## AUTOMATIC

## MODEL SELECTION

## The linear regression model

Let

$$
\mathrm{y}=\left(\begin{array}{c}
\mathrm{y}_{1} \\
\vdots \\
\mathrm{y}_{\mathrm{n}}
\end{array}\right)
$$

be an n-dimensional random vector with mean vector $\mu=E y$ and covariance matrix $\sum=\operatorname{var}(y)$.

For the standard linear model, we assume that
$\mu=\left(\begin{array}{c}E y_{1} \\ \vdots \\ E y_{n}\end{array}\right)=\left(\begin{array}{c}\beta_{1} x_{11}+\ldots+\beta_{k} x_{1 k} \\ \vdots \\ \beta_{1} x_{n 1}+\ldots+\beta_{k} x_{n k}\end{array}\right)=\underbrace{\left(\begin{array}{ccc}x_{11} & \cdots & x_{1 k} \\ \vdots & \ddots & \vdots \\ x_{n 1} & \cdots & x_{n k}\end{array}\right)}_{x} \underbrace{\left(\begin{array}{c}\beta_{1} \\ \vdots \\ \beta_{k}\end{array}\right)}_{\beta}=X \beta$
and $\begin{aligned} \sum & =\left(\begin{array}{cccc}\operatorname{Var}\left(\mathrm{y}_{1}\right) & \operatorname{Cov}\left(\mathrm{y}_{1}, \mathrm{y}_{2}\right) & \cdots & \operatorname{Cov}\left(\mathrm{y}_{1}, \mathrm{y}_{\mathrm{n}}\right) \\ \operatorname{Cov}\left(\mathrm{y}_{2}, \mathrm{y}_{1}\right) & \operatorname{Var}\left(\mathrm{y}_{2}\right) & \cdots & \operatorname{Cov}\left(\mathrm{y}_{2}, \mathrm{y}_{\mathrm{n}}\right) \\ \vdots & \vdots & \ddots & \vdots \\ \operatorname{Cov}\left(\mathrm{y}_{\mathrm{n}}, \mathrm{y}_{1}\right) & \operatorname{Cov}\left(\mathrm{y}_{\mathrm{n}}, \mathrm{y}_{2}\right) & \cdots & \operatorname{Var}\left(\mathrm{y}_{\mathrm{n}}\right)\end{array}\right) \\ & =\left(\begin{array}{cccc}\sigma^{2} & 0 & \cdots & 0 \\ 0 & \sigma^{2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sigma^{2}\end{array}\right)=\sigma^{2}\left(\begin{array}{cccc}1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1\end{array}\right)=\sigma^{2} \mathrm{I},\end{aligned}$
where the k columns of the matrix X (the k regressors) are linearly independent.

## Likelihood function of the linear model

If $\mathrm{y}=\left(\mathrm{y}_{1}, \ldots, \mathrm{y}_{\mathrm{k}}\right)^{\mathrm{T}}$ has a multivariate normal distribution with a diagonal covariance matrix, the multivariate normal density $f\left(y_{1}, \ldots, y_{k}\right)$ factors into $n$ univariate normal densities:

$$
\begin{aligned}
f\left(y_{1}, \ldots, y_{k}\right) & =\prod_{t=1}^{n} f_{t}\left(y_{t}\right) \\
& =\prod_{t=1}^{n} \frac{1}{\sqrt{2 \pi \operatorname{Var}\left(y_{t}\right)}} \exp \left(-\frac{\left(y_{t}-E y_{t}\right)^{2}}{2 \operatorname{Var}\left(y_{t}\right)}\right)
\end{aligned}
$$

Under the assumptions $E y=X \beta$ and $\operatorname{var}(y)=\sigma^{2} I$ of the linear model we have

$$
\begin{aligned}
f\left(y_{1}, \ldots, y_{k}\right) & =\prod_{t=1}^{n} \frac{1}{\sqrt{2 \pi \sigma^{2}}} \exp \left(-\frac{\left(y_{t}-E y_{t}\right)^{2}}{2 \sigma^{2}}\right) \\
& =\left(2 \pi \sigma^{2}\right)^{-\frac{n}{2}} \exp \left(-\frac{1}{2 \sigma^{2}} \sum_{t=1}^{n}\left(y_{t}-\beta_{1} x_{t 1}-\ldots-\beta_{k} x_{t k}\right)^{2}\right)
\end{aligned}
$$

This density is a function of $\mathrm{y}_{1}, \ldots, \mathrm{y}_{\mathrm{k}}$ with fixed model parameters $\beta_{1}, \ldots, \beta_{\mathrm{k}}$, and $\sigma^{2}$. When we want to stress the dependence of the density on the model parameters, we write $f\left(y_{1}, \ldots, y_{k} ; \beta_{1}, \ldots, \beta_{\mathrm{k}}, \sigma^{2}\right)$ instead of $f\left(y_{1}, \ldots, y_{k}\right)$.
Viewing $f\left(y_{1}, \ldots, y_{k} ; \beta_{1}, \ldots, \beta_{\mathrm{k}}, \sigma^{2}\right)$ as a function of $\beta_{1}, \ldots, \beta_{\mathrm{k}}$, and $\sigma^{2}$ with $\mathrm{y}_{1}, \ldots, \mathrm{y}_{\mathrm{k}}$ fixed, we obtain the likelihood function of the linear model:

$$
\mathrm{L}\left(\beta_{1}, \ldots, \beta_{\mathrm{k}}, \sigma^{2} ; \mathrm{y}_{1}, \ldots, \mathrm{y}_{\mathrm{k}}\right)=\mathrm{f}\left(\mathrm{y}_{1}, \ldots, \mathrm{y}_{\mathrm{k}} ; \beta_{1}, \ldots, \beta_{\mathrm{k}}, \sigma^{2}\right)
$$

## ML estimators for the model parameters

The maximum likelihood (ML) estimators for the model parameters are obtained by maximizing the likelihood function or equivalently the log likelihood function

$$
\begin{aligned}
& \log L\left(\beta_{1}, \ldots, \beta_{k}, \sigma^{2} ; y_{1}, \ldots, y_{k}\right) \\
& \quad=-\frac{n}{2} \log \left(2 \pi \sigma^{2}\right)-\frac{1}{2 \sigma^{2}} \sum_{t=1}^{n}\left(y_{t}-\beta_{1 x_{t 1}-\ldots-\beta_{k} x_{t k}}\right)^{2} .
\end{aligned}
$$

Setting the partial derivatives of the log likelihood with respect to $\beta_{1}, \ldots, \beta_{\mathrm{k}}$, and $\sigma^{2}$ to zero gives

$$
\begin{gathered}
-\frac{1}{2 \sigma^{2}} \sum_{\mathrm{t}=1}^{\mathrm{n}} 2\left(\mathrm{y}_{\mathrm{t}}-\beta_{1 \mathrm{x}} \mathrm{x}_{\mathrm{t}}-\ldots-\beta_{\mathrm{k}} \mathrm{x}_{\mathrm{t}}\right)\left(-\mathrm{x}_{\mathrm{tj}}\right)=0, \mathrm{j}=1, \ldots, \mathrm{k}, \\
-\frac{\mathrm{n}}{2} \frac{1}{\sigma^{2}}+\frac{1}{2 \sigma^{4}} \sum_{\mathrm{t}=1}^{\mathrm{n}}\left(\mathrm{y}_{\mathrm{t}}-\beta_{\left.1 \mathrm{x}_{\mathrm{t} 1}-\ldots-\beta_{\mathrm{k}} \mathrm{x}_{\mathrm{tk}}\right)^{2}=0,} .\right.
\end{gathered}
$$

which is equivalent to

$$
-\frac{1}{\sigma^{2}}(y-X \beta)^{\mathrm{T}} X=0,-\frac{n}{\sigma^{2}}+\frac{1}{\sigma^{4}}(y-X \beta)^{\mathrm{T}}(y-X \beta)=0
$$

and also to

$$
X^{T}(y-X \beta)=0,-n \sigma^{2}+(y-X \beta)^{T}(y-X \beta)=0
$$

and finally also to

$$
X^{T} y=X^{T} X \beta,(y-X \beta)^{T}(y-X \beta)=n \sigma^{2} .
$$

Thus

$$
\hat{\beta}=\left(\hat{\beta}_{1}, \ldots, \hat{\beta}_{k}\right)^{\mathrm{T}}=\left(X^{\mathrm{T}} X\right)^{-1} X^{\mathrm{T}} y, \hat{\sigma}^{2}=\frac{1}{n}(\mathrm{y}-\mathrm{X} \hat{\boldsymbol{\beta}})^{\mathrm{T}}(\mathrm{y}-\mathrm{X} \hat{\boldsymbol{\beta}}) .
$$

## Geometrical interpretation

$\mathrm{X} \hat{\beta}=\mathrm{X}\left(\mathrm{X}^{\mathrm{T}} \mathrm{X}\right)^{-1} \mathrm{X}^{\mathrm{T}} \mathrm{y}$ is the projection of y onto the subspace of $\mathbb{R}^{n}$ spanned by the columns $\mathrm{x}_{1}, \ldots, \mathrm{x}_{\mathrm{k}}$ of X because

$$
X \hat{\beta}=\left(\begin{array}{c}
\hat{\beta}_{1} x_{11}+\ldots+\hat{\beta}_{k} x_{1 k} \\
\vdots \\
\hat{\beta}_{1} x_{n 1}+\ldots+\hat{\beta}_{k} x_{n k}
\end{array}\right)=\hat{\beta}_{1}\left(\begin{array}{c}
x_{11} \\
\vdots \\
x_{n 1}
\end{array}\right)+\ldots+\hat{\beta}_{\mathrm{k}}\left(\begin{array}{c}
x_{1 \mathrm{k}} \\
\vdots \\
x_{\mathrm{nk}}
\end{array}\right)
$$

is an element of $\operatorname{span}\left(\mathrm{x}_{1}, \ldots, \mathrm{x}_{\mathrm{k}}\right)$ and

$$
\left(\begin{array}{c}
x_{1}^{T} \\
\vdots \\
x_{k}^{T}
\end{array}\right)(y-X \hat{\beta})=X^{T}(y-X \hat{\beta})=X^{T} y-X^{T} X\left(X^{T} X\right)^{-1} X^{T} y=0,
$$

which implies that $y-X \hat{\beta}$ is an element of the orthogonal complement of $\operatorname{span}\left(\mathrm{x}_{1}, \ldots, \mathrm{x}_{\mathrm{k}}\right)$.
Analogously, $y-X \hat{\beta}=\left(I-X\left(X^{T} X\right)^{-1} X^{T}\right) y$ is the projection of $y$ onto the orthogonal complement of $\operatorname{span}\left(\mathrm{x}_{1}, \ldots, \mathrm{x}_{\mathrm{k}}\right)$ because

$$
y-X \hat{\beta} \in\left(\operatorname{span}\left(x_{1}, \ldots, x_{k}\right)\right)^{\perp}
$$

and

$$
y-(y-X \hat{\beta})=X \hat{\beta} \in \operatorname{span}\left(x_{1}, \ldots, x_{k}\right)=\left(\left(\operatorname{span}\left(x_{1}, \ldots, x_{k}\right)\right)^{\perp}\right)^{\perp} .
$$

Exercise: Show that the matrices

$$
P_{X}=X\left(X^{T} X\right)^{-1} X^{T}, P_{X^{\perp}}=I-X\left(X^{T} X\right)^{-1} X^{T}
$$

are symmetric and idempotent.

## Expected values of the ML estimators

$\hat{\beta}=\left(X^{T} X\right)^{-1} X^{T} y$ is an unbiased estimator for $\beta$ because

$$
E \hat{\beta}=\left(X^{T} X\right)^{-1} X^{T} E y=\left(X^{T} X\right)^{-1} X^{T} X \beta=\beta .
$$

Furthermore, using

$$
E P_{x^{\perp}} y=E(y-X \hat{\beta})=E y-E X \hat{\beta}=X \beta-X E \hat{\beta}=X \beta-X \beta=0
$$

we obtain

$$
\begin{aligned}
& E(y-X \hat{\beta})^{T}(y-X \hat{\beta})=E\left(P_{x^{\perp}} y\right)^{T}\left(P_{x^{\perp}} y\right)=E \operatorname{tr}\left(P_{x^{\perp}} y\right)^{T} P_{x^{\perp}} y \\
& =E \operatorname{tr} \mathrm{P}_{\mathrm{x}^{\perp}} \mathrm{y}\left(\mathrm{P}_{\mathrm{x}^{\perp}} \mathrm{y}\right)^{\mathrm{T}}=\operatorname{trE} \mathrm{P}_{\mathrm{x}^{\perp}} \mathrm{y}\left(\mathrm{P}_{\mathrm{x}^{\perp}} \mathrm{y}\right)^{\mathrm{T}} \\
& =\operatorname{trvar}\left(\mathrm{P}_{\mathrm{x}^{\perp}} \mathrm{y}\right)=\operatorname{tr} \mathrm{P}_{\mathrm{x}^{\perp}} \operatorname{var}(\mathrm{y}) \mathrm{P}_{\mathrm{x}^{\perp}}^{\mathrm{T}} \\
& =\operatorname{tr}_{\mathrm{X}^{\perp}} \sigma^{2} \mathrm{IP}_{\mathrm{X}^{\perp}}=\sigma^{2} \operatorname{tr} \mathrm{P}_{\mathrm{X}^{\perp}} \mathrm{P}_{\mathrm{X}^{\perp}} \\
& =\sigma^{2} \operatorname{tr}_{\mathrm{X}^{\perp}}=\sigma^{2} \operatorname{tr}\left(\mathrm{I}-\mathrm{X}\left(\mathrm{X}^{\mathrm{T}} \mathrm{X}\right)^{-1} \mathrm{X}^{\mathrm{T}}\right) \\
& =\sigma^{2}\left(\operatorname{trI}-\operatorname{tr} X\left(\mathrm{X}^{\mathrm{T}} \mathrm{X}\right)^{-1} \mathrm{X}^{\mathrm{T}}\right) \\
& =\sigma^{2}(\operatorname{tr} \underbrace{I}_{n \times n}-\operatorname{tr} \underbrace{X^{T} X\left(X^{T} X\right)^{-1}}_{k \times k})=\sigma^{2}(n-k) \text {. }
\end{aligned}
$$

Thus

$$
E \hat{\sigma}^{2}=E \frac{1}{n}(y-X \hat{\beta})^{T}(y-X \hat{\beta})=\frac{n-k}{n} \sigma^{2}
$$

Exercise: Show that

$$
\operatorname{Cov}(X \hat{\beta}, y-X \hat{\beta})=0 .
$$

## The final prediction error criterion

Let y and z be independent and identically distributed (i.i.d.) normal random vectors with mean vector $X \beta$ and covariance matrix $\sigma^{2}$ I.
Using the ML estimate $\hat{\beta}=\left(X^{T} X\right)^{-1} X^{T} y$ obtained from y we may predict $z$ by $X \hat{\beta}$. It follows from

$$
\begin{aligned}
& 2 \sigma^{2} \mathrm{I}=\operatorname{Var}(\mathrm{z})+\operatorname{Var}(\mathrm{y})=\operatorname{Var}(\mathrm{z}-\mathrm{y})=\operatorname{Var}((\mathrm{z}-\mathrm{X} \hat{\beta})-(\mathrm{y}-\mathrm{X} \hat{\beta})) \\
= & \operatorname{Var}(\mathrm{z}-\mathrm{X} \hat{\beta})-2 \operatorname{Cov}(\mathrm{z}-X \hat{\beta}, \mathrm{y}-X \hat{\beta})+\operatorname{Var}(\mathrm{y}-X \hat{\beta}) \\
= & \operatorname{Var}(\mathrm{z}-\mathrm{X} \hat{\beta})-2 \operatorname{Cov}(\mathrm{z}, \mathrm{y}-X \hat{\beta})+2 \operatorname{Cov}(X \hat{\beta}, y-X \hat{\beta})+\operatorname{Var}(y-X \hat{\beta}) \\
= & \operatorname{Var}(\mathrm{z}-X \hat{\beta})+\operatorname{Var}(y-X \hat{\beta}) \\
= & \mathrm{E}(\mathrm{z}-X \hat{\beta})(\mathrm{z}-X \hat{\beta})^{\mathrm{T}}+\mathrm{E}(\mathrm{y}-\mathrm{X} \hat{\beta})(\mathrm{y}-X \hat{\beta})^{\mathrm{T}}
\end{aligned}
$$

that

$$
\begin{aligned}
& 2 \mathrm{n} \sigma^{2}=\operatorname{tr}\left(2 \sigma^{2} \mathrm{I}\right)=\mathrm{Etr}(\mathrm{z}-\mathrm{X} \hat{\beta})(\mathrm{z}-\mathrm{X} \hat{\boldsymbol{\beta}})^{\mathrm{T}}+\mathrm{Etr}(\mathrm{y}-\mathrm{X} \hat{\boldsymbol{\beta}})(\mathrm{y}-\mathrm{X} \hat{\boldsymbol{\beta}})^{\mathrm{T}} \\
& =E \operatorname{tr}(z-X \hat{\beta})^{T}(z-X \hat{\beta})+E \operatorname{tr}(y-X \hat{\beta})^{T}(y-X \hat{\beta}) \\
& =E(z-X \hat{\beta})^{T}(z-X \hat{\beta})+E(y-X \hat{\beta})^{T}(y-X \hat{\beta}) \\
& =E(z-X \hat{\beta})^{T}(z-X \hat{\beta})+(n-k) \sigma^{2} \text {. }
\end{aligned}
$$

Thus, the mean squared prediction error is given by

$$
\frac{1}{n} E(z-X \hat{\beta})^{T}(z-X \hat{\beta})=\frac{n+k}{n} \sigma^{2}
$$

and an unbiased estimator for it is

$$
\operatorname{FPE}(\mathrm{k})=\frac{\mathrm{n}+\mathrm{k}}{\mathrm{n}} \frac{\mathrm{n}}{\mathrm{n}-\mathrm{k}} \hat{\sigma}^{2}=\frac{\mathrm{n}+\mathrm{k}}{\mathrm{n}-\mathrm{k}} \hat{\sigma}^{2}=\left(1+\frac{2 \mathrm{k}}{\mathrm{n}-\mathrm{k}}\right) \hat{\sigma}^{2} .
$$

## The corrected AIC

Let $y$ and $z$ be i.i.d. $N\left(X \beta, \sigma^{2} I\right)$ and

$$
\hat{\beta}=\left(X^{T} X\right)^{-1} X^{T} y, \hat{\sigma}^{2}=\frac{1}{n}(y-X \hat{\beta})^{T}(y-X \hat{\beta})
$$

A measure that is somehow related to the mean squared prediction error is

$$
\mathrm{E}\left(-2 \log \mathrm{f}\left(\mathrm{z} ; \hat{\beta}, \hat{\sigma}^{2}\right)\right)=\mathrm{E}\left(\mathrm{n} \log (2 \pi)+\mathrm{n} \log \hat{\sigma}^{2}+\frac{\left(\mathrm{z}-\mathrm{X} \hat{)^{\mathrm{T}}}(\mathrm{z}-\mathrm{X} \hat{\beta})\right.}{\hat{\sigma}^{2}}\right)
$$

Here $f\left(z ; \hat{\beta}, \hat{\sigma}^{2}\right)$ is viewed as a function of $z, \hat{\beta}$, and $\hat{\sigma}^{2}$. Clearly, the naïve estimator

$$
-2 \log \mathrm{f}\left(\mathrm{y} ; \hat{\beta}, \hat{\sigma}^{2}\right)
$$

underestimates $\mathrm{E}\left(-2 \log \mathrm{f}\left(\mathrm{z} ; \hat{\beta}, \hat{\sigma}^{2}\right)\right)$. It follows from

$$
\begin{aligned}
& \mathrm{E}\left[-2 \log \mathrm{f}\left(\mathrm{z} ; \hat{\beta}, \hat{\sigma}^{2}\right)\right]-\mathrm{E}\left[-2 \log \mathrm{f}\left(\mathrm{y} ; \hat{\beta}, \hat{\sigma}^{2}\right)\right] \\
= & \mathrm{E} \frac{(\mathrm{z}-\mathrm{X} \hat{\beta})^{\mathrm{T}}(\mathrm{z}-\mathrm{X} \hat{\beta})}{\hat{\sigma}^{2}}-\mathrm{E} \frac{\left(\mathrm{y}-\mathrm{X} \hat{)^{T}}(\mathrm{y}-\mathrm{X} \hat{\beta})\right.}{\hat{\sigma}^{2}} \\
= & \mathrm{E}(\mathrm{z}-\mathrm{X} \hat{\beta})^{\mathrm{T}}(\mathrm{z}-\mathrm{X} \hat{\beta}) \frac{\mathrm{n}}{\sigma^{2}} \mathrm{E}\left(\frac{1}{\frac{n \hat{\sigma}^{2}}{\sigma^{2}}}\right)-\mathrm{n} \\
= & \operatorname{tr}(\operatorname{var}(\mathrm{z})+\operatorname{var}(\mathrm{X} \hat{\beta})) \frac{\mathrm{n}}{\sigma^{2}} \frac{1}{\mathrm{n}-\mathrm{k}-2}-\mathrm{n} \\
= & (\mathrm{n}+\mathrm{k}) \sigma^{2} \frac{\mathrm{n}}{\sigma^{2}} \frac{1}{n-k-2}-\mathrm{n} \\
= & 2(\mathrm{k}+1)+\frac{2 \mathrm{k}^{2}+6 \mathrm{k}+4}{\mathrm{n}-\mathrm{k}-2}
\end{aligned}
$$

that

$$
\operatorname{AIC}_{C}(\mathrm{k})=-2 \log \mathrm{f}\left(\mathrm{y} ; \hat{\beta}, \hat{\sigma}^{2}\right)+2(\mathrm{k}+1)+\frac{2 \mathrm{k}^{2}+6 \mathrm{k}+4}{\mathrm{n}-\mathrm{k}-2}
$$

is an unbiased estimator for $\mathrm{E}\left[-2 \log \mathrm{f}\left(\mathrm{z} ; \hat{\boldsymbol{\beta}}, \hat{\sigma}^{2}\right)\right]$.

Exercise: Check each step in the derivation of $\mathrm{AIC}_{\mathrm{C}}$. You may use the following facts:
(i) The statistics $\hat{\beta}$ and $\hat{\sigma}^{2}$ are independent.
(ii) $\hat{\beta} \sim N\left(\beta, \sigma^{2}\left(X^{T} X\right)^{-1}\right), n \hat{\sigma}^{2} / \sigma^{2} \sim \chi^{2}(n-k)$
(iii) $\mathrm{X} \sim \chi^{2}(\mathrm{j}) \Rightarrow \mathrm{E} \frac{1}{\mathrm{X}}=\frac{1}{\mathrm{j}-2}$

Up to now we have never questioned the assumption that the design matrix X containing the regressors is given. In practice, we rarely know a priori which regressors should be included in a regression model and must therefore select the design matrix from a set of candidate matrices. A possible strategy is to select that $\mathrm{n} \times \mathrm{k}$ matrix which minimizes $\operatorname{FPE}(\mathrm{k})$ or $\mathrm{AIC}_{\mathrm{C}}(\mathrm{k})$.
While $\hat{\sigma}^{2}$ can only decrease if additional variables are included, the terms

$$
1+\frac{2 \mathrm{k}}{\mathrm{n}-\mathrm{k}}
$$

and

$$
2(k+1)+\frac{2 k^{2}+6 k+4}{n-k-2}
$$

occurring in $\operatorname{FPE}(\mathrm{k})$ and $\mathrm{AIC}_{\mathrm{C}}(\mathrm{k})$, respectively, increase as the number of regressors k increases and therefore serve as penalty terms to prevent overparametrization.
An apparent flaw of this model selection approach is that $\operatorname{FPE}(\mathrm{k})$ and $\mathrm{AIC}_{\mathrm{C}}(\mathrm{k})$ have been derived under the assumption that the mean of y can be written as a linear combination of the columns of X. Why should all candidate matrices satisfy this assumption?

At second glance, model selection with $\operatorname{FPE}(\mathrm{k})$ or $\mathrm{AIC}_{\mathrm{C}}(\mathrm{k})$ is not so absurd after all, because the chances of selecting a too small (misspecified) model disappear as n increases. So the real challenge is to avoid choosing a too large model. But FPE(k) and $\mathrm{AIC}_{\mathrm{C}}(\mathrm{k})$ are particularly suitable for comparing the correct model with larger models, because all of these models are correctly specified.

Exercise: Show that the minimization of

$$
\operatorname{AIC}_{C}(k)=-2 \log f\left(y ; \hat{\beta}, \hat{\sigma}^{2}\right)+2(k+1)+\frac{2 k^{2}+6 k+4}{n-k-2}
$$

is equivalent to the minimization of

$$
n \log \hat{\sigma}^{2}+2(k+1)+\frac{2 k^{2}+6 k+4}{n-k-2} .
$$

If we ignore the last term occurring in $\operatorname{AIC}_{\mathrm{C}}(\mathrm{k})$, which vanishes as n increases, we obtain

$$
\operatorname{AIC}(\mathrm{k})=-2 \log \mathrm{f}\left(\mathrm{y} ; \hat{\beta}, \hat{\sigma}^{2}\right)+2(\mathrm{k}+1)
$$

Here the penalty term is just two times the number of model parameters. (The parameters in the linear regression model are $\beta_{1}, \ldots, \beta_{\mathrm{k}}$, and $\sigma^{2}$.)

Exercise: Show that the minimization of

$$
\operatorname{FPE}(\mathrm{k})=\left(1+\frac{2 \mathrm{k}}{\mathrm{n}-\mathrm{k}}\right) \hat{\sigma}^{2}
$$

is roughly equivalent to the minimization of $\operatorname{AIC}(\mathrm{k})$.
Hint: $\log (1+\varepsilon) \approx \varepsilon$

We might expect that

$$
\operatorname{AIC}(\mathrm{k})=-2 \log \mathrm{f}\left(\mathrm{y} ; \hat{\beta}, \hat{\sigma}^{2}\right)+2(\mathrm{k}+1)
$$

which has been derived as an asymptotically unbiased estimator for

$$
\mathrm{E}\left[-2 \log \mathrm{f}\left(\mathrm{z} ; \hat{\mathrm{\beta}}, \hat{\sigma}^{2}\right)\right]
$$

in the framework of the linear regression model

$$
y_{\mathrm{t}}=\beta_{1} \mathrm{x}_{\mathrm{t} 1}+\ldots+\beta_{\mathrm{k}} \mathrm{x}_{\mathrm{tk}}+\mathrm{u}_{\mathrm{t}}
$$

can also be used when $y=\left(y_{1}, \ldots, y_{n}\right)^{T}$ comes from $a$ Gaussian AR(p) model

$$
y_{t}=\phi_{1} y_{t-1}+\ldots+\phi_{p} y_{t-p}+u_{t}
$$

with parameters $\phi_{1}, \ldots, \phi_{p}$, and $\sigma^{2}=\operatorname{var}\left(u_{t}\right)$.
Indeed, if $\hat{\phi}=\left(\hat{\phi}_{1}, \ldots, \hat{\phi}_{\mathrm{p}}\right)^{\mathrm{T}}$ and $\hat{\sigma}^{2}$ are the ML estimators for the model parameters and $\mathrm{z}=\left(\mathrm{z}_{1}, \ldots, \mathrm{z}_{\mathrm{n}}\right)^{\mathrm{T}}$ is an independent series from the same $\operatorname{AR}(\mathrm{p})$ model, then

$$
\operatorname{AIC}(p)=-2 \log \mathrm{f}\left(\mathrm{y} ; \hat{\phi}, \hat{\sigma}^{2}\right)+2(\mathrm{p}+1)
$$

is an approximately unbiased estimator for

$$
\mathrm{E}\left[-2 \log \mathrm{f}\left(\mathrm{z} ; \hat{\phi}, \hat{\sigma}^{2}\right)\right]
$$

Analogously, in the case of an ARMA(p,q) model

$$
\mathrm{y}_{\mathrm{t}}=\phi_{1} \mathrm{y}_{\mathrm{t}-1}+\ldots+\phi_{\mathrm{p}} \mathrm{y}_{\mathrm{t}-\mathrm{p}}+\mathrm{u}_{\mathrm{t}}+\theta_{1} \mathrm{u}_{\mathrm{t}-1}+\ldots+\theta_{\mathrm{q}} \mathrm{u}_{\mathrm{t}-\mathrm{q}}
$$

we may use

$$
\operatorname{AIC}(\mathrm{p}, \mathrm{q})=-2 \log \mathrm{f}\left(\mathrm{y} ; \hat{\phi}, \hat{\theta}, \hat{\sigma}^{2}\right)+2(\mathrm{p}+\mathrm{q}+1)
$$

## The likelihood function for an AR(1) model

Suppose that $\mathrm{y}=\left(\mathrm{y}_{1}, \ldots, \mathrm{y}_{\mathrm{n}}\right)^{\mathrm{T}}$ comes from a Gaussian AR(1) model represented by

$$
y_{t}=\phi y_{t-1}+u_{t}
$$

or, equivalently, by

$$
y_{t}=\phi\left(\phi y_{t-2}+u_{t-1}\right)+u_{t}=\phi\left(\phi\left(\phi y_{t-3}+u_{t-2}\right)+u_{t-1}\right)+u_{t}=\ldots=\sum_{j=0}^{\infty} \phi^{j} u_{t-j}
$$

where $\mid \phi<1$ and the errors $u_{t}$ are i.i.d. $\mathrm{N}\left(0, \sigma^{2}\right)$. Then

$$
E y_{\mathrm{t}}=\sum_{\mathrm{j}=0}^{\infty} \phi^{\mathrm{j}} E \mathrm{u}_{\mathrm{t}-\mathrm{j}}=0
$$

and for $\mathrm{h} \geq 0$

$$
\begin{aligned}
\gamma(\mathrm{h}) & =\operatorname{cov}\left(y_{t}, \mathrm{y}_{\mathrm{th}}\right)=E \mathrm{E}_{\mathrm{t}} \mathrm{y}_{\mathrm{t}-\mathrm{h}} \\
& =\mathrm{E}\left(\mathrm{u}_{\mathrm{t}}+\phi \mathrm{u}_{\mathrm{t}-1}+\phi^{2} \mathrm{u}_{\mathrm{t}-2}+\ldots\right)\left(\mathrm{u}_{\mathrm{th}}+\phi \mathrm{u}_{\mathrm{th}-1}+\phi^{2} \mathrm{u}_{\mathrm{th}-2}+\ldots\right) \\
& =\sigma^{2}\left(\phi^{\mathrm{h}} \phi^{0}+\phi^{\mathrm{h}+1} \phi^{1}+\phi^{\mathrm{h}+2} \phi^{2}+\ldots\right)=\sigma^{2} \phi^{\mathrm{h}} \sum_{\mathrm{j}=0}^{\infty}\left(\phi^{2}\right)^{\mathrm{j}}=\frac{\sigma^{2}}{1-\phi^{2}}{ }^{\mathrm{h}} .
\end{aligned}
$$

The ML estimates are obtained by finding the values of $\phi$ and $\sigma^{2}$ which maximize

$$
\mathrm{f}\left(\mathrm{y}_{1}, \ldots, \mathrm{y}_{\mathrm{n}} ; \phi, \sigma^{2}\right)=(2 \pi)^{-\frac{\mathrm{n}}{2}}(\operatorname{det} \Gamma)^{-\frac{1}{2}} \exp \left(-\frac{1}{2} \mathrm{y}^{\mathrm{T}} \Gamma^{-1} \mathrm{y}\right)
$$

where $\Gamma=$ Eyy ${ }^{\text {T }}$ depends on $\phi$ and $\sigma^{2}$.
This maximization problem can only be solved numerically but not analytically.

Exercise: Show that

$$
\Gamma=\frac{\sigma^{2}}{1-\phi^{2}}\left(\begin{array}{cccc}
1 & \phi & \cdots & \phi^{n-1} \\
\phi & 1 & \cdots & \phi^{n-2} \\
\vdots & \vdots & \ddots & \vdots \\
\phi^{n-1} & \phi^{n-2} & \cdots & 1
\end{array}\right)
$$

and

$$
\Gamma^{-1}=\frac{1}{\sigma^{2}}\left(\begin{array}{ccccc}
1 & -\phi & 0 & \cdots & 0 \\
-\phi & 1+\phi^{2} & -\phi & \cdots & 0 \\
0 & -\phi & 1+\phi^{2} & \cdots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & \cdots & 1
\end{array}\right) .
$$

Exercise: Show that $\Gamma^{-1}=L^{T} L$, where

$$
\mathrm{L}=\frac{1}{\sigma}\left(\begin{array}{ccccc}
\sqrt{1-\phi^{2}} & 0 & 0 & \cdots & 0 \\
-\phi & 1 & 0 & \cdots & 0 \\
0 & -\phi & 1 & \cdots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & \cdots & 1
\end{array}\right) .
$$

Exercise: Show that $\operatorname{det} \Gamma=\frac{\sigma^{2 n}}{1-\phi^{2}}$.

## The conditional likelihood function

The joint density of a sample $y=\left(y_{1}, \ldots, y_{n}\right)^{T}$ from a Gaussian AR(1) model represented by

$$
y_{t}=\phi y_{t-1}+u_{t}
$$

can be written as

$$
\begin{aligned}
f\left(y_{1}, \ldots, y_{n}\right) & =f\left(y_{n} \mid y_{1}, \ldots, y_{n-1}\right) f\left(y_{1}, \ldots, y_{n-1}\right) \\
& =f\left(y_{n} \mid y_{1}, \ldots, y_{n-1}\right) f\left(y_{n-1} \mid y_{1}, \ldots, y_{n-2}\right) f\left(y_{1}, \ldots, y_{n-2}\right) \\
& \vdots \\
& =f\left(y_{n} \mid y_{1}, \ldots, y_{n-1}\right) \ldots f\left(y_{2} \mid y_{1}\right) f\left(y_{1}\right) .
\end{aligned}
$$

If $u_{t} \sim N\left(0, \sigma^{2}\right), y_{t-1}$ is fixed, and $y_{t}=\phi y_{t-1}+u_{t}$, then

$$
y_{t} \sim N\left(\phi y_{t-1}, \sigma^{2}\right) .
$$

Thus,

$$
\begin{aligned}
\mathrm{f}\left(\mathrm{y}_{\mathrm{t}} \mid \mathrm{y}_{1}, \ldots, \mathrm{y}_{\mathrm{t}-1}\right) & =\mathrm{f}\left(\mathrm{y}_{\mathrm{t}} \mathrm{y}_{\mathrm{t}-1}\right) \\
& =\left(2 \pi \sigma^{2}\right)^{-\frac{1}{2}} \exp \left(-\frac{1}{2 \sigma^{2}}\left(\mathrm{y}_{\mathrm{t}}-\phi \mathrm{y}_{\mathrm{t}-1}\right)^{2}\right)
\end{aligned}
$$

and

$$
\begin{aligned}
f\left(y_{n}, \ldots, y_{2} \mid y_{1}\right) & =f\left(y_{n} \mid y_{1}, \ldots, y_{n-1}\right) \ldots f\left(y_{2} \mid y_{1}\right) \\
& =f\left(y_{n} \mid y_{n-1}\right) \ldots f\left(y_{2} \mid y_{1}\right) \\
& =\left(2 \pi \sigma^{2}\right)^{-\frac{n-1}{2}} \exp \left(-\frac{1}{2 \sigma^{2}} \sum_{t=2}^{n}\left(y_{t}-\phi y_{t-1}\right)^{2}\right) .
\end{aligned}
$$

Exercise: Show that maximizing

$$
\log \mathrm{f}\left(\mathrm{y}_{\mathrm{n}}, \ldots, \mathrm{y}_{2} \mid \mathrm{y}_{1}\right)=-\frac{\mathrm{n}-1}{2} \log \left(2 \pi \sigma^{2}\right)-\frac{1}{2 \sigma^{2}} \sum_{\mathrm{t}=2}^{\mathrm{n}}\left(\mathrm{y}_{\mathrm{t}}-\phi \mathrm{y}_{\mathrm{t}-1}\right)^{2}
$$

gives the ordinary least squares (OLS) estimate

$$
\widehat{\phi}=\frac{\sum_{\mathrm{t}=2}^{\mathrm{n}} \mathrm{y}_{\mathrm{t}} \mathrm{y}_{\mathrm{t}-1}}{\sum_{\mathrm{t}=2}^{\mathrm{n} y_{\mathrm{t}-1}^{2}}}
$$

Multiplying the conditional likelihood function by $f\left(y_{1}\right)$ we obtain the full likelihood function, i.e.,

$$
\mathrm{f}\left(\mathrm{y}_{1}, \ldots, \mathrm{y}_{\mathrm{n}}\right)=\mathrm{f}\left(\mathrm{y}_{\mathrm{n}}, \ldots, \mathrm{y}_{2} \mid \mathrm{y}_{1}\right) \mathrm{f}\left(\mathrm{y}_{1}\right)
$$

It follows from $\operatorname{Var}\left(\mathrm{y}_{1}\right)=\frac{\sigma^{2}}{1-\phi^{2}}$ that

$$
\mathrm{f}\left(\mathrm{y}_{1}\right)=\left(2 \pi \frac{\sigma^{2}}{1-\phi^{2}}\right)^{-\frac{1}{2}} \exp \left(-\frac{1-\phi^{2}}{2 \sigma^{2}} \mathrm{y}_{1}^{2}\right)
$$

