AUNET (Attention-based Unified Network): Leveraging Attention Based N-BEATS for Enhanced Univariate Time Series Forecasting

by

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Declaration

It is hereby declared that

1. The thesis submitted is my original work while completing my degree at BRAC University.
2. The thesis does not contain material previously published or written by a third party, except where this is appropriately cited through full and accurate referencing.
3. The thesis does not contain material that has been accepted, or submitted, for any other degree or diploma at a university or other institution.
4. We have acknowledged all main sources of help.

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Ethics Statement

This research adheres to ethical guidelines by ensuring the responsible use of data and maintaining integrity throughout the experimentation process. The dataset used for this study was obtained from publicly available sources, and no personally identifiable information (PII) was involved. All analyses were conducted transparently, and the findings were presented without bias. The research complies with ethical standards in machine learning and deep learning, including proper data handling, model evaluation, and fair reporting of results.

Abstract

This study presents AUNET, an enhanced version of the N-BEATS model specifically designed for univariate time series forecasting by incorporating a multi-head self-attention mechanism. The motivation behind AUNET is to address key limitations of the traditional N-BEATS model, such as redundancy in feature learning, inefficiency in capturing temporal dependencies, and over-complexity for univariate datasets. The proposed model aims to improve the representation of temporal features by selectively focusing on relevant parts of the input sequence, thus enhancing predictive accuracy while maintaining computational efficiency.

The AUNET architecture leverages multi-head self-attention layers to capture both short-term fluctuations and long-term dependencies effectively. By integrating attention mechanisms, AUNET dynamically focuses on significant time intervals, minimizing redundancy and improving generalization capabilities. The model's modular structure allows for an interpretable approach to time series forecasting, providing insights into critical temporal patterns.

Experimental results demonstrate that AUNET outperforms the original N-BEATS and other attention-based variations, achieving lower **Mean Absolute Error (MAE) 0.8857** and **Root Mean Squared Error (RMSE) 0.9896**, along with a higher **R^2 score 0.9948**, indicating improved prediction accuracy and robustness. Comparisons with models incorporating Neural Attention Memory (NAM), ProbSparse Attention, and Multi-Query Attention further highlight the superiority of AUNET in terms of capturing diverse temporal relationships while balancing model complexity.

The findings suggest that AUNET offers a powerful solution for accurate, interpretable, and efficient time series forecasting, particularly applicable in domains such as finance, climate modeling, and energy demand prediction. Future work will explore expanding AUNET's applicability to multivariate time series and enhancing its interpretability for real-time forecasting applications.

Keywords: AUNET, N-BEATS, Time Series Forecasting, Multi-Head Self-Attention, Univariate Forecasting, Deep Learning, Temporal Dependencies, Interpretability

Dedication

This work is dedicated to my family and supervisor Dr. Md. Golam Rabiul Alam, whose guidance, encouragement, and unwavering support have been so important to getting this research done. Honestly, their belief in me was what kept me going throughout this journey, even when things got tough. I couldn't have done it without them.

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Chapter 1

Introduction

Forecasting time series predicts the upcoming values from data points of the past and is applied across domains like weather forecasting, finance, economics, and healthcare. It plays a crucial role in weather prediction by analyzing past atmospheric data, such as temperature, humidity, and pressure, to forecast future conditions. Accurate weather predictions are essential for planning daily activities, disaster management, and agricultural practices [37]. In finance, time series forecasting is used for predicting stock prices, foreign exchange rates, and market trends, which helps financial institutions manage risks and optimize trading strategies [8]. In healthcare, forecasting assists in resource allocation, predicting disease outbreaks, and improving patient care through early detection [27] [31]. In general, time series forecasting helps optimize processes and make strategic decisions. With growing data availability, improving forecast accuracy has become increasingly important, particularly for real-time applications [22].

1.1 Overview of Time Series Forecasting

Recently, time series forecasting has become one of the basic techniques to encourage many kinds of predictions based on past data. Its applications are found in finance, energy management, meteorology, and public health. Traditional statistical methods have long been a cornerstone for time series analysis and forecasting; among these stands the ARIMA model developed by Box and Jenkins [1]. All of these methods are based on the stationarity assumption and apply best in conditions of linearity in the relationship between variables in the series [2]. However, real-time data in time series is mostly non-linear in features and has complex patterns, which requires more sophisticated modeling techniques such as artificial neural networks (ANNs) [9] [21].
In particular, studies show that ANNs can outperform traditional models (e.g., ARIMA) when their architecture is enriched by seasonal components for some contexts, such as electricity consumption or energy demand forecasting [25] [3]. ANNs are capable of learning non-linear relationships, and adding seasonal and trend components has further improved their accuracy, especially for fluctuating and high-frequency data [7]. Additionally, the inclusion of advanced architectures like Convolutional Neural Networks (CNNs) for feature extraction has further boosted the capabilities of ANN models by identifying intricate patterns in data [5]. Moreover, deep learning methods such as Recurrent Neural Networks (RNNs) and Long Short-

Term Memory (LSTM) networks have attracted much attention due to their ability to model long-term dependencies and manage huge volumes of data in an effective way [35] [17] [6]. LSTMs, in particular, have been successful in overcoming issues like the vanishing gradient problem, which allows them to retain information over long sequences and predict complex temporal patterns effectively.
Recent works have also integrated neural network architectures with attention mechanisms to enhance the accuracy of multivariate time series forecasting, especially when working with intricate, nonlinear data [18] [19]. Attention mechanisms have been particularly effective in improving the performance of LSTMs by allowing models to focus on the relevant portions of historical data, which helps capture dependencies across longer time intervals [28] [29]. In addition, attention mechanisms have enabled models to assign different weights to input features, which has proven beneficial for tasks involving multivariate time series [26]. Techniques like causal inference have also been employed to estimate the effects of certain interventions and exogenous variables in time series, allowing for more robust predictions and better decision-making in practical applications, such as public health and economic policy planning [24] [15]. Although machine learning and deep learning methodologies have shown great promise, selecting appropriate models while balancing complexity and interpretability remains a long-standing challenge. Hybrid models, such as those combining ARIMA with neural networks, have been explored by scholars to capitalize on the strengths of both statistical and machine learning methods, providing a more flexible approach for modeling complex time series data [23] [32].
The N-BEATS algorithm has been designed specifically for the purpose of performing univariate time series forecasting based on neural networks [25]. The N-BEATS model leverages a neural network architecture for the extraction of patterns in trends and seasonality from historical data. N-BEATS achieves this by using fully connected layers, residual connections between layers, and block segments, which allows it to perform both back-cast and forecast operations effectively [25]. This in turn helps the model capture complex patterns present in the time series data. Furthermore, the model's tuning flexibility and its ability to provide highly accurate performance across a wide range of datasets have made it an important and dependable tool for analyzing time series data [25] [32].

1.2 Research Problem

Over recent years, attention mechanisms have become a more prominent part of various neural network applications [18] [12]. Attention mechanisms often allow models to concentrate on the most important parts of the input to produce a more accurate and reliable output. Applications in text analysis, image classification, and language translation have leveraged attention mechanisms to generate better results, as the models can dynamically assess the importance of various input features [13] [20]. These mechanisms have proven crucial for handling long sequences and understanding complex interactions in data [30].
Likewise, infusing attention mechanisms also helps time-series forecasting models to highlight required time intervals and concentrate on relevant patterns, resulting in more dependable predictions [28] [26]. Recent research suggests that combining attention mechanisms with N-BEATS can significantly improve its capacity to handle univariate time series forecasting, as attention provides an additional mechanism

for focusing on relevant temporal elements within the data [29] [34]. The N-BEATS model, although successful for forecasting, still faces some challenges when used for univariate data:

- **Redundancy and Inefficiency**: Fully connected networks result in increasing parameter counts, adding more complexity than required and increasing the risk of overfitting. This is especially true for univariate data.
- **Lacking Temporal Mechanisms**: N-BEATS struggles to capture long-term temporal dependencies effectively without components like RNNs, convolutions, or attention mechanisms.
- **Over Complexity of Model**: The model runs the risk of being over-parameterized for univariate time series, which hinders its ability to generalize, especially with small datasets, resulting in increased resource requirements.
- **Limited Interpretability**: The block-based approach used in N-BEATS lacks clear interpretability, making it harder for domain experts to analyze results.

Thus, there is a key scope to improve N-BEATS for univariate time series by attempting to reduce complexity, enhance temporal representation, increase generalization, and improve interpretability overall. Adding an attention-based approach seems to be a promising way to handle these issues, as it allows the model to dynamically assign importance to specific parts of the input components, leading to a more effective, interpretable, and accurate prediction [36].

1.3 Research Contribution

This study introduces AUNET, an improved version of the N-BEATS model designed specifically for univariate time series forecasting, featuring a multi-head self-attention mechanism. The key contributions are outlined below:

- **Enhanced Temporal Dependency Representation**: By using multi-head self-attention, AUNET can capture both short-term variations and long-term dependencies effectively, which helps overcome some of the weaknesses of the original N-BEATS model [33].
- **Improved Parameter Efficiency and Generalization**: The attention mechanism enables the model to selectively focus on the most relevant time steps, reducing redundancy and enhancing its generalization capabilities, leading to improved parameter efficiency and minimized risk of overfitting [30].
- **Enhanced Interpretability**: Attention provides insights into the importance of different time steps, improving model interpretability for domain experts [34].
- **Better Handling of Complex Dynamics**: Attention helps AUNET adaptively focus on critical parts of the input, enhancing its ability to handle nonlinear dynamics and complex temporal relationships [33].

- **Reduced Model Complexity**: Multi-head self-attention replaces some fully connected layers, reducing model complexity without compromising prediction quality [30].
- **Superior Predictive Performance**: Experimental results show that AUNET outperforms the original N-BEATS in metrics like MAE, RMSE, and R^2, providing more accurate and robust forecasts, especially for nonlinear dependencies [11].

1.4 Thesis Organization

The thesis is structured as follows:

- **Chapter 1: Introduction** - This chapter introduces the concept of time series forecasting, its importance, and various applications across different domains such as weather forecasting, finance, and healthcare. It discusses the limitations of traditional forecasting methods and presents the motivation behind improving the N-BEATS model by integrating attention mechanisms.
- **Chapter 2: Related Work** - This chapter reviews existing literature on traditional statistical approaches, machine learning methods, and deep learning models used for time series forecasting. Special emphasis is placed on attention mechanisms and their application to enhance forecasting accuracy.
- **Chapter 3: Background Study** - This chapter details the N-BEATS architecture and attention mechanisms, providing an overview of how the original model operates and the role of attention in improving temporal representation.
- **Chapter 4: Proposed AUNET Scheme** - The chapter describes the proposed AUNET model, including its architecture, which integrates multi-head self-attention mechanisms to address limitations found in the original N-BEATS. The step-by-step implementation and details of the model's components are also covered.
- **Chapter 5: Implementation** - This chapter explains the dataset preparation, feature extraction, and training procedures used for implementing AUNET. Details about preprocessing, feature engineering, hyperparameter tuning, and system configuration are included to provide a complete understanding of the experimental setup.
- **Chapter 6: Performance Evaluation** - The performance of AUNET is evaluated against baseline models, including the original N-BEATS and other variants incorporating different attention mechanisms. The evaluation metrics used are Mean Absolute Error (MAE), Root Mean Squared Error (RMSE), and the Coefficient of Determination (R^2). Comparisons are made through error metrics, visualizations, and detailed discussions.
- **Chapter 7: Conclusion** - This chapter summarizes the findings of the research, highlighting the improvements achieved with AUNET. It also discusses the limitations of the proposed model and suggests potential future research

directions to further enhance forecasting accuracy and applicability in different domains.

This organization ensures a comprehensive exploration of the research problem, methodologies, and findings, while presenting the contributions of AUNET in the context of time series forecasting.

Chapter 2

Related Work

Traditional forecasting methods have long been the cornerstone of time series analysis, providing a fundamental approach to understanding temporal data. Techniques such as Autoregressive Integrated Moving Average (ARIMA), Exponential Smoothing (ETS), and Seasonal Decomposition of Time Series (STL) have been extensively utilized due to their ability to handle linear relationships and decompose data into meaningful components. Despite their success, these methods have inherent limitations, particularly in capturing non-linear trends, handling volatile data, and managing intricate temporal dependencies. These shortcomings have necessitated the development of more advanced methods, paving the way for modern approaches, such as deep learning and hybrid models, which aim to overcome the complexities that traditional methods struggle to address.
This chapter provides an overview of these conventional techniques, highlighting their strengths, limitations, and the motivation for advancing towards more sophisticated time series forecasting methodologies.

2.1 Traditional Forecasting Methods

Conventional methods of time series forecasting have served as the foundational framework for time series analysis for numerous decades. Among the most prevalent models are Autoregressive Integrated Moving Average (ARIMA), Exponential Smoothing (ETS), and Seasonal Decomposition of Time Series (STL). The ARIMA model, developed by Box and Jenkins, has garnered significant popularity owing to its capacity to capture linear relationships via autoregressive and moving average components, while simultaneously accommodating trends and seasonal variations [1], [21].
Notwithstanding its prevalent application, the ARIMA model presumes that the underlying data is stationary, signifying that its statistical characteristics remain constant throughout time. This assumption may present challenges in contexts where time series data display non-linear trends or encounter structural breaks or shifts in the fundamental trajectory [10]. To address these challenges, transformations such as differencing are often applied to stabilize the data; however, these transformations can be complex and may not always provide satisfactory results. Conversely, Exponential Smoothing methods, including Holt-Winters, provide alternative methodologies by emphasizing trend and seasonal components; however, they also operate under the assumption of relatively uncomplicated data structures

[3], [25]. These methods are computationally efficient and perform well for short-term forecasting, particularly for univariate time series data.
The Seasonal Decomposition of Time Series (STL) is another common technique, which decomposes the time series into seasonal, trend, and residual components. STL is advantageous because of its robustness and flexibility in handling complex seasonal patterns that evolve over time [4]. However, similar to ARIMA and ETS, STL is limited when it comes to capturing non-linear relationships or dealing with highly volatile data.
The conventional techniques, although efficient in handling linear and stationary datasets, encounter difficulties when tasked with modeling non-linear relationships, intricate seasonal fluctuations, or long-term dependencies. These shortcomings have driven the development of more sophisticated methodologies capable of capturing complex patterns over extended periods, consequently leading to the exploration of machine learning and deep learning frameworks [9], [22], [23]. Furthermore, these traditional methods often require substantial manual feature engineering and domain expertise to achieve optimal performance, which limits their scalability and applicability to more complex datasets.

2.2 Deep Learning Based Time Series Forecasting

Deep learning-based approaches have become prominent in time series forecasting due to their capacity to model complex patterns and dependencies in sequential data. Traditional models, like ARIMA, are often limited by their linear assumptions, while deep learning models can handle non-linear relationships and multivariate data effectively [2], [14]. Recurrent Neural Networks (RNNs), particularly Long Short-Term Memory (LSTM) networks, were early applications in deep learning-based forecasting. LSTMs address the vanishing gradient problem, making them suitable for long-term dependencies, which is essential in applications such as finance and climate modeling [6], [19], [35]. LSTMs are particularly well-suited for capturing long-term temporal dependencies in sequential data, which makes them a natural fit for time series forecasting tasks where historical patterns influence future values.
Convolutional Neural Networks (CNNs) have also been applied to time series forecasting, particularly for capturing local temporal dependencies. By treating time series data similarly to image data, CNNs enhance pattern recognition in short-term intervals, enabling them to identify local trends and seasonality [5], [15]. The use of CNNs has been particularly effective in applications such as energy consumption forecasting and anomaly detection, where capturing localized changes is crucial.
More recently, hybrid models combining CNNs and LSTMs have shown superior performance by leveraging the strengths of both architectures in capturing both local and sequential dependencies [15], [17]. These hybrid models provide a more holistic approach by using CNNs to extract local features and LSTMs to model the sequential nature of time series data.
Another breakthrough in time series forecasting is the application of Transformer models, which are known for their self-attention mechanism that enables capturing long-range dependencies more efficiently than RNNs and LSTMs. Transformers have proven to be highly effective in handling long sequences due to their ability to attend to all time steps simultaneously, making them well-suited for large-scale forecasting tasks [18], [27]. The ability of Transformers to parallelize training has

also led to significant reductions in computational cost, making them a popular choice for tasks requiring scalability, such as multivariate forecasting and anomaly detection. Transformers have found applications in fields like healthcare, where modeling patient data over long periods is essential, and in finance, where they help predict market trends by analyzing vast amounts of historical data.
Recent research has also explored neural basis expansion architectures like N-BEATS, which are specifically designed for time series forecasting without requiring traditional decomposition techniques for trend and seasonality. N-BEATS utilizes a stack of fully connected layers with residual connections, allowing the model to learn complex patterns directly from the raw data [25]. Its modular architecture has demonstrated robustness across a wide range of forecasting tasks. A recent study explored the integration of N-BEATS with the Temporal Fusion Transformer to predict surface temperature, contributing to the understanding of global warming trends and showcasing the adaptability of N-BEATS in integrating advanced attention-based models for improved long-term forecasting performance [29], [36]. The use of attention mechanisms in N-BEATS and other architectures has further enhanced performance by allowing models to focus selectively on significant time steps, leading to more accurate forecasts [26], [28].

2.3 Refined Attention Techniques in Forecasting Time Series

Recently, there has been much emphasis on the attention mechanisms within neural networks, especially within disciplines such as NLP and computer vision. The attention mechanism enables the model to focus its attention on specific parts of the input during the prediction rather than considering the entire input sequence as being equally important [12], [13], [18]. This targeted emphasis allows the model to identify connections that may extend across various segments of the input, thereby enhancing its effectiveness in tasks where contextual understanding and relational dynamics are essential.
The self-attention mechanism, introduced in the Transformer architecture by Vaswani et al. (2017), has had a profound impact on sequence modeling [18]. The self-attention mechanism allows every element of the input sequence to interact with every other element, thereby capturing both local and global dependencies. This has been revolutionary in tasks like machine translation, where understanding relationships between words across a sentence is crucial. Self-attention has also enabled parallel processing of input sequences, making models like Transformers highly scalable and efficient. In time series forecasting, attention mechanisms have been incorporated into models like RNNs and LSTMs to enhance their ability to focus on relevant time steps, which helps capture long-range dependencies and improves prediction accuracy. For instance, attention can enable the model to pay more attention to specific past time steps where similar patterns occurred, which is particularly useful for scenarios involving recurring seasonal or cyclical patterns [17], [26], [28].
The integration of attention mechanisms in time series forecasting has been an area of active research. Traditional models like ARIMA and ETS are limited by their linear assumptions and struggle to handle complex dependencies. To address this, researchers have explored combining attention mechanisms with deep learning models

such as Recurrent Neural Networks (RNNs) and Long Short-Term Memory (LSTM) networks [17], [35]. Qin et al. (2017) introduced a dual-stage attention-based RNN model that leverages both temporal attention and feature-based attention, enabling the model to focus on relevant features and time steps for more accurate predictions [17]. This approach demonstrated significant improvements over standard LSTMs, especially in multivariate time series forecasting where different features contribute to the prediction. The use of attention mechanisms allowed the model to capture important temporal patterns without being overwhelmed by irrelevant data points.
Further advancements were seen with the introduction of Transformer-based models for time series forecasting. Unlike RNNs, which process sequences sequentially, Transformers use self-attention mechanisms to process all time steps in parallel, making them more efficient and capable of capturing long-range dependencies [18], [20], [27]. Transformers have been adapted for various time series tasks, including anomaly detection and multivariate forecasting, by treating time steps as "tokens" similar to words in a sentence.
Despite these successes, applying attention mechanisms within architectures like N-BEATS is still a developing area. Some attempts have been made to combine the strengths of N-BEATS' block-based architecture with attention to improve its focus on relevant time steps, but challenges remain. For instance, integrating attention effectively requires balancing the model's ability to generalize across different datasets while maintaining interpretability and efficiency [26], [28].
Hybrid models that combine the robust forecasting capabilities of N-BEATS with the dynamic focus of attention mechanisms represent a promising direction for future research. These models aim to capture both short-term and long-term dependencies more effectively, enabling more accurate and robust predictions across various domains, from weather forecasting to financial analysis [19], [26], [28].
A recent comparison between the topological attention approach [16], [31] and the proposed model highlights key differences in their application of attention mechanisms. While both models enhance forecasting by focusing on significant parts of the input, the proposed model utilizes multi-head self-attention for capturing different temporal dependencies, aiming to improve prediction accuracy. In contrast, topological attention also leverages structural features of the data, which enhances interpretability and is particularly advantageous for datasets with clear cyclic patterns. Depending on the data characteristics and the need for interpretability, either approach may offer distinct advantages.

Chapter 3

Background Study

This section covers the N-BEATS architecture, designed for univariate time series forecasting, and the significance of attention mechanisms in neural networks. It explains how N-BEATS leverages stacked blocks to improve forecast accuracy, and explores key attention mechanisms like scaled dot-product and multi-head attention. The discussion also includes attention-based models such as Transformers and their applications in tasks like machine translation and text summarization, demonstrating their effectiveness in handling complex temporal and sequential data.

3.1 N-BEATS Architecture

The N-BEATS is a neural network-based architecture explicitly fabricated for univariate time series forecasting. The key components of this architecture are explained below.
An illustration of the N-BEATS (Neural Basis Expansion Analysis Time Series) architecture, intended for time series forecasting, may be found in the above figure 3.1. The architecture seen in the illustration can be explained as follows:

1. Overall Structure: The process of creating forecasts from time series data using the N-BEATS architecture is depicted in the image. Several blocks and stacks are used in the initial processing of the input time series, each of which adds to the final forecast. Both a "backcast" (a reconstruction of the input) and a "forecast" (a prediction of future values) are the intended outputs of the model [25] [19] [32]. The backcast helps in effectively modeling residuals, which are then passed on to subsequent blocks for refining the forecasts. This approach allows the model to gradually improve the accuracy of the predictions by learning from the residual errors at each block [14].

2. Fully Connected Stack (FC Stack) and Block Input: The block receives the time series data as input. A fully connected (FC) stack, usually consisting of several layers (four layers are displayed here), makes up each block. To reconstruct the portion of the input time series that the block was in charge of, the block creates a backcast. In addition, the block produces a forecast, which is the time series's estimated future values based on the model. The actions carried out by the FC stack to generate the prediction and backcast are represented by the functions θ^b and θ^f, respectively [19] [27] [29]. The backcast and forecast are essential components for

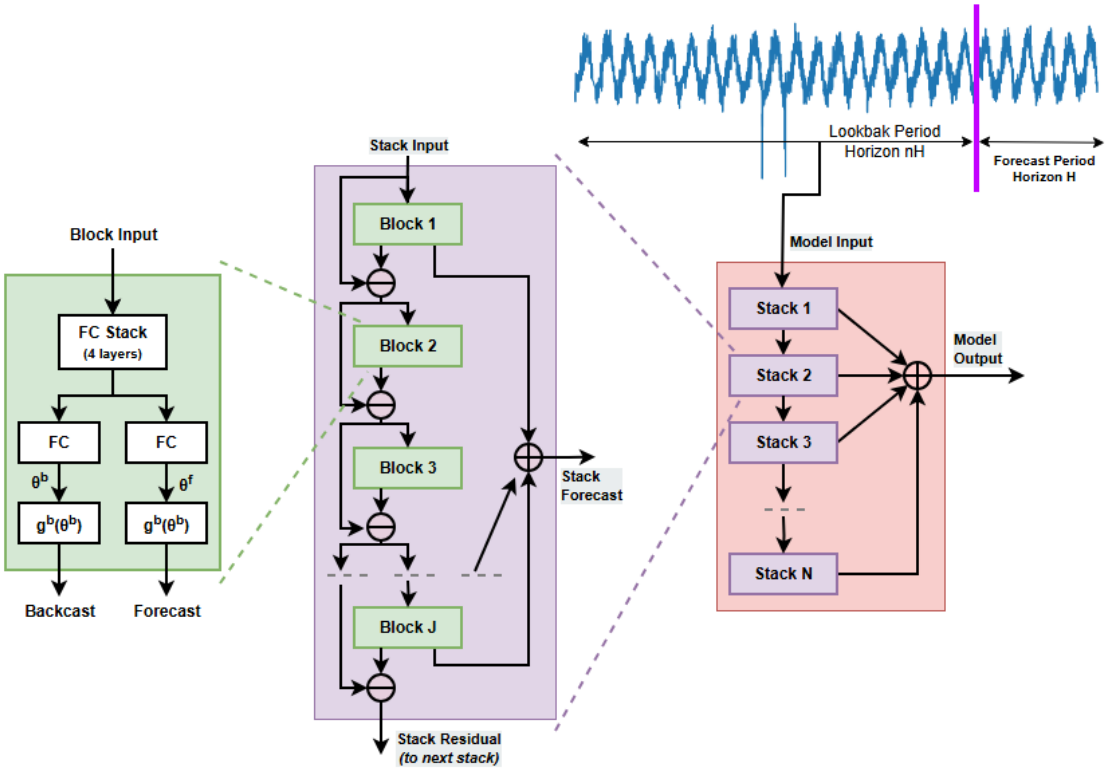

Figure 3.1: Structure of N-BEATS Architecture [25]

capturing both the short-term and long-term dynamics in time series, providing a more robust modeling of residuals [10].

3. Stack of Blocks: A stack is created by placing several blocks on top of one another. Every block in the stack handles the residual from the block before it, which is the difference between the input and the backcast. Block 1 creates a forecast and backcast based on the original input. The following block receives the residual or the difference between the input and backcast. Block by block, from Block 2 to Block K, the forecast is further refined by operating on the residual from the preceding block. The forecasts from each block in the stack are combined to create the stack forecast [25] [23] [31]. This iterative refinement process helps capture both linear and non-linear aspects of the time series, thereby improving the model's overall forecasting capabilities [16].

4. Multiple Stacks: The architecture has multiple stacks, each of which could have a distinct focus on a particular aspect of the time series (trend, seasonality, etc.). Each stack, from Stack 1 to Stack M, builds upon the residuals from the one before it, gradually improving the forecast. The global prediction is created by combining the output from each stack [19] [23] [30]. Different stacks focusing on trend and seasonality allow the model to adapt to various types of time series data and improve the overall performance of the forecast, especially in data with complex seasonal patterns [4].

5. Final Forecast: The global forecast, which is derived by adding the contributions from each stack, is the N-BEATS model's ultimate output. Based on the

model's construction and training, the architecture enables both short- and long-term forecasts [22], [27]. The combination of multiple stack outputs provides flexibility in capturing a wide range of temporal dependencies, allowing for accurate forecasting across different types of time series with varying properties [11].
6. Lookback and Forecast Periods: The upper portion of the figure displays a time series that is separated into two periods: the forecast period, which is the model's output, and the lookback period, which is the model's input. To produce forecasts for the forecast period, the model looks backward in time, or the "lookback period" [3], [25], [27]. The model's ability to effectively utilize the lookback period for generating meaningful future predictions is crucial for applications in domains such as finance, healthcare, and energy management [7].
In conclusion, N-BEATS is a deep learning architecture wherein the input data is processed through several stackable fully connected layers (blocks) for time series forecasting. A backcast (reconstruction) and a forecast (prediction) are generated by each block in a stack. A final global forecast is produced by combining many stacks of blocks to refine the original forecast. The architecture works well for a variety of forecasting jobs since it is adaptable, comprehensible, and able to handle complex time series data [19], [23], [29], [32]. The ability to combine multiple stacks and blocks provides the flexibility to model a wide range of time series patterns, including non-stationary and highly volatile datasets, making N-BEATS suitable for various applications such as finance, climate modeling, and energy forecasting [6], [22], [27].

3.2 Attention mechanism

Nowadays, attention mechanisms are an essential aspect of many neural network topologies, especially for tasks involving computer vision and natural language processing (NLP). The fundamental principle of attention is to provide a model the ability to choose focus on certain input components while making decisions, as opposed to considering every component of the input to be equally significant. Tasks like text summarization, image labeling, and machine translation have significantly improved as a result of this [18] [12].
Nowadays, attention mechanisms are an essential aspect of many neural network topologies, especially for tasks involving computer vision and natural language processing (NLP). The fundamental principle of attention is to provide a model the ability to choose focus on certain input components while making decisions, as opposed to considering every component of the input to be equally significant. Tasks like text summarization, image labeling, and machine translation have significantly improved as a result of this [12], [18].
Attention mechanisms have fundamentally transformed how neural networks operate by enabling models to prioritize different parts of the input sequence. This capability is particularly important in applications where understanding contextual relationships is crucial, such as speech recognition, machine translation, and text summarization [20], [28]. The concept of attention originated from the idea of replicating the human ability to selectively concentrate on relevant information, which allows neural networks to better mimic human cognitive functions. Attention mechanisms help tackle problems such as long-term dependencies and complex relationships in sequential data [13].

1. The Fundamental Idea of Attention: A model that uses attention techniques can dynamically determine how important various input components are. By learning to give varying attention scores to different sections of the input, the model effectively focuses on the most relevant parts while producing an output, as opposed to processing the full input sequence evenly [13], [18]. This selective focus leads to more efficient use of computational resources and enhances the model's ability to generalize to complex patterns in data. For example, in machine translation, the model can give more attention to words in the source sentence that are highly relevant to predicting the next word in the target sentence [12].

2. Self-Attention (Scaled Dot-Product Attention): Self-attention, also known as scaled dot-product attention, is a specific attention mechanism where a sequence's elements attend to other elements within the same sequence. This mechanism is a key component of the Transformer architecture.
How Self-Attention Works:
Inputs: A sequence of vectors (e.g., word embeddings).
Queries, Keys, and Values: The input sequence is transformed into three sets of vectors: queries (Q), keys (K), and values (V) shown in equation 3.1. These are typically linear projections of the input vectors [18] [13]. The queries, keys, and values represent different aspects of the input that the model uses to calculate relevance between various parts of the sequence.
Attention Score Calculation: The attention score for each pair of input elements is computed by taking the dot product of the query vector for one element and the key vector for another element. This results in a matrix of attention scores [13], [18], [20]. These scores determine the relationships between the elements in the sequence, allowing the model to identify which parts are most relevant for generating the output.
Softmax Normalization: The attention scores are then normalized using the softmax function, ensuring that the weights sum to 1 across each row [12], [20]. This normalization process helps the model weigh the importance of each element relative to the others, enhancing its focus on more significant parts of the sequence.
Weighted Sum: Finally, the normalized attention scores are used to compute a weighted sum of the value vectors. This produces a new sequence of vectors where each vector is a mixture of the input vectors, weighted by the attention scores [13], [28]. This weighted sum allows the model to create a context-aware representation of the input sequence, which is crucial for capturing complex dependencies.

The formula for Scaled Dot-Product Attention:

$$\text{Attention}(Q, K, V) = \text{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right)V \tag{3.1}$$

Multi-Head Attention: Multi-Head Attention (MHA) [18] allows a model to focus on different parts of an input sequence simultaneously, which helps it better capture complex relationships. The process starts by transforming input embeddings into three components: Queries (Q), Keys (K), and Values (V). These components each have a specific role in determining which parts of the input are most important.
For each attention head, a mechanism called **Scaled Dot-Product Attention** is used to decide where to focus. This is achieved by calculating attention scores using

the formula:

$$\text{head}_i = \text{softmax}\left(\frac{(QW_i^Q)(KW_i^K)^T}{\sqrt{d_k}}\right)(VW_i^V) \tag{3.2}$$

In the equation 3.2, $Q \cdot K^T$ represents the similarity between the queries and keys, giving an indication of how much focus each part of the input should receive. To keep the values from becoming too large, the result is scaled by $\sqrt{d_k}$. The softmax function then converts these scores into probabilities, emphasizing the most relevant parts of the input. These probabilities are used to compute a weighted sum of the values (V), which produces the output for that particular attention head.
To capture different aspects of the input, multiple attention heads are used in parallel (equation 3.3). Each head has its own set of learnable weights (W_i^Q, W_i^K, and W_i^V), allowing it to focus on different information. The outputs from all attention heads are then concatenated and transformed using a final set of weights:

$$\text{MHA}(Q, K, V) = \text{Concat}(\text{head}_1, \text{head}_2, \ldots, \text{head}_h)W^O \tag{3.3}$$

This final output is refined with another set of weights, W^O, to produce the final result. This design enables MHA to understand a wide range of patterns and relationships within the input sequence, making it particularly effective for tasks like language modeling and machine translation.

Neural Attention Memory: Neural Attention Memory is an extension of the attention mechanism aimed at enhancing the model's ability to retain long-term dependencies. It combines memory components with attention to keep track of crucial information over long input sequences. By using attention to selectively update and retrieve from an external memory, models employing neural attention memory can achieve better performance in tasks requiring complex reasoning and understanding of long-term dependencies [30]. Neural Attention Memory has proven effective in tasks such as question-answering and dialogue systems, where maintaining information over long contexts is essential [12].
The formula for Neural Attention Memory can be represented as follows in equation 3.4:

$$M_t = f(M_{t-1}, x_t, A_t) \tag{3.4}$$

Where M_t represents the memory state at time t, M_{t-1} is the previous memory state, x_t is the input at time t, and A_t is the attention mechanism that decides how much of the memory should be updated.

ProbSparse Attention: ProbSparse Attention is an efficient variant of the original self-attention mechanism. It is particularly designed to improve scalability for long input sequences, where the quadratic complexity of traditional self-attention becomes impractical. ProbSparse reduces computational requirements by focusing attention only on the most informative parts of the input sequence. By sparsifying the attention map, the model retains high accuracy while significantly reducing the computational load [33]. This makes ProbSparse Attention suitable for applications in which efficiency and scalability are key concerns, such as large-scale time series forecasting [15].

The formula for ProbSparse Attention is represented in equation 3.5:

$$\text{Attention}(Q, K, V) = \sum_{k \in S} \text{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right)_k V_k \tag{3.5}$$

Where S represents the set of the most informative keys chosen probabilistically to reduce the computational complexity.

Multi-Query Attention: Multi-Query Attention is a modification of the multi-head attention mechanism in which a single set of keys and values is shared across multiple queries, unlike traditional multi-head attention where each head has separate keys and values. This reduces memory and computational requirements while maintaining the diversity of information captured by multiple queries. Multi-Query Attention is highly useful for scaling up Transformer models in applications like machine translation, where efficiency is crucial [20], [34].
The formula for Multi-Query Attention is represented in equation 3.6:

$$\text{MultiQueryAttention}(Q, K, V) = \text{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right) V \tag{3.6}$$

Where the same K and V are shared across multiple query vectors Q to reduce the computation while preserving the expressiveness of attention.

3. Attention in Transformers: Transformers are a type of neural network architecture that relies entirely on self-attention mechanisms and forgoes recurrence and convolution. Transformers have become the foundation for state-of-the-art models in NLP, such as BERT and GPT [18] [20] [28]. Their reliance on attention allows them to efficiently capture relationships between different elements of a sequence, irrespective of their distance from each other, which is a significant limitation in RNNs [6].
Key Components of the Transformer:
Multi-Head Self-Attention: Instead of using a single attention mechanism, Transformers use multiple attention "heads" to capture different types of relationships in the data. Each head performs self-attention independently, and the results are concatenated and linearly transformed to form the final output [20] [28]. This multi-head mechanism enables the model to jointly attend to information from different representation subspaces, providing a richer representation of the input sequence [18].

Positional Encoding: Since Transformers do not have recurrence or convolution to capture the order of the sequence, they add positional encodings to the input embeddings to provide information about the position of each element in the sequence [18] [20]. These encodings allow the model to differentiate between elements based on their positions, which is crucial for preserving sequential information [14].

Feed-Forward Networks: After the self-attention layers, Transformers apply position-wise feed-forward networks (fully connected layers) to further process the attended representations [28]. These feed-forward layers help transform the attended representations into more complex feature spaces, enhancing the model's ability to

learn abstract patterns.
Layer Normalization and Residual Connections: Transformers use layer normalization and residual connections to stabilize and improve training [12] [20]. Residual connections help mitigate the vanishing gradient problem by providing a direct path for gradients to flow, while layer normalization ensures consistent scaling of inputs, which accelerates training convergence [13].

4. Types of Attention: Beyond self-attention, there are several other types of attention mechanisms:
Bahdanau Attention (Additive Attention): Introduced by Bahdanau et al. in 2015, this was one of the first attention mechanisms used in sequence-to-sequence models. It computes attention scores using a feed-forward neural network [18]. Bahdanau Attention is particularly useful for aligning elements of different sequences, such as in translation tasks where source and target sequences need to be aligned effectively.

Luong Attention (Multiplicative Attention): Proposed by Luong et al. in 2015, this method computes attention scores using the dot product of the query and key vectors, similar to scaled dot-product attention but without scaling [12] [13]. Luong Attention is computationally efficient and is often used in machine translation models where the computational overhead needs to be minimized.

5. Applications of Attention Mechanisms: Attention mechanisms are widely used in various tasks, including:
Machine Translation: Transformers use attention to translate sentences from one language to another [12], [18]. By focusing on relevant words in the source language while generating each word in the target language, attention allows for more fluent and accurate translations.
Text Summarization: Attention helps models focus on the most important parts of a document to generate a summary [13], [18]. This selective focus is crucial for capturing the key ideas in lengthy documents, thereby enabling concise and informative summaries.
Image Captioning: In computer vision, attention mechanisms allow models to focus on specific regions of an image when generating a descriptive caption [12], [28]. This allows the model to generate more contextually relevant and accurate descriptions by selectively attending to different parts of the image.
Speech Recognition: Attention is used to focus on relevant parts of an audio sequence when transcribing speech [20]. This helps the model dynamically adjust its focus as it processes audio input, improving accuracy in recognizing spoken words.
Interpretability: Attention mechanisms provide insights into which parts of the input are most important for the model's predictions, making the models more interpretable [28]. This transparency is particularly valuable in fields like healthcare, where understanding model decisions is critical.
Scalability: Attention mechanisms, particularly in Transformers, allow for parallel computation, making them highly scalable and efficient for processing large sequences [18], [20]. The parallel nature of attention makes it possible to train models on large datasets in less time compared to traditional sequential models like RNNs [27].

Flexibility: Attention can be applied to a wide range of tasks across different domains, from text and speech to images and video [12], [20], [28]. This versatility makes attention mechanisms a core component of modern AI applications.
Attention mechanisms, especially self-attention, have revolutionized the way neural networks process sequential data. They allow models to focus on the most relevant parts of the input, leading to significant improvements in performance across various tasks. The introduction of Transformers, which relies heavily on self-attention, has set new benchmarks in NLP and continues to influence advancements in other areas of AI [13], [18], [28]. As AI research progresses, the application of attention mechanisms is expected to expand, driving further innovations in domains such as healthcare, finance, and autonomous systems [27] [6].

Chapter 4

Proposed AUNET Scheme

The proposed model extends the traditional N-BEATS architecture by incorporating a multi-head self-attention mechanism. This enhancement improves the model's ability to identify significant patterns in the input time series, capturing both short-term fluctuations and long-term dependencies. The overall architecture is depicted in Figure 4.1, and the step-by-step implementation is outlined in Algorithm 1.

4.1 Model Architecture

The Attention-based Unified Network (AUNET) model in Figure 4.1 is designed as a comprehensive architecture for time series forecasting, combining advanced attention mechanisms and fully connected layers to generate both short-term and long-term forecasts. The network architecture is composed of three main components: blocks, stacks, and a multi-stack aggregation module. Below, we describe each component and its contribution to the overall model output.

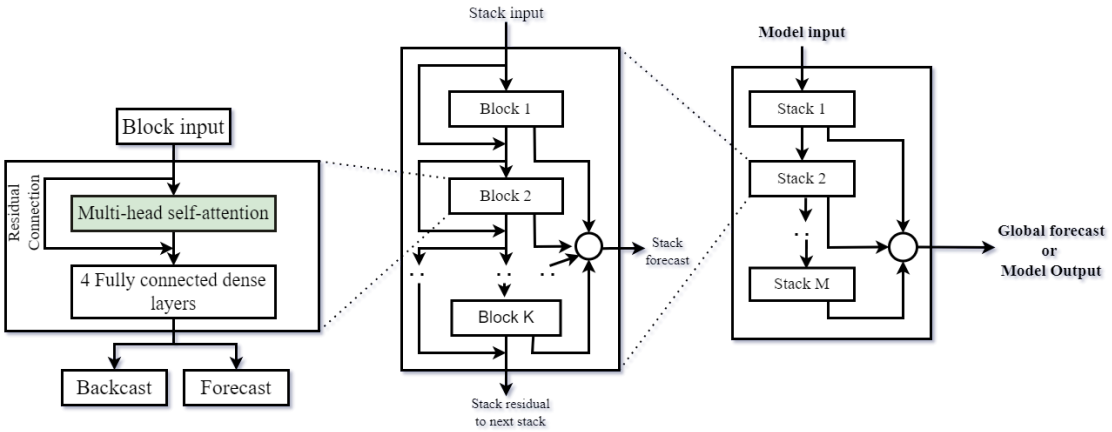

Figure 4.1: Overview of the Attention-based Unified Network (AUNET) Architecture

4.1.1 Block Structure

The smallest fundamental unit of AUNET is the **Block**. Each block in the architecture processes a segment of the input sequence using a set of distinct operations:

- **Block Input**: The input sequence is first received by the block. This sequence could either be the original input or a residual from previous blocks.
- **Multi-Head Self-Attention**: The block starts by applying a *multi-head self-attention* mechanism, which allows the model to focus on different parts of the input sequence simultaneously. This mechanism computes several attention scores to capture a wide range of dependencies, ensuring that the model can identify relevant features across the entire input sequence. The multi-head self-attention layer enhances the model's ability to account for diverse aspects of the input, capturing local and global relationships.
- **Residual Connection**: The output from the self-attention layer is connected back to the input via a *residual connection*. This helps to stabilize the training and preserve useful information, preventing the vanishing gradient problem and allowing the model to learn efficiently from deep layers.
- **Fully Connected Dense Layers**: Following the attention mechanism, the output is processed by *four fully connected dense layers*. These layers serve to extract features and transform the attended representation into a useful format for generating outputs. The dense layers help to model complex dependencies in the data, contributing to the robustness of the predictions.
- **Backcast and Forecast**: The block produces two main outputs:
  - **Backcast**: A reconstruction of the input signal. The backcast helps minimize the residuals between the input and the block's learned representation.
  - **Forecast**: A prediction of future values based on the current input. This forecast is passed on to subsequent blocks for refinement.

4.1.2 Stack of Blocks

A stack is composed of several blocks organized sequentially. The input to a stack can either be the original sequence or a residual derived from a previous stack:

- **Stack Input**: Each **stack** receives the input sequence and processes it through multiple blocks. Each **Block (e.g., Block 1, Block 2, ..., Block K)** handles a portion of the residual input from the previous block. The goal of each block within a stack is to progressively minimize the residual, focusing only on the parts of the sequence that have not yet been accurately forecasted.
- **Residual Passing**: Each block generates a *residual*, which is passed forward to the subsequent block. This approach helps in sequentially reducing the discrepancy between the actual input and the backcasted signal, allowing later blocks to concentrate on the difficult-to-model portions of the data.
- **Stack Forecast**: Each stack produces a *stack forecast* by aggregating the outputs of all blocks within the stack. This forecast is passed on to subsequent stacks or directly used in the final aggregation.

4.1.3 Multiple Stacks and Model Output

The architecture consists of multiple stacks (e.g., **Stack 1, Stack 2, ..., Stack M**), each focused on refining different features of the input data. The motivation for using multiple stacks is to enable specialization, where each stack may focus on modeling specific components such as trend, seasonality, or noise:

- **Model Input**: The input to the entire model is fed through multiple stacks, where each stack builds upon the residuals of the previous stack.
- **Stack Residuals**: As each stack processes the input, it produces *stack residuals*, which are passed forward to subsequent stacks, allowing each stack to refine the prediction further.
- **Global Forecast (Model Output)**: The *global forecast* is computed by aggregating the contributions from each stack. Each stack's forecast is combined to produce a final model output. The resulting **Global Forecast** is a unified prediction that takes into account all the information processed through the various blocks and stacks, offering a holistic forecast of future values.

The AUNET architecture is a highly modular and adaptable approach for time series forecasting, leveraging the power of attention mechanisms and deep learning techniques. Its *multi-head self-attention* enhances the model's capacity to capture complex temporal dependencies, while *fully connected dense layers* provide robust feature extraction. By organizing these blocks into *stacks* and using *residual learning*, the model is capable of progressively refining predictions. The final *global forecast* is an aggregation of forecasts from all stacks, effectively capturing both short-term and long-term patterns in the data.
The *residual connections* and *stacked structure* ensure that the model efficiently learns and improves its forecasts iteratively, allowing it to focus more precisely on aspects of the time series that have not yet been adequately predicted. Overall, AUNET provides a flexible and powerful framework for accurate time series prediction, benefiting applications that require dynamic and interpretable forecasting.

4.2 AUNET Procedure

The process of building the AUNET model starts with preparing the dataset to extract meaningful temporal features. Initially, the data is divided into training, validation, and test sets. To help the model understand the underlying patterns in the time series data, temporal features like year, month, lagged values, and moving averages (MA) are extracted. These features add valuable context about the seasonal trends and recurring behaviors within the data, making it easier for the model to learn.
After the data preparation step, the model architecture is constructed. It begins with input layers that receive these extracted features, followed by a multi-head self-attention mechanism. This mechanism is crucial as it allows different parts of the input sequence to interact, helping the model focus dynamically on the most significant patterns. The attention mechanism essentially gives the model the ability to identify and focus on the features that matter the most during prediction. After

the attention layer, there are fully connected dense layers with ReLU activation functions and dropout layers to prevent overfitting. These dense layers process the attended data further, helping to extract abstract and meaningful features that improve the robustness of the predictions. The model then produces two types of outputs: one for backcasting (reconstructing input) and another for forecasting (making future predictions).

The model is compiled using the Adam optimizer, chosen because of its ability to adapt to different learning rates. Mean Squared Error (MSE) is used as the loss function to measure how well the model is performing, while metrics like Mean Absolute Error (MAE) and Root Mean Squared Error (RMSE) are used to evaluate its performance more comprehensively.

During training, validation monitoring is employed to ensure the model does not overfit the training data. To achieve this, early stopping is used, which stops the training process if no further improvements are observed on the validation set. This helps in reducing overfitting. Additionally, learning rate scheduling is applied to dynamically adjust the learning rate during training, ensuring optimal convergence.

Once training is complete, the model's performance is evaluated using the test set, with MAE and RMSE metrics providing a clear picture of its accuracy. Additionally, the training process and model performance are visualized through loss curves, and comparisons between actual and predicted values are plotted to highlight the model's capabilities. Finally, the results are documented to understand the model's strengths and areas for improvement.

Algorithm 1 AUNET Algorithm

1: **Input:** Dataset D, Target Y
2: **Output:** Forecast $\hat{Y}$
3: **Steps:**
4: Load D, convert dates, extract features $\{year, month, lag, MA\}$
5: Split $\{train, val, test\}$, normalize with `StandardScaler`
6: Design N-BEATS:
- Input: Features
- Attention: Multihead mechanism
- Dense: 4 layers, ReLU + dropout
- Output: $\hat{Y}$

7: Compile: Optimizer `Adam`, Loss MSE, Metrics $\{MAE, RMSE\}$
8: Train: Monitor validation, use early stopping
9: Test: Compute $\{MAE, RMSE\}$ on $test$
10: Visualize: Plot loss, compare Y vs $\hat{Y}$
11: Save model, report results

The AUNET model is designed to be smarter and more adaptable when it comes to forecasting time series data. One of the key features that sets it apart is the use of a multi-head self-attention mechanism. This feature allows the model to focus on the most critical parts of the input data, leading to more precise predictions. Imagine having multiple eyes that can each look at a different aspect of the data at once—that is what the multi-head attention does, and it makes the model much better at understanding complex relationships.

Another important aspect is the use of residual connections. These connections help the model learn more effectively by ensuring that the information flows smoothly through all the layers, even in very deep networks. This way, the model doesn't lose valuable details during training, which can be a big challenge in deep learning models. The residual connections also prevent common issues like vanishing gradients, making the learning process more stable and efficient.
The hierarchical design of AUNET means that the model can capture both the big picture—the overall trends in the data—and the finer details, like local variations. This makes AUNET particularly powerful for time series forecasting, as it can adapt to both long-term patterns and short-term fluctuations, providing more accurate and reliable predictions.

4.3 Integration of Attention Mechanism

Figure 4.2 shows an attention-based setup mixed with the N-BEATS model, which is used for time series forecasting. The left side of the image explains scaled dot-product attention, which is an important part of transformer models. In this setup, we use three matrices called Q (Query), K (Key), and V (Value) to calculate attention scores. To do this, Q is multiplied by the transpose of K, giving us a score that shows how similar the queries and keys are. This score is then scaled by the square root of the size of the keys (d_k) to keep numbers stable. Sometimes, a mask is also used to control which positions in the sequence get attention, such as avoiding attention to future steps in autoregressive tasks. The scores are then passed through a softmax function to get weights, and these weights are used to multiply V, giving the final result.

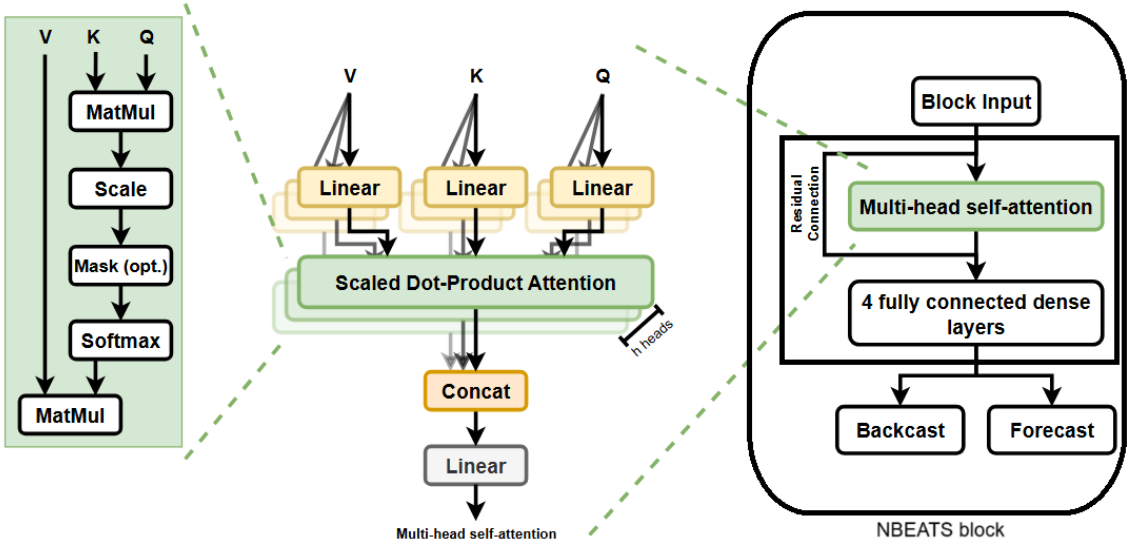

Figure 4.2: N-BEATS block with Multi-Head Attention, Residual Connections, and Dense Layers for Backcast and Forecast

When using **Multihead Attention** in the **N-BEATS** model for time series forecasting, Q (Query), K (Key), and V (Value) have specific meanings. These ideas, which started in Transformer models, are very helpful in working with time-based data like temperature readings over days. Let's connect these terms to the dataset,

which has daily temperatures and features like lagged values, rolling averages, and other time information.

Query (Q): The Query is the current data you want to predict or understand. For this dataset, it could be the latest temperature, past temperatures, and moving averages. It helps the model focus on what it needs to predict right now.

Key (K): The Key is the past data that the model uses to compare against the current information. In this dataset, it could be temperatures from earlier days and other features. Keys help the model figure out which past data points are important for making predictions.

Value (V): The Value holds the real historical data used to make the final prediction. In this dataset, Values include temperatures and other features from past days. The model weighs and combines these Values based on their importance, which helps it make better predictions.

In scaled dot-product attention, Q is multiplied by the transpose of K, and the result is scaled and passed through a softmax function to create attention weights. These weights are used to combine the **Value** vectors, which helps the model decide which past data points are most relevant for predicting the future.

Figure 4.2 also includes the **multi-head attention mechanism**, which is shown in the middle part of the image. This mechanism extends scaled dot-product attention by using several attention heads in parallel. Q, K, and V are each passed through their own linear transformations, allowing each head to learn different relationships. Each head computes scaled dot-product attention on its own, and the results are then joined and passed through a linear layer to merge the information. This allows the model to focus on multiple parts of the data at once, capturing more complex patterns between elements.

In this dataset, each head can focus on different parts of the time series. One head might look at short-term trends, like lag1 or rolling_mean_3, while another head might focus on longer trends, like rolling_mean_7 or yearly patterns. This helps the model learn about both short-term and long-term relationships at the same time, which is important for forecasting complicated time series.

The right part of Figure 4.2 shows an **N-BEATS block** that includes multi-head self-attention. This block starts with an input sequence and runs it through multi-head self-attention to capture connections across time steps. A **residual connection** is added to combine the input with the output from the attention layer, keeping key information and helping stable learning. The output then goes through four fully connected dense layers to process the data further, and is then split into **backcast** and **forecast** parts. The backcast part reconstructs the history of the input, while the forecast part predicts future values. This way, the model learns from both the past and future, which makes it good for time series forecasting.

Overall, using **scaled dot-product attention**, **multi-head self-attention**, and **N-BEATS blocks** with residual connections helps the model understand both short-term and long-term relationships. This setup is especially good for forecasting tasks, as it uses past data to make reliable predictions. By combining attention mechanisms with dense layers and residuals, the model can learn complicated patterns in time-based data, which improves its ability to make accurate forecasts.

The table 4.1 shows that the multi-head self-attention mechanism is used in this block for its effectiveness in capturing diverse relationships within the input sequence, significantly improving the learning of both local and global dependencies.

Table 4.1: Summary of Attention Mechanism Integration

Attention Mechanism	**Description**	**Key Features**
Self-Attention	Enhances focus on temporal features	Dynamic focus on time steps
Neural Attention Memory	Improves prediction accuracy	Memory module integration
ProbSparse Attention	Reduces computational overhead	Selective emphasis on elements
Multi-Query Attention	Increases computational efficiency	Shared queries across heads
Multi-Head Attention	*Captures diverse temporal relationships*	*Multiple attention heads for richer feature representation*

Self-attention enhances the model's focus on relevant temporal features by allowing it to learn which time steps are most influential, while multi-head attention extends this by utilizing multiple attention heads to capture different aspects of the sequence. This nuanced representation is crucial for time series with complex, nonlinear dependencies. This approach is favored over alternatives like Neural Attention Memory (NAM), ProbSparse Attention, and Multi-Query Attention.

Neural Attention Memory is designed to improve long-term memory retention, making it suitable for scenarios with repeating long-term patterns. However, its primary focus is on memory storage and retrieval, while the priority in this block is to enhance immediate feature extraction and representation, which multi-head self-attention does more effectively. ProbSparse Attention, on the other hand, reduces computational overhead by focusing on only the most critical parts of a sequence, which makes it efficient for longer inputs but potentially less expressive for capturing all relevant features. Multi-Query Attention is computationally efficient by sharing queries across heads, but it lacks the richness of representation offered by independent queries in multi-head attention. Therefore, multi-head self-attention is selected for its ability to provide a comprehensive view of temporal relationships without compromising on detail.

The placement of the multi-head self-attention mechanism directly after the block input is crucial for prioritizing significant temporal dependencies before further processing through the fully connected dense layers. By positioning attention at this point, the model can immediately learn dependencies and interactions between different time steps of the input sequence, ensuring that subsequent dense layers receive a representation that emphasizes the most relevant temporal features. This positioning ensures that when the dense layers process the data, they are operating on an enriched representation that already highlights the important aspects of the sequence, leading to more effective feature extraction.

The dense layers that follow attention are responsible for further processing and transforming the input features. By applying attention first, the dense layers can focus on extracting high-level, abstract features from a representation that already emphasizes the most significant temporal relationships. Furthermore, the residual connection from the input directly to the output of the attention mechanism improves stability by providing a direct path for gradient flow, mitigating the risk of

vanishing gradients during training. This is particularly important for deep architectures where gradient issues can hinder effective learning.
If attention were placed later in the sequence, such as after the fully connected layers, the model might end up processing noisy or irrelevant features before determining which parts of the sequence are most important. This could reduce the efficiency of both attention and feature extraction. By placing attention at the beginning, the model benefits from a clear separation between identifying the focus (attention) and transforming features (dense layers), which enhances both the backcast and forecast outputs.
The backcast output aims to reconstruct the input sequence, minimizing the residuals between the actual input and the learned representation, thereby refining the understanding of what has already been observed. The forecast output, on the other hand, leverages the attention-refined features to predict future values, allowing for accurate forecasting by focusing on the most significant aspects of past data. Overall, the integration of multi-head attention, residual connections, and fully connected dense layers allows the block to effectively capture both local and global patterns in the data, leading to more accurate time series forecasts.

Chapter 5

Implementation

5.1 Dataset

The dataset utilized in this study was sourced from the California Irrigation Management Information System (CIMIS) [37] and contains daily average air temperature observations. It includes two main attributes: the 'Date' column, recorded in the 'MM/DD/YYYY' format, which represents the temporal component of the data, and the 'Avg Air Temp (F)' column, which provides the daily average air temperature in Fahrenheit. The dataset focuses exclusively on air temperature as the target variable, with no additional predictors, classifying it as a univariate time series. It contains 9081 entries for the Date column, while the Avg Air Temp (F) column has 8989 non-null entries, indicating some missing values. These gaps, likely due to inconsistencies in data collection or recording, require careful preprocessing through imputation or exclusion to ensure data quality. The dataset spans multiple years, offering a detailed temporal resolution that captures both short-term fluctuations and long-term trends, making it highly suitable for univariate time series forecasting. This dataset forms the basis for evaluating the performance of the N-BEATS model with Multi-Head Attention in predicting temperature patterns.

5.2 Dataset Preprocessing

When working with the Attention-Based N-BEATS model, data preprocessing plays a vital role in making sure the time series data is properly formatted, normalized, and ready for analysis. The dataset used in this study consists of daily average air temperature readings, and to prepare it for the model, we applied several preprocessing steps, as illustrated in Figure 5.1:

1. Data Loading and Parsing: We began by loading the dataset, which included columns for Date and Avg Air Temp (F). The Date column was then converted into a datetime format to make it easier to carry out time-series analysis tasks.

2. Lagged and Rolling Features: To capture the temporal relationships in the data, we created lagged features (temperatures from one and two days before) as well as moving average features (3-day and 7-day averages). These additional features help smooth out fluctuations and bring out short-term trends, making it easier for the model to learn important patterns.

3. Handling Missing Values: Adding lagged and rolling features introduced

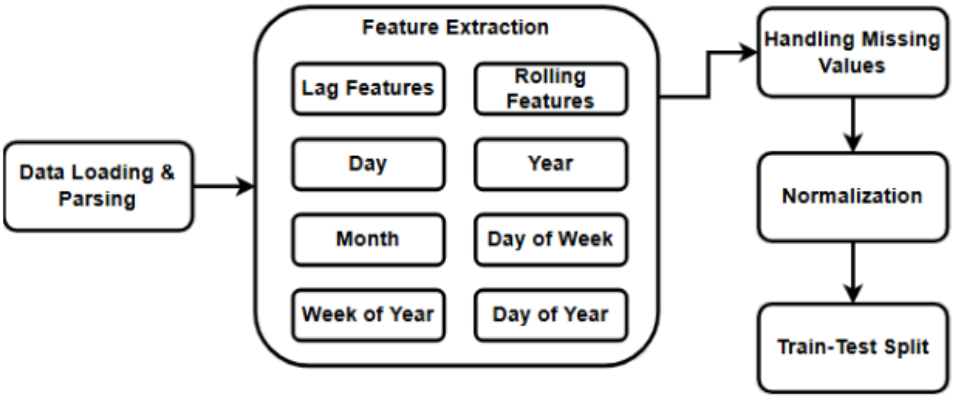

Figure 5.1: Visual Representation of Dataset Preprocessing Steps

some missing values at the beginning of the dataset. To deal with this, we removed these rows to ensure we had a clean dataset for training.
4. Normalization: Next, we normalized the target variable, Avg Air Temp (F), using a standard scaler. This step was essential for keeping the scaling consistent and helping the model converge more effectively during training. All the input features were also normalized independently to prevent data leakage and to maintain a consistent scale throughout.
5. Train-Test Split: Finally, we split the dataset into training (80%) and testing (20%) subsets. This split provided enough data for training while ensuring that we had a fair way to evaluate the model's performance on unseen data.
This preprocessing pipeline ensured that the dataset was consistent and enriched with meaningful statistical features, providing a solid foundation for accurate time-series forecasting.

5.3 Feature Extraction

To boost the predictive power of our dataset, we engineered several new features from the Date and Avg Air Temp (F) columns. First, we created lagged features (lag1, lag2) to capture recent temperature trends, essentially incorporating the temperatures from one and two days earlier. These features help the model understand short-term dependencies in the data. In addition, we computed moving averages (rolling mean 3, rolling mean 7) to help smooth out short-term fluctuations and highlight the underlying trends more clearly.
We also derived several temporal features from the Date column to account for seasonal and periodic variations. These included attributes like the year, month, day, day of the week, day of the year, and week of the year. Together, these features provided valuable insights into annual, monthly, and weekly temperature patterns, as detailed in Table 5.1.
Overall, this feature engineering process enriched the dataset by adding both statistical and temporal attributes. These features ensured that the model could leverage both short-term dependencies and long-term seasonal trends, leading to more accurate forecasting results.

Table 5.1: Feature Engineering for Extracting Temporal and Statistical Features

Feature	Description
Lag Features	`lag1` and `lag2` represent the temperatures from one and two days prior, respectively.
Rolling Features	`rolling mean 3` is the 3-day moving average, and `rolling mean 7` is the 7-day moving average.
Year	Extracted from the `Date` column to represent the year of observation.
Month	Extracted from the `Date` column to represent the month of observation (1–12).
Day	Extracted from the `Date` column to represent the day of the month (1–31).
Day of Week	Encoded as an integer (0–6) representing Monday through Sunday.
Day of Year	The ordinal day of the year (1–365 or 366 for leap years).
Week of Year	The ISO week number of the year (1–53).

5.4 Training & Hyperparameter Tuning

In this section, we discuss how the training and hyperparameter tuning strategies were used to boost the performance of the AUNET and N-BEATS models for time series forecasting. The key goals were to ensure stable convergence, minimize overfitting, and improve the models' ability to generalize. To achieve this, we used techniques like adaptive learning rate schedules, efficient optimizers, and validation monitoring.

Adaptive learning rate schedules helped the models adjust their learning pace throughout training, allowing them to converge more effectively. We used efficient optimizers like Adam, which is known for adapting learning rates during the training process. Additionally, validation monitoring was employed to evaluate model performance on unseen data, helping to prevent overfitting. Early stopping was also applied, meaning that training was halted as soon as further improvements on the validation set were no longer observed. This way, we avoided unnecessary training that could lead to overfitting.

We also performed a comparative analysis of the AUNET and N-BEATS models, highlighting the advantages of using a multi-head attention mechanism in AUNET. The analysis, illustrated through training and validation learning curves, shows that AUNET, with its multi-head attention feature, provides better generalization and accuracy—particularly when it comes to capturing complex temporal relationships.

5.4.1 Training

The training of the N-BEATS model with Multi-Head Attention was designed to ensure stable convergence and optimal performance using adaptive learning rates, validation monitoring, and early stopping to enhance robustness and accuracy. **Table 5.2** summarizes the training process used for all models. The optimization relied on the Adam optimizer, which is widely recognized for its ability to adaptively adjust the learning rate during training. The Mean Squared Error (MSE) loss function

was employed to penalize larger deviations, enhancing predictive accuracy. A batch size of 16 was selected to balance computational efficiency with precise weight updates. Training spanned 300 epochs, offering sufficient opportunities for the models to learn while monitoring generalization using a validation split of 20% of the training data. Furthermore, callbacks such as early stopping and ReduceLROnPlateau were applied. Early stopping halted training when the validation loss stagnated (patience = 10), while ReduceLROnPlateau dynamically adjusted the learning rate during plateaus (patience = 3) to improve learning efficiency.

Table 5.2: Training Process Details

Aspect	**Description**
Optimizer	Adam optimizer with an initial learning rate of 0.0001, known for adaptive learning rate capabilities.
Loss Function	Mean Squared Error (MSE) to penalize larger deviations and minimize prediction errors.
Batch Size	Set to 16 to achieve a balance between computational efficiency and weight update precision.
Number of Epochs	Trained over 300 epochs, ensuring sufficient learning opportunities while monitoring validation performance.
Validation Split	20% of the training data reserved for validation to monitor generalization during training.
Callbacks	Early stopping (patience = 10) to halt training when validation loss stagnates; ReduceLROnPlateau (patience = 3) to adjust learning rate during plateaus.

The comparison of the learning curves across AUNET and different variations of N-BEATS with attention mechanisms highlights clear differences in model performance, stability, and generalization capabilities.

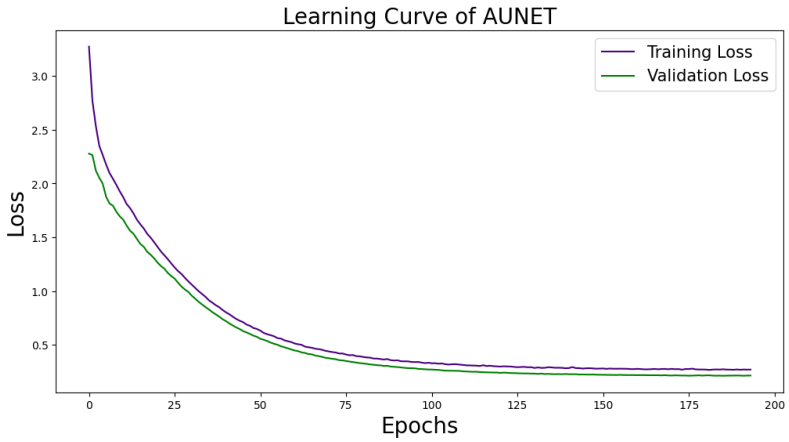

Figure 5.2: Learning Curve of AUNET showing stable convergence of training and validation loss.

The **AUNET learning curve** (Figure 5.2) stands out due to its smooth and stable convergence in both training and validation loss over 200 epochs. Both losses decrease steadily and in near-perfect alignment, with no noticeable divergence between the two. This indicates excellent generalization and minimal overfitting, as

the model effectively captures relevant patterns in the data without being overly biased towards the training dataset. The absence of instability or significant fluctuations in the validation loss further reinforces AUNET's robustness and reliability during optimization. Moreover, AUNET reaches lower loss values overall, suggesting superior predictive accuracy compared to the other models.

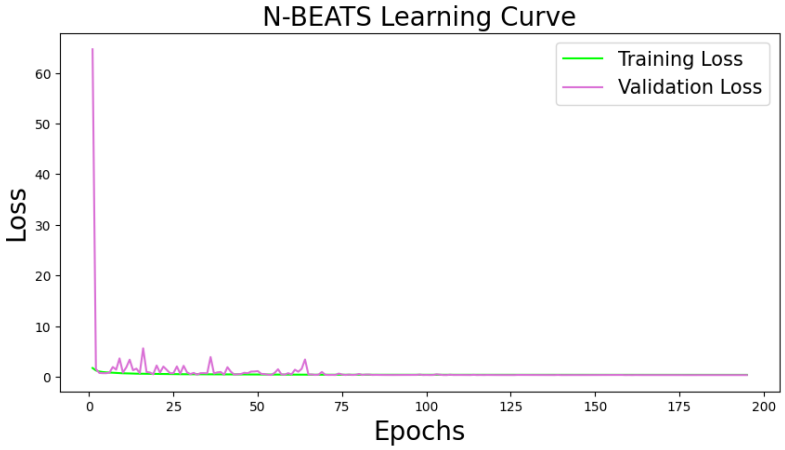

Figure 5.3: Learning Curve of standalone N-BEATS without additional attention mechanisms.

On the other hand, the **standalone N-BEATS model** (Figure 5.3) exhibits a rapid initial decline in both training and validation losses. However, the validation loss shows some fluctuations throughout the training process, signaling moderate overfitting or sensitivity to validation data distribution. While this model demonstrates strong learning ability, its performance on unseen data is less consistent compared to AUNET.

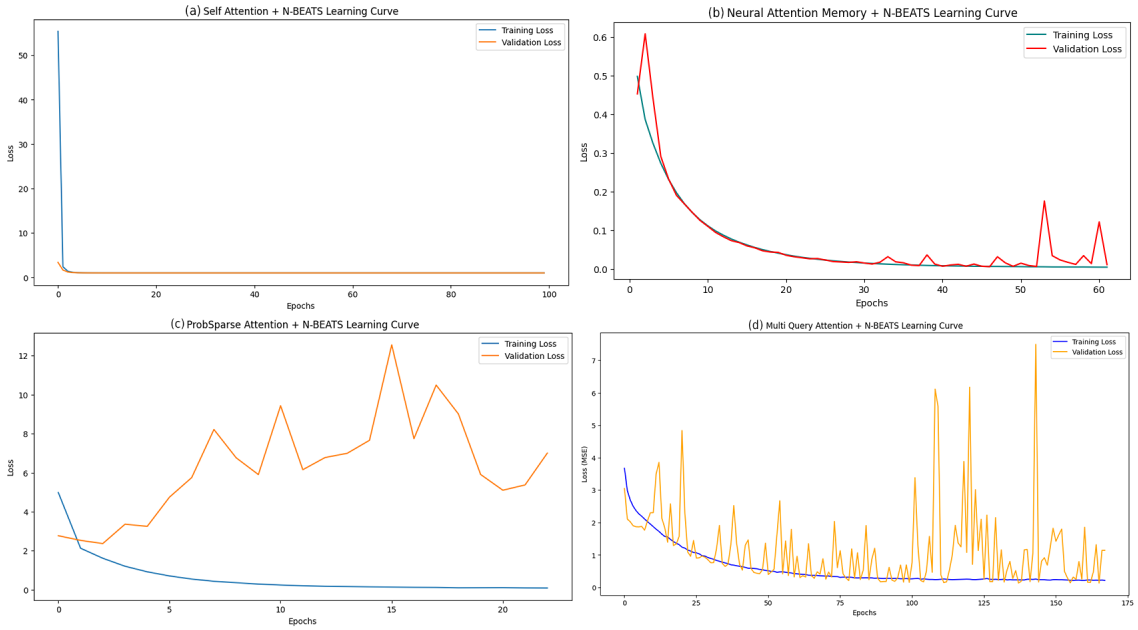

Figure 5.4: Learning curves of N-BEATS variants with attention mechanisms: (a) Self-Attention, (b) Neural Attention Memory, (c) ProbSparse Attention, (d) Multi-Query Attention.

Among the N-BEATS variants enhanced with attention mechanisms, significant performance disparities are evident (Figure 5.4). The **Self-Attention + N-BEATS model** converges quickly in training loss but maintains a relatively high and static validation loss, indicating severe overfitting. The model appears to prioritize minimizing training loss at the expense of generalization. Similarly, the **ProbSparse Attention + N-BEATS model** suffers from erratic validation loss behavior, which oscillates significantly despite steady reductions in training loss. These fluctuations suggest instability in the optimization process, potentially caused by ineffective attention integration or an imbalance between model complexity and data size.
The **Multi-Query Attention + N-BEATS model** also fails to generalize effectively, as evidenced by the extreme volatility in validation loss throughout training. Although the training loss decreases smoothly, the erratic validation performance indicates poor robustness to unseen data, making this model unreliable despite its capacity to minimize training error. In contrast, the **Neural Attention Memory + N-BEATS model** achieves better generalization. During training, both the training and validation losses declined at similar rates, although there were occasional spikes in the validation loss. This model performed better than other attention-based N-BEATS variants, but it still showed more instability compared to AUNET.
In summary, **AUNET stands out by outperforming all other models thanks to its consistently smooth and stable learning curve** (Figure 5.2). The small gap between training and validation losses suggests strong generalization with no overfitting, and the lack of significant fluctuations in the validation loss underscores its robustness during training. AUNET's ability to steadily reduce loss over time and achieve lower final values demonstrates superior learning efficiency and predictive accuracy compared to the standalone N-BEATS (Figure 5.3) and its attention-augmented variants (Figure 5.4). The combination of stability, generalization, and minimal validation error fluctuations makes AUNET the most reliable and effective model in this comparison.

5.4.2 Hyperparameter Tuning

We fine-tuned the N-BEATS model with different attention mechanisms, like Multi-Head Attention, to get the best performance without overfitting or underfitting. Tables 5.3 and 5.4 summarize the chosen hyperparameters, which were carefully selected to balance computational efficiency, training speed, and the ability to capture both short- and long-term dependencies.
For the model with Multi-Head Attention, we started with an initial learning rate of 0.00591715275954413, which was adjusted during training using Bayesian Optimization Strategy. This allowed the model to learn fast initially and then gradually fine-tune as it progressed. We used a batch size of 16, which provided a good trade-off between efficiency and precise updates. The training ran for 300 epochs, with early stopping in place to save resources when the validation loss stopped improving for 10 straight epochs.
To avoid overfitting, we used L2 regularization and a dropout rate of 0.5, where random neurons were deactivated during training to make the model more robust. We also used a ReduceLROnPlateau strategy to halve the learning rate when the validation loss plateaued for three consecutive epochs, helping the model escape

local minima and continue improving.

Table 5.3: Hyperparameter Tuning Details

Hyperparameter	**Description**
Learning Rate	Initial learning rate set to 0.00591715275954413, dynamically adjusted using Bayesian Optimization Strategy.
Batch Size	Training batch size set to 16 to balance computational efficiency and precise weight updates.
Number of Epochs	Model trained for 300 epochs with early stopping to monitor and halt if no improvement in validation loss.
Regularization	L2 regularization with $\lambda = 0.005$ applied to dense layers to penalize large weights and reduce overfitting.
Dropout Rate	Dropout rate set to 0.3725669863572014 to deactivate random neurons during training, encouraging redundancy and improving generalization.
Early Stopping	Training stopped if validation loss failed to improve for 10 consecutive epochs to avoid overfitting and unnecessary computation.
ReduceLROnPlateau	Learning rate reduced by half if validation loss plateaued for three consecutive epochs to escape local minima.

The table 5.4 shows the results of tuning the hyperparameters for the AUNET model, which uses a combination of Multihead Attention and the N-BEATS architecture. This tuning was done using the Optuna tool to find the best settings that give the lowest validation loss, meaning better performance. The hyperparameters tuned include learning rate, dropout rate, number of attention heads, and batch size.
The learning rate controls how much the model's weights are adjusted with each training step. We tried a range of values—from very small ones like 1.01e-05 to larger ones like 0.006047—to find the best way for the model to learn. The dropout rate is used to prevent the model from overfitting, meaning it prevents the model from memorizing instead of learning general patterns. It does this by randomly turning off parts of the model during training. The dropout rate values we tried ranged from 0.20 to 0.69, helping us find the right balance between learning and overfitting.
The attention heads are part of the Multihead Attention mechanism, and they help the model focus on different parts of the input data at the same time. We experimented with 1 to 8 attention heads to see which works best for capturing the important information. Batch size is the number of data samples the model processes before updating its weights. We tried small sizes, like 8 and 16, and larger ones, like 64. Smaller batch sizes often make the model learn better but can be a bit unstable, while larger batch sizes can be more stable but might not always generalize well.
The trial value in the table is the validation loss for each trial, which tells us how well the model is doing at each step. The best trial value is the lowest loss value found so far, showing which settings worked best. For example, Trial 11 achieved the best result with a validation loss of 0.0040, using a learning rate of 4.21e-05, a dropout rate of 0.3726, 2 attention heads, and a batch size of 16. This means that this set of hyperparameters gave the best performance in minimizing errors.

Table 5.4: Summary of Optimization Trials for AUNET Model

Trial	Learning Rate	Dropout Rate	Attention Head	Batch Size	Trial Value	Best Trial Value
0	0.005917	0.5374	8	32	0.05888	0.05888
1	0.000179	0.3461	6	16	0.00962	0.00962
2	0.000253	0.5802	7	32	0.01054	-
3	0.000808	0.3265	3	16	0.01504	-
4	0.001019	0.5158	8	32	0.01439	-
5	0.001901	0.6149	1	8	0.03316	-
6	2.29e-05	0.2468	6	64	0.05380	-
7	0.001136	0.5129	7	8	0.01869	-
8	0.000258	0.6365	6	32	0.01104	-
9	0.006047	0.4414	4	32	0.05766	-
10	4.48e-05	0.3806	3	16	0.00487	0.00487
11	**4.21e-05**	**0.3726**	**2**	**16**	**0.00401**	**0.00401**
12	2.98e-05	0.4147	2	16	0.00442	-
13	1.01e-05	0.2013	1	16	0.02339	-
14	6.73e-05	0.4319	2	16	0.00648	-
15	7.60e-05	0.2928	2	64	0.00694	-
16	1.02e-05	0.3926	4	16	0.03860	-
17	2.80e-05	0.4779	2	16	0.00769	-
18	0.000111	0.2927	3	16	0.00481	-
19	2.14e-05	0.3987	1	8	0.00742	-
20	0.000453	0.4731	5	64	0.00882	-
21	0.000120	0.6906	3	16	0.01082	-
22	0.000112	0.2885	2	16	0.00667	-
23	4.77e-05	0.3417	3	16	0.00460	-
24	3.66e-05	0.3467	4	16	0.00761	-

From the results, we can see some patterns. Smaller learning rates generally helped the model learn more steadily, while moderate dropout rates were good for avoiding overfitting. Fewer attention heads, especially 2 or 3, were enough to help the model capture the necessary information, and using too many heads did not make a big difference. Smaller batch sizes often led to better results, which matches the idea that smaller batches, though noisier, can help the model learn more effectively. Overall, the tuning showed that using lower learning rates, moderate dropout, fewer attention heads, and smaller batch sizes led to the best results. This means that careful selection of these hyperparameters is key to making the model work well, without overfitting or underperforming.

5.5 System Configuration

The experiments and model development for this research were carried out using Python in the Visual Studio Code (VS Code) editor, which offered a robust environment for coding, debugging, and script management. Several essential Python

libraries supported the project, including Pandas for data manipulation, NumPy for numerical operations, and Matplotlib for visualizations. TensorFlow and Keras were key to building, training, and optimizing the neural network models, with modules such as layers, models, and optimizers used for designing and training the architecture. Additionally, StandardScaler from sklearn.preprocessing ensured consistent data scaling, while LearningRateScheduler dynamically adjusted learning rates during training.

The hardware setup included an AMD Ryzen 5 3600 processor, 64GB of RAM, and a Zotac AMP Extreme GTX 2060 Super GPU. This configuration allowed for efficient data processing and accelerated deep learning tasks. The multi-core processor facilitated parallel computations, the large memory capacity managed extensive datasets seamlessly, and the GPU significantly shortened training times by leveraging parallel processing. This combination of software and hardware created an optimized environment for model development, experimentation, and accurate training of both the N-BEATS model and its attention-enhanced variant.

Chapter 6

Performance Evaluation

Evaluating time series forecasting models involves examining every step, from data preprocessing to assessing how well the models perform based on various error metrics. In this section, we introduce the experimental design and summarize the results for two forecasting models: AUNET and N-BEATS. Both models were used to predict daily average air temperature by utilizing different temporal features and incorporating attention mechanisms.
Our analysis includes both qualitative and quantitative comparisons of the models' predictive performance, focusing on important metrics like Mean Absolute Error (MAE), Root Mean Square Error (RMSE), and the Coefficient of Determination (R^2). The following sections present the outcomes of these experiments, highlighting how AUNET's attention-based architecture captures temporal dependencies more effectively and outperforms traditional deep learning models in this specific forecasting task.

6.1 Performance Metrics

When it comes to evaluating forecasting models, we often rely on well-known error metrics like Mean Absolute Error (MAE), Root Mean Square Error (RMSE), and the Coefficient of Determination (R^2). These metrics are crucial for checking how accurate and reliable the predictions are, especially in univariate time series data.
1. Mean Absolute Error (MAE): MAE measures the average size of the errors between predicted and actual values, without worrying about whether the errors are positive or negative. It's calculated as:

$$\text{MAE} = \frac{1}{n}\sum_{i=1}^{n}|y_i - \hat{y}_i| \tag{6.1}$$

where y_i is the observed value, $\hat{y}_i$ is the predicted value, and n is the number of observations [11]. Since MAE is in the same units as the target variable, it gives an easy-to-understand measure of the average error, making it especially useful for univariate time series forecasting.
2. Root Mean Square Error (RMSE): RMSE takes into account larger errors more seriously by squaring them before averaging. It is defined as:

$$\text{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2} \tag{6.2}$$

RMSE puts more emphasis on bigger errors, which makes it ideal for situations where large prediction errors could be problematic [8]. In univariate time series forecasting, RMSE helps highlight significant deviations, which might be crucial depending on the forecasting application.

3. R^2**:** R^2 measures how much of the variance in the observed data is explained by the model. It is calculated as:

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y_i - \hat{y}i)^2}{\sum i = 1^n (y_i - \bar{y})^2} \tag{6.3}$$

where $\bar{y}$ is the mean of the observed values [7]. An R^2 value close to 1 means the model explains most of the variability in the data, while a value near 0 indicates that the model has limited predictive power. For univariate time series analysis, R^2 is useful to see how well the model captures the trends in the observed data.

These metrics are widely used in univariate time series forecasting because they are easy to interpret and relevant. MAE gives a simple average error measure, RMSE emphasizes the impact of large deviations, and R^2 shows how well the model explains the data's variability. Together, they provide a complete assessment of model performance, helping to evaluate and compare different forecasting models [11] [8] [7].

6.2 Experimental Setup

In this experiment, we used two different models, AUNET and N-BEATS, to predict daily average air temperatures based on a dataset of daily temperature records. We extracted several temporal features from the date variable, such as the year, month, day, day of the week, day of the year, and week of the year, to help capture the underlying seasonality and temporal patterns in the data. To give the models more context, we also added lag features (lag1, lag2) and moving averages (rolling mean 3, rolling mean 7) to provide information about recent temperature trends.

Next, we cleaned the dataset by dropping any missing values and normalized the features and target variable separately. This step ensured that the data was standardized, making it easier for the models to learn effectively without being affected by differences in scale between the input data.

The dataset was partitioned into training (80%) and testing (20%) sets. Two models were constructed and evaluated: the N-BEATS model, consisting of dense fully connected layers to predict target values, and the AUNET model, which utilized a multi-head attention mechanism to enhance learning by focusing on important temporal features. The models were trained with the Adam optimizer using a learning rate of 0.0001, and mechanisms such as L2 regularization and dropout were employed to address overfitting. Model training was conducted with the aid of early stopping to prevent over-training.

The performance of the models was assessed on the testing set using metrics including Mean Absolute Error (MAE), Root Mean Squared Error (RMSE), and R-squared

(R^2). All predicted values were de-normalized for comparability with the actual target values, and visual inspection was performed through scatter and residual plots to analyze the prediction accuracy of each model.

6.3 Prediction Comparison

Based on the prediction graphs, AUNET demonstrates clear advantages over N-BEATS in modeling the specific characteristics of this dataset. We used both models to predict daily average temperatures, focusing on how well they could capture complex temporal relationships and short-term changes in the dataset. As you can see in Figure 6.1, AUNET ended up doing a much better job overall, especially when it came to picking up those short-term ups and downs and capturing local patterns better than N-BEATS could. AUNET really seemed to shine in identifying those little changes, while N-BEATS was more about giving smoother, generalized predictions.
In this section, we dive deep into how each model did when predicting temperatures, looking at the key differences between them. We emphasize how they handled fluctuations and anomalies, and the way they each approached capturing the temporal dynamics present in the data. AUNET seemed to be more in tune with the finer details, while N-BEATS had a broader, more generalized take.

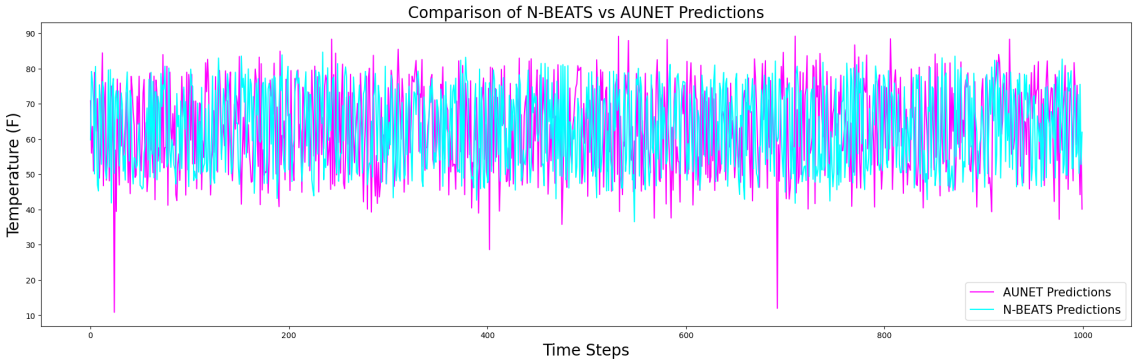

Figure 6.1: Comparison of AUNET and N-BEATS predictions using the first 1000 data points for a clearer picture. This plot shows the predicted temperature values over time. AUNET's predictions (pink) react more to the fluctuations, while N-BEATS (cyan) provides smoother and more generalized results

In the figure 6.1 above, AUNET's predictions showed more sensitivity to the fluctuations, especially those short-term temperature swings, compared to N-BEATS. You could see this in how closely AUNET tracked those local peaks and dips, which shows it can handle intricate patterns better. N-BEATS, on the other hand, seemed to smooth things out, often missing those subtle ups and downs in the data. This is mostly because N-BEATS relies on a fully connected setup that doesn't have an explicit way to adjust focus on certain time steps, which makes its predictions more generalized and less capable of capturing short-term deviations.
AUNET's edge in picking up short-term changes makes it super useful in situations where accuracy over short time periods is really important—like in agriculture, energy management, or public safety where sudden temperature spikes or drops matter a lot. In those cases, AUNET's precision in keeping up with sudden changes

gives it a real advantage over N-BEATS. To help visualize this, we used the first 1000 data points in the graph to make it easier to see the differences between the two models clearly.
The attention mechanisms built into AUNET allow it to zero in on the most relevant parts of the input, which is a big reason why it performs so well. These mechanisms help AUNET decide which time steps are the most important, so it can prioritize those and improve accuracy. You can see this adaptability in Figure 6.2, where AUNET handles variability in the data much better. Unlike N-BEATS, which often ends up smoothing out sharp changes due to its static approach, AUNET manages to capture extreme values and anomalies effectively. This ability is especially valuable in data with irregular patterns or anomalies, like sudden temperature changes, which can be crucial for making informed decisions.

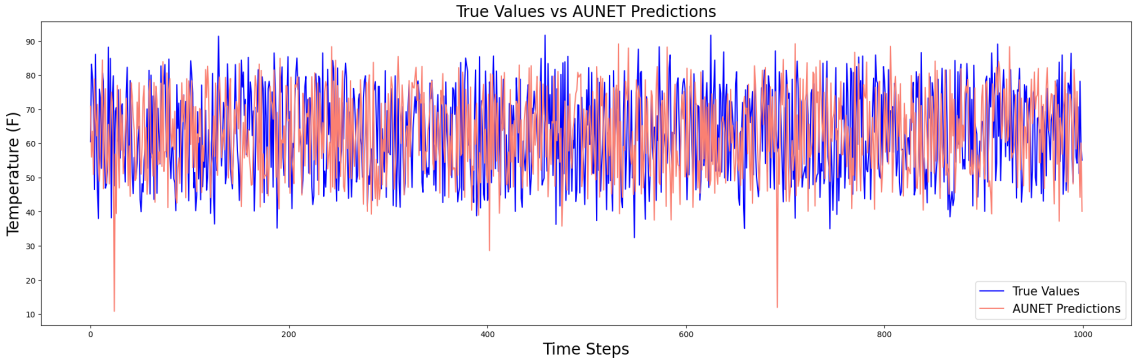

Figure 6.2: The comparison of true values and AUNET predictions is depicted using the first 1000 data points for clarity. The plot illustrates the actual temperature values (blue) alongside the predictions from the AUNET model (orange). The close alignment between the AUNET predictions and the true values demonstrates the model's ability to effectively capture both short-term fluctuations and long-term trends.

We're looking at how AUNET's predictions stack up against the actual temperature values, using the first 1000 data points to keep things clear. In the graph (Figure 6.2), you can see that AUNET's predictions (orange) pretty much follow the real temperature values (blue) closely. This shows that AUNET does a good job of capturing both quick changes and long-term trends in the data.
This happens because AUNET uses a multi-head attention mechanism, which lets the model look at different aspects of the input sequence at the same time. By doing this, AUNET can pick up on key time-based features that might be missed if it only used a single attention head. This means it can effectively capture both detailed fluctuations and the bigger picture.
AUNET's attention mechanism also helps it make predictions that are detailed and aware of the context by focusing on the most relevant parts of the input sequence. You can really see this in Figure 6.2, where AUNET's predictions not only line up well with the true values but also catch subtle fluctuations that N-BEATS tends to miss. Because AUNET can dynamically focus on important time intervals, it adapts well to changes in the dataset. For instance, during times when the temperature changes rapidly, AUNET can give more weight to those periods, making sure its predictions accurately reflect these critical shifts.

On the other hand, N-BEATS gives us more generalized and smoother predictions that follow the overall trend but lack the nuanced adaptability that AUNET shows. While the smoother output from N-BEATS can be useful when we're only interested in the general trend and not so much in short-term deviations, it falls short in situations where precise local accuracy is important—like predicting short-term weather patterns or forecasting energy demand. This limitation becomes more pronounced when the dataset has frequent fluctuations or anomalies that require the model to be highly responsive to short-term changes.

AUNET's better performance comes down to its multi-head attention mechanism, which lets the model focus on different parts of the time series all at once. Each attention head can hone in on a different subset of the input sequence, picking up diverse patterns and time-based relationships that help make the overall prediction more accurate. This multi-faceted approach gives AUNET a more complete understanding of how the data changes over time, leading to predictions that are both accurate and context-aware. In contrast, N-BEATS relies only on a stack of fully connected layers and doesn't have this dynamic focus, which results in a more uniform and less responsive output.

All in all, the graphs highlight how AUNET is better at capturing short-term variations, adapting to anomalies, and delivering accurate, context-aware predictions. For this dataset, AUNET's attention-driven architecture makes sure it performs well in situations that require precise modeling of time-based fluctuations and complex dependencies. Its ability to dynamically focus on key features, capture both short-term and long-term trends, and adapt to irregularities makes it a better choice for univariate time series forecasting tasks. N-BEATS, while good at capturing general trends, doesn't have the flexibility and precision needed for applications that demand high accuracy and responsiveness to sudden changes.

The benefits of AUNET are especially clear in applications where accurate short-term predictions are crucial. In temperature forecasting, for example, sudden changes can significantly impact agricultural planning, energy consumption, and public health efforts. By effectively capturing these short-term fluctuations, AUNET provides a more reliable tool for people who rely on precise, timely forecasts. Plus, the use of attention mechanisms not only boosts prediction accuracy but also makes the model easier to interpret by showing which time steps are most influential for the forecast. This interpretability is a bonus in real-world applications, where understanding why a prediction was made can be just as important as the prediction itself.

In conclusion, AUNET's attention-based approach significantly improves upon N-BEATS in modeling the complex time-based characteristics of the dataset. The combination of enhanced short-term accuracy, the ability to capture anomalies, and better interpretability makes AUNET a superior choice for univariate time series forecasting tasks, especially those involving complex and fluctuating data patterns. The detailed comparisons we've presented here underscore the importance of incorporating attention mechanisms into time series forecasting models to achieve high levels of accuracy and robustness.

6.4 Performance Comparison

AUNET beats N-BEATS across all error metrics, as shown in Table 6.1, proving it's better at making predictions and is more robust. We used several evaluation metrics

in this study—Mean Absolute Error (MAE), Root Mean Square Error (RMSE), and the Coefficient of Determination (R^2)—to get a full picture of how well each model predicts the time series data. AUNET's consistent performance across all these metrics shows it's able to give more accurate and reliable forecasts compared to N-BEATS.

Looking at the Mean Absolute Error (MAE), AUNET has a much lower value (0.8857) than N-BEATS (2.7391). MAE measures the average size of the errors in the predictions, without worrying about whether they're over or under the actual values. It's a straightforward way to see how far off the predictions are, on average. The lower MAE for AUNET means its predictions are, on average, closer to the true values than those of N-BEATS. This shows that AUNET can make precise predictions, keeping the typical errors small, which is important in applications where even small deviations matter like in temperature forecasting, where small errors can have big impacts.

Table 6.1: Comparison of Error Metrics for AUNET and NBEATS

Error Metric	**AUNET**	**NBEATS**
MAE	0.8857	2.7391
RMSE	0.9896	3.5588
R^2 Score	0.9948	0.9271

AUNET outperforms N-BEATS in all the error metrics, as shown in Table 6.1, proving it's better at making predictions and is more robust. We used Mean Absolute Error (MAE), Root Mean Square Error (RMSE), and the Coefficient of Determination (R^2) to see how well each model predicts the time series data. AUNET's consistent performance across these metrics shows it's more accurate and reliable compared to N-BEATS.

The MAE for AUNET is much lower (0.8857) than for N-BEATS (2.7391). MAE measures the average size of the errors in the predictions, without worrying about whether they're over or under the actual values. A lower MAE for AUNET means its predictions are, on average, closer to the true values than those of N-BEATS. This shows that AUNET makes more precise predictions, keeping errors small, which is important in areas like temperature forecasting where even small mistakes can have big impacts.

Similarly, the RMSE is a lot lower for AUNET (0.9896) compared to N-BEATS (3.5588). RMSE emphasizes larger errors by squaring the differences between predicted and actual values before averaging them. So, a lower RMSE for AUNET means it's better at reducing big errors compared to N-BEATS. This is important because large deviations can lead to wrong conclusions or bad decisions, especially in critical applications like climate modeling or financial forecasting. AUNET's ability to keep RMSE low shows it's robust in maintaining prediction accuracy even when there are irregular or extreme data points.

Moreover, AUNET achieves a much higher R^2 score of 0.9948 compared to N-BEATS' score of 0.9271. The R^2 score measures how much of the variance in the observed data is explained by the model. An R^2 score closer to 1 means the model accounts for most of the variability in the data. AUNET's high R^2 score means it captures nearly all the variance in the temperature data, showing a strong model fit and making it reliable for forecasting. In contrast, N-BEATS explains less of the

variability, which means it might miss some underlying patterns or trends in the data. This makes AUNET the better choice when high reliability and precision are needed.
These results show that AUNET not only gives more accurate predictions but is also more robust and reliable. Its lower MAE means it consistently stays closer to the actual values, which is crucial when precision is key. The lower RMSE indicates that AUNET is good at minimizing big errors, making sure that large mistakes, which can be harmful, are less common. This makes AUNET effective in real-world situations where large prediction errors could have serious consequences.
Also, the higher R^2 score shows that AUNET understands and models the underlying relationships in the data better than N-BEATS. Capturing nearly all the variance in the data ensures that AUNET's predictions are not only accurate but also align well with the real patterns and trends in the temperature data. This makes the model reliable for decision-making, as it can be trusted to provide insights that accurately reflect actual conditions. For example, in temperature forecasting, capturing the full variability of the data is crucial for things like agricultural planning, energy forecasting, or public health, where accurate temperature predictions can significantly affect planning and resource allocation.
So, AUNET is the better choice for this forecasting task over N-BEATS. The combination of lower MAE, reduced RMSE, and a higher R^2 score shows AUNET's superior predictive performance. Its ability to provide accurate forecasts, reduce large prediction errors, and explain most of the data's variance makes it a highly robust and reliable model for time series forecasting tasks. The attention mechanisms in AUNET play a key role in helping it focus on important temporal features, which further boosts its performance compared to models like N-BEATS.

6.5 Ablation Study

This section shows the best hyperparameters for the attention integrated models and also digs deeper into how N-BEATS models perform when they're combined with different attention mechanisms like Self-Attention, Neural Attention Memory (NAM), ProbSparse Attention, Multi-Query Attention, and AUNET's Multi-Head Attention. We analyze their performance using visual comparisons and some key metrics, highlighting what each approach does well and where it might fall short—especially when it comes to prediction accuracy, how fast they compute results, and how well they capture time-based dependencies in the data. What we find really shows how important it is to pick the right attention mechanism to boost the N-BEATS model's forecasting abilities.
For the other attention mechanisms integrated into the N-BEATS model, hyperparameter settings were carefully chosen based on extensive experimentation, as summarized in Table 6.2. These settings allowed each attention mechanism to contribute effectively to the model's performance by capturing temporal dependencies in the time series data.
The hyperparameter configurations for different attention mechanisms were carefully chosen to achieve stable training and optimal performance in time series forecasting. For the **Self-Attention Mechanism**, we set a learning rate of 0.0001 and a dropout rate of 0.5 to maintain stability. We used four attention heads to capture various

Table 6.2: Hyperparameter Tuning Summary of Other Attention Based N-BEATS Models

Attention Mechanism	Learning Rate	Dropout Rate	Attention Heads	Batch Size
Self-Attention	0.0001	0.5	4	16
NAM Attention	0.0001	0.4	3	32
ProbSparse Attention	0.0001	0.5	8	16
Multi-Query Attention	0.0001	0.5	6	32

temporal dependencies, and a batch size of 16 was selected to balance training speed and memory use.

The **Neural Attention Memory (NAM)** used a learning rate of 0.0001 with a slightly lower dropout rate of 0.4, which helped the model retain important information while minimizing overfitting. We used three attention heads and a batch size of 32 for efficient learning.

For the **ProbSparse Attention Mechanism**, we maintained a learning rate of 0.0001 and a dropout rate of 0.5. Eight attention heads were employed to manage the sparse attention mechanism effectively, focusing on the key parts of the sequence. We used a batch size of 16 to promote generalization.

The **Multi-Query Attention Mechanism** had a learning rate of 0.0001 and a dropout rate of 0.5, similar to other mechanisms. Six attention heads were used to balance capturing dependencies and reducing computational load, and a batch size of 32 was chosen for faster training without sacrificing accuracy.

These configurations helped ensure efficient convergence while capturing both short-term and long-term dependencies, contributing to the overall robustness and reliability of the N-BEATS model.

Figure 6.3, 6.4, 6.5 & 6.6 feature four plots that compare the predictions of N-BEATS models using different attention mechanisms. Each plot gives us a visual snapshot of how each model handles the data. By looking at these, we can see patterns in how well each attention mechanism helps the model predict the time series.

For instance, some attention mechanisms might help the model better capture quick fluctuations in the data, while others might smooth out the predictions too much, missing some of the finer details. Self-Attention could excel at identifying important patterns over various time scales, whereas ProbSparse Attention might speed up computations but at the cost of some accuracy.

By comparing these different approaches side by side, we get a clearer picture of how each attention mechanism affects the model's ability to learn from the data. This helps us understand which mechanisms are better suited for specific types of forecasting tasks, depending on what's most important—be it accuracy, speed, or the ability to catch complex temporal relationships.

In the end, this comprehensive comparison highlights that choosing the right attention mechanism isn't just a technical detail—it's a crucial decision that can significantly enhance the performance of N-BEATS models in time series forecasting. It shows that by carefully selecting the attention mechanism, we can improve how well the model predicts future data points, making our forecasts more reliable and effective.

In Figure 6.3, we compare the predictions of the standard N-BEATS model with those from the N-BEATS model enhanced with Self-Attention. Both sets of predictions (in green) overlap a lot, suggesting that while Self-Attention helps highlight

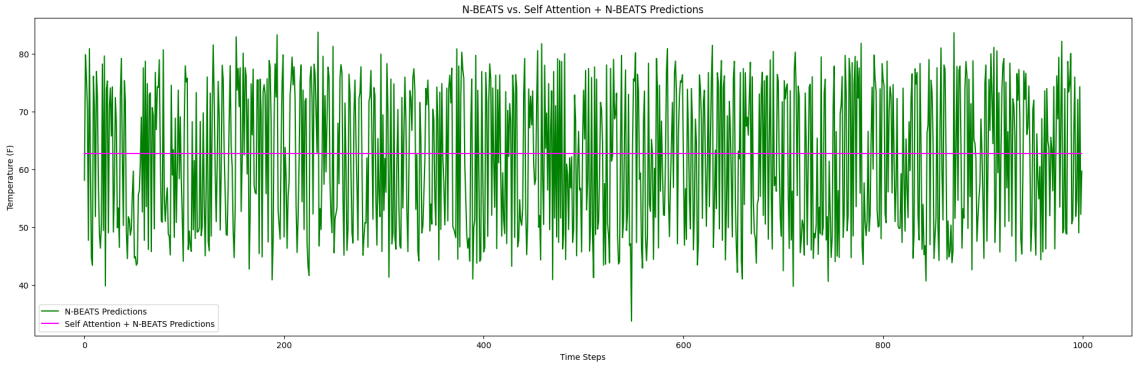

Figure 6.3: Comparison of N-BEATS Predictions with Self Attention + N-BEATS Prediction

important time points, it doesn't make a big difference in prediction accuracy for this dataset. This might be because the dataset doesn't have strong periodic features that Self-Attention can latch onto effectively. Also, since the predictions are so similar, the extra computational effort of using Self-Attention might not be worth it here if it doesn't significantly boost accuracy.

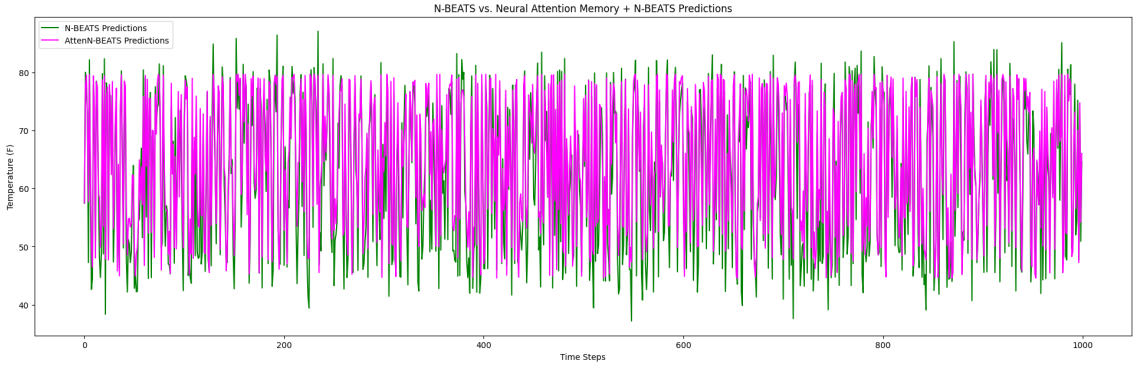

Figure 6.4: Comparison of N-BEATS Predictions with Neural Attention Memory + N-BEATS Prediction

In Figure 6.4, we contrast the standard N-BEATS model with the one integrated with Neural Attention Memory (NAM). The NAM-enhanced predictions, shown in magenta, seem to capture more of the underlying patterns, indicating a better ability to use key temporal features and reduce prediction errors. This suggests that NAM gives the model a stronger way to remember and leverage important information over time. By keeping a memory component, the NAM-enhanced model effectively holds onto and reuses past information, leading to more accurate short-term and long-term predictions. This is especially clear in how well it captures the quick temperature fluctuations that the standard N-BEATS model often misses.
Figure 6.5 compares the baseline N-BEATS model with the one using ProbSparse Attention. The magenta predictions from ProbSparse Attention show bigger deviations from the baseline, indicating that focusing on sparsity might have caused the model to miss crucial temporal information, reducing overall prediction accuracy. While ProbSparse Attention aims to concentrate on the most critical parts of the time series, this seems to come at the cost of losing some important details, leading to less accurate predictions. This trade-off between computational efficiency and

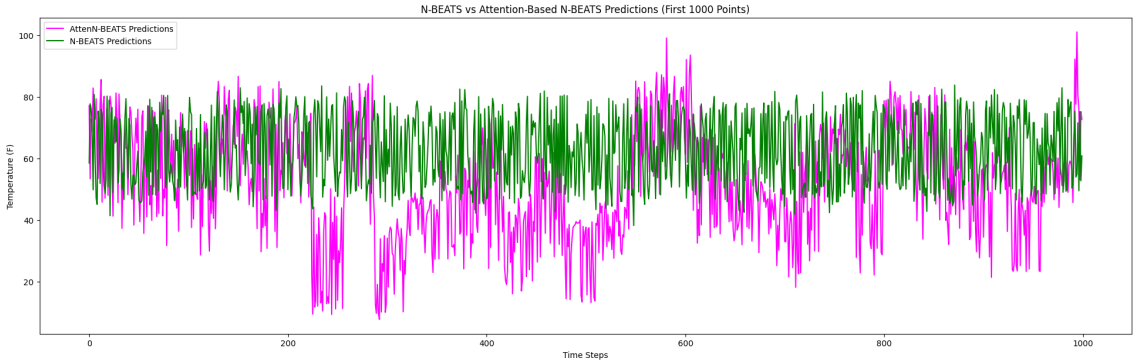

Figure 6.5: Comparison of N-BEATS Predictions with ProbSparse Attention + N-BEATS Prediction

prediction quality is evident in the differences between the ProbSparse-enhanced predictions and the actual data, especially during periods of rapid temperature changes. Even though ProbSparse Attention helps cut down computational complexity, its tendency to ignore non-critical information might lead to weaker performance in datasets that need a thorough analysis of all data points.

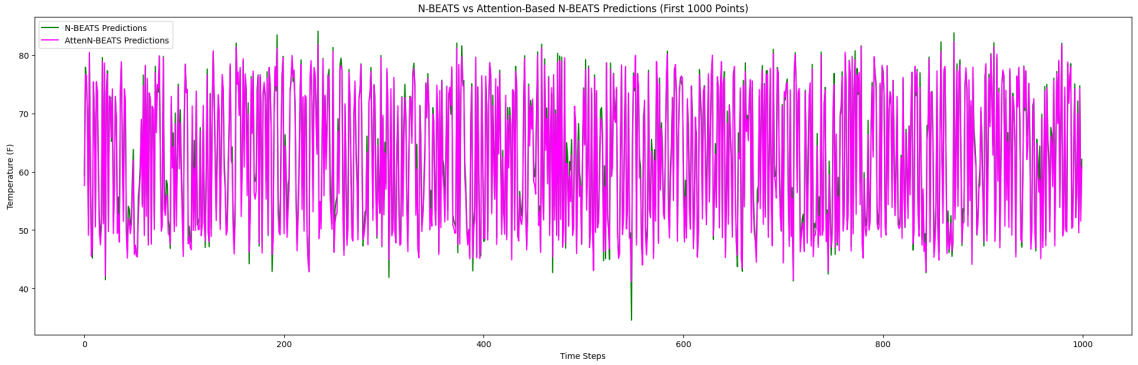

Figure 6.6: Comparison of N-BEATS Predictions with Multi-Query Attention + N-BEATS Prediction

Lastly, figure 6.6 shows a comparison between the baseline N-BEATS and the model enhanced with Multi-Query Attention. In this plot, the magenta predictions closely follow the green ones, showing that Multi-Query Attention keeps high accuracy while improving computational efficiency by sharing queries across multiple heads. This mechanism not only captures the key dependencies in the data but also reduces the model's complexity, making it an effective and balanced solution. By cutting down the number of attention queries while still maintaining multiple perspectives on the time series data, Multi-Query Attention offers an efficient way to boost N-BEATS's forecasting abilities without significantly increasing computational load.
Overall, each attention mechanism performs differently. NAM and Multi-Query Attention (Figure 6.4 & 6.6) show improved predictive performance compared to the baseline. Their predictions closely match the actual data, highlighting their effectiveness in enhancing the model's ability to predict future values accurately. On the other hand, ProbSparse Attention (Figure 6.5) deviates more noticeably, suggesting it may not be as good at capturing the full temporal structure of the dataset. These plots underline the importance of choosing the right attention mechanism, as

some, like NAM and Multi-Query Attention, clearly boost predictive performance, while others, like ProbSparse Attention, involve a trade-off between computational efficiency and accuracy.
The differences shown in these plots suggest that attention mechanisms like NAM and Multi-Query Attention add significant value by increasing the focus on key temporal patterns and improving overall accuracy. NAM excels when memory retention and recognizing recurring patterns are essential, while Multi-Query Attention offers a good balance between accuracy and computational demands. In contrast, mechanisms like ProbSparse Attention, although efficient in reducing computational burden, might not focus enough on all relevant time points, leading to weaker performance in datasets with complex temporal dynamics.
Compared to methods like ProbSparse Attention, which tries to reduce computational complexity by focusing on only a subset of time steps, AUNET's Multi-Head Attention maintains accuracy by ensuring no crucial information is lost. The multi-head structure lets AUNET assign different attention heads to different parts of the input sequence, capturing various temporal relationships. This not only boosts accuracy but also makes the predictions more robust, as the model can effectively pay attention to both short-term fluctuations and long-term trends at the same time. Additionally, mechanisms like Self-Attention and NAM, while good at enhancing temporal focus, don't benefit from the same level of efficiency and diverse pattern recognition that AUNET's multiple attention heads provide. This makes AUNET not just a powerful choice for boosting accuracy but also for maintaining computational efficiency, leading to consistently better performance across different types of time series data.

Table 6.3: Performance Metrics for Attention Mechanisms Integrated with N-BEATS

Attention Mechanism	**MAE**	**RMSE**	**R^2 Score**
Self-Attention	11.520	13.184	-0.000056
Neural Attention Memory (NAM)	5.196	6.457	0.760
ProbSparse Attention	13.711	17.086	-0.540
Multi-Query Attention	3.307	4.243	0.896

In Table 6.3, the **Self-Attention Mechanism** got a **Mean Absolute Error (MAE)** of 11.52 and a **Root Mean Squared Error (RMSE)** of 13.18, with an **R-squared (R^2)** value of -0.000056. Even though self-attention could focus on important time steps, overall it didn't improve much over the baseline—maybe because of overfitting from too many attention parameters. So, the self-attention approach wasn't that impactful here, showing that adding complexity doesn't always lead to better results in datasets without strong time patterns.
The **Neural Attention Memory (NAM)** mechanism made the model work a lot better, achieving an **MAE** of 5.20 and an **RMSE** of 6.46, with an R^2 value of 0.76. NAM let the model keep and use crucial past info effectively, making predictions more accurate compared to the self-attention mechanism. Being better at remembering and leveraging key features over time helps NAM shine, especially in datasets where past info plays a big role in future outcomes.
The **ProbSparse Attention** mechanism ended up with an **MAE** of 13.71 and an **RMSE** of 17.09, and an R^2 score of -0.54. Its performance was noticeably worse

than the other variants, probably because the sparsity constraint made it miss some critical time info. This suggests that while ProbSparse attention can cut down on computation, it might not be the best for complex datasets that need richer representations. The trade-off between saving on computational cost and losing key temporal info shows how important it is to pick attention mechanisms based on the dataset's complexity and nature.

The **Multi-Query Attention** mechanism got the best results among all the variants, with an **MAE** of 3.31, an **RMSE** of 4.24, and an R^2 value of 0.90. Sharing queries allowed for computational efficiency while still capturing essential time dependencies, leading to better forecasting accuracy. This shows that cutting down the number of queries can boost efficiency without hurting prediction quality. Multi-Query Attention strikes a good balance between accuracy and computational cost, making it great for situations that need efficient and accurate forecasting.

On the other hand, AUNET (Multi-Head Attention + N-BEATS) stands out as the best-performing model because of its top-notch accuracy across all evaluation metrics. In Table 6.1, it shows the lowest **Root Mean Squared Error (RMSE)** of **0.9896** and the lowest **Mean Absolute Error (MAE)** of **0.8857**, meaning its predictions are way more precise compared to other models. Plus, AUNET achieves an **R^2 score** of **0.9948**, which is really close to 1, showing it explains almost all the variance in the data effectively.

AUNET does so well because of its **Multi-Head Attention** mechanism, which lets the model focus on multiple features of the time series at the same time, grabbing both long-term trends and short-term changes. Unlike models like **ProbSparse Attention**, which gives up some time info for efficiency, or **Self-Attention**, which doesn't improve much here, AUNET's multi-head approach gets a richer representation of the temporal patterns. So, AUNET balances efficiency with a detailed focus on key time features, leading to consistently better predictions compared to the other attention-based N-BEATS models.

Overall, this section points out the strengths and limits of each attention mechanism when used with the N-BEATS model. NAM and Multi-Query Attention gave significant performance boosts, while ProbSparse Attention showed potential trade-offs between computational efficiency and prediction accuracy. AUNET, with Multi-Head Attention, showed the best performance, highlighting the value of dynamic attention for optimal accuracy in time series forecasting.

Chapter 7

Conclusion

This study introduced AUNET, an improved version of the N-BEATS model that uses different attention mechanisms to enhance univariate time series forecasting. The results showed that adding attention mechanisms, like Multi-Head Attention, helped the model understand both short-term and long-term patterns better, leading to more accurate forecasts compared to the original N-BEATS and other variations. AUNET had fewer prediction errors and proved to be reliable, making it a good choice for different time series tasks in various domains. This study proves that choosing the right attention mechanism can really boost the performance of forecasting models, as it allows the model to focus on the most important parts of the data, capturing both subtle changes and broader trends effectively.

7.1 Limitations

AUNET, while effective, has some drawbacks. It was only tested for univariate time series forecasting, so it is unclear how well it would work on multivariate data where multiple factors need to be considered simultaneously. The added attention mechanisms make the model more complex, which means training takes longer and needs more computational power. This could be a limitation for users with limited resources or those needing faster model updates. Also, the model can be hard to interpret, especially with the complex attention layers, which may make it difficult for domain experts to understand how the model makes decisions and to trust its predictions in critical applications.

7.2 Future Work

Future work could explore expanding AUNET to handle multivariate time series data, allowing it to work with datasets that have multiple features and dependencies. Making the model easier to understand would also be important so that it can be used more widely in real-life applications where interpretability is key. Researchers could develop lighter attention mechanisms to reduce computing power, making the model suitable for real-time use and edge deployment. Applying the model to areas like finance, healthcare, and climate science could show its effectiveness across different fields and highlight the practical benefits of advanced attention mechanisms for time series forecasting.

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