

# Unit 3: Introduction Spectral Analysis of Time Series Analysis

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#### Introduction

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- Introduction
- Stationarity
- The Periodogram and the Spectral Density Periodogram and Regression
  - Spectral Density
- Smoothing and Tapering Smoothing
  - Tapering
- Example

#### **Stationarity**



- The assumption of stationarity imposes regularity on a time series model.
- We will need repeated observations with the same or similar relationship to one another in order to estimate the underlying relationships between observations.
- There are other ways to do this, but stationarity is the most common and perhaps most basic.

#### **Strictly Stationary**



A time series ...,  $x_{-1}$ ,  $x_0$ ,  $x_1$ ,  $x_2$ , ... is *strictly stationary* if for a sequence of times  $t_k$ 

$$\{x_{t_1}, ..., x_{t_k}\}$$

has the same distributions as

$$\{X_{t_1+h}, ..., X_{t_k+h}\}$$

for every integer h. In other words,

$$P\{x_{t_1} \leq c_1, ..., x_{t_k} \leq c_k\} = P\{x_{t_1+h} \leq c_1, ..., x_{t_k+h} \leq c_k\}.$$

## **Weak Stationarity**



- An important measure of dependency in time series is autocovariances.
- This is defined as

• 
$$y(t, s) = E(x_t - \mu_t)(x_s - \mu_s)$$

- where  $\mu_t = Ex_t$ .
- The time series  $x_t$  is weakly stationary if  $\mu_t$  is constant and  $\gamma(s, t)$  depends only on the distance |s t|.
- In the case of Gaussian time series, these two concepts of stationarity overlap.

#### **Autocovariances Notation**



- For a weakly stationary time series, the notation used for auto covariance uses only lag:
- $\gamma(h) = E(x_t \mu)(x_{t-h} \mu)$  where  $\mu$  is the constant variance.
- We also have a concept of the autocorrelation function which we saw in the first section in the ACF plot. The autocorrelation function is defined as

$$\rho(h) = \frac{\gamma(h)}{\gamma(0)}$$

#### **Discrete Fourier Transform of the Time Series**



- What if we are less interested in how our underlying process evolves in time and are more interested in the variance of the time series at certain frequencies?
- We may attempt to apply a Fourier transform to the data. For our time series,  $x_1, ..., x_n$ , the discrete Fourier transform would be

• where  $\omega_j = 0, 1/n, ..., (n-1)/n$ .

$$d(\omega_j) = n^{-1/2} \sum_{\substack{n \text{ } x t exp(-2\pi i t \omega_j) \\ t=1}}^{\sum}$$

#### **An Alternate Representation**



• Note that we can break up  $d(\omega_j)$  into two parts

$$d(\omega_j) = n^{-1/2} \sum_{t=1}^{n} x_t \cos(2\pi i \omega_j t) - i n^{-1/2} \sum_{t=1}^{n} x_t \sin(2\pi i \omega_j t)$$

which we could write as a cosine component and a sine component

$$d(\omega_j) = d_c(\omega_j) - id_s(\omega_j)$$

#### **An Alternate Representation**



We may use an inverse Fourier transform to rewrite the data as

$$x_{t} = n^{-1/2} \sum_{j=1}^{2^{n}} d(\omega_{j}) e^{2\pi i \omega_{j} t}$$

$$= n^{-1/2} \sum_{j=1}^{2^{n}} d(\omega_{j}) e^{2\pi i \omega_{j} t}$$

$$= a +_{0} n^{-1/2} \sum_{j=1}^{2^{n}} d(\omega_{j}) e^{2\pi i \omega_{j} t} + n^{-1/2} \sum_{j=m+1}^{2^{n}} d(\omega_{j}) e^{2\pi i \omega_{j} t}$$

$$= a +_{0} \sum_{j=1}^{2^{n}} \frac{2d_{c}(\omega_{j})}{n^{-1/2}} \cos(2\pi i \omega_{j} t) + \sum_{j=1}^{2^{n}} \frac{2d_{s}(\omega_{j})}{n^{-1/2}} \sin(2\pi i \omega_{j} t)$$

$$\text{where } m = \lfloor \frac{\pi}{2} \rfloor$$

#### The Periodogram



The Periodogram is defined as

$$I(\omega_j) = |d(\omega_j)|^2 = d_c^2(\omega_j) + d_c^2(\omega_j)$$

- If there is no periodic trend in the data, then  $Ed(\omega_j) = 0$ , and the Periodogram expresses the variance of  $x_t$  at frequency  $\omega_j$ .
- If a periodic trend exists in the data, then  $Ed(\omega_j)$  will be the contribution to the periodic trend at the frequency  $\omega_i$ .

#### The Periodogram



- What are we trying to estimate with the Periodogram?
- We can use the Periodogram to find periodic trends in the data.
- Is there information left in the Periodogram after the trend is removed?
- Assuming that we have a stationary time series, what does the Periodogram estimate?

#### **The Spectral Density**



The spectral density is the Fourier transform of the auto covariance function

$$f(\omega) = \sum_{h=-\infty}^{h=\infty} e^{-2\pi i \omega h} \gamma(h)$$

• for  $\omega \in (-0.5, 0.5)$ . Note that this is a population quantity. (i.e. This is a constant quantity defined by the model.)

#### **The Spectral Density**

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- Why is the Periodogram an estimate for the spectral density?
- Let m be the sample mean of our data.

$$I(\omega_{j}) = |d(\omega)| = n^{2} \qquad -1 \qquad x_{t}e^{-2\pi i\omega_{f}} \qquad x_{t}e^{-2\pi i\omega_{f}}$$

$$= |d(\omega)|_{j} = n^{2} \qquad -1 \qquad x_{t}e^{-2\pi i\omega_{f}} \qquad x_{t}e^{-2\pi i\omega_{f}}$$

$$= |d(\omega)|_{j} = n^{2} \qquad -1 \qquad (x_{t} - m)(x_{s} - m)e^{-2\pi i\omega_{f}}(t - s)$$

$$= n^{-1} \qquad (x_{t+|h|} - m)(x_{t} - m)e^{-2\pi i\omega_{f}}(h)$$

$$= n^{-(n-1)} \qquad (x_{t+|h|} - m)(x_{t} - m)e^{-2\pi i\omega_{f}}(h)$$

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#### **The Spectral Density**



- Is the Periodogram a good estimator for the spectral density?
- Not really!
- The Periodogram,  $I(\omega_1)$ , ...,  $I(\omega_m)$ , attempt to estimate parameters  $f(\omega_1)$ , ...,  $f(\omega_m)$ . We have nearly the same number of parameters as we have data.
- Moreover, the number of parameters grow as a constant proportion of the data. Therefore, the Periodogram is NOT a consistent estimator of the spectral density.

## **Moving Average**



A simple way to improve our estimates is to use a moving average

smoothing technique

$$\hat{f}(\omega_j) = \frac{1}{2m+1} \sum_{k=-m}^{m} I(\omega_{j-k})$$

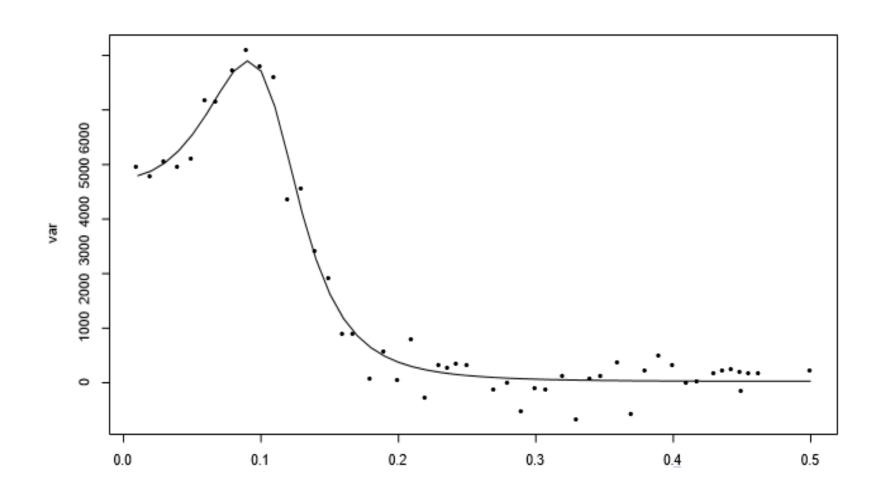
 We can also iterate this procedure of uniform weighting to be more weight on closer observations.

$$\hat{u}_t = \frac{1}{3}u_{t-1} + \frac{1}{3}u_t + \frac{1}{3}u_{t+1}$$

$$\hat{\hat{u}}_t = \frac{1}{3}\hat{u}_{t-1} + \frac{1}{3}\hat{u}_t + \frac{1}{3}\hat{u}_{t+1}$$

- Then, we iterate.
- Then, substitute to obtain better weights.

## **Moving Average**





#### **Smoothing Summary**



- Smoothing decreases variance by averaging over the Periodogram of neighboring frequencies.
- Smoothing introduces bias because the expectation of neighboring Periodogram values are similar but not identical to the frequency of interest.
- Beware of over smoothing!

## **Tapering**



- Tapering corrects bias introduced from the finiteness of the data.
- The expected value of the Periodogram at a certain frequency is not quite equal to the spectral density.
- It is affected by the spectral density at neighboring frequency points.
- For a spectral density which is more dynamic, more tapering is required.

#### Why do we need to taper?

- Our theoretical model ...,  $x_{-1}$ ,  $x_0$ ,  $x_1$ , ... consists of a doubly infinite time series on the series of the series
- We could think of our data,  $y_t$  as the following transformation of the model
- $y_t = h_t x_t$
- where  $h_t$ = 1 for t = 1, ..., n and zero otherwise. This has repercussions on the expectation of the Periodogram of our data.

$$E[I_{y}(\omega_{j})] = \int_{-0.5}^{0.5} W_{n}(\omega_{j} - \omega) f_{x}(\omega) d\omega$$

• where  $W_n(\omega) = |H_n(\omega)|^2$  and  $H_n(\omega)$  is the Fourier transform of the sequence  $h_t$ .

#### The Taper



Specifically,

$$H_n(\omega) = \frac{1}{\sqrt{n}} \sum_{t=1}^n h_t e^{-2\pi i \omega t}$$

When we put in the  $h_t$  above, we obtain a spectral window of

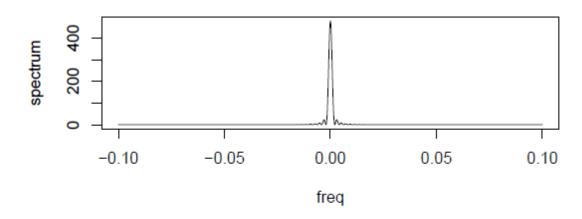
$$W_n(\omega) = \frac{\sin^2(n2\pi\omega)}{\sin^2(\pi\omega)}.$$

We set  $W_n(0) = n$ .

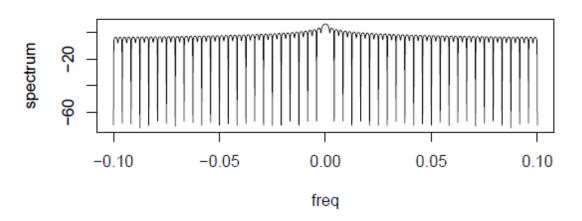
#### **Smoothing and Tapering**

 There are problems with this spectral window, namely there is too much weight on neighboring frequencies (sidelobes).

#### Fejer window, n=480



#### Fejer window (log), n=480

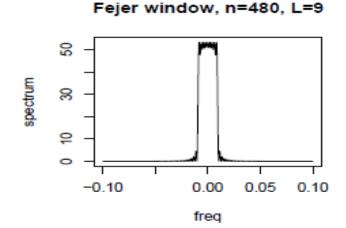


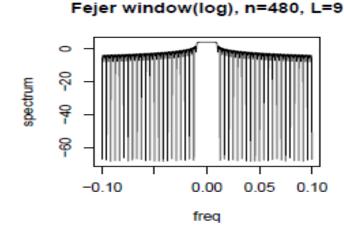


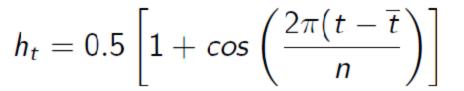
#### **Smoothing and Tapering**



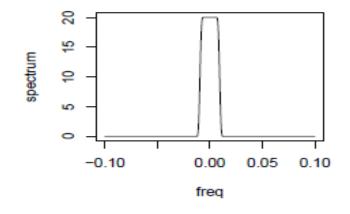
#### One way to fix this is to use a Cosine taper. We select a transform $h_t$ to be

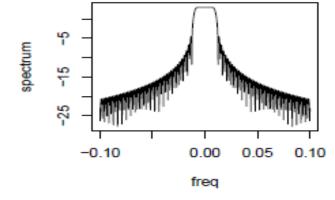






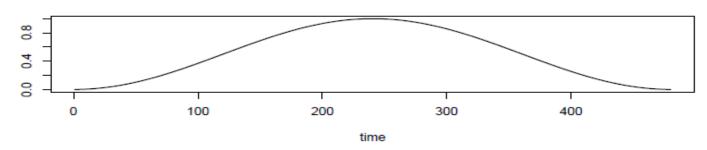
#### Full Tapering Window, n=480, L=9 Full Tapering Window(log), n=480, L



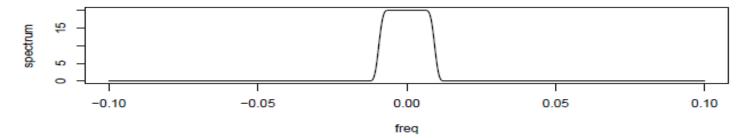


#### **Smoothing and Tapering**

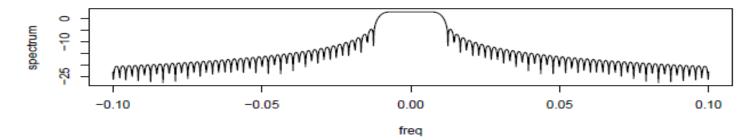
#### Full Tapering, n=480, transformation in time domain



#### Full Tapering Window, n=480, L=9



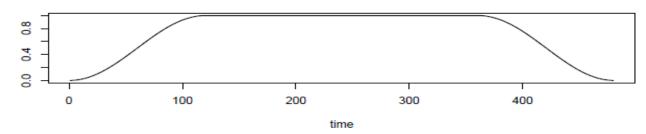
#### Full Tapering Window(log), n=480, L=9



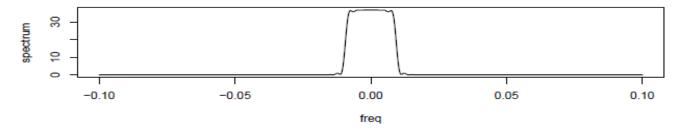


#### **Smoothing and Tapering**

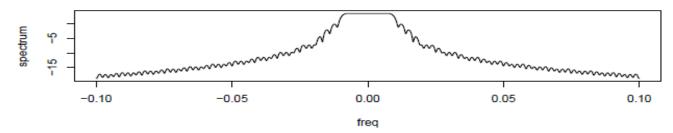
#### 50% Tapering, n=480, transformation in time domain



#### 50% Tapering Window, n=480, L=9



#### 50% Tapering Window(log), n=480, L=9





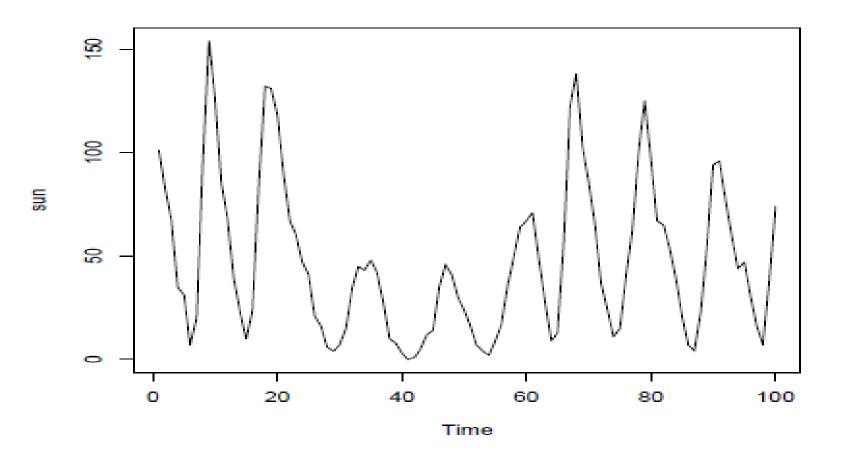
#### **Smoothing and Tapering**



- Smoothing introduces bias, but reduces variance.
- Smoothing tries to solve the problem of too many "parameters".
- Tapering decreases bias and introduces variance.
- Tapering attempts to diminish the influence of sidelobes that are introduced via the spectral window.

## **Examples**

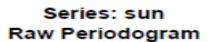
## Wolfer sunspots 1770-1869

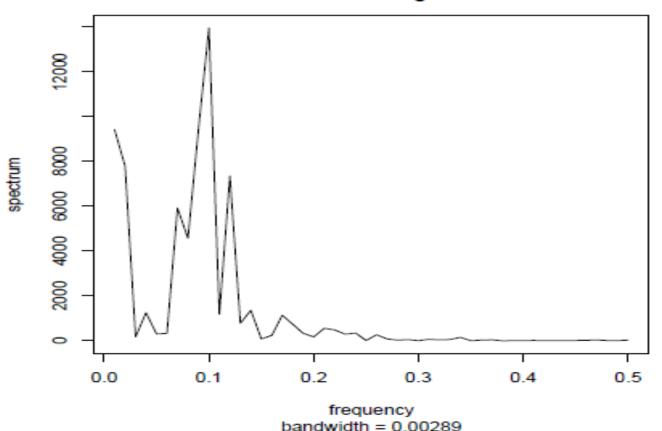




## **Examples**

# Raw Periodogram

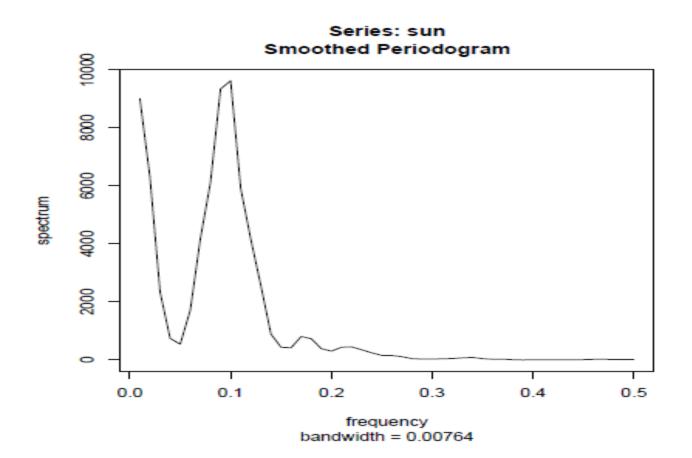






#### **Examples**

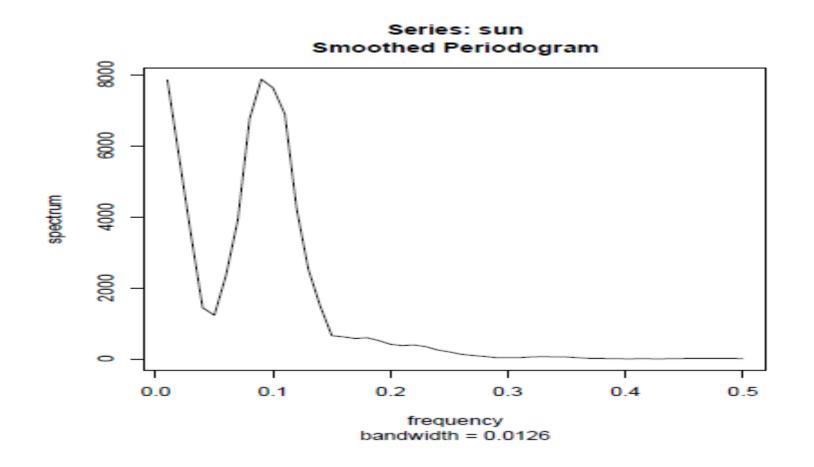
## Periodogram with Smoothing Window of 3





#### **Examples**

#### Periodogram with Smoothing Window of 5

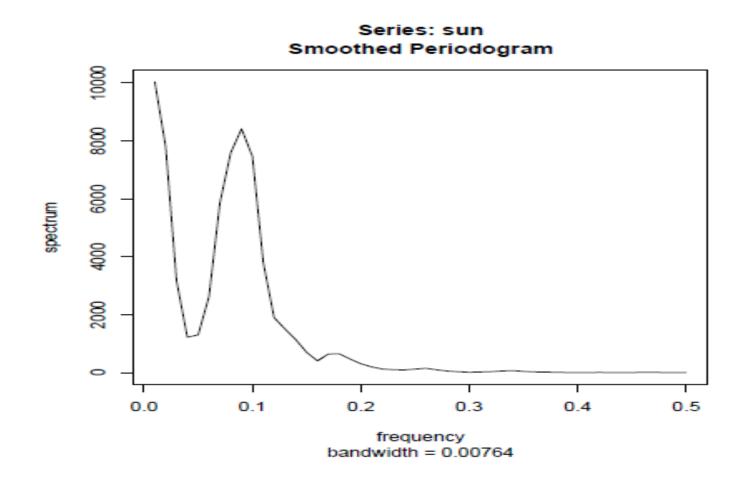




#### **Examples**



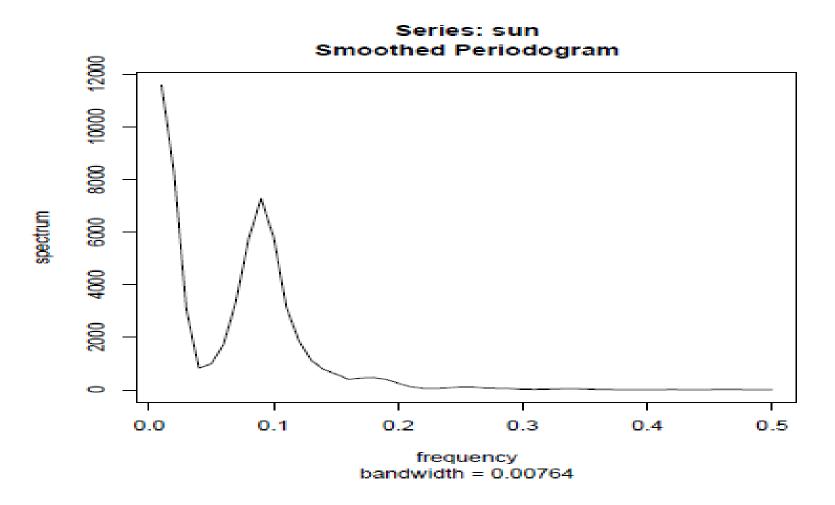
Periodogram with Smoothing Window of 3 with Some Tapering



#### **Examples**

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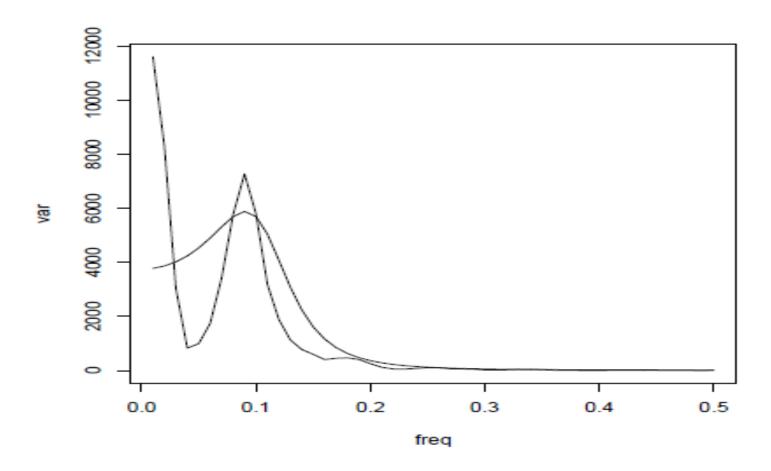
#### Periodogram with Smoothing Window of 3 with More Tapering



## **Smoothed Periodogram with ARMA Spectral Density**



The smoothed Periodogram of the sun spot data with the spectral density of the AR(3) model overlayed



#### **Dynamic Fourier Analysis**



- What can be done for non-stationary data?
- One approach is to decompose our time series as a sum of a non-constant (deterministic) trend plus a stationary "noise" term:
  - $X_t = \mu_t + y_t$
- What if our data instead appears as a stationary model locally, but globally the model appears to shift? One approach is to divide the data into shorter sections (perhaps overlapping) and
- This approach is developed in Shumway and Stoffer. One essentially looks at how the spectral density changes over time.

#### **Wavelets**



- We have been using Fourier components as a basis to represent stationary processes and seasonal trends.
- Since we are dealing with finite data, we must use a finite number of terms, and perhaps one could use an alternative basis.
- Wavelets are one option to accomplish this goal. They are particularly well suited to the same situation as Dynamic Fourier analysis.

#### **Introduction to Spectral Analysis**



#### **Spectral Analysis**

- 1. Spectral density: Facts and examples.
- 2. Spectral distribution function.
- 3. Wold's decomposition.

#### A periodic time series

Consider

• 
$$X_t = A \sin(2\pi vt) + B \cos(2\pi vt)$$

• = 
$$C \sin(2\pi vt + \varphi)$$
,

- where A, B are uncorrelated, mean zero, variance  $\sigma^2 = 1$ , and
- $C^2 = A^2 + B^2$ ,  $\tan \varphi = B/A$ . Then

• 
$$\mu_t = E[X_t] = 0$$

• 
$$\gamma(t, t+h) = \cos(2\pi vh)$$
.

• So  $\{X_t\}$  is stationary.



# An aside: Some trigonometric identities



$$\tan \theta = \frac{\sin \theta}{\cos s}$$

$$\sin^2 \theta + \cos^2 \theta = 1_{\theta}$$

$$\sin(a+b) = \sin a \cos b + \cos a \sin b,$$

$$\cos(a+b) = \cos a \cos b - \sin a \sin b.$$

## A periodic time series



- For  $X_t = A \sin(2\pi vt) + B \cos(2\pi vt)$ , with uncorrelated A, B
- (mean 0, variance  $\sigma^2$ ),  $\gamma(h) = \sigma^2 \cos(2\pi vh)$ .
- The auto covariance of the sum of two uncorrelated time series is the sum of their auto covariances. Thus, the auto covariance of a sum of random sinusoids is a sum of sinusoids with the corresponding frequencies:

$$X_{t} = \sum_{j=1}^{k} (A_{j} \sin(2\pi v_{j}t) + B_{j} \cos(2\pi v_{j}t)),$$

$$y(h) = \sum_{j=1}^{k} \sum_{j=1}^{k} \text{where } A_{j}, B_{j} \text{ are uncorrelated, mean zero,}$$

$$\alpha_{j}^{2} \cos(2\pi v_{j}h), \text{and } Var(A_{j}) = Var(B_{j}) = \sigma^{2}. j$$

## A periodic time series



$$X_{t} = \sum_{j=1}^{k} (A_{j} \sin(2\pi v_{j}t) + B_{j} \cos(2\pi v_{j}t)), \quad \gamma(h) = \sum_{j=1}^{k} \sigma_{j}^{2} \cos(2\pi v_{j}h).$$

- Thus, we can represent  $\gamma(h)$  using a Fourier series. The coefficients are the variances of the sinusoidal components.
- The spectral density is the continuous analog: the Fourier transform of γ.
- (The analogous spectral representation of a stationary process X<sub>t</sub> involves a stochastic integral—a sum of discrete components at a finite number of frequencies is a special case. We won't consider this representation in this course.)

# **Spectral density**

If a time series  $\{X_t\}$  has autocovariance  $\gamma$  satisfying

$$\sum_{h=-\infty}^{\infty} |\gamma(h)| < \infty$$
, then we define its spectral density as

$$f(v) = \sum_{h=-\infty}^{\infty} \gamma(h)e^{-2\pi i v h}$$

for 
$$-\infty < v < \infty$$
.



# **Spectral density: Some facts**



1. We have 
$$\sum_{h=-\infty}^{\infty}$$
  $: \gamma(h)e^{-2\pi i vh} : < \infty$ .

This is because  $|e^{i\theta}| = |\cos \theta + i \sin \theta| = (\cos^2 \theta + \sin^2 \theta)^{1/2} = 1$ , and because of the absolute summability of  $\gamma$ .

2. *f* is periodic, with period 1.

This is true since  $e^{-2\pi i vh}$  is a periodic function of v with period 1.

Thus, we can restrict the domain of f to  $-1/2 \le v \le 1/2$ . (The text does this.)

# **Spectral density: Some facts**



3. f is even (that is, f(v) = f(-v)). To see this, write

$$f(v) = \sum_{h=-\infty}^{\Sigma-1} \gamma(h)e^{-2\pi i v h} + \gamma(0) + \sum_{h=1}^{\infty} \gamma(h)e^{-2\pi i v h},$$

$$f(-v) = \sum_{h=-\infty}^{\Sigma-1} \gamma(h)e^{-2\pi i v (-h)} + \gamma(0) + \sum_{h=1}^{\infty} \gamma(h)e^{-2\pi i v (-h)},$$

$$= \sum_{h=1}^{\infty} \sum_{h=1}^{\infty} \sum_{h=1}^{\Sigma-1} \gamma(-h)e^{-2\pi i v h} + \gamma(0) + \sum_{h=1}^{\infty} \gamma(-h)e^{-2\pi i v h}$$

$$= f(v).$$

4. 
$$f(v) \ge 0$$
.

## **Spectral density: Some facts**



5. 
$$\gamma(h) = \int_{-1/2}^{1/2} e^{2\pi i v h} f(v) dv$$
.

$$\int_{-1/2}^{1/2} e^{2\pi i v h} f(v) dv = \int_{-1/2 = -\infty}^{1/2} \sum_{j=-\infty}^{\infty} e^{-2\pi i v (j-h)} \gamma(j) dv$$

$$= \int_{-1/2 = -\infty}^{\infty} \int_{-1/2 = -\infty}^{1/2} e^{-2\pi i v (j-h)} dv$$

$$= \gamma(j) \int_{-1/2}^{\infty} e^{-2\pi i v (j-h)} dv$$

$$= \gamma(h) + \sum_{\substack{j \neq j = -\infty \\ j \neq j = -\infty \\ k}} \frac{\gamma(j)}{2\pi i (j-h)} \cdot e^{\pi i (j-h)} - e^{-\pi i (j-h)}$$

$$= \gamma(h) + \sum_{\substack{j \neq j = -\infty \\ k}} \frac{\gamma(j) \sin(\pi(j-h))}{\pi(j-h)} = \gamma(h).$$

## **Example: White noise**



For white noise  $\{W_t\}$ , we have seen that  $\gamma(0) = \sigma^2$  and  $\gamma(h) = 0$  for  $h \neq 0$ 

Thus,

$$f(v) = \sum_{h=-\infty}^{\infty} \gamma(h)e^{-2\pi i v h}$$
$$= \gamma(0) = \sigma^{2}_{w}$$

 That is, the spectral density is constant across all frequencies: each frequency in the spectrum contributes equally to the variance. This is the origin of the name white noise: it is like white light, which is a uniform mixture of all frequencies in the visible spectrum.

# **Example: AR(1)**



For 
$$X_t = \varphi_1 X_{t-1} + W_t$$
, we have seen that  $\gamma(h) = \sigma^2 \varphi_w^{|h|} / (1 - \varphi^2)$ . Thus, 
$$f(v) = \sum_{h=-\infty}^{\infty} \gamma(h) e^{-2\pi i v h} = \frac{\sigma_w^2}{1 - \varphi_1^2} \sum_{h=-\infty}^{\infty} \varphi_1^{|h|} e^{-2\pi i v h}$$

$$= \frac{\sigma_{w}^{2}}{1 - \varphi_{1}^{2}} \cdot \sum_{h=1}^{\infty} \varphi_{1}^{h} \cdot e^{-2\pi i v h} + e^{2\pi i v h} \sum_{h=1}^{\infty} \varphi_{1}^{h} \cdot e^{-2\pi i v h} + e^{2\pi i v h}$$

$$= \frac{\sigma_{\rm w}^2}{1 - \varphi_1^2} \cdot 1 + \frac{\varphi_1 e^{-2\pi i v}}{1 - \varphi_1 e^{-2\pi i v}} + \frac{\varphi_1 e^{2\pi i v}}{1 - \varphi_1 e^{2\pi i v}} \sum_{n=0}^{\infty} \frac{1}{1 - \varphi_1 e^{2\pi i v}} \frac{1}{1 - \varphi_1 e^{2\pi i v}}$$

$$= \frac{\sigma_{\rm w}^2}{(1-\varphi_1^2)} \frac{1-\varphi_1 e^{-2\pi {\rm i} v} \varphi_1 e^{2\pi {\rm i} v}}{(1-\varphi_1 e^{-2\pi {\rm i} v})(1-\varphi_1 e^{2\pi {\rm i} v})}$$

$$= \frac{\sigma_{\rm w}^2}{1 - 2\varphi_1 \cos(2\pi v) + \varphi_1^2}.$$

# **Examples**

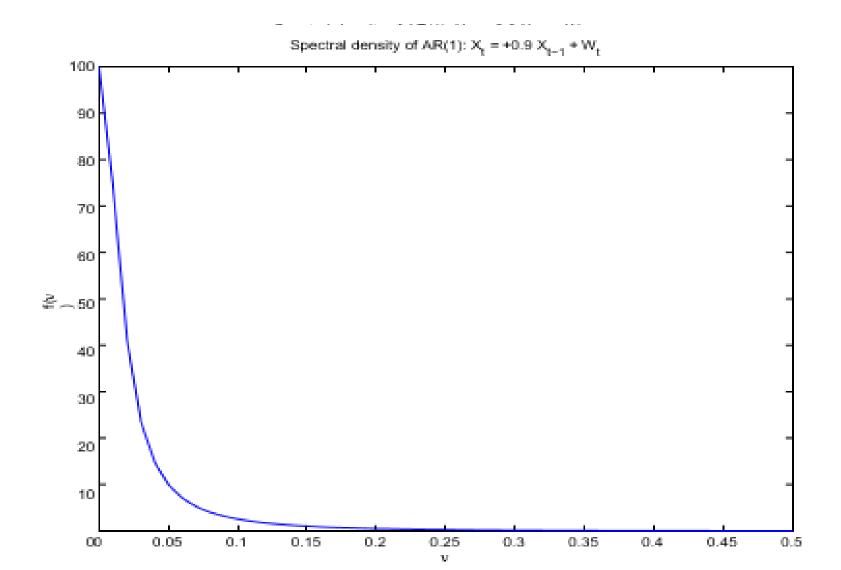


White noise: 
$$\{W_t\}$$
,  $\gamma(0) = \sigma^2_{w}$  and  $\gamma(h) = 0$  for  $h = 0$   
 $f(v) = \gamma(0) = \sigma^2_{w}$ .

AR(1):  $X_t = \varphi_1 X_{t-1} + W_t$ ,  $\gamma(h) = \sigma^2 \varphi_w^{|h|} / (1 - \varphi^2)$ . 1
$$f(v) = \frac{\sigma_w^2}{1 - 2\varphi_1 \cos(2\pi v) + \varphi_1^{-2}}$$

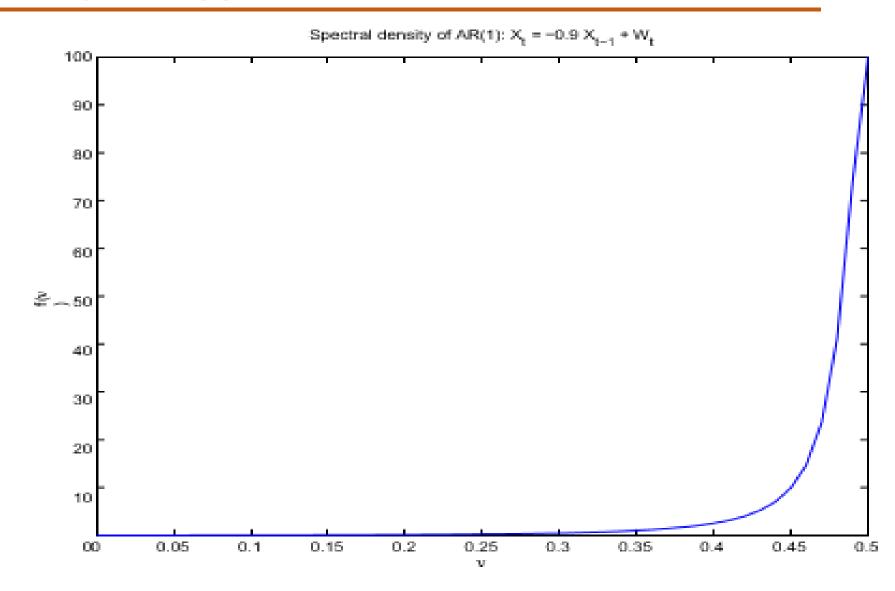
- If  $\varphi_1 > 0$  (positive autocorrelation), spectrum is dominated by low frequency components—smooth in the time domain.
- If  $\varphi_1 < 0$  (negative autocorrelation), spectrum is dominated by high frequency components—rough in the time domain.

# **Example: AR(1)**





# **Example: AR(1)**





## A periodic time series

Consider

• 
$$X_t = A \sin(2\pi vt) + B \cos(2\pi vt)$$

• = 
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• 
$$\gamma(t, t+h) = \cos(2\pi vh)$$
.



## A periodic time series

Consider

• 
$$X_t = A \sin(2\pi vt) + B \cos(2\pi vt)$$

• = 
$$C \sin(2\pi vt + \varphi)$$
,

- where A, B are uncorrelated, mean zero, variance  $\sigma^2 = 1$ , and
- $C^2 = A^2 + B^2$ ,  $\tan \varphi = B/A$ . Then

• 
$$\mu_t = E[X_t] = 0$$

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$$\gamma(t, t+h) = \cos(2\pi vh)$$
.





# Artificial Intelligence for Time-Series and Sequential Decision Making

## **Outline**

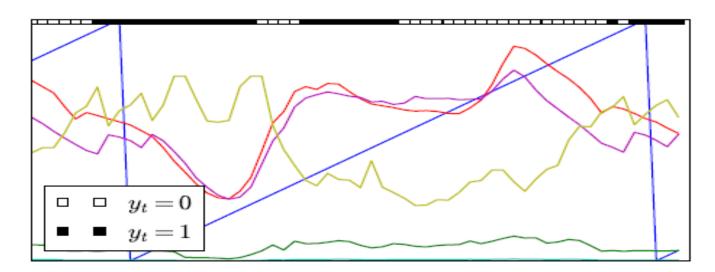


- Time Series
- Filtering
- Forecasting
- Embedding
- Classifier and Repressor Chains
- Sequential Decision Making

## **Time Series**



- $X_1, X_2, ..., X_t, ...$
- Generated by some process  $\mathbf{x} \sim p(X)$  in the domain we are interested in.
- Measurements may be continuous,  $\mathbf{x}_t \in \mathbb{R}^D$  or discrete,  $\mathbf{x}_t \in \mathbb{N}_+^D$ ; across time t.
- May be associated with unobserved signal  $\mathbf{y}_t$ .



Time series  $\mathbf{x}_t \in \mathbb{R}^{\mathbf{5}}$  associated with state  $y_t \in \{0, 1\}$ .

## Examples of time series data:

- Electricity demand for a city
  - Sensor measurements on equipment in an aircraft
     Number of calls to an insurance service
  - Light-sensor measurements (and movement through a room)
  - Smartphone GPS and signal strength measurements of urban travellers (and their predicted trajectory)
  - EEG and ECG signals obtained during sleep
     Cellular growth in trees



Environmental measurements (temperature, humidity)



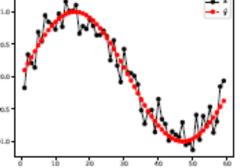
## **Time Series Tasks**

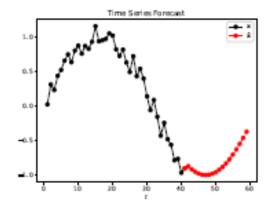


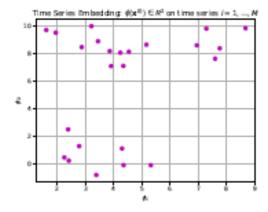
- Filtering (estimate)  $y_1, \ldots, y_{t-1}, y_t$  from observations
- $X_1, \ldots, X_{t-1}, X_t$
- Forecasting (*predict*)  $\mathbf{x}_{t+1}$ ,  $\mathbf{x}_{t+2}$ , . . . from time t. Embedding: Describe a time series  $\{\mathbf{x}_1, \ldots, \mathbf{x}_T\}$  as a vector  $\boldsymbol{\varphi} = [\varphi_1, \ldots, \varphi_N]$

of fixed length N.









Motif extraction

Clustering

- Novelty/anomaly detection
- Query by content

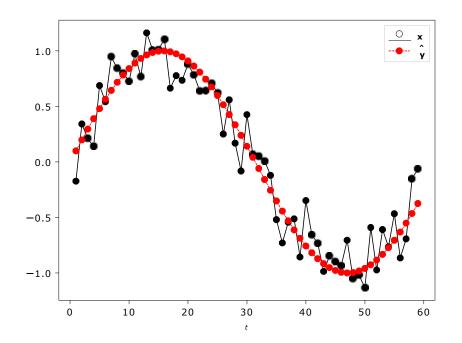
# **Filtering**

Given observations (time series) $\{x_1, x_2, \dots, x_t, \dots\}$ 

we want a model f to predict corresponding

$$\{^{\wedge}y_1, ^{\wedge}y_2, \ldots, ^{\wedge}y_t, \ldots\}$$

Time Series Filtering





#### **Traditional Methods**



- Finite impulse response (FIR) filter
- Moving average, exponential smoothing (low-pass filters) Kalman filter, particle filters
- ARIMA (Auto-Regressive Integrated Moving Average)

$$y_1$$
 $y_2$ 
 $y_3$ 
 $y_4$ 
 $x_1$ 
 $x_2$ 
 $x_3$ 
 $x_4$ 

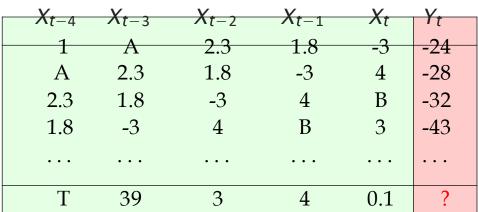
• 
$$y_t = f(w_1 x_{t-0} + \cdots + w_k x_{t-k}) + s_t$$

- with some weights  $\mathbf{w} = [w_1, \dots, w_k]$  (window size k). This is a convolution with kernel  $\mathbf{w}$ .
- Robust and well-understood
- Need to be hand-crafted, calibration by domain expert else not suitable for multiple dimensions; complex problems

## **Machine Learning for Filtering**

• Given training data, we can design a machine learning approach (e.g., artificial

neural networks, decision trees, . . . ), on



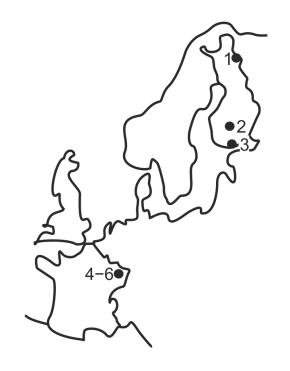
i.e., model 
$$y_t = f(x_{t-4}, \dots, x_t; \theta) + s$$

The decision making and interpretation is relegated to the learner.



# **Example: Predicting Cellular Growth in Scots Pine**

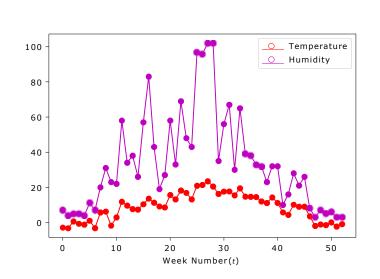
- 6 sites in Finland and France, of Scots pine
- Interested in modelling cellular growth under different latitude, altitude, . . .
- Models must be carefully crafted, parametrized, and adjusted by domain experts, per site.

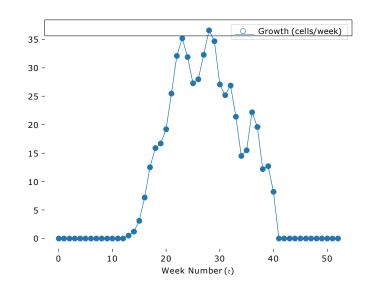




# **Example: Predicting Cellular Growth in Scots Pine**







- Environmental measurements (temperature, humidity, . . . ).
- Some cell-growth data (from micro-core samples and counts during growth season) over
   3–4 years

## **Outline**



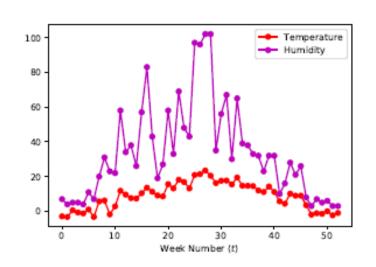
Domain experts were

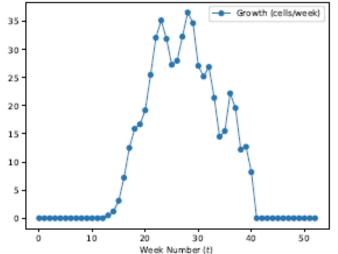
functions, e.g., growth

timing variable (left) and

using numerous

heat sum (right),





Σ

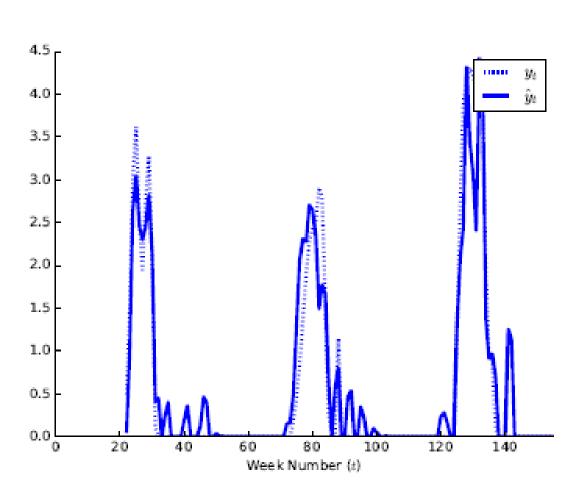
e.g., where  $\tau_t$  = temperature and week t,  $\sum_{t=1}^{\infty} \frac{1}{1+\exp(-\beta \tau_t)}$  and t, t are per-site parameters.

Assembled into a differential equation

About 4-5 parameters to be hand-selected *per site* 

#### Outline

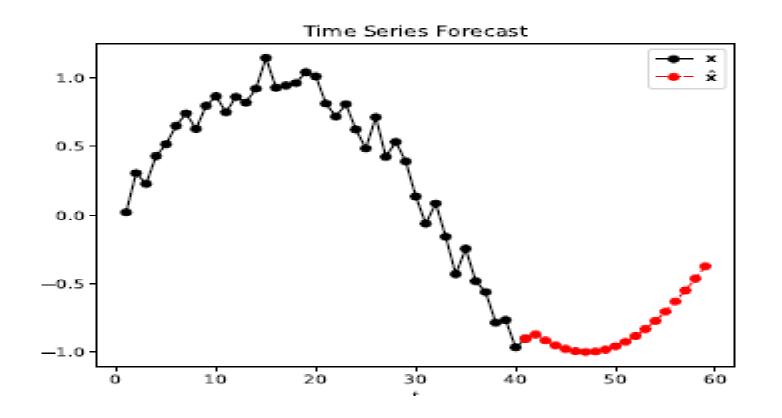




- Data-driven model to parametrize and combine expert-inspired functions, for each site
- Achieved accuracy to within a fraction of a cell per week
- Using decision tree learners,
   interpretation was possible (e.g., how
   far back to take into account
   temperature measurements)

# **Time-Series Forecasting (Prediction)**

Given  $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_t$ we want a model fto predict  $^{\mathbf{x}_{t+1}, ^{\mathbf{x}_{t+2}, \dots, ^{\mathbf{x}_{t+A}}}$ 





#### **Traditional Methods**



- Naive Forecasting (rain today = rain tomorrow)  $\hat{x}_{t+1} = x_t$
- Moving average (mean of last k observations)

$$\hat{x}_{t+1} = \mathbf{w}^{\mathsf{T}} \mathbf{x}$$

$$\mathbf{x} = [x_{t-(k-1)}, \dots, x_t], \ \mathbf{w} = [\frac{1}{k}, \dots, \frac{1}{k}].$$

on window

Auto-regressive linear fit on previous k points, and extrapolate.

# **Machine Learning for Forecasting**



Formulating a data-driven supervised learning problem:

$X_{t-AE}$	V	V	V	ν.	V
^t−Æ	Λ	$X_{t-2}$	$\lambda t-1$	$\wedge t$	$X_{t+1}$
1	Λ	2 3	1.2	3	4
1	$\Gamma$	2.0	1.0	-3	<b>T</b>
A	2.3	1.8	<b>-</b> 3	4	В
2.3	1.8	-3	4	В	3
1.8	-3	4	В	3	-7
				• • •	• • •
T	39	3	4	0.1	?

$$\hat{\mathbf{x}}_{t+1} = f(\mathbf{x}_{t-4}, \ldots, \mathbf{x}_t; \theta)$$

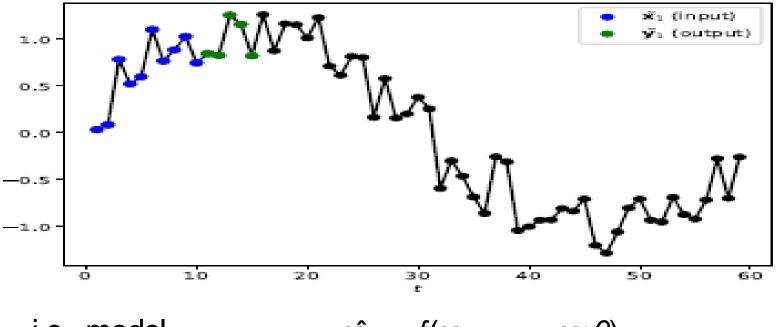
(we can plug in  $x_{t+1}$  and propagate); or estimate a window directly:

$$x^{\hat{t}+1},...,x^{\hat{t}+k}=f(x_{t-4},...,x_t)$$

## **Machine Learning for Forecasting**



• Formulating a data-driven supervised learning problem:



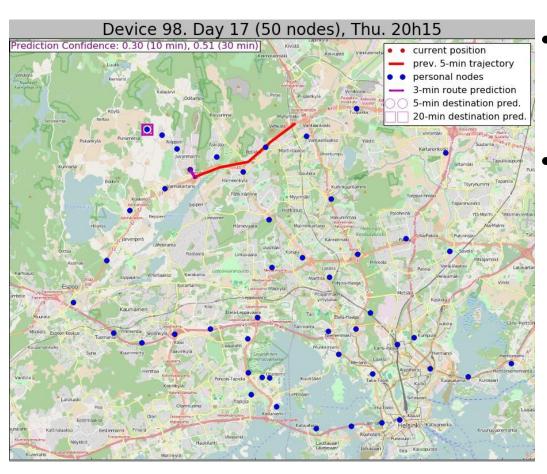
i.e., model  $\hat{x}_{t+1} = f(x_{t-4}, \dots, x_t; \theta)$ 

(we can plug in  $\hat{x}_{t+1}$  and propagate); or estimate a window directly:

$$\hat{x}_{t+1},\ldots,\hat{x}_{t+k}=f(x_{t-4},\ldots,x_t)$$

# **Machine Learning for Forecasting**



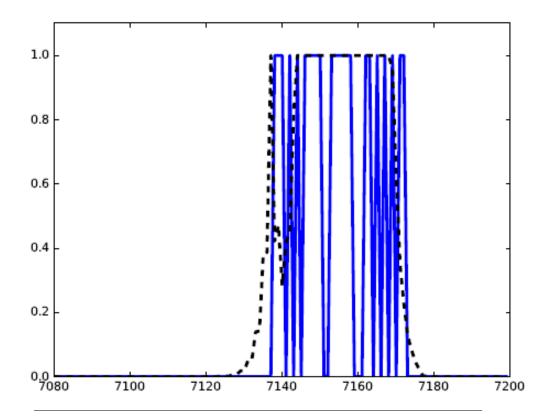


- Collected data of travellers<sup>1</sup>: GPS coordinates, signal strength, battery level, current time, . . .
- Predict future trajectory from current trajectory

<sup>&</sup>lt;sup>1</sup>All participants volunteered to install App; share data Work with Jaakko Hollmèn et al. @Aalto University

## **Example: Predictive Maintenance of Aircraft**

- Sensor readings from aircraft and textual description of observations
- Predict warnings/required replacement of components

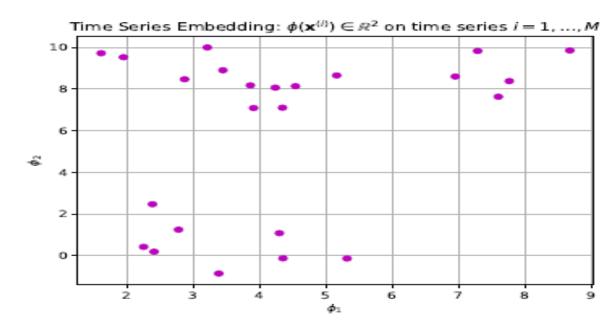




## **Embedding Time Series**



We seek to turn variable-length time series  $\{\mathbf{x}_1^{(i)}, \dots, \mathbf{x}_{T_i}^{(i)}\}_{i=1}^{M}$  into fixed-length vectors  $\boldsymbol{\varphi}^{(i)} = [\varphi_1, \dots, \varphi_{\nu_J}]$ .



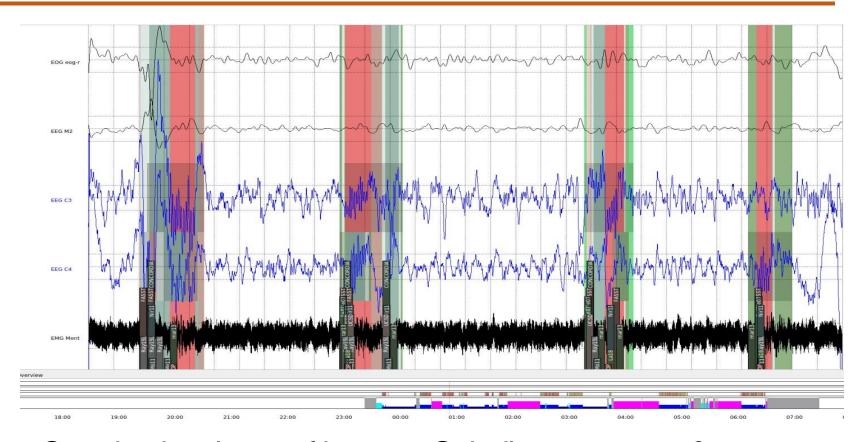
• This lets us compare and cluster time series/look for anomalies, (and classify, if we have the label): measure similarity/distance between  $\varphi(\mathbf{x}^{(i)})$  and  $\varphi(\mathbf{x}^{(2)})$ .

## **Example: Modelling and Treating Chronic Insomnia**

- Goal: (semi-)automate clinical assessment; what kind of insomnia + treatment recommendation.
- Data from patients:
  - Psychological questionnaires (MMPI, CAS) EEG and ECG data overnight
  - Some labels: follow-up tests/questionnaires and *biofeedback* results (some patients found success without pharmaceutical intervention, others not)
- Questionnaire data: can take 'standard' machine learning approach,  $f: X \to Y$ , and inspect feature importance, statistical correlation wrt to label variable (extent of insomnia, and improvement); cluster into groups, etc.
- Time-series data: different lengths, contains artifacts, subjects fall asleep at different times, . . . . How to compare?

## **Example: Modelling and Treating Chronic Insomnia**

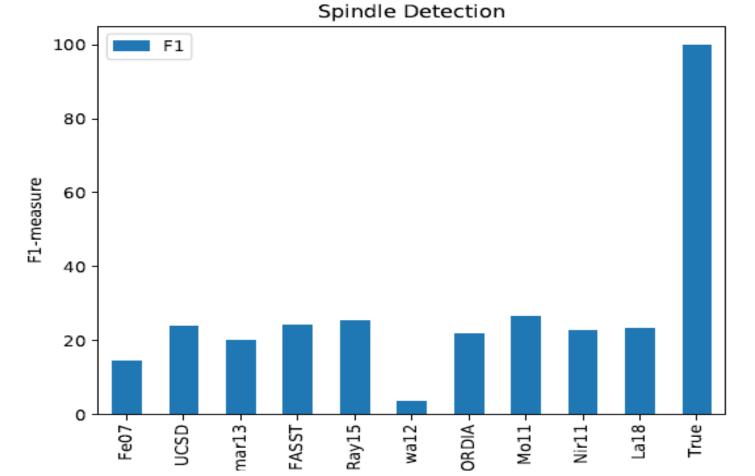




- Certain signals are of interest: Spindles,  $\alpha$ -waves,  $\beta$ -waves, . . . Simple embeddings, e.g.,
- $\varphi(\mathbf{x}^{(i)}) = [\text{spindles/hour}, \text{ avg freq of spindle}]$ . Detection and labelling by an expert is labour intensive.

### **Outline**

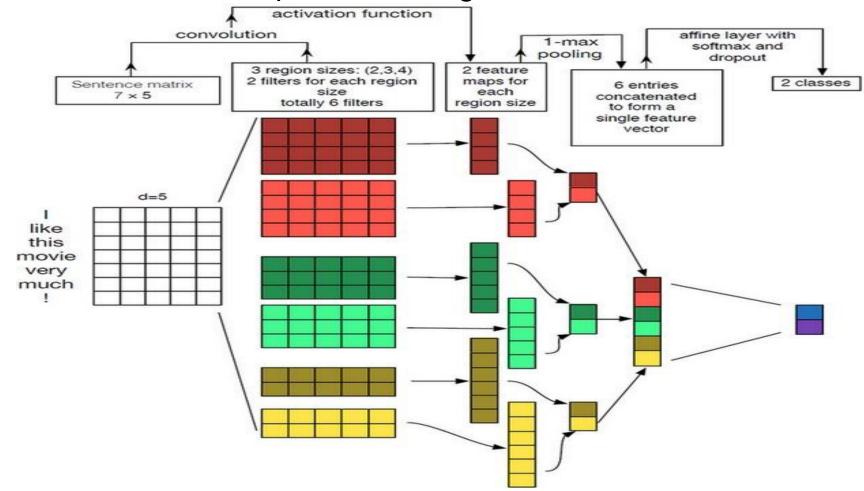
There exist many rule-based methods, e.g., wavelet analysis But predictive performance is insufficient in many practical settings





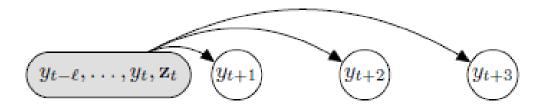
### **Deep learning**

- Many current solutions are inspired by / related to NLP.
- Similar to a 'simple' embedding, but more data-driven.

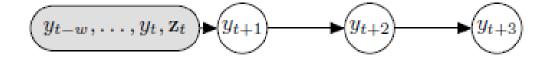




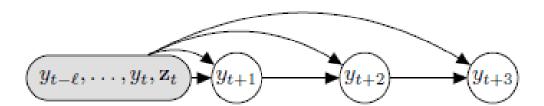
# **Multi-Step-Ahead Forecasting**



#### Direct



Iterated

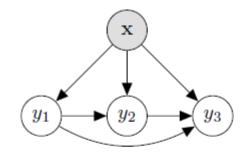


Classifier/Regressor Chain cascade

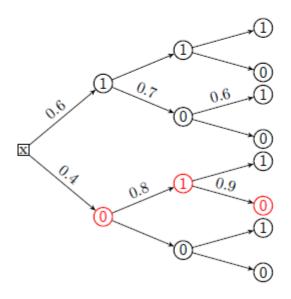


### **Classifier Chains**





For example, where each  $y_t \in \{0,1\}$ 



- Predictions become input, across a cascade/chain
- Efficient
- Probabilistic interpretation:

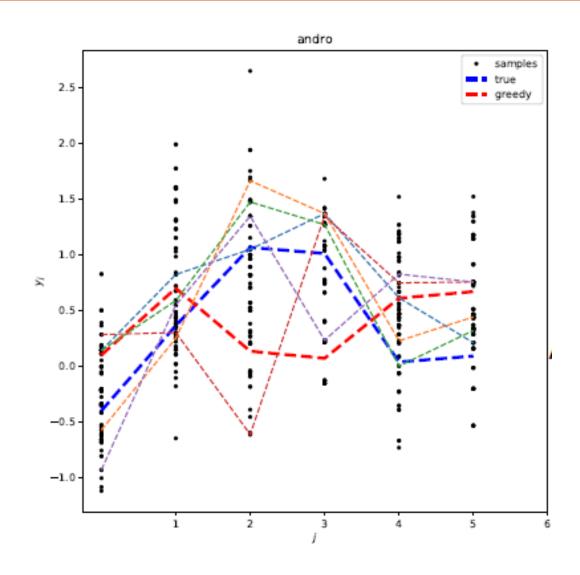
$$P(\mathbf{y}|\mathbf{x}) = \prod_{t=1}^{T} P(y_t|\mathbf{x}, y_1, \dots, y_{t-1})$$

$$\mathbf{\hat{y}} = f(\mathbf{x}) = \underset{\mathbf{y} \in \{0,1\}^3}{\operatorname{argmax}} P(\mathbf{y}|\mathbf{x})$$

- Search probability tree (for best prediction) with Al-search techniques (Monte-Carlo search, beam search, A\* search, . . . )
- Explore structure

# **Regressor Chains**





- e.g., where  $y \in \mathbb{R}^6$ ,
  - Sample down the chain
  - $y_{t+1} \sim p(y_{t+1}|y_1, \ldots, y_t, \mathbf{x})$
  - More samples = more hypotheses
  - Consider different loss functions
- Applications:
  - Multi-output regression
     Tracking
  - Forecasting

# **One-Step Decision Theory**



Under uncertainty, we wish to assign  $y = f^*(\mathbf{x})$ , the best label/hypothesis,  $y \in Y$ , given  $\mathbf{x} \in \mathbb{R}^D$ 

# .Minimizing conditional expected loss

$$f^* = \underset{f \in \mathcal{F}}{\operatorname{argmin}} \sum_{y \in \mathcal{Y}} \ell(f(\mathbf{x}), y) P(y|\mathbf{x})$$
$$\mathbb{E}_{Y \sim P(Y|\mathbf{x})} [\ell(\hat{y}, Y)|\mathbf{x}]$$

under loss function A, which describes our preferences. In the case of 0/1 loss (1 if  $y f = \hat{y}$ , else 0),

#### **Maximum a Posteriori**

$$y^* = \underset{y \in \mathcal{Y}}{\operatorname{argmax}} p(\mathbf{x}|y)P(y) = \underset{y \in \{0,1\}}{\operatorname{argmax}} P(y|\mathbf{x})$$

We can estimate P from the training data.

### **Expected Utility**



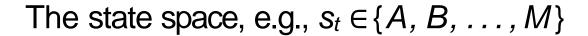
- An intelligent agent wishes to make a decision to achieve a goal.
  - The decision which involves the least risk. Another way of looking at the problem: utility.
  - A rational agent maximizes their expected utility, not necessarily a simple payoff (e.g.,
  - amount of money):

Expected Utility 
$$U(y) = \sum_{y \in \mathcal{Y}} u(y)p(y)$$

- with satisfaction/utility u(y) for outcome y. Different agents may have different utility functions, even when 'payoff' is the same item. Instead of labels given input, we can deal with actions given evidence and belief.
  - A risk-prone agent will tend to gamble higher stakes A conservative (riskadverse) agent will not
  - A risk-neutral agent only cares about payoff y directly

### What about sequential decisions?

In a Deterministic Environment (e.g., board games – chess, etc.)



An initial state, e.g.,  $s_0 = S$ 

A goal state, e.g.,  $s_t = M$ 

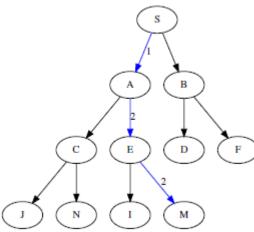
A set of actions, e.g.,  $a_t \in \{1, 2\}$ 

A cost for each branch, e.g., Cost(S, A) = 1

It's just a search! Al-search techniques applicable (DFS, A\*, .







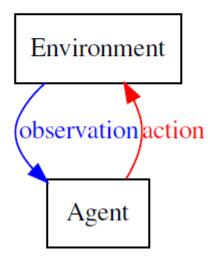
# Markov Decision Processes (MDP)

PES UNIVERSITY ONLINE

MDPs are models that seek to provide optimal solutions for stocastic sequential

decision problems.

MDP = Markov Chain + One-step Decision Theory



#### **Outline**

#### Now we have a model with

 $P(s^{j}|s, a)$  transition function

 $R(s^{j}, a, s)$  reward function

Objective: obtain a policy

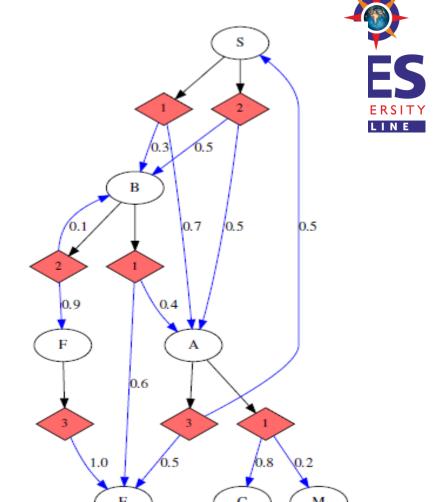
$$\pi: \mathcal{S} \mapsto \mathcal{A}$$

which maximizes expected reward:

$$\mathbb{E}[R_0|s_0=s] = \mathbb{E}\left[\sum_{t=0}^{\infty} \gamma^t r_t(s_t, a_t)\right]$$

solution can be found via dynamic programming!

Just need the model . . .



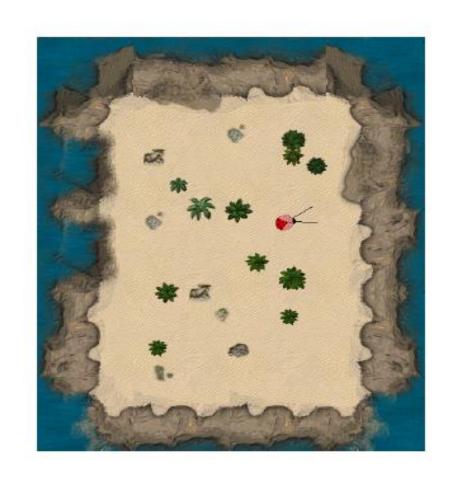
### **Reinforcement Learning**

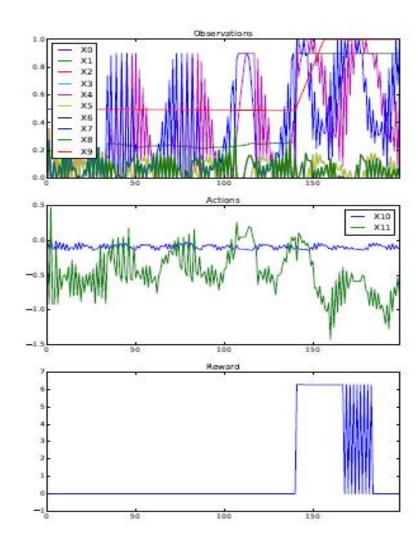
- We don't have the model!
- Don't have transition/reward functions.
- No input-output training pairs, just reward signal.
- The agent needs to experiment! Exploration vs exploitation. Deep neural net can learn a model
- ...over millions of iterations. Emerging applications:
  - Gameplay
  - Robotics (usually trained in simulation) Parameter-tuning, etc. (as a tool)
- Transfer learning is promising



# Outline







### References



### **Text Book:**

"Business Analytics, The Science of Data-Driven Making", U. Dinesh Kumar, Wiley 2017

# **Image Courtesy**



https://www.abs.gov.au/websitedbs/D3310114.nsf/home/Time+Series+Analysis:+The+Basics

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# **THANK YOU**

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