School of MATHEMATICAL AND STATISTICAL SCIENCES
Clemson University

Parameter Estimation
Model Diagnostics and Selection

Lecture 10

ARMA Models: Estimation, Diagnostics, and Model Selection

Reading: Bowerman, O'Connell, and Koehler (2005): Capter 10.1-10.2; Cryer and Chen (2008): Chapter 7.3-7.5; Chapter 8.1

MATH 4070: Regression and Time-Series Analysis

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Agenda

1. **Parameter Estimation**

2. **Model Diagnostics and Selection**

Estimation of the ARMA Process Parameters

Suppose we choose an ARMA(p, q) model for a zero-mean $\{\eta_t\}$

- Need to estimate the $p + q + 1$ parameters:
  - AR component $\{\phi_1, \cdots, \phi_p\}$
  - MA component $\{\theta_1, \cdots, \theta_q\}$
  - $\mathrm{Var}(Z_t) = \sigma^2$
- One strategy:
  - Do some preliminary estimation of the model parameters (e.g., via Yule-Walker estimates)
  - Follow-up with maximum likelihood estimation with Gaussian assumption

The Yule-Walker Method

Suppose η_t is a causal AR(p) process

$$\eta_t - \phi_1 \eta_{t-1} - \cdots - \phi_p \eta_{t-p} = Z_t$$

To estimate the parameters $\{\phi_1, \cdots, \phi_p\}$, we use a method of moments estimation scheme:

- Let $h = 0, 1, \cdots, p$. We multiply η_{t-h} to both sides

$$\eta_t \eta_{t-h} - \phi_1 \eta_{t-1} \eta_{t-h} - \cdots - \phi_p \eta_{t-p} \eta_{t-h} = Z_t \eta_{t-h}$$

- Taking expectations:

$$\mathbb{E}(\eta_t \eta_{t-h}) - \phi_1 \mathbb{E}(\eta_{t-1} \eta_{t-h}) - \cdots - \phi_p \mathbb{E}(\eta_{t-p} \eta_{t-h}) = \mathbb{E}(Z_t \eta_{t-h}),$$

we get $\boxed{\gamma(h) - \phi_1 \gamma(h-1) - \cdots - \phi_p \gamma(h-p) = \mathbb{E}(Z_t \eta_{t-h})}$

The Yule-Walker Equations

- When $h = 0$, $\mathbb{E}(Z_t \eta_{t-h}) = \mathrm{Cov}(Z_t, \eta_t) = \sigma^2$ (Why?) Therefore, we have

$$\gamma(0) - \sum_{j=1}^{p} \phi_j \gamma(j) = \sigma^2$$

- When $h > 0$, Z_t is uncorrelated with η_{t-h} (because the assumption of causality), thus $\mathbb{E}(Z_t \eta_{t-h}) = 0$ and we have

$$\gamma(h) - \sum_{j=1}^{p} \phi_j \gamma(h - j) = 0, \quad h = 1, 2, \cdots, p$$

- The Yule-Walker estimates are the solution of these equations when we replace $\gamma(h)$ by $\hat{\gamma}(h)$

The Yule-Walker Equations in Matrix Form

Let $\hat{\boldsymbol{\phi}} = (\hat{\phi}_1, \cdots, \hat{\phi}_p)^T$ be an estimate for $\boldsymbol{\phi} = (\phi_1, \cdots, \phi_p)^T$ and let

$$\hat{\boldsymbol{\Gamma}} = \begin{bmatrix} \hat{\gamma}(0) & \hat{\gamma}(1) & \cdots & \hat{\gamma}(p-1) \\ \hat{\gamma}(1) & \hat{\gamma}(0) & \cdots & \hat{\gamma}(p-2) \\ \vdots & \vdots & \ddots & \vdots \\ \hat{\gamma}(p-1) & \hat{\gamma}(p-2) & \cdots & \hat{\gamma}(0) \end{bmatrix}.$$

Then the Yule-Walker estimates of ϕ and σ^2 are

$$\hat{\boldsymbol{\phi}} = \hat{\boldsymbol{\Gamma}}^{-1}\hat{\boldsymbol{\gamma}},$$

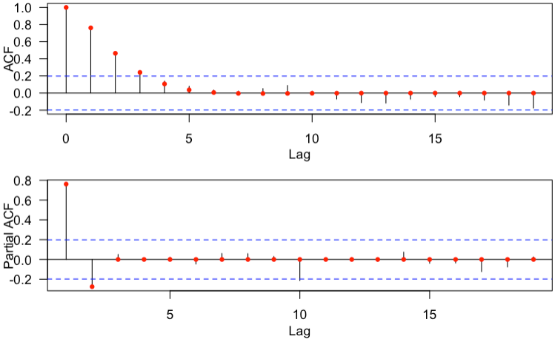
and

$$\hat{\sigma}^2 = \hat{\gamma}(0) - \hat{\boldsymbol{\phi}}^T\hat{\boldsymbol{\gamma}},$$

where $\hat{\boldsymbol{\gamma}} = (\hat{\gamma}(1), \cdots, \hat{\gamma}(p))^T$

Lake Huron Example in R

```
```{r}
YW_est <- ar(lm$residuals, aic = F, order.max = 2, method = "yw")
# plot sample and estimated acf/pacf
par(las = 1, mgp = c(2.2, 1, 0), mar = c(3.6, 3.6, 0.6, 0.6), mfrow = c(2, 1))
acf(lm$residuals)
acf_YWest <- ARMAacf(ar = YW_est$ar, lag.max = 23)
points(0:23, acf_YWest, col = "red", pch = 16, cex = 0.8)
pacf(lm$residuals)
pacf_YWest <- ARMAacf(ar = YW_est$ar, lag.max = 23, pacf = T)
points(1:23, pacf_YWest, col = "red", pch = 16, cex = 0.8)
```
```



Remarks on the Yule-Walker Method

- For large sample size, Yule-Walker estimator have (approximately) the same sampling distribution as maximum likelihood estimator (MLE), but with small sample size Yule-Walker estimator can be far less efficient than the MLE

[1] See **Least Squares Estimation** in Chapter 7.2 of Cryer and Chan (2008).

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- The Yule-Walker method is a poor procedure for MA(q) and ARMA(p,q) processes with $q > 0$ (see Cryer Chan 2008, p. 150-151)

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Remarks on the Yule-Walker Method

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- The Yule-Walker method is a poor procedure for MA(q) and ARMA(p,q) processes with $q > 0$ (see Cryer Chan 2008, p. 150-151)
- We move on the more versatile and popular method for estimating ARMA(p,q) parameters–maximum likelihood estimation[1]

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Maximum Likelihood Estimation

- The setup:

Maximum Likelihood Estimation

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  - Model: $\boldsymbol{X} = (X_1, X_2, \cdots, X_n)$ has joint probability density function $f(\boldsymbol{x}; \boldsymbol{\omega})$ where $\boldsymbol{\omega} = (\omega_1, \omega_2, \cdots, \omega_p)$ is a vector of p parameters

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  - Data: $\boldsymbol{x} = (x_1, x_2, \cdots, x_n)$
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$$L_n(\boldsymbol{\omega}) = f(\boldsymbol{x}; \boldsymbol{\omega})$$

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- The maximum likelihood estimate (MLE) is the value of $\boldsymbol{\omega}$ which maximizes the likelihood, $L_n(\boldsymbol{\omega})$, of the data $\boldsymbol{x}$:

$$\hat{\boldsymbol{\omega}} = \underset{\boldsymbol{\omega}}{\operatorname{argmax}} \, L_n(\boldsymbol{\omega}).$$

It is equivalent (and often easier) to maximize the log likelihood,

$$\ell_n(\boldsymbol{\omega}) = \log L_n(\boldsymbol{\omega})$$

The MLE for an i.i.d. Gaussian Process

Suppose $\{X_t\}$ be a Gaussian i.i.d. process with mean μ and variance σ^2. We observe a time series $\boldsymbol{x} = (x_1, \cdots, x_n)^T$.

- The likelihood function is

$$
\begin{aligned}
L_n(\mu, \sigma^2) &= f(\boldsymbol{x}|\mu, \sigma^2) \\
&= \prod_{t=1}^{n} f(x_t|\mu, \sigma) \\
&= \prod_{t=1}^{n} \left\{ \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(x_t - \mu)^2}{2\sigma^2} \right] \right\} \\
&= (2\pi)^{-n/2} (\sigma^2)^{-n/2} \exp\left[-\frac{\sum_{t=1}^{n} (x_t - \mu)^2}{2\sigma^2} \right]
\end{aligned}
$$

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- The log-likelihood function is

$$\begin{aligned} \ell_n(\mu, \sigma^2) &= \log L_n(\mu, \sigma^2) \\ &= -\frac{n}{2} \log(2\pi) - \frac{n}{2} \log(\sigma^2) - \frac{\sum_{t=1}^{n} (x_t - \mu)^2}{2\sigma^2} \end{aligned}$$

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$$\Rightarrow \hat{\mu}_{\text{MLE}} = \frac{\sum_{t=1}^{n} X_t}{n} = \bar{X}, \qquad \hat{\sigma}^2_{\text{MLE}} = \frac{\sum_{t=1}^{n} (X_t - \bar{X})^2}{n}$$

Likelihood for Stationary Gaussian Time Series Models

Suppose $\{X_t\}$ be a mean zero stationary Gaussian time series with ACVF $\gamma(h)$. If $\gamma(h)$ depends on p parameters, $\boldsymbol{\omega} = (\omega_1, \cdots, \omega_p)$

- The likelihood of the data $\boldsymbol{x} = (x_1, \cdots, x_n)$ given the parameters $\boldsymbol{\omega}$ is

$$L_n(\boldsymbol{\omega}) = (2\pi)^{-n/2} |\boldsymbol{\Gamma}|^{-1/2} \exp\left(-\frac{1}{2}\boldsymbol{x}^T \boldsymbol{\Gamma}^{-1} \boldsymbol{x}\right),$$

  where $\boldsymbol{\Gamma}$ is the covariance matrix of $\boldsymbol{X} = (X_1, \cdots, X_n)^T$, $|\boldsymbol{\Gamma}|$ is the determinant of the matrix $\boldsymbol{\Gamma}$, and $\boldsymbol{\Gamma}^{-1}$ is the inverse of the matrix $\boldsymbol{\Gamma}$

- The log-likelihood is

$$\ell_n(\boldsymbol{\theta}) = -\frac{n}{2}\log(2\pi) - \frac{1}{2}\log|\boldsymbol{\Gamma}| - \frac{1}{2}\boldsymbol{x}^T \boldsymbol{\Gamma}^{-1} \boldsymbol{x}$$

  Typically need to solve it numerically

Decomposing Joint Density into Conditional Densities

A joint distribution can be represented as the product of conditionals and a marginal distribution

- The simple version for $n = 2$ is:

$$f(x_1, x_2) = f(x_2|x_1)f(x_1)$$

Decomposing Joint Density into Conditional Densities

A joint distribution can be represented as the product of conditionals and a marginal distribution

- The simple version for $n = 2$ is:

$$f(x_1, x_2) = f(x_2|x_1)f(x_1)$$

- Extending for general n we get the following expression for the likelihood:

$$L_n(\boldsymbol{\theta}) = f(\boldsymbol{x};\boldsymbol{\theta}) = f(x_1)\prod_{t=2}^{n} f(x_t|x_{t-1},\cdots,x_1;\boldsymbol{\theta}),$$

and the log-likelihood is

$$\ell_n(\boldsymbol{\theta}) = \log f(\boldsymbol{x};\boldsymbol{\theta}) = \log(f(x_1)) + \sum_{t=2}^{n} \log f(x_t|x_{t-1},\cdots,x_1;\boldsymbol{\theta}).$$

AR(1) Log-likelihood

Let $\{\eta_1, \eta_2, \cdots, \eta_n\}$ be a realization of a zero-mean stationary AR(1) Gaussian time series. Let $\boldsymbol{\theta} = (\phi, \sigma^2)$

$$\ell_n(\boldsymbol{\theta}) = \underbrace{\log(f(\eta_1))}_{\ell_{n,1}} + \underbrace{\sum_{t=2}^{n} \log f(\eta_t | \eta_{t-1}, \cdots, \eta_1; \boldsymbol{\theta})}_{\ell_{n,2}}.$$

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Note that for $t \geq 2$, $f(\eta_t|\eta_{t-1}, \cdots, \eta_1) = f(\eta_t|\eta_{t-1})$, where $[\eta_t|\eta_{t-1}] \sim \mathrm{N}(\phi\eta_{t-1}, \sigma^2) \Rightarrow \ell_{n,2} =$

$$-\frac{(n-1)}{2}\log 2\pi - \frac{(n-1)}{2}\log\sigma^2 - \frac{\sum_{t=2}^{n}(\eta_t - \phi\eta_{t-1})^2}{2\sigma^2}$$

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Also, we know $[\eta_1] \sim \mathrm{N}\left(0, \frac{\sigma^2}{(1-\phi^2)}\right) \Rightarrow \ell_{1,n} =$

$$\frac{-\log 2\pi}{2} - \frac{\log\sigma^2}{2} + \frac{\log(1-\phi^2)}{2} - \frac{(1-\phi^2)\eta_1^2}{2\sigma^2}$$

Parameter Estimation

Model Diagnostics and Selection

AR(1) Log-likelihood

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$$\ell_n(\boldsymbol{\theta}) = \underbrace{\log(f(\eta_1))}_{\ell_{n,1}} + \underbrace{\sum_{t=2}^{n} \log f(\eta_t|\eta_{t-1}, \cdots, \eta_1; \boldsymbol{\theta})}_{\ell_{n,2}}.$$

Note that for $t \geq 2$, $f(\eta_t|\eta_{t-1}, \cdots, \eta_1) = f(\eta_t|\eta_{t-1})$, where $[\eta_t|\eta_{t-1}] \sim \mathrm{N}(\phi\eta_{t-1}, \sigma^2) \Rightarrow \ell_{n,2} =$

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$$\Rightarrow \ell_n(\boldsymbol{\theta}) = -\frac{n}{2}\log 2\pi - \frac{n}{2}\log\sigma^2 - \frac{\sum_{t=2}^{n}(\eta_t - \phi\eta_{t-1})^2}{2\sigma^2} + \frac{\log(1-\phi^2)}{2} - \frac{(1-\phi^2)\eta_1^2}{2\sigma^2}$$

AR(1) Log-likelihood Cont'd

$$\ell_n(\boldsymbol{\theta}) = -\frac{n}{2}\log 2\pi - \frac{n}{2}\log\sigma^2 + \frac{\log(1-\phi^2)}{2} - \frac{S(\phi)}{2\sigma^2},$$

where $S(\phi) = \sum_{t=2}^{n}(\eta_t - \phi\eta_{t-1})^2 + (1-\phi^2)\eta_1^2$

- For given value of ϕ, $\ell_n(\phi, \sigma^2)$ can be maximized analytically with respect to σ^2

$$\hat{\sigma}^2 = \frac{S(\hat{\phi})}{n}$$

AR(1) Log-likelihood Cont'd

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- Estimation of ϕ can be simplified by maximizing the **conditional sum-of-squares** ($\sum_{t=2}^{n}(\eta_t - \phi\eta_{t-1})^2$)

AR(1) Log-likelihood Cont'd

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- Estimation of ϕ can be simplified by maximizing the **conditional sum-of-squares** ($\sum_{t=2}^{n}(\eta_t - \phi\eta_{t-1})^2$)
- **Standard errors** can be obtained by computing the inverse of the **Hessian matrix**: $\mathrm{Var}(\hat{\boldsymbol{\theta}}) = H(\hat{\boldsymbol{\theta}})^{-1}$, where $H(\boldsymbol{\theta}) = \frac{\partial^2\ell_n(\boldsymbol{\theta})}{\partial\boldsymbol{\theta}\partial\boldsymbol{\theta}^T}$

`arima` in `R` with the Lake Huron Example

arima: ARIMA Modelling of Time Series

Description

Fit an ARIMA model to a univariate time series.

Usage

```
arima(x, order = c(0L, 0L, 0L),
      seasonal = list(order = c(0L, 0L, 0L), period = NA),
      xreg = NULL, include.mean = TRUE,
      transform.pars = TRUE,
      fixed = NULL, init = NULL,
      method = c("CSS-ML", "ML", "CSS"), n.cond,
      SSinit = c("Gardner1980", "Rossignol2011"),
      optim.method = "BFGS",
      optim.control = list(), kappa = 1e6)
```

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      optim.method = "BFGS",
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```

````
```{r}
(MLE_est1 <- arima(lm$residuals, order = c(2, 0, 0), method = "ML"))
```
````

```
Call:
arima(x = lm$residuals, order = c(2, 0, 0), method = "ML")

Coefficients:
         ar1      ar2  intercept
      1.0047  -0.2919     0.0197
s.e.  0.0977   0.1004     0.2350

sigma^2 estimated as 0.4571:  log likelihood = -101.25,  aic = 210.5
```

Inference for the ARMA Parameters

Motivating example: What is an approximate 95% CI for ϕ_1 in an AR(1) model?

- Let $\boldsymbol{\phi} = (\phi_1, \cdots, \phi_p)$ and $\boldsymbol{\theta} = (\theta_1, \cdots, \theta_q)$ denote the ARMA parameters (excluding σ^2), and let $\hat{\boldsymbol{\phi}}$ and $\hat{\boldsymbol{\theta}}$ be the ML estimates of $\boldsymbol{\phi}$ and $\boldsymbol{\theta}$. Then for "large" n, $(\hat{\boldsymbol{\phi}}, \hat{\boldsymbol{\theta}})$ have approximately a joint normal distribution:

$$\begin{bmatrix} \hat{\boldsymbol{\phi}} \\ \hat{\boldsymbol{\theta}} \end{bmatrix} \dot{\sim} \mathrm{N}\left(\begin{bmatrix} \boldsymbol{\phi} \\ \boldsymbol{\theta} \end{bmatrix}, \frac{V(\boldsymbol{\phi}, \boldsymbol{\theta})}{n} \right)$$

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$$\begin{bmatrix} \hat{\boldsymbol{\phi}} \\ \hat{\boldsymbol{\theta}} \end{bmatrix} \dot{\sim} \mathrm{N}\left(\begin{bmatrix} \boldsymbol{\phi} \\ \boldsymbol{\theta} \end{bmatrix}, \frac{V(\boldsymbol{\phi}, \boldsymbol{\theta})}{n} \right)$$

- $V(\boldsymbol{\phi}, \boldsymbol{\theta})$ is a known $(p+q) \times (p+q)$ matrix depending on the ARMA parameters

$V(\phi, \theta)$ for AR Processes

- For an AR(p) process

$$V(\phi) = \sigma^2 \Gamma^{-1},$$

where Γ is the $p \times p$ covariance matrix of the series $(\eta_1, \cdots, \eta_p)$

- AR(1) process:

$$V(\phi_1) = 1 - \phi_1^2$$

- AR(2) process:

$$V(\phi_1, \phi_2) = \begin{bmatrix} 1 - \phi_2^2 & -\phi_1(1 + \phi_2) \\ -\phi_1(1 + \phi_2) & 1 - \phi_2^2 \end{bmatrix}$$

Other Examples of $V(\phi, \theta)$

- MA(1) process:

$$V(\theta_1) = 1 - \theta_1^2$$

- MA(2) process:

$$V(\theta_1, \theta_2) = \begin{bmatrix} 1 - \theta_2^2 & \theta_1(1 - \theta_2) \\ \theta_1(1 - \theta_2) & 1 - \theta_2^2 \end{bmatrix}$$

- Casual and invertible ARMA(1,1) process

$$V(\phi, \theta) = \frac{1 + \phi\theta}{(\phi + \theta)^2} \begin{bmatrix} (1 - \phi^2)(1 + \phi\theta) & -(1 - \phi^2)(1 - \theta^2) \\ -(1 - \phi^2)(1 - \theta^2) & 1 - \theta_2^2 \end{bmatrix}$$

- More generally, for "small" n, the covariance matrix of $(\hat{\phi}, \hat{\boldsymbol{\theta}})$ can be approximated using the second derivatives of the log-likelihood function, known as the Hessian matrix

MLE for Trend and Temporal Correlation in One Step

```{r}
(MLE_est4 <- arima(LakeHuron, order = c(2, 0, 0), xreg = yr))
```

```
Call:
arima(x = LakeHuron, order = c(2, 0, 0), xreg = yr)

Coefficients:
         ar1      ar2  intercept     xreg
      1.0048  -0.2913   620.5115  -0.0216
s.e.  0.0976   0.1004    15.5771   0.0081

sigma^2 estimated as 0.4566:  log likelihood = -101.2,  aic = 210.4
```

Fitted model:

$$Y_t = 620.51 - 0.022\text{Year} + \eta_t,$$

where

$$\eta_t = 1.00\eta_{t-1} - 0.29\eta_{t-2} + Z_t, \quad Z_t \sim \mathrm{N}(0, \sigma^2 = 0.46^2).$$

What About Non-Gaussian Processes?

It is more challenging to express the joint distribution of X_t for non-Gaussian processes. Instead, we often rely on the Gaussian likelihood as an approximate likelihood

- In practice:
  - Transform the data to make the series as close to Gaussian as possible (e.g., using a log, square-root, or Box-Cox transformation)
  - Then use the Gaussian likelihood to estimate parameters, assuming the transformed series follows a near-Gaussian structure
  - For many real-world applications, this approximation works well and simplifies estimation. However, residual diagnostics are needed to ensure the model fits the data adequately

Assessing Fit / Comparing Different Time Series Models

- We can use diagnostic plots for the “residuals” of the fitted time series, along with Box tests to assess whether an i.i.d. process is reasonable

```
> Box.test(YW_est$resid[-(1:2)], type = "Ljung-Box")

        Box-Ljung test

data:  YW_est$resid[-(1:2)]
X-squared = 0.56352, df = 1, p-value = 0.4528
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- Use confidence intervals for the parameters. Intervals that contain zero may indicate that we can simplify the model
- We can also use model selection criteria, such as AIC, to compare between different models

Diagnostics via the Time Series Residuals

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- Define the residuals $\{R_t\}$ by

$$R_t = \frac{U_t}{\sqrt{r_{t-1}}} = \frac{X_t - \hat{X}_t}{\sqrt{r_{t-1}}}$$

Under Gaussian model $R_t \stackrel{i.i.d}{\sim} \mathrm{N}(0, \sigma^2)$

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- To choose the order (p and q) of ARMA model it makes sense to penalize models with a large number of parameters
- Here we consider an information based criteria to compare models

Akaike Information Criterion (AIC)

- The Akaike information criterion (AIC) is defined by

$$\text{AIC} = -2\ell_n(\hat{\boldsymbol{\phi}}, \hat{\boldsymbol{\theta}}, \hat{\sigma}^2) + 2(p+q+1)$$

- We choose the values of p and q that minimizes the AIC value

- For AR(p) models, AIC tends to overestimate p. The bias corrected version is

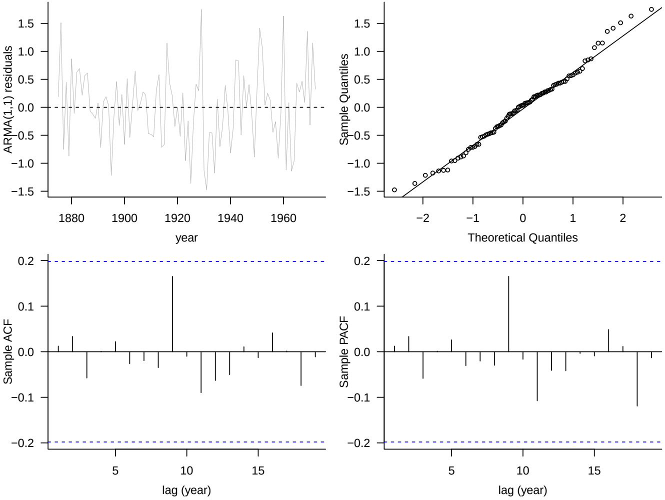
$$\text{AICc} = 2\ell_n(\hat{\boldsymbol{\phi}}, \hat{\boldsymbol{\theta}}, \hat{\sigma}^2) + \frac{2n(p+q+1)}{(n-1)-(p+q+1)}$$

Lake Huron Example: AIC and AICc

```
m1 <- arima(LakeHuron, order = c(1, 0, 0), xreg = yr)
m2 <- arima(LakeHuron, order = c(1, 0, 1), xreg = yr)
m3 <- arima(LakeHuron, order = c(2, 0, 0), xreg = yr)
m4 <- arima(LakeHuron, order = c(2, 0, 1), xreg = yr)
AIC(m1); AIC(m2); AIC(m3); AIC(m4)
library(MuMIn)
AICc(m1); AICc(m2); AICc(m3); AICc(m4)
```

```
[1] 218.4501
[1] 212.3954
[1] 212.3965
[1] 214.0638
[1] 218.8803
[1] 213.0476
[1] 213.0487
[1] 214.9868
```

Lake Huron Model Diagnostics




```
> Box.test(resids, lag = 10, type = "Ljung-Box")

        Box-Ljung test

data:  resids
X-squared = 3.7882, df = 10, p-value = 0.9564
```