Systematic Trading Strategies with Machine Learning Algorithms

Time Series Forecasting with Neural Networks



June 12, 2025

Outline



Position of the Problem

Temporal Processing using RNNs

The Transformer Architecture

The Variable Selection Network

The TFT Architecture

Programming Session: Forecasting daily realized volatility of 31 stock indices

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- Goal: Predict multiple future time steps for a target variable (y^t_i) using:
 - Past observations of the target variable.
 - Additional features that provide context and improve forecasting accuracy.
- Multiple time series:
 - We consider several entities i ∈ {1,..., N}, each associated with its own time series (y_i^t)_{t-T_b+1≤t≤t+T_f.}
 - Examples of entities:
 - Finance: Volatility for different stocks in financial markets.
 - **Energy:** Consumption or production across multiple regions.
 - Traffic: Flow rates at various locations.

Position of the Problem



- Let us consider an entity *i* at time *t*:
- We aim to predict the future values of the univariate time series (y^t_i)_{t−T_b+1≤t≤t+T_f}:
 - The past values in a T_b sized window of the target time series: $(y_i^{t-T_b+1}, \dots, y_i^t)$
 - The future values up to the horizon $T_f: (y_i^{t+1}, \ldots, y_i^{t+T_f})$
- There are 3 possible inputs:

Name	Notation
Static attributes	$s_i \in \mathbb{R}^{d_s}$
Time varying unknown	$(z_i^{t-\mathcal{T}_b+1},\ldots,z_i^t)\in\mathbb{R}^{\mathcal{T}_b imes d_z}$
Time varying known	$(x_i^{t+1},\ldots,x_i^{t+T_f}) \in \mathbb{R}^{T_f imes d_x}$

Table: Types of Inputs



Features for Prediction:

Static Attributes:

- Fixed characteristics of each financial asset.
- Example: Industry sector or market capitalization of a stock.

Time-Varying Known Features:

- Features whose future values are available or predictable.
- Example: Economic calendar events, such as interest rate decisions or earnings announcements.
- Time-Varying Unknown Features:
 - Sequential features observed only up to the present time.
 - Example: Recent trends in stock price movements or realized volatility.



- Let Q be the set of quantiles that interest us. For this example, Q = {0.1, 0.5, 0.9}.
- ► The model outputs for each time step t + t_f (for t_f ∈ {1,..., T_f}) the prediction associated with each quantile q ∈ Q, denoted as ŷ_i^{t+t_f}(q).
- ► Thus, for each t_f ∈ {1,..., T_f}, the output vector at each time step t + t_f is given by:

$$\hat{y}_{i}^{t+t_{f}} = \begin{bmatrix} \vdots \\ \hat{y}_{i}^{t+t_{f}}(q) \\ \vdots \end{bmatrix}_{q \in \mathcal{Q}}$$

Position of the Problem



Example: The following graph summarizes the previous notations:



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The Learning Problem



- ► To train the model, we compare the predictions $\hat{y}_i^{t+t_f} \in \mathbb{R}^{|\mathcal{Q}|}$ to the true values $y_i^{t+t_f}$ for all $t_f \in \{1, \ldots, T_f\}$.
- The loss function is defined as:

$$\mathcal{L}(\mathcal{B}, \theta) = \sum_{i \in \mathcal{B}} \sum_{q \in \mathcal{Q}} \sum_{t_f=1}^{T_f} \frac{QL_q\left(y_i^{t+t_f}, \hat{y}_i^{t+t_f}(q)\right)}{|\mathcal{B}| T_f}$$

Where:

- B is the batch of training data.
- ► $\forall y, \hat{y} \in \mathbb{R}, \ QL_q(y, \hat{y}) = q(y \hat{y})_+ + (1 q)(\hat{y} y)_+$

Equivalently:

$$QL_q(y,\hat{y}) = \max\left((q-1)(y-\hat{y}), q(y-\hat{y})\right)$$





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Hidden Markov Models (HMMs):

- Popular in the 1980s for sequence modeling (e.g., speech recognition [10]).
- Relied on the Markov assumption for hidden states, limiting their ability to model long-range dependencies.

Recurrent Neural Networks (RNNs):

- Introduced to overcome HMM limitations.
- Achieved state-of-the-art performance in tasks such as speech recognition [4].

Introduction to Vanilla RNNs



- Feed-forward neural networks assume data is independent and identically distributed (i.i.d).
- Recurrent Neural Networks (RNNs) [11] process data sequentially, making them suitable for time-series and other sequence-based tasks.





- Objective: Process an input sequence of *D*-dimensional vectors x₁,..., x_T to generate *d*-dimensional hidden states h₁,..., h_T.
- Model Parameters:
 - ▶ $W_{xh} \in \mathbb{R}^{D \times d}$: Input-to-hidden weights.
 - ▶ $W_{hh} \in \mathbb{R}^{d \times d}$: Hidden-to-hidden weights.
- Hidden state at time t:

$$h_t = anh\left(W_{hh}^T h_{t-1} + W_{xh}^T x_t
ight)$$



Exploding Gradients:

 Occur when gradients become excessively large, destabilizing model training.

Vanishing Gradients:

- Occur when gradients diminish during backpropagation, preventing the model from learning long-term dependencies.
- Often observed in deep or sequential networks when dealing with long input sequences.



Solutions to Exploding Gradients:

- Gradient Clipping: Caps gradients to stabilize training [9].
- Solutions to Vanishing Gradients:
 - Regularization: Preserves norm consistency during training [9].
 - Gated Architectures:
 - Long Short-Term Memory (LSTM) [5]: Introduces gates to manage information flow.
 - Gated Recurrent Unit (GRU) [3]: Simplified alternative to LSTM.

Overview of LSTMs



- LSTMs were state-of-the-art for tasks like:
 - Machine Translation [13, 3, 1].
 - Language Modeling [12].
 - Time Series Prediction [6].
 - Robot Reinforcement Learning [2].
- Core Idea: Maintain long-term dependencies through a cell state regulated by gates.
- Gates are responsible for filtering information flow:
 - Input: New information to add.
 - Forget: Remove irrelevant information.
 - Output: Decide what to expose to the hidden state.

The Concept of Gates in LSTMs



Gates use a sigmoid function to scale values between 0 and 1:

$$\sigma(z) = \frac{1}{1 + e^{-z}}$$

 Point-wise multiplication adjusts information based on gate values.



(a) Filtering a signal using a sigmoid function and a neural network







Each time step has:

Cell State C^t: Preserves long-term memory.

Hidden State *h*^{*t*}: Represents short-term output.

- ▶ Transition from (h^{t-1}, C^{t-1}) to (h^t, C^t) involves:
 - 1. Filtering with input and forget gates.
 - 2. Generating a memory candidate \tilde{C}^t .
 - 3. Updating the cell state and computing the hidden state.



Each time step has:

Cell State *C*^{*t*}: Preserves long-term memory.

Hidden State *h*^{*t*}: Represents short-term output.

▶ Transition from (h^{t-1}, C^{t-1}) to (h^t, C^t) involves:

1. Filtering with input and forget gates.

2. Generating a memory candidate \tilde{C}^t :

$$\tilde{C}^t = \tanh\left(W_C[h^{t-1}, x^t] + b_C\right)$$

3. Updating the cell state and computing the hidden state.

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Forget Gate: Filters irrelevant past memory.

$$f^{t} = \sigma \left(W_{f}[h^{t-1}, x^{t}] + b_{f} \right)$$

Input Gate: Filters new memory candidate.

$$i^{t} = \sigma \left(W_{i}[h^{t-1}, x^{t}] + b_{i} \right)$$

• **Output Gate:** Determines visible parts of the cell state.

$$o^{t} = \sigma \left(W_{o}[h^{t-1}, x^{t}] + b_{o} \right)$$



Cell State Update:

$$C^t = f^t \circ C^{t-1} + i^t \circ \tilde{C}^t$$

$$h^t = o^t \circ \tanh(C^t)$$

- Result: LSTMs Handle long-term dependencies better than vanilla RNNs. LSTMs can:
 - **Write:** Add new information via the input gate.
 - **Erase:** Remove irrelevant information via the forget gate.
 - **Read:** Expose relevant memory via the output gate.

The LSTM Architecture





Figure: LSTM architecture.





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- Section 1: Temporal Processing using RNNs
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- LSTM/GRU models in Many-to-Many settings require input and output sequences of the same length (e.g., POS tagging [15]).
- ► For applications where $T_x \neq T_y$ (e.g., machine translation), we need the Sequence to Sequence (Seq2Seq) framework.
- Seq2Seq maps an input sequence of length T_x to an output sequence of length T_y using two components:
 - 1. **Encoder:** Encodes the input sequence into a fixed-length representation.
 - 2. **Decoder:** Generates the output sequence from the encoded representation.

Sequence to Sequence Framework







Encoder:

Maps the input sequence (X¹_i,...,X^{T_x}) ∈ ℝ^{T_x×D_x</sub> into hidden states h¹_i,...,h^{T_x}.}

Final hidden state $h_i^{T_x}$ summarizes the input sequence.

Decoder:

Takes the encoder's last hidden state h_i^{T_x} as its initial hidden state s_i⁰.



Example: Seq2seq for machine translation







Challenges with Seq2Seq Framework:

- Encoder compresses all input information into a fixed-length vector, leading to information loss.
- Performance degrades for long input sequences.
- No mechanism for aligning input and output sequences.

Alignment Intuition:

- For each output Y^t_i, the model should selectively focus on relevant parts of the input sequence X^{t'}_i.
- Alignment helps determine how much of each X_i^{t'} contributes to generating Y_i^t.

The Need for Alignment



The following figure shows the desired alignment matrix, where scores indicate the relevance of each input vector to a specific output.



Figure: Matrix of alignment scores.

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Key Challenges of Seq2Seq:

No explicit mechanism to focus on relevant parts of the input.

Why Attention?

Allows models to dynamically focus on relevant input parts.

 Combines perception with a selective memory mechanism for reasoning.

Applications:

- Machine translation.
- Time series prediction.
- Speech-to-text.

Attention: Query-Retrieval Modeling



- Attention mechanisms are inspired by database Query-Retrieval Problems:
 - A query is matched against keys to retrieve values.
 - The following figure shows a classic hard query retrieval system.



- In attention mechanisms:
 - Multiple keys can match a query (soft query retrieval).
 - The result is a weighted sum of values, called the attention vector.

Soft Query Retrieval: Steps



- ▶ Given: a query $q \in \mathbb{R}^{d_q}$, keys $(k_i)_{1 \leq i \leq n} \in \mathbb{R}^{n \times d_k}$, and values $(v_i)_{1 \leq i \leq n} \in \mathbb{R}^{n \times d_v}$.
- Steps:
 - 1. Compute alignment scores a_i between the query and each key:

$$a_i = a(q, k_i) \quad \forall i \in \{1, \ldots, n\}.$$

Normalize scores to get attention weights α_i using a distribution function (e.g., softmax):

$$\alpha_i = \frac{e^{a_i}}{\sum_{j=1}^n e^{a_j}}.$$

3. Compute the attention vector as a weighted sum of values:

$$A(q, K, V) = \sum_{i=1}^{n} \alpha_i v_i.$$



Alignment functions compute similarity between query q and keys k_i:

Function	Equation
Dot Product	$a(q,k_i) = q^T k_i$
Scaled Dot Product	$a(q,k_i) = rac{q^T k_i}{\sqrt{d_k}}$
Luong's	
Multiplicative	$a(q,k_i) = q^T W k_i$
Bahdanau's	7 · · · · · · · · · · · · · · · · · · ·
Additive	$a(q,k_i)=v_a^{\prime} ext{ tanh}(W_1q+W_2k_i)$
Feature-based	$a(q,k_i) = W_{imp}^{\mathcal{T}} \operatorname{act}(W_1\phi_1(k_i) + W_2\phi_2(q) + b)$
Kernel Method	$a(q,k_i)=\phi(q)^{\mathcal{T}}\phi(k_i)$

Table: Common Alignment Functions.

Soft and Sparse Attention



Soft Attention:

Uses dense alignments with a softmax function:

$$\alpha_i = \frac{e^{a_i}}{\sum_{j=1}^n e^{a_j}}.$$

Sparse Attention:

Assigns non-zero probabilities to only a few values.

Examples:

- Sparsemax [7].
- Sparse Entmax [8].

The attention vector combines weighted values:

$$A(q, K, V) = \sum_{i=1}^{n} \alpha_i v_i.$$
Soft Query Retrieval Summary







Objective: Learn a mapping function Φ_θ from input sequences to output sequences.

$$(\hat{Y}_i^1,\ldots,\hat{Y}_i^{T_y})=\Phi_{\theta}(X_i^1,\ldots,X_i^{T_x}).$$

• Components of Φ_{θ} :

- 1. **Encoder:** Maps input sequence to hidden states $h_i^1, \ldots, h_i^{T_x}$.
- 2. **Attention Layer:** Computes context vector $c_i^{t_y}$ for each output step.
- 3. **Decoder:** Generates output sequence using attention and decoder states.

Sequence to Sequence with Attention





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The Encoder



- ▶ The encoder can be a GRU model or an LSTM model that transforms input sequence $(X_i^1, \ldots, X_i^{T_x})$ into hidden states $(h_i^1, \ldots, h_i^{T_x})$.
- The GRU Model



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The Attention Layer

Assigns weights to encoder hidden states to compute a context vector c_i^{ty}:

$$c_i^{t_y} = \sum_{t_x=1}^{T_x} \alpha_i^{\langle t_y, t_x \rangle} h_i^{t_x}.$$

Steps:

- 1. Compute alignment scores $e_i^{\langle t_y, t_x \rangle}$ between decoder hidden state $s_i^{t_y-1}$ and encoder hidden states $h_i^{t_x}$.
- 2. Normalize scores into attention weights $\alpha_i^{\langle t_y, t_x \rangle}$ using a distribution function (e.g., softmax).
- 3. Calculate context vector $c_i^{t_y}$ as a weighted sum of encoder hidden states.





▶ Calculating the weights: $\alpha_i^{\langle t_y, t_x \rangle}$ for all $t_x \in \{1, \ldots, T_x\}$:



The Decoder and Application-Specific Final Layer Imperial College

Decoder: Combines:

- Previous hidden state $s_i^{t_y-1}$,
- Context vector $c_i^{t_y}$ (from the attention mechanism),

• To generate the decoder hidden state $s_i^{t_y}$.

Final Layer: Maps $s_i^{t_y}$ to the output prediction $\hat{Y}_i^{t_y}$.

The nature of the final layer depends on the application:

- Machine Translation: Dense layer with a softmax activation to predict the next word in a target language.
- Text Generation: Softmax-based layer for generating characters or tokens.
- Time Series Forecasting: Regression output layer for predicting continuous values, such as stock prices or energy consumption.





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Programming Session: Forecasting daily realized volatility of 31 stock indices



- The paper "Attention is All You Need" [14] introduced a groundbreaking model called the Transformer.
- Key contributions:
 - Eliminates the need for recurrent units (e.g., RNNs, LSTMs) in sequence-to-sequence tasks.
 - Fully relies on self-attention mechanisms for capturing dependencies.
- The Transformer model has revolutionized sequence modeling tasks such as machine translation, text summarization, and more.

Introduction to the Transformer



The following figure illustrates the full Transformer architecture.



Figure: The Transformer Architecture [14].

Creating a Contextual Embedding with Self-Attentionaria College

- ► Given a sequence of *D*-dimensional input vectors (X^t)_{1≤t≤T}, we project each vector X^t into:
 - Query space: $q^t = W_Q^T X^t$, $W_Q \in \mathbb{R}^{D \times d_q}$,
 - Key space: $k^t = W_K^T X^t$, $W_K \in \mathbb{R}^{D \times d_k}$,
 - ► Value space: $v^t = W_V^T X^t$, $W_V \in \mathbb{R}^{D \times d_v}$.
- ▶ **Objective**: Create a **contextual embedding** for each query q^t , leveraging all keys $(k^{t'})_{1 \le t' \le T}$ and values $(v^{t'})_{1 \le t' \le T}$.
- Intuition: Compute the attention weights α^{<t,t'>} to determine how much each value v^{t'} contributes to the embedding A (q^t, (k^{t'})_{1≤t'≤T}, (v^{t'})_{1≤t'≤T}).

Creating a Contextual Embedding with Self-Attentionerial College



Computing the Contextual Embedding



Use the scaled dot product alignment function [14] to compute similarity scores:

$$e^{< t,t'>} = rac{q^t \cdot k^{t'}}{\sqrt{d_k}}$$

Convert similarity scores to attention weights using the softmax distribution:

$$\alpha^{\langle t,t'\rangle} = \frac{\mathsf{e}^{\langle t,t'\rangle}}{\sum_{s=1}^{T} \mathsf{e}^{\langle t,s\rangle}}$$

Compute the contextual embedding:

$$A\left(q^{t}, (k^{t'})_{1 \le t' \le T}, (v^{t'})_{1 \le t' \le T}\right) = \sum_{t'=1}^{T} \alpha^{< t, t' > v^{t'}}$$



► To compute contextual embeddings for all input vectors (X^t)_{1≤t≤T}, we define:

$$Q = \begin{bmatrix} q^1 \\ \vdots \\ q^T \end{bmatrix} \in \mathbb{R}^{T \times d_q}, \ \mathcal{K} = \begin{bmatrix} k^1 \\ \vdots \\ k^T \end{bmatrix} \in \mathbb{R}^{T \times d_k}, \ V = \begin{bmatrix} v^1 \\ \vdots \\ v^T \end{bmatrix} \in \mathbb{R}^{T \times d_v}.$$

Each q^t, k^t, v^t is computed using projection matrices:

$$q^t = W_Q^T X^t, \quad k^t = W_K^T X^t, \quad v^t = W_V^T X^t.$$

 Q, K, V represent the query, key, and value matrices, respectively.

Scaled Dot Product Attention Matrix



Definition:

$$A(Q, K, V) := \operatorname{Softmax}\left(rac{QK^T}{\sqrt{d_k}}
ight) V.$$

Explanation:

- $\frac{QK^{T}}{\sqrt{d_k}}$: Computes pairwise similarities between queries and keys.
- Softmax: Converts similarities into attention weights.
- Multiplication with V: Aggregates values using attention weights.
- Each row of A(Q, K, V) corresponds to:

$$\mathcal{A}(q^t,\mathcal{K},\mathcal{V}) = \sum_{t'=1}^T lpha^{< t,t'>} \mathbf{v}^{t'}, \quad \forall t \in \{1,\ldots,T\}.$$

MultiHead Attention (MHA)



- Objective: Extend the attention mechanism to multiple heads to capture diverse notions of similarity.
- Attention mechanism is applied *h* times:

$$A\left(\mathcal{QW}_Q^{h'},\mathcal{KW}_K^{h'},\mathcal{VW}_V^{h'}
ight) \quad ext{for } h'\in\{1,\ldots,h\}.$$

Projection matrices for each head h':

$$W_Q^{h'} \in \mathbb{R}^{d_q imes p_q}, \quad W_K^{h'} \in \mathbb{R}^{d_k imes p_k}, \quad W_V^{h'} \in \mathbb{R}^{d_v imes p_v}$$

Outputs are concatenated and projected:

$$P = \operatorname{concat}(A_1, \ldots, A_h) W_o \in \mathbb{R}^{T_q \times p_o}.$$

Scaled Dot Product Attention Generalization



▶ The following figure illustrates MHA with *h* attention heads



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Positional Encoding: Intuition and Key Idea



 Objective: Incorporate positional information into the permutation-invariant attention mechanism to reflect the order of sequence elements.

Intuition:

- Positions in a sequence need a unique representation to differentiate elements based on their location.
- Shifting a positional encoding by k steps results in a consistent transformation that preserves relative distances.

Key Idea:

- Add positional encoding vectors $p^1, \ldots, p^T \in \mathbb{R}^D$ to input embeddings X^1, \ldots, X^T .
- Use periodic functions (sine and cosine) to define the positional encodings in a way that captures relative positions effectively.

Positional Encoding: Method and Properties



Method:

Positional encoding at step t:

$$p_d^t = \begin{cases} \sin(w_d t), & \text{if } d \text{ is odd,} \\ \cos(w_d t), & \text{if } d \text{ is even.} \end{cases}$$

Where $w_d = \frac{1}{10000\frac{2d}{D}}$ ensures unique frequencies for different dimensions.

Positional encodings are added to input embeddings:

$$\tilde{X}^t = X^t + p^t.$$

Properties:

- Shift Consistency: Shifting p^t by k steps aligns with p^{t+k} .
- Relative Distance Encoding: The sine and cosine functions ensure relative positional information is preserved across sequences.

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- Sequence-to-Sequence Model: Built entirely on attention mechanisms, eliminating recurrent units.
- **Core Components:**
 - Multi-Head Attention Layer: Captures different notions of similarity.
 - **Feed-Forward Layer:** Applies pointwise transformations.
 - Normalization Layer: Ensures stability and accelerates convergence.
- Architecture Overview: Combines stacked encoder and decoder layers to process and generate sequences efficiently.

The Encoder Layer



Objective: Generate attention-based contextual embeddings that focus on relevant parts of the input sequence.

Structure:

- Stack of N = 6 identical layers.
- Each layer consists of:
 - Multi-Head Self-Attention: Re-averages value vectors for contextual embeddings.
 - **Feed-Forward Layer:** Fully connected, applied pointwise.
 - Residual Connections and Normalization: Added after each sub-layer.

• **Output Dimension:** $d_{\text{model}} = 512$ for all layers.

The Encoder Layer in the Transformer







 Objective: Retrieve and use information from encoder outputs to generate target sequences.

Structure:

- Stack of N = 6 identical layers.
- Each layer includes:
 - Masked Multi-Head Self-Attention: Prevents information leakage (look-ahead masking).
 - Multi-Head Attention: Queries the encoder outputs.
 - **Feed-Forward Layer:** Applies pointwise transformations.
 - Residual Connections and Normalization: Enhance gradient flow and stability.

The Decoder Layer in the Transformer







Input Processing:

- Input sequence X = (X¹,..., X^{T_x}) embedded and combined with positional encodings.
- Encoder outputs context-aware representations $H = (h^1, \dots, h^{T_x}).$
- Decoding Process:
 - Decoder uses:
 - Self-Attention: Processes previously generated tokens with masked attention.
 - Encoder-Decoder Attention: Focuses on encoder outputs H to generate context for predictions.
 - Outputs generated step-by-step using linear and softmax layers.

The Transformer Architecture









Programming Session 7: Section 2

- Section 2: Coding the Transformer Architecture
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Variable Selection Network (VSN)



Explore the Variable Selection Network (VSN): Click here for the detailed implementation



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Temporal Fusion Transformer Architecture



Overview: A specialized deep learning model for time series forecasting with the following components:

Variable Selection Networks (VSN):

- Dynamically select the most relevant features from static, time-varying known features, and time-varying unknown features.
- Employ Gated Residual Networks for feature transformation and importance estimation.

Sequence-to-Sequence Framework:

- Encoder-decoder architecture for multi-step forecasting.
- Encoder processes historical data, while the decoder generates future predictions.



Masked Multi-Head Attention:

- Enables context-aware forecasting by focusing on relevant time steps in the past.
- Prevents information leakage by masking future time steps during decoding.
- Gated Residual Networks (GRN):
 - Adds non-linear transformations and flexible gating mechanisms.
 - Regularizes and improves robustness across diverse datasets.

TFT Architecture: High-Level View





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Outline



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Programming Session: Forecasting daily realized volatility of 31 stock indices



- Objective: Implement and experiment with the Temporal Fusion Transformer (TFT) for forecasting realized volatility.
- **Dataset:** Realized volatility data from 31 financial indices.

► Goals:

- Build the TFT model architecture.
- Train the model on time series data with static, time-varying known, and time-varying unknown features.
- Evaluate predictions and interpret model outputs.


Task: Forecast realized volatility for 31 indices.

 Outcome: Example of predicted vs. actual realized volatility for two indices.





 Objective: Understand how the model uses historical data for forecasting by highlighting the most influential historical time steps.



Results: Feature Importance



Objective: Quantify the impact of input features on predictions.



Feature Importance Analysis by Section

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Thank you.

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