
Enforcing Interpretability using Concept Bottleneck Transformer Layers for Time Series

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Abstract

Neurosymbolic AI, which combines deep learning with symbolic reasoning, aspires to yield models that are more explainable than pure deep learning models, and yet maintain or improve their performance. In this effort, temporal data, and specifically time series, are of particular interest: many important application domains involve changes over time that require dynamically changing concepts, but only few approaches have addressed this challenge. In this paper, we introduce a *Concept Bottleneck Transformer Layer* (CBTL), an encoder layer whose hidden representations are trained to encode predefined, human-interpretable concepts. We employ a Centered Kernel Alignment (CKA) regularizer to allow the learned representations to be similar to the concepts, *without requiring exact identity*. We apply our framework to a common time series transformer (Autoformer) and use a simple linear surrogate model and time-of-day information as interpretable concepts. We evaluate on synthetic data and six long-term time series benchmarks and find that predictive performance remains largely unaffected while interpretability is substantially improved. In particular, using activation patching, we causally intervene on the CBTL and obtain evidence that its components represent the predefined concepts. This illustrates how high-level concepts can be localized in a dedicated transformer layer and directly intervened on, rather than relying solely on post-hoc explanations.

Keywords

Concept Bottleneck Models, Time Series Forecasting, Transformers, Interpretability by Design, Neuro-Symbolic AI

Introduction

Deep time-series forecasting models can achieve high predictive performance, but their internal computations are often difficult to interpret (Benidis et al. 2022). In particular, it can be unclear whether forecasts rely on plausible temporal structure, such as autoregressive dynamics or calendar-related periodicity. Post-hoc methods can associate internal activations with such properties, but these interpretations are not guaranteed to be faithful (Ismail et al. 2020; Zschech et al. 2026).

An alternative approach ensures model interpretability by carefully constraining the model before or during training (Zschech et al. 2026). Concept bottleneck models (CBMs) are an example of such *inherently interpretable* models. In CBMs, deep learning is still applied, but used to first find intermediate concepts, which are predefined and human-interpretable concepts. These concepts then subsequently determine the predictions and, in some settings, support debugging or interventions (Koh et al. 2020; Poeta et al. 2023). CBMs can be thought of as providing a neurosymbolic interface: neural representations are used in between input and concept activations, but concepts whose activations reach a threshold can then be input to symbolic rules. For example, concept-level variables may be used to construct syntactic rule structures, learn logic rules, or model causal relations (Barbiero et al. 2023; Debot et al.; Moreira et al. 2024).

In this paper, we explore how this approach to inherent interpretability can be applied to time-series forecasting. This domain poses particular challenges, because the relevant human interpretable concepts are diverse – discrete, continuous, not-precisely delineated – or even partially lacking. We explore potential sources of ‘concepts’, and address the problem of **concept forcing**: encouraging information about a predefined concept to be represented in a designated model component. Rather than locating concepts post hoc, we encourage their localization during training and subsequently test whether the corresponding components are functionally relevant.

In particular, we propose a **symbolic training framework** for time series transformers using time series specific, yet domain-agnostic concepts, as shown in Figure 1. A key aspect of our training framework is to encourage the learned representations of the **concept bottleneck transformer layer (CBTL)** to be similar, but not identical, to the interpretable concepts. The interpretable concepts are enforced with the similarity measure Centered Kernel Alignment (CKA; Kornblith et al. 2019), which is included in the loss function as a regularizer. We additionally make a minimal but essential architectural modification by removing the residual connection around the bottleneck. This makes sure that all feature representations pass through the bottleneck.

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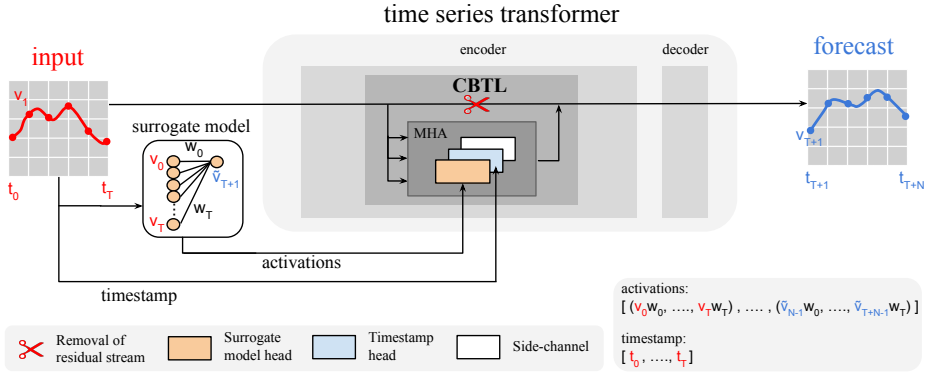


Figure 1. Overview of the symbolic training framework using a concept bottleneck transformer layer (CBTL). The CBTL is one encoder layer which is trained to be similar to predefined, interpretable concepts. The residual stream around the bottleneck is removed, such that all information passes through the bottleneck.

In our implementation of this framework, we choose as a first concept a simple, linear surrogate model and the second is time information (e.g. hour-of-day). Note that our definition of an interpretable concept is a higher-level concept represented by a vector rather than a scalar. Because each input is a time series, concepts must be defined across the temporal dimension and should therefore have a corresponding vector representation. Scalar concepts are too restrictive to capture this temporal structure, making the original concept bottleneck model (CBM) formulation infeasible for our setting (Koh et al. 2020). Although the concept vectors themselves are not necessarily human-understandable, encouraging the representations learned by the CBTL to resemble these vectors yields concept-aligned representations. This enables the localisation of concepts within specific model components, thereby improving the overall interpretability of the model.

We apply our concept bottleneck framework to Autoformer (Wu et al. 2021), which is a common time series transformer. We perform extensive experiments on seven datasets in the domains of electricity, traffic, weather, illness, exchange rate and (physical) electricity transformers. We show that our setup results in models that are more transparent while the overall performance remains largely unaffected. Furthermore, we causally test the obtained interpretations with an intervention study using activation patching.

Our contributions are summarized as follows:

1. We propose a novel training framework using a concept bottleneck transformer layer (CBTL) to enhance the interpretability of transformers for time series.
2. We demonstrate the feasibility of applying this framework to time series transformers by conducting extensive experiments on seven datasets for Autoformer, and identify interpretable concepts in each of these transformers.
3. We assess the faithfulness of the interpretability analysis by performing an activation patching experiment on the electricity dataset, and obtain evidence that

the identified components (in the concept bottleneck transformer layer) indeed have the hypothesized unique and causal role in the predictions of the target model.

Background and Related Work

This paper combines and builds upon foundational works from different fields, including neuro-symbolic AI, CBMs, knowledge transfer with CKA and time series transformers. CBMs have been applied to time series before (Ferfoglía et al. 2024), but not with the same interpretable concepts. Likewise, the similarity index CKA has been used before to transfer knowledge between models (Tian et al. 2023), yet, to the best of our knowledge, it has not been used to construct a CBM. This makes our work a unique contribution at the intersection of (mechanistic) interpretability, concept learning, and neuro-symbolic AI.

Concept Bottleneck Models

Concept bottleneck models (CBMs; Koh et al. 2020) have emerged as promising interpretable models, but are not usually considered neuro-symbolic AI (Poeta et al. 2023). Here, the concept bottleneck constrains the model to first predict interpretable concepts, and then to use only these concepts in the final downstream task. They are shown to be useful in multiple applications, such as model debugging and human intervention. The bottleneck allows for explaining which information the model is using and when it makes an error due to incorrect concept predictions.

One of the shortcomings of standard CBMs is that concept annotations are needed during training to learn the bottleneck, and concept labels do not necessarily contain all information needed to accurately perform the downstream task, and can therefore decrease the task accuracy (Mahinpei et al. 2021). Therefore, Zarlenga et al. (2022) propose Concept Embedding Models, where concepts are represented as vectors, such that richer and more meaningful concept semantics can be captured. CBMs and their variants are usually applied to the field of computer vision, and less frequently to natural language (Tan et al. 2024), graphs (Barbiero et al. 2023) or tabular data (Zarlenga et al. 2022).

Interpretability for Time Series

Applying CBMs to time series is challenging because meaningful high-level concepts must be defined. Ferfoglía et al. (2024) use Signal Temporal Logic formulas as concept embeddings for time series anomaly detection, and convert the concept embeddings into natural language. More recently, concurrent and subsequent work has explored alternative CBM approaches for time series, including concepts learned through input masking (Forest et al. 2025) and a small set of physically motivated concepts (Ma et al. 2025). Our earlier preprint (Sprang et al. 2025) introduced the CBTL framework for localizing pre-defined concepts in transformer components. This manuscript extends our earlier preprint in additional evaluations (the ablation and probing experiments) and in clarifying the conceptual contributions.

Centered Kernel Alignment

Inspired by neuroscience, **Centered Kernel Alignment** (CKA) measures the similarity between different representations from neural networks (Kornblith et al. 2019). By factoring out differences in scaling or orthogonal transformations, CKA captures intuitive notions of similarity between representations. To obtain the score, firstly, the similarity between every pair of examples in each representation separately is measured using a predefined kernel, and then the obtained similarity structures are compared. A kernel virtually maps data into a feature space such that the relative positions in the space are meaningful (Cristianini et al. 2001). There are different ways to learn the kernel from the data, and centered alignment is introduced as a similarity between kernels (Cortes et al. 2012). We use a linear kernel, which makes the CKA score defined as follows for representations X and Y using the Frobenius norm:

$$\text{CKA}(X, Y) = \frac{\|Y^\top X\|_F^2}{\|X^\top X\|_F \|Y^\top Y\|_F}. \quad (1)$$

Here, $X \in \mathbb{R}^{n \times p}$ and $Y \in \mathbb{R}^{n \times q}$ are representations of the same n observations, with each feature column centered by subtracting its mean across observations. CKA permits different feature dimensions p and q , since it compares similarity structures across observations rather than individual feature coordinates.

The CKA score can be used to transfer knowledge between different models when included in the loss function (Tian et al. 2023). In this work, the authors study knowledge distillation between a teacher and student model, and incorporate CKA into the loss function to transfer feature representation knowledge from the pretrained model to the incremental learning model (Parisi et al. 2019). The CKA score can also be used to measure alignment between the model representations and human-interpretable concepts in CBMs (Almudevar et al. 2026).

Method

We propose a training framework to make any transformer model interpretable by including a bottleneck based on knowledge transfer with CKA (Kornblith et al. 2019), as shown in Figure 2. The main idea is that we assign one of the encoder layers to be the CBTL, whose representations are subject to a soft constraint of being as similar as possible to predefined interpretable concepts. To this end, we calculate CKA scores with the interpretable concepts, and include these scores in the loss function. To introduce our method, we first formalise time series transformers.

Time Series Transformers

Time series transformers for long-term time series forecasting, such as Autoformer, obtain two types of input: (1) data values $\mathbf{X} \in \mathbb{R}^{I \times d}$, and (2) timestamps $\mathbf{T} \in \mathbb{R}^{I \times 4}$. More specifically, they can be regarded as a function $f: \mathbb{R}^{I \times d} \times \mathbb{R}^{I \times 4} \times \mathbb{R}^{O \times 4} \rightarrow \mathbb{R}^{O \times d}$, where I is the number of input time steps, O is the number of future time steps,

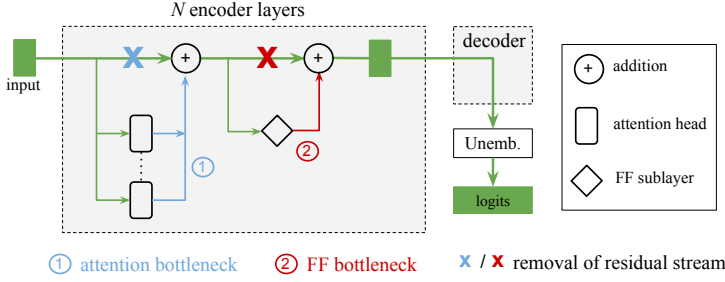


Figure 2. The CBTL can be on the attention (blue) or the feed-forward (red) module.

Note that the residual connection is removed at the location of the bottleneck (and the residual stream thus interrupted). Visualisation inspired by [Rai et al. 2024](#).

and d is the number of variables in the time series. The additional four dimensions of timestamps T represent four time features, namely hour-of-day, day-of-week, day-of-month, and day-of-year. The future timestamps are also provided, for which the model should forecast the future data values. Note that we explicitly introduce a notation for the timestamps to later define the CKA scores and the **activation patching** experiment.

Loss Function

The loss function encourages the model to represent the interpretable concepts in the bottleneck layer. Therefore, we add a term $\mathcal{L}_{CKA}$ based on the CKA scores of the bottleneck and the interpretable concepts (Eq. 3). In particular, low similarity between the bottleneck and the interpretable concepts results in a higher value for $\mathcal{L}_{CKA}$. The total loss function $\mathcal{L}_{Total}$ (Eq. 2), then, is a weighted average of the Mean Squared Error (MSE) loss $\mathcal{L}_{MSE}$ and the CKA loss $\mathcal{L}_{CKA}$:

$$\mathcal{L}_{Total} = (1 - \alpha) \mathcal{L}_{MSE} + \alpha \mathcal{L}_{CKA}, \quad (2)$$

$$\mathcal{L}_{CKA} = 1 - \frac{1}{c} \sum_{i=1}^c CKA_i, \quad (3)$$

where α is a hyperparameter, c is the number of concepts, and $CKA_i \in [0, 1]$ is the CKA score (using a linear kernel) between the model's representation and concept i (see Interpretability Analysis Section).

Interpretable Concepts in the Bottleneck

In this section, we describe how to calculate the CKA score to measure the presence of a concept. We refer to the Appendix for a more detailed description of the concept bottleneck framework.

Location bottleneck. We assign one encoder layer to be the bottleneck layer, because the encoder focuses on modelling seasonal information. Within the bottleneck layer, the

latent representations can be taken from two different types of blocks: the attention block ($\tau = Att$) and the feed-forward block ($\tau = FF$). These two options are illustrated in Figure 2. We assign c interpretable concepts over the latent representations, with the goal of teaching the corresponding model component to represent the predefined interpretable concepts.

Since the attention block is multi-headed, different heads naturally form the components of the attention bottleneck. Moreover, the components need to be divided between the heads, which would be convenient when the number of heads is a multiple of the total number of concepts to maintain a uniform **heads per concept** ratio. For the feed-forward bottleneck, we define the components to be slices from its output, such that stacking the components results in the original output.

Interpretable concepts. For the real-world time series, we use two domain-agnostic interpretable concepts which can be used for forecasting, namely: (1) a simple, human-interpretable surrogate forecasting model, (2) the input timestamps recorded with the time series. Note that each model token (time step) should map to each concept to calculate the CKA score.

1. We use a simple autoregressive model (AR) as a surrogate model, which predicts the next future value as a linear combination of its past values. This model is transparent, and the attribution of each input feature to the output can be simply interpreted by its weight. This concept can also be regarded as a baseline for the forecasting performance. The model is fit to the same training data as the transformer (with its order being the length of the input). **We fit a separate univariate model on the target variate of each dataset.** We use the model’s “activations” to calculate the CKA score. **In this context, “activations” mean the stacked coefficient-weighted values of the rolling input window at each step during long-term prediction. The model’s prediction equals its sum with a bias term. This representation captures both the input and the model’s coefficients for each step in long-term prediction.**
2. We use the hour-of-day feature from the timestamps T as interpretable time concept, denoted by $T_{hour\ of\ day}$. This provides the bottleneck with a simplified notion of time. **The observations are all input tokens in a mini-batch, resulting in target scalar values $Y \in \mathbb{R}^{n \times 1}$ using Equation 1.**

Removal of residual connection. Any transformer layer contains residual connections around the attention and feed-forward blocks. To ensure that all information passes through the bottleneck, we remove the residual connection around the bottleneck, potentially at the cost of a loss in performance. Otherwise, any concept, including the interpretable concepts, can be passed through the residual connection and compromise the bottleneck.

In the scenario that the number of components is equal to the number of interpretable concepts ($c = 2$), the construction of the bottleneck limits learning domain-specific features from the data, other than the interpretable concepts. Therefore, we perform experiments where we allow an extra component in the bottleneck to not learn any predefined concept ($c = 3$). In other words, the extra component serves as a *side-channel*

or *free component*, on which no CKA loss is calculated. The free component may partly restore the information lost by removing the residual connection, but with the advantage that we can monitor which information goes through it, and even visualize it (see Interpretability Analysis Section).

Implementation details.

In our experiments, we use transformer models with three encoder layers, of which the bottleneck layer is the second layer. **All other settings remain similar to the original Autoformer paper, which include** one decoder layer, the Adam optimizer (Kingma and Ba 2017) with an initial learning rate of 10^{-4} , and a batch size of 32. The training process is early stopped within 25 epochs. All experiments are repeated five times on different seeds, using hyperparameter $\alpha = 0.3$. Each model is trained on 1 Nvidia GeForce GTX 1080 Ti for approximately 30 minutes.

Experiments

We evaluate our framework on seven datasets, including synthetic and real-world data. The six real-world benchmarks consider the domains of energy, traffic, economics, weather, and disease (similar to Wu et al. 2021, see Table 1). These datasets are multivariate, and the task is to predict the future values of all variates. For example, the electricity dataset consists of hourly measurements of the electricity consumption of 321 customers from 2012 to 2014.

We apply our experiments to the Autoformer. First, we train a simple AR model on the same data, so that its outputs can be used to align the representations of the bottleneck. Then, we train the transformers with and without bottleneck, using different configurations for the bottleneck.

Synthetic Data

To show the general applicability of the bottleneck framework, we first train an Autoformer on a synthetic time series. In particular, we generate the dataset as the sum of different sines using the function f_{Total} with time t as follows:

$$f_{Total}(t) = f_1(t) + f_2(t) + f_3(t),$$

where:

$$\begin{aligned} f_1(t) &= \sin(2\pi t), \\ f_2(t) &= \frac{1}{2} \sin(4\pi t + \frac{\pi}{4}), \\ f_3(t) &= \frac{1}{4} \sin(6\pi t + \frac{\pi}{2}) + \epsilon_t. \end{aligned}$$

Note that all functions f_1 , f_2 and f_3 follow a periodic structure, and f_3 contains random noise ϵ from a normal distribution with standard deviation of 0.2. See Figure 3 for a visualization of the functions.

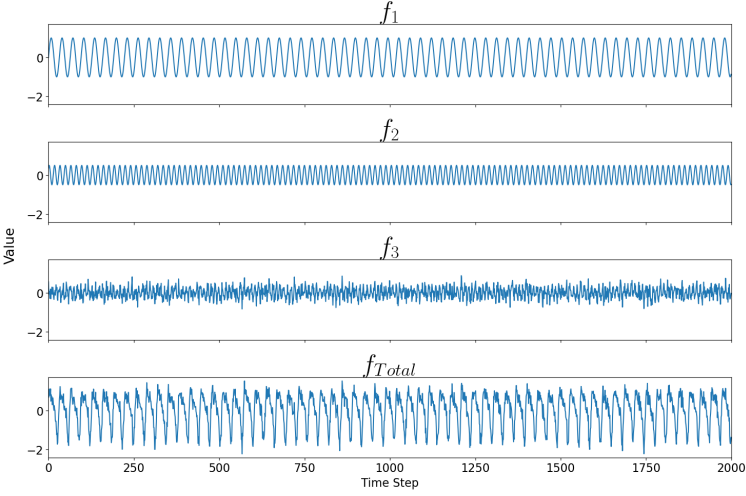


Figure 3. The synthetic time series dataset consists of three sines and a noise component.

Each concept in the bottleneck is defined as one of the underlying functions (i.e., f_1 , f_2 or f_3), for which the ground-truth is known by construction. For hyperparameter $\alpha = 0.8$ (see Method Section), we find that the model is able to forecast well, while achieving very high similarity scores. That is, the model obtains a Mean Squared Error (MSE) of 0.36 ± 0.17 and Mean Absolute Error (MAE) of 0.46 ± 0.12 on 5 different seeds. See Figure 4 for a sample forecast on the test data and the CKA scores of the model’s representations with the concept representations. The heads in the bottleneck `layer1` show high similarity for their respective concepts, e.g., a score of 0.93 for the head trained on f_1 (recall that CKA scores range from 0 for totally dissimilar to 1.0 for identical, although potentially scaled and rotated).

These results indicate that the model is successfully learning the **intended** interpretable concepts (high CKA scores), while maintaining downstream performance. Interestingly, when using lower values for hyperparameter α , we find that the performance slightly decreases (Figure 5). This suggests that properly chosen concepts improve the performance of the model, at least when the ground-truth underlying functions are known. Note that a low forecasting error cannot be expected for $\alpha = 1$, because in this edge case the loss function does not contain any term that represents the forecasting error.

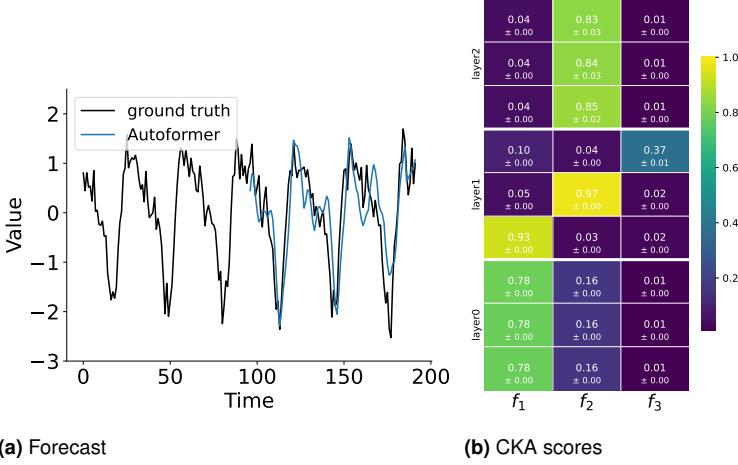


Figure 4. The CBTL successfully captures the interpretable concepts, while maintaining high forecasting performance. The CKA scores are given for three heads per layer (vertically) across the three concept vectors (horizontally) regarding the attention CBTL Autoformer on synthetic data.

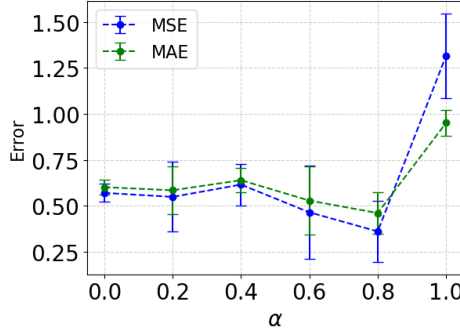


Figure 5. Increasing the weight of the CKA loss on the CBTL enhances model performance for the synthetic dataset. The forecasting error on the synthetic dataset decreases for α , for an Autoformer with attention CBTL (across 5 seeds).

Real-world data

Table 2 shows the performance of the Autoformer with and without our bottleneck on the benchmark datasets, compared to the AR surrogate model (i.e., the first interpretable concept) and Wu et al. (2021) (i.e., the original Autoformer model).

We find that including a bottleneck (either **Att bottleneck** or **FF bottleneck**) outperforms Wu et al. for three datasets (traffic, exchange rate and ETT), and stays within 5% of the MSE and MAE for the other three datasets. Surprisingly, the surrogate

Table 1. Descriptions of the datasets, as given by Zhou et al. (2022) and shared online. ‘Pred len’ denotes the prediction length used in our experiments. The input length for Illness is 36 and 96 for the others.

Dataset	Pred len	Description
Electricity	96	Hourly electricity consumption of 321 customers from 2012 to 2014.
Traffic	96	Hourly data from California Department of Transportation, which describes the road occupancy rates measured by different sensors on San Francisco Bay area freeways.
Weather	96	Recorded every 10 minutes for 2020 whole year, which contains 21 meteorological indicators, such as air temperature, humidity, etc.
Illness	24	Includes the weekly recorded influenza-like illness (ILI) patients data from Centers for Disease Control and Prevention of the United States between 2002 and 2021, which describes the ratio of patients seen with ILI and the total number of the patients.
Exchange rate	96	Daily exchange rates of eight different countries ranging from 1990 to 2016.
ETT	96	Data collected from electricity transformers, including load and oil temperature that are recorded every 15 minutes between July 2016 and July 2018.

Table 2. Error scores of different Autoformer models. For both metrics, it holds that a lower score indicates a better performance, where the best results are **bold**, and the second-best are underlined. Note that ‘No bottleneck’ is a baseline of the same size as the bottleneck (3 attention heads, 3 encoder layers), and ‘Wu et al.’ is not (8 attention heads, 2 encoder layers).

	Att bottleneck		FF bottleneck		No bottleneck		AR		Wu et al.	
	MSE	MAE	MSE	MAE	MSE	MAE	MSE	MAE	MSE	MAE
Electricity	0.231	0.338	<u>0.207</u>	<u>0.320</u>	0.280	0.368	0.497	0.522	0.201	0.317
Traffic	0.642	0.393	0.393	0.377	0.619	<u>0.387</u>	0.420	0.494	0.613	0.388
Weather	0.290	0.354	0.271	0.341	0.269	0.344	0.006	0.062	<u>0.266</u>	<u>0.336</u>
Illness	3.586	1.313	3.661	1.322	<u>3.405</u>	1.295	1.027	0.820	3.483	<u>1.287</u>
Exchange rate	0.195	0.323	0.155	0.290	<u>0.152</u>	0.283	0.082	0.230	0.197	<u>0.323</u>
ETT	0.177	0.282	0.174	0.280	<u>0.155</u>	<u>0.265</u>	0.034	0.117	0.255	0.339

AR model outperforms the other models for most datasets w.r.t. both MSE and MAE, even though this model is very simple. Note that the phenomenon that simple models sometimes beat time series transformers (Zeng et al. 2022) has been observed before*; for our purposes, the setup remains useful to investigate whether Transformer-based models

*There has been a vivid discussion about the relevance of these results, for instance here: <https://huggingface.co/blog/autoformer>. More information on the effect of AR as surrogate model can be found in the Appendix.

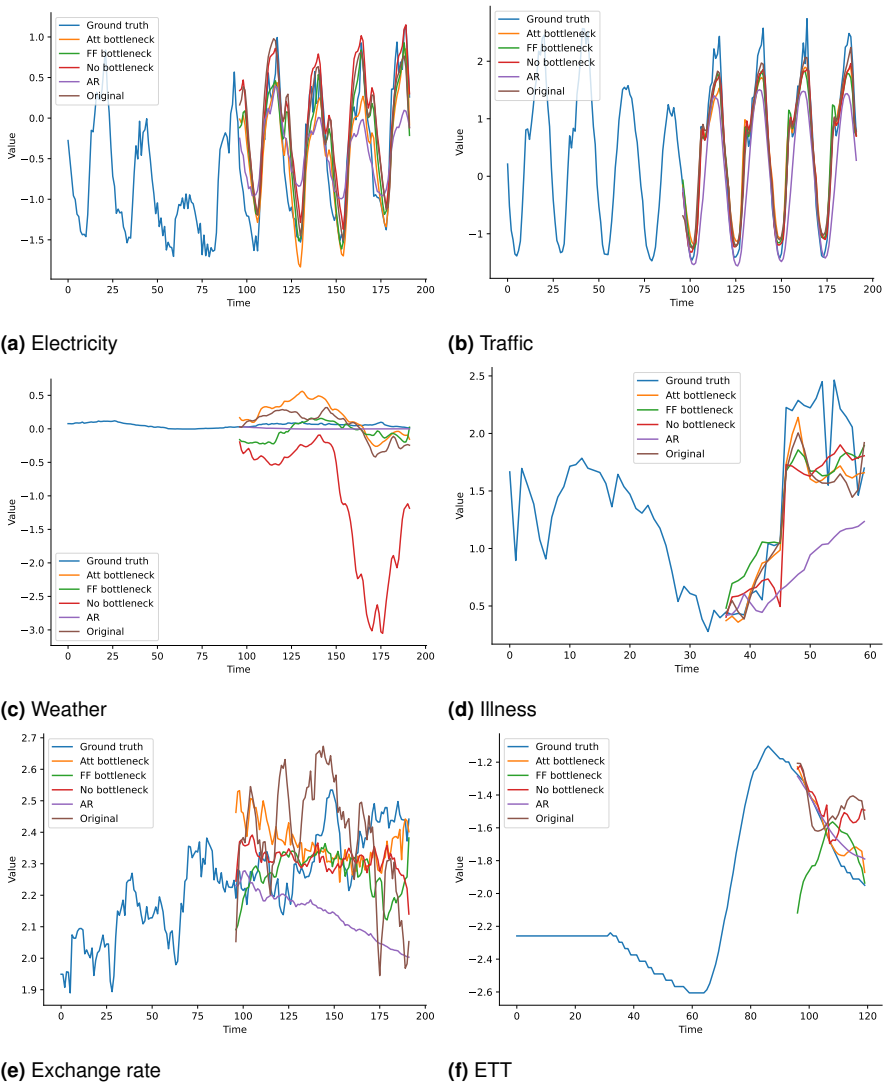


Figure 6. Models with or without CBTL obtain similar results. Forecasts of different models are given across datasets. The first part of the ground truth (shown in blue) is the input for the models.

can be made more interpretable. Visualizations of the forecasts from these models are shown in Figure 6.

Ablation Experiment Training a concept bottleneck layer involves two modifications: adding the CKA loss and removing the residual connection. To isolate these effects, we perform an ablation experiment where we remove the residual connection, but do not include the CKA loss. Table 3 reports results for removing the residual connection at the attention block (**No Resid Att**) and the feed-forward block (**No Resid FF**). We find that the effect of the residual removal is mixed across datasets and depends on the location (attention vs. feed-forward block). In particular, the performance of these no-CKA models does not necessarily approach that of the bottleneck models, for example on the Traffic dataset. This indicates that the behavior of the bottleneck layers cannot solely be attributed to removing the residual connection. Notably, the residual removal does not uniformly harm the forecasting performance. Across several datasets, the residual-removal models are comparable to, or outperform, the baseline no-bottleneck model (**No bottleneck**). One possible explanation is that removing the residual connection encourages the affected component to learn a more informative representation, rather than relying on information from the residual connection.

Table 3. Residual-removal ablation. Lower error scores are better, with **best** and second-best results.

	Att bottleneck CKA + removal		FF bottleneck CKA + removal		No bottleneck no CKA, no removal		No Resid Att no CKA, removal		No Resid FF no CKA, removal	
	MSE	MAE	MSE	MAE	MSE	MAE	MSE	MAE	MSE	MAE
Electricity	0.231	0.338	0.207	0.320	0.280	0.368	0.218	0.325	0.203	0.319
Traffic	0.642	0.393	0.393	0.377	0.619	0.387	0.655	0.401	0.672	0.407
Weather	0.290	0.354	0.271	0.341	0.269	0.344	0.249	0.319	0.245	0.321
Illness	3.586	1.313	3.661	1.322	3.405	1.295	3.718	1.355	3.499	1.291
Exchange rate	0.195	0.323	0.155	0.290	0.152	0.283	0.167	0.299	0.148	0.279
ETT	0.177	0.282	0.174	0.280	0.155	0.265	0.097	0.218	0.103	0.225

Analysis Extensions We extended the analysis using different training set-ups, and obtained similar results. In particular, we repeated the experiments for different transformer architectures (vanilla **transformer** and FEDformer), for different values of hyperparameter α and with excluding the free component.

Interpretability Analysis

To demonstrate the impact of the bottleneck on model interpretability, we first conduct a CKA analysis on the bottleneck layer with the corresponding interpretable concepts, and then visually demonstrate how each component contributes to the final forecast.

CKA Analysis To test the extent to which the bottleneck represents the interpretable concepts, we calculate the CKA scores of the model’s representations with the concept representations. The scores of the feed-forward bottleneck on the electricity dataset are shown in Figure 7. Note that the bottom, middle and upper layer of `layer1` correspond to the AR, hour-of-day, and free component of the bottleneck, respectively.

The scores show that the representations in the bottleneck layer are much more similar to the intended concepts than the representations from the model without bottleneck:

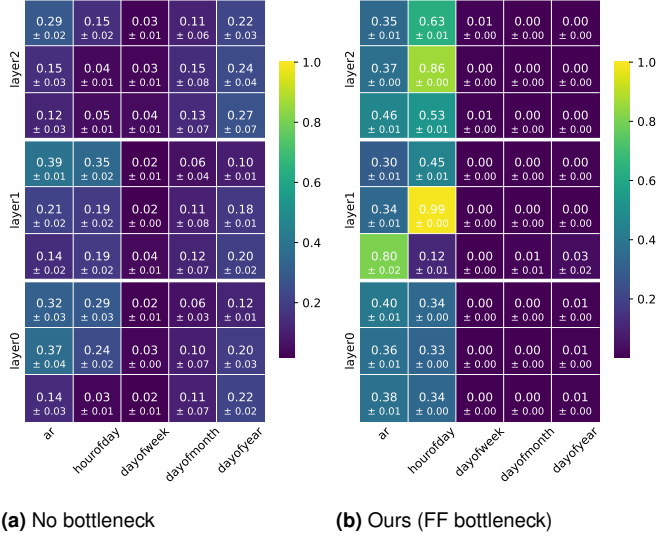


Figure 7. CBTL components learn representations that are similar to the interpretable concepts. CKA scores on different concepts for the encoder of the Autoformer without bottleneck and with FF bottleneck. The first component of *layer1* (lower row) of the CBTL is trained to be similar to AR, and the second component (middle row) to the hour-of-day concept. The scores are calculated on three batches of size 32 from the electricity test data. Recall that CKA is defined on a scale from 0 to 1, where 1 denotes perfect similarity.

0.80 for the AR model, and 0.99 for the hour-of-day feature, whereas the model without bottleneck does not show high similarity to the interpretable concepts. This indicates that the training framework can encourage the components to form representations that are perfectly similar to the interpretable concepts. Additionally, note that the CKA scores of other layers than the bottleneck layer are also higher in Fig. 7b, which indicates that these other model components also learn to represent the interpretable concepts. This does not affect the interpretability of the bottleneck layer itself (see Activation Patching Section below).

Component Visualizations Because the model components all read and write from the residual stream (Elhage et al. 2021), we can visualize the contributions to the final prediction of each component separately by applying the entire decoder to the component representations (Decoder Lens method, Langedijk et al. (2023)). This way, we obtain visualizations of the contributions of each component in the bottleneck, see Figure 8. We obtain the output from the full bottleneck by applying the decoder to the output of the bottleneck (after performing layer normalization). The output from each component individually is obtained by masking the other components with zero (close to the mean).

From Figure 8a and 8b we see that the different bottleneck components are similar to the concepts they were trained on. In particular, the first component shows a forecast

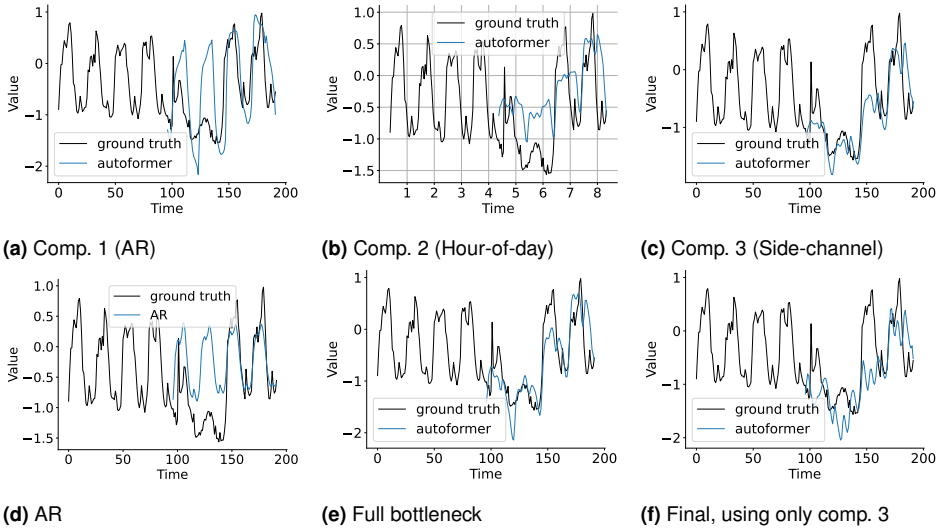


Figure 8. The CBTL components individually predict their interpretable concept.

Forecasts from individual bottleneck components by masking the other components with zero in 8a, 8b and 8c (FF bottleneck Autoformer on electricity data). The first half of the ground truth forms the input to the model. Note that the horizontal axes are the same across all figures, but Fig. 8b contains a grid of days instead of numbered hours. Fig. 8d shows the forecast made by the surrogate model AR; Fig. 8e shows the forecast of the entire layer (i.e., all components together), and 8f shows the forecast of the final layer when only the third component is used in the bottleneck layer. Note the difference between Figures 8c and 8f, where we decode from the bottleneck and the final layer, respectively.

with correct periodicity and few irregularities, similar to the actual forecast from the AR model. Likewise, the second component shows a periodicity to the actual hour-of-day feature. The third component is not trained to be similar to an interpretable concept, and seems to pick up on the high-frequency patterns in the data, e.g., the low, second peak in the forecast. This observation is further strengthened by Figure 8f, which shows that the final forecast consists of many high-frequency patterns when using only the third component from the bottleneck.

Probing Additionally, we evaluate the presence of the pre-defined concepts with diagnostic probes. For each input window, we extract frozen activations from each bottleneck component and train linear probes to predict their respective concept targets.

The concept labels are not naturally scalar labels. Rather, they are sequences and are aligned with the window of the input time series. To simplify the set-up, we opt for tasks to test whether the designated model components contain *some* of the information. In particular, we train (1) a probe on predicting the hour-of-day associated with the final input time step (a 24-class classification task), and (2) a probe on predicting the final value of the forecast horizon for the same input window (a regression task). These probes

Table 4. Linear probes on bottleneck representations. Hour-of-day probes predict the hour at the final input time step. AR probes predict the final value of the AR surrogate forecast; values are reported as probe / matched training-mean baseline. Hour-of-day information is (almost) perfectly decodable on electricity, traffic and ETT and substantially decodable on weather. AR-related information is strongly decodable on traffic, while results on the remaining datasets are mixed or below the matched constant baseline.

	Hour-of-day		AR / baseline		
	Acc $\uparrow$	Macro-F1 $\uparrow$	MSE $\downarrow$	MAE $\downarrow$	R2 $\uparrow$
Electricity	1.000	1.000	0.845 / 0.392	0.748 / 0.509	-1.157 / -0.001
Traffic	1.000	1.000	0.231 / 1.496	0.376 / 1.091	0.846 / -0.002
Weather	0.779	0.780	0.000 / 0.000	0.001 / 0.002	-1.423 / -2.259
Illness	N.A.	N.A.	82.747 / 4.499	5.604 / 1.987	-149.586 / -7.188
Exchange rate	N.A.	N.A.	7.492 / 2.638	2.147 / 1.475	-15.139 / -4.684
ETT	0.990	0.990	92.875 / 1.430	5.261 / 1.066	-274.703 / -3.244

do not measure whether the model has learned a complete or unique representation of either concept. Instead, they provide evidence of whether the designated component contains some linearly decodable information about the pre-defined concepts.

Table 4 reports the performance of the linear probes. The hour-of-day classification probe is evaluated using accuracy and macro-F1, i.e., the unweighted mean of the per-class F1 scores. The AR regression probe is evaluated using MSE, MAE and R^2 . The coefficient of determination R^2 compares the probe’s squared prediction error with that of a predictor that always outputs the mean of the test set (where $R^2 = 1$ is a perfect prediction, $R^2 = 0$ is the same squared error as predicting the test-set mean, and $R^2 < 0$ is when the probe has more squared error than the mean predictor). The hour-of-day probe achieves perfect accuracy and macro-F1 on electricity, traffic and ETT, indicating that the designated representation contains linearly decodable information about the final hour-of-day feature of the input. Performance is lower, but remains substantial, on weather. Hour-of-day labels are not evaluated for illness and exchange rate, because their temporal granularity does not support the 24-class task.

The AR probe results are more dataset-dependent. On traffic, the representation strongly predicts the final AR forecast value, obtaining $R^2 = 0.846$ and substantially improving over the matched training-mean baseline (MSE = 0.231 vs. 1.496). This result indicates that the traffic bottleneck contains information relevant to predicting the final forecast of the AR surrogate. On weather, the probe equals or improves on the matched baseline in all metrics, although its negative R^2 indicates that it remains worse than a predictor that outputs the mean of the held-out targets. For the other datasets, the learned AR probe performs worse than the constant baseline. Note that the constant baseline also obtains negative R^2 values on several datasets. Because this baseline predicts the mean target value of the training data, these negative values are consistent with a distribution shift of the train and test data of the final-AR target. Although the final AR value is not consistently linearly decodable across datasets, it is only one scalar summary of the vector-valued AR concept. Its train-test shift on several datasets may

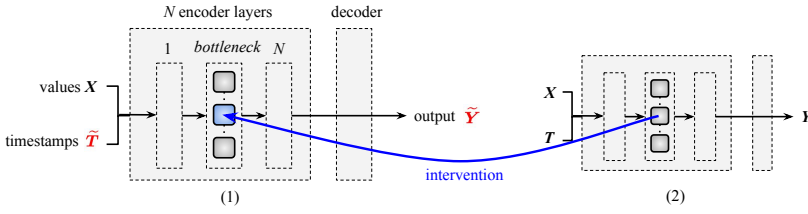


Figure 9. Activation patching allows for mechanistically testing the interpretations of the CBTL. In the **activation patching** experiment we run the model on time-shifted input (1), but replace the activations of the hour-of-day component with those from a run (2) on unshifted timestamps T .

make it an unstable target for probing, and alternative trajectory summaries may be more stable and better aligned with information encoded in the bottleneck.

In conclusion, the probing results confirm that our concept forcing setup is indeed effective, as the hour-of-the-day and AR features can, mostly, be successfully decoded from the concept bottleneck layer that our training objective targeted. However, probing analyses by themselves cannot establish that the identified representations are causally involved in the behavior of the model, leading us to explore activation patching next.

Activation Patching

The main benefit of interpreting trained models is gaining a deeper understanding and, possibly, more control of the model’s behavior. This can be useful in the scenario of out-of-distribution data at inference time. If the data changes in features that can be interpreted in the model, it is feasible to intervene locally in these concepts to exclusively employ the model with data from its training distribution. Additionally, an **activation patching** experiment can be regarded as a causal interpretability test, where successful patching indicates a successful representation of the concept of interest.

To show such benefit of our framework, we perform activation patching (or causal tracing, Meng et al. 2023), where causal effects of hidden state activations are researched by evaluating the model on clean and corrupted inputs. We evaluate the trained model on data with shifted timestamps and compare it with performing patching on the shifted concept.

More specifically, we delay the input timestamps $T \in \mathbb{R}^{I \times 4}$ with a fixed number of hours to obtain the shifted timestamps $\hat{T}$, so that the learned patterns associated to the hour-of-day feature are misleading. We run the model on both types of timestamps, and perform **activation patching** in the bottleneck by substituting the activations based on the shifted time with the activations based on the original, see Figure 9 for an overview.

We perform the **activation patching** experiment with the electricity dataset, and perform shifts of up to and including 23 hours. We compare the performance of the **activation patching** with out-of-the-box performance of the same model on the shifted dataset (see Figure 10).

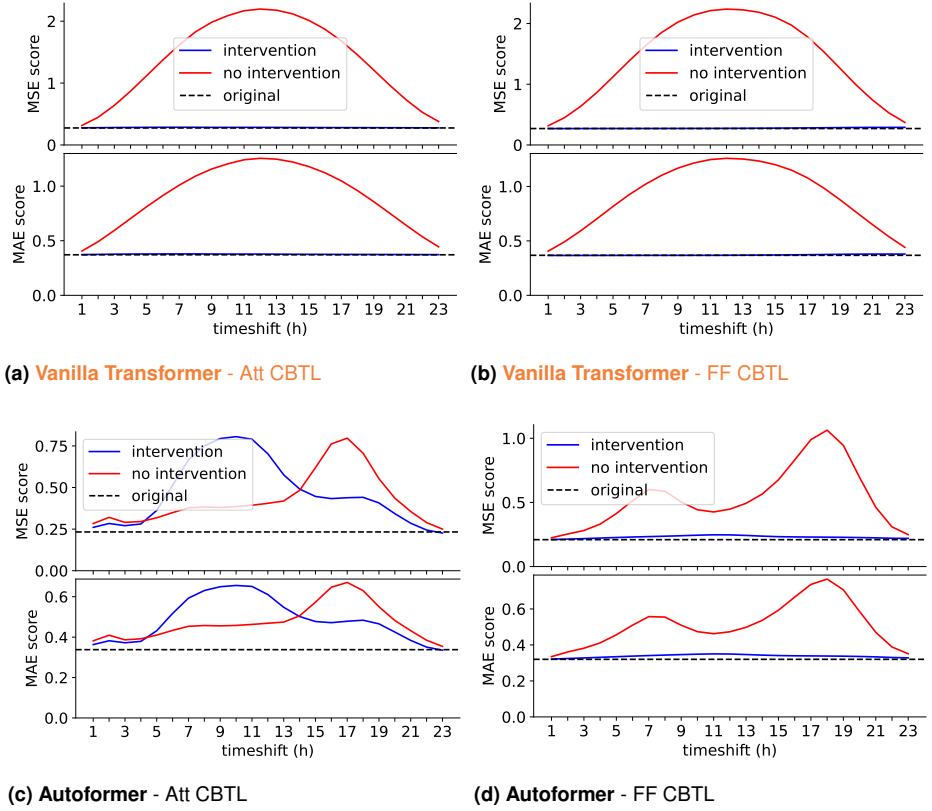


Figure 10. The hour-of-day concept is successfully learned and used downstream by the vanilla Transformer and Autoformer FF CBTL. The dashed line represents the performance on the data without timeshift. The **activation patching** experiment shows the performance of the model on electricity data with shifted timestamps. Patching retrieves the original performance almost perfectly.

Remarkably, **activation patching** on the vanilla Transformer and Autoformer feed-forward CBTL achieves similar results to the original performance for all timeshifts. This indicates that the bottleneck can effectively learn to represent the hour-of-day concept in the dedicated bottleneck component. Most interestingly, the models only utilise this interpretable concept in the CBTL and *not* in other encoder layers (because the experiment only intervenes in the bottleneck).

Note that activation patching hurts the performance for smaller timeshifts in the attention bottleneck of the Autoformer. This indicates that the choice of bottleneck location is relevant for the Autoformer, and suggests that the concept of time might be represented in a more complex manner in those attention heads. Presumably, the

architectural changes to the attention head by the Autoformer (which include auto-correlation), increase the complexity of the representations. This could result in more downstream consequences when patching compared to patching in the slice of a linear layer (as done in the FF CBTL) or in the vanilla attention heads.

Discussion and Conclusions

In this work, we propose a training framework based on Concept Bottleneck Models to enforce interpretability of time series transformers. We introduce a new loss function based on the similarity score CKA of the model’s representations and interpretable concepts. We apply our framework to Autoformer using synthetic data and six benchmark datasets. Our results indicate that the overall performance remains unaffected, while the model’s components become more interpretable. Additionally, it becomes possible to perform local **activation patching** when employing the model after a temporal data shift.

The main limitation of our concept bottleneck framework is that interpretable concepts have to be decided on before training, which might require domain knowledge. Representations for these concepts have to be available during training. However, domain-agnostic concepts such as the AR surrogate model and hour-of-day information are sufficient. Additionally, our framework increases computational complexity. This might be problematic if the size of the architecture increases.

Another limitation is the problem of concept leakage, which is a known problem with CBMs (Mahinpei et al. 2021). In standard settings, the concept bottleneck encodes more information than the intended concepts. Our results show that the designated model components learn the concepts, and while allowing a side-channel in the bottleneck, it is plausible that the designated model components have additionally learned to represent other information than the intended concepts.

An interesting direction for future research would be to optimize the number and type of interpretable concepts in the bottleneck, and extend the framework to other modalities. We trained mostly using two domain-agnostic concepts (AR and hour-of-day), but including more concepts, possibly domain-specific, would be very interesting. For example, one could consider choosing speech and music concepts for audio time series. Additionally, the framework should also work for transformers in other modalities, e.g., language and vision, although these models are usually of larger size. We hope our work contributes to a deeper understanding of (time series) transformers and their behavior in different fields. In particular, recent progress in the field of mechanistic interpretability is based on the observation that the residual stream of the transformer encourages modular solutions, which enables localized concepts or specialized circuitry to perform a specific task. Instead of relying on post-hoc localization of these concepts, our paper presents a demonstration that we can encourage locality of concepts, without a significant loss in performance.

Regarding societal impact, this work enables transparent time series forecasting models, which enable explainable forecasts. However, in the case of malicious use, biases could be included in the models. Harm could be prevented by developing mechanistic interpretability techniques for bias detection in time series models.

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Appendix

Formalization of Concept Bottleneck Framework

Any time series transformer obtains two types of input: (1) data values $\mathbf{X} \in \mathbb{R}^{I \times d}$, and (2) timestamps $\mathbf{T} \in \mathbb{R}^{I \times 4}$. The transformer consists of an encoder and a decoder, which are both constructed from one or multiple layers. Any encoder layer contains two sub-layers: a multi-head attention mechanism (Att) and a fully connected neural network (FF). Every sub-layer contains a residual connection around it. More specifically, the output $\mathbf{X}^\ell$ of any encoder layer ℓ is:

$$\begin{aligned}\mathbf{X}^\ell &= \text{Encoder}(\mathbf{X}^{\ell-1}) \\ &= \text{LayerNorm}(\text{FF}(\mathbf{S}^\ell) + \mathbf{S}^\ell), \\ \mathbf{S}^\ell &= \text{LayerNorm}(\text{Att}(\mathbf{X}^{\ell-1}) + \mathbf{X}^{\ell-1}),\end{aligned}$$

where

$$\begin{aligned}\text{FF}(\mathbf{x}) &= \max(0, \mathbf{x}\mathbf{W}_1 + \mathbf{b}_1) \mathbf{W}_2 + \mathbf{b}_2, \\ \text{Att}(\mathbf{x}) &= \mathbf{W}_0 \cdot \text{Concat}(\mathbf{h}_1(\mathbf{x}), \dots, \mathbf{h}_h(\mathbf{x})).\end{aligned}$$

For future reference, we denote the output of the feed-forward module as follows: $\text{FF}(\mathbf{S}^\ell) = \mathbf{Z}^\ell \in \mathbb{R}^{d_1 \times d_2}$. We omit the definition of the decoder, because our bottleneck framework does not include it. Note that the exact implementation of each (sub-)layer depends on the type of transformer.

Concept Bottleneck Transformer Layer

We assign one encoder layer to be the bottleneck and construct it such that it contains c latent representations or *components*, i.e., $(\mathbf{H}_i)_{i=1}^c$. Depending on the bottleneck type τ , these latent representations are either taken from the attention mechanism or the feed-forward module. More specifically:

$$\mathbf{H}_i = \begin{cases} \mathbf{h}_i(\mathbf{x}) & \text{if bottleneck type } \tau = \text{Att}, \\ \mathbf{Z}_i & \text{if bottleneck type } \tau = \text{FF}. \end{cases}$$

Since the attention block is multi-headed, different heads naturally form the components of the attention bottleneck. For the feed-forward bottleneck, we define the components to be slices (in d_1) from its output $\mathbf{Z}$, such that stacking the components results in the original output.

Note that the residual connection around the corresponding bottleneck component is removed, and that each component $\mathbf{H}_i$ should represent a predefined interpretable concept.

Activation Patching

In the **activation patching** experiment, we shift the time stamps $\mathbf{T}$ to obtain $\tilde{\mathbf{T}}$. The key aspect of the experiment is to run the transformer on the shifted time stamps $\tilde{\mathbf{T}}$, and

replace the input representations $\widetilde{\mathbf{X}}^{b-1}$ of the bottleneck layer b with $\mathbf{X}^{b-1}$ (based on $\mathbf{T}$), but only in the component that represents the time concept.

More specifically, if type $\tau = \text{Att}$, we intervene on the attention block in the bottleneck as follows:

$$\text{Att}(\mathbf{x}, \widetilde{\mathbf{x}}) = \mathbf{W}_0 \cdot \text{Concat}(\mathbf{h}_1(\widetilde{\mathbf{x}}), \mathbf{h}_2(\mathbf{x}), \mathbf{h}_3(\widetilde{\mathbf{x}})),$$

and, if type $\tau = \text{FF}$, as follows:

$$\text{FF}(\mathbf{x}, \widetilde{\mathbf{x}}) = \text{Stack}(\widetilde{\mathbf{Z}}_1, \mathbf{Z}_2, \widetilde{\mathbf{Z}}_3).$$

In both functions we make use of the fact that the time concept is represented in the second component, and there are three components in total. This **activation patching** can be done in the bottleneck only, because, by construction, the location of its concept representations is known.

Detailed results

Table 5. Performance of different models in Mean Squared Error (MSE) and Mean Absolute Error (MAE). The bottlenecks **do** contain a free component ($c = 3$), and use AR as surrogate model. The model with no bottleneck is an original Autoformer of similar size (**meaning 3 attention heads, and 3 encoder layers**). For all datasets, the shortest prediction lengths from Wu et al. (2021) are used, see Table 1. The standard deviation is determined using five different seeds.

Free component	Att bottleneck		FF bottleneck		No bottleneck		AR		Wu et al.	
	MSE	MAE	MSE	MAE	MSE	MAE	MSE	MAE	MSE	MAE
Electricity	0.231 ± 0.009	0.338 ± 0.005	<u>0.207</u> ± 0.005	<u>0.320</u> ± 0.005	0.280 ± 0.165	0.368 ± 0.111	0.497 ± 0.000	0.522 ± 0.000	0.201 ± 0.003	0.317 ± 0.004
Traffic	0.642 ± 0.022	0.393 ± 0.013	0.393 ± 0.013	0.377 ± 0.006	0.619 ± 0.015	<u>0.387</u> ± 0.005	<u>0.420</u> ± 0.000	0.494 ± 0.000	0.613 ± 0.028	0.388 ± 0.012
Weather	0.290 ± 0.027	0.354 ± 0.020	0.271 ± 0.016	0.341 ± 0.011	0.269 ± 0.000	0.344 ± 0.000	0.006 ± 0.000	0.062 ± 0.000	<u>0.266</u> ± 0.007	<u>0.336</u> ± 0.006
Illness	3.586 ± 0.241	1.313 ± 0.040	3.661 ± 0.237	1.322 ± 0.050	<u>3.405</u> ± 0.208	1.295 ± 0.044	1.027 ± 0.000	0.820 ± 0.000	3.483 ± 0.107	<u>1.287</u> ± 0.018
Exchange rate	0.195 ± 0.029	0.323 ± 0.025	0.155 ± 0.010	0.290 ± 0.013	<u>0.152</u> ± 0.003	0.283 ± 0.003	0.082 ± 0.000	0.230 ± 0.000	0.197 ± 0.019	<u>0.323</u> ± 0.012
ETT	0.177 ± 0.003	0.282 ± 0.004	0.174 ± 0.006	0.280 ± 0.005	<u>0.155</u> ± 0.004	<u>0.265</u> ± 0.002	0.034 ± 0.000	0.117 ± 0.000	0.255 ± 0.020	0.339 ± 0.020

Table 6. Performance on different datasets, where the bottlenecks **do not** contain a free component ($c = 2$). AR is used as surrogate model in the bottlenecks. The model with no bottleneck is an original Autoformer of similar size (**meaning 2 attention heads, 3 encoder layers**). For all datasets, the shortest prediction lengths from Wu et al. (2021) are used, see Table 1. The standard deviation is determined using five different seeds.

No free component	Att bottleneck		FF bottleneck		No bottleneck		AR		Wu et al.	
	MSE	MAE	MSE	MAE	MSE	MAE	MSE	MAE	MSE	MAE
Electricity	0.224 ± 0.006	0.332 ± 0.003	0.206 ± 0.009	0.321 ± 0.009	<u>0.202</u> ± 0.006	<u>0.318</u> ± 0.007	0.497 ± 0.000	0.522 ± 0.000	0.201 ± 0.003	0.317 ± 0.004
Traffic	0.629 ± 0.023	0.394 ± 0.015	0.627 ± 0.031	0.392 ± 0.025	<u>0.613</u> ± 0.018	0.378 ± 0.007	0.420 ± 0.000	0.494 ± 0.000	0.613 ± 0.028	0.388 ± 0.012
Weather	0.281 ± 0.025	0.348 ± 0.018	0.260 ± 0.015	0.333 ± 0.013	<u>0.257</u> ± 0.004	<u>0.332</u> ± 0.005	0.006 ± 0.000	0.062 ± 0.000	0.266 ± 0.007	0.336 ± 0.006
Illness	3.966 ± 0.296	1.401 ± 0.073	3.721 ± 0.268	1.351 ± 0.053	3.585 ± 0.331	1.333 ± 0.070	1.027 ± 0.000	0.820 ± 0.000	<u>3.483</u> ± 0.107	<u>1.287</u> ± 0.018
Exchange rate	0.208 ± 0.026	0.333 ± 0.022	0.158 ± 0.009	0.293 ± 0.009	<u>0.152</u> ± 0.006	<u>0.284</u> ± 0.007	0.082 ± 0.000	0.230 ± 0.000	0.197 ± 0.019	0.323 ± 0.012
ETT	0.178 ± 0.011	0.283 ± 0.007	0.174 ± 0.01	0.283 ± 0.009	<u>0.165</u> ± 0.004	<u>0.274</u> ± 0.004	0.034 ± 0.000	0.117 ± 0.000	0.255 ± 0.020	0.339 ± 0.020