Employment in age band 15 - 64 years, Number of people</td>
<td>1</td>
</tr>
<tr>
<td>Employment rate, % employment age 15 - 64 over working age population 15 - 64</td>
<td>1</td>
</tr>
<tr>
<td>Employment rate, % employment age 15 - max. over working age population 15 - max.</td>
<td>1</td>
</tr>
<tr>
<td>Employment rate growth, 15 years old and over, Index (2001=100)</td>
<td>1</td>
</tr>
<tr>
<td>Employment rate growth, 15 years old and over, Index (2007=100)</td>
<td>1</td>
</tr>
</tbody>
</table>
Figure S1. An illustration of the architecture of the AME presented in the medical prescription demand forecasting experiment. The AME consists of $M = 6$ (architecturally equivalent) experts $E_i$ that each operate on their own distinct input feature group $x_i$ of dimensionality $D_i$ after collapsing the temporal dimension (see S1 for the exhaustive list of inputs for each expert). The "..." layer indicates the input-dependant data transformation that collapses the temporal dimension for those input features that have a temporal dimension. Each expert has its own respective number of units per hidden layer $N_i$ with the hidden blocks repeated $L$ times. Note that the evaluated feedforward neural networks (FNNs) use the same architecture as a single expert $E_i$ of the AME that receives all inputs $x_i$ at once and does not have its output modulated by an attentive gating network. For the evaluated recurrent neural networks (RNNs), we use the same architecture as for the FNNs but do not collapse the input features $x$ in time and replace the first fully connected hidden block with a bidirectional long short-term memory (BLSTM) layer. The numbers in parentheses indicate the dimensionality of the connections between components of the AME.
References


