Chapter 5. Parameter estimation and model identification for ARMA models

Objectives

1. Develop likelihood-based inference in the context of ARMA models.
2. Discuss maximum likelihood parameter estimation and alternative methods.
3. Investigate strategies for model selection, also known as model identification, in the context of ARMA models.
4. Work on practical computational approaches for implementing these methods.

Background on likelihood-based inference

- For any data $y_{1:N}$ and any probabilistic model $f_{Y_{1:N}}(y_{1:N}\,;\theta)$ we define the likelihood function to be

$$\mathcal{L}(\theta) = f_{Y_{1:N}}(y_{1:N}\,;\theta).$$

- It is often convenient to work with the logarithm to base e of the likelihood, which we write as

$$\ell(\theta) = \log \mathcal{L}(\theta).$$

- Using the likelihood function as a statistical tool is a very general technique, widely used since Fisher (1922)] (`wikipedia.org/wiki/Likelihood_function`).
- Time series analysis involves various situations where we can, with sufficient care, compute the likelihood function and take advantage of the general framework of likelihood-based inference.

- Computation of the likelihood function for ARMA models is not entirely straightforward.
- Computationally efficient algorithms exist, using a state space model representation of ARMA models that will be developed later in this course.
- For now, it is enough that software exists to evaluate and maximize the likelihood function for a Gaussian ARMA model. Our immediate task is to think about how to use that capability.

- Before evaluation of the ARMA likelihood became routine, it was popular to use a method of moments estimator called **Yule-Walker** estimation. This is described by Shumway and Stoffer (Section 3.6) but is nowadays mostly of historical interest.
- There are occasionally time series situations where massively long data or massively complex models mean that it is computationally infeasible to work with the likelihood function. However, we are going to focus on the common situation where we can (with due care) work with the likelihood.
- Likelihood-based inference (meaning statistical tools based on the likelihood function) provides tools for parameter estimation, standard errors, hypothesis tests and diagnosing model misspecification.
- Likelihood-based inference often (but not always) has favorable theoretical properties. Here, we are not especially concerned with the underlying theory of likelihood-based inference. On any practical problem, we can check the properties of a statistical procedure by simulation experiments.

The maximum likelihood estimator (MLE)

- A maximum likelihood estimator (MLE) is

$$\hat{\theta}(y_{1:N}) = \arg\max_{\theta} f_{Y_{1:N}}(y_{1:N}\,;\theta),$$

  where $\arg\max_\theta g(\theta)$ means a value of argument θ at which the maximum of the function g is attained, so $g\big(\arg\max_\theta g(\theta)\big) = \max_\theta g(\theta)$.
- If there are many values of θ giving the same maximum value of the likelihood, then an MLE still exists but is not unique.
- The maximum likelihood estimate (also known as the MLE) is

$$\begin{aligned} \hat{\theta} &= \hat{\theta}(y_{1:N}) && (1) \\ &= \arg\max_{\theta} \mathcal{L}(\theta) && (2) \\ &= \arg\max_{\theta} \ell(\theta). && (3) \end{aligned}$$

Question 5.1. Why are $\arg\max_\theta \mathcal{L}(\theta)$ and $\arg\max_\theta \ell(\theta)$ the same?

- We can write $\hat{\theta}_{MLE}$ and $\hat{\theta}_{MLE}$ if we are considering various alternative estimation methods. However, in this course, we will most often be using maximum likelihood estimation so we let $\hat{\theta}$ and $\hat{\theta}$ correspond to this approach.

Standard errors for the MLE

- As statisticians, it would be irresponsible to present an estimate without a measure of uncertainty!
- Usually, this means obtaining a confidence interval, or an approximate confidence interval.
- It is good to say **approximate** when you present something that is not exactly a confidence interval with the claimed coverage. For example, remind yourself of the definition of a 95
- Saying "approximate" reminds you that there is some checking that could be done to assess how accurate the approximation is in your particular situation.
- It also helps to remind you that it may be interesting and relevant to explain why the interval you present is an approximate confidence interval rather than an exact one.
- There are three main approaches to estimating the statistical uncertainty in an MLE.

  1. The Fisher information. This is computationally quick, but works well only when $\hat{\theta}(Y_{1:N})$ is well approximated by a normal distribution.
  2. Profile likelihood estimation. This is a bit more computational

Standard errors via the observed Fisher information

- We suppose that $\theta \in \mathbb{R}^D$ and so we can write $\theta = \theta_{1:D}$.
- The Hessian matrix of a function is the matrix of its second partial derivatives. We write the Hessian matrix of the log likelihood function as $\nabla^2 \ell(\theta)$, a $D \times D$ matrix whose (i,j) element is
$$\big[\nabla^2 \ell(\theta)\big]_{ij} = \frac{\partial^2}{\partial\theta_i \partial\theta_j} \ell(\theta).$$
- The observed Fisher information is
$$\hat{I} = -\nabla^2 \ell(\hat{\theta}).$$
- A standard asymptotic approximation to the distribution of the MLE for large N is
$$\hat{\theta}(Y_{1:N}) \approx N\left[\theta, [\hat{I}]^{-1}\right],$$
where θ is the true parameter value. This asserts that the MLE is asymptotically unbiased, with variance asymptotically attaining the Cramer-Rao lower bound. Thus, we say the MLE is **asymptotically efficient**. Here, we interpret $\approx$ to mean "one could write a limit statement formally justifying this approximation in a suitable limit."

Confidence intervals via the profile likelihood

- Let's consider the problem of obtaining a confidence interval for θ_d, the dth component of $\theta_{1:D}$.
- The **profile log likelihood function** of θ_d is defined to be

$$\ell_d^{\text{profile}}(\theta_d) = \max_{\phi \in \mathbb{R}^D : \phi_d = \theta_d} \ell(\phi).$$

  In general, the profile likelihood of one parameter is constructed by maximizing the likelihood function over all other parameters.
- Check that $\max_{\theta_d} \ell_d^{\text{profile}}(\theta_d) = \max_{\theta_{1:D}} \ell(\theta_{1:D})$. Maximizing the profile likelihood $\ell_d^{\text{profile}}(\theta_d)$ gives the MLE, $\hat{\theta}_d$.
- An approximate 95

$$\big\{\theta_d : \ell(\hat{\theta}) - \ell_d^{\text{profile}}(\theta_d) < 1.92\big\}.$$

- This is known as a profile likelihood confidence interval. The cutoff 1.92 is derived using **Wilks's theorem**, which we will discuss in more detail when we develop likelihood ratio tests.
- Although the asymptotic justification of Wilks's theorem is the same limit that justifies the Fisher information standard errors, profile likelihood confidence intervals tend to work better than Fisher

Bootstrap methods for constructing standard errors and confidence intervals

- Suppose we want to know the statistical behavior of the estimator $\hat{\theta}(y_{1:N})$ for models in a neighborhood of the MLE, $\theta = \hat{\theta}(y_{1:N})$.
- In particular, let's consider the problem of estimating uncertainty about θ_1. We want to assess the behavior of the maximum likelihood estimator, $\hat{\theta}(y_{1:N})$, and possibly the coverage of an associated confidence interval estimator, $\big[\hat{\theta}_{1,\mathrm{l}o}(y_{1:N}), \hat{\theta}_{1,\mathrm{h}i}(y_{1:N})\big]$. The confidence interval estimator could be constructed using either the Fisher information method or the profile likelihood approach.
- The following simulation study lets us address the following goals:
  (A) Evaluate the coverage of a proposed confidence interval estimator, $[\hat{\theta}_{1,\mathrm{l}o}, \hat{\theta}_{1,\mathrm{h}i}]$,
  (B) Construct a standard error for $\hat{\theta}_1$,
  (C) Construct a confidence interval for θ_1 with exact local coverage.
  1. Generate J independent Monte Carlo simulations,

$$Y^{[j]}_{1:N} \sim f_{Y_{1:N}}(y_{1:N}\,; \hat{\theta}) \text{ for } j \in 1:J.$$

  2. For each simulation, evaluate the maximum likelihood estimator,

Question 5.2. Local coverage as an approximation to actual coverage for a confidence interval

- A true 95
- The local coverage probability at a value $\theta = \tilde{\theta}$ is the chance that the confidence interval covers $\tilde{\theta}$ when the true parameter value is $\tilde{\theta}$. Typically, we compute local coverage at $\theta = \hat{\theta}$.
- Local coverage can be evaluated or calibrated via simulation; the actual (global) coverage is usually hard to work with.
- What properties of the model and data make local coverage a good substitute for global coverage? How would you check whether or not these properties hold?

Likelihood-based model selection and model diagnostics

1. Likelihood ratio tests for nested hypotheses
   - The whole parameter space on which the model is defined is $\Theta \subset \mathbb{R}^D$.
   - Suppose we have two **nested** hypotheses

$$H^{\langle 0 \rangle} \; : \; \theta \in \Theta^{\langle 0 \rangle}, \tag{4}$$

$$H^{\langle 1 \rangle} \; : \; \theta \in \Theta^{\langle 1 \rangle}, \tag{5}$$

   defined via two nested parameter subspaces, $\Theta^{\langle 0 \rangle} \subset \Theta^{\langle 1 \rangle}$, with respective dimensions $D^{\langle 0 \rangle} < D^{\langle 1 \rangle} \leq D$.

   - We consider the log likelihood maximized over each of the hypotheses,

$$\ell^{\langle 0 \rangle} = \sup_{\theta \in \Theta^{\langle 0 \rangle}} \ell(\theta), \tag{6}$$

$$\ell^{\langle 1 \rangle} = \sup_{\theta \in \Theta^{\langle 1 \rangle}} \ell(\theta). \tag{7}$$

- A useful approximation asserts that, under the hypothesis $H^{\langle 0\rangle}$,

$$\ell^{\langle 1\rangle} - \ell^{\langle 0\rangle} \approx (1/2)\chi^2_{D^{\langle 1\rangle} - D^{\langle 0\rangle}},$$

  where χ^2_d is a chi-squared random variable on d degrees of freedom and $\approx$ means "is approximately distributed as."
- We will call this the **Wilks approximation**.
- The Wilks approximation can be used to construct a hypothesis test of the null hypothesis $H^{\langle 0\rangle}$ against the alternative $H^{\langle 1\rangle}$.
- This is called a **likelihood ratio test** since a difference of log likelihoods corresponds to a ratio of likelihoods.
- When the data are IID, $N \to \infty$, and the hypotheses satisfy suitable regularity conditions, this approximation can be derived mathematically and is known as **Wilks's theorem**.
- We therefore have two different interpretations of $\approx$. One is "one could write a limit statement formally justifying this approximation in a suitable limit" and another is "this approximation is useful in the finite sample situation at hand." These interpretations may both be appropriate!
- The chi-squared approximation to the likelihood ratio statistic may be useful, and can be assessed empirically by a simulation study, even in

Using a likelihood ratio test to construct profile likelihood confidence intervals

- Recall the duality between hypothesis tests and confidence intervals: The estimated parameter θ does not lead us to reject a null hypothesis of $\theta = \theta^{\langle 0 \rangle}$ at the 5

  $$\Updownarrow$$

  $\theta^{\langle 0 \rangle}$ is in a 95
- We can check what the 95% cutoff is for a chi-squared distribution with one degree of freedom,

```r
qchisq(0.95,df=1)
## [1] 3.841459
```

- We can now see how the Wilks approximation suggests a confidence interval constructed from parameter values having a profile likelihood within 1.92 log units of the maximum.
- It is a exercise to write out more details (to your own satisfaction) on how to use the Wilks approximation, together with the duality between hypothesis tests and confidence intervals, to derive a profile likelihood confidence interval

Akaike's information criterion (AIC)

- Likelihood ratio tests provide an approach to model selection for nested hypotheses, but what do we do when models are not nested?
- A more general approach is to compare likelihoods of different models by penalizing the likelihood of each model by a measure of its complexity.
- Akaike's information criterion **AIC** is given by

  $$AIC = -2 \times \ell(\theta) + 2D$$

  "Minus twice the maximized log likelihood plus twice the number of parameters."
- We are invited to select the model with the lowest AIC score.
- AIC was derived as an approach to minimizing prediction error. Increasing the number of parameters leads to additional **overfitting** which can decrease predictive skill of the fitted model.
- Viewed as a hypothesis test, AIC may have weak statistical properties. It can be a mistake to interpret AIC by making a claim that the favored model has been shown to provides a superior explanation of the data. However, viewed as a way to select a model with reasonable

Comparing AIC with likelihood ratio tests

- Suppose we are in a situation in which we wish to choose between two nested hypotheses, with dimensions $D^{\langle 0 \rangle} < D^{\langle 1 \rangle}$. Suppose the Wilks approximation is valid.
- Consider the strategy of selecting the model with the lowest AIC value.
- We can view this model selection approach as a formal statistical test.
- Find an expression for the size of this AIC test (i.e, the probability of rejecting the null hypothesis, $H^{\langle 0 \rangle}$, when this null hypothesis is true).
- Evaluate this expression for $D^{\langle 1 \rangle} - D^{\langle 0 \rangle} = 1$.

Implementing likelihood-based inference for ARMA models in R

- The Great Lakes are an important resource for leisure, agriculture and industry in this region.
- A past concern has been whether human activities such as water diversion or channel dredging might be leading to a decline in lake levels.
- An additional current concern is the effects of climate change. The physical mechanisms are not always obvious: for example, evaporation tends to be highest when the weather is cold but the lake is not ice-covered.
- We look at monthly time series data on the depth of Lake Huron.

Reading in the data

Here is the head of the file `huron_depth.csv`

```
# downloaded on 1/24/16 from
# http://www.glerl.noaa.gov/data/dashboard/data/levels/mGauge/
# Lake Michigan-Huron:, Monthly Average Master Gauge Water Lev
# Source:, NOAA/NOS
Date, Average
01/01/1860,177.285
02/01/1860,177.339
03/01/1860,177.349
04/01/1860,177.388
05/01/1860,177.425
```

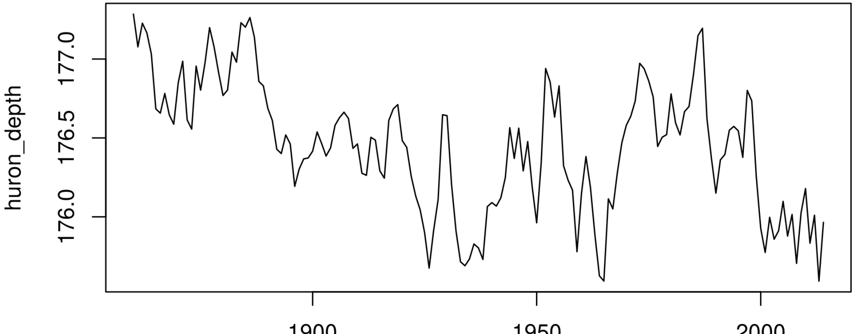
- A bit of work has to be done manipulating the Date variable.
- Moving between date formats is a necessary skill for time series analysis!
- A standard representation of time is POSIXct, which is a signed real number representing the number of seconds since the beginning of 1970.
- The raw data have a character string representing date. We convert this into the standard format using strptime. Than we can extract whatever we need. See ?DateTimeClasses for more on manipulating date and time formats in R.

```
dat <- read.table(file="huron_depth.csv",sep=",",header=TRUE)
dat$Date <- strptime(dat$Date,"%m/%d/%Y")
dat$year <- as.numeric(format(dat$Date, format="%Y"))
dat$month <- as.numeric(format(dat$Date, format="%m"))
head(dat)

##         Date Average year month
## 1 1860-01-01 177.285 1860     1
## 2 1860-02-01 177.339 1860     2
## 3 1860-03-01 177.349 1860     3
## 4 1860-04-01 177.388 1860     4
```

- For now, let's avoid monthly seasonal variation by considering an annual series of January depths. We will investigate seasonal variation later in the course, but sometimes it is best avoided.

```
dat <- subset(dat,month==1)
huron_depth <- dat$Average
year <- dat$year
plot(huron_depth~year,type="l")
```



Fitting an ARMA model

- Later, we will consider hypotheses of trend. For now, let's start by fitting a stationary ARMA(p, q) model under the null hypothesis that there is no trend. This hypothesis, which asserts that nothing has substantially changed in this system over the last 150 years, is not entirely unreasonable from looking at the data.
- We seek to fit a stationary Gaussian ARMA(p,q) model with parameter vector $\theta = (\phi_{1:p}, \psi_{1:q}, \mu, \sigma^2)$ given by

$$\phi(B)(Y_n - \mu) = \psi(B)\epsilon_n,$$

  where

$$\begin{aligned} \mu &= \mathbb{E}[Y_n] && (8) \\ \phi(x) &= 1 - \phi_1 x - \cdots - \phi_p x^p, && (9) \\ \psi(x) &= 1 + \psi_1 x + \cdots + \psi_q x^q, && (10) \\ \epsilon_n &\sim \text{iid}\, N[0, \sigma^2]. && (11) \end{aligned}$$

- We need to decide where to start in terms of values of p and q. Let's tabulate some AIC values for a range of different choices of p and q.
- In the code below, note the use of kable for formatting HTML tables

```
aic_table <- function(data,P,Q){
  table <- matrix(NA,(P+1),(Q+1))
  for(p in 0:P) {
    for(q in 0:Q) {
       table[p+1,q+1] <- arima(data,order=c(p,0,q))$aic
    }
  }
  dimnames(table) <- list(paste("<b> AR",0:P, "</b>", sep=""),paste
  table
}
huron_aic_table <- aic_table(huron_depth,4,5)
require(knitr)
kable(huron_aic_table,digits=2)
```

	MA0	MA1	MA2	MA3	MA4	MA5
¡b¿ AR0¡/b¿	166.75	46.60	7.28	-14.97	-18.64	-26.09
¡b¿ AR1¡/b¿	-38.00	-37.41	-35.46	-33.82	-34.13	-32.20
¡b¿ AR2¡/b¿	-37.33	-38.43	-36.90	-34.93	-34.35	-33.08
¡b¿ AR3¡/b¿	-35.52	-35.17	-32.71	-31.38	-31.13	-32.98
¡b¿ AR4¡/b¿	-33.94	-34.91	-34.43	-36.27	-31.31	-30.90

Question 5.3. What do we learn by interpreting the results in the above table of AIC values?

Question 5.4. In what ways might we have to be careful not to over-interpret the results of this table?

- Let's fit the ARMA(2,1) model recommended by consideration of AIC.

```
huron_arma21 <- arima(huron_depth,order=c(2,0,1))
huron_arma21

##
## Call:
## arima(x = huron_depth, order = c(2, 0, 1))
##
## Coefficients:
##          ar1     ar2     ma1  intercept
##      -0.0525  0.7910  1.0000   176.4603
## s.e.  0.0522  0.0526  0.0242     0.1210
##
## sigma^2 estimated as 0.04188:  log likelihood = 24.21,  aic = -38
```

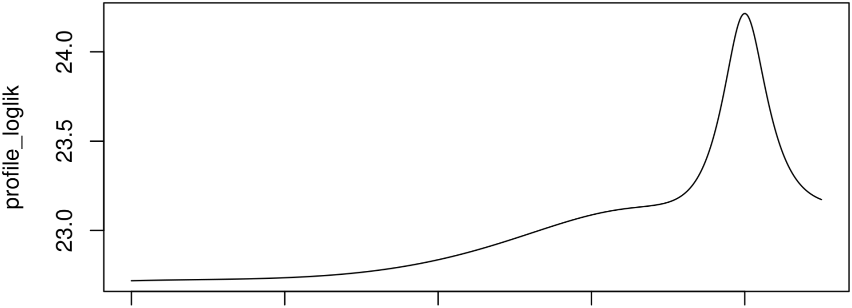
- We can examine the roots of the AR polynomial,

```
AR_roots <- polyroot(c(1,-coef(huron_arma21)[c("ar1","ar2")]))
AR_roots

## [1]  1.158084-0i -1.091669+0i
```

- These are just outside the unit circle, suggesting we have a stationary

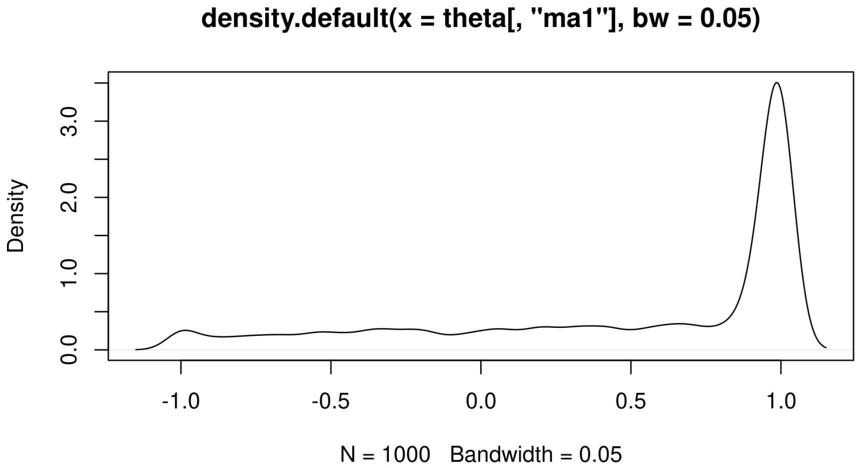
```r
K <- 500
ma1 <- seq(from=0.2,to=1.1,length=K)
profile_loglik <- rep(NA,K)
for(k in 1:K){
   profile_loglik[k] <- logLik(arima(huron_depth,order=c(2,0,1),
      fixed=c(NA,NA,ma1[k],NA)))
}
plot(profile_loglik~ma1,ty="l")
```



A simulation study

```
set.seed(57892330)
J <- 1000
params <- coef(huron_arma21)
ar <- params[grep("^ar",names(params))]
ma <- params[grep("^ma",names(params))]
intercept <- params["intercept"]
sigma <- sqrt(huron_arma21$sigma2)
theta <- matrix(NA,nrow=J,ncol=length(params),dimnames=list(NULL,nar
for(j in 1:J){
   Y_j <- arima.sim(
      list(ar=ar,ma=ma),
      n=length(huron_depth),
      sd=sigma
   )+intercept
   theta[j,] <- coef(arima(Y_j,order=c(2,0,1)))
}
hist(theta[,"ma1"],freq=FALSE)
```

```
plot(density(theta[,"ma1"],bw=0.05))
```



- Here, We look at the raw plot for instructional purposes. For a report, one should improve the default axis labels and title.
- Note that `arima` transforms the model to invertibility. Thus, the

```
require(doParallel)
registerDoParallel()
```

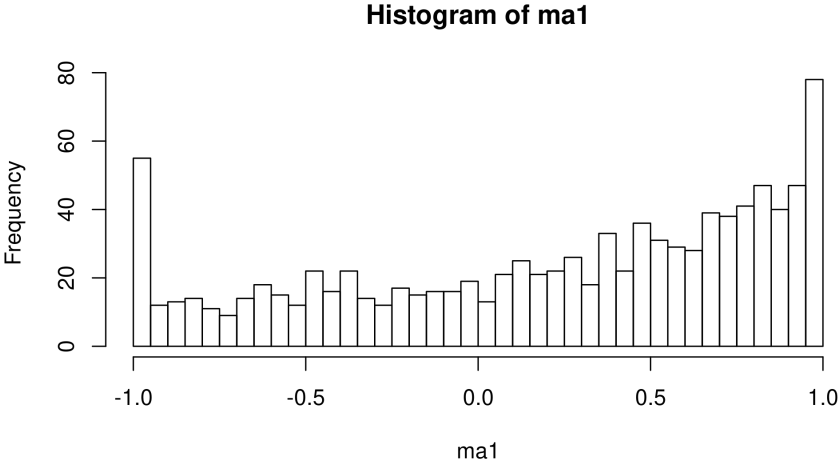
We can use foreach to carry out a parallel for loop where jobs are sent to different processors.

```
J <- 1000
huron_ar1 <- arima(huron_depth,order=c(1,0,0))
params <- coef(huron_ar1)
ar <- params[grep("^ar",names(params))]
intercept <- params["intercept"]
sigma <- sqrt(huron_ar1$sigma2)
t1 <- system.time(
  huron_sim <- foreach(j=1:J) %dopar% {
     Y_j <- arima.sim(list(ar=ar),n=length(huron_depth),sd=sigma)+i
     try(coef(arima(Y_j,order=c(2,0,1))))
  }
)
```

- Some of these arima calls did not successfully produce parameter estimates. The try function lets the simulation proceed despite these errors. Let's see how many of them fail:

- Now, for the remaining ones, we can look at the resulting estimates of the MA1 component:

```
ma1 <- unlist(lapply(huron_sim,function(x) if(!inherits(x,"try-erro
hist(ma1,breaks=50)
```



Question 5.6. What else could we look for to help diagnose, and understand, this kind of model fitting problem? Hint: pay some more attention to the roots of the fitted ARMA(2,1) model.

Assessing the numerical correctness of evaluation and maximization of the likelihood function

- We can probably suppose that `arima` has negligible numerical error in evaluating the likelihood.
- Likelihood evaluation is a linear algebra computation which should be numerically stable away from singularities.
- Possibly, numerical problems could arise for models very close to reducibility (canceling AR and MA roots).
- Numerical optimization is more problematic.
- `arima` calls the general purpose optimization routine `optim`.
- We know the likelihood surface can be multimodal and have nonlinear ridges; both these are consequences of the possibility of reducibility or near reducibility (AR and MA roots which almost cancel).
- No optimization procedure is reliable for maximizing awkward, non-convex functions.
- Evidence for imperfect maximization (assuming negligible likelihood evaluation error) can be found in the above AIC table, reproduced here:

	MA0	MA1	MA2	MA3	MA4	MA5
¡b¿ AR0¡/b¿	166.75	46.60	7.28	-14.97	-18.64	-26.09
¡b¿ AR1¡/b¿	-38.00	-37.41	-35.46	-33.82	-34.13	-32.20
¡b¿ AR2¡/b¿	-37.33	-38.43	-36.90	-34.93	-34.35	-33.08
¡b¿ AR3¡/b¿	-35.52	-35.17	-32.71	-31.38	-31.13	-32.98
¡b¿ AR4¡/b¿	-33.94	-34.91	-34.43	-36.27	-31.31	-30.90

Question 5.7. How is this table inconsistent with perfect maximization? Here are two hints:

- Recall that, for nested hypotheses $H^{\langle 0\rangle} \subset H^{\langle 1\rangle}$, the likelihood maximized over $H^{\langle 1\rangle}$ cannot be less than the likelihood maximized over $H^{\langle 0\rangle}$.
- Recall also the definition of AIC,
  AIC $=$ -2$\times$ maximized log likelihood $+$ 2$\times$ number of parameters

Acknowledgments and License

- These notes build on previous versions at `ionides.github.io/531w16` and `ionides.github.io/531w18`.