Interpretable Mixture of Experts for Structured Data

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Abstract

With the growth of machine learning for structured data, the need for reliable model explanations is essential, especially in high-stakes applications. We introduce a novel framework, Interpretable Mixture of Experts (IME) that provides interpretability for structured data while preserving accuracy. IME consists of an assignment module and a mixture of interpretable experts such as linear models where each sample is assigned to a single interpretable expert. This results in an inherently-interpretable architecture where the explanations produced by IME are the exact descriptions of how the prediction is computed. In addition to constituting a standalone inherently-interpretable architecture, an additional IME capability is that it can be integrated with existing Deep Neural Networks (DNNs) to offer interpretability to a subset of samples while maintaining the accuracy of the DNNs. Experiments on various structured datasets demonstrate that IME is more accurate than a single interpretable model and performs comparably to existing state-of-the-art deep learning models in terms of accuracy while providing faithful explanations.

1 Introduction

Structured data, often with a time component3, appear in numerous applications, including healthcare, finance, retail, environmental sciences and cybersecurity [11]. Deep neural networks (DNNs) have recently shown state-of-the-art performance for structured data [6, 37, 43, 31, 22, 58] and are being deployed in the real world. Yet, one challenge hindering their widespread use is their black-box nature [38] – humans are unable to understand the complex decision-making process behind their predictions. For most applications, explainability is crucial [8, 39] – physicians need to understand why a drug would help, and retail data analysts need to gain insights on the trends in the predicted sales.

In an attempt to produce explanations for structured data, various interpretable architectures have been proposed. Attention-based DNNs are growing in popularity [6, 37] with attention weights being used as explanations; however, recent works [29, 47, 45] show the limitations of such explanations. Differentiable neural versions of generalized additive models [5, 9] and soft decision trees (DTs) [41] are among approaches for tabular data, and trend-seasonality decomposition based architectures [42] for univariate time-series data. Recently, [46] proposed DNNs with explanations in the form of continued fractions, whose interpretation complexity increases with the addition of network layers. Overall, a systematic interpretable DNN framework remains an important direction for exploration.

We propose a novel framework for inherently-interpretable modeling, with the idea of combining multiple interpretable models in a mixture of experts (ME) framework. ME frameworks are composed

∗Work done while at Google Cloud AI
IME implementation can be found at: https://github.com/google-research/google-research/tree/master/ime
3Structured data are usually referred as ‘tabular data’ when only features from a single timestep affect the output, and ‘time-series data’ when features from multiple time steps affect the output.

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of multiple “experts” and an assignment module that decides which expert should be picked for each sample. Recent works [49, 16] have used ME to replace layers of DNNs to scale the model capacity efficiently. In contrast, we use a single ME to fit different data subsets by interpretable experts. Intuitively, although complex distributions cannot be fit by simple interpretable models, small subsets of them can be fit with low-capacity interpretable models. By following such an approach, one could preserve accuracy while providing useful interpretability capabilities by replacing black-box models with multiple interpretable models. The key contributions can be summarized as follows:

- Enabled by innovations in its design, IME constitutes a new class of interpretable models that can replace or encapsulate DNNs to achieve accuracy on par with or better than the state-of-the-art on multiple real-world tabular and time-series datasets.
- We propose multiple options for IME that offer flexibility depending on the interpretability needs of particular applications. Single-level assignment S-IME\(_{ii}\) & S-IME\(_{di}\) (Fig.1 (a) & (b)) employs an assignment module that can be interpretable (yielding both assignment and expert interpretability) or a DNN (yielding only expert interpretability) with interpretable experts. Hierarchical assignment H-IME\(_{ii}\) & H-IME\(_{di}\) (Fig.1 (c) & (d)) first selects between a pretrained black-box expert and an IME, and then between different interpretable experts.
- S-IME\(_{ii}\) (Fig.1 (a)) can generate explanations in the form of the exact description of predictions with an easy-to-digest concise formula, enabling its use in high-stakes applications.
- S-IME\(_{di}\) (Fig.1 (b)) can be used for local interpretability, as a separate interpretable function expresses the predictions in each cluster.
- H-IME\(_{ii}\) & H-IME\(_{di}\) (Fig.1 (c) & (d)) offer interpretable decision making for a subset of samples while maintaining accuracy. E.g., we show that on one real-world Retail task, \(\sim 40\%\) of samples can be assigned to an interpretable expert while preserving the same accuracy. The trade-off can be adjusted by the user, enabling the ability to trade between interpretability and accuracy based on application needs. This can be used to identify ‘difficult’ samples (i.e., samples requiring a DNN for an accurate prediction) and ‘easy’ samples (i.e., samples that can be predicted by a simple interpretable model), offering another form of explainability.

2 IME Framework

Fig. 2 shows the proposed IME architecture. IME consists of a set of ‘interpretable experts’ and an ‘assignment module’. The experts can be any interpretable differentiable model, each with its own
Figure 2: IME consists of a set of ‘interpretable experts’ (3 in this example) and an ‘assignment module’. The input to IME can be time-series or tabular data. Each expert produces a single prediction. The input to the assignment module is both a feature embedding and the past error made by the experts (when the time dimension exists). The assignment module selects a single expert during inference to make the final prediction. We define various losses (shown in red boxes) that are used to supervise the assignment module and expert weights.

IME can be used for any structured data, including tabular data (where a sample consists of a single observation at a given timestep) or time-series (where a sample consists of multiple observations over a time period). Broadly, consider a regression problem for input data with \( S \) samples \( \{(X_i, Y_i)\}_{i=1}^S \); with \( X = [x_1, \ldots, x_T] \in \mathbb{R}^{N \times T} \), where \( T \) is the number of timesteps (for tabular data, we have \( T = 1 \)) and \( N \) is the number of features. Outputs are \( Y = [y_1, \ldots, y_H] \in \mathbb{R}^H \), where \( H \) is the horizon (for tabular data \( H = 1 \)). For notational simplicity, we denote \( X_t \) as the input until timestep \( t \). For an IME with \( n \) experts, we denote each expert as \( f_i \) where \( i \) is the expert index. The prediction made by the expert \( i \) is given as \( f_i(X) = \hat{Y}_i \) and the corresponding prediction error at a given horizon \( h \), for which we use mean squared error (MSE), is denoted as \( \epsilon_{i,h} = \frac{1}{S} \sum_{i=1}^S (y_h - \hat{y}_h)^2 \). The errors made by all experts at time \( t \) are denoted as \( E_t = [\epsilon_{1,t}, \ldots, \epsilon_{n,t}] \). The assignment module \( A \) outputs prediction \( \hat{Y}_A \) along with an \( n \)-dimensional vector representing the weight \( w_i \) as the probability of choosing a particular expert such that \( \sum_{i=1}^n w_i = 1 \).

2.1 Learning from past errors

IME is applicable to general tabular data without any time-related feature. However, in cases where time-related features are available, IME benefits from incorporating past errors (as shown in...
We design IME with the following goals: [a] Overall model accuracy should be high. [b] The assignment module should be accurate in selecting the most appropriate experts. [c] Utilization of individual experts should not be imbalanced; it is desired to avoid all samples being assigned to a single expert. [d] Experts should yield diverse predictions and not converge to same models, helping the assignment module to better choose between the experts. [e] For inputs with time information, assignments should be smooth over time for consecutive inputs. Smoother assignment is also beneficial for interpretability. Correspondingly, we propose the following objective:

$$
L(f, A, X, Y) = \mathcal{L}_{\text{pred}}(f, A, X, Y) + \beta \mathcal{L}_{\text{util}}(A, X) + \gamma \mathcal{L}_{\text{div}}(f, X) + \\
\delta \mathcal{L}_{\text{smooth}}(A, X) + \lambda \mathcal{L}_{A, \text{pred}}(A, X, Y),
$$

where $\beta, \gamma, \delta$ and $\lambda$ are hyperparameters. $\mathcal{L}_{\text{pred}}, \mathcal{L}_{\text{util}}, \mathcal{L}_{\text{div}}$ and $\mathcal{L}_{A, \text{pred}}$ refer to overall accuracy loss, expert utilization loss, expert diversity loss, assignment smoothness loss and assignment accuracy loss, respectively. Next, we explain each term in detail.

**[a] Prediction accuracy:** We adopt the maximum likelihood loss under a Mixture of Gaussians modeling assumption:

$$
\mathcal{L}_{\text{pred}}(f, A, X, Y) = -\log \sum_{i=1}^{n} A(X)_i k e^{-\frac{1}{2}\|Y-f_i(X)\|^2},
$$

where $k = 1/\sqrt{2\pi}$ is a normalizing constant. This loss was used for ME models by [28] to encourage expert specialization by comparing each expert separately with the target and training to reduce the average of all these discrepancies.

**[b] Expert utilization:** The assignment module can converge to a state where it produces large assignment weights for the same few experts, which results in some experts being trained more rapidly and selected even more by the assignment module. This phenomenon is also observed in previous works. To circumvent this, [15] uses hard constraints at the beginning of training to avoid local minimum, [7] uses soft constraints on the batch-wise average of each expert, and [49] encourages all experts to have equal importance (i.e., uniform expert utilization) by penalizing the coefficient of variation between different expert utilization. For IME, we propose that each expert should focus on a subset of the distribution. These subsets do not have to be equal in size, so all experts should be utilized but not necessarily in a uniform manner. Given this, we propose the following utilization objective:

$$
\mathcal{L}_{\text{util}} = (1/N) \sum_{i=1}^{N} e^{-kU_i} - e^{-k},
$$

where $U_i$ is the utilization of expert $i$ such that $U_i = 1/N \sum_{j=1}^{N} w_{i,j}$ and $k$ is a hyperparameter to encourage utilization without enforcing uniformity across experts.

**[c] Expert diversity:** Ideally, each expert should produce different predictions as they focus on different subsets and specialize in them. Diversity in predictions would also help the assignment module to choose between different experts. To promote diversity between the outputs of experts, we propose using contrastive loss which is based on minimizing the distance between similar samples, and maximizing the distance between different samples. For IME, we adapt it as minimizing the distance between outputs from the same expert and maximizing the distance between outputs from different experts. We add Gaussian noise $\eta$ with zero mean and unit variance to the inputs, and define positive pairs as outputs coming from the same expert (with and without the noise) and negative pairs as outputs coming from two different experts (both without noise). We propose the loss function:

$$
\mathcal{L}_{\text{div}}(f, X) = -\sum_{i=1}^{n} \log \frac{\exp \left( S(f_i(X), f_i(X + \eta)) / \tau \right)}{\sum_{k=1}^{n} \mathbb{1}_{[k \neq i]} \exp \left( S(f_i(X), f_k(X)) / \tau \right)},
$$

where $S(\cdot, \cdot)$ refers to overall model accuracy should be high.
where \( S(u, v) = u^T v / \| u \| \| v \| \) denote the dot product between \( l_2 \) normalized \( u \) and \( v \), \( \mathbb{1}_{[k \neq i]} \in \{0, 1\} \) is an indicator function such that 1 if \( k \neq i \), and \( \tau \) denotes the temperature parameter.

**[d] Assignment smoothness:** For data with time component, consecutive inputs have mostly overlapping information, so one would expect mostly similar assignment for them. To promote smooth transition of assignments over time, we adopt the Kullback–Leibler (KL) divergence \([33]\) between the weights output by the assignment module for consecutive timesteps \( t-1 \) and \( t \):

\[
\mathcal{L}_{\text{smooth}}(A, \bar{X}) = D_{\text{KL}} \left( A(\bar{X}_{t-1}) \parallel A(\bar{X}_t) \right),
\]

where \( D_{\text{KL}}(P \parallel Q) \) denote the KL divergence between two distributions \( P \) and \( Q \) defined on the same probability space \( \mathcal{X} \). Assignment smoothness can also be helpful for improving the interpretability, as users can build more reliable insights.

**[e] Assignment module accuracy:** We propose to have the assignment module produce a prediction (only used during training) along with the weights, and encourage it to be accuracy via error minimization:

\[
\mathcal{L}_{A,\text{pred}}(A, \bar{X}, Y) = (1/N) \sum_{i=1}^{N} (Y - A(\bar{X}))^2.
\]

Although such a loss isn’t typical for ME, we observe that it helps improving assignment accuracy.

### 2.3 Training procedure

The model first is trained in an end-to-end way to minimize the loss in Eq. 1 until convergence. Then, the experts are frozen, and the assignment module is trained independently to minimize the loss in Eq. 2. This alternating optimization approach first promotes expert specialization, and then improves the assignment module accuracy on trained experts. Since experts and the assignment module might have different architectures, they may converge at different rates \([27]\). Hence, different learning rates are employed for them. More details are provided in the Appendix.

### 2.4 Interpretability capabilities

IME offers different forms of interpretability:

- **[S-IME\(_{di}\)] Single-level interpretable assignment & interpretable experts:** Each prediction can be expressed as a switch statement with the cases specifying the prediction functions of experts, and the case conditions specifying the assignment predicate corresponding to each expert. Thus, we effectively have a single interpretable function defining each prediction as a globally-interpretable model. This can be useful for regulation-sensitive applications where the exact input-output relationships are needed, such as criminal justice systems.

- **[S-IME\(_{d}\)] Single-level DNN assignment & interpretable experts:** When the assignment logic isn’t interpretable, the stability property of IME allows the data to be clustered into \( n \) subsets such that the prediction in each subset comes from a single interpretable expert. This can be likened to local interpretability, as a separate interpretable function expresses the prediction in each cluster. Post-hoc interpretability methods can be used to assess feature importance for different assignments. This can be used for model debugging to verify that each expert’s logic is correct.

- **[H-IME\(_{di}\)] Hierarchical interpretable assignment with DNN & interpretable experts & [H-IME\(_{d}\)] Hierarchical DNN assignment with DNN & interpretable experts:** For hierarchical assignment, the DNN assignment module decides whether a sample are easy i.e. it can be accurately predicted by simple interpretable models vs. difficult i.e. it requires complex models. Similar to S-IME\(_{d}\), one can obtain local interpretations for the easy samples. If explainability for the difficult samples is desired, post-hoc interpretability methods such as \([40]\) may be adapted, however, their fidelity and faithfulness would be worse than the explanations coming from the inherently-interpretable experts. In addition, understanding why particular samples are assigned as easy vs. difficult can give insights into different data distribution modes (e.g. different seasonal climates and clothing sales), significant regime changes over time (e.g. after an ad campaign is launched for a product), and data anomalies (e.g. when pandemic outbreak occurs).

### 2.5 Accuracy-interpretability trade-off with H-IME

The main difference between H-IME and S-IME is using a pretrained DNN as an expert. To avoid all samples being assigned to the pretrained DNN expert, an additional loss term is added to Eq. 1

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\mathcal{L}_{\text{smooth}}(A, \bar{X}) = D_{\text{KL}} \left( A(\bar{X}_{t-1}) \parallel A(\bar{X}_t) \right),
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\( \alpha U_{\text{DNN}} \), where \( U_{\text{DNN}} \) is the DNN expert utilization as described in Sec. 2.2. Increasing \( \alpha \) yields less samples being assigned to the DNN expert, and hence constitutes a mechanism to increase the ratio of samples for which we use interpretable decision making. The effect of changing the value of \( \alpha \) is empirically shown in Sec. 3. For some real-world datasets, H-IME can be highly valuable in preserving the accuracy (better than fully-interpretable S-IME) while utilizing interpretable models for a significant majority of samples.

### 3 Tabular Data Performance

We conduct experiments on the Rossmann Store Sales data [1], which has 30 features. We perform a 70/10/20 train/validation/test split. Detailed description is available in Appendix.

**Baselines:** We compare IME to black-box models including Multi-layer Perceptron (MLP) [18], CatBoost [13], LightGBM [32] and XGBoost [10], and Inherently-interpretable Neural Additive models (NAM) [5], linear regression (LR) and shallow DTs. Our goal is to analyze the achievable performance and the accuracy vs. interpretability trade-off.

**Training and evaluation:** We use \( n=20 \) experts that are modeled as either LR, shallow soft DTs [17], or a mixture of both. For interpretable assignment, a LR is used as the assignment module. For DNN assignment, an MLP is used. We run hyperparameter tuning using a random grid search. For more details, please refer to the Appendix.

**Results:** Table 1 shows the performance of baselines and IME in RMSE. The best-performing black-box model is MLP. There is a huge performance gap between a single interpretable model and any black box model. Using S-IME\(_{\text{di}}\) with an interpretable assignment module (the first two rows in the IME section in Table 1), we observe significant outperformance compared to a single interpretable model, but underperformance compared to black-box models – as expected. The performance becomes comparable to black-box models with S-IME\(_{\text{di}}\), using a DNN assignment module. This underlines the importance and value of high capacity assignment for some problems. IME with hierarchical-level assignment, H-IME\(_{\text{di}}\) and H-IME\(_{\text{di}}\), yields the the best accuracy, while offering partial interpretability. This partial interpretability is demonstrated in Fig. 3 and is achieved by changing the penalty for assigning samples to the DNN expert. As expected, the more samples are assigned to interpretable experts, the less accurate the model becomes. Surprisingly, we observe that 20% of samples can be assigned to interpretable models with LR experts and 40% with soft DT experts, with almost no loss in accuracy. This shows that a large portion of the data is sufficiently easy to be captured by interpretable models.

| Model category     | Model name     | RMSE  |
|--------------------|----------------|-------|
| Black-box models   | MLP            | 457.72|
|                    | CatBoost       | 520.07|
|                    | LightGBM       | 490.57|
|                    | XGBoost         | 567.80|
| Interpretable models | Linear        | 1499.45|
|                    | Soft DTs (SDT) | 1181.17|
|                    | NAM            | 1497.47|

Table 1: Performance on Rossmann. S-IME\(_{\text{di}}\) performs better than a single interpretable model but worse than black-box models. S-IME\(_{\text{di}}\) is comparable with black-box models. H-IME\(_{\text{di}}\) outperforms all, while offering partial interpretability.

### 4 Time-Series Data Performance

We conduct experiments on multiple real-world time-series datasets, including Electricity [2], Climate [1] and ETT [59]. We perform a 70/10/20 train/validation/test split for each dataset. Detailed descriptions of datasets, hyperparameter tuning and additional experiments are available in Appendix.
Expert interpretability: All IME options provide local expert interpretability. Explanations can be given as equations for each expert, or can be conveniently visualized as plots when there is a higher number of features or experts. Fig. 4 exemplifies this for Rossmann – “Expert 1” puts high positive weights on ‘the number of customers’, ‘open’ and ‘competition distance’; “Expert 2” puts high negative weights on ‘assortment’; and “Expert 3” makes its prediction mainly based on ‘the number of customers’. We also show sample-wise interpretability examples in Appendix.

Identifying data distribution modes: We use \( n=10 \) LR experts for IME. We use either LR and LSTM as assignment modules for S-IME\(_{11}\) and S-IME\(_{id}\) respectively. We conduct hyperparameter tuning using a grid search based on the validation performance. For more details on hyperparameters, please refer to Appendix. To measure performance in Table 2 we use MSE.

Table 2: The MSE of baselines and IME for various time-series datasets at different forecasting horizons.

| Features | Datasets | Forecast horizon | Black Box Models | White Box Models | IME |
|----------|----------|------------------|------------------|------------------|-----|
|          |          |                  | LSTNN | Transformer | TCNN | AR | LR | S-IME\(_{11}\) | S-IME\(_{id}\) |
|          |          |                  | Electricity | Climate | Electricity | Climate | Electricity | Climate | Electricity | Climate | Electricity |
| Univariate | 24 | 178 .159 | 163 | 172 | 173 | 167 | 158 | 158 |
|          | 48 | 204 | 188 | 199 | 195 | 198 | 188 | 180 | 180 |
|          | 168 | 251 | 234 | 252 | 235 | 242 | 224 | 217 | 224 |
| Multivariate | 24 | 094 | 106 | 094 | 092 | 095 | 098 | 099 | 091 |
|          | 48 | 128 | 176 | 131 | 134 | 140 | 141 | 137 | 140 |
|          | 168 | 230 | 313 | 242 | 209 | 228 | 254 | 222 | 220 |
| ETTh1 | 48 | 085 | 075 | 077 | 084 | 030 | 034 | 027 | 027 |
|          | 168 | 202 | 109 | 131 | 133 | 049 | 054 | 040 | 042 |
| ETTh1 | 24 | 098 | 119 | 216 | 095 | 171 | 106 | 097 | 097 |
|          | 48 | 204 | 220 | 252 | 188 | 285 | 197 | 192 | 191 |
|          | 168 | 518 | 1.027 | 303 | 172 | 1.788 | 142 | 1.24 | 1.44 |

Table 2 shows the MSE for different datasets at different forecasting horizons. For univariate forecasting, IME outperforms black-box models. For multivariate forecasting IME performance is comparable with black-box models (second-best accuracy after TCN). We also observe that using an interpretable assignment doesn’t degrade the accuracy.

5 Interpretability Results

Global interpretability: In S-IME\(_{11}\), where both the assignment module and experts are interpretable, explanations are reduced to merely the equations of assignment and experts. We use the 

\[
A_{expert_1} = -0.05x_{t-1} + 0.03x_{t-2} + 0.9x_{t-3} + 3.86c_1 - 0.02c_2 \\
A_{expert_2} = -0.03x_{t-1} + 0.11x_{t-2} + 0.08x_{t-3} + 2.36c_1 + 0.5e_2
\]

if \( A_{expert_1} > A_{expert_2} \) then

\[
y_{t+1} = -0.049x_{t-1} - 0.29x_{t-2} + 1.17x_{t-3};
\]

else

\[
y_{t+1} = -0.081x_{t-1} - 0.23x_{t-2} + 1.13x_{t-3}
\]

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Identifying data distribution modes: We construct a synthetic dataset (Fig. 5a) to showcase additional interpretability capabilities offered by IME. We run S-IME\(_{11}\) with LR assignment (Fig. 5b)
and S-IME$_{di}$ with MLP assignment (Fig. 1b). Fig. 5 shows that both S-IME$_{ii}$ and S-IME$_{di}$ assign most samples so that $Y = x_1$ are assigned to Expert 1, $Y = x_2$ to Expert 2 and $Y = x_3$ to Expert 3. In this way, IME gives insights into how different subsets can be split based on unique characteristics – e.g. different seasonal climates and clothing sales in Retail.

**Identifying temporal regime changes:** Fig. 6a shows a synthetic univariate dataset where the feature distribution changes over time. S-IME$_{ii}$ with an LR assignment module and S-IME$_{di}$ with an LSTM assignment module are used, and all interpretable experts are simple auto-regressive models. Fig. 6b and 6c show that IME can identify changes over time and uses different experts for distribution modes. This capability can be used to get insights into temporal characteristics and major events, e.g. to understand the impact of introducing new drugs for disease prediction.

**Identifying incorrect model behavior:** Another use case for interpretability is model debugging and identifying undesired behaviours. To showcase IME for use case, we use synthetic data from Fig. 5b. Fig. 5c shows the weights for the experts for S-IME with interpretable (top) and DNN assignment (bottom) respectively. S-IME$_{ii}$ yields almost ideal behavior; Expert 1 assigns highest weight to feature $x_1$, Expert 2 to $x_2$ and Expert 3 to $x_3$. However, Expert 1 in S-IME$_{di}$ incorrectly assigns the highest weights to feature $x_2$. Investigating different weights in this way can help verify whether the expert logic is correct. Model builders can benefit from this insights to debug and improve model performance, e.g. by replacing or down-weighing certain experts.

**User study on IME explanations:** IME offers faithful local explanations, as the actual interpretable models behind each prediction are known. This is in contrast to post-hoc methods used to explain black-box methods such as SmoothGrad [53], SHAP [40], Integrated Gradients [54], DeepLift [51]. Such post-hoc methods may be unreliable [4, 24, 20], especially so for time series [26]. To demonstrate the quality of IME’s explanations, we design a user study that focuses on comparisons with the commonly-used post-hoc method, SHAP [40]. We base the objective component on human-grounded metrics [14], where the tasks conducted by users are simplified versions of the original task. We use sales prediction on Rossmann as the task, and experiment with S-IME$_{ii}$ (LR assignment & 20 experts) and MLP as the black-box model. First, we consider a counterfactual simulation scenario: for each sample, the users are given an input and an explanation (along with access to training data for analyses) and asked how the model output (sales prediction) would change with the input changes. The user can choose: no change, increase or decrease. Explanations are provided by the chosen interpretable expert of IME vs. SHAP [40]. We collect 77 samples from 15 users. When provided with IME explanations, users can predict model behavior with an accuracy of 69% vs. 42% of SHAP. This shows that explanations provided by IME can be easily understood by users and are more faithful. Next, we also ask the users which explanations they trust more for each sample: explanation A/B, both, or neither. IME is chosen in 87% of the cases vs. 6.5% of SHAP (and neither gets 6.5%), demonstrating the trustworthiness of IME’s explanations.
6 Performance Analyses

Comparison to black-box model performance: Table 2 shows that IME can outperform black-box models. To further shed light on when this is the case, we investigate the effect of changing the interpretable model’s capacity. For LR models, as we increase the input sequence length (and hence the number of learnable coefficients), the model accuracy increases as shown in Fig. 7. Note that increasing the sequence length doesn’t affect the number of parameters for an LSTM. IME outperforms a single interpretable model for any sequence length, and starts outperforming LSTM when the accuracy gap between LR and LSTM gets smaller (e.g. with 160 timesteps). IME’s performance depends on the performance of its experts. It has been shown [21] that interpretable models perform particularly well for time-series forecasting, explaining why IME may outperform DNNs for time-series.

Effect of the number of experts: Fig. 8 shows the effect of changing the number of experts on IME’s accuracy on the Rossmann dataset. As the number of experts increases, the accuracy increases until the optimal number of experts is reached (40 for LR experts, 20 for soft DTs). After this value, increasing the number of experts causes a slight decrease in accuracy as experts become underutilized. The number of experts can be treated as a hyperparameter that can be optimized on a validation dataset. Note that IME with fewer experts is desirable for improving overall model interpretability.

Ablation studies: We perform ablation studies on the performance benefits brought by each component. Table 3 shows that removing various IME components yields worse performance. Note that IME can be used for any tabular dataset without a time component by removing the past error from the input to the assignment module, i.e \( A([X_t; E_{t-1}]) \rightarrow A(X) \). However, the availability of errors over time improves the performance of the assignment module.

IME in comparison to other ME variants: Sparsely-gated ME [49] assigns samples to a subset of experts and then combines the outputs of gates. Switch ME [16] assigns each sample to a single expert. For fair comparison, at inference a single expert is used. Table 3 shows that IME’s assignment mechanism yields superior results.

7 Related Work

Mixture of experts: [28] introduced ME over three decades ago. Since then many expert architectures have been proposed such as SVMs [12], Dirichlet Processes [48] and Gaussian Processes [55]. [30] introduced hierarchical assignment for MEs. [49] proposed an effective deep learning method that stacked ME as a layer between LSTM layers. [50, 35, 16] incorporated ME as a layer in Transformers. [44] introduced human-ML ME where the assignment module depends on human-based rules, and the experts themselves are black-box DNNs. IME combines interpretable experts with DNNs to produce an inherently-interpretable architecture with accuracy comparable to DNNs.

Interpretable DNNs for structured data: [5] proposed NAM which uses a DNN per feature; it does not consider feature-feature interactions and thus is not suitable for high-dimensional data. To address this, NODE-GAM [9] was introduced, modifying NODE [43] into a generalized additive model. Both NAM and NODE-GAM are only applicable to tabular data. [42] proposed the use of a soft DT to make DNNs more interpretable. N-Beats [42] was created for univariate time-series with a residual stack of MLP layers constraining to trend and seasonality functional forms.
to generate interpretable stacks. IME creates a per-user decision tree for tabular data recommendation systems. In contrast to these methods, IME (1) provides explanations that accurately describe the overall prediction process with minimal loss in accuracy, (2) supports both tabular and time-series data, and (3) can be easily used for complex large-scale real-world datasets.

8 Conclusion

We propose IME, a novel inherently-interpretable framework for structured data. IME has different forms: while one can provide explanations that are the exact description of how prediction is computed via interpretable models, the other can be used to adjust what ratio of samples can be predicted with interpretable models. We show that on real-world tabular and time-series data, while achieving useful interpretability capabilities, the accuracy of IME is on par with, and in some cases even better than, state-of-the-art black-box DNNs. Future work can address current limitations of IME, for example by enabling feature sparsity for easier-to-understand explanations with a high number of features, and making model selection more efficient with the multiple loss functions.

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A Appendix

IME Training procedure

Algorithm 2 overviews the training procedure. First, the model is trained in an end-to-end way to minimize the overall loss until convergence. Then, the experts are frozen, and the assignment module is trained independently to minimize the prediction loss. This alternating optimization approach first promotes expert specialization, and then improves the assignment module accuracy on trained experts. Since experts and the assignment module might have different architectures, they may converge at different rates [27]; hence, different learning rates are employed for each.

Algorithm 2: Training Interpretable Mixture of Experts

Input: Features $X$, targets $Y$, expert learning rate $\tau$, assignment learning rate $\rho$, hyperparameters $\beta, \gamma, \delta, \lambda$

Initialize: All experts parameters $f_\theta$, the assignment module $A_\phi$ & set previous error $E = 0$

while not converged do
  $X = [X; E]$;
  $\mathcal{L} = \mathcal{L}_{\text{pred}}(f, A, X, X, Y) + \beta \mathcal{L}_{\text{util}}(A, X) + \gamma \mathcal{L}_{\text{div}}(f, X) + \delta \mathcal{L}_{\text{smooth}}(A, X) + \lambda \mathcal{L}_{A,\text{pred}}(A, X, Y)$;
  $f_\theta = f_\theta - \tau \nabla \mathcal{L}$;
  $A_\phi = A_\phi - \rho \nabla \mathcal{L}$;

Update E;

Freeze experts and train assignment module;

while not converged do
  $\mathcal{L} = \mathcal{L}_{\text{pred}}(f_\theta, A_\phi, X, X, Y)$;
  $A_\phi = A_\phi - \rho \nabla \mathcal{L}$;

Interpretability Results

Sample-wise expert interpretability:

Fig. 9 shows feature weights of the interpretable LR model for different samples on Rossmann. For the first sample shown in Fig. 9a, the most influential feature was the number of customers entering the store. Whereas for the second sample shown in Fig. 9b, multiple features influence the model output.

(a) For this sample, the most influential feature was the number of customers.

(b) For this sample, multiple features influence the model output.

Figure 9: Sample-wise feature weights on Rossmann dataset.
User study details:

The users were given instructions as shown in Fig. 10.

Interpretability User Study Sample 1

The goal of this user study is to test two explanation methods generated from two different models. The task is to predict the model output given an explanation.

To test both explanations we will present examples from the Rossmann dataset. This is a retail dataset with the goal of predicting the daily sales of a store. Store sales are influenced by many factors, including promotions, competition, school and state holidays, seasonality, and locality. The dataset is available here

(https://docs.google.com/spreadsheets/d/1fmvh9UZLqEipf3dOqiKz6Bzy8KEpEUEHlyGSOpfDco0/edit?usp=sharing)

Sales - the turnover for any given day (this is what you are predicting)

Store - a unique Id for each store
Customers - the number of customers on a given day
Open - an indicator for whether the store was open: 0 = closed, 1 = open
StateHoliday - indicates a state holiday. Normally all stores, with few exceptions, are closed on state holidays. Note that all schools are closed on public holidays and weekends. 1 = public holiday, 2 = Easter holiday, 3 = Christmas, 0 = None
School holiday - indicates if the (Store, Date) was affected by the closure of public schools
Store Type - differentiates between 4 different store models: 1, 2, 3, 4
Assortment - describes an assortment level: 1 = basic, 2 = extra, 3 = extended
Competition Distance - the distance in meters to the nearest competitor store
Competition Open Since [Month/Year] - gives the approximate year and month of the time the nearest competitor was opened
Promo - indicates whether a store is running a promo on that day
Promo2 - Promo2 is a continuing and consecutive promotion for some stores: 0 = store is not participating, 1 = store is participating
Promo2 Since [Year/Week] - describes the year and calendar week when the store started participating in Promo2
Promo2 [month] - describes if Promo2 was running in that month it takes a boolean value 0/1

Use the training data to answer the following questions (you can try to find the nearest example and sort values to get the general trends on how input features affect the output).

Based on the training dataset and your understanding of the problem please answer the questions in the following sections. In each section, you will be given a training example and previous input values (if any), then you will be asked a series of questions on that sample. In the first question, we ask you to guess the correct output given the sample. Then assume that you are given a model explanation and asked to guess the model output given multiple explanations.

Figure 10: User study instructions
Then, a data-sample from Rossmann was provided as shown in Fig. 11 and the users were asked to answer questions based on two explanations.

Using the training data, predict the daily sales of the store in the sample below.

| Features          | Time Step 1 |
|-------------------|-------------|
| Store             | 1           |
| Day Of Week       | 1           |
| # Customers       | 712         |
| Open              | 1           |
| Promo             | 1           |
| State Holiday     | 0           |
| School Holiday    | 1           |
| Year              | 2015        |
| Month             | 1           |
| Day               | 5           |
| Store Type        | 1           |
| Assortment        | 1           |
| Competition Distance | 570       |
| Competition Open Since Month | 11     |
| Competition Open Since Year | 2007 |
| Promo2           | 1           |
| Promo2 Since Week | 13          |
| Promo2 Since Year | 2010        |
| Promo2 Jan       | 1           |
| Promo2 Feb       | 0           |
| Promo2 Mar       | 0           |
| Promo2 Apr       | 1           |
| Promo2 May       | 0           |
| Promo2 Jun       | 0           |
| Promo2 Jul       | 1           |
| Promo2 Aug       | 0           |
| Promo2 Sept      | 0           |
| Promo2 Oct       | 1           |
| Promo2 Nov       | 0           |
| Promo2 Dec       | 0           |

Below are two model explanations each from a different model where each feature value represents the importance of a feature to the model prediction, positive values indicate that as the value of this feature increases the sales values increase, and vice-versa for the negative values.

Use the explanations to answer the questions below.

Figure 11: Data-sample from Rossmann dataset.
Explanations from different models, and sample questions are shown in Fig. 12 and Fig. 13.

**Figure 12:** Explanation from Model A and sample question.

Given the above input and explanation A shown above (not your own intuition) if the number of customers changes from 712 to 800 how will the model A output change?

- [ ] Increase
- [ ] Decrease
- [ ] No change

**Figure 12:** Explanation from Model A and sample question.
Given the above input and explanation B (shown below) please predict model B’s output.

| Features                  | Time Step 1 | Explanation (feature importance weights) |
|---------------------------|-------------|------------------------------------------|
| Store                     | -0.14       |                                          |
| Day Of Week               | 0.47        |                                          |
| # Customers               | -0.82       |                                          |
| Open                      | 0.13        |                                          |
| Promo                     | 0.10        |                                          |
| State Holiday             | 0.02        |                                          |
| School Holiday            | 0.05        |                                          |
| Year                      | 0.00        |                                          |
| Month                     | 0.00        |                                          |
| Day                       | 0.03        |                                          |
| Store Type                | -0.08       |                                          |
| Assortment                | -0.10       |                                          |
| Competition Distance      | -0.10       |                                          |
| Competition Open Since Month | 0.56   |                                          |
| Competition Open Since Year | -0.13 |                                          |
| Promo2                    | -0.13       |                                          |
| Promo2 Since Week         | -0.08       |                                          |
| Promo2 Since Year         | -0.01       |                                          |
| Promo2 Jan                | -0.06       |                                          |
| Promo2 Feb                | 0.05        |                                          |
| Promo2 Mar                | 0.09        |                                          |
| Promo2 Apr                | -0.28       |                                          |
| Promo2 May                | 0.03        |                                          |
| Promo2 Jun                | 0.00        |                                          |
| Promo2 Jul                | -0.03       |                                          |
| Promo2 Aug                | 0.05        |                                          |
| Promo2 Sept               | 0.05        |                                          |
| Promo2 Oct                | -0.12       |                                          |
| Promo2 Nov                | 0.01        |                                          |
| Promo2 Dec                | -0.03       |                                          |

Given the above input and explanation B shown above (not your own intuition) if the number of customers changes from 712 to 800 how will the model B output change?

- [ ] Increase
- [ ] Decrease
- [ ] No change

**Figure 13:** Explanation from Model B and sample question.
Finally, the user was asked which model he trusts more as shown in Fig. 14.

**Experimental details**

All experiments were ran on a NVIDIA Tesla V100 GPU. We perform experiments in two settings – multivariate and univariate forecasting. The multivariate setting involves multivariate inputs and a single output. The univariate setting involves univariate inputs and outputs, which are the target values described below. We use MSE as the evaluation metric.

**Datasets**

- **Rossmann**: The dataset consists of samples from 1115 stores. The goal is to predict daily product sales based on sales history and other factors, including promotions, competition, school and state holidays, seasonality, and locality. Overall, the dataset consists of 30 different features.
- **Electricity**: The dataset measures the electricity consumption of 321 clients. We convert the dataset into hourly-level measurements and forecast the consumption of different clients over time.
- **Climate**: The dataset consists of 14 different quantities (air temperature, atmospheric pressure, humidity, wind direction, etc.), recorded every 10 minutes between 2009-2016. We convert the dataset into hourly-level measurements and forecast the hourly temperature over time.
- **ETT**: We conduct experiments on ETT (Electricity Transformer Temperature) [59]. This consists three datasets: two hourly-level datasets (ETTh) and one 15-minute-level dataset (ETTm), measuring six power load features and “oil temperature”, the chosen target value for univariate forecasting. Results for ETTh1 are available in main paper Table 2, results for ETTh2 and ETTm1 can be found in Table 7.

**Hyperparameters**

All baselines were tuned using [36] with at least 20 trials. Hyperparameter search grid used for each model is available in table [4]. To avoid overfitting, dropout and early stopping were used. The best hyperparameters were chosen based on the validation dataset while the results reported in the table are on the test dataset. For all IME experiments we set $k = 1$ for $L_{util}$. For $L_{div}(f, X)$, we set $\tau = 0.2$. All models were trained using Adam optimizer, and the batch size and learning rate values were modified at each experiment.

- **Rossmann** For CatBoost, LightGBM and XGBoost, we used parameters specified by benchmark [1].
  - *LR*: The batch size is 512 and learning rate is .001. *Soft DT (SDT)*: The batch size is 512, learning rate is .0001 and the depth is 5. *MLP*: The batch size is 512, 5 layers are used, each containing 128 hidden units with a learning rate .001. *NAM*: Each feature is modeled using a MLP with 2 hidden layers each with 32 hidden units, with a batch size 512 and learning rate .001.

- **Electricity** Hyperparameters for baseline are in Table [5]. For IME, we use a batch size of 512 and a sequence length 336. The remaining hyperparameters are available below:

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Figure 14: User study questions

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https://github.com/catboost/benchmarks/blob/master/kaggle/rossmann-store-sales/README.md
| Learning rate | LSTM | TCN | Transformer | Informer |
|---------------|------|-----|-------------|---------|
| 0.00001 to 0.1 | 64,128,256 | 64,128,256 | 64,128,256 | 64,128,256 |
| Batch size    | 64,128,256 | 64,128,256 | 64,128,256 | 64,128,256 |
| Hidden units  | 128, 256, 512 | 128, 256, 512 | 128, 256, 512 | 2048 |
| Encoder layers | 2 to 6 | N/A | 2 to 6 | 1 to 3 |
| Decoder layers | N/A | N/A | 2 to 6 | N/A |
| Levels        | N/A | 1 to 10 | N/A | N/A |
| Kernal        | N/A | 5 to 15 | N/A | N/A |
| Attention heads | N/A | N/A | 2.4, 8 | 8 |
| Embedding sizes | N/A | N/A | 128, 256, 512 | 512 |

Table 4: Hyperparameter search grid used for different models

| IME                  | Number of experts | Learning rates | Model Hyperparameters |
|----------------------|-------------------|----------------|-----------------------|
|                       |                   | τ | ρ | β | γ | δ | λ |
| IME                  | Linear Assign. LR Expert | 20 | .0001 | .001 | 10 | 0 | .1 | 1 |
| IME                  | Linear Assign. SDT Expert | 20 | .0001 | .001 | .1 | 0 | .1 | 1 |
| IME                  | MLP Assign. LR Expert | 20 | .0001 | .001 | .1 | 0 | .1 | 1 |
| IME                  | MLP Assign. SDT Expert | 20 | .0001 | .001 | .1 | 0 | .1 | 1 |

Table 5: Hyperparameters for Electricity dataset.
Climate Hyperparameters for baseline are in table 6. For IME, 512 batch size and a sequence length 336 the remaining hyperparameters are available below:

| Features      | IME          | Number of Experts | Learning rates | Model Hyperparameters |
|---------------|--------------|-------------------|----------------|-----------------------|
| Univariate    | Linear Assigner LR Expert | 2                | .002 .005   | τ ρ β γ δ λ            |
|               | LSTM Assigner LR Expert    | 2                | .001 .01    | 1 0 .1 1              |
| Multivariate  | Linear Assigner LR Expert | 10               | .00001 .001 | 1 .001 10 1           |
|               | LSTM Assigner LR Expert    | 10               | .00001 .001 | 1 0 10 1              |

| Univariate Model | Forecast horizon | Batch size | Sequence length | Learning rate |
|------------------|------------------|------------|-----------------|---------------|
| Auto-regressive   | 24               | 256        | 336             | .001          |
|                  | 48               | 256        | 336             | .005          |
|                  | 168              | 256        | 336             | .005          |
| LR                | 24               | 256        | 336             | .005          |
|                  | 48               | 256        | 336             | .001          |
|                  | 168              | 256        | 336             | .005          |
| LSTM              | 24               | 1024       | 24              | .01           |
|                  | 48               | 256        | 24              | .01           |
|                  | 168              | 256        | 24              | .01           |
| TCN               | 24               | 256        | 96              | .0005         |
|                  | 48               | 1024       | 96              | .0001         |
|                  | 168              | 1024       | 96              | .0005         |
| Transformer       | 24               | 64         | 168             | .0005         |
|                  | 48               | 64         | 168             | .001          |
|                  | 168              | 128        | 168             | .0005         |
| Transformer       | 24               | 128        | 168             | .0005         |
|                  | 48               | 128        | 168             | .001          |
|                  | 168              | 128        | 168             | .0005         |
| Transformer       | 24               | 1024       | 96              | .001          |
|                  | 48               | 1024       | 96              | .001          |
|                  | 168              | 1024       | 96              | .001          |
| Transformer       | 24               | 128        | 96              | .0005         |
|                  | 48               | 128        | 168             | .0005         |
|                  | 168              | 128        | 168             | .0005         |
| Transformer       | 24               | 512        | 168             | .0001         |
|                  | 48               | 512        | 168             | .0001         |
|                  | 168              | 512        | 336             | .0001         |

Table 6: Hyperparameters for Climate dataset.
### Additional Experiments

#### More ETT dataset results

| Methods | Black Box Models | White Box Models | Interpretable Mixture of Experts |
|---------|-----------------|-----------------|----------------------------------|
| LSTM    | Informer        | Transformer     | TCN                              |
| AR      | LR              | Interpretable Assignment | DNN Assignment                   |
| ETTh2   | 24   | .093 | .121 | .073 | .076 | .067 | .071 | **.065** | .066 |
|         | 48   | .122 | .145 | .108 | .110 | .104 | .101 | **.096** | .096 |
|         | 168  | .256 | .253 | .169 | .248 | .176 | .173 | **.167** | .167 |
| ETTm1   | 24   | .017 | .055 | .017 | .017 | .013 | .011 | .012 | **.011** |
|         | 48   | .029 | .056 | .361 | .362 | **.020** | .020 | .021 | **.020** |
|         | 168  | .161 | .117 | .166 | .110 | .060 | .049 | .047 | **.044** |

| Methods | Black Box Models | White Box Models | Interpretable Mixture of Experts |
|---------|-----------------|-----------------|----------------------------------|
| LSTM    | Informer        | Transformer     | TCN                              |
| AR      | LR              | Interpretable Assignment | DNN Assignment                   |
| ETTh2   | 24   | .224 | .385 | .346 | .263 | .244 | .105 | .098 | **.091** |
|         | 48   | .590 | 1.557 | .582 | .772 | .738 | .390 | **.260** | .263 |
|         | 168  | .923 | 2.110 | 1.124 | .817 | .770 | .578 | **.477** | .548 |
| ETTm1   | 24   | .034 | .070 | .029 | .035 | .024 | .022 | .017 | **.017** |
|         | 48   | .065 | .109 | .074 | .038 | .067 | .031 | **.029** | **.029** |
|         | 168  | .242 | .371 | .430 | .127 | .929 | **.069** | .078 | .078 |

**Table 7:** MSE for ETT datasets for different forecasting horizons. Best results are highlighted in bold.