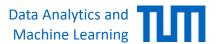
#### **Machine Learning for Graphs and Sequential Data**

Sequential Data – Autoregressive Models

Lecturer: Prof. Dr. Stephan Günnemann

cs.cit.tum.de/daml

Summer Term 2024



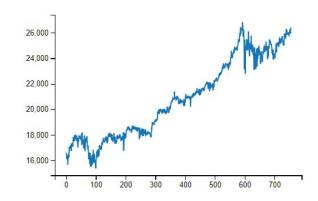
#### Roadmap

- Chapter: Temporal Data / Sequential Data
  - 1. Autoregressive Models
    - Motivation & Definitions
    - Parameter Learning
    - Stationarity
  - 2. Markov Chains
  - 3. Hidden Markov Models
  - 4. Neural Network Approaches
  - 5. Temporal Point Processes

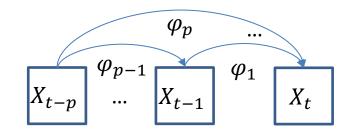
#### **Motivation**

- Autoregressive (AR) models for sequences of observations  $X_1, X_2, ..., X_T$ .
  - The index t can correspond to time, location, etc.
  - For now, we focus on the case of continuous observations occurring at discrete time-steps
- Example: Time-series forecasting
  - $-X_t$  = measurement of a sensor at time-step t
  - Applications in weather forecasting,
     e.g.,  $X_t$ = temperature on t-th day
  - Applications in the field of economics, e.g.,  $X_t$ = stock market quotations on t-th day

Observations are not independent → non-i.i.d. data



#### **AR model - Definition**



Definition: An autoregressive model AR(p) of order p is defined as:

$$X_t = c + \sum_{i=1}^{p} \varphi_i X_{t-i} + \varepsilon_t$$

where  $\varphi_1, ..., \varphi_p$  are the parameters, c is a constant and  $\varepsilon_t \sim N(0, \sigma)$  is a **white noise**. The variable  $X_{t-i}$  is the **lagged value** at time i.

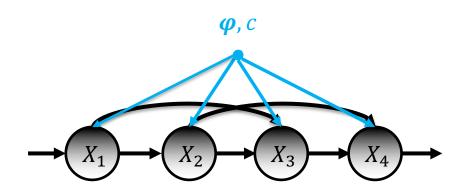
- Intuitively, we perform a regression where the lags  $([X_{t-1}, ..., X_{t-p}])_t$  are the inputs and  $(X_t)_t$  are the outputs.
- Remark that a modification (or shock) on  $X_t$  will have a repercussion far into the future. The variables  $(X_t)_t$  are not independent.

# **AR model – Graphical Model**

We can rewrite the AR model:

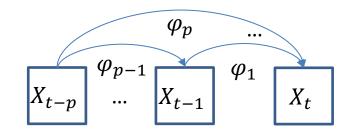
$$P(X_t|X_{t-1},...X_{t-p}) \sim N(c + \sum_{i=1}^p \varphi_i X_{t-i}, \sigma)$$

- The graphical model representation of the AR model is:
  - The parameters  $\phi$ , c are shared through time



 AR model can be viewed as a probabilistic model for continuous observations

#### **AR model - Definition**



- The **mean function** of an AR model is  $\mu(t) = E[X_t]$ . By default, it depends on t.
- The autocovariance  $\gamma(t,i) = Cov(X_t,X_{t-i})$ . By default, it depends on t and i.
- The autocovariance function can be normalized to give the **Pearson** autocorrelation function  $\rho(t,i) = \frac{Cov(X_t,X_{t-i})}{\sqrt{Var(X_t)}\sqrt{Var(X_{t-i})}}$ . It lies in [-1,1].
- The autocorrelation and autocovariance are indicators of the dependence of the variable  $X_t$  with respect to the past variables  $X_{t-i}$

#### Roadmap

- Chapter: Temporal Data / Sequential Data
  - 1. Autoregressive Models
    - Motivation & Definitions
    - Parameter Learning
    - Stationarity
  - 2. Markov Chains
  - 3. Hidden Markov Models
  - 4. Neural Network Approaches
  - 5. Temporal Point Processes

## **AR model – Parameter Learning (1)**

■ The parameters can be learned with classic least squares regression:

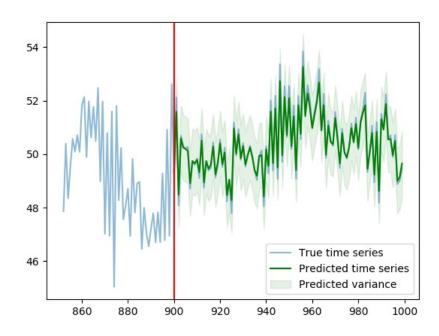
$$\begin{bmatrix} \varphi_1 \\ \varphi_2 \\ \vdots \\ \varphi_{p-1} \\ \varphi_p \end{bmatrix} = (X^T X)^{-1} X^T y$$

where 
$$\mathbf{X} = \begin{bmatrix} X_{p-1} & \cdots & X_0 \\ X_p & \cdots & X_1 \\ \vdots & \cdots & \vdots \end{bmatrix}$$

and 
$$y = \begin{bmatrix} X_p \\ X_{p+1} \\ \vdots \end{bmatrix}$$

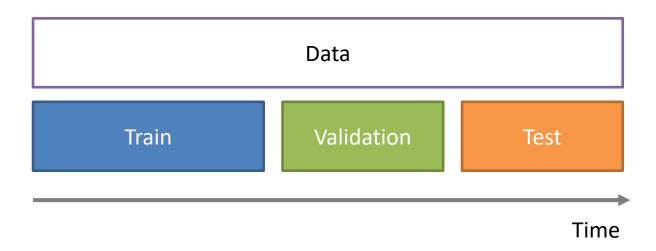
## **AR model – Parameter Learning**

- Example:  $X_t = 5 + 0.8 * X_{t-1} + 0.1 * X_{t-2} + N(0,1)$ 
  - 1. We learn parameters and the variance on the 900 first samples
    - Estimated parameters:  $\varphi_1=0.82$ ,  $\varphi_2=0.07$ ,  $\sigma=1.21$
  - 2. We predict on the last 100 samples



## **General Remark: Data split**

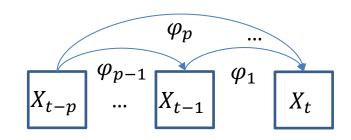
- An important part of training is model selection
  - Usually we split data into train, validation and test set
- With time series and sequential data these sets should be split in such a way to keep the temporal ordering
- A model should be tested only on the data from the future



#### Roadmap

- Chapter: Temporal Data / Sequential Data
  - 1. Autoregressive Models
    - Motivation & Definitions
    - Parameter Learning
    - Stationarity
  - 2. Markov Chains
  - 3. Hidden Markov Models
  - 4. Neural Network Approaches
  - 5. Temporal Point Processes

## **AR model - Stationarity**



Definition: A process is said to be stationary if

1. 
$$E[X_t] = E[X_{t-i}] = \mu, \forall t, \forall i$$

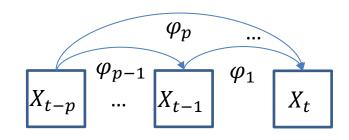
2. 
$$Cov(X_t, X_{t-i}) = \gamma_i, \forall t, \forall i$$

3. 
$$E[|X_t|^2] < \infty, \forall t$$

- The mean function  $E[X_t]$  is constant.
- The autocovariance  $Cov(X_t, X_{t-i})$  only depends on the lagged value at time i. It does not depend on t.

Remark: we have  $\gamma_i = Cov(X_t, X_{t-i}) = Cov(X_{t-i}, X_t) = \gamma_{-i}$ 

## **AR model - Stationarity**



Definition: A process is said to be stationary if

1. 
$$E[X_t] = E[X_{t-i}] = \mu, \forall t, \forall i$$

2. 
$$Cov(X_t, X_{t-i}) = \gamma_i, \forall t, \forall i$$

3. 
$$E[|X_t|^2] < \infty, \forall t$$

#### Benefits:

- Stationarity is often a good modeling assumption (like i.i.d. assumption).
- For stationary processes, it is possible to estimate mean and autocovariance by averaging measures over time.
- In other words: Parameters learned from past observations will generalize to future observations.

# **AR model – Parameter Learning (2)**

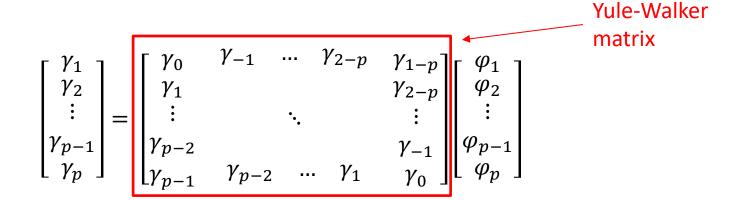
Assuming stationarity, the parameters can also be learned by using the Yule Walker equations:

$$\gamma_{0} = \sum_{j=1}^{p} \varphi_{j} \gamma_{-j} + \sigma^{2}$$

$$\gamma_{1} = \sum_{j=1}^{p} \varphi_{j} \gamma_{1-j}$$

$$\gamma_{2} = \sum_{j=1}^{p} \varphi_{j} \gamma_{2-j}$$
...
$$\gamma_{p} = \sum_{j=1}^{p} \varphi_{j} \gamma_{p-j}$$

- 1. Estimate the moments  $\gamma_0, \gamma_1, ..., \gamma_p$
- 2. Inverse Yule-Walker matrix to estimate  $\varphi_1, \dots, \varphi_p$
- 3. Use  $\gamma_0$  equation to estimate  $\sigma$



#### **Questions – AR**

- 1. What is the mean  $E[X_t]$  of the following processes:
  - a)  $X_t = \sin(t/10) + \varepsilon_t$  where  $\varepsilon_t \sim N(0, \sigma)$
  - b)  $X_t = 4 0.8 * X_{t-1} 0.1 * X_{t-2} + \varepsilon_t$  where  $\varepsilon_t \sim N(0, \sigma)$
  - c)  $X_t = 4 + X_{t-1} + \varepsilon_t$  where  $\varepsilon_t \sim N(0, \sigma)$  and  $X_0 \sim N(0, \sigma)$
- 2. Why does Yule Walker parameter learning require stationarity?

## **Reading Material**

- [1] Stationary Models lecture, Matthieu Stigler:
   <a href="http://matthieustigler.github.io/Lectures/Lect2ARMA.pdf">http://matthieustigler.github.io/Lectures/Lect2ARMA.pdf</a>
- [2] Time Series lecture, Rauli Susmel:
   <a href="https://www.bauer.uh.edu/rsusmel/phd/ec2-3.pdf">https://www.bauer.uh.edu/rsusmel/phd/ec2-3.pdf</a>
- [3] Introduction on AR Model lecture, Rob Reider:
   <a href="https://s3.amazonaws.com/assets.datacamp.com/production/course\_4267/slides/chapter3.pdf">https://s3.amazonaws.com/assets.datacamp.com/production/course\_4267/slides/chapter3.pdf</a>