

# Time Series Analysis

## Forecasting

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**Informatik**



# Outline

- Forecasting
- Forecasting with baselines, ARIMA
- Underfitting and overfitting
- Evaluation workflow
- Splitting time series data
- Residual analysis
- Confidence intervals
- Information criteria
- Performance metrics
- Back-transforms

# Forecasting

**Extrapolating** past observations to predict future data.

- Works well provided future data follows past patterns.
- Strong signals (low noise) can lead to accurate forecasts.
- Noise increases **uncertainty**, making predictions reliable only for the **short term**.

Sources of uncertainty

- Data: unexpected **disruption** from past patterns.
- Model: chosen model may not represent the **true data-generating process**.
- Parameters: even with the correct model, estimated **parameters may be inaccurate**.
- Forecasts: model typically yield an estimate of the **conditional mean** of future instances, which may be strongly influenced by future **unpredictable innovations**.

Forecasts must be complemented with a measure of the model uncertainty, typically **prediction intervals**.

# Forecasting

Given a time series realization  $\{x_1, x_2, \dots, x_T, \dots, x_n\}$ ,

The  $h$ -step forecast of  $x_{T+h}$  based on the data  $\{x_1, x_2, \dots, x_T\}$  is represented as  $\hat{x}_{T+h|T}$ .

- $T$  is the **forecast time**.
- $h$  is the **forecast horizon** i.e., how far into the future the forecast is made.
- $T + h$  is the **target time** i.e., the time point of the forecast.

Considering a monthly time series and a 1-year forecast horizon,

- **Point** forecast is  $\hat{x}_{T+12|T}$ .
- **Multi-step** forecast is  $\{\hat{x}_{T+1|T}, \dots, \hat{x}_{T+12|T}\}$ .

# Forecasting baselines

**Mean:** forecasts are equal to the average of the observed data,  $\hat{x}_{T+h|T} = \frac{1}{T} \sum_{i=1}^T x_i$

**Naïve:** forecasts are equal to the last observed value of the series,  $\hat{x}_{T+h|T} = x_T$

- Naïve is optimal for random walk process.

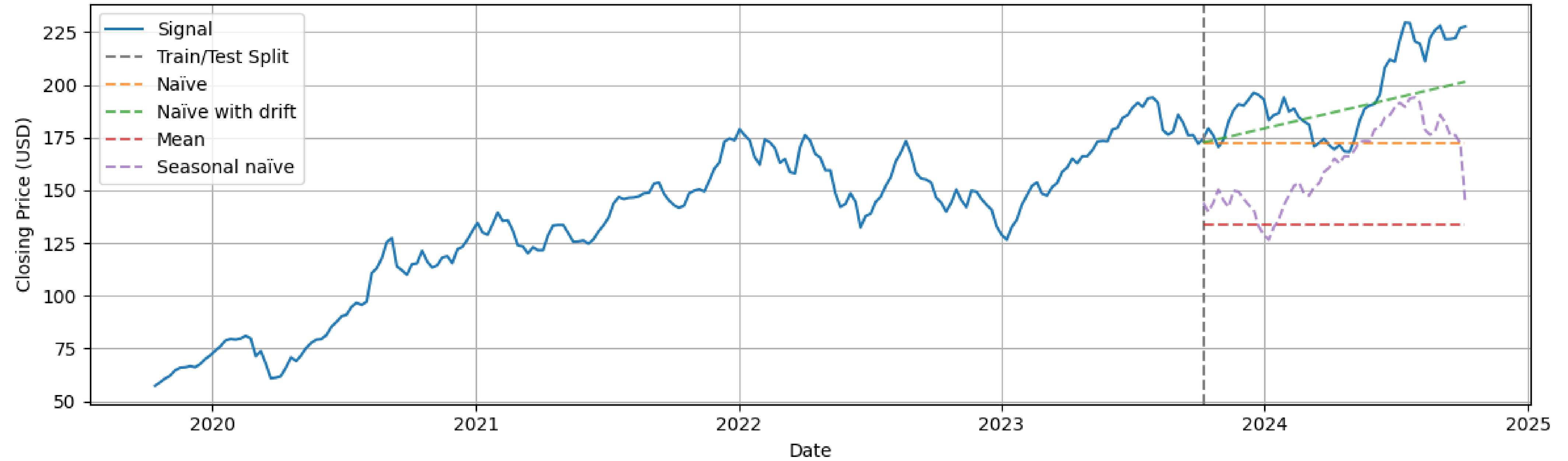
**Seasonal naïve:** forecasts are equal to the last observed value from the same season,  $\hat{x}_{T+h|T} = x_{T+h-[h/P]P}$

- Setting  $P = 1$  (non-seasonal data) results in the naïve forecast

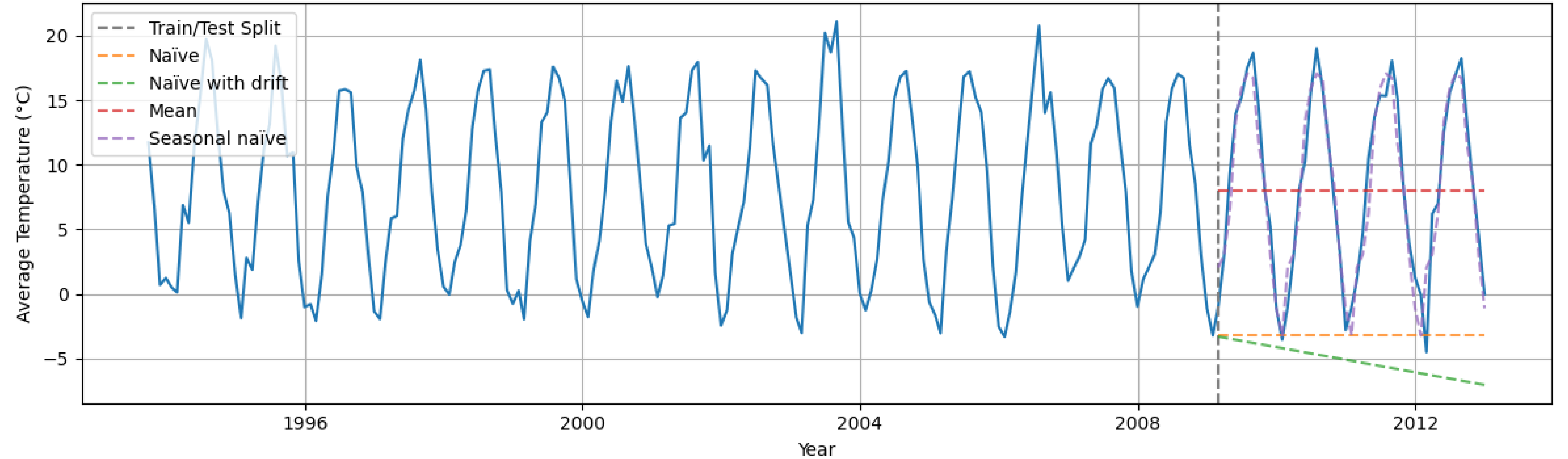
**Naïve with drift:** naïve forecast with linear drift,  $\hat{x}_{T+h|T} = x_T + h \frac{x_T - x_1}{T-1}$

Baselines serve as **benchmark** to evaluate the added value of more complex methods.

Time plot: Weekly Apple Inc. (AAPL) Closing Prices



Time plot: Monthly Average Temperature in Switzerland



# Forecasting with ARIMA

The forecast  $\hat{x}_{T+h|T}$  from an ARIMA model can be computed as follows:

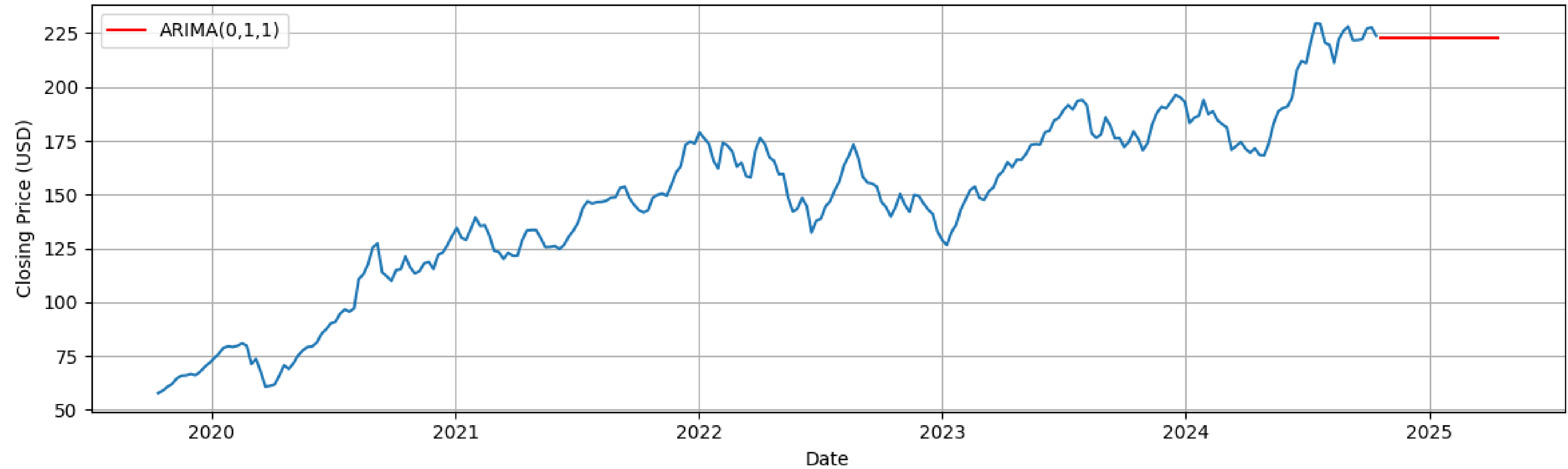
1. Rewrite the ARIMA equation  $\Phi(B)\nabla^d X_t = \Phi(B)(1-B)^d X_t = c + \Theta(B)W_t$  with  $x_t$  on the left-hand side.

- For an ARIMA(1,1,1):  $(1 - \hat{\phi}B)(x_T - x_{T-1}) = \hat{c} + (1 + \hat{\theta}B)w_T \Leftrightarrow x_T = \hat{c} + w_T + \hat{\theta}w_{T-1} + (\hat{\phi} + 1)x_{T-1} - \hat{\phi}x_{T-2}$

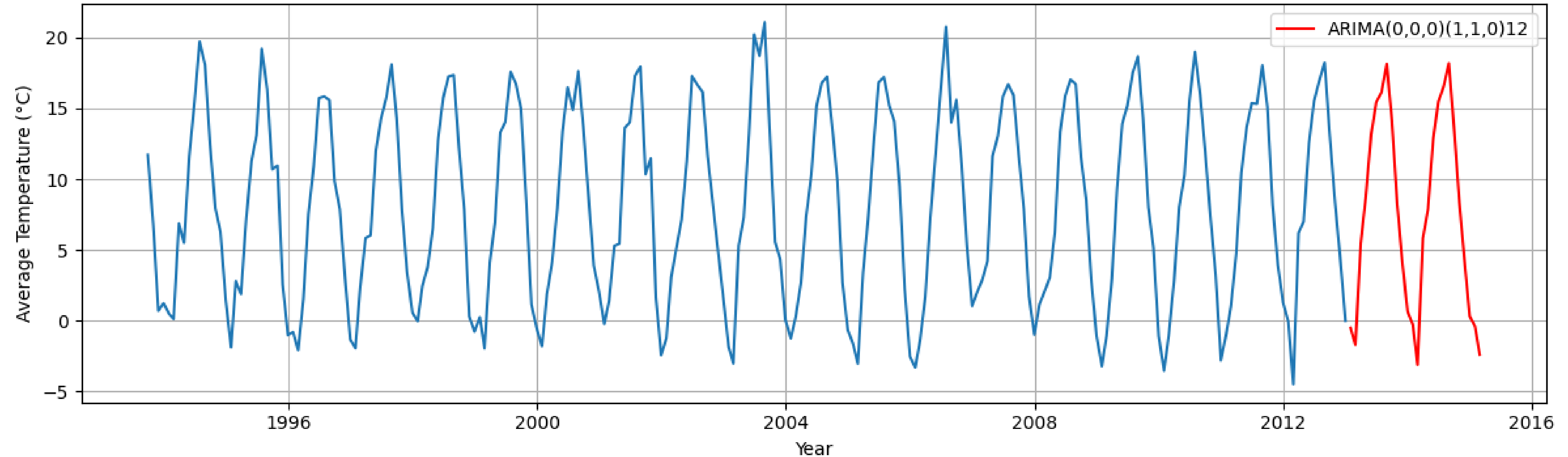
2. Replace future observations with their forecast, future errors with zero, and past errors with the ARIMA residuals.

- $T + h \rightarrow x_{T+h} = \hat{c} + w_{T+h} + \hat{\theta}w_{T+h-1} + (\hat{\phi} + 1)x_{T+h-1} - \hat{\phi}x_{T+h-2}$
- $h = 1 \rightarrow \hat{x}_{T+1|T} = \hat{c} + 0 + \hat{\theta}\hat{w}_T + (\hat{\phi} + 1)x_T - \hat{\phi}x_{T-1}$
- $h = 2 \rightarrow \hat{x}_{T+2|T} = \hat{c} + 0 + 0 + (\hat{\phi} + 1)\hat{x}_{T+1|T} - \hat{\phi}x_T$
- $h = 3 \rightarrow \hat{x}_{T+3|T} = \hat{c} + 0 + 0 + (\hat{\phi} + 1)\hat{x}_{T+2|T} - \hat{\phi}\hat{x}_{T+1|T}$
- ...

Time plot: Forecast of Monthly Average Apple Closing Prices



Time plot: Forecast of Monthly Average Temperature in Switzerland





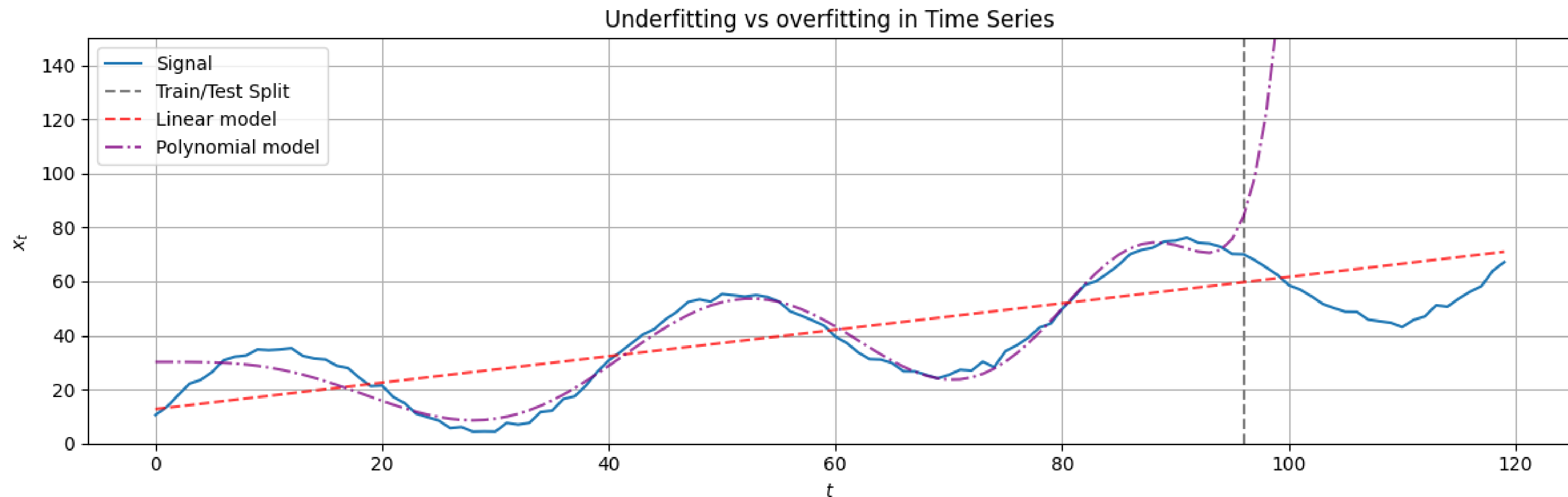
# Underfitting and overfitting

**Underfitting** occurs when a model fits training data poorly and fails to generalize to new data.

- Model is too simple to capture the underlying patterns in the data.

**Overfitting** occurs when a model fits training data very well but fails to generalize to new data.

- Model is too complex and learns to reproduce the training data exactly.
- Training data is too small.
- Training procedure does not involve regularization (discussed in following lectures).



# Evaluation workflow

Given a time series realization  $\{x_1, x_2, \dots, x_T, \dots, x_V, \dots, x_n\}$ ,

1. **Split dataset** into **training**  $\{x_1, \dots, x_T\}$ , **validation**  $\{x_{T+1}, \dots, x_V\}$ , and **test**  $\{x_{V+1}, \dots, x_n\}$  sets.
  - Validation set is required either when model fitting involves hyperparameters tuning or when model selection is based on performance metrics.
  - Multiple versions of training and validation sets can be considered with cross-validation.
2. **Train** candidate models on training set.
  - Tune hyperparameters using the validation set.
3. **Select model** based on model fit, complexity and performance on the validation set.
  - Information criteria, residual analysis, uncertainty, performance metrics
4. **Train selected model** on training + validation sets then **evaluate performance** on test set.
  - Metrics provide an indication of how well the model will forecast new data.

# Splitting time series data & rolling cross-validation

**Split dataset** into **training**  $\{x_1, \dots, x_T\}$ , **validation**  $\{x_{T+1}, \dots, x_V\}$ , and **test**  $\{x_{V+1}, \dots, x_n\}$  sets

- Time series must be split **chronologically** → **no random splits**.
- **Seasonality and trends**: ensure the splits account for any patterns in the data.
- Validation and test set should be at least as large as the **forecast horizon** i.e.,  $h \leq V - T$  and  $h \leq n - V$ .

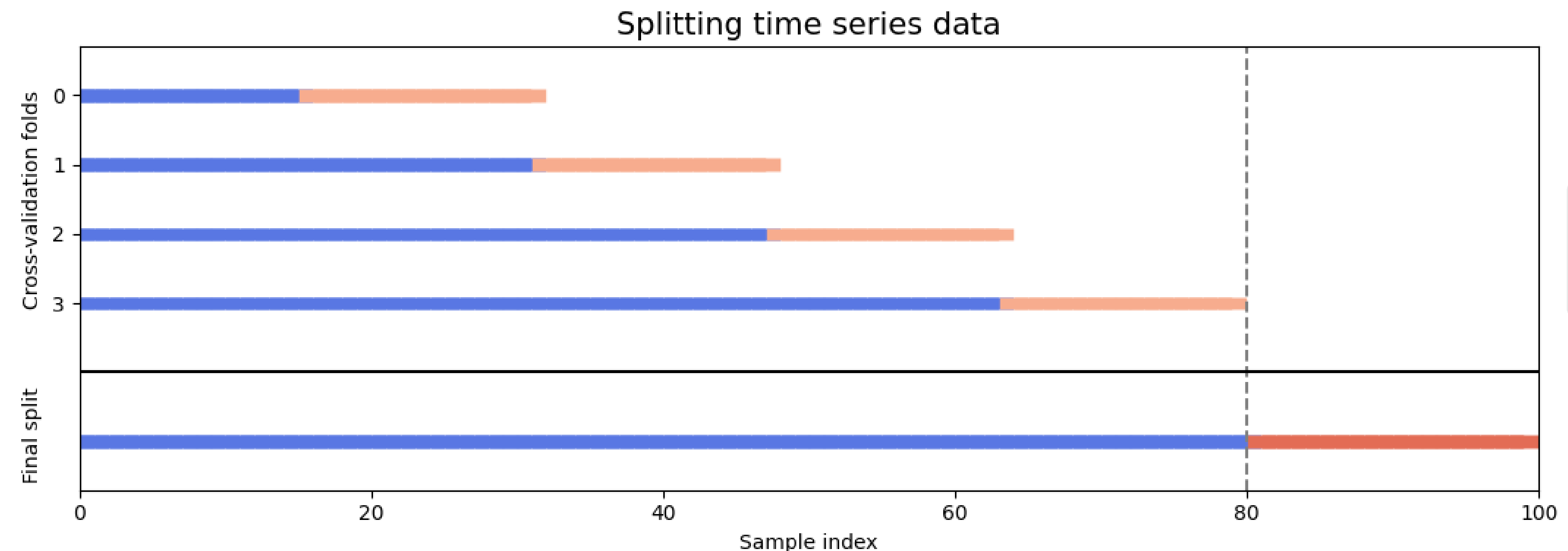
**Use test data once for final evaluation**, otherwise risk of **over-estimating** performance on new data

→ compare candidate models performance on the validation set.

## Rolling Cross-Validation:

sequentially increase the training set, while moving the validation set forward.

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# Residual analysis

**Residuals** are the difference between observed values and predicted values:  $e_i = x_i - \hat{x}_{i|T}$  for  $i = 1, \dots, T$ .

- Also called **training set errors**, it is an estimate of the noise/innovation component of the data.
- Residuals are expected to be **normal, uncorrelated, zero-mean, and homoscedastic**.
- Analyse **standardized residuals**  $\tilde{e}_i = e_i / \hat{\sigma}_e$

**Identify patterns or autocorrelations** that the model did not capture.

- Time plot, correlogram
- Ljung-Box test: null hypothesis ( $H_0$ ) states that residuals are **uncorrelated** up to a certain lag.

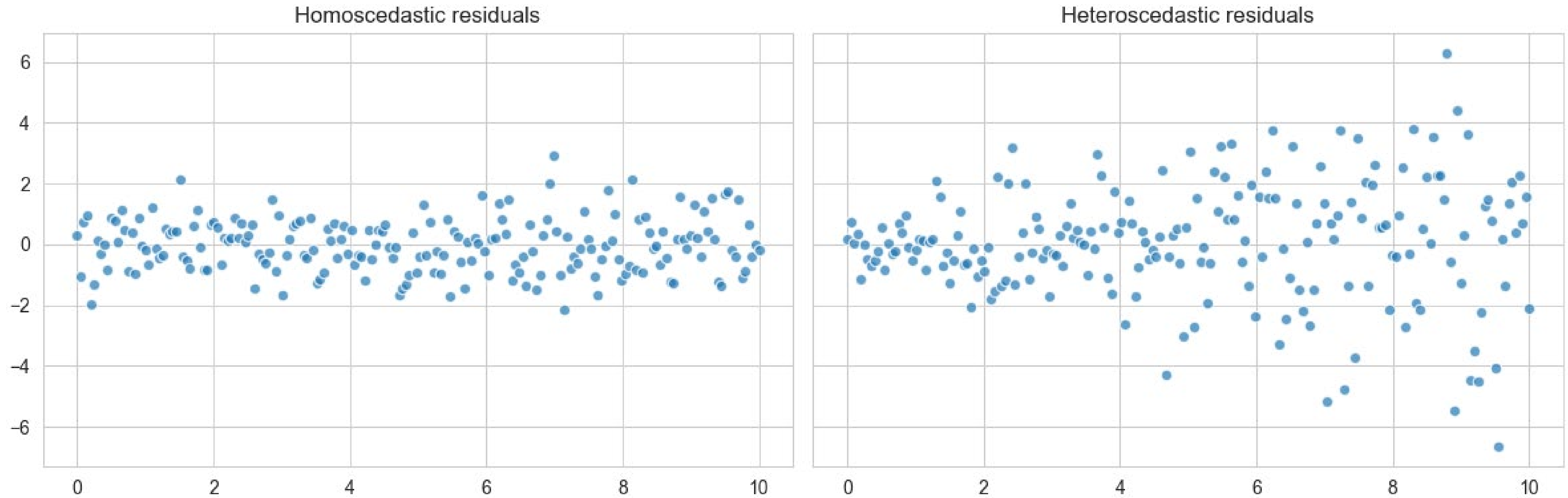
**Validate model assumptions**, typically  $E_t \sim \mathcal{N}(0, \sigma^2)$ .

- Q-Q plot: compare the residuals quantiles with normal quantiles.
- Histogram: visual representation of the residuals distribution.

Evaluate how well a model **utilizes available signal** in the data but **does not help with model selection**.

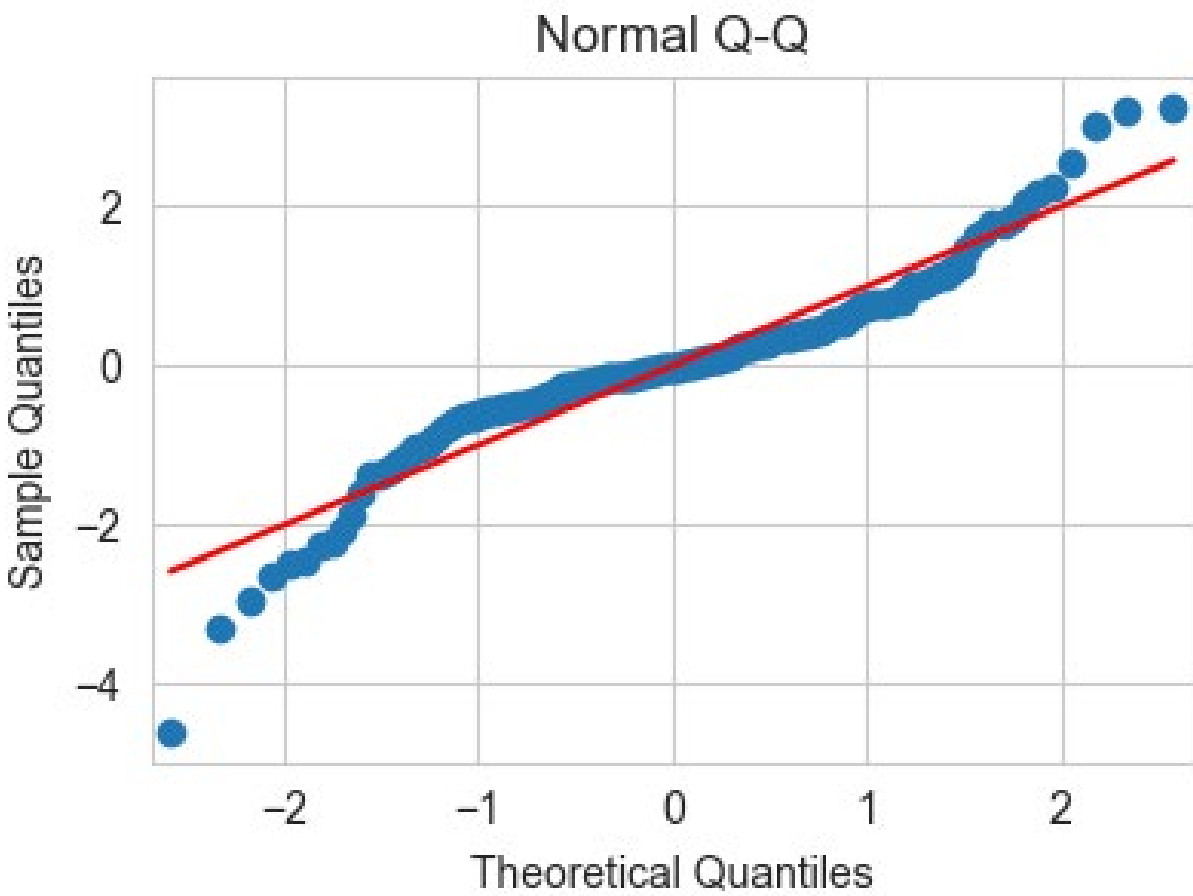
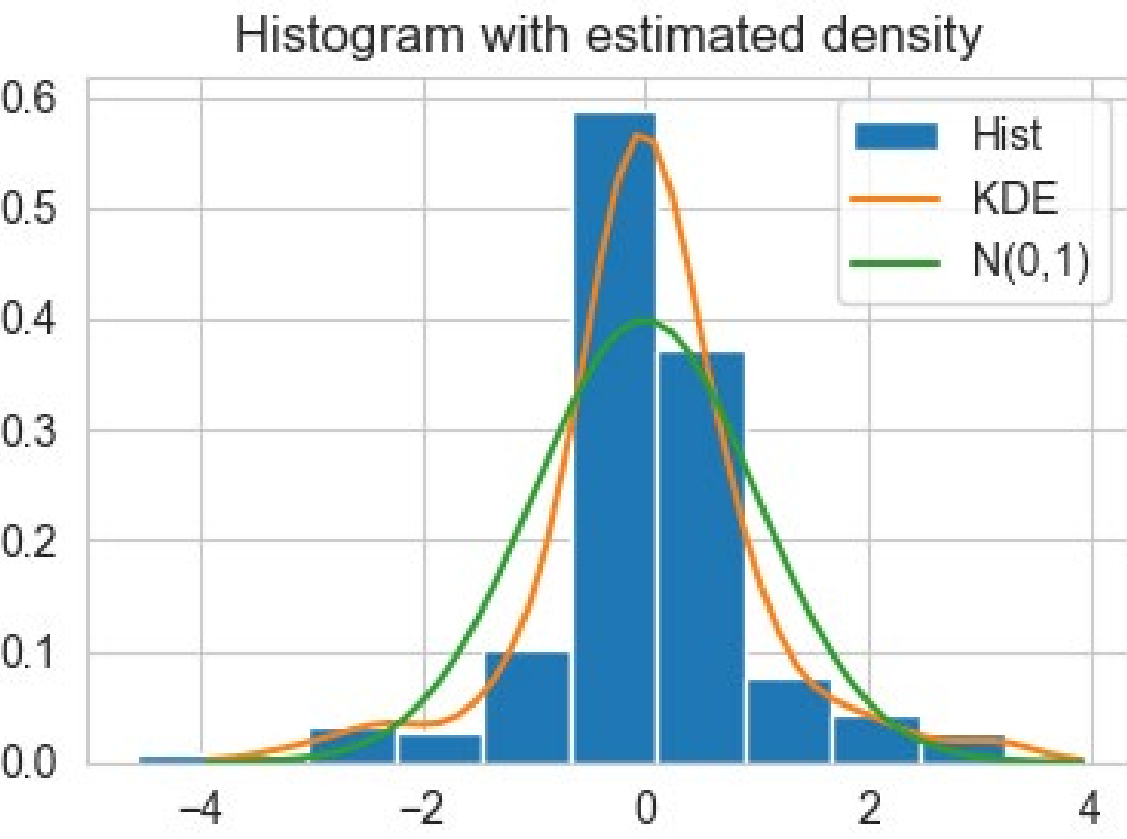
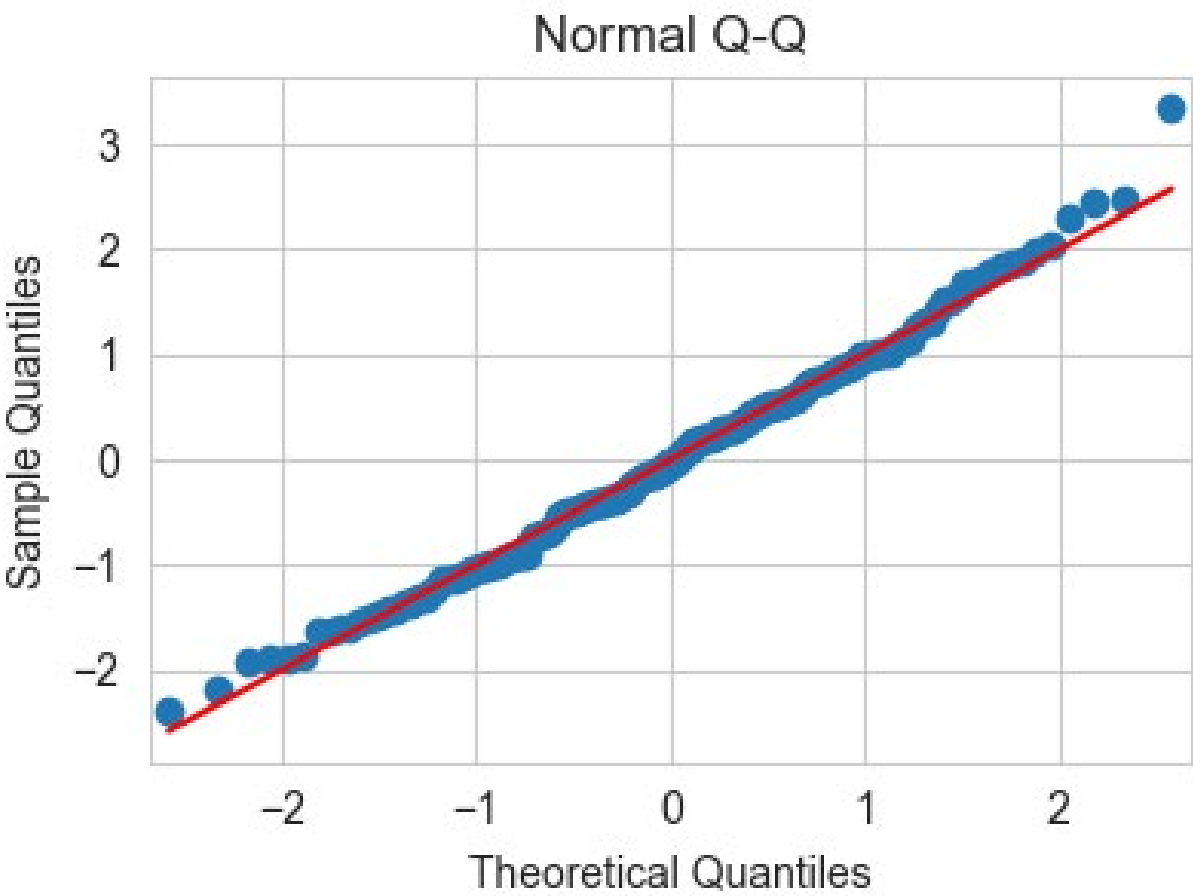
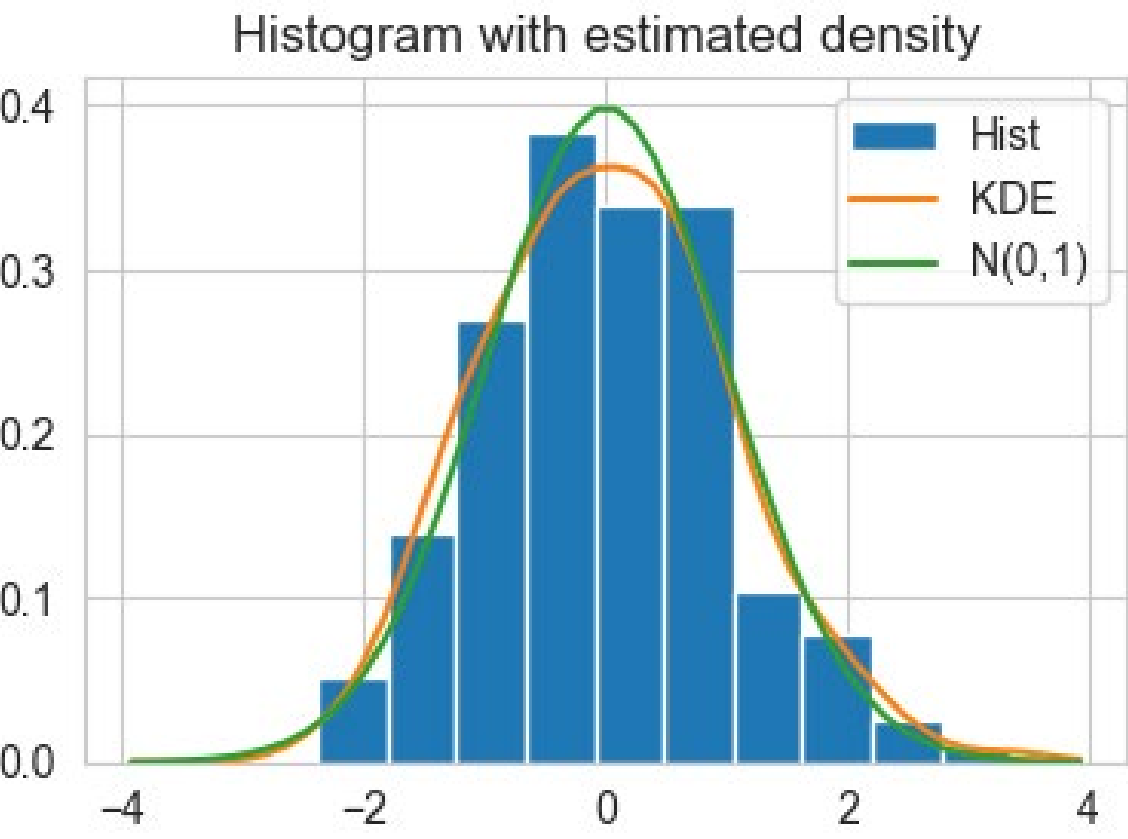
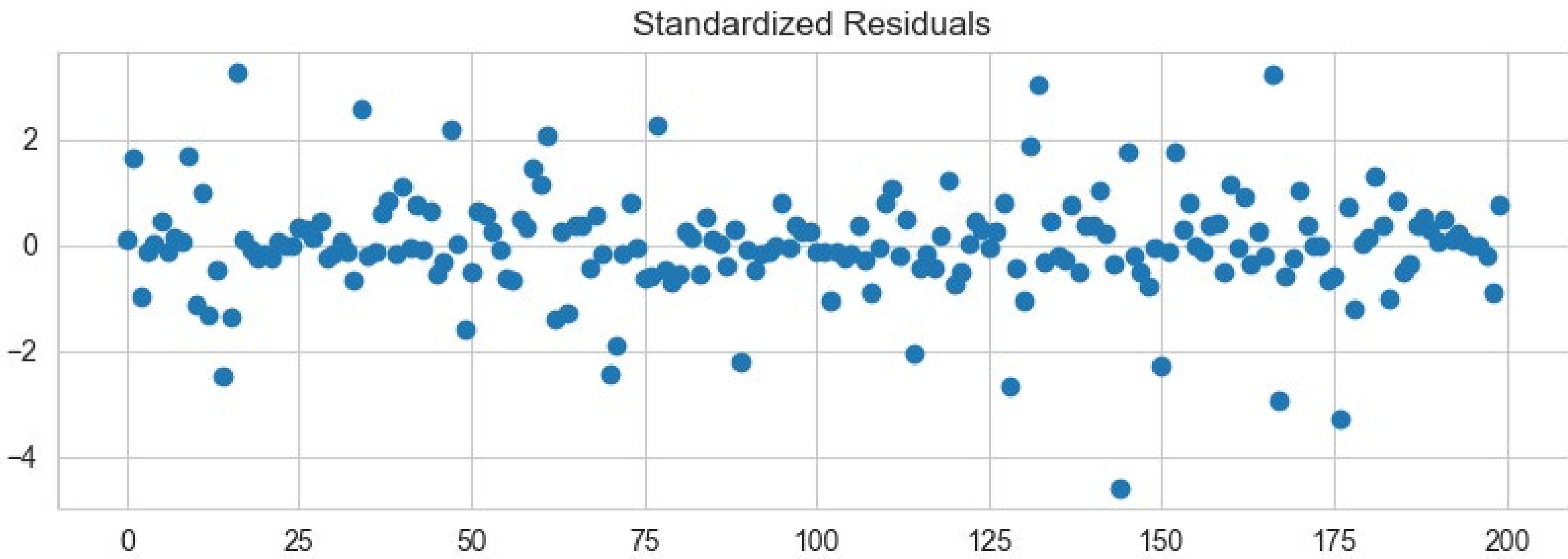
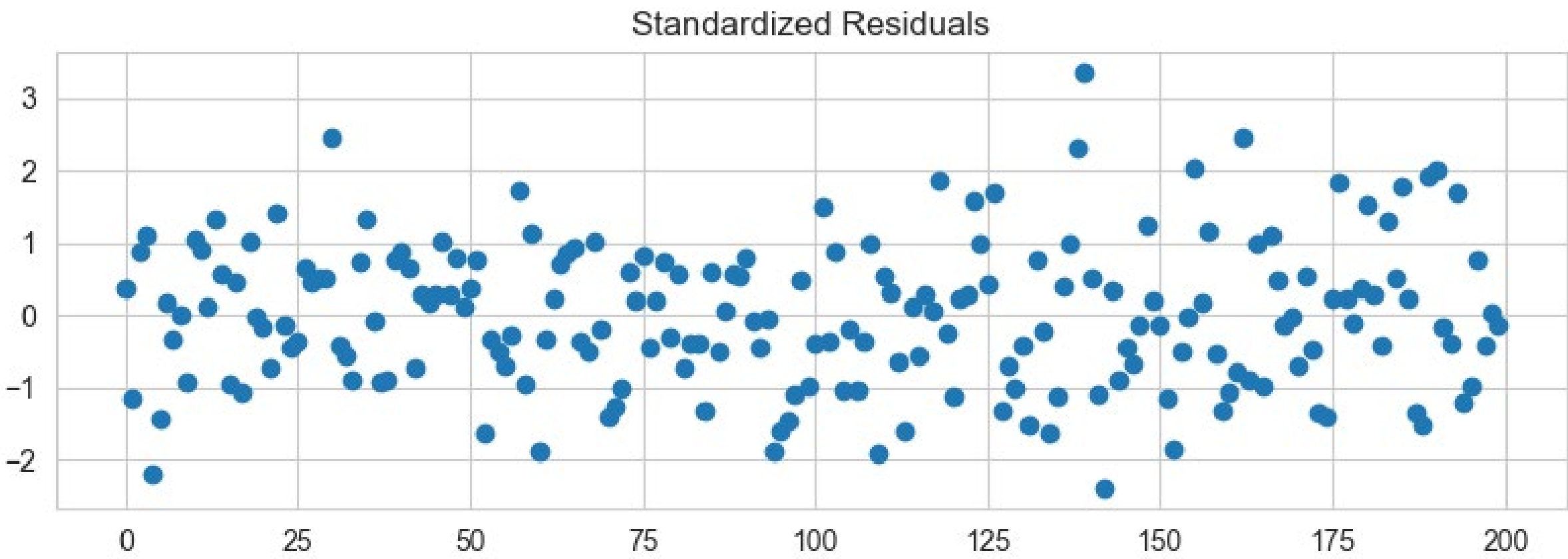
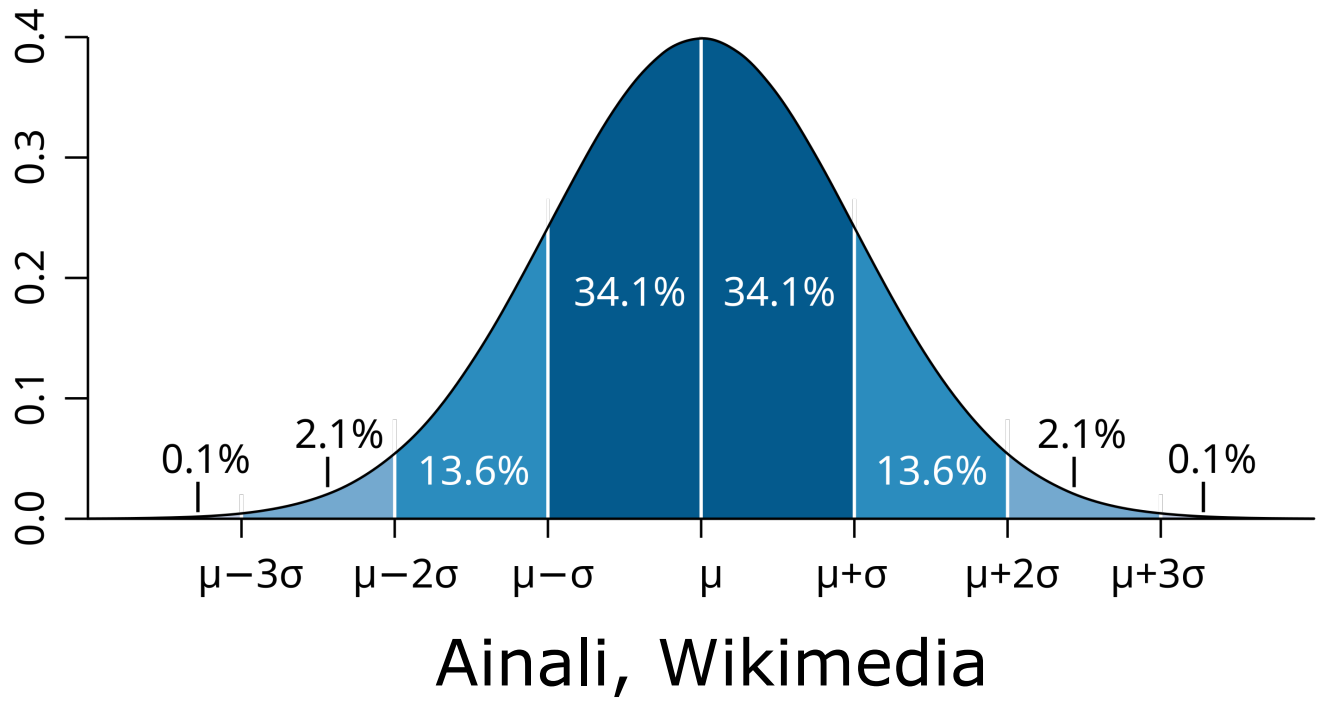
## Recap – Homoscedasticity

The variance of the error is **constant** over the entire feature space.

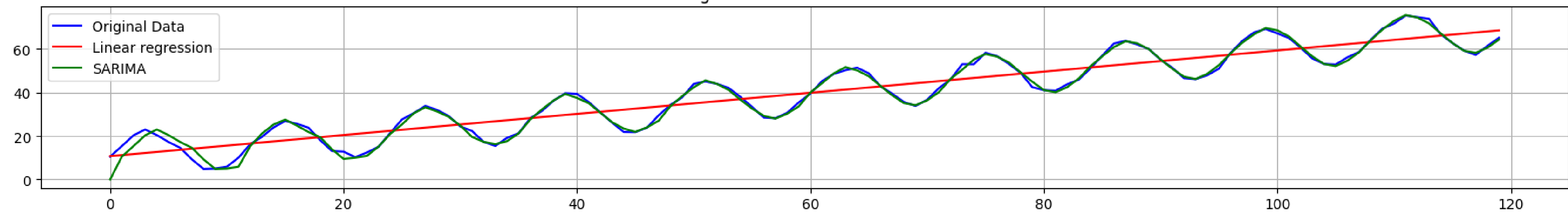


# Recap – Normality

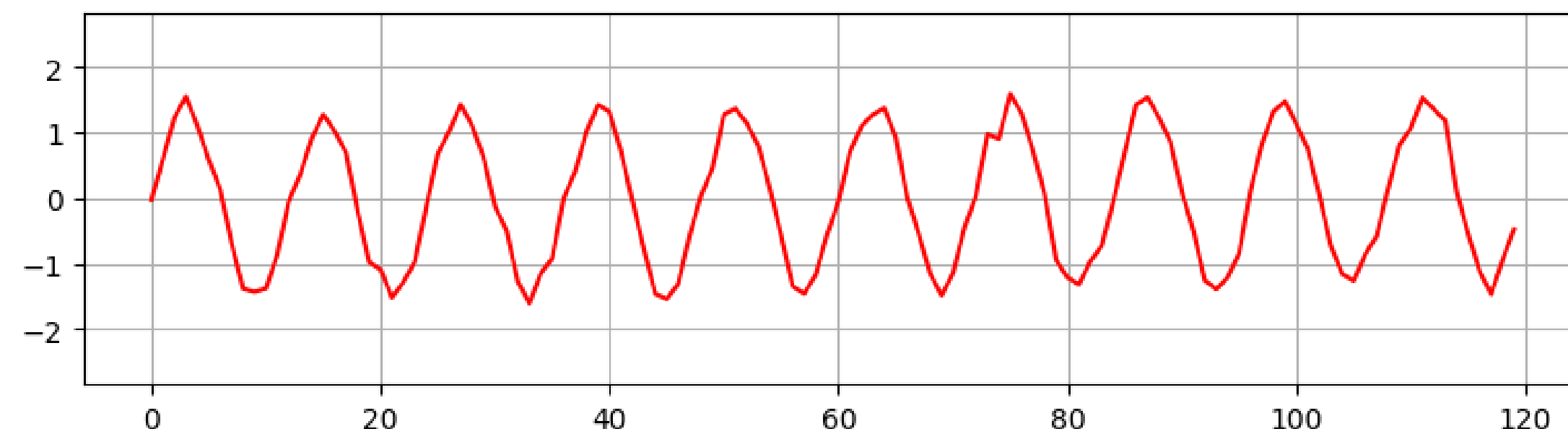
The model error given the features follows a **normal distribution**  $\epsilon | X \sim \mathcal{N}(0, \sigma^2)$ .



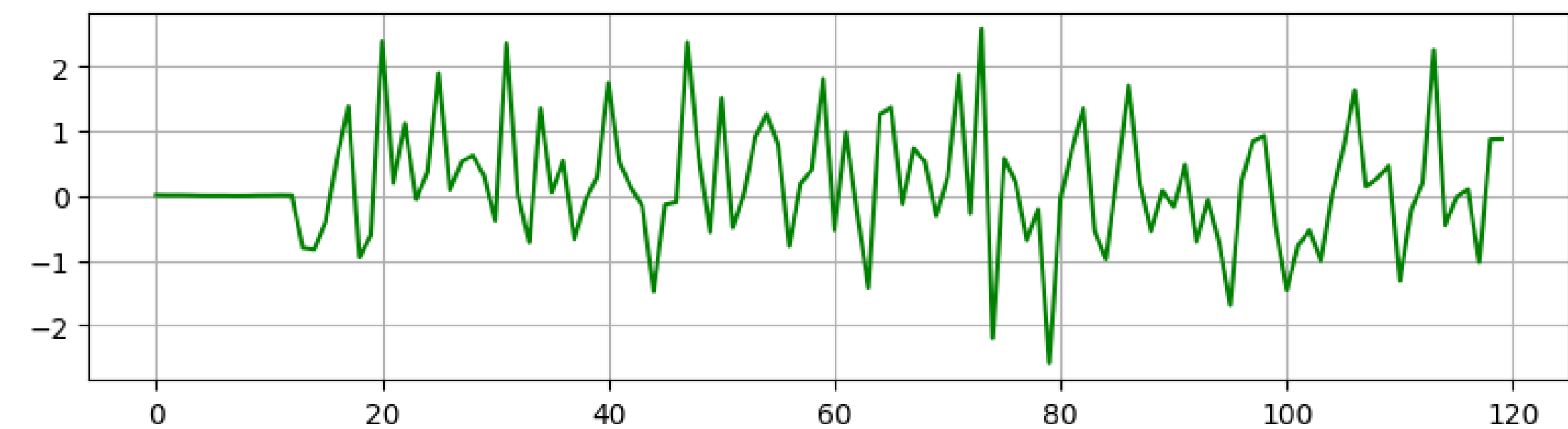
Original Data and Fitted Values



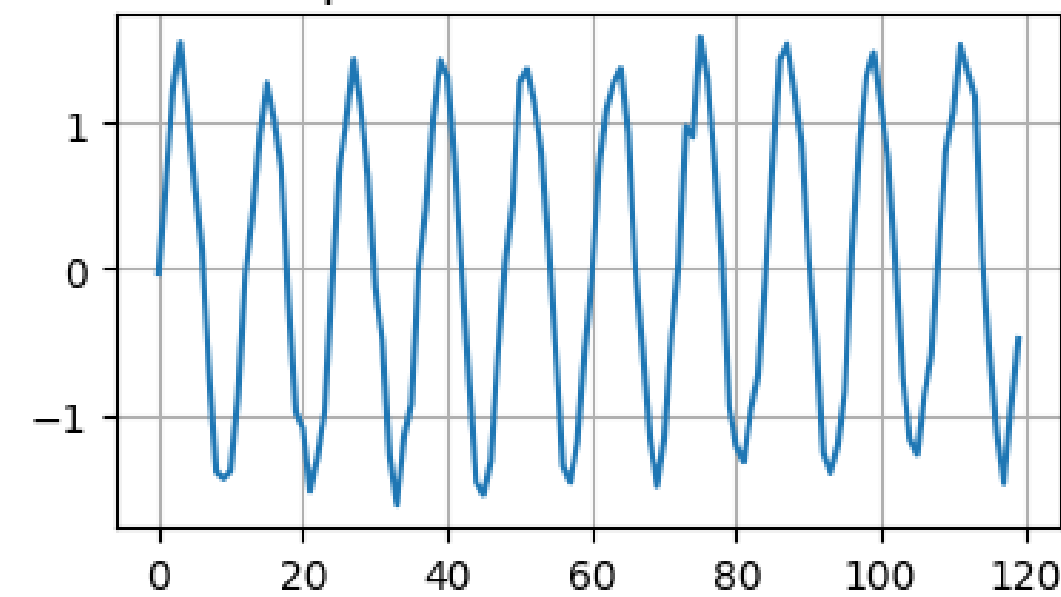
Standardized residuals of the linear model



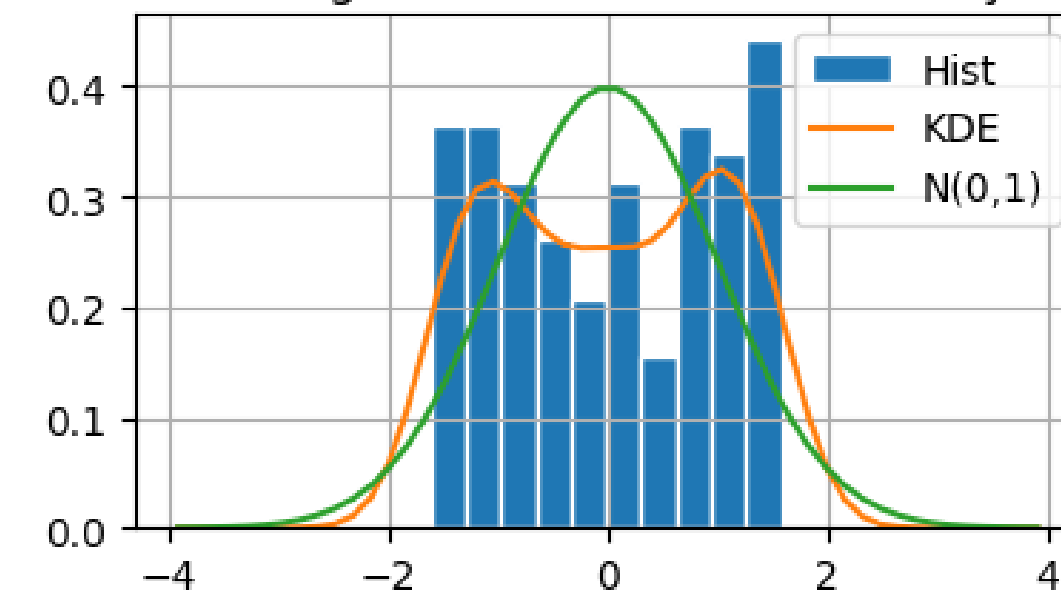
Standardized residuals of the SARIMA model



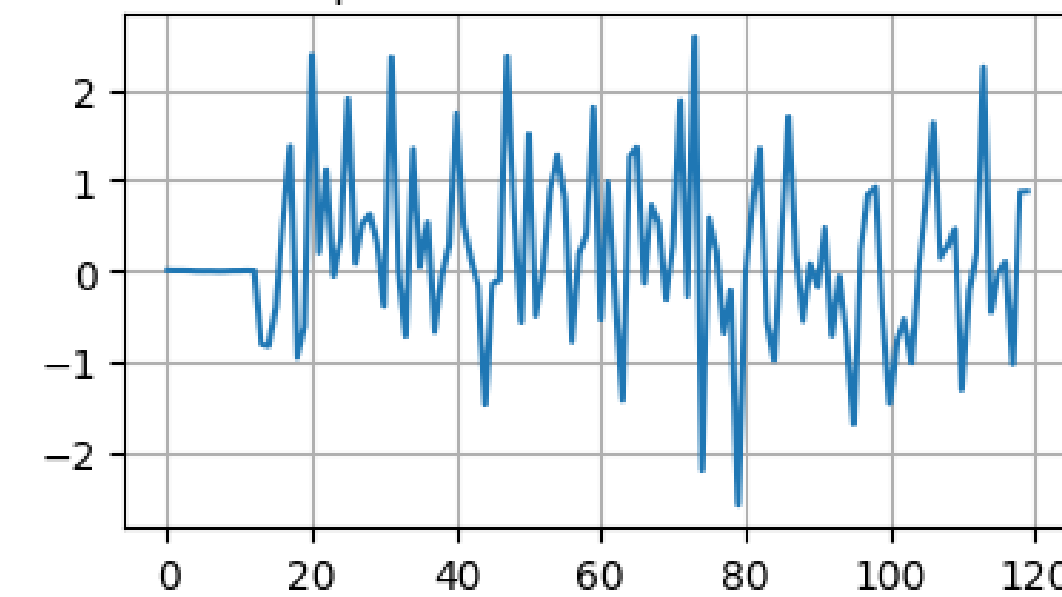
Time plot: Standardized residuals



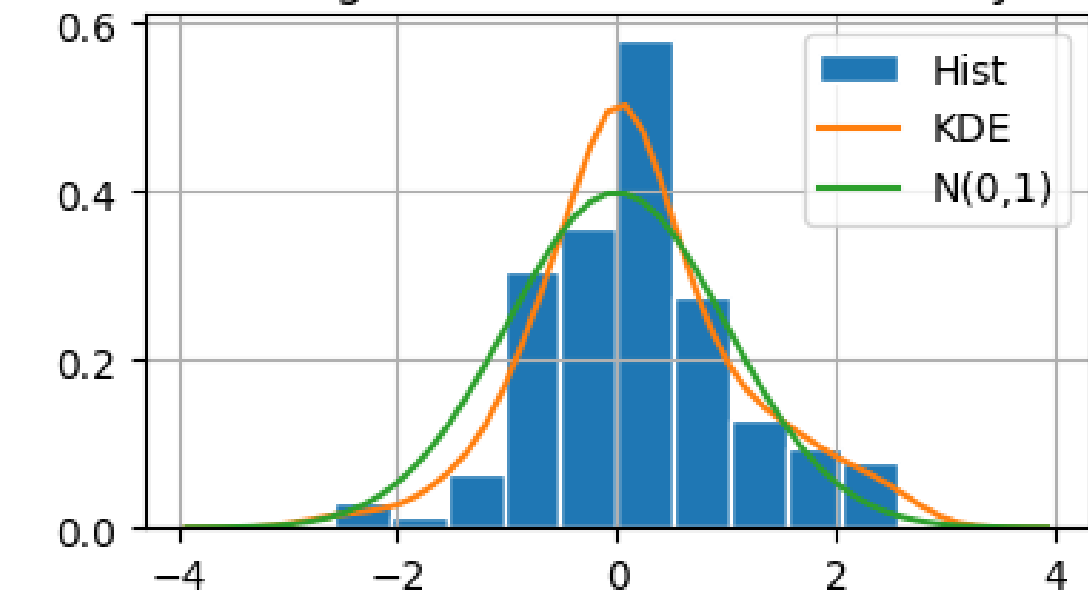
Histogram with estimated density



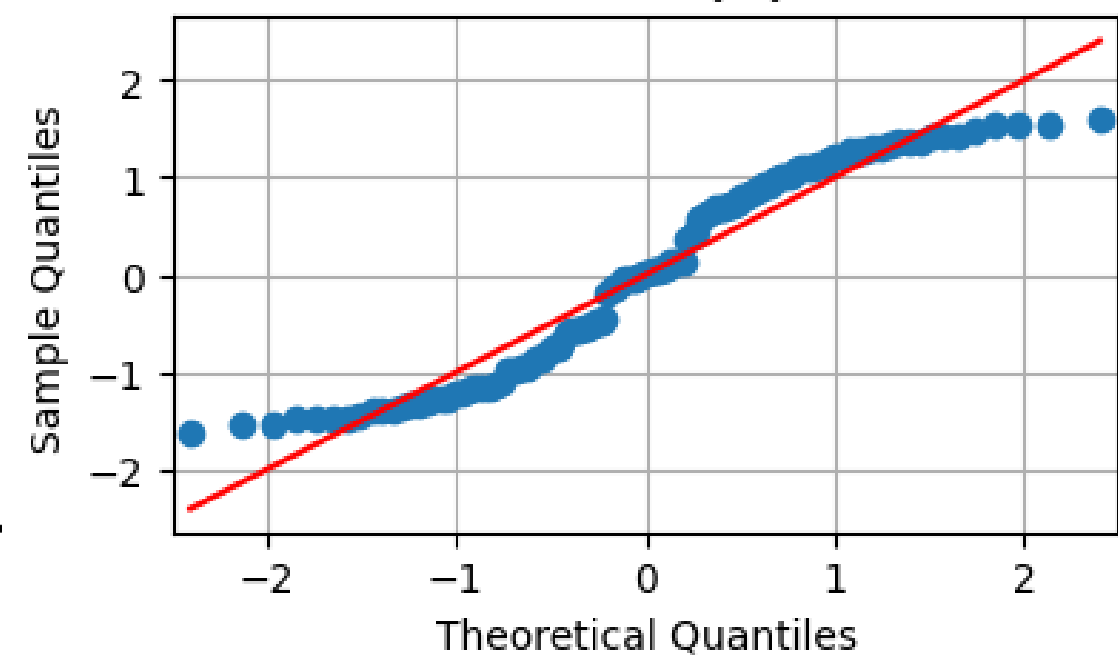
Time plot: Standardized residuals



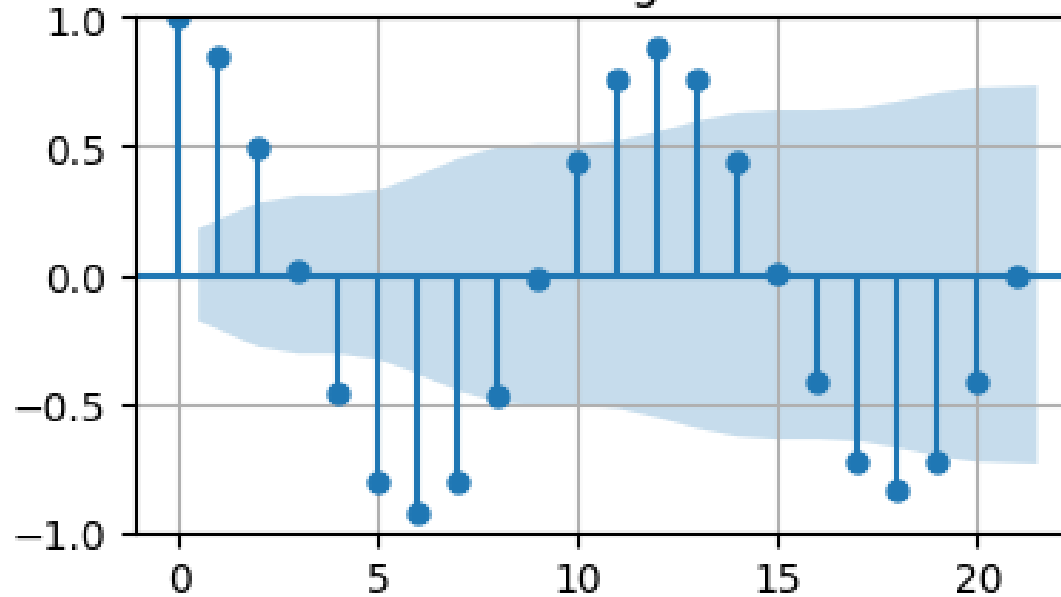
Histogram with estimated density



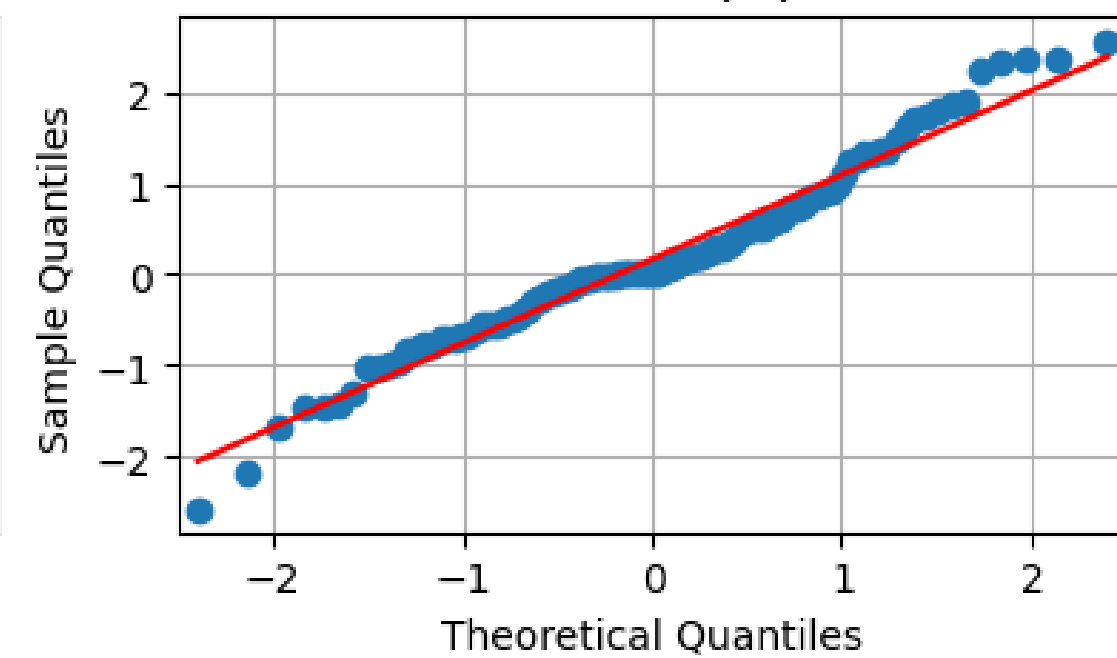
Normal Q-Q



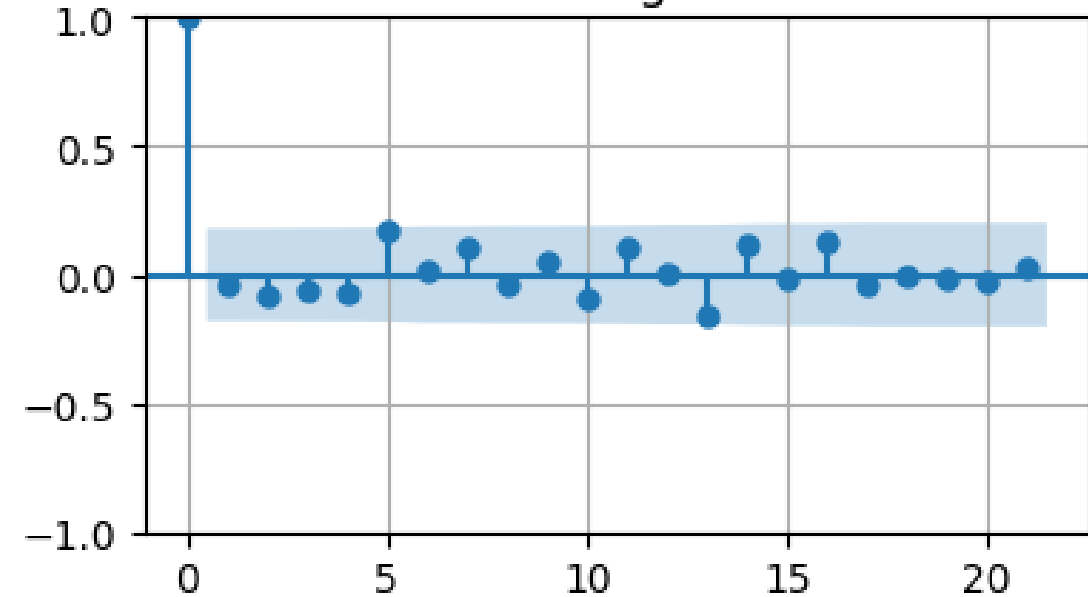
Correlogram



Normal Q-Q



Correlogram



# Confidence intervals (CI) for normal residuals

Confidence intervals provide a measure of **forecast uncertainty**.

When the residuals are **normally distributed**, the CI of  $\hat{x}_{T+h|T}$  is  $\hat{x}_{T+h|T} \pm z_{1-\alpha/2} \hat{\sigma}_{h|T}$

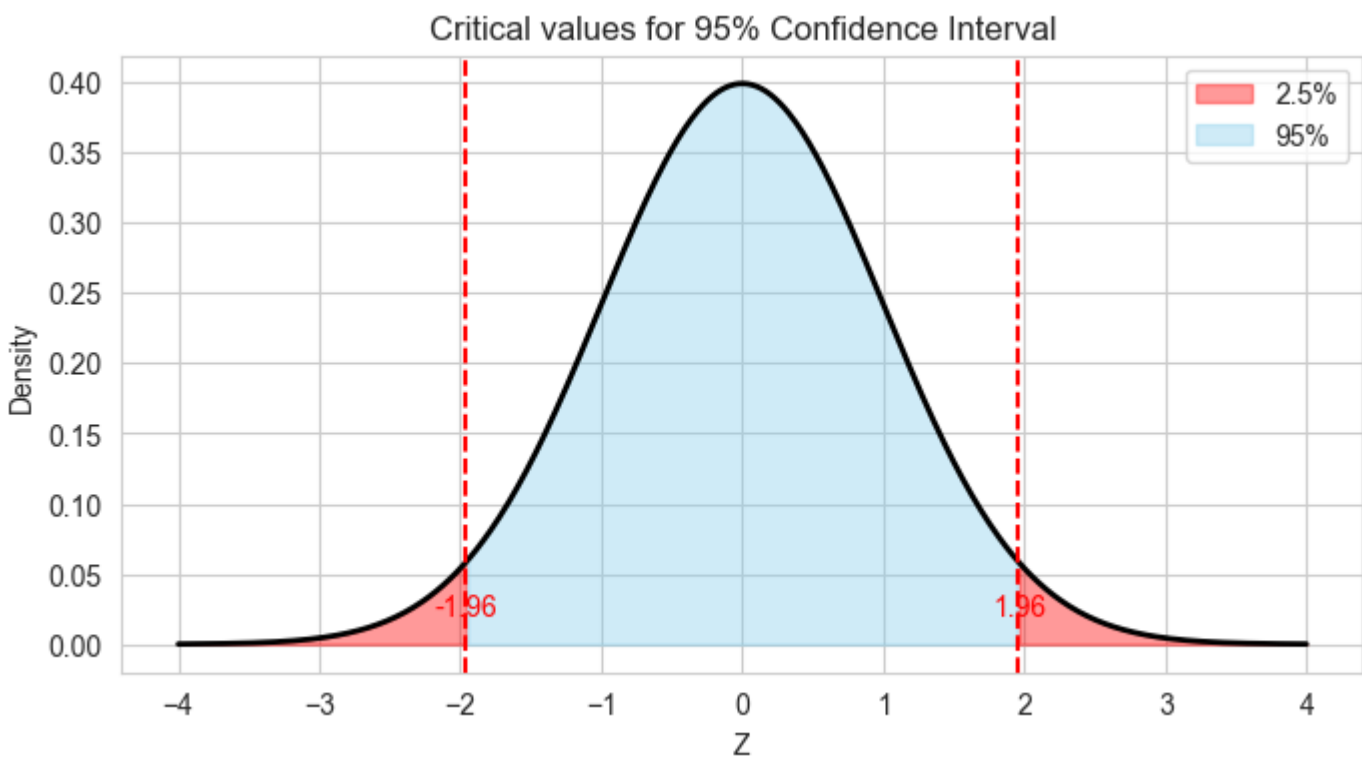
- $z_{1-\alpha/2}$  is the critical value of the normal distribution e.g., for 95% CI  $z_{1-\alpha/2} = 1.96$
- $\hat{\sigma}_{h|T}$  is an **estimate of the standard deviation** of the  $h$ -step forecast with  $\hat{\sigma}_1 = \hat{\sigma}_e$  (residuals std)

$$\hat{\sigma}_e = \sqrt{\frac{1}{T-k-m} \sum_{i=m+1}^T e_i^2}$$

with  $k$  the number of model parameters and  $m$  the number of missing residuals due to initialization.

For  $h > 1$ ,  $\hat{\sigma}_h$  depends on the forecasting method and how the **innovations accumulate**:

| Mean                                                         | Naïve                                          | Seasonal naïve                                                 | Naïve with drift                                                                |
|--------------------------------------------------------------|------------------------------------------------|----------------------------------------------------------------|---------------------------------------------------------------------------------|
| $\hat{\sigma}_{h T} = \hat{\sigma}_e \sqrt{1 + \frac{1}{T}}$ | $\hat{\sigma}_{h T} = \hat{\sigma}_e \sqrt{h}$ | $\hat{\sigma}_{h T} = \hat{\sigma}_e \sqrt{\lceil h/P \rceil}$ | $\hat{\sigma}_{h T} = \hat{\sigma}_e \sqrt{h \left( 1 + \frac{h}{T-1} \right)}$ |





# Confidence intervals (CI) for non-normal residuals

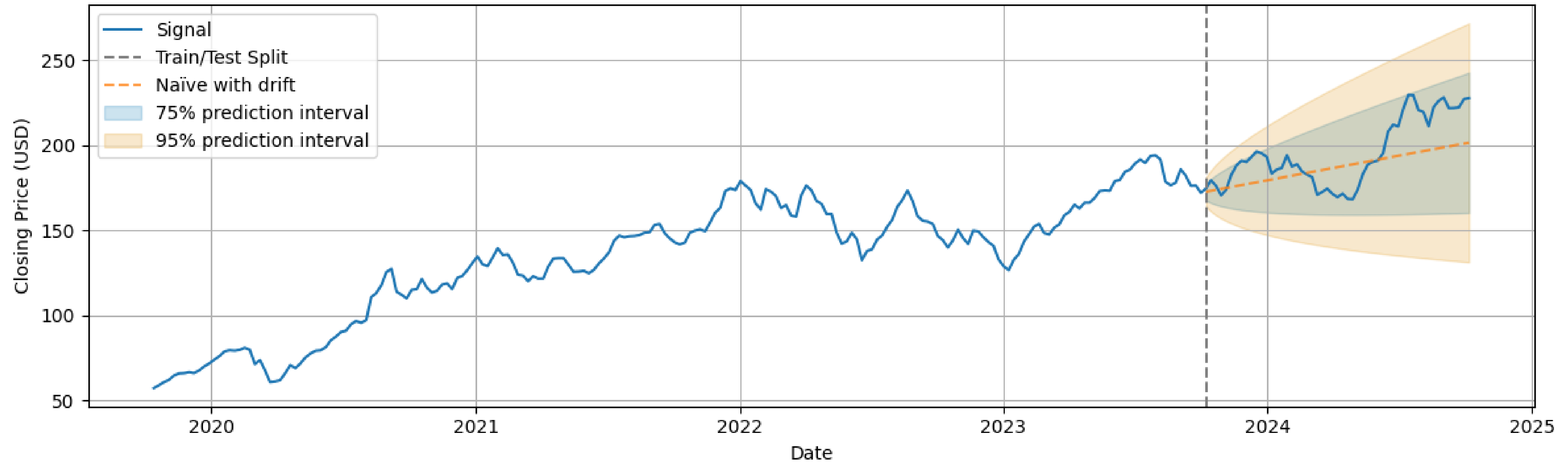
Use **bootstrapping** when the residuals are **uncorrelated** and have **constant variance**.

Assuming future and past errors will be similar, generate possible futures:

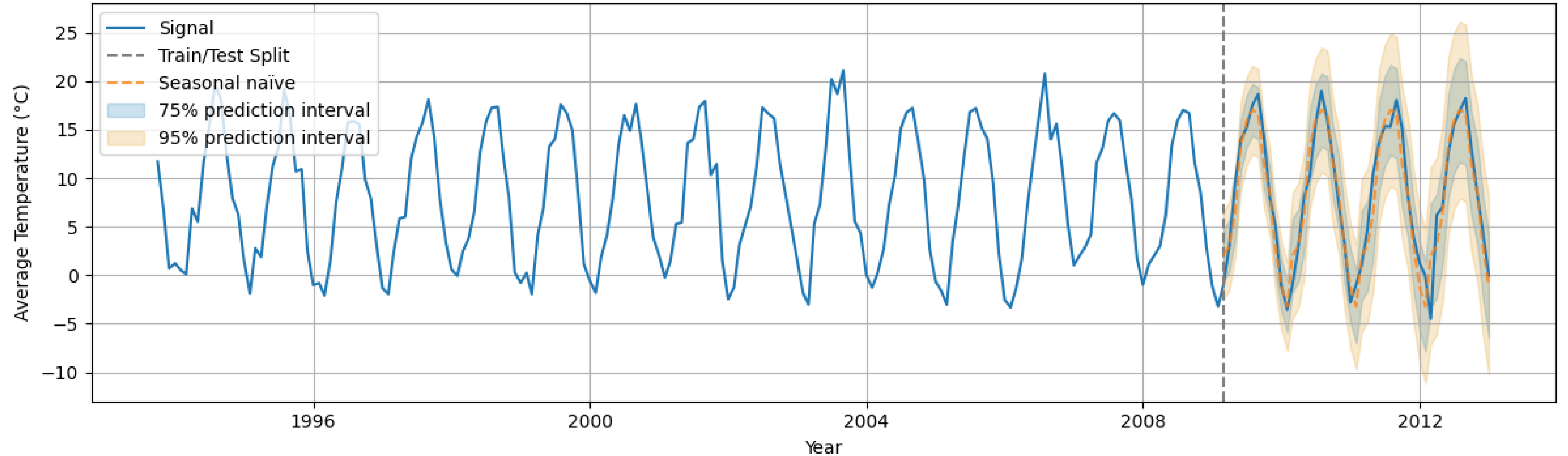
1. Fit forecasting model on  $\{x_1, x_2, \dots, x_T\}$  and compute residuals  $\{e_1, e_2, \dots, e_T\}$ .
2. **Resample residuals with replacement** to simulate future forecast errors  $\{e_{k_1}, e_{k_2}, \dots, e_{k_h}\}$ .
3. Generate futures by adding resampled residuals to model forecasts  $\{\hat{x}_{T+1|T} + e_{k_1}, \hat{x}_{T+2|T} + e_{k_2}, \dots, \hat{x}_{T+h|T} + e_{k_h}\}$ .
4. Repeat step 2, 3 multiple times e.g., 1000 iterations.
5. Derive confidence intervals by computing the **percentiles**.
  - e.g., for 95% CI use the 2.5<sup>th</sup> and 97.5<sup>th</sup> percentiles.

Note that the bootstrapped confidence intervals are **not symmetric**.

Time plot: Weekly Apple Inc. (AAPL) Closing Prices



Time plot: Monthly Average Temperature in Switzerland



# Information criteria

Measure of the **goodness of fit** of a model while penalizing for **model complexity**.

Goodness of fit is measured by the **likelihood** of the data under the model:

$$L = \prod_{i=1}^T \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{e_i^2}{2\sigma^2}\right) \text{ with } e_i = x_i - \hat{x}_{i|T} \text{ and assuming } e_i \sim \mathcal{N}(0, \sigma^2)$$

**Akaike's Information Criterion:**  $AIC = 2k - 2\log(L)$  with  $k$  the number of model parameters.

**Bayesian Information Criterion:**  $BIC = \log(T) k - 2\log(L)$

For ARIMA  $e_i = \hat{w}_i$  and  $k = \begin{cases} p + q & \text{if } c = 0 \\ p + q + 1 & \text{if } c \neq 0 \end{cases}$

Select model **minimizing either AIC or BIC** (for models in the same class)

- BIC tends to favor simpler models than AIC due to a larger penalty term.
- AIC prioritizes **model fit** (potentially better performance), while BIC emphasizes **model simplicity** (faster inference, simpler model interpretation).

# Performance metrics

Given a validation set  $\{x_{T+1}, \dots, x_V\}$ , the forecast performance can be evaluated based on

- **Scale-dependent errors:**  $e_i = x_i - \hat{x}_{i|T}$  (same unit as the data  $\rightarrow$  not comparable for TS with different units)
- **Scaled errors:**  $e_i = (x_i - \hat{x}_{i|T}) / \left( \frac{1}{T} \sum_{j=1}^T |x_j - \hat{x}'_{j|T}| \right)$  with  $\hat{x}'_{j|T}$  a baseline **training** forecasts.

Considering the **multi-step** forecasts  $\{\hat{x}_{T+1|T}, \dots, \hat{x}_{V|T}\}$ , the errors can be aggregated as follows:

- Mean absolute (scaled) error MAE/MASE:  $\frac{1}{T-V} \sum_{i=T+1}^V |e_i|$   $\rightarrow$  robust to outliers
- Root mean squared (scaled) error RMSE/RMSSE:  $\sqrt{\frac{1}{T-V} \sum_{i=T+1}^V e_i^2}$   $\rightarrow$  sensitive to outliers

When units has a **meaningful zero**, consider the mean absolute **percentage errors** MAPE  $\frac{1}{T-V} \sum_{i=T+1}^V \left| \frac{100(x_i - \hat{x}_{i|T})}{x_i} \right|$

# Rolling forecast performance

When the validation set encompasses multiple forecast horizons  $\{x_{T+1}, \dots, x_h, \dots, x_V\}$ ,

1. With  $i = 0$  for the first iteration, forecast  $\{\hat{x}_{T+i+1|T}, \dots, \hat{x}_{T+i+h|T}\}$ .
2. Compute performance metrics of the forecast.
3. Increment  $i = i + k$  with  $k$  the chosen step-size, typically  $k = h$ .
4. Refit model with the newly available values  $\{x_{T+i+1}, \dots, x_{T+i+h}\}$ .
  - On the test set choosing between **refit** vs **update** strategy depends on the training objective.
  - Update: recalculate model internal state given new data points **without refitting its parameters**.
5. Repeat until the end of the validation set and then aggregate performance.

# Back-transforms

To obtain forecasts on the **original scale**, we need to **reverse transformations** applied to the data.

The back-transform for differencing is

- First-order:  $\hat{x}_{T+h|T} = x_T + \sum_{i=1}^h \hat{y}_{T+i|T}$  with  $y_t = \nabla x_t$
- Seasonal differencing:  $\hat{x}_{T+(kP+n)|T} = x_{T+n} + \sum_{i=1}^k \hat{y}_{T+iP+n|T}$  with  $y_t = \nabla_P x_t$

Reversing non-linear transforms does **not** preserve the **mean** from the transformed scale but the **median** (assuming the distribution on the transformed scale is symmetric)

- Considering a log-normal distribution  $y_t = \log(x_t)$ , the mean of  $y_t$  corresponds to the median of  $x_t$ .
- **Bias correction** is needed to account for the variance in the transformed space.

| Reverse Box-Cox transform                                                                                                                                                                                              | Bias adjusted reverse Box-Cox transform                                                                                                                                                                                                          |
|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| $\hat{x}_{T+h T} = \begin{cases} \exp(\hat{y}_{T+h T}) & \text{if } \lambda = 0 \\ \text{sign}(\lambda \hat{y}_{T+h T} + 1)  \lambda \hat{y}_{T+h T} + 1 ^{\frac{1}{\lambda}} & \text{if } \lambda \neq 0 \end{cases}$ | $\hat{x}_{T+h T}^* = \begin{cases} \hat{x}_{T+h T} (1 + \sigma_h^2/2) & \text{if } \lambda = 0 \\ \hat{x}_{T+h T} \left( 1 + \frac{\sigma_h^2 (1 - \lambda)}{2 (\lambda \hat{y}_{T+h T} + 1)^2} \right) & \text{if } \lambda \neq 0 \end{cases}$ |

# Exercise

## Forecasting

- Split real-world time series into train/test sets.
- Fit ARIMA on training, forecast test observations.
- Plot forecasts vs. actuals, what patterns does your model capture or miss?
- Perform residual analysis
- Generate 80% / 95% forecast intervals. Are values within the intervals? What does this imply?

## Evaluation workflow

- Use cross-validation to generate different validation folds
- Compute rolling forecast performance. Which metric is best suited for your data?
- Compare ARIMA with baseline models (mean, naïve, seasonal naïve).
- Review [sktime forecasting notebook](#) and test different [forecasting approaches](#).
- Select best model and evaluate performance on the test set.