Time Series Analysis

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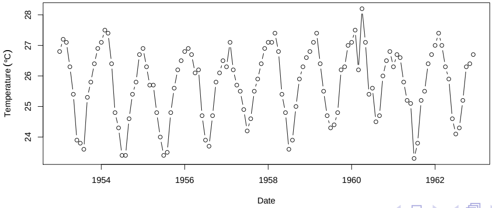
Outline

Introduction

- A Time Series is a collection of observations made sequentially through time
- A continuous time series is one where observations are made continuously through time
  - *Continuous* refers to the measurement of observations not the type of variable that is observed
- A discrete time series is one where the observations are taken at specific time points
  - Sampling points are generally equally spaced in time
- **deterministic** vs. **stochastic**



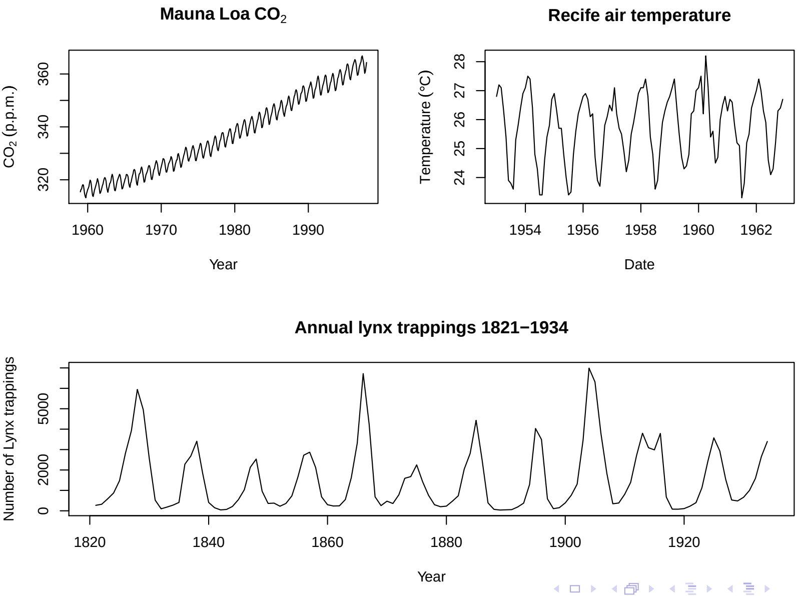
Objectives of time series analysis

- Description
  - Time plots of observations; a simple way to describe temporal patterns in a time series
  - regular **seasonal effects** or **cyclicity**, presence of a **trends**, **outliers**, **sudden changes** or **breaks**
- Explanation
  - Observations on one variable in time may be used to explain the variation in another series
  - May help understand the **mechanisms** that generated a given time series
- Prediction
  - Given an observed time series one may want to predict future values of the series — also called **forecasting**
- Control
  - Time series often collected to improve *control* over a physical process
  - Monitoring to alert when conditions exceed an *a priori* determined threshold

Descriptive Techniques — types of variations

- Traditional time series methods are often concerned with decomposing variation in a time series in components representing **trend**, **seasonal** or other **cyclic** variation. Remaining variation is attributed to **irregular** fluctuations
- **Seasonal variation**
  - Variation that is **annual** in period
  - Easily estimated if of interest, or removed — deseasonalised
- **Cyclic variation**
  - Variation that is **fixed** in period — diurnal temperature variation
  - Oscillations without a fixed period but are predictable to some extent
- **Trend**
  - **Long term change in the mean level**
  - Trend is a function of the length of the record
- Other **irregular** fluctuations
  - Variation remaining after removal of trend and cyclic variations
  - May or may not be **random**

Types of variation



Transformations 1

- Transform time series for similar reasons as for any other type of data
  - to stabilise the variance
    - If trend present and variance of series increases with mean; $\log$ transform
    - If no trend but variance increases with mean then a transformation is of little use
  - to make seasonal component additive
    - If seasonal component increases with the mean in presence of a trend, said to be **multiplicative**
    - Transform (e.g. $\log$) to make the seasonal component constant from year to year; **additive**
    - Transformation will only stabilise the variance if the error term is also multiplicative
  - to make the data normally distributed
    - Model building usually assumes data are normally distributed
    - 'spikes' in the time plot will show up as skew in the distribution — can be difficult to remove
- Inherently difficult, however...

Transformations 2

- Seasonal components
  - Additive: $X_t = m_t + S_t + \varepsilon_t$
  - Multiplicative: $X_t = m_t S_t + \varepsilon_t$
  - Multiplicative: $X_t = m_t S_t \varepsilon_t$
  - Only the latter will be improved by a transformation
- A transformation that makes the seasonal component additive may fail to stabilise the variance
- As such we may not be able to achieve all the aims on previous slide
- A model constructed on transformed data less useful than one fitted to raw data
  - May be more difficult to interpret to models fitted to transformed data
  - Forecasts need to be back transformed
- Avoid transformation where possible, though use them if they make physical sense (e.g. $\log$ or square root for abundances or percentages)

Filtering

- A **linear filter** is used to convert a times series $\{x_t\}$ into another $\{y_t\}$ via a linear operation

$$y_t = \sum_{r=-q}^{+s} a_r x_{t+r}$$

- $\{a_r\}$ are a set of weights
- To smooth out local fluctuations and estimate local mean, choose $\{a_r\}$ so $\sum a_r = 1$; **moving average**
- Simple moving average; $a_r = 1/(2q+1)$ for $r = -q, \ldots, +q$ so that

$$y_t = \frac{1}{2q+1} \sum_{r=-q}^{+q} x_{t+r}$$

- Moving average over monthly data has 13 weights, and is symmetric $\{1/24, 1/12, \ldots, 1/12, 1/24\}$
- Apply other functions; for example moving SD to measure changes in variance of $\{x_t\}$

Differencing

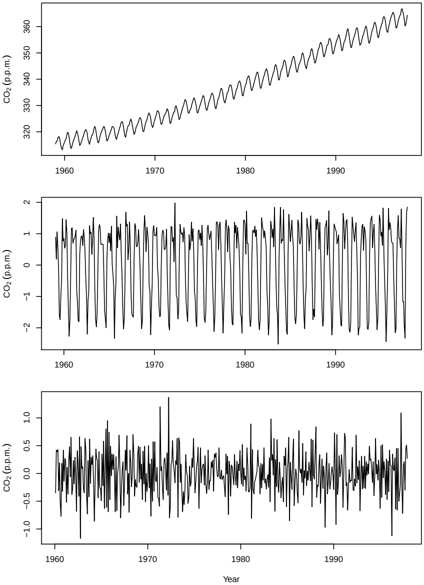
- **Differencing** is a special type of filtering useful for removing trends and seasonality to produce a stationary series
- First order differencing; new series formed by subtracting x_{t-1} from x_t

$$\nabla x_t = x_t - x_{t-1}$$

- **Seasonal differencing**; e.g. for monthly data

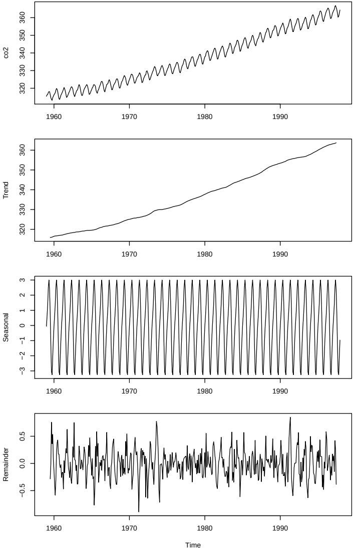
$$\nabla_{12} x_t = x_t - x_{t-12}$$

- Raw CO_2 data (upper); $\nabla_1 CO_2$ (middle); $\nabla_1 \{\nabla_{12} CO_2\}$ (lower)



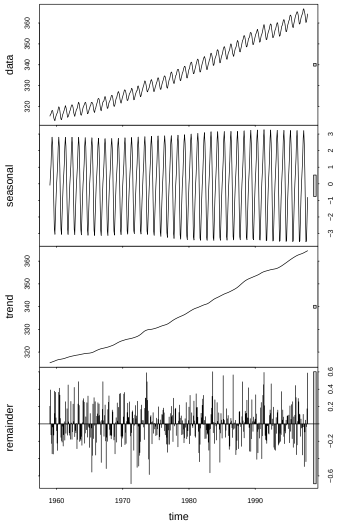
Decomposing time series — classical approach

- Decompose series into **trend**, **seasonal**, and **random** components
- $x_t = \mathrm{Trend}_t + \mathrm{Seasonal}_t + \mathrm{remainder}_t$
- Moving average filter used to identify the trend
- Compute seasonal component as the average over the detrended series of each period (e.g. month or quarter)
- Seasonal component is formed from the period averages repeated to match the length of the original series
- Random component is the remainder once the trend and the seasonal components have been subtracted from the original series



Decomposing time series — LOESS approach (STL)

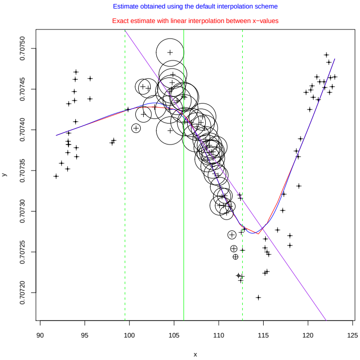
- Decompose series into **trend**, **seasonal**, and **random** components using LOESS
- The seasonal component is found by LOESS smoothing of the seasonal sub-series (e.g. series of January values)
- x_t is deseasonalised and this series is smoothed to find the trend
- Overall level subtracted from seasonal series and added to the trend
- This process is repeated a few times until convergence
- Remainder is the residuals of the trend + seasonal components



Lowess — Locally weighted regression

Locally weighted regression scatterplot smoother

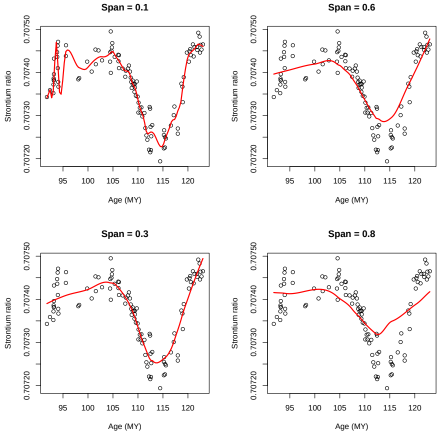
- Decide how smooth relationship should be (span or size of bandwidth window)
- For target point assign weights to observations based on adjacency to target point
- Fit linear (polynomial) regression to predict target using weighted least squares; repeat
- Compute residuals & estimate robustness weights based on residuals; well-fitted points have high weight
- Repeat Loess procedure with new weights based on robustness and distance weights



Try different span and degree of polynomial to optimise fit

Lowess — Locally weighted regression

- Two key choices in Loess
- α is the span or bandwidth parameter, controls the size of the window about the target observation
- Observation outside the window have 0 weight
- Larger the window the more global the fit — smooth
- The smaller the window the more local the fit — rough
- λ is the degree of polynomial using the the weighted least squares
- $\lambda = 1$ is a linear fit, $\lambda = 2$ is a quadratic fit



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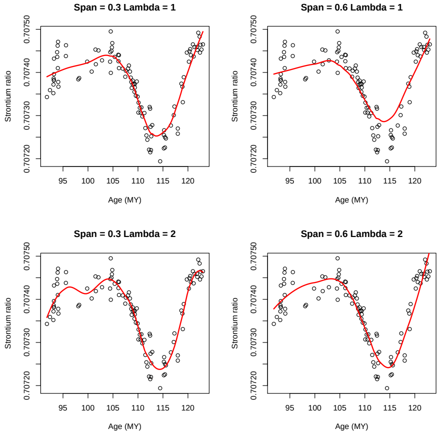


Lowess — Locally weighted regression

"In any specific application of LOESS, the choice of the two parameters α and λ must be based upon a combination of judgement and trial and error. There is no substitute for the latter"

Cleveland (1993) Visualising Data. AT&T Bell Laboratories

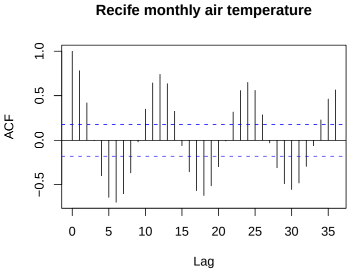
- CV can be used to optimise α and λ to guard against overfitting the local pattern by producing too rough a smoother or missing local pattern by producing too smooth a smoother
- Loess is perhaps most useful as an exploratory technique as part of EDA
- Cleveland, W.S. (1979) J. Amer. Stat. Assoc. **74**, 829–836
- Cleveland, W.S. (1994) The Elements of Graphing Data. AT&T Bell Laboratories
- Efron, B & Tibshirani, R (1981) Science **253**, 390–395

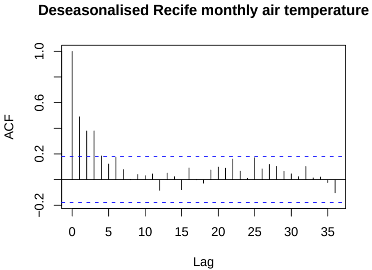
Autocorrelation function

- **Sample autocorrelation coefficients** are an important guide to the properties of time series
- Measure the correlation between observations at different distances apart

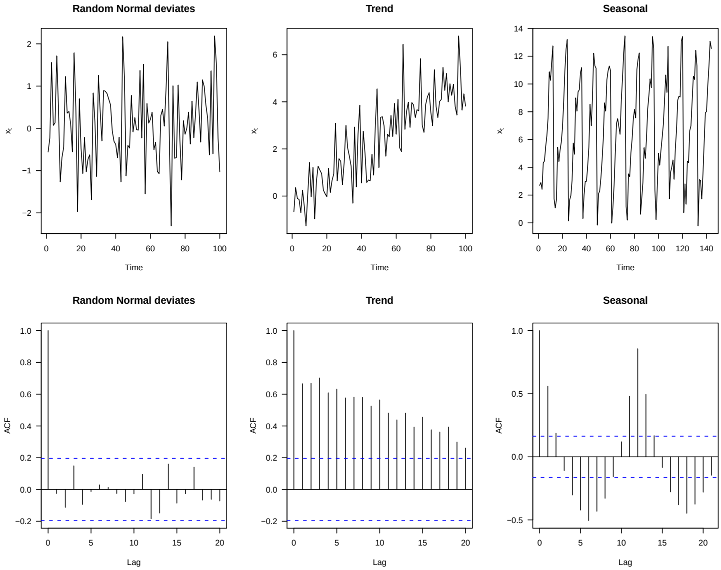
$$r_k = \frac{\sum_{t=1}^{n-k} (x_t - \bar{x})(x_{t+k} - \bar{x})}{\sum_{t=1}^{n} (x_t - \bar{x})^2}$$

- Computed for small number of lags k
- Use min. of 36 lags to view several seasonal cycles
- Dashed lines drawn at $\pm 2/\sqrt{n}$ enclose insignificant correlations
- Display on a **correlogram**





Example correlograms 1

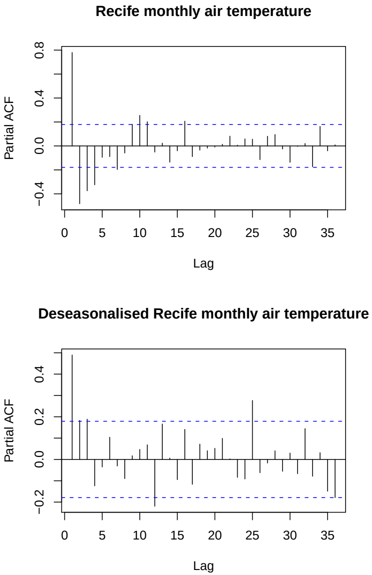


Partial autocorrelation function

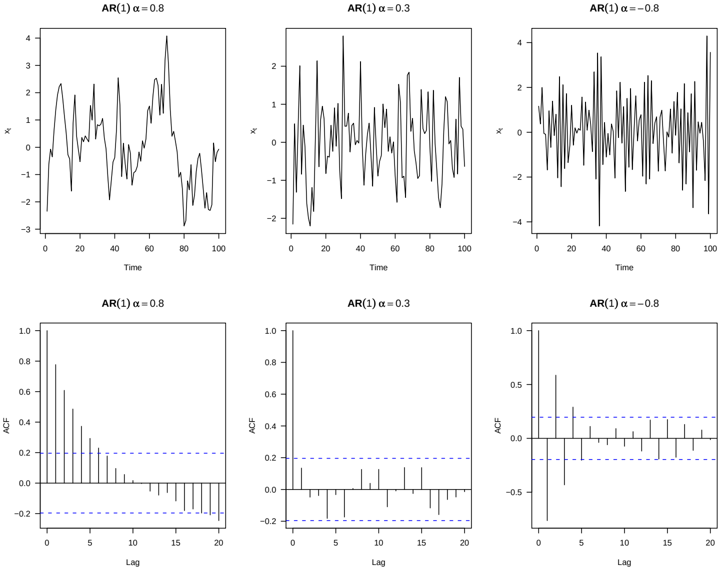
- If x_t and x_{t-1} are highly correlated then x_{t-1} and x_{t-2} will also be highly correlated
- Because x_t and x_{t-2} are highly correlated with x_{t-1}, it is likely that x_t and x_{t-2} are also highly correlated
- It would be nicer if we could estimate correlation between x_t and x_{t-2} after removing the effect of x_{t-1}
- This is the **partial autocorrelation**
- The partial autocorrelation α_k is obtained as coefficient β_k from the regression

$$x_t = \beta_0 + \beta_1 x_{t-1} + \beta_2 x_{t-2} + \cdots + \beta_k x_{t-k}$$

- This is an **autoregressive** (AR) process of order k

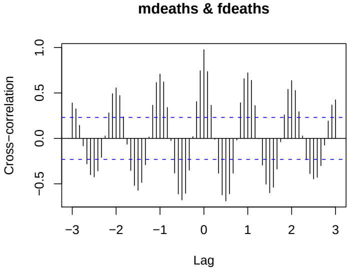


Example correlograms 2



Cross-correlation function

- **Sample cross-correlation function** measures the correlation between observations of two series at different lags



$$r_{xy}(k) = \begin{cases} \dfrac{1}{n} \dfrac{\sum_{t=1}^{n-k} (x_t - \bar{x})(y_{t+k} - \bar{y})}{s_x s_y} & k = 0, 1, \ldots, n-1 \\ \dfrac{1}{n} \dfrac{\sum_{t=1-k}^{n} (x_t - \bar{x})(y_{t+k} - \bar{y})}{s_x s_y} & k = -1, -2, \ldots, -(n-1) \end{cases}$$

Outline

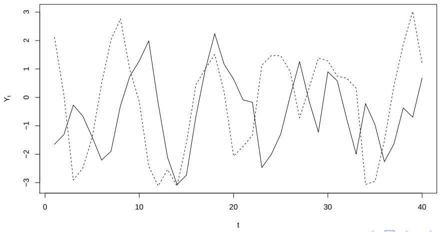
Stochastic Trends

- Tend to think of a trend as a deterministic one polluted by noise

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

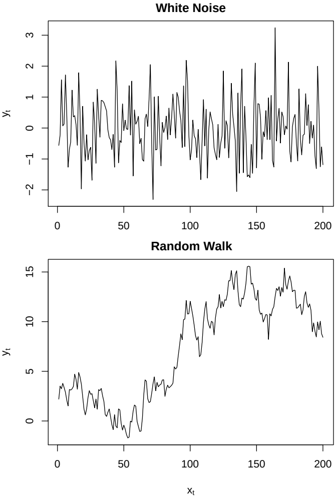
- Other types of trend may be at work; stochastic trends
- Here, variation in a time series is determined solely via dependence between successive observations rather than a fixed, deterministic trend
- Two stochastic trends fitted from the model

$$Y_t = 0.9959 Y_{t-1} + -0.5836 Y_{t-2} + \varepsilon_t$$



Useful time series models — purely random processes

- Several stochastic processes are useful for modelling time series
- A **purely random process** consists of mutually independent random variables, distributed normal with zero mean and variance σ^2
- Such a process has constant mean and variance
- Often termed **white noise**
- Different values are uncorrelated; $\rho(k) = 1$ if $k = 0$, otherwise $\rho(k) = 0$
- As the mean and autocovariance function do not depend on time, the process is second order stationary
- Independence implies the series is strictly stationary



Useful time series models — random walks

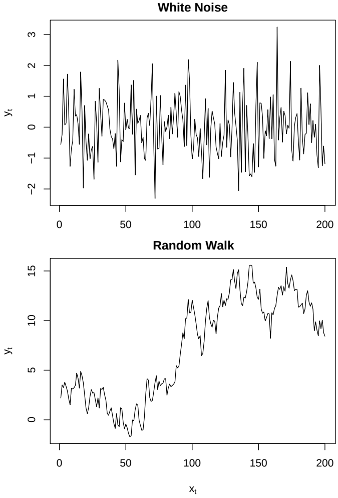
- Several stochastic processes are useful for modelling time series
- Suppose $\{z_t\}$ is a purely random process with mean μ and variance σ_z^2
- A time series is said to be a **random walk** if

$$x_t = x_{t-1} + z_t$$

- If started at 0 when $t = 0$ then $x_1 = z_1$ and

$$x_t = \sum_{i=1}^{t} z_i$$

- x_t is the cumulative sum of the random process up to time t
- The first differences of a random walk yield a purely random process

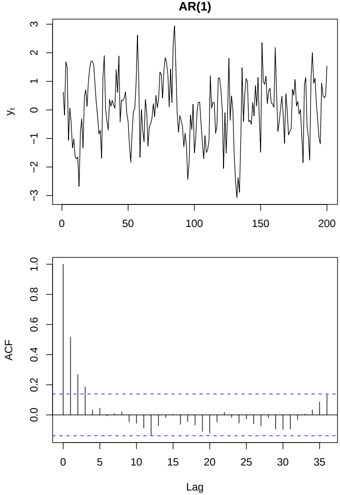


Useful time series models — autoregressive processes

- Several stochastic processes are useful for modelling time series
- A series x_t is said to be an **autoregressive** process if

$$x_t = \alpha_0 x_{t-1} + \cdots + \alpha_p x_{t-p} + z_t$$

- x_t is a function of past observations plus a purely random process (z_t)
- An **AR(p)** is a function of the p previous observations — said to be of order p
- AR(1) is the simplest such function, where $x_t = \alpha_1 x_{t-1} + z_t$
- An AR(1) is also called a **Markov process**
- Can have a non-zero mean and then the AR(p) contains an intercept (mean) term

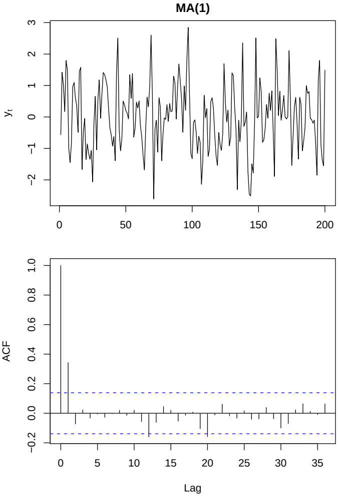


Useful time series models — moving average processes

- Several stochastic processes are useful for modelling time series
- A series x_t is said to be a **moving average** process if

$$x_t = \beta_0 z_t + \beta_1 z_{t-1} + \cdots + \beta_q z_{t-q}$$

- x_t is modelled as a function of the current and past values of a purely random process
- An **MA(**q**)** is of order q
- MA(1) is the simplest such function, where $x_t = \beta_0 z_t + \beta_1 z_{t-1}$
- Can have a non-zero mean and then the MA(q) contains an intercept (mean) term
- The ACF of a MA(q) has a sharp cut-off

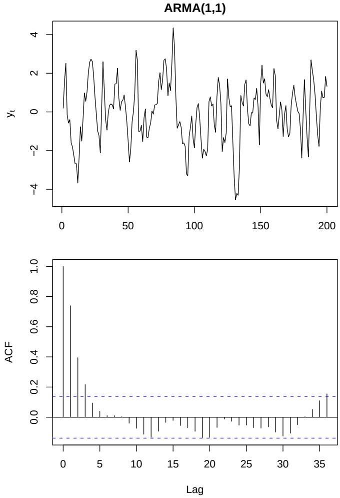


Useful time series models — ARMA models

- An **autoregressive moving average** process combines both AR(p) and MA(q) terms into a general model for time series

$$x_t = \sum_{l=1}^{p} \alpha_l x_{t-l} + z_t + \sum_{j=1}^{q} \beta_j z_{t-j}$$

- In shorthand we have ARMA(p,q)
  - p refers to the order of the AR process
  - q refers to the order of the MA process

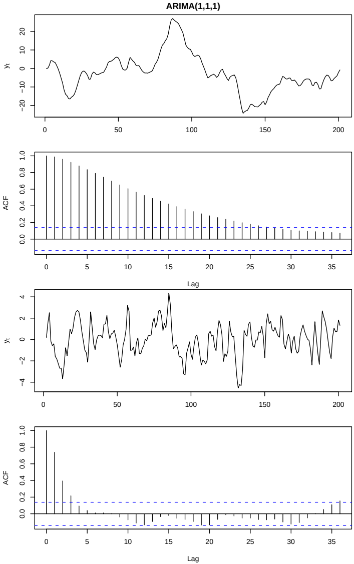


Useful time series models — ARIMA models

- An **autoregressive integrated moving average** process combines both AR(p) and MA(q) terms, *and* differencing into a general model for time series

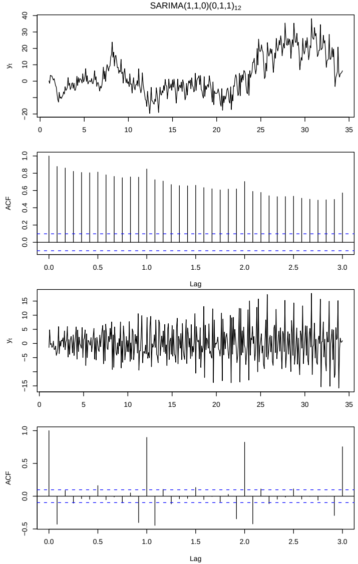
$$\nabla^d x_t = \sum_{l=1}^{p} \alpha_l \nabla^d x_{t-l} + z_t + \sum_{j=1}^{q} \beta_j z_{t-j}$$

- In shorthand we have ARIMA(p,d,q)
  - p refers to the order of the AR
  - q refers to the order of the MA
  - d refers to the order of the differencing applied to the original x_t
- First-order differencing is usually sufficient so generally $d = 1$
- A random walk can be regarded as an ARIMA(0,1,0)



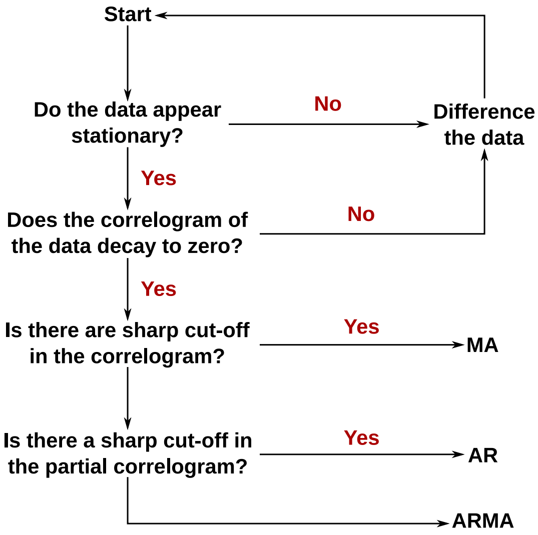
Useful time series models — SARIMA models

- A **seasonal autoregressive integrated moving average**, or SARIMA, model acknowledges that in practice many time series contain seasonal components
- In a monthly series we expect x_t to depend on x_{t-12} and perhaps x_{t-24} as well as on more recent non-seasonal values such as x_{t-1} and x_{t-2}
- SARIMA$(p,d,q)(P,D,Q)_s$
  - p: order of the AR
  - q: order of the MA
  - d: order of the differencing
  - P: seasonal order of the AR
  - Q: seasonal order of the MA
  - D: order of seasonal differencing
  - s: the period of seasonality
- E.g. SARIMA$(1{,}1{,}0)(0{,}1{,}1)_{s=12}$



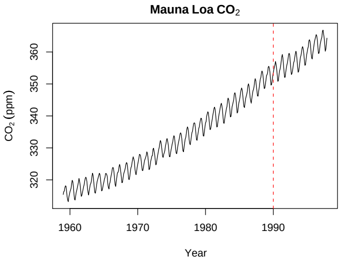
Choosing between ARMA models

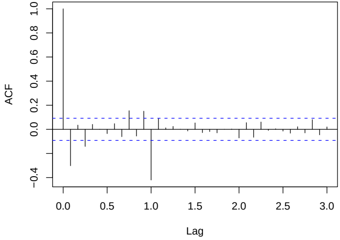
- First step; are the data stationary?
- If not difference them
- Then compute the correlogram (ACF)
- If sharp cut-off then MA
- If not, compute partial-ACF
- If sharp cut-off then AR
- If not, ARMA
- If differenced, then use ARIMA choosing AR, MA or ARMA selected above
- If seasonal data, use SARIMA



Example — Mauna Loa CO_2 concentrations

- CO_2 concentrations (ppm) measured at Mauna Loa 1959–1997
- Develop an appropriate SARIMA model for these data
- Fit model for 1957–1990
- Features:
  - Trend (differencing)
  - Seasonal component (seasonal differencing require)
  - Sharp cut-off in ACF suggests MA
  - ∇^{12} not removed all seasonal component; SAR or SMA
- Fit several models (36) and select using BIC
- p(0-2), d(1), q(0-2), P(0-1), D(1), Q(0-1), $s = 12$





Example — Mauna Loa CO_2 concentrations

- Optimal model has BIC = 151.46
  - $p(0)$, $d(1)$, $q(1)$, $P(0)$, $D(1)$, $Q(1)$, $s = 12$
- Diagnostics suggest no major problems with residuals

```
Call:
arima(x = CO2, order = c(0, 1, 1),
      seasonal = c(0, 1, 1))

Coefficients:
          ma1     sma1
      -0.3605  -0.8609
s.e.   0.0545   0.0313

sigma^2 estimated as 0.08031:
log likelihood = -66.8,  aic = 139.61
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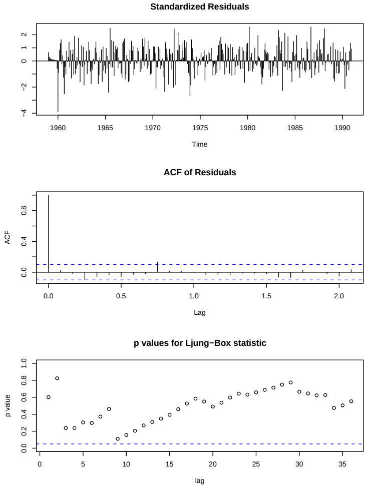
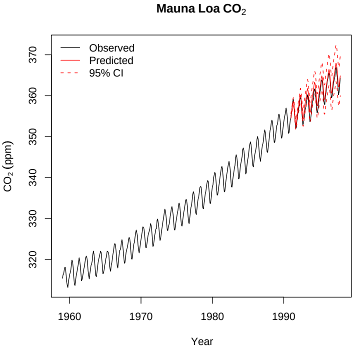


Example — Mauna Loa CO_2 concentrations

- Using the fitted SARIMA model, predict for the years 1991-1997
- Predicted values are in general agreement with the observed trend and seasonality
- Model over predicts for the "unobserved" period slightly
- The observed data, however lie within the 95% confidence interval of the predictions



Outline

Regression models for time series

- The SARIMA family of models allows us to model properties of a single time series
- They help us to understand the stochastic processes that might underlie the observations
- They don't help explain which factors may be driving the observed time series
- If we have additional time series on explanatory variables we can use these to try to explain the response time series
- Can extend (S)ARIMA model to include exogenous variables (S)ARIMAX...
- ... but regression provides a more familiar and powerful way of modelling time series and the effects of predictor variables
- ARIMA-type models assume equally-spaced observations; can have missing data, and hence an irregular sequence
- This means they are of limited use for lots of ecological and palaeoecological data

Regression models for time series

- Ordinary least squares regression makes assumptions about the model residuals — i.i.d.
  - Residuals are **independent** and **identically** distributed
  - Normally distributed, with mean 0 and known variance σ^2
- GLMs and GAMs allow us to relax the distributional assumptions to take account of Poisson or binomial data, etc.
- To model time series with regression techniques we need to account for the lack of independence of the observations in some way
- We can extend the linear regression case through the use of **generalised least squares** GLS
- Going further, we can extend GLS to use smoothers and model non-normal responses using **generalised additive mixed models** GAMMs
- This is achieved, primarily, by relaxing the assumptions about the variance, σ^2

Assumptions of least squares regression

1. The linear model correctly describes the functional relationship between y and X
   - If violated the estimate of predictor variances (σ^2) will be inflated
   - Incorrect model specification can show itself as patterns in the residuals
2. x_i are measured without error
   - Allows us to isolate the error component as random variation in y
   - Estimates $\hat{\beta}$ will be biased if there is error in X — often ignored!
3. For any given value of x_i, the sampled y_i values are independent with normally distributed errors
   - Independence and normality of errors allows us to use parametric theory for confidence intervals and hypothesis tests on the F-ratio.
4. Variances are constant along the regression line/model
   - Allows a single constant variance σ^2 for the variance of the regression line/model
   - Non-constant variances can be recognised through plots of residuals (amongst others) — i.e. residuals get wider as the values of y increase.

Generalised Least Squares

- The familiar least squares regression model can be written

$$y = \beta_0 + \beta_1 x_1 + \cdots + \beta_i x_i \qquad \varepsilon \sim N(0, \sigma^2 \mathbf{\Lambda})$$

- $\mathbf{\Lambda} \equiv \mathbf{I}$
- $\mathbf{I}$ is the identity matrix
- When multiplied by σ^2 we get the following covariance matrix

$$\mathbf{I} = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{pmatrix} \qquad \begin{pmatrix} \sigma^2 & 0 & \cdots & 0 \\ 0 & \sigma^2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sigma^2 \end{pmatrix}$$

- σ^2 same for all observations (variance), and all are independent (0 covariance)

Generalised Least Squares

- In least squares, the β are estimated by

$$\hat{\beta} = (X^{\mathsf{T}}X)^{-1}X^{\mathsf{T}}y$$

- If we now allow for correlated errors and set $\sigma^2\mathbf{I}$ from the previous slide to be $\Sigma_{\varepsilon\varepsilon}$, the coefficients in GLS are estimated by

$$\hat{\beta} = (X^{\mathsf{T}}\Sigma_{\varepsilon\varepsilon}^{-1}X)^{-1}X^{\mathsf{T}}\Sigma_{\varepsilon\varepsilon}^{-1}y$$

- We now need to choose a simple enough form for $\Sigma_{\varepsilon\varepsilon}$ so that we can estimate it and all the other parameters in the model from the data in a parsimonious manner
- As $\Sigma_{\varepsilon\varepsilon}$ is not known, estimation of model is done by ML
- It is worth noting that if the diagonal of $\Sigma_{\varepsilon\varepsilon}$ contains different values it indicates different variances for the residuals

Generalised Least Squares — correlated errors

- We can assume that the covariance of two errors depends only on their separation in time
- In which case we can use the autocorrelation function and define the autocorrelation at lag s as ρ_s, the correlation between two errors that are separated by $|s|$ time periods
- This results in an error covariance matrix with the following pattern

$$\mathbf{\Sigma}_{\varepsilon\varepsilon} = \sigma_{\varepsilon}^2 \begin{pmatrix} 1 & \rho_1 & \rho_2 & \cdots & \rho_{n-1} \\ \rho_1 & 1 & \rho_1 & \cdots & \rho_{n-2} \\ \rho_2 & \rho_1 & 1 & \cdots & \rho_{n-3} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \rho_{n-1} & \rho_{n-2} & \rho_{n-3} & \cdots & 1 \end{pmatrix} = \sigma^2 \mathbf{P}$$

- This allows quite a flexible correlation structure, but comes at the costs of estimating n distinct parameters (σ^2 and $\rho_1, \cdots, \rho_{n-1}$)
- Too many!

Generalised Least Squares — correlated errors

- To simplify the model further, we restrict the order of the autocorrelations to a small number of lags
- Usually the first-order AR process is used: $\varepsilon_s = \rho\varepsilon_{s-1} + \eta_s$
- The correlation between two errors at times t and s is

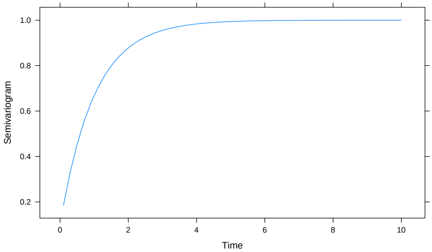
$$\mathrm{cor}(\varepsilon_s \varepsilon_t) = \begin{cases} 1 & \text{if } s = t \\ \rho^{|t-s|} & \text{else} \end{cases}$$

- This results in an error covariance matrix with the following pattern

$$\boldsymbol{\Sigma}_{\varepsilon\varepsilon} = \sigma^2_{\varepsilon} \begin{pmatrix} 1 & \rho & \rho^2 & \cdots & \rho^{n-1} \\ \rho & 1 & \rho & \cdots & \rho^{n-2} \\ \rho^2 & \rho & 1 & \cdots & \rho^{n-3} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \rho^{n-1} & \rho^{n-2} & \rho^{n-3} & \cdots & 1 \end{pmatrix} = \sigma^2 \mathbf{P}$$

Smoothing and correlated errors

- Can also use MA or ARMA processes for the model errors
- This is fine for equally-spaced observations, for irregularly spaced observations we need to turn to spatial correlation structures
- Use a 1-D spatial correlation structure to model correlations between two errors that are arbitrary distances apart in time
- Several structures, simplest is Exponential spatial correlation structure
- In 1-D, this is also known as the Continuous-time AR(1) (CAR(1))



Additive models

- Additive models are a generalization of linear models that replace the sum of regression coefficients $\times$ covariates by a sum of smooth functions of the covariates X
- Such a model has the following form

$$y = \beta_0 + \sum_{p=1}^{j} f_j(X_j) + \varepsilon, \quad \varepsilon \sim N(0, \sigma^2 \mathbf{\Lambda})$$

- where the f_j are arbitrary smooth functions
- Additive models are more flexible than the linear model but remain interpretable as the f_j can be plotted to show the marginal relationship between the predictor and the response

Using statistical models on times series data — trends

- Approach follows closely that of Ferguson et al (2006, 2007)
- A linear model for a trend component in the data might be

$$y = \beta_0 + \beta_1 time + \varepsilon, \quad \varepsilon \sim N(0, \sigma^2 \mathbf{\Lambda})$$

- An additive model for a trend component in the data might be

$$y = \beta_0 + f_1(time) + \varepsilon, \quad \varepsilon \sim N(0, \sigma^2 \mathbf{\Lambda})$$

- We can compare these two models to select between a linear or smooth (non-linear) trend
- We can also test for the presence of a trend by comparing this model to a null model

$$y = \beta_0 + \varepsilon, \quad \varepsilon \sim N(0, \sigma^2 \mathbf{\Lambda})$$

- Model testing is does via **likelihood ratio test** (LRT) and information statistics

Using statistical models on times series data — trends

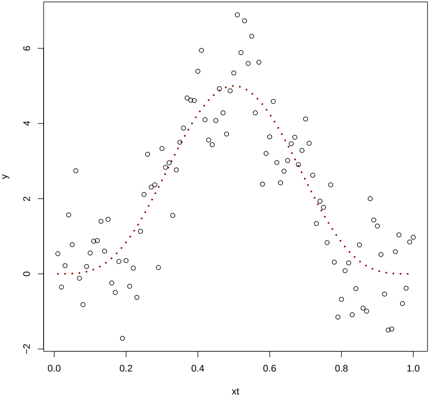
- Additionally, we can include additional predictor variables into the linear predictor to model changes in the response time series as a function of the explanatory variables
- We can also test whether the autocorrelation structure is required using LRT
- As these models are just regression models, use existing, well-developed theory for fitting models
- Using smoothers allows very flexible models to be fitted that include non-linear trends, seasonal smoothers etc.
- However, fitting these models in software is demanding and not for the faint hearted

Smoothing and correlated errors

- Data generated from the model

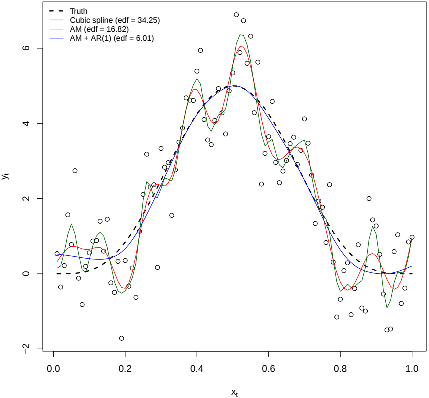
$$y_t = (1280 \times x_t^4) \times (1 - x_t)^4$$

- Added AR(1) noise; $\alpha = 0.3713$
- Task is to retrieve the trend y_t from the noisy data
- The data exhibit a non-linear trend and we can use a smoother to model this feature of the data
- A problem in smoothing is selecting the bandwidth or complexity of fitted spline
- The usual methods for smoothness selection assume the observations are independent



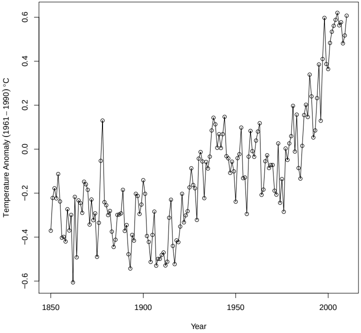
Smoothing and correlated errors

- Fit three separate models to the data
  1. Cubic smoothing spline (GCV)
  2. Additive model (GCV)
  3. Additive model with AR(1) errors (LMM)
- The two models that assume independent errors over fit the data
- Identify structure that is sampling artefact of the data at hand
- Additive model with AR(1) errors fits actual trend will
- $\hat{\phi} = 0.403$ (0.169, 0.594 95% CI)



NH Global Temperature

- Much interest in the patterns shown in temperature records, esp. in the most recent period
- Classic diagram used in the most recent IPCC Assessment Reports demonstrating trends and rates of change in temperature
- Mann and colleagues filtered the timeseries so had to pad the series at the ends to allow estimates of trends and rates in most recent period
- Padding the series done in several ways, but all involved inventing data for most recent period
- Can we do better with a regression model? — AM

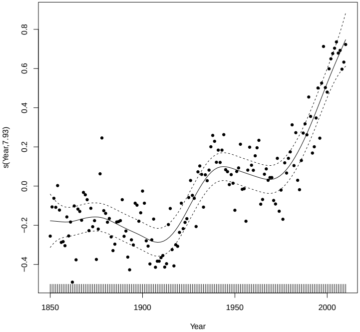


NH Global Temperature — additive model

- Annual mean global NH temperature anomaly (1960-1990)
- Fitted additive model of form

$$y = \beta_0 + f_1(year) + \varepsilon,\ \varepsilon \sim N(0, \sigma^2 \mathbf{\Lambda})$$

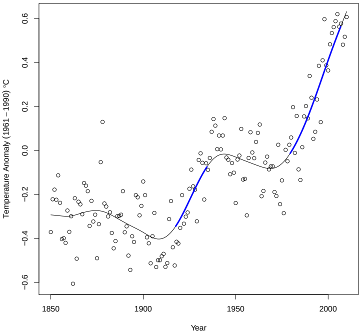
- Estimated the model with $\mathbf{\Lambda} \equiv \mathbf{I}$



- $\mathbf{\Lambda}$ assumed to be simple $\mathrm{AR(p)}$ or $\mathrm{MA(q)}$ or combinations for p and $q \in (1, 2, 3)$
- Fitted ARMAs to the residuals of this model to identify best model for residuals — AR(1)
- Refitted AM with an AR(1) correlation structure
- Checked for residual correlation

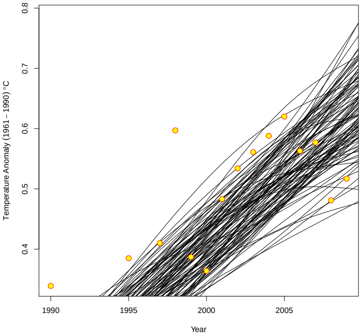
NH Global Temperature — additive model

- Interested in rates of change in temperature
- Also in the trend in the most recent period
- Can estimate the first derivatives of the fitted trend to show periods where the first derivative is statistically different from 0
- Use the method of finite differences
- Colour the fitted trend according to periods of significant change
  - Red — significantly decreasing
  - Blue — significantly increasing
  - (*c.f.* Sizer)



NH Global Temperature — additive model

- Uncertainty in fitted trend?
- Recall that the smoother is a spline for which we estimate coefficients $\hat{\beta}^s$
- Each $\hat{\beta}^s$ estimated with uncertainty
- The set of $\hat{\beta}^s$ form a MVN distribution
- Simulate new values for $\hat{\beta}^s$ from the MVN to generate trends consistent with the fitted model
- Sampling from the posterior distribution of the model parameters
- Only a tiny proportion of 1000 samples from the posterior distribution suggest that, given these data, there is little support for claims that the planet is cooling



Practicalities of fitting models using mgcv

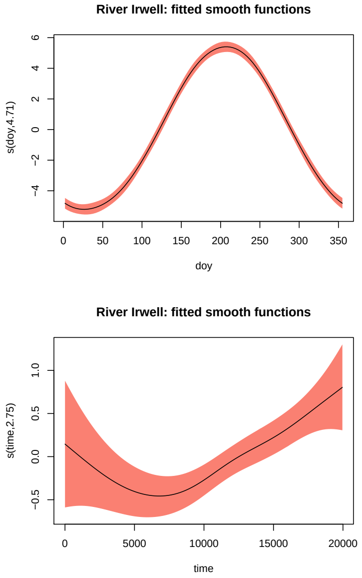
- Simple model for seasonal data

```
gamm(y ~ s(time, bs = "cr") + s(doy, bs = "cc", k = 12),
     data = foo,
     correlation = corCAR1(form = ~ time),
     knots = list(doy = seq(1, 366, length = 12)))
```

- For seasonal smooth, do not want discontinuity between Dec and Jan
- Use a cyclic smoothing spline (`bs = "cc"`)
- End points have common first and second derivatives — the end points are "joined"
- Only some types of smoother available in cyclic forms (here using cubic splines)
- `k` is the number of knots to use
- If data don't cover start and end of year, specify knots at days 1 and 366 and evenly in between

Practicalities of fitting models using mgcv

- Figure shows the two fitted smoothers
- Estimated degrees of freedom given on y-axis
- Shaded region is an approximate, 95% point-wise confidence interval on fitted smooths
- `plot(mod, pages = 1, scale = 0)`



Using by variables

- Sometimes we might want to fit separate trends within seasons
- Or fit trends to several sites in a single model
- Can use the by argument for this

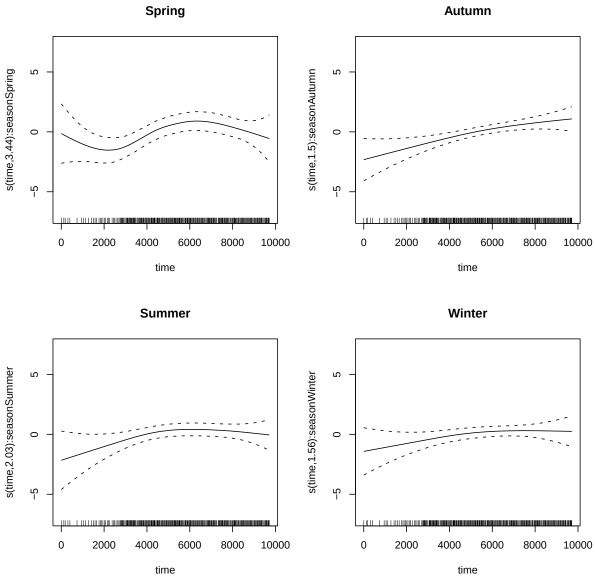
```
gamm(y ~ season + s(time, bs = "cr", by = season) +
         s(doy, bs = "cc", k = 12),
     data = foo,
     correlation = corCAR1(form = ~ time),
     knots = list(doy = seq(1, 366, length = 12)))
```

- season is a factor coding for season
- Included as a main term to centre each smooth about that season mean value

```
gamm(y ~ season + s(time, bs = "cr") + s(time, bs = "cr", by = season) +
         s(doy, bs = "cc", k = 12),
     data = foo,
     correlation = corCAR1(form = ~ time),
     knots = list(doy = seq(1, 366, length = 12)))
```

- Different parametrisation, by smoothers now represent deviations from global trend

Using by variables



Fitting multivariate models

- Might want a model that allows seasonal component to vary with the trend
- Use a mutivariate smooth; must get models properly nested to compare them

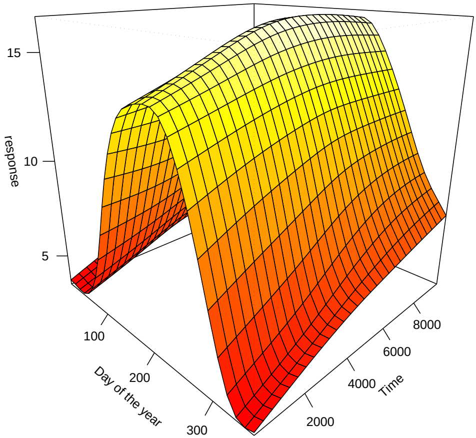
```
m1 <- gamm(y ~ s(time, bs = "cr") + s(doy, bs = "cc", k = 12), ...)
m2 <- gamm(y ~ te(time, doy, bs = c("cr", "cc")), data = foo, ...)
```

- m1 is not strictly nested in m2 because may use different basis
- Need te() smooth to allow different bs for each variable
- To get proper nesting fit models as

```
m3 <- gamm(y ~ s(time, bs = "cr", k = 10) + s(doy, bs = "cc", k = 12), ...)
m4 <- gamm(y ~ s(time, bs = "cr", k = 10) + s(doy, bs = "cc", k = 12) +
           te(time, doy, bs = c("cr", "cc"), k = c(10,12)), data = foo, ...)
```

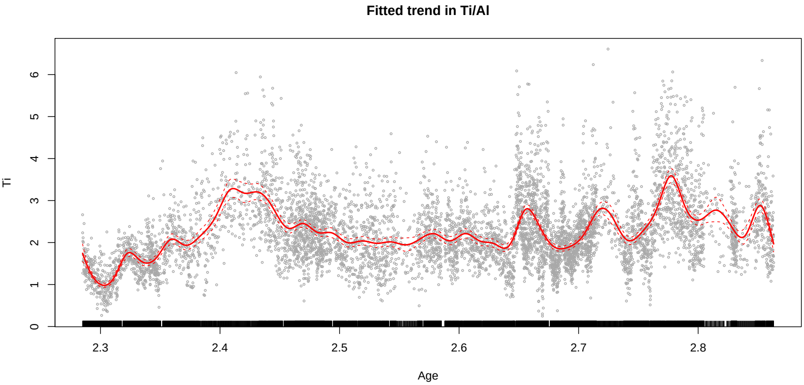
- In m4 2d smoother represents how trend and seasonal smooths deviate from global smooths
- If m4 fits better than m3, refit model as in m2 so smooth is easier to interpret/use

Fitting multivariate models



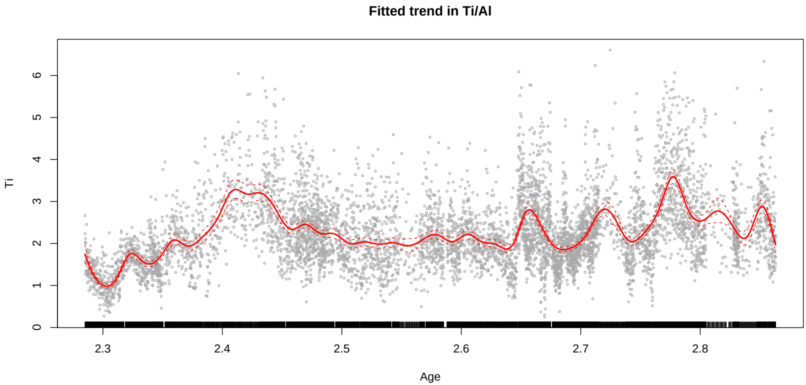
Katy's crazy amounts of data

- Lots, and lots, and lots of XFR data
- Model takes a week to fit
- How can we deal with data like this?



Katy's crazy amounts of data

- Realise that we might have to be subjective here
- Fix the degree of smoothness — or force use of fewer DF, and
- Use and adaptive smoother



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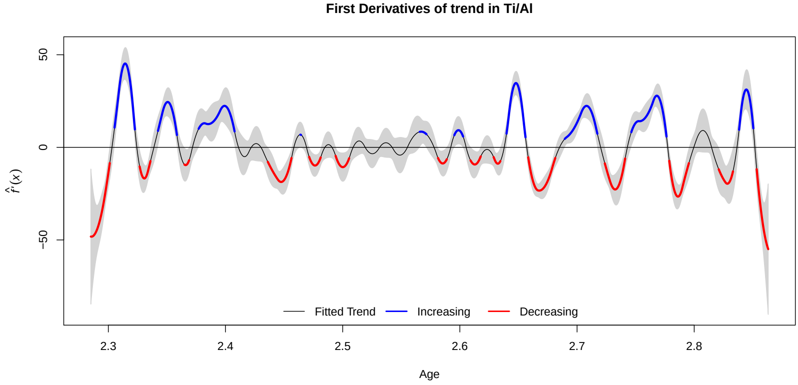

Katy's crazy amounts of data

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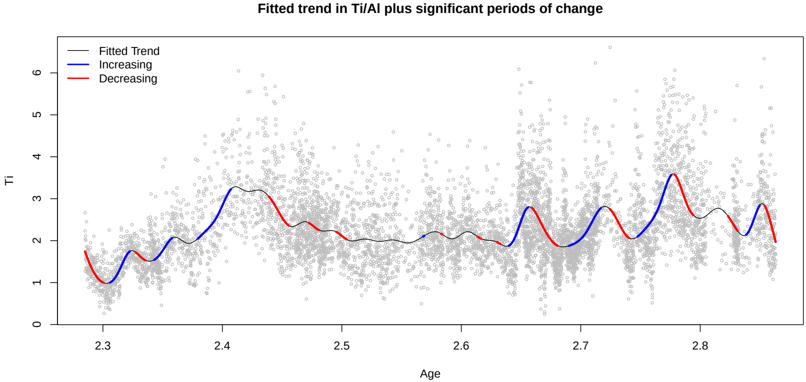


lmeControl

- To control the fitting process, say to print out details of the iterations or to increase number of iterations, we need to use a control object
- Import to set `niterEM = 0` when using `gamm()`
- See `?lmeControl` and `?gamm` for details

```
## need a control object
ctrl <- lmeControl(msVerbose = TRUE,
                   maxIter = 400,
                   msMaxIter = 400,
                   niterEM = 0,      ## this is VERY important for gamm()!
                   tolerance = 1e-8,
                   msTol = 1e-8,
                   msMaxEval = 400)

## pass the control object as part of your model fitting call
mod <- gamm(y ~ s(time) + s(doy, bs = "cc", k = 10), data = foo,
            ...., ## other arguments here
            control = ctrl)
```

Protocols for fitting GLS and (G)AMM

- Model selection now involves finding the correct fixed effects formulation *and* the correct specification for the model errors
- A protocol for model selection could take the following form
  1. Fit the fixed effects model you think is plausible without the autocorrelation — don't worry too much at this stage about getting a minimal, adequate model for the fixed effects
  2. Now add the autocorrelation structure to the model and refine that — LRT to see if the correlation is required
  3. Finally, revisit the fixed effects and remove variables not required
- When fitting the correlation structure, don't worry about getting this part exactly correct
- The aim is to add a structure that plausibly accounts for the autocorrelation, not to model it exactly
- In general, this means AR(1) for equally-spaced observations and CAR(1) for unequally-spaced observations

Outline

Spectral Analysis

- Spectral analysis: methods of estimating the spectral density function, or spectrum, of a given time series
- Spectral analysis can be used to detect periodic signals corrupted by noise
- Periodic signals; a repeating pattern in a series is periodic, with **period** equal to the length of the pattern
- The sine wave is the fundamental periodic signal in mathematics
- Joseph Fourier (1768–1830) showed that good approximations to most periodic signals can be achieved using sums of sine waves
- Spectral analysis is based on sine waves and a decomposition of variation in series into waves of various frequencies

Sine waves

- A sine wave of frequency ω, amplitude A, and phase ψ for time t is

$$A \sin(\omega t + \psi)$$

- A general sine wave can be expressed as a weighted sum of sine and cosine functions

$$A \sin(\omega t + \psi) = A \cos(\psi) \sin(\omega t) + A \sin(\psi) \cos(\omega t)$$

- A sampled sine wave of any amplitude and phase can be fitted by a linear regression model with the sine and cosine functions as predictor variables

Sine waves

- Suppose we have a time series of length n, $\{x_t : t = 1, \ldots, n\}$ (n is even)
- Fit time series regression with x_t as response and $n - 1$ predictor variables

$$\cos\left(\frac{2\pi t}{n}\right), \sin\left(\frac{2\pi t}{n}\right), \cos\left(\frac{4\pi t}{n}\right), \sin\left(\frac{4\pi t}{n}\right)$$

$$\cos\left(\frac{6\pi t}{n}\right), \sin\left(\frac{6\pi t}{n}\right), \ldots \cos\left(\frac{2(n/2-1)\pi t}{n}\right), \sin\left(\frac{2(n/2-1)\pi t}{n}\right)$$

$$\cos(\pi t)$$

Sine waves

- Estimated coefficients denoted by $a_1, b_1, a_2, b_2, \ldots, a_{n/2-1}, b_{n/2-1}, a_{n/2}$
- As many coefficients as observations
- No degrees of freedom for errors
- a_0 is the intercept, and is the mean of x
- Lowest frequency is one cycle (or 2π radians) per record length, $2\pi/n$ radians per sampling interval (RPSI)
- General frequency, m cycles per sampling interval ($2\pi m/n$ RPSI), m is integer between 1 and $n/2$
- highest frequency, 0.5 cycles per sampling interval (π RPSI), $n/2$ cycles in the series
- Sine wave that makes m cycles in series length is the mth harmonic
- Amplitude of mth harmonic is $A_m = \sqrt{a_m^2 + b_m^2}$

Raw Periodogram

- Amplitude of mth harmonic is $A_m = \sqrt{a_m^2 + b_m^2}$
- Parseval's Theorem expresses variance of a series as a sum of $n/2$ components at integer frequencies $1, \ldots, n/2$

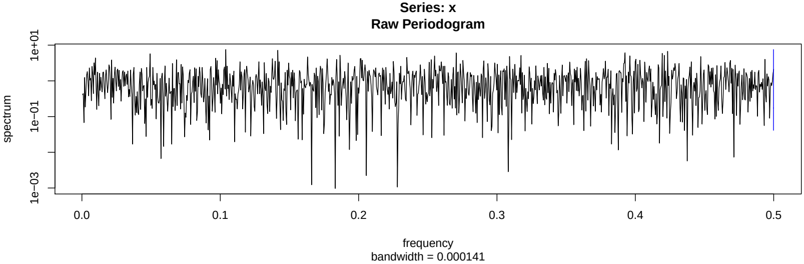
$$\mathrm{Var}(x) = \frac{1}{2} \sum_{m=1}^{(n/2)-1} A_m^2 + A_{n/2}^2$$

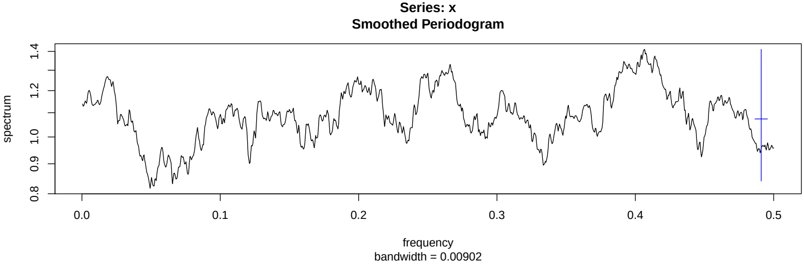
- In general, instead of via a regression, the calculations above are usually performed with the fast fourier transform (FFT) algorithm
- A plot of A_m^2 as spikes against m is a Fourier line spectrum
- Raw periodogram is produced by joining the tips of the spikes in the Fourier line spectrum and scaling area equal to the variance

Smoothed Periodogram

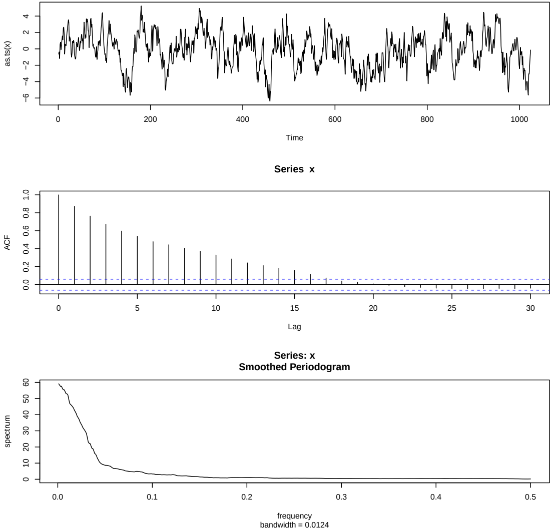
- Periodogram distributes variance over frequency but has two drawbacks
  - Precise set of frequencies is arbitrary, depends on series length
  - Periodogram does not get smoother as series length increases — just gets more packed
- The remedy to this is to smooth the periodogram
- Smooth the spikes of the Fourier line spectrum using moving averages before joining the tips
- Smoothed periodogram also known as the (sample) spectrum
- Smoothing will reduce the heights of the peaks and excessive smoothing will blur the features we are interested in
- In practice try several degrees of smoothing

Example Periodograms — white noise

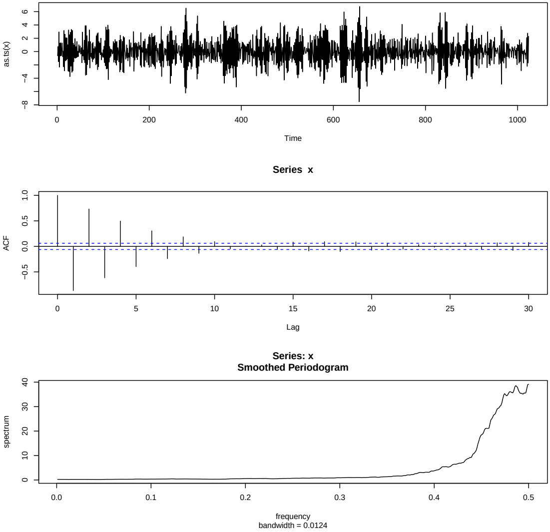




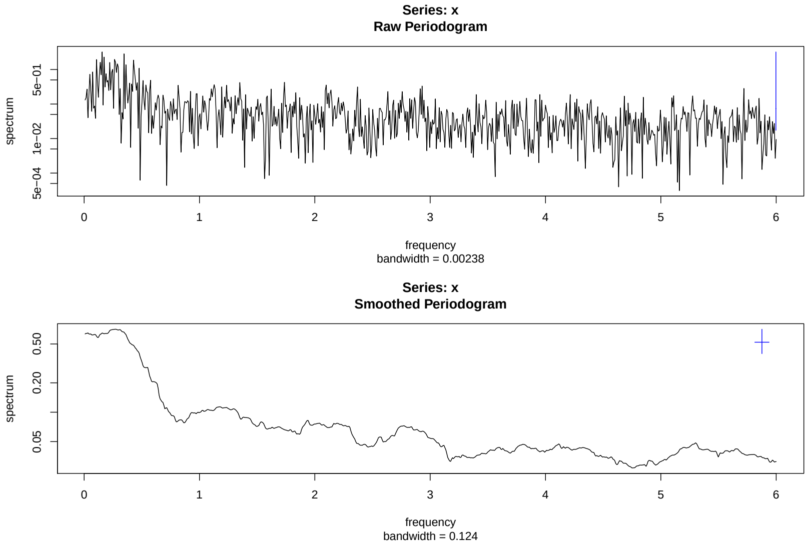
Example Periodograms — AR(1) v1



Example Periodograms — AR(1) v2



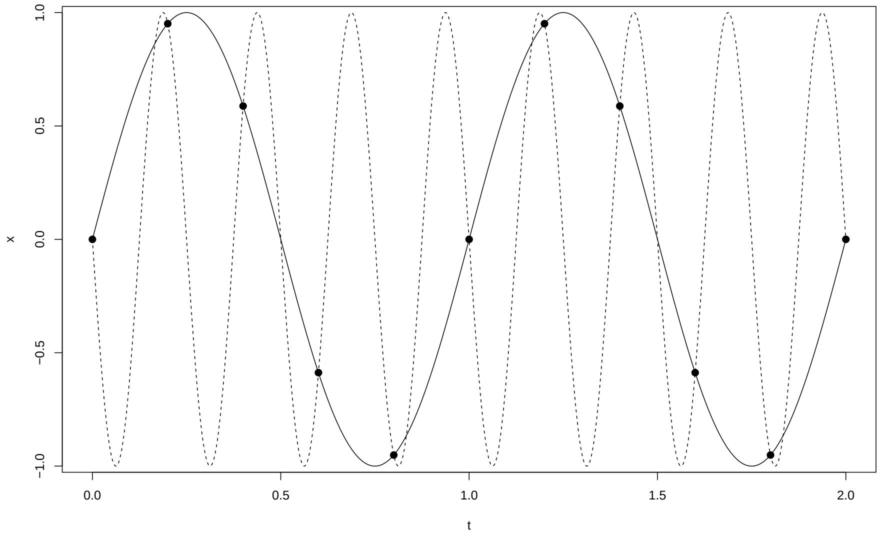
Southern Oscillation Index



Aliasing and the Nyquist frequency

- Many time series are discrete measurements of a continuous process
- Important to sample at high enough frequency to capture highest frequency oscillations in process
- If sampling frequency is too low, miss information
- Also, real high frequency variation will show up as lower frequency variation
- This is known as aliasing
- The Nyquist frequency is half the sampling frequency and is the maximum frequency we can recover from the data series collected

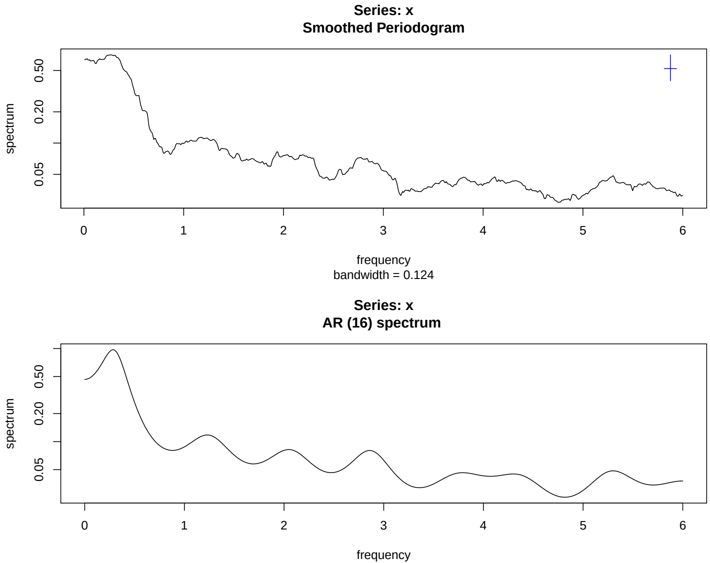
Aliasing



Autoregressive spectrum estimation

- An alternative method for estimating the spectrum of a time series is to fit an ARMA(p, q) model to the series
- They one can use the theoretical spectrum of the ARMA(p, q) model to compute the spectrum
- In general, a high-order AR(p) model is used
- In `spectrum()` we can use this via `method = "ar"`
- Tends to give a very smooth estimate of the spectrum as p becomes large
- `spectrum()` estimates the order p using AIC

Autoregressive spectrum — SOI



Further reading

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