PSTAT 126

Regression Analysis

Laura Baracaldo

Lecture 8
Transformations and Generalized Least Squares

Violation of Assumptions

We can order model assumptions according to their importance:

- The systematic form of the model. Wrong assumptions lead to inaccurate predictions.
- ② Dependence of errors. We may overlook information about more complex structures.
- Non-constant variance. Wrong quantification of of prediction uncertainty, however, inference may not be seriously compromised.
- Normality. For large data sets, the inference will be robust to a lack of normality (due to the Central limit theorem (CLT)), unless the errors are extremely abnormal.

Laura Baracaldo PSTAT 126 2 / 35

How to overcome Assumptions Violations?

- When linear dependence between the response y and the predictors X is violated we can opt for **Transformations** of the response and/or predictors.
- Dependence and heteroscedasticity of the errors can be fixed by changing the covariance matrix structure of the errors - Generalized Least Squares (GLS).

Laura Baracaldo PSTAT 126 3 / 35

Transforming the Response

Suppose that the true response-predictors relationship can be written as:

$$y = \exp(\beta_0 + \beta_1 x_1 + \ldots + \beta_p x_p) \exp(\epsilon)$$

- The dependency between the response and the set of predictors is not linear.
- The random error ϵ enters the model *multiplicatively* and not additively.

Applying what we have learned on MLR models (Inference/prediction/diagnosis) could be problematic.

Laura Baracaldo PSTAT 126 4 / 35

Transforming the Response

By taking the log transformarion on both sides of the previous model:

$$log(y) = \beta_0 + \beta_1 x_1 + \ldots + \beta_p x_p + \epsilon$$

We can use results from MLR models on the transformed response loq(y). In practice, we may not know:

- How the errors enter the model.
- What transformation on the response guarantees a linear relationship with the set of predictors. The best approach is to try different transforms, then check the residuals to see whether they satisfy the conditions required for linear regression.

PSTAT 126 5/35

Interpretation and Back Transformation

If we are interested in prediction we may need to obtain those predictions in the original scale, which requires back transforming. For example in the logged model the prediction in the transformed scale is:

$$log(\hat{y}) = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \ldots + \hat{\beta}_p x_p$$

However in the original scale the prediction would be:

$$\hat{y} = \exp(\hat{\beta}_0 + \hat{\beta}_1 x_1 + \ldots + \hat{\beta}_p x_p)$$

Prediction intervals: For a prediction interval in the transformed scale [l,u], the prediction interval in the original scale would be: [exp(l),exp(u)]. Note that this interval may not be symmetric.

Laura Baracaldo PSTAT 126 6/35

Interpretation and Back Transformation

Interpretation of Coefficients β_j : Regression coefficients will need to be interpreted with respect to the transformed scale. When you use a log transformation on the response, the regression coefficients have a particular interpretation:

$$\hat{y} = e^{\hat{\beta}_0} e^{\hat{\beta}_1 x_1} \dots e^{\hat{\beta}_p x_p}$$

An increase of one in x_j would multiply the predicted response (in the original scale) by $e^{\hat{\beta}_j}$. Thus when a log scale is used, the regression coefficients can be interpreted in a multiplicative rather than additive manner.

Laura Baracaldo PSTAT 126 7 / 35

The Box-Cox method is a popular tool to determine the most suitable transformation for the response. The method transforms **strictly positive** response $y \to g_{\lambda}(y)$, where the family of transformations indexed by λ is:

$$g_{\lambda}(y) = \begin{cases} \frac{y^{\lambda} - 1}{\lambda} & \lambda \le 0\\ \log(y) & \lambda = 0 \end{cases}$$

For y > 0, $g_{\lambda}(y)$ is continuous in λ .

Assumptions:

- $E(g_{\lambda}(y)) = \beta_0 + \beta_1 x_1 + \ldots + \beta_p x_p = x^T \beta$
- $Var(g_{\lambda}(y)) = \sigma^2$
- $g_{\lambda}(y)$ is approximately normal.

We estimate λ via maximum likelihood estimation. Under normality of the errors the likelihood is written as:

$$L(\lambda) = (2\pi\sigma^2)^{-\frac{n}{2}} \exp\left\{-\frac{1}{2\sigma^2} \sum_{i=1}^n (g_{\lambda}(y_i) - x_i^T \beta)^2\right\} \prod_{i=1}^n y_i^{\lambda - 1}$$

Therefore, the log-likelihood is:

$$l(\lambda) = -\frac{n}{2}\log(SSR_{\lambda}/n) + (\lambda - 1)\sum_{i=1}^{n}\log(y_i)$$

 SSR_{λ} is the SSR when $g_{\lambda}(y)$ is the response.

PSTAT 126 9/35

Transforming the response can make the model harder to interpret so we try to avoid it unless it is necessary. The way we can check this is by using a confidence interval for λ . An approximate $100(1-\alpha)\%$ CI for λ is:

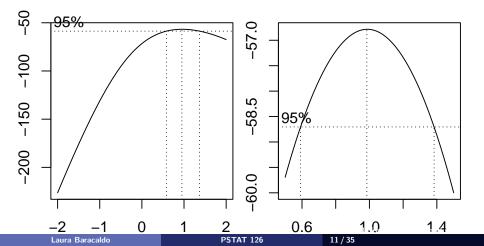
$$\left\{\lambda: l(\lambda) > l(\hat{\lambda}) - \frac{1}{2}\chi_{1,1-\alpha}^2\right\}$$

- If the confidence interval contains $\hat{\lambda}=1$, no transformation is necessary.
- If the purpose of the regression analysis is interpretation, round off $\hat{\lambda}$. For instance if $\hat{\lambda} = 0.48$ round to the nearest interpretable value $\hat{\lambda} = 0.5$, as $g_{0.5} \propto \sqrt{y}$ is easier to explain.

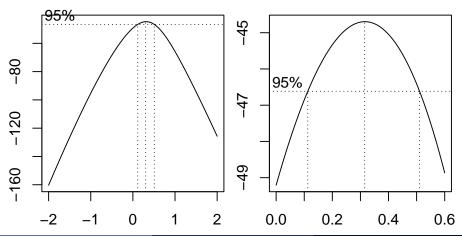
PSTAT 126 10 / 35

```
## Loading required package: MASS
```

```
lmod<- lm(sr - pop15 + pop75+ dpi+ ddpi, savings)
par(mfrow=c(1,2), mar = c(2, 2, 0.8, 0.5))
boxcox(lmod, plotit =TRUE);boxcox(lmod, plotit =TRUE, lambda=seq(0.5, 1.5, by=0.5))</pre>
```



```
lmod1<- lm(Species -Area + Elevation+ Nearest+ Scruz+Adjacent, gala)
par(mfrow=c(1,2), mar = c(2, 2, 0.8, 0.5))
boxcox(lmod1, plotit =TRUE);boxcox(lmod1, plotit =TRUE, lambda=seq(0.0, 0.6, by=0.2))</pre>
```



Laura Baracaldo PSTAT 126 12 / 35

General Considerations

- ① The Box-Cox method gets greatly impacted by outliers, if you find that $\hat{\lambda} \geq 5$, you may want to check for outliers that justify this extreme transformation.
- ② If $y_i < 0$, we can add a constant to all the responses, This is a reasonable solution when the constant added is small.
- **3** If $\max_i y_i / \min_i y_i$ is small, then the Box-Cox method will not have much real effect.
- **①** There are other methods for transforming the response (Example: The log family $g_{\alpha} = \log(y + \alpha)$).

Laura Baracaldo PSTAT 126 13 / 35

Extensions for Linear Models - Predictors Transformation

Recall that the relationship between the response and the predictors is assumed to be *linear* and *additive*.

• **Polynomial Regression:** One way to generalize the linear structure is by including polynomial terms. In the one-predictor case, we have:

$$y = \beta_0 + \beta_1 x + \beta_2 x^2 + \ldots + \beta_d x^d + \epsilon$$

Which allows for a more flexible relationship. Note y is no longer linear in x, however it is linear in the z_k 's, $z_k = x^k$:

$$y = \beta_0 + \beta_1 z_1 + \beta_2 z_2 + \ldots + \beta_d z_d + \epsilon$$

There are two commons ways to choose d.

- Keep adding terms until the added term is not statistically significant
- ② Start with a large d, remove non-statistically significant terms starting with the highest order term.

Laura Baracaldo PSTAT 126 14 / 35

Polynomial Regression

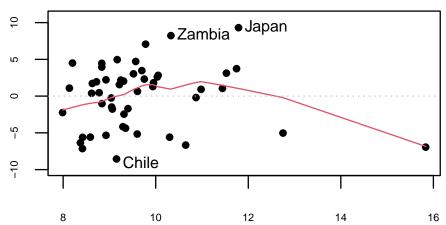
```
summary(m1<-lm(sr~ddpi, savings))$coefficients
##
              Estimate Std. Error t value Pr(>|t|)
## (Intercept) 7.883021 1.0110011 7.797243 4.464697e-10
## ddpi
              0.475830 0.2146166 2.217117 3.138509e-02
summary(m2<-lm(sr~ddpi + I(ddpi^2), savings))$coefficients #We add quadratic term
               Estimate Std. Error t value Pr(>|t|)
##
## (Intercept) 5.13038069 1.43471517 3.575888 0.0008211413
## ddpi
            1.75751897 0.53772368 3.268443 0.0020258542
## I(ddpi^2) -0.09298521 0.03612318 -2.574115 0.0132617330
summary(m3<-lm(sr~ddpi + I(ddpi^2)+ I(ddpi^3), savings))$coefficients #We add cubic term
##
                  Estimate Std. Error t value Pr(>|t|)
## (Intercept) 5.145360e+00 2.19860644 2.340282237 0.02366212
## ddpi
             1.746017e+00 1.38045499 1.264812459 0.21230898
## I(ddpi^2) -9.096724e-02 0.22559835 -0.403226554 0.68864973
## I(ddpi^3)
              -8.496955e-05 0.00937393 -0.009064453 0.99280691
```

We stick with the quadratic term.

Polynomial Regression

```
par(mar = c(3, 2, 1.5, 0.5))
plot(m1, cex.main=1, cex.lab=0.5, cex.axis=0.5, pch=20)
```

Residuals vs Fitted

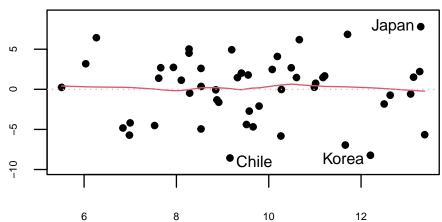


Laura Baracaldo PSTAT 126 16 / 35

Polynomial Regression

```
par(mar = c(3, 2, 1.5, 0.5))
plot(m2, cex.main=1, cex.lab=0.5, cex.axis=0.5, pch=20)
```





Laura Baracaldo PSTAT 126 17 / 35

Polynomial Regression for p > 1

 Interaction Effects: We can extend the additive assumption by including non-additive structures through interactions between predictors:

$$y = \beta_0 + \sum_{i=1} \beta_j x_j + \sum_{i \le j} \alpha_{ij} x_i x_j + \epsilon$$

For p=2:

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \alpha_1 x_1^2 + \alpha_2 x_2^2 + \alpha_{12} x_1 x_2 + \epsilon$$

Interactions between x_i and x_j accounts for the impact of x_i on y in the presence of x_j and vice versa.

Laura Baracaldo PSTAT 126 18 / 35

Polynomial Regression for p > 1

Estimate Std. Error t value Pr(>|t|)

(Intercept) 7.59867182 4.49133342 1.6918521 0.09743877 -0.01520380 0.11373407 -0.1336785 0.89423995 ## ddpi 2.59309111 1.05992616 2.4464828 0.01830752 ## pop15:ddpi -0.05464617 0.02651832 -2.0606951 0.04501275

Generalized Additive Models

Polynomial Regression is not the only nonlinear prediction transformation. We have also piece wise polynomials and regression splines among others.

Searching for a good transformation of the predictors is difficult when p>1, since changing the transformation on one predictor may change the choice of transformation for other predictors. We can use the generalized additive models to simultaneously choose the transformation. An additive model takes the form:

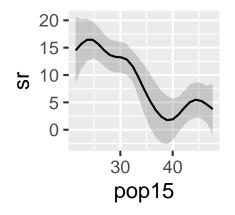
$$y = \alpha + f_1(x_1) + \ldots + f_p(x_p) + \epsilon$$

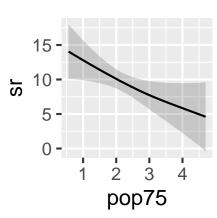
The linear terms were replaced with more flexible functional forms.

Laura Baracaldo PSTAT 126 20 / 35

Generalized Additive Models

```
require(mgcv); require(ggplot2); require(tidymv); library("gridExtra")
par(mar = c(3, 2, 0.5, 0.5))
gamod<- gam(sar - s(pop15) + s(pop75) + s(dpi) + s(ddpi), data=savings)
p1<-plot_smooths(gamod, pop15); p2<-plot_smooths(gamod, pop75)
grid.arrange(p1, p2, ncol = 2, nrow = 1)</pre>
```



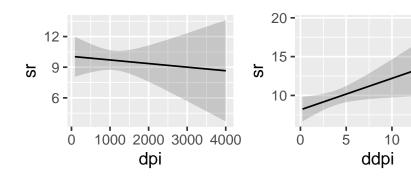


Laura Baracaldo PSTAT 126 21 / 35

Generalized Additive Models

```
p1<-plot_smooths(gamod, dpi); p2<-plot_smooths(gamod, ddpi)
library("gridExtra")
grid.arrange(p1, p2, ncol = 2, nrow = 1)</pre>
```

15



Laura Baracaldo PSTAT 126 22 / 35

Generalized Least Squares

Until now we have assumed that $Var(\epsilon) = Cov(\epsilon) = \sigma^2 I$, which means that the errors have constant variance and are uncorrelated:

$$Cov \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{bmatrix} = \begin{bmatrix} \sigma^2 & 0 & \dots & 0 \\ 0 & \sigma^2 & \dots & 0 \\ \vdots & \vdots & \dots & \vdots \\ 0 & 0 & \dots & \sigma^2 \end{bmatrix}$$

However this may not be the case. A more generalized framework assumes $Var(\epsilon)=Cov(\epsilon)=\sigma^2\Sigma$ with $\Sigma\neq I$. Although σ^2 is unknown, we assume Σ is known.

Laura Baracaldo PSTAT 126 23 / 35

Generalized Least Squares (GLS)

By using the *Cholesky decomposition*, which can be seen as the "square root" of a matrix, Σ can be written as: $\Sigma = LL^T$, with L a lower triangular matrix. We can transform the regression model as follows:

Note that:

 $Var(\tilde{\boldsymbol{\epsilon}}) = Var(\boldsymbol{L}^{-1}\boldsymbol{\epsilon}) = \boldsymbol{L}^{-1}Var(\boldsymbol{\epsilon})(\boldsymbol{L}^{-1})^T = \sigma^2\boldsymbol{L}^{-1}\boldsymbol{L}\boldsymbol{L}^T\boldsymbol{L}^{-T} = \sigma^2\boldsymbol{I}.$ This means we can reduce GLS to ordinary least squares OLS.

Laura Baracaldo PSTAT 126 24 / 35

Generalized Least Squares (GLS)

As we have transformed the problem to the standard case, we can find estimate for β by minimizing the SSR of the model:

$$SSR = (\tilde{\boldsymbol{y}} - \tilde{\boldsymbol{X}}\boldsymbol{\beta})^{T}(\tilde{\boldsymbol{y}} - \tilde{\boldsymbol{X}}\boldsymbol{\beta})$$

$$= (\boldsymbol{L}^{-1}\boldsymbol{y} - \boldsymbol{L}^{-1}\boldsymbol{X}\boldsymbol{\beta})^{T}(\boldsymbol{L}^{-1}\boldsymbol{y} - \boldsymbol{L}^{-1}\boldsymbol{X}\boldsymbol{\beta})$$

$$= (\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta})^{T}\boldsymbol{L}^{-T}\boldsymbol{L}^{-1}(\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta})$$

$$= (\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta})^{T}\boldsymbol{\Sigma}^{-1}(\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta})$$

Which is minimized by: $\hat{\boldsymbol{\beta}} = (\boldsymbol{X}^T \boldsymbol{\Sigma}^{-1} \boldsymbol{X})^{-1} \boldsymbol{X}^T \boldsymbol{\Sigma}^{-1} \boldsymbol{y}$. (Prove this!)

Laura Baracaldo PSTAT 126 25 / 35

Generalized Least Squares (GLS)

Under normality of the errors it can be proved that:

$$\hat{\boldsymbol{\beta}} \sim N(\boldsymbol{\beta}, \sigma^2(\boldsymbol{X}^T \boldsymbol{\Sigma}^{-1} \boldsymbol{X})^{-1})$$

- Inference on β : Confidence Intervals and Hypothesis Testing are constructed as in previous lectures.
- Regression Diagnostics: Since $\tilde{\epsilon} = L^{-1} \epsilon \sim N(\mathbf{0}, \sigma^2 I)$, diagnostics should be applied to the residuals $\tilde{\epsilon}$.
- Practical Consideration: The main problem in applying GLS in practice is that Σ may not be known and we have to estimate it using the data.

PSTAT 126 26 / 35

Sometimes is reasonable to assume that the errors are uncorrelated $Cov(\epsilon_i,\epsilon_j)=0, \quad i\neq j$ with unequal variance $Var(\epsilon_i)=\sigma_i^2.$

$$Cov \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{bmatrix} = \begin{bmatrix} \sigma_1^2 & 0 & \dots & 0 \\ 0 & \sigma_2^2 & \dots & 0 \\ \vdots & \vdots & \dots & \vdots \\ 0 & 0 & \dots & \sigma_n^2 \end{bmatrix} = \mathbf{\Sigma}$$

Thus, the Cholesky decomposition of the covariance matrix is written as $\Sigma = LL^T$. With:

$$\boldsymbol{L} = \begin{bmatrix} \sigma_1 & 0 & \dots & 0 \\ 0 & \sigma_2 & \dots & 0 \\ \vdots & \vdots & \dots & \vdots \\ 0 & 0 & \dots & \sigma_n \end{bmatrix}$$

Laura Baracaldo PSTAT 126 27 / 35

We transform the model as in the case of GLS:

$$egin{aligned} oldsymbol{L}^{-1}oldsymbol{y} &= oldsymbol{L}^{-1}oldsymbol{X}eta + oldsymbol{L}^{-1}\epsilon \ & ilde{oldsymbol{y}} &= ilde{oldsymbol{X}}eta + ilde{\epsilon} \end{aligned}$$

Note that \tilde{y} can be seen as a vector of weighted responses:

$$\tilde{m{y}} = m{L}^{-1} m{y} = \begin{bmatrix} \sigma_1^{-1} & 0 & \dots & 0 \\ 0 & \sigma_2^{-1} & \dots & 0 \\ \vdots & \vdots & \dots & \vdots \\ 0 & 0 & \dots & \sigma_n^{-1} \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} y_1/\sigma_1 \\ y_2/\sigma_2 \\ \vdots \\ y_n/\sigma_n \end{bmatrix}$$

Laura Baracaldo PSTAT 126 28 / 35

We transform the model as in the case of GLS:

$$egin{aligned} oldsymbol{L}^{-1}oldsymbol{y} &= oldsymbol{L}^{-1}oldsymbol{X}eta + oldsymbol{L}^{-1}oldsymbol{\epsilon} \ & ilde{oldsymbol{y}} &= ilde{oldsymbol{X}}eta + ilde{oldsymbol{\epsilon}} \end{aligned}$$

And $ilde{m{X}}$ can be seen as a matrix of weighted predictor variables:

$$\boldsymbol{L}^{-1}\boldsymbol{X} = \begin{bmatrix} 1/\sigma_1 & 0 & \dots & 0 \\ 0 & 1/\sigma_2 & \dots & 0 \\ \vdots & \vdots & \dots & \vdots \\ 0 & 0 & \dots & 1/\sigma_n \end{bmatrix} \begin{bmatrix} 1 & x_{11} & \dots & x_{1p} \\ 1 & x_{21} & \dots & x_{2p} \\ \vdots & \vdots & \dots & \vdots \\ 1 & x_{n1} & \dots & x_{np} \end{bmatrix} = \begin{bmatrix} 1/\sigma_1 & \dots & x_{1p}/\sigma_1 \\ 1/\sigma_2 & \dots & x_{2p}/\sigma_2 \\ \vdots & \dots & \vdots \\ 1/\sigma_n & \dots & x_{np}/\sigma_n \end{bmatrix}$$

Laura Baracaldo PSTAT 126 29 / 35

We transform the model as in the case of GLS:

$$egin{aligned} m{L}^{-1}m{y} &= m{L}^{-1}m{X}m{eta} + m{L}^{-1}m{\epsilon} \ & ilde{m{y}} &= ilde{m{X}}m{eta} + ilde{m{\epsilon}} \end{aligned}$$

Similarly, $\tilde{\epsilon}$ can be written as a vector of weighted errors:

$$\tilde{\boldsymbol{\epsilon}} = \boldsymbol{L}^{-1} \boldsymbol{\epsilon} = \begin{bmatrix} \sigma_1^{-1} & 0 & \dots & 0 \\ 0 & \sigma_2^{-1} & \dots & 0 \\ \vdots & \vdots & \dots & \vdots \\ 0 & 0 & \dots & \sigma_n^{-1} \end{bmatrix} \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{bmatrix} = \begin{bmatrix} \epsilon_1/\sigma_1 \\ \epsilon_2/\sigma_2 \\ \vdots \\ \epsilon_n/\sigma_n \end{bmatrix}$$

Laura Baracaldo PSTAT 126 30 / 35

By minimizing the SSR of this model we obtain the Least Squares Estimates:

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

Where $oldsymbol{W}$ is deemed as the weight matrix:

$$\boldsymbol{W} = \begin{bmatrix} W_1 & 0 & \dots & 0 \\ 0 & W_2 & \dots & 0 \\ \vdots & \vdots & \dots & \vdots \\ 0 & 0 & \dots & W_n \end{bmatrix} = \begin{bmatrix} 1/\sigma_1 & 0 & \dots & 0 \\ 0 & 1/\sigma_2 & \dots & 0 \\ \vdots & \vdots & \dots & \vdots \\ 0 & 0 & \dots & 1/\sigma_n \end{bmatrix}$$

Laura Baracaldo PSTAT 126 31/35

Example: Divorce in the US 1920 - 1996

Response: Year (1920-1996), **Predictor**: Divorce (Divorce per women 18 years or more)

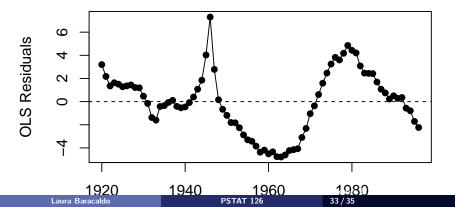
```
lmodt<- lm(divorce ~vear, data=divusa)</pre>
summary(lmodt)
##
## Call:
## lm(formula = divorce ~ vear, data = divusa)
##
## Residuals:
      Min
              10 Median
                                     Max
## -4 7828 -1 8092 0 1592 1 6292 7 3048
## Coefficients:
                Estimate Std. Error t value Pr(>|t|)
## (Intercept) -422.97530 27.29465 -15.50 <2e-16 ***
## year
                 0.22280
                         0.01394 15.98 <2e-16 ***
## ---
## Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' 1
##
## Residual standard error: 2.719 on 75 degrees of freedom
## Multiple R-squared: 0.7731, Adjusted R-squared: 0.77
## F-statistic: 255.5 on 1 and 75 DF, p-value: < 2.2e-16
```

data(divusa)

Laura Baracaldo PSTAT 126 32 / 35

Example: Years vs Residuals

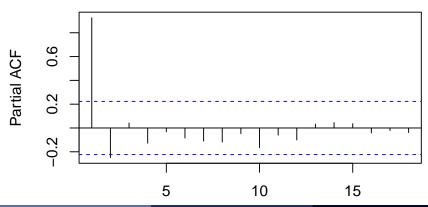
plot(divusa\$year, residuals(lmodt), type="o", pch=16, xlab="Year", ylab="OLS Residuals")
abline(h=0, lty=2)



Example: Autocorrelation

acf(residuals(lmodt), type="partial")

Series residuals(Imodt)



Laura Baracaldo PSTAT 126 34 / 35

Example: GLS

```
require(nlme);gmod<- gls(divorce -year, correlation=corAR1(form=-year),data=divusa)
summary(gmod)</pre>
```

```
## Generalized least squares fit by REML
    Model: divorce ~ year
    Data: divusa
         ATC
##
                  BIC
                       logLik
    216 2057 225 4756 -104 1028
##
## Correlation Structure: AR(1)
  Formula: ~vear
   Parameter estimate(s):
        Phi
## 0 9955474
##
## Coefficients:
                   Value Std.Error t-value p-value
## (Intercept) -283.78012 195.07262 -1.454741 0.1499
                 0.15192 0.09952 1.526571 0.1311
## year
##
   Correlation:
       (Intr)
## year -0.999
##
## Standardized residuals:
         Min
                     Ω1
                                Med
                                                      Max
## -0.4900705 -0.2675280 -0.1277208 0.2248171 0.6060676
##
## Residual standard error: 9.972029
## Degrees of freedom: 77 total; 75 residual
```

Laura Baracaldo PSTAT 126 35 / 35