DYNASTEE DYNamic Analysis. Simulation and Testing applied to the Energy and Environmental performance of buildings

Free On-Line Training Webinars; 22 and 29 September, 6 and 13 October 2021

Dynamic Calculation Methods for Building Energy Performance Assessment

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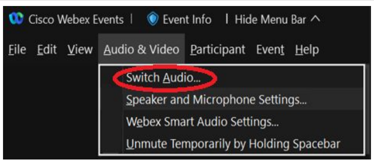

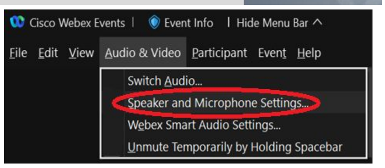

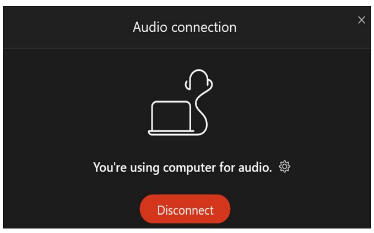

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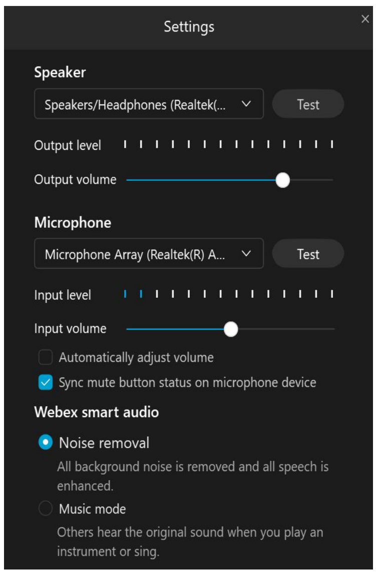

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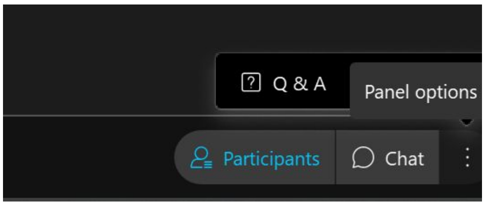
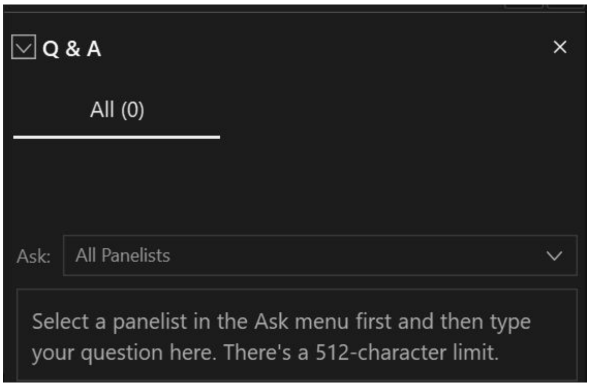
How to ask questions during the webinar

Note: Please DO NOT use the chat box to ask your questions!

Locate the **Q&A box**

Select **All Panelists** | Type your question | Click on Send





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NOTES:

1. The questions addressed to the speakers during this webinar- via the Q&A box- will be gathered and answered **during the last webinar of the series on October 13th**
2. After the end of the webinar you can also send further questions you might have, via email to Hans Bloem at: hans.bloem@inive.org
3. The webinar will be recorded and published at https://dynastee.info/ within a couple of weeks, along with the presentation slides.

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Introduction to statistical modelling of dynamical systems

Peder Bacher

DYNASTEE On-line Training for Dynamic Calculation Methods for Building Energy Performance Assessment

Webinar 2020

October 6, 2021

Overview

Data analysis and statistics

Statistical inference

- "Everything should be made as simple as possible, but not simpler" (Einstein)
- **Which model**? and **how complex** should it be? **Depends on data!**
- Statistics provide the techniques to:
  - **Estimate model parameters** and their uncertainties
  - Verify and argue that you have found the best model (or rather there is not one best model, so we call it a **suitable model**)

We can: Extract information and draw conclusions from data

We can: Train models for prediction and use them as basis for optimization

Time series analysis

Statistical modeling of dynamical systems

- Called time series analysis
- Tons of literature (and software):
  - Wiener, N. (1949). Extrapolation, Interpolation, and Smoothing of Stationary Time Series. The MIT Press
  - Box, G., Jenkins, G. (1976). *Time series analysis: forecasting and control*
  - ...
- Used in any thinkable application!

Time series models

General types of models *(can all be tweaked!)*:

- Static model *no dynamics*
- ARMAX, *discrete models* based on transfer functions
- Grey-box, *continuous time models*, combination of physics and statistics (stochastic differential equations (SDEs))

Static model *(linear function)*

$$\text{Measurements} = \text{Function}(\text{Inputs}) + \text{Error}$$

Discrete ARX model *(Auto-Regressive with eXogenous input)*

$$\text{Measurements} = \text{TransferFun}(\text{Inputs}) + \text{Error}$$

Discrete ARMAX model *(Auto-Regressive Moving Average with eXogenous input)*

Statistical model validation: examine the residuals

Residuals from a *simple linear regression model*

$$Y_t = \beta_0 + \beta_1 x_t + \varepsilon_t$$

$$y_t = \hat{\beta}_0 + \hat{\beta}_1 x_t + \hat{\varepsilon}_t$$

$$y_t = \hat{y}_t + \hat{\varepsilon}_t$$

$$\hat{\varepsilon}_t = y_t - \hat{y}_t$$

$$\text{Residual}_t = \text{Observation}_t - \text{Prediction}_t$$

Two assumptions:

1. The error is normal distributed: $\varepsilon_t \sim N(0, \sigma^2)$ (less important with many obs.)
2. The error is *independent and identically distributed* (i.i.d.):
   - Check $\hat{\varepsilon}_t$ is not dependent on other variables

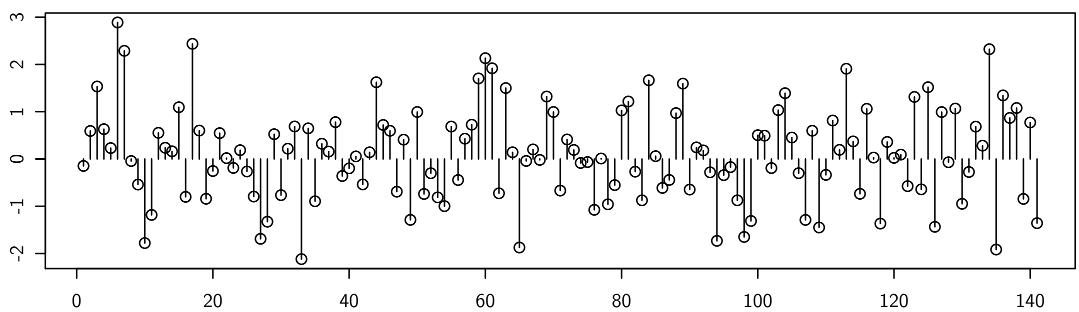
   - Check $\hat{\varepsilon}_t$ is not dependent on $\hat{\varepsilon}_{t-k}$ for any k

Do you know about:

- White noise?
- AutoCorrelation Function (ACF)?

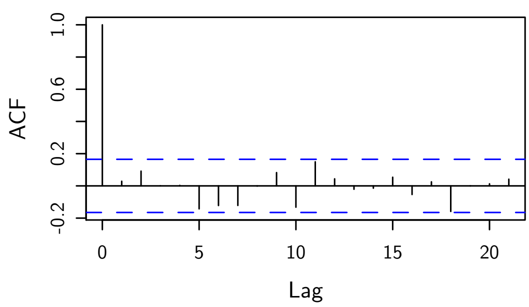
ACF of white noise

```
## Plot
x <- rnorm(141)
plot(x, type="n", xlab="Time", ylab="")
points(x)
lines(x, type='h')
```



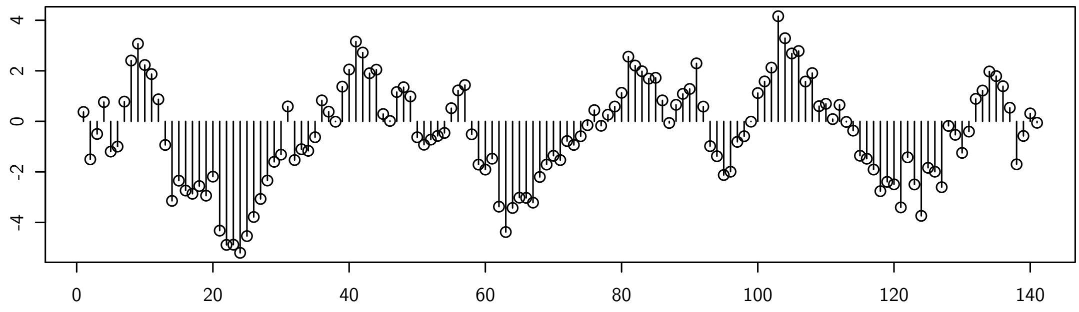
The ACF:

```
## Autocorrelation function
acf(x)
```



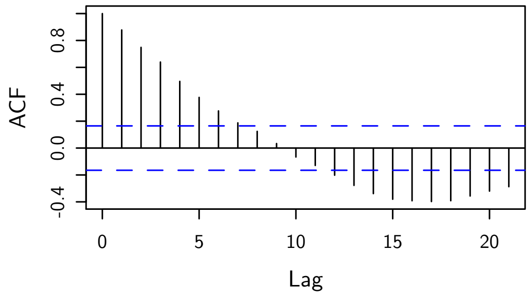
ACF of non-white noise

```
## Plot
x <- filter(rnorm(141), 0.9, "recursive")
plot(x, type="n", xlab="Time", ylab="")
points(x)
lines(x, type='h')
```



The ACF:

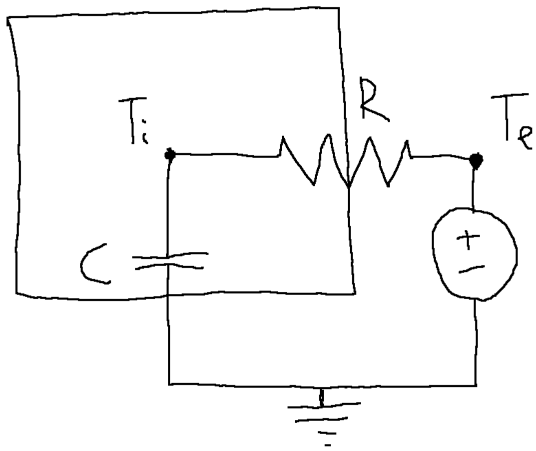
```
## Autocorrelation function
acf(x)
```



We want white noise!

- We fit the model and then analyze the residuals
- If they are *not* white noise, then we can still improve the model!

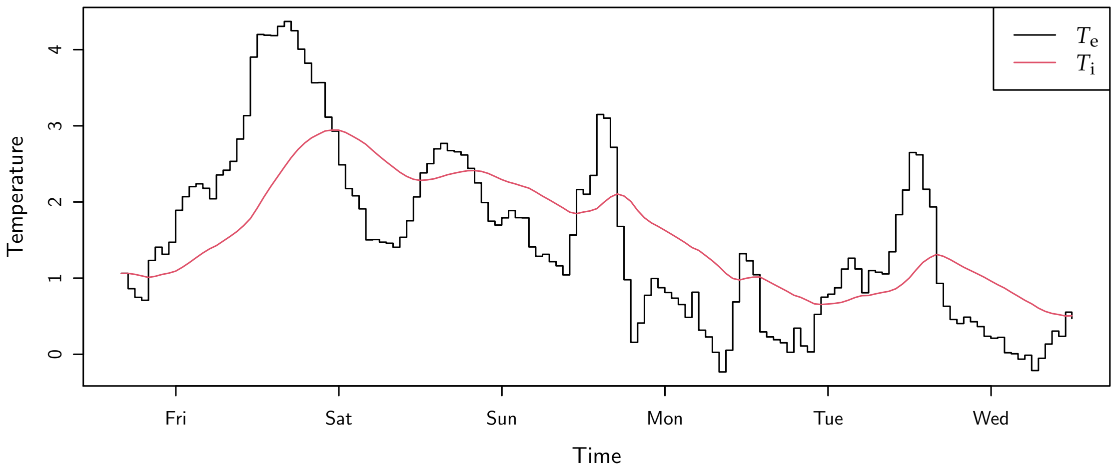
Simplest first order RC-system



Simplest RC-system

- T_t^{e} external and T_t^{i} internal temperature at time $t = [1, 2, \ldots, n]$
- ODE model

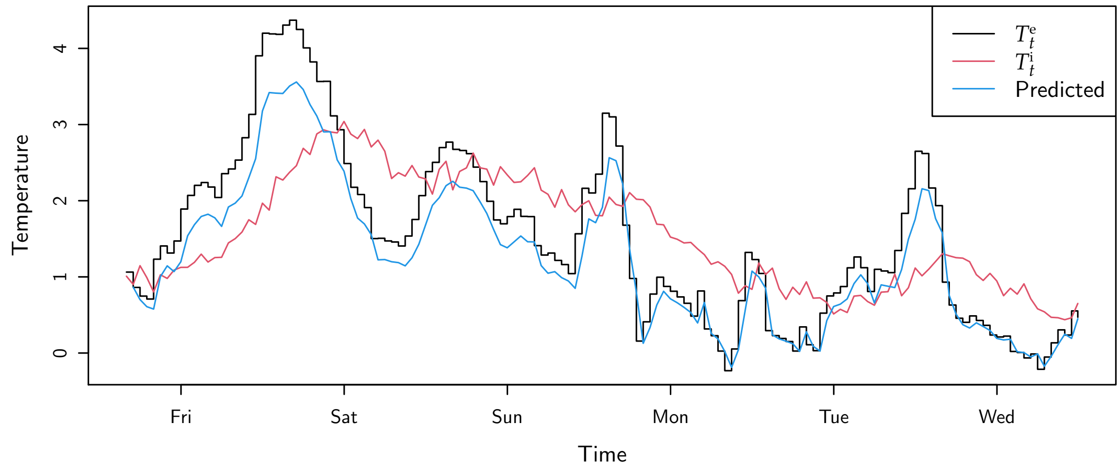
$$\frac{dT_{\mathrm{i}}}{dt} = \frac{1}{RC}(T_{\mathrm{e}} - T_{\mathrm{i}})$$



Try a static model

- A simple linear regression model (ε_t is the error)
- Not describing dynamics

$$T^{\mathrm{i}}_t = \omega_{\mathrm{e}} T^{\mathrm{e}}_t + \varepsilon_t$$



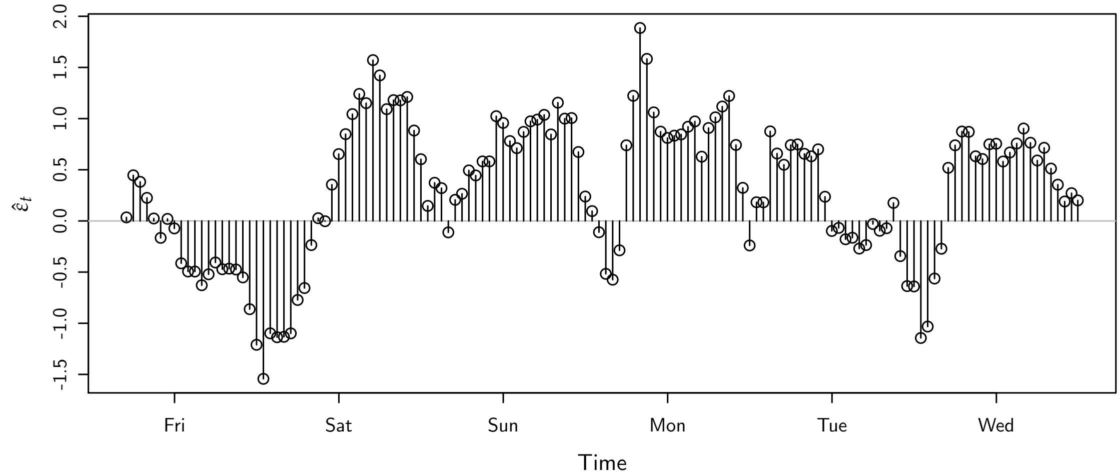
White noise and autocorrelation function

Model validation: check i.i.d. of residuals

Are residuals like white noise?

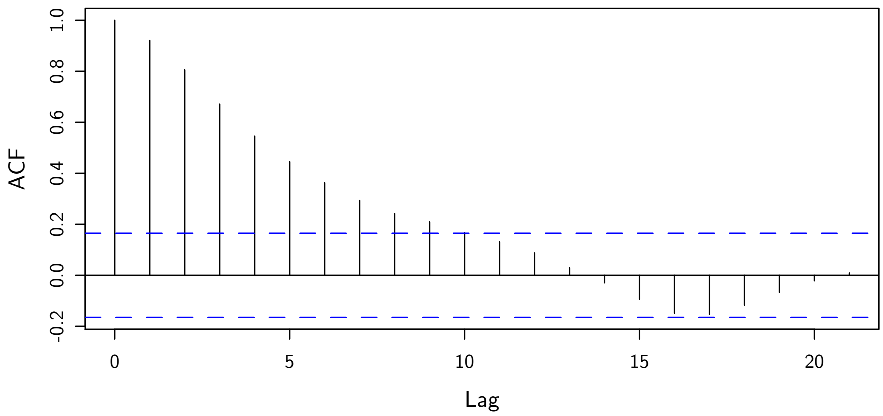
- Check if they are *independent and identically distributed*
- Is $\hat{\varepsilon}_t$ independent of $\hat{\varepsilon}_{t-k}$ for all t and k?

Nope! There is a pattern left...



Model validation: Test for i.i.d. with ACF

TEST if residuals independent of each other using the *Auto Correlation Function*?



It's not white nose! How do we find a better model?

Discretize the ODE

$$\frac{dT_\mathrm{i}}{dt} = \frac{1}{RC}(T_\mathrm{e} - T_\mathrm{i})$$

It has the solution

$$T_\mathrm{i}(t+\Delta t) = T_\mathrm{e}(t) + e^{-\frac{\Delta t}{RC}}\big(T_\mathrm{i}(t) - T_\mathrm{e}(t)\big)$$

if $\Delta t = 1$ and T_e is constant between the sample points then

$$T^\mathrm{i}_{t+1} = e^{-\frac{1}{RC}} T^\mathrm{i}_t + (1 - e^{-\frac{1}{RC}}) T^\mathrm{e}_t$$

since $e^{-\frac{1}{RC}}$ is between 0 and 1, then write it as

$$T^\mathrm{i}_{t+1} = \phi_1 T^\mathrm{i}_t + \omega_1 T^\mathrm{e}_t$$

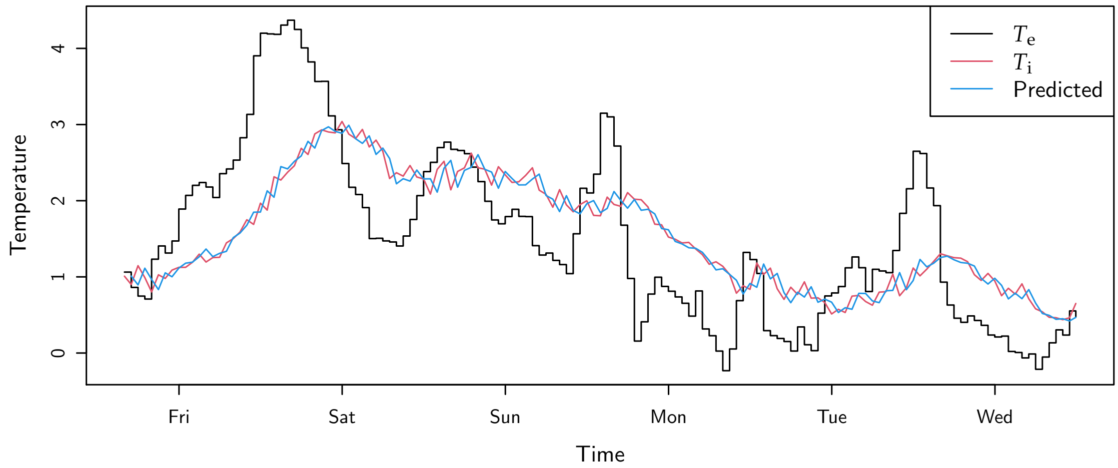
where ϕ_1 and ω_1 are between 0 and 1.

Add a noise term and we have the ARX model

$$T^\mathrm{i}_{t+1} = \phi_1 T^\mathrm{i}_t \quad + \omega_1 T^\mathrm{e}_t \quad + \varepsilon_{t+1} T^\mathrm{i}_t \qquad = \phi_1 T^\mathrm{i}_{t-1} + \omega_1 T^\mathrm{e}_{t-1} + \varepsilon_t$$

An ARX model

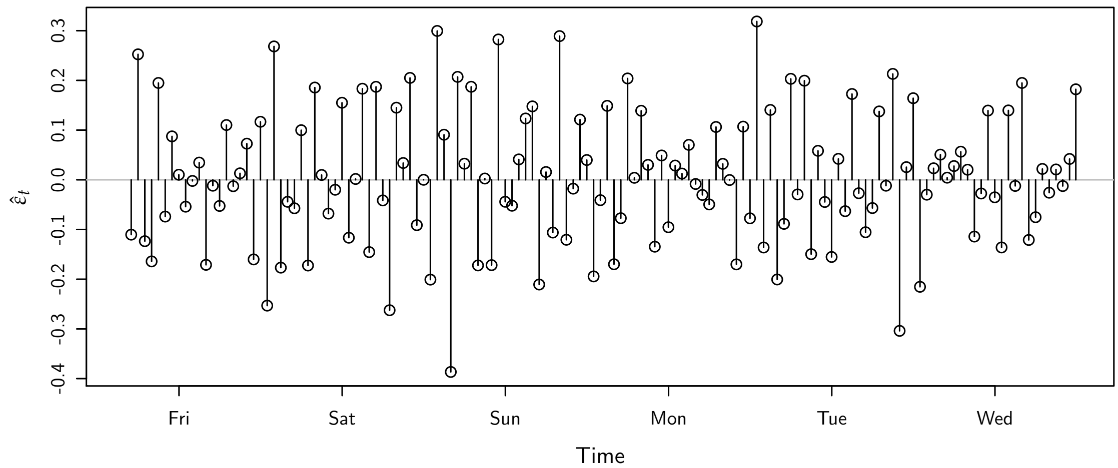
$$T^{\mathrm{i}}_t = \phi_1 T^{\mathrm{i}}_{t-1} + \omega_1 T^{\mathrm{e}}_{t-1} + \varepsilon_t$$



ARX model

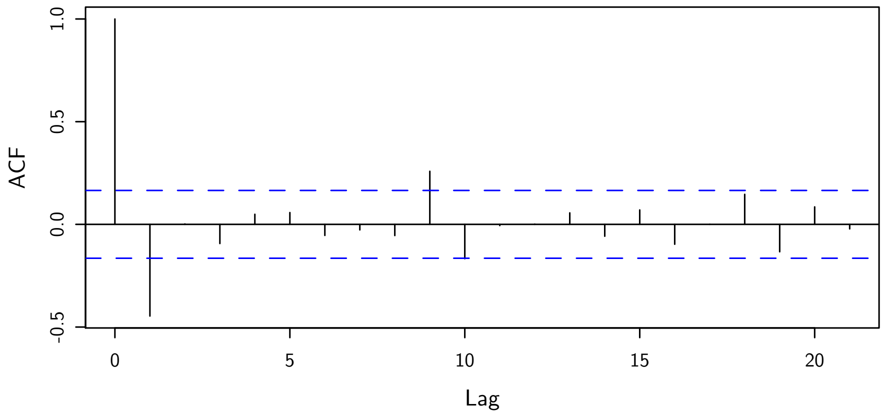
The residuals

$$\hat{\varepsilon}_t = T^{\mathrm{i}}_t - \frac{\hat{\omega}_1 \mathrm{B}}{1 - \hat{\phi}_1 \mathrm{B}} T^{\mathrm{e}}_t$$



Check for i.i.d. of residuals

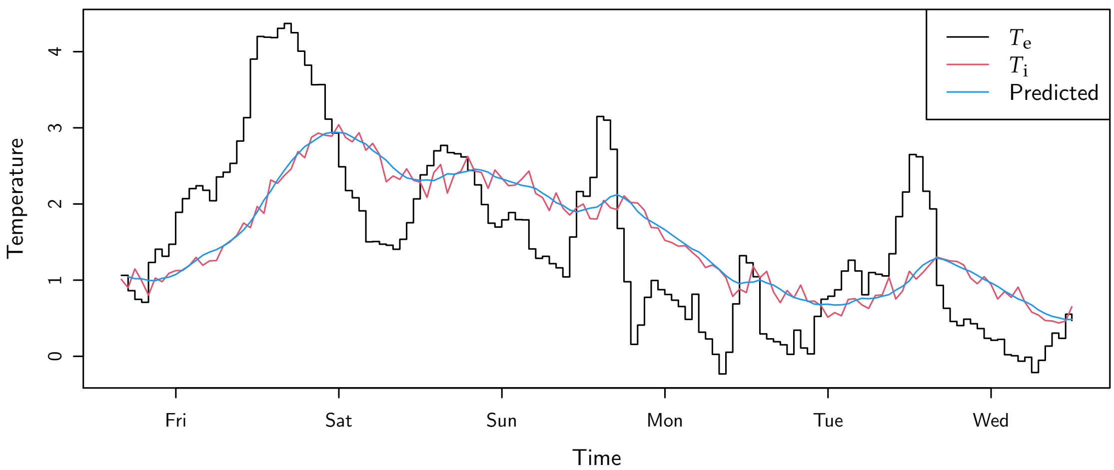
Is it likely that this is white noise? Almost!



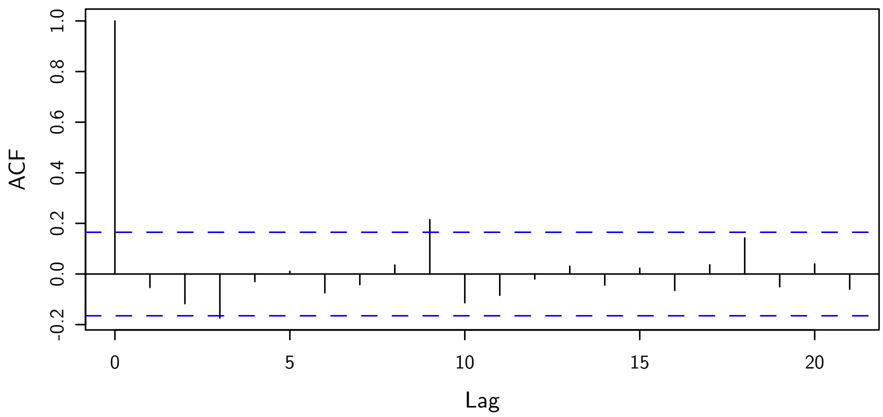
Actually we miss an MA part!

An ARMAX model

$$T_t^{\mathrm{i}} = \phi_1 T_{t-1}^{\mathrm{i}} + \omega_1 T_t^{\mathrm{e}} + \varepsilon_t + \theta_1 \varepsilon_{t-1}$$



Validate the model with the residuals ACF



Now we have *white noise residuals*, that is want to have after applying the model!

Note that we are validating the *one-step prediction* residuals: $\hat{\varepsilon}_{t+1} = y_{t+1} - \hat{y}_{t+1|t}$
$\hat{\varepsilon}_t \; = y_t - \hat{y}_{t|t-1}$

Auto-regressive (AR) model

AR model of order 1

$$Y_t = \phi_1 Y_{t-1} + \varepsilon_t$$

ARX model of order 1

$$Y_t = \phi_1 Y_{t-1} + \omega_1 X_{t-1} + \varepsilon_t$$

ARMAX model of order 1

$$Y_t = \phi_1 Y_{t-1} + \omega_1 X_{t-1} + \varepsilon_t + \theta_1 \varepsilon_{t-1}$$

where $\varepsilon_t \sim N(0, \sigma^2)$ and i.i.d.
Use either X or U as the input (just a variable name in the generalized form).

Discrete linear time series models

AR model of order p

$$Y_t = \phi_1 Y_{t-1} + \phi_2 Y_{t-2} + \ldots + \phi_p Y_{t-p} + \varepsilon_t$$

ARX model of order p

$$Y_t = \phi_1 Y_{t-1} + \ldots + \phi_p Y_{t-p} + \omega_1 X_{t-1} + \ldots + \omega_p X_{t-p} + \varepsilon_t$$

ARMAX model of order p

$$Y_t = \phi_1 Y_{t-1} + \ldots + \phi_p Y_{t-p} + \omega_1 X_{t-1} + \ldots + \omega_p X_{t-p} + \varepsilon_t + \theta_1 \varepsilon_{t-1} + \ldots + \theta_p \varepsilon_{t-p}$$

where $\varepsilon_t \sim N(0, \sigma^2)$ and i.i.d.
Doesn't need to have same order p for the AR, X and MA parts.

Discrete linear time series models

AR model

$$\phi(B) Y_t = \varepsilon_t$$

ARX model

$$\phi(B) Y_t = \omega(B) X_t + \varepsilon_t$$

ARMAX model

$$\phi(B) Y_t = \omega(B) X_t + \theta(B) \varepsilon_t$$

- $\varepsilon_t \sim N(0, \sigma^2)$ and i.i.d.
- B is the back-shift operator $\mathrm{B}^k Y_t = Y_{t-k}$
- $\phi(B) = 1 + \phi_1 B + \phi_2 B^2 + \ldots + \phi_p B^p$
- $\omega(B) = \omega_1 B + \omega_2 B^2 + \ldots + \omega_p B^p$
- $\theta(B) = 1 + \theta_1 B + \theta_2 B^2 + \ldots + \theta_q B^q$

Discrete linear time series models

On transfer function form

ARMAX model

$$Y_t = \frac{\omega(B)}{\phi(B)} X_t + \frac{\theta(B)}{\phi(B)} \varepsilon_t$$

$$\Leftrightarrow$$

$$Y_t = H_\omega(B) X_t + H_\theta(B) \varepsilon_t$$

where $H_\omega(B)$ and $H_\theta(B)$ are a transfer functions

How to estimate parameters in discrete TS models

Fit (in R)

- ARX models with linear regression (closed form optimization, always give the optimum, in R `lm()`)
- ARMA in R is in `arima()`
- ARMAX in R can be fitted with the `marima` and several other packages

And we can tweak and also make non-linear discrete models in many ways!

Continuous time series models

Introduction to grey-box modelling and **ctsmr**

ctsmr

Continuous Time Stochastic Modelling in R

more correctly

Continuous-Discrete Time Stochastic Modelling in R

Grey-box modelling

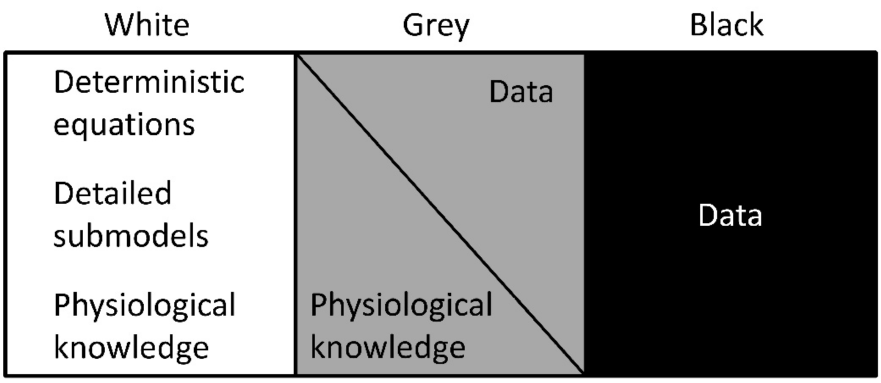


Figure: Ak et al. 2012

Bridges the gap between physical and statistical modelling.
THERE is a manual on ctsm.info

The model class

ctsmr implements a state space model with:

Continuous time stochastic differential system equations (SDE)

$$dX_t = f(X_t, U_t, t, \theta)dt + g(X_t, U_t, t, \theta)dB_t$$

Discrete time measurement equations

$$Y_k = h(X_{t_k}, u_t, t, \theta) + e_k \quad , \quad e_k \in N(0, S(u_k, t_k, \theta))$$

- Underlying physics (system, states) modelled using continuous SDEs.
- Some (or all) states are observed in discrete time.

Write up the physical model!

This is easier to work with (if you know the physics behind the system)!

The ODE

$$\frac{dT_{\mathrm{i}}}{dt} = \frac{1}{RC}(T_{\mathrm{e}} - T_{\mathrm{i}})$$

Just needs a diffusion term to make into the *system equation*

state drift term diffusion term

$$dT_{\mathrm{i}} = \frac{1}{RC}(T_{\mathrm{e}} - T_{\mathrm{i}})dt + \sigma_{\mathrm{i}} d\omega$$

and together with the *measurement equation*

observation state error

$$Y_{T_{\mathrm{i}},k} = T_{\mathrm{i},t_k} + e_k \quad , \quad e_k \in N(0, \sigma) \text{ and i.i.d.}$$

it forms a *grey-box model*.

Wuuups

This particular models are actually unidentifiable!!

R and C cannot be separated (change one, then the other accordingly and the model prediction is equal (same goes for ϕ_1 and ω_1))

The time constant $RC = \tau$ is used instead

$$dT_{\mathrm{i}} = \frac{1}{RC\tau}(T_{\mathrm{e}} - T_{\mathrm{i}})dt + \sigma_{\mathrm{i}} d\omega$$

Define a GB model

Install the `ctsm-r` package from `ctsm.info`.

Define the model:

```
## Generate a new object of class ctsm
model <- ctsm$new()
## Add a system equation and thereby also a state
model$addSystem(dTi ~ ( 1/tau*(Te-Ti) )*dt + exp(p11)*dw1)
## Set the names of the inputs
model$addInput(Te)
## Set the observation equation: Ti is the state, yTi is the measured output
model$addObs(yTi ~ Ti)
## Set the variance of the measurement error
model$setVariance(yTi ~ exp(e11))
```


Fit the model

Set initial values and bounds for the estimation:

```
## Set the initial value (for the optimization) of the value of the state at the starting time point
model$setParameter(  Ti = c(init=5     ,lb=-5   ,ub=20 ) )
## Set the initial value for the optimization
model$setParameter( tau = c(init=10    ,lb=1E-2 ,ub=200 ) )
model$setParameter( p11 = c(init=0.01 ,lb=-30   ,ub=10 ) )
model$setParameter( e11 = c(init=0.01 ,lb=-50   ,ub=10 ) )
```

Run the parameter estimation:

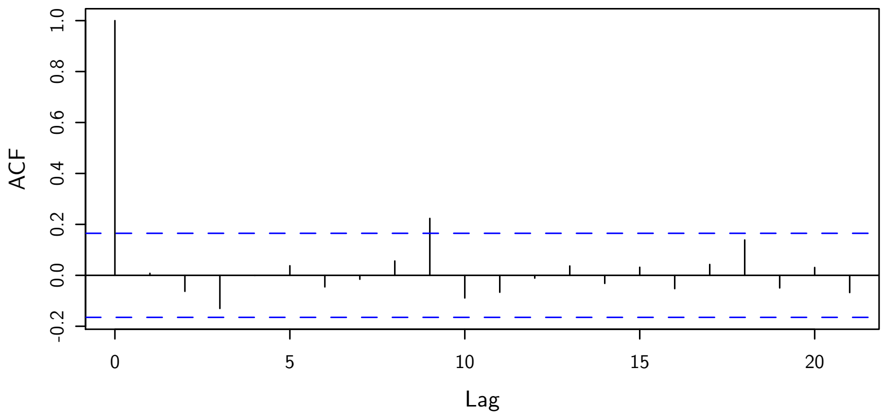
```
fit <- model$estimate(X)
```

Validate the model

Check the *one-step prediction* residuals:

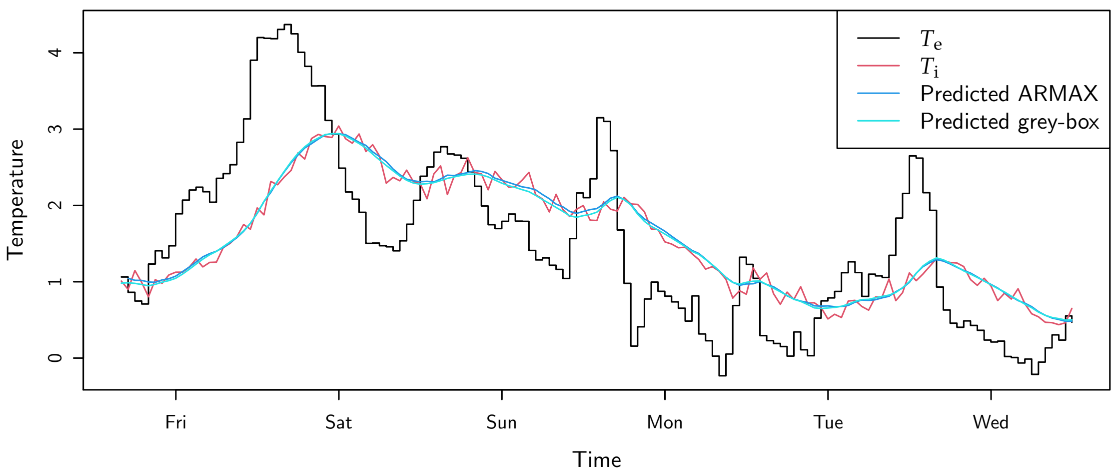
```
# Teke the one-step predictions from the fit
val <- predict(fit)[[1]]
# Calculate the residuals
residualsgb <- unlist(X$yTi - val$output$pred)

# The autocorrelation function
acf(residualsgb)
```



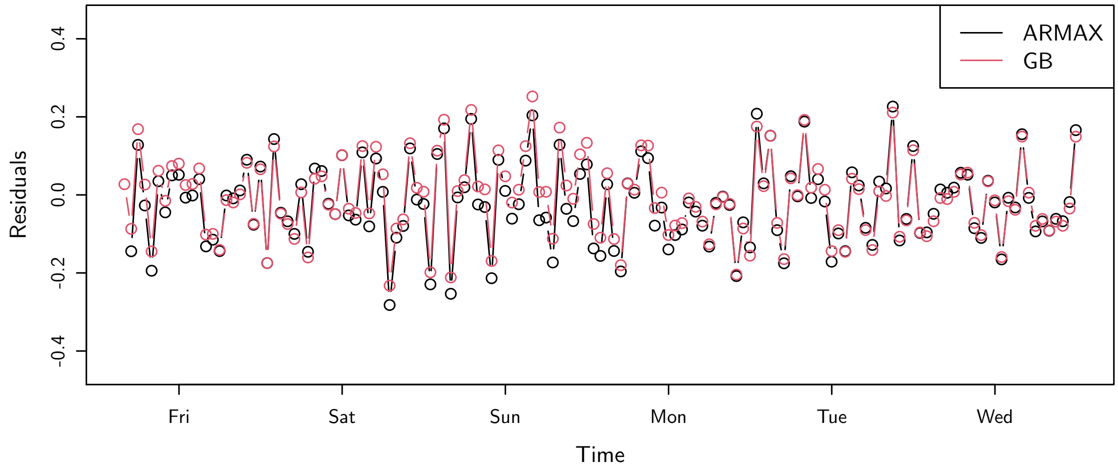
Discrete ARMAX is equivalent to continuous SDE model

One-step predictions of ARMAX and grey-box are almost equal:



Discrete ARMAX is equivalent to continuous SDE model!

Plot the ARMAX and GB residuals:



Parameter estimation with the likelihood

An example, we have:

- A model with two parameters $Y_i \sim N(\mu, \sigma^2)$
- n observations $(y_1, y_2, \ldots, y_n)$

The likelihood is defined by the joint probability density function (pdf) of the observations

$$L(\mu, \sigma) = p(y_1, y_2, \ldots, y_n | \mu, \sigma)$$

Hence, the model defines the pdf as a function of the parameters (the observations are not varying).

Independence of the observations simplifies it to

$$L(\mu, \sigma) = \prod_{i=1}^{n} p(y_i | \mu, \sigma)$$

Maximum likelihood estimation

Maximum likelihood estimation (MLE)

Parameter estimation by maximizing the likelihood function

$$\hat{\theta} = \arg\max_{\theta \in \Theta} \left(L(\theta) \right)$$

Due to numerical properties we always minimize the negative log-likelihood

$$\hat{\theta} = \arg\min_{\theta \in \Theta} \left(-\ln(L(\theta)) \right)$$

So in the example $\theta = (\mu, \sigma)$

Likelihood for time correlated data

Given a time series of measurements $\mathcal{Y}_N$

$$\begin{aligned} L(\theta) &= p(\mathcal{Y}_N | \theta) \\ &= p(y_N, y_{N-1}, \dots, y_0 | \theta) \\ &= \left(\prod_{k=1}^{N} p(y_k | \mathcal{Y}_{k-1}, \theta) \right) p(y_0 | \theta) \end{aligned}$$

Essentially, $p(y_k | \mathcal{Y}_{k-1}, \theta)$ is the pdf of the one-step ahead prediction

Thus assuming independence of the one-step predictions (so i.i.d. error)

Likelihood for time correlated data

If Gaussian

$$\hat{y}_{k|k-1} = E[y_k|\mathcal{Y}_{k-1}, \theta]$$
$$P_{k|k-1} = V[y_k|\mathcal{Y}_{k-1}, \theta]$$
$$\varepsilon_k = y_k - \hat{y}_{k|k-1}$$

then the likelihood is

$$L(\theta) = \left(\prod_{k=1}^{N} \frac{\exp(-\frac{1}{2}\varepsilon_k^T P_{k|k-1}^{-1} \varepsilon_k)}{\sqrt{|P_{k|k-1}|}\sqrt{2\pi}^l} \right)$$

Kalman filter

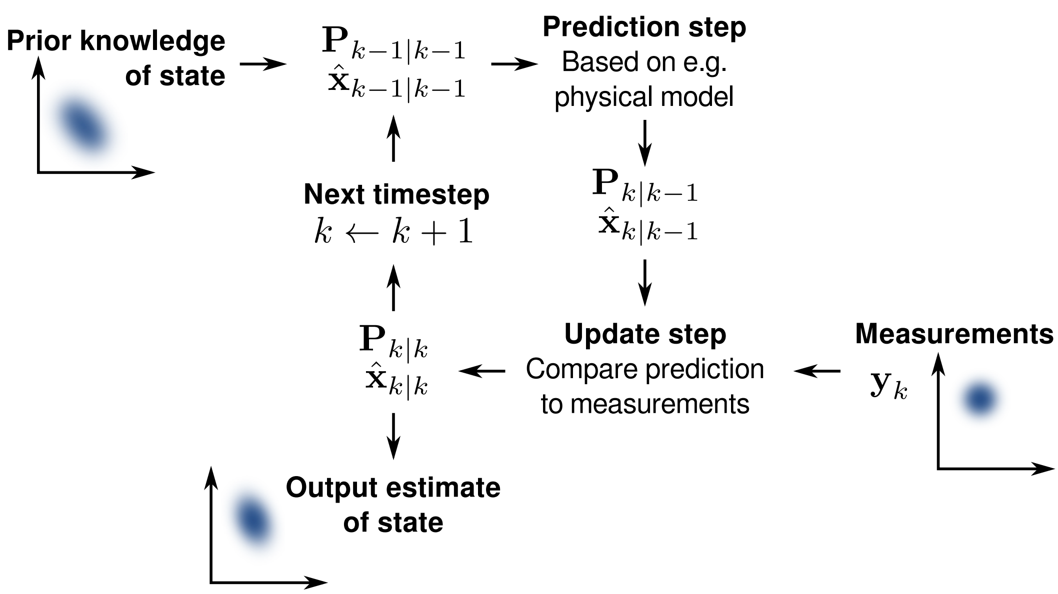


Figure: "Basic concept of Kalman filtering" by Petteri Aimonen. Wikipedia

Grey-box model MLE

Steps for maximum likelihood estimation of a grey-box model

1. Load data
2. Define a model
3. Define initial values and parameter bounds
4. Run an optimizer to find the parameter values maximizing the likelihood (run the Kalman filter many times)
5. Interpret and validate the result:
   - Check the optimizer convergence (e.g. no parameters at bounds)
   - Check estimated values and statistics
   - Validate the model by analyzing residuals

Show an example in R

Model complexity

The big question!!

How to select a *suitable* model complexity, neither underfitted nor overfitted! Both which inputs, the structure. Number of parameters increase complexity.

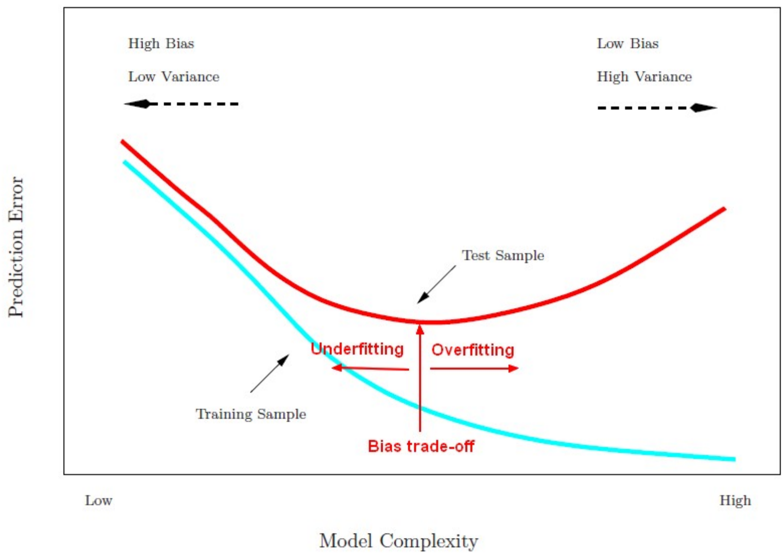


Figure from https://gerardnico.com/data_mining/bias_trade-off.

Model selection

The suitable model is a *compromise*:

- Not too complex (overfitted) and not too simple (underfitted).
- Use statistical tests to find out which model is better:
  - Nested models, use e.g. F-test or *likelihood ratio-test*
  - Un-nested models, use e.g. AIC or BIC

Different strategies:

- Forward selection: Start with the simplest model and extend step-wise
- Backward selection: Start with the full model and remove terms step-wise

ctsmr R package

See the website ctsm.info

- Installation needs compilers
- Documentation and examples
- Nice tricks
- Literature list with overview of studies where ctsm has been used