CHEMICAL ENGINEERING EDUCATION

Time series Modelling and analysis

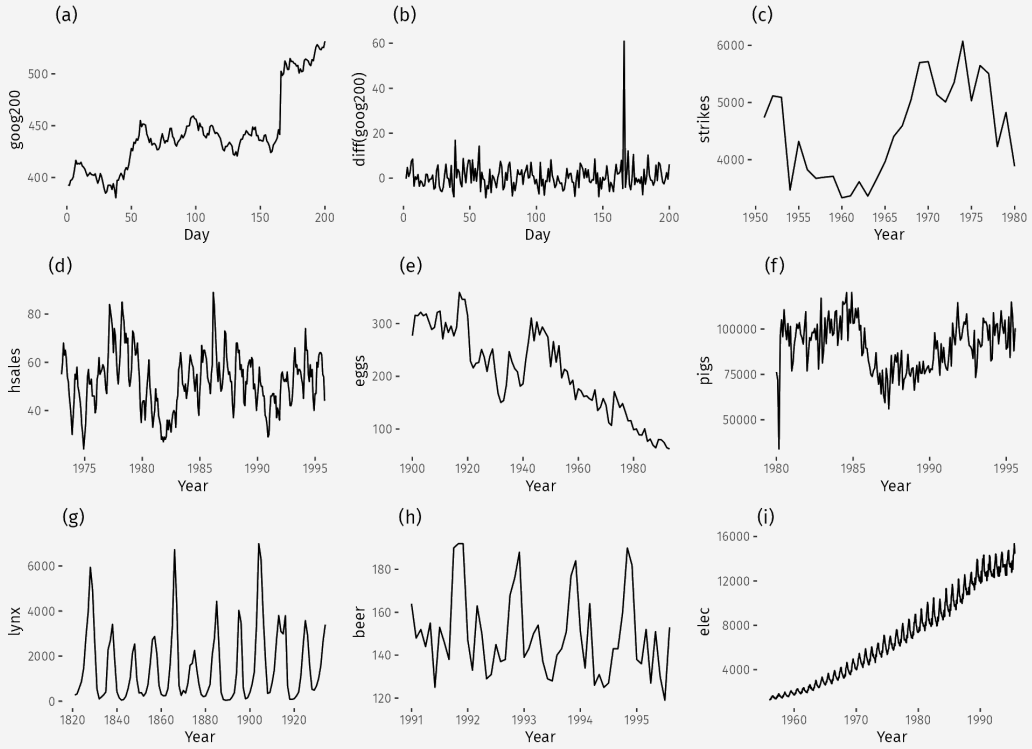
Advanced Modeling and Control

Outline

- Introduction & Motivation
- Basics of Time Series
- Transfer Function Models
- Autoregressive (AR) Models
  - ARX Models
  - ARMAX Models
  - ARMA/ARIMA Models
- Model Evaluation & Selection
- Summary & Reflection

What is Time Series?

- A time series is a sequence of observations recorded at successive points in time
- Each observation is ordered, meaning the position in time matters
- Data is often collected at regular intervals:
  - Seconds, minutes, hours (process monitoring sensors)
  - Days, months, years (economic, environmental, health data)



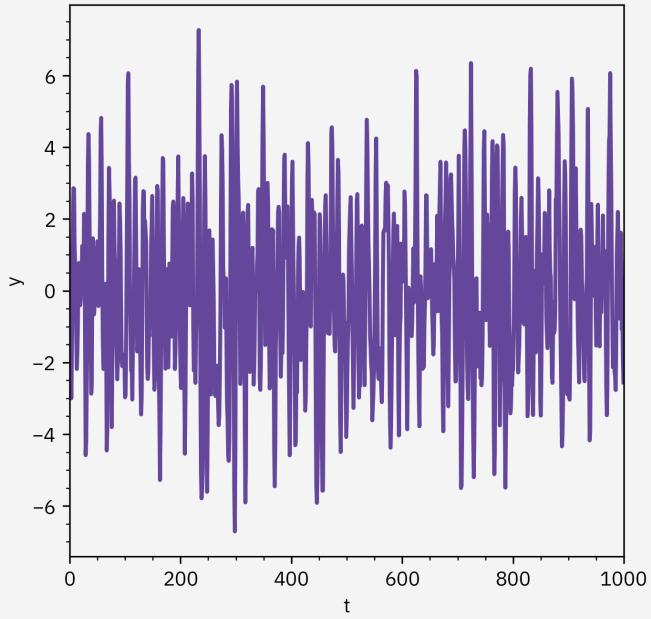
Importance

- Provides patterns and forecasts to support decisions
- Anticipates specification violations in process industries
- Typical applications:
  - Process control
  - Energy demand forecasting
  - Equipment health monitoring
  - Economic and financial trends
  - Climate and agriculture planning
  - Public health surveillance

Stationary vs Non-stationary

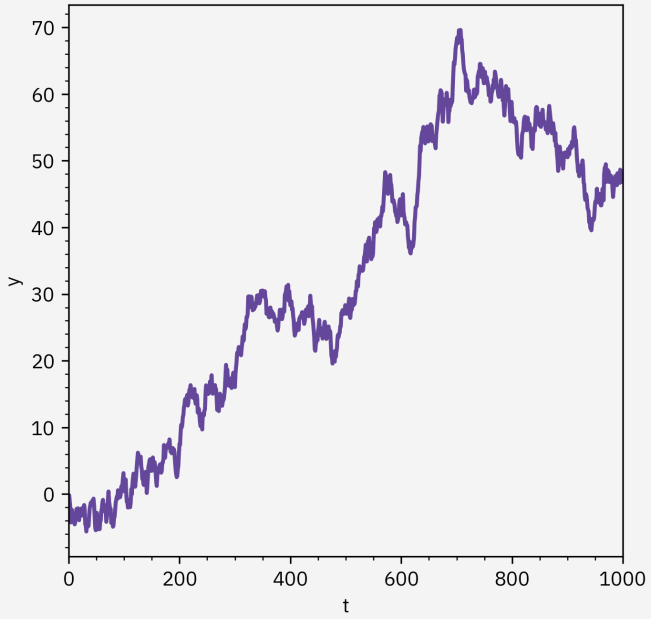
Stationary series

- Mean and variance constant over time
- Fluctuates around a stable level
- Easier to model and forecast



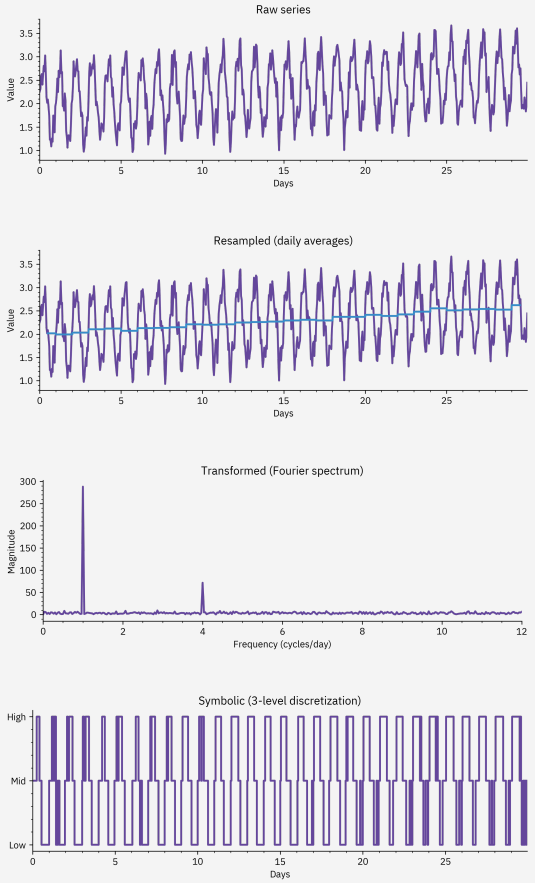
Non-stationary series

- Mean or variance changes with time
- Shows trend, seasonality, or shifts
- Requires differencing or detrending



Time Series Representation

- Time series often large and high-dimensional
- Representation helps simplify analysis and comparison
- Common approaches:
  - Raw series (original data)
  - Resampling (reducing data points, e.g., daily → monthly)
  - Transformation (Fourier, wavelets, PCA)
  - Symbolic representation (grouping values into categories)

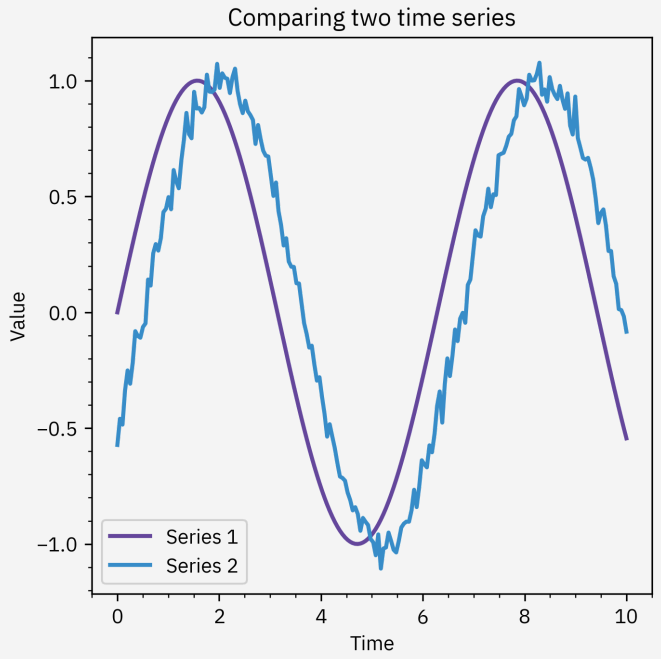


Benefits

- Reduces dimensionality while preserving essential patterns
- Enables efficient similarity search and clustering
- Provides basis for further tasks:
  - Pattern discovery, Classification, Forecasting

Similarity Measures

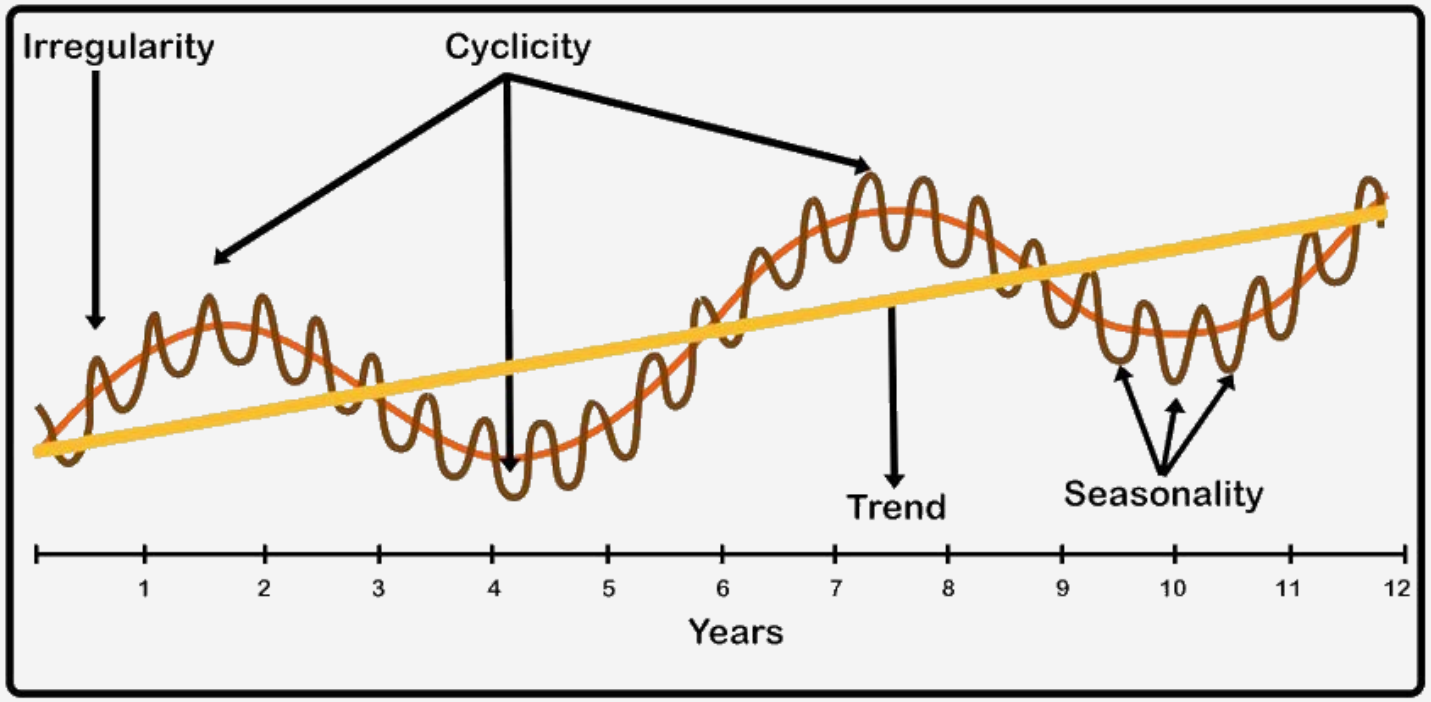
- Used to compare two or more time series
- Important for:
  - Clustering and classification
  - Pattern discovery
  - Anomaly detection
- Common measures:
  - Euclidean distance
  - Correlation-based distance
  - Dynamic Time Warping (DTW) for misaligned series



- Euclidean distance works if sequences are aligned
- DTW allows matching when sequences are stretched or shifted
- Correlation-based measures capture shape similarity
- Choice of similarity measure affects clustering, anomaly detection, and forecasting

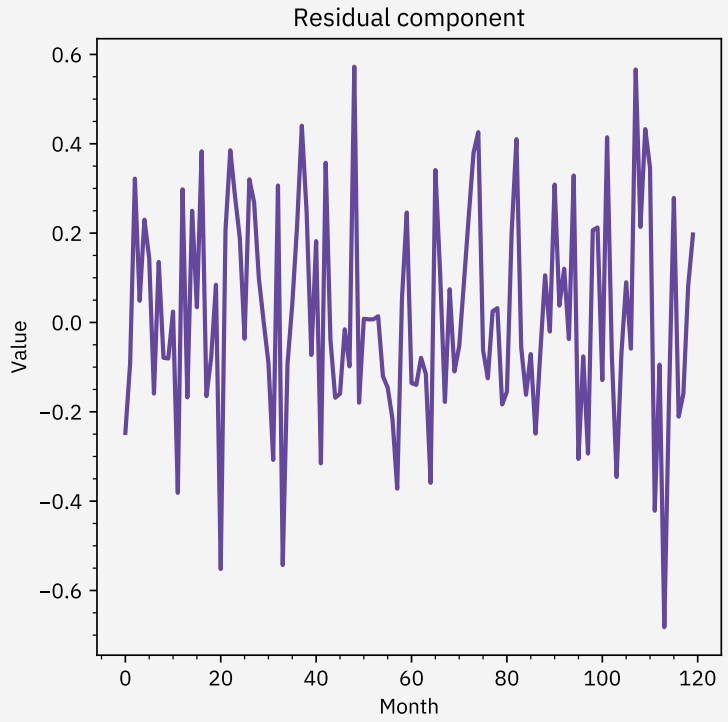
Characteristics of Time Series

- Temporal dependence: current values often depend on past values
- Directionality: useful for forecasting forward in time
- Patterns may include:
  - Trend (long-term increase or decrease)
  - Seasonality (repeated cycles, e.g., daily, monthly, yearly)
  - Random fluctuations (noise)



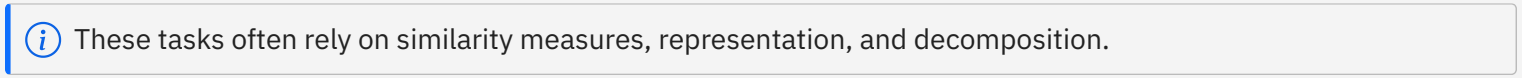
Time-Series Decomposition

- A time series can be expressed as the sum of underlying components
  - Trend: long-term direction
  - Seasonality: repeating cycles
  - Cyclic variation: slower, irregular fluctuations
  - Residual: noise or unexpected shocks



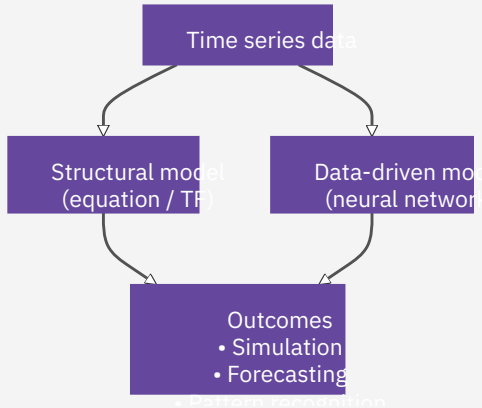
Mining in Time Series

- Goal: discover hidden information or patterns
- Common tasks:
  - Pattern discovery and clustering
  - Classification (e.g., healthy vs faulty sensor data)
  - Rule discovery (if X happens, Y follows)
  - Summarization and anomaly detection



What Do We Mean by Modelling?

- A model is a simplified description used to explain and predict data
- Two perspectives:
  - Structural: parameters have physical meaning (equation / transfer function)
  - Data-driven: parameters capture patterns (e.g., neural network)
- What models enable: simulation, forecasting, pattern recognition



Structural vs Data-Driven Models

Structural models

- Based on physical laws and first principles
- Parameters have physical interpretation
- Examples:
  - Transfer functions
  - Differential equations

Pros: interpretability, extrapolation
Cons: need detailed knowledge

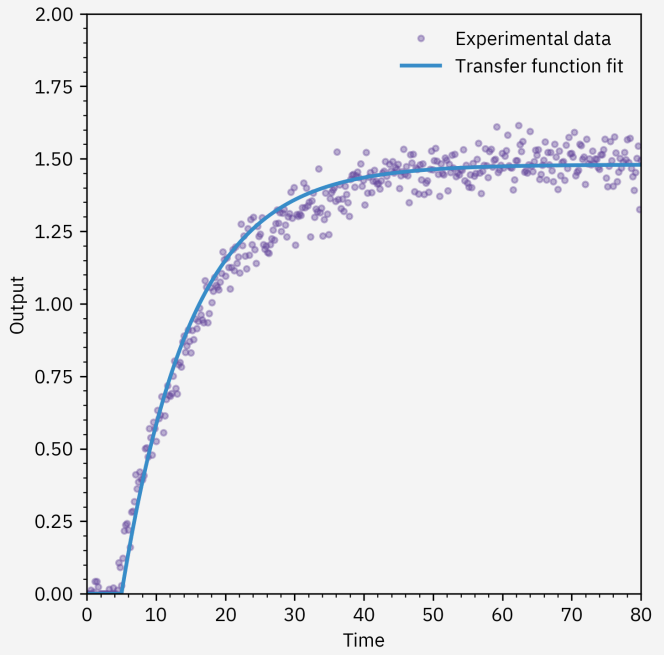
Data-driven models

- Based on observed data patterns
- Parameters capture correlations, not physics
- Examples:
  - AR, ARX, ARMAX
  - Neural networks

Pros: flexible, captures complex patterns
Cons: less interpretable, may overfit

Transfer Function Models

- Many physical processes can be represented by transfer functions in the Laplace domain
- Transfer function relates input → output dynamics
- Useful for:
  - Capturing process gain, time constant, and delay
  - Providing a baseline for time-series model comparison
- Often estimated from input–output data (system identification)



Transfer Functions as a Starting Point

- Physics-based intuition: order, delay, stability
- Provides initial guess for data-driven models (ARX, ARMAX)
- Bridges between first-principles modeling and time-series modeling

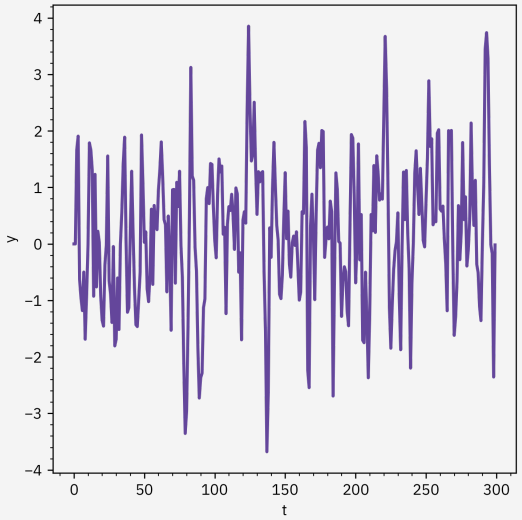
Activity 1: Estimating Transfer Function Models for a Heat Exchanger.

Autoregressive (AR) Models

- Concept
  - Current value depends on a linear combination of past values
  - AR(p):

$$y_t = \phi_1 y_{t-1} + \phi_2 y_{t-2} + \cdots + \phi_p y_{t-p} + e_t$$

  - Captures short-term correlations in stationary data
- MATLAB
  - `ar(data, order)` estimates AR model
  - Order selection via AIC / FPE
- Applications
  - Forecasting short horizon
  - Identifying dominant lags
  - Noise modeling in ARMAX



Autoregressive (AR) Models

- Present value depends on past values in discrete time
- General AR(n):

$$y_t = c + \sum_{i=1}^{n} \alpha_i y_{t-i} + \varepsilon_t$$

  - Where: c: constant; α_i: AR coefficients; n: model order; ε_t: white noise
- Example for AR(2):

$$y_t = c + \alpha_1 y_{t-1} + \alpha_2 y_{t-2} + \varepsilon_t$$

- Properties of AR models
  - Short-term memory, good for capturing autocorrelation
  - Flexible building block for ARX, ARMAX, ARIMA

AR model with backshift operator z^{-k}

- AR(2) in operator notation:

$$y_t = c + \alpha_1 y_{t-1} + \alpha_2 y_{t-2} + \varepsilon_t$$

  can be written as

$$(1 + \alpha_1 z^{-1} + \alpha_2 z^{-2}) y_t = c + \varepsilon_t$$

$$y_t = \frac{c + \varepsilon_t}{1 + \alpha_1 z^{-1} + \alpha_2 z^{-2}} = \frac{c + \varepsilon_t}{A(z)}$$

- Interpretation
  - The AR model acts like a filter that takes in random noise and produces the series.
  - The filter has only poles (all-pole system), so the effect of a shock gradually fades but never ends completely (infinite impulse response, IIR).
  - In contrast, some models have responses that die out completely after a fixed time (finite impulse response, FIR).

> **In-class Activity 2**
>
> Fit an AR model to *Australia COVID-19 infection data* (`Australia_covid_cases.xlsx`) and evaluate order selection.

ARX Models

- ARX: Autoregressive with Exogenous Input
- Exogenous Input
  - Many processes are driven by outside factors (inputs, e.g. manipulated variables, disturbances)
  - In a distillation column, the feed composition or coolant flow are exogenous inputs that affect the impurity (output).
  - In finance, the interest rate might be an exogenous input affecting stock prices.

  👉 Exogenous input = something external you can measure and that drives the system.
- Why ARX?
  - AR models only use past outputs → good for forecasting trends
  - ARX extends AR by including the exogenous inputs explicitly

ARX Model

Structure

$$A(q^{-1})y(t) = B(q^{-1})u(t - n_k) + e(t)$$

- $A(q^{-1})$: polynomial in past outputs
- $B(q^{-1})$: polynomial in past inputs
- n_k: input delay
- $e(t)$: noise

- Interpretation
  - Captures cause–effect between input and output
  - Useful for system identification with I/O data

MATLAB

`m = arx(data, [na nb nk])`
where `na` = AR order, `nb` = input order, `nk` = input delay.

> Activity 3: Develop an ARX Model for a Given Transfer Function

ARMA Models

- ARMA: Autoregressive Moving Average
  - AR models capture dependence on past outputs
  - But sometimes random shocks persist for several steps (noise is not white)
  - ARMA = AR + MA, adds a moving average (MA) term for noise

Structure

$$A(q^{-1})y(t) = C(q^{-1})e(t)$$

- $A(q^{-1})$: polynomial in past outputs
- $C(q^{-1})$: polynomial in past noise (MA part); $e(t)$: white noise

- Interpretation
  - Models a stationary time series without external input
  - Captures both memory in outputs and persistence in shocks
  - Building block for ARIMA models (to handle non-stationarity)

MATLAB

```
m = arima(p,0,q)
```

where `p` = AR order, `q` = MA order.
Use `estimate(m, data)` to fit.

ARMAX Models

- ARMAX: Autoregressive Moving Average with Exogenous Input
  - ARX models assume the disturbance is white noise
  - In practice, noise often has its own dynamics (colored noise)
  - ARMAX extends ARX by adding a **moving average (MA) term** for noise

Structure

$$A(q^{-1})y(t) = B(q^{-1})u(t - n_k) + C(q^{-1})e(t)$$

- $A(q^{-1})$: past outputs; $B(q^{-1})$: past inputs (exogenous input)
- $C(q^{-1})$: noise dynamics (MA part); n_k: input delay

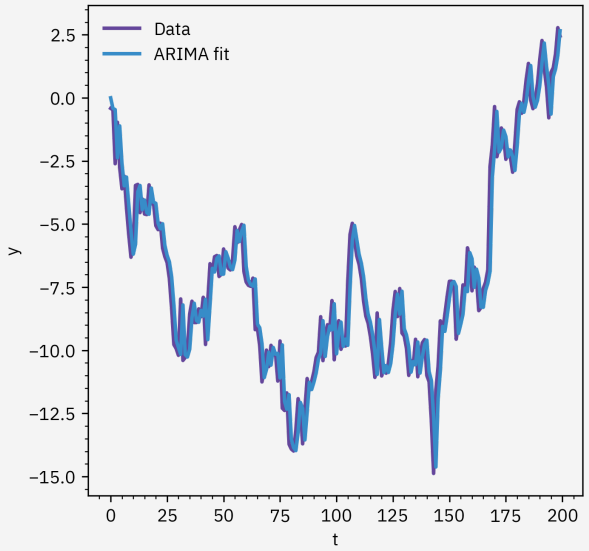
- Interpretation
  - Captures both input–output dynamics and structured noise
  - More flexible and realistic than ARX
  - Often needed when residuals of ARX show correlation

ARIMA Models

- ARIMA = Autoregressive Integrated Moving Average
- Extends ARMA for non-stationary series
  - Integration differencing step

    $$\nabla y(t) = y(t) - y(t-1)$$

  - Makes the series stationary before ARMA modeling
- Interpretation
  - AR: memory of past values
  - I: removes trends and seasonality
  - MA: corrects random shocks



MATLAB

`m = arima(p,d,q)`

`p` = AR order; `d` = number of differences (integration order); `q` = order of MA part

Activity 4: Iron Ore Prices – ARIMA Modeling

Model Evaluation and Selection

- Many possible models → need criteria to choose the best one
- Avoid overfitting (too complex) and underfitting (too simple)
- Common criteria
  - Residual analysis (should look like white noise)
  - Goodness of fit (%) to validation data
  - Information criteria (Akaike information criteria (AIC), Final prediction error (FPE))
  - Prediction accuracy (on test data)
- Best practice
  - Compare several models with different orders
  - Choose the simplest model that explains the data well
  - Validate with unseen (test) data if available

> ⓘ In MATLAB
>
> - `goodnessOfFit`
> - `compare(data, model1, model2, ...)` → compare fit visually
> - `aic`, `fpe` → return information criteria
> - `resid(data, model)` → check residuals

Summary

- Time-series data can be broken into components: trend, seasonality, cyclic variation, and residuals
- Models help us explain and predict time-series behavior
  - AR models: depend on past outputs
  - ARX models: extend AR by including exogenous inputs
  - ARMA/ARMAX: combine autoregression with moving average, noise modeling
  - ARIMA: adds differencing for non-stationary data
- Model evaluation and selection
  - Check residuals (should look like white noise)
  - Use metrics like AIC, FPE, fit percentage
  - Validate using unseen data

📌 Different models suit different needs — forecasting, simulation, or understanding system dynamics.