

## Lecture 2 Transformations and the Specification of Econometric Models

A fundamental aspect of interpreting any parametric statistical model is choice of functional form. Let's begin a consideration of this topic with the following simple example. Suppose

$$\log y_i = \alpha + \beta \log x_i + u_i$$

but unaware of this convenient formulation we instead estimate

$$y_i = a + bx_i + v_i.$$

What relationship does  $(\hat{a}, \hat{b})$  bear to  $(\alpha, \beta)$  in the original model and can we hope to say anything reasonable having made this initial specification error?

In Figure 1, we can examine a specific version of this situation in which  $(\alpha, \beta) = (1, .5)$  and the variance of  $u_i$  is quite small. Clearly we don't do a very good job of estimating the curve represented by the observed points by the line indicating the least squares fit, but it is useful to look at this more carefully.\* On a more optimistic note it might appear that the slope of the linear fit might provide a decent approximation to the tangent of the curve at a point roughly corresponding to  $\bar{x}$ . Figure 2 illustrates this phenomenon on the elasticity scale. Were we to estimate the log-linear model we would have an easily interpreted constant elasticity estimate. However, since we have estimated the model in the linear form, the implied elasticity of  $y$  with respect to  $x$  varies as we move along the fitted line. More explicitly, the elasticity is defined as

$$\eta = \frac{dy}{dx} \frac{x}{y}$$

and according to the linear specification the derivative,  $dy/dx = b$  is constant, so the natural estimate of the elasticity of  $y$  with respect to  $x$ , at any point  $x$ , is given by

$$\hat{\eta}(x) = \hat{b} \cdot \frac{x}{\hat{y}(x)}$$

where  $\hat{y}(x) = \hat{a} + \hat{b}x$ . If we were going to offer only one such elasticity estimate for expository purposes, we would typically choose  $x = \bar{x}$ , but sometimes it is useful to choose several such points of evaluation for purposes of comparison. Recall  $\hat{y}(\bar{x}) = \bar{y}$  as long as the estimated model has an intercept. This is done for each of the observed values of  $x$  in Figure 2. The horizontal line at  $\beta = .5$  is the "true" elasticity according to which the data was generated, while the dots represent  $\hat{\eta}(x)$  at the various observed  $x$ 's. Obviously these estimates are rather poor in the extremes, but reasonably good in the center of the  $x$ 's. The two vertical lines represent the arithmetic and geometric means of  $x$  and we note that one yields a small overestimate while the other yields a small underestimate of  $\beta$ . This is the first of many lessons which can be roughly formulated by the

*Maxim:* It is dangerous to draw inferences too far away from the center of your data.

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\*One way to do this is to ask: suppose the  $x_i$ 's are generated randomly from some distribution,  $F$ , and that  $E(y|x) = g(x)$ , then  $(\hat{a}, \hat{b})$  solves  $\min E_x(g(x) - a - bx)^2$ , i.e.,  $\hat{a} + \hat{b}x$  is the best linear approximation to  $g(x)$  in quadratic mean.

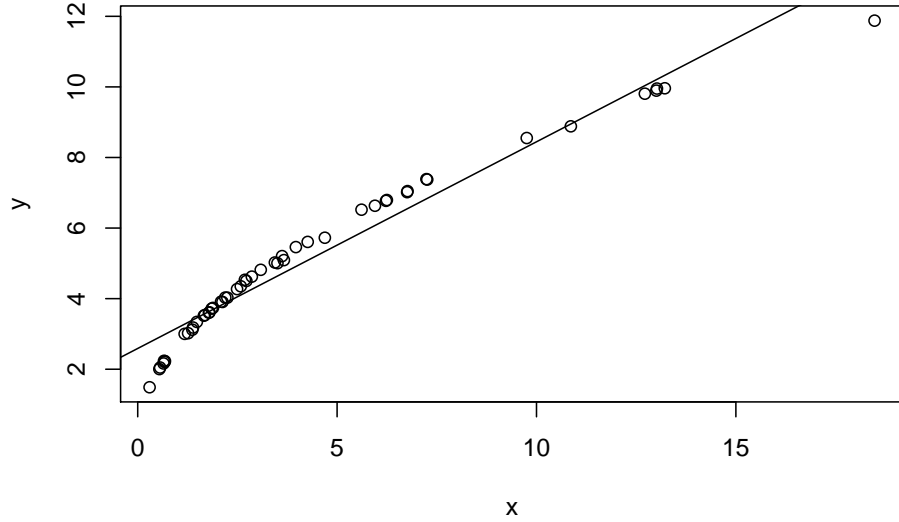


FIGURE 1. A linear fit to a log-linear model: The figure illustrates 50 observations from a log-linear model and a superimposed least-squares linear fit of the observations. Note that the fit provides a rough estimate of the tangent of the curve near the “center” of the  $x$ ’s, but cannot be considered very reliable unless the range of the  $x$ ’s is quite restricted.

A corollary, which is often offered as advice to young novelists is “Write what you know,” another pithy corollary is “Extrapolate at your peril.” A nice introduction to a more general formulation of these issues is White (1980).

A common error in applied work when estimating log-linear models involves the transition back to predictions about expectations of the response variable in the original scale. If we have the log-linear specification in our first equation and if as would be commonly assumed  $u_i$ ’s were assumed to be homoscedastic and normal, then in the original scale we would have  $y_i = e^\alpha x_i^\beta e^{u_i}$  with  $e^{u_i}$  a lognormal random variable. If we were interested in estimating  $E(y|x)$  then we would need to consider the mean of this lognormal random variable. If  $u$  is normal, then  $v = e^u$  is lognormal, so

$$Ev^j = \int v^j d\Lambda(v) = \int e^{ju} d\Phi(u) = Ee^{ju} = \exp\{ju + \sigma^2 j^2/2\}$$

where the last equality follows by the (familiar!) computation for the moment generating function of the normal distribution. Here  $\Lambda$  and  $\Phi$  denote generic lognormal and normal distribution functions, respectively. In our case we are typically only interested in the case  $\mu = 0$  and  $j = 1$  but even in this simple case we see that our expectation needs to account for the contribution of the variability of  $u$  as well as the mean contribution from the systematic portion of the model.

Another common difficulty with the log-linear specification involves treatment of zero observations, for which it is difficult to compute logs. A common “fix” is to replace zeros by some arbitrary  $\epsilon$  and then compute logs, but this can be dangerous since results can be very sensitive to the choice of  $\epsilon$ , for which there is rarely an obvious a priori choice.

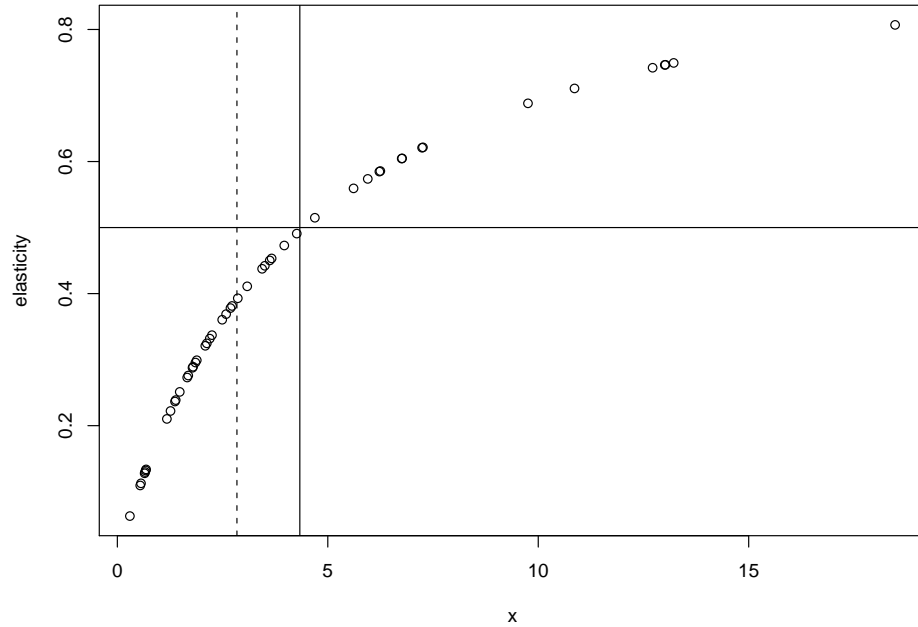


FIGURE 2. A linear fit to a log-linear model: This figure illustrates the bias introduced in estimating the elasticity parameter of the log-linear model by using the estimated linear model. The points in the figure represent elasticities implied by the fitted *linear* model at each of the observed  $x$ 's. The horizontal line at  $\beta = .5$  represents the true, constant elasticity for the model, and the two vertical lines indicate the mean (solid) and geometric mean (dotted) of the  $x$ 's. Thus, at the mean of the  $x$ 's the linear model slightly overestimates the elasticity, and at the geometric mean it slightly underestimates it.

Having seen this example it is natural to ask whether there is a systematic strategy for deciding on appropriate functional forms. This is obviously a big topic and I will try only to briefly survey the basic idea in the simplest bivariate regression setting.

The classical approach to dealing with this ‘transformation problem’ involves the family of power transformations

$$h(x, \lambda) = \begin{cases} \frac{x^\lambda - 1}{\lambda} & \lambda \neq 0 \\ \log x & \lambda = 0 \end{cases}$$

Applying this transformation to the response variable  $y$  and/or the independent variable(s)  $x$  yields a rich class of potential models. It is useful to consider a few special cases. We will consider  $\lambda = 0$  which is somewhat peculiar in detail, but  $\lambda = -1$  is also of interest.

*Exercise:* Verify using L'Hôpital's rule that

$$\lim_{\lambda \rightarrow 0} \frac{x^\lambda - 1}{\lambda} = \log x$$

Answer:

$$\begin{aligned} \lim_{\lambda \rightarrow 0} \frac{x^\lambda - 1}{\lambda} &= \frac{\frac{d}{d\lambda}(e^{\lambda \log x} - 1)}{1} \Big|_{\lambda=0} \\ &= e^{\lambda \log x} \cdot \log x \Big|_{\lambda=0} \\ &= \log x \end{aligned}$$

The family of Box-Cox transformations is illustrated in Figure 3 for 6 different values of  $\lambda$ . The

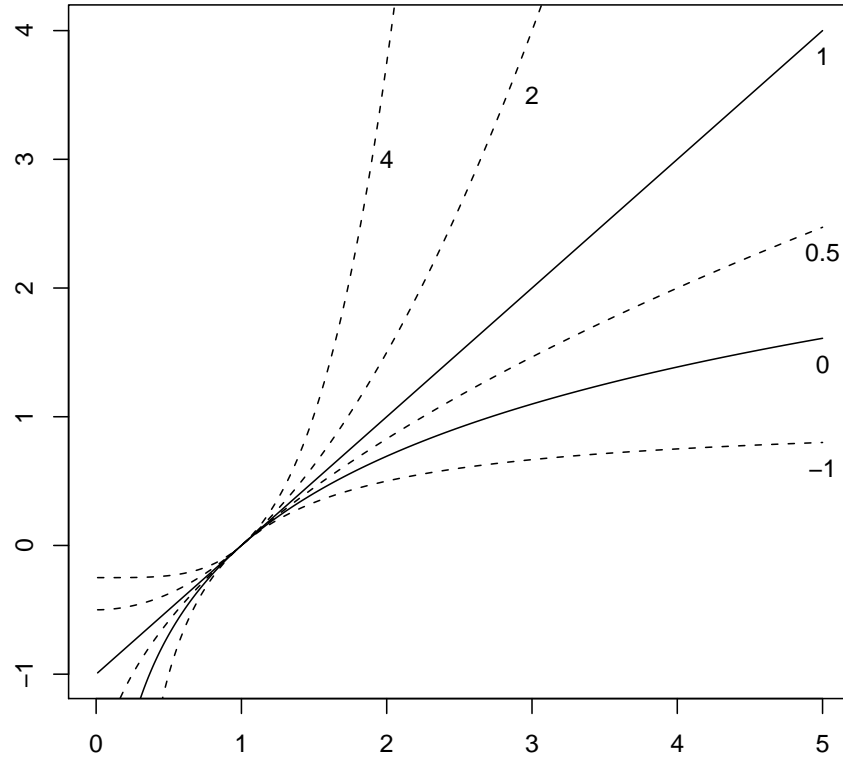


FIGURE 3. The Box-Cox Power Transformations: The Figure illustrates 6 versions of the Box-Cox Power family of transformations. Note that the log transformation fits nicely into the family with  $\lambda = 0$ .

family is quite flexible and useful, but it is somewhat limited because it is only fully applicable for  $x \geq 0$ . It has been suggested that one might extend the definition using

$$\lambda(x) = (|x|^\lambda \operatorname{sgn}(x) - 1)/\lambda$$

but this behaves rather strangely and is rarely used in applications.

As an exercise in reviewing some basic ideas about maximum likelihood estimation, let's consider, following Box and Cox (1964), the problem of estimating the model

$$h(y_i, \lambda) = x_i \beta + u_i$$

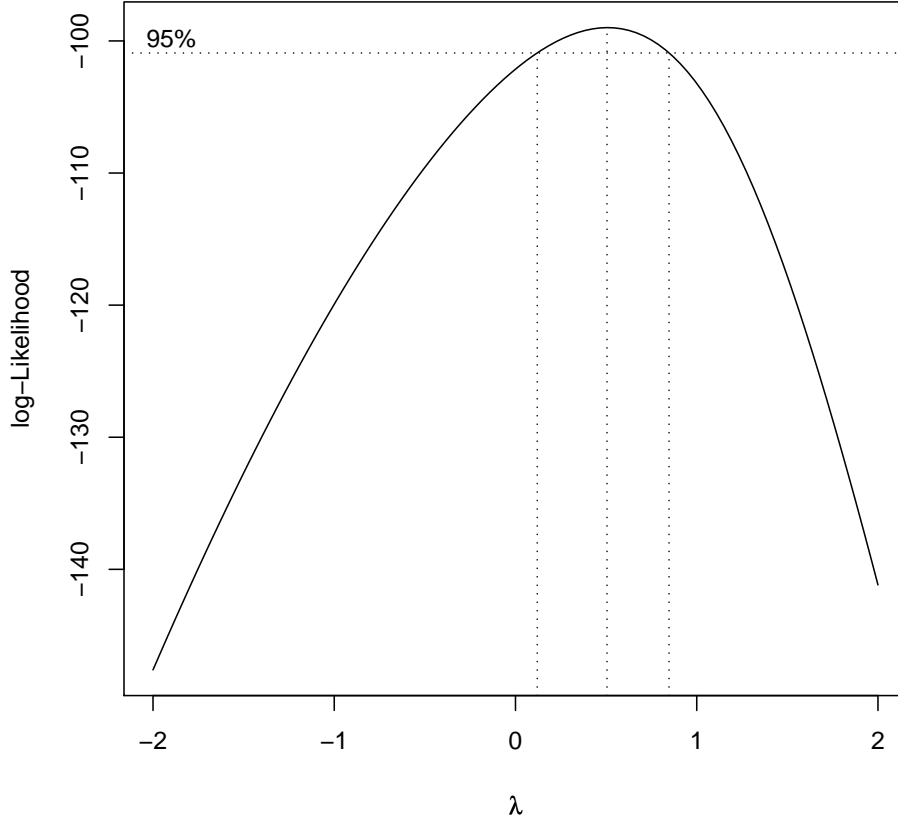


FIGURE 4. The Box-Cox Power Transformation: The Figure illustrates the profile log likelihood for a simple bivariate linear model, the confidence interval indicated for  $\lambda$  is based on the asymptotic theory of the likelihood ratio statistic.

assuming that  $\{u_i\}$  is iid  $\mathcal{N}(0, \sigma^2)$ . The log likelihood is

$$\ell(\beta, \lambda, \sigma) = -\frac{n}{2} \log(2\pi\sigma^2) - \frac{1}{2\sigma^2} \sum (h(Y_i, \lambda) - x_i\beta)^2 + \log |J|$$

where  $J = \prod_{i=1}^n |\partial h(y_i)/\partial y_i|$  is the determinant of the transformation from  $u$  to  $h(y, \lambda)$ . Note that

$$\frac{\partial h(y_i, \lambda)}{\partial y_i} = y_i^{\lambda-1}$$

so

$$\log |J| = (\lambda - 1) \sum_{i=1}^n \log(y_i).$$

Concentrating the likelihood we have

$$\ell(\lambda, \sigma) = -\frac{n}{2} \log \hat{\sigma}^2 + \log |J| + K$$

where  $K$  doesn't depend on the parameters. Now note that if we had been very lucky and the response observations  $y_i : i = 1, \dots, n$  happened to have geometric mean of zero, then the Jacobian term would have been zero. Alternatively, suppose we, with malice aforethought, transform the observed  $y_i$ 's:  $y_i \rightarrow \tilde{y}_i \equiv y_i/\tilde{y}$  where  $\tilde{y} = (\prod y_i)^{1/n}$  denotes the geometric mean of  $y_i$ 's. Then,

$$\log |J| = (\lambda - 1) \sum \log(\tilde{y}_i) = (\lambda - 1) \sum \log(y_i/\tilde{y}) = (\lambda - 1) \sum (\log(y_i) - \log(\tilde{y})) = 0.$$

How convenient! Having made this transformation the Jacobian term vanishes and we can focus on the simple classical idea of minimizing the sum of squared errors, or equivalently, minimizing  $\log(\hat{\sigma}^2)$  since it becomes the only relevant term in the likelihood. One might still worry about whether there are any serious side effects resulting from the transformation of the response observations? A useful exercise would be to convince yourself that a.) in the case that  $\lambda = 0$  so we had the log transformation then dividing by the geometric mean would have only the effect of shifting the intercept of the model, or b.) in the case that  $\lambda = 1$ , dividing the  $y_i$ 's by a constant rescales *all* the coordinates of the  $\hat{\beta}$  vector by the same factor. These so-called "equivariance" properties of the least-squares estimator will arise periodically throughout the course.

The function  $\ell(\lambda)$  which we used to call the concentrated log likelihood we now call the profile (log) likelihood, terminology I believe introduced by Cox. The profile likelihood provides an extremely convenient and powerful means of doing inference in many problems. In the simple Box-Cox problem under consideration we would often like to test the hypothesis  $H_0 : \lambda = \lambda_0$ . This is effectively done using the fact (whose proof is deferred to 574) that under  $H_0$ ,

$$(*) \quad \tau(\lambda_0) = 2(\ell(\hat{\lambda}) - \ell(\lambda_0)) \rightsquigarrow \chi_1^2$$

where  $\hat{\lambda}$  denotes the maximum likelihood estimate of  $\lambda$ . The limiting behavior of this likelihood ratio statistic can also be used to construct confidence intervals for  $\lambda$ : we simply find the set of  $\lambda_0$  such that  $\tau(\lambda_0)$  fails to reject at a specified level of confidence. This is illustrated in Figure 4.

A more challenging problem related to the Box-Cox transformation is the problem of testing whether a Box-Cox transformed covariate belongs in the model. This is a very classical problem with several proposed solutions. I like the one proposed by Harold Hotelling in 1939. If there is time, I'll provide some supplementary notes on this and discuss Hotelling's approach in class.

Sometimes we would rather not go to the bother of estimating the Box-Cox model, but instead we would like to estimate some "preferred" form and then test whether this choice of  $\lambda$  is reasonable. A simple test suggested by David Andrews (1971) handles this situation, and since it nicely illustrates an important principle of diagnostic test design we will develop it in some detail. Consider

$$h(y, \lambda) = x_i^\top \beta + u_i$$

with  $\lambda = 1$  as our "preferred" value. Expanding in Taylor series we have

$$\begin{aligned} h(y, \lambda) &\simeq y - 1 + (\lambda - 1) \frac{dh(y, \lambda)}{d\lambda} \Big|_{\lambda=1} \\ &= (y - 1) + (\lambda - 1)[y \log y - (y - 1)] \end{aligned}$$

Thus, for  $\lambda$  close to one, we have for some mysterious constant,  $\kappa$ ,

$$\kappa(y - 1) \simeq x^\top \beta + ((1 - \lambda)/\lambda)y \log y$$

this seems rather strange since it suggests that we should regress  $y$  on  $y \log y$  - this is clearly unsound. But if we instead proceed in two steps:

- (1) Estimate the linear model and compute  $\hat{y}_i = x_i^\top \hat{\beta}$  for  $i = 1, \dots, n$  and then

(2) Reestimate the augmented model

$$y_i = x_i^\top \beta + \gamma \hat{y}_i \log \hat{y}_i$$

and test  $H_0 : \gamma = 0$ .

This procedure, in effect provides one-step approximation to the mle for  $\lambda$  i.e.,  $\hat{\lambda} = \hat{\gamma} + 1$ .

*Question:* What about the  $\kappa$  and the 1? Are they really needed, if so how would it affect the result if you ignored it? More generally suppose in the usual linear regression setting you transform the response variable  $y \rightarrow ay + b$  how does this change the estimated coefficients and their estimated standard errors? Consider this question first when  $X$  “contains an intercept” and then when it does not.

*Exercises (Review)* For the OLSE  $\hat{\beta}$  show (1.)  $\hat{\beta}(\sigma y + X\gamma, X) = \sigma \hat{\beta}(y, X) + \gamma$ , and (2.)  $\hat{\beta}(y, XA) = A^{-1} \hat{\beta}(y, X)$ .

On the other hand if  $H_0 : \lambda = 0$  is the preferred version, then at  $\lambda = 0$ , we have,

$$\left. \frac{dh(y, \lambda)}{d\lambda} \right|_{\lambda=0} = \frac{1}{2} (\log y)^2$$

so now we would fit

$$\log(y) = x^\top \beta + \delta \cdot (\widehat{\log y})^2$$

so here  $\delta$  estimates  $(1/2)\lambda$  under the alternative hypothesis.

Another useful and important aspect of diagnostic evaluation of transformation models is the partial residual plot. We illustrate this for the gasoline data of PS 2 in the next two figures. In the first group of 4 figures I plot in the upper two figures the scatterplots of percapita US gasoline demand vs percapita income and price respectively. Note that neither of these plots look like something a reasonable person would want to fit with a straight line. Nevertheless, we need to become accustomed to the idea that the *multivariate* relationship may be approximately linear even if the bivariate relationships are not. In this case this is (encouragingly!) roughly true.

The partial residual plot is a device for representing the final step of a multivariate regression result as a bivariate scatterplot. To accomplish this slightly mysterious feat, we need somehow to “remove” the effect of the “other” variables before doing the scatterplot. The natural way of doing this is to regress the two variables of primary interest on the “other” variables of the model, and then plotting the resulting residuals against one another. This can be formalized in the following way.

Consider the model

$$y = X\beta + z\gamma + u$$

and the least squares fitted values,  $\hat{y} = X\hat{\beta} + z\hat{\gamma}$ , where  $Z = [X : z]$ . and  $M_Z = I - P_Z$ , and  $P_Z = Z(Z^\top Z)^{-1}Z^\top$

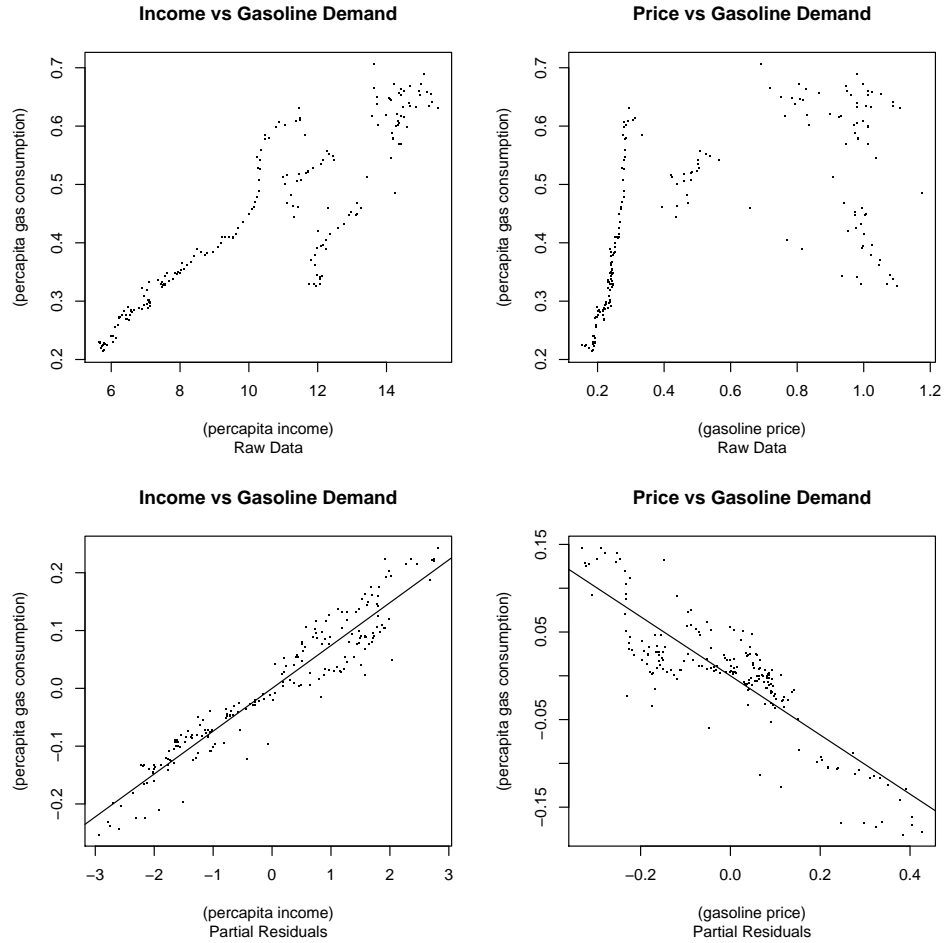
*Theorem* (Gauss-Frisch-Waugh)  $\hat{\gamma} = (z^\top M_X z)^{-1} z^\top M_X y$  where  $M_X = I - P_X$ , and  $P_X = X(X^\top X)^{-1}X^\top$ .

*Proof* Write

$$z^\top M_X \hat{y} = z^\top M_X X \hat{\beta} + z^\top M_X z \hat{\gamma}$$

but  $M_X X = 0$ , so it only remains to show that

$$z^\top M_X P_Z y = z^\top M_X y.$$



Note that

$$M_X P_Z = (I - P_X) P_Z = P_Z - P_X P_Z = P_Z - P_X.$$

In the last step note that  $X^\top P_Z = (P_Z X)^\top = X^\top$  (Why?) so  $P_X P_Z = P_X$ . Finally, we can compute,

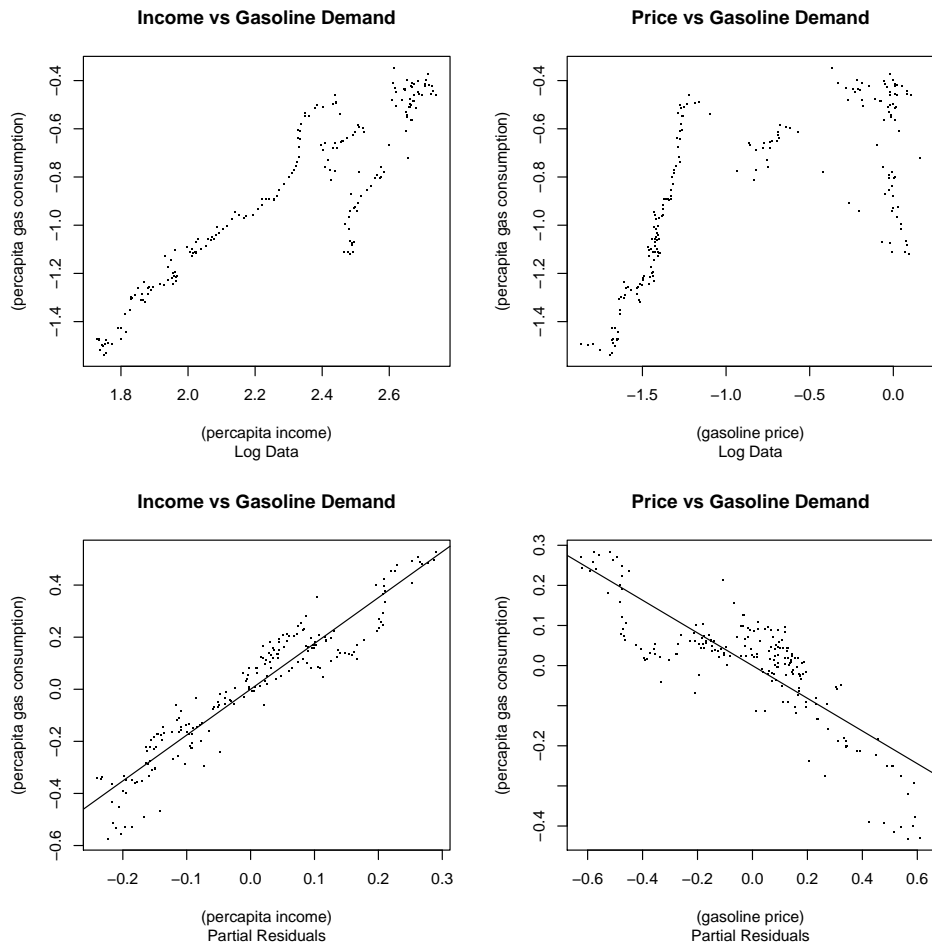
$$z^\top M_X P_Z y = z^\top (P_Z - P_X) y = z^\top y - z^\top P_X y = z^\top (I - P_X) y = z^\top M_X y$$

which concludes the argument.

An additional feature of this approach is that the standard errors that would be computed by the last step are exactly the same as those that come out of full regression. So not only does the scatter plot give an accurate assessment of the position of the least squares fit of the bivariate relationship, it also provides an accurate visual assessment of the precision of this estimate.

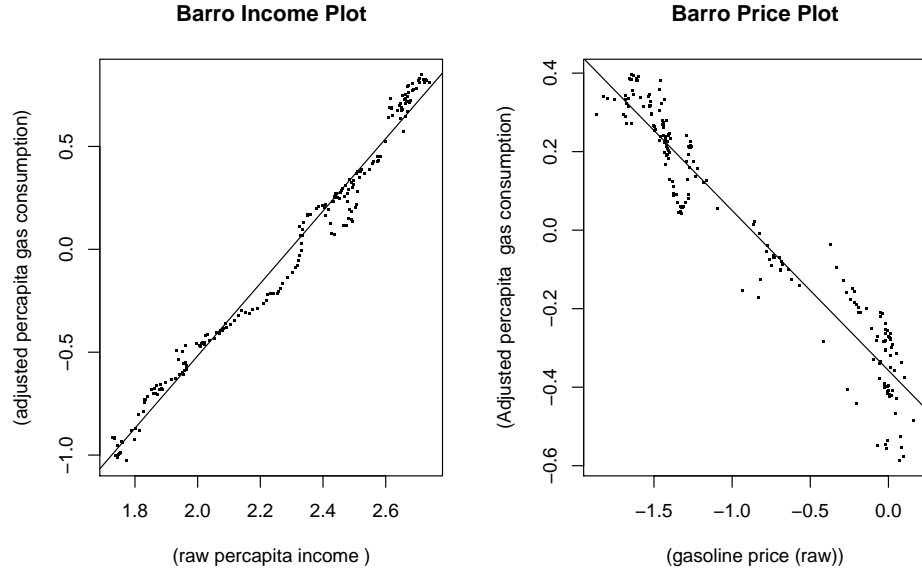
This last point inevitably recalls an amusing “fiasco of econometrics” perpetrated here by Robert Barro in his 1997 David Kinley lecture. Barro presented some “growth regressions” of the type described in his monograph with Sala i Martin. But to illustrate the results for a “general audience” he chose to spend a considerable portion of the talk showing slides of the bivariate relationship between various explanatory variables and his “national growth” variable, after controlling for the effect of other variables. Barro’s approach was, however, somewhat





idiosyncratic. For each of the possible  $z$  variables of interest, he computed  $\tilde{y} = \hat{u} + z_i \hat{\beta}_i$ , that is the residuals from the full regression plus the estimated effect of the  $i$ th variable, and then this variable was centered at zero and plotted against  $z_i$ . This approach is easily shown to produce the correct point estimate of the coefficient  $\hat{\beta}_i$ , (it would be a useful exercise for you to show this), however the visual impression of the scatterplot is much more optimistic than one would expect to get from the partial residual plot method described above. In effect, the denominator effect in the t-statistics of  $z_i^\top M_X z_i$  is replaced in the Barro approach by  $z_i^\top M_1 z_i$  – regression on only an intercept. Since the former can be very small, compared to the later the result is a picture that has an implied standard error that appears considerably smaller than would the standard error in the full regression. In the next panel of two figures, I illustrate the effect of the Barro approach for the gasoline data. As one can see, these figures suggest a much more precise estimate of the two effects than that conveyed by the conventional partial residual plots appearing above. This is good, of course, if the object is to impress the audience with the precision of the fit, but bad if one is interested in conveying an accurate assessment of that precision.

Another apparent example of this sort of statistical shenanigans can be found in the PNAS paper Alvergne et al (2010), see Figure 1.



### *Conflicting Objectives of Transformations*

We have 3 possibly conflicting objectives in choosing a transformation. We would like the transformation to (simultaneously) yield a model

- (i) which is linear in parameters
- (ii) homoscedastic
- (iii) has approximately “normal” conditional density

Carroll and Ruppert have proposed a more general strategy which they call “transforming both sides”. We begin with a model like

$$E(y_t|x_t) = f(x_t, \beta).$$

One might think of this as the *systematic* part of the model before any noise is introduced. Now we might consider models based on the Box-Cox transformation of the form,

$$h(y_t, \lambda) = h(f(x_t, \beta), \lambda) + u_t$$

But this is different than the Box-Cox models we considered above. Here  $f(x_t, \beta)$  is intended to deal with the non-linearity, while  $h$  is *hopefully* going to transform to homoscedastic and normal errors. How does  $h(\cdot)$  work?

Suppose  $y_i$  has  $E(y_i|x_i) = \mu_i$ ,  $V(y_i|x_i) = \sigma_i^2$  and  $\sigma_i = \sigma g(\mu_i)$ , then

$$\begin{aligned} V(h(y_i)) &\simeq E(h(y_i) - h(\mu_i))^2 \\ &\simeq (h'(\mu_i))^2 E(y_i - \mu_i)^2 \\ &= (h'(\mu_i))^2 \sigma^2 (g(\mu_i))^2 \end{aligned}$$

Note these approximations depend on  $\sigma$  being “small!” This is our first contact with the so-called  $\delta$ -method, but it will appear in various guises throughout the course. Now, if we were to choose  $h$  so that

$$h'(\mu_i) = \frac{1}{g(\mu_i)}$$

then we would have (approximate) homoscedasticity. For example, in Poisson cases

$$g(\mu) = \mu^{1/2}$$

so

$$h(\mu) = 2\mu^{1/2} \Rightarrow h'(\mu) = \frac{1}{\mu^{1/2}}$$

and

$$g(\mu) = \mu \Rightarrow h(\mu) = \log(\mu) \Rightarrow h'(\mu) = \frac{1}{\mu}$$

and

$$g(\mu) = \mu^{(1-\lambda)} \Rightarrow h(\mu) = y^{(\lambda)} \Rightarrow h'(\mu) = \mu^{\lambda-1}$$

Here we use the common notational convention that  $y^{(\lambda)} = (y^\lambda - 1)/\lambda$ . Another way to look at this is to say that if  $\sigma^2$  is small relative to the variability of  $\mu_i$ 's, then

$$h(y_i) = h(\mu_i) + h'(\mu_i)(y_i - \mu)$$

For this order of approximation we are back to a “simple” heteroscedastic model,

$$y_i = \mu_i + \sigma h'(\mu_i)\varepsilon_i$$

Note that the interpretation of the  $\beta$ 's is quite different in this setup than in the classical Box-Cox setup. There the  $\beta$ 's don't mean much independent of  $\lambda$  – recall  $\partial y/\partial x$  expression, – but here they do.

Transformation *and* weighting: Consider the model

$$h(y_i, \lambda) = h(f(y_i, \beta), \lambda) + \sigma g(\mu_i(\beta), z_i\theta)\varepsilon_i$$

Now we can think of  $g(\cdot)$  as modeling the heteroscedasticity and  $h(\cdot)$  being exclusively for achieving normality, while  $f(\cdot)$  fixes the non-linearity in the conditional mean relationship. This model is considerably more complicated to estimate, but may arise naturally in the process of diagnostic checking.

### *Interpreting Transformed Models*

It is very important to be clear about what parameters “*mean*” in transformation models, In the normal linear model

$$y_i = x_i\beta + \sigma\varepsilon_i \quad \varepsilon_i \sim \mathcal{N}(0, 1)$$

$$P(y_i < y|x_i) = \Phi((y - x_i\beta)/\sigma)$$

$$Q_{y_i}(p|x_i) = x_i\beta + \sigma\Phi^{-1}(p)$$

In the Box-Cox framework we have,

$$h(y, \lambda) = x_i\beta + \sigma\varepsilon$$

so the  $p$ th quantile of  $y_i|x_i$  is

$$y_i = h_\lambda^{-1}(x_i\beta + \sigma\varepsilon)$$

$$Q_{y_i}(p|x_i) = h_\lambda^{-1}(x_i\beta + \sigma\Phi^{-1}(p))$$

Thus if we wanted to estimate the effect of a change in  $x_{ij}$  on the  $p$ th quantile of  $y_i$ , we would write

$$\frac{\partial}{\partial x_{ij}} Q_{y_i}(p|x_i) = \frac{\partial}{\partial x_{ij}} [h_\lambda^{-1}(x_i\beta + \sigma\Phi^{-1}(p))]$$

For example, if

$$h_\lambda(y_i) = \frac{y_i^\lambda - 1}{\lambda}$$

then,

$$\begin{aligned} y_i^\lambda &= \lambda h_i + 1 \\ y_i &= (\lambda h_i + 1)^{1/\lambda} \\ Q_{y_i}(p|x) &= (\lambda(x_i\beta + \sigma\Phi^{-1}(p)) + 1)^{1/\lambda} \\ \frac{\partial y_i}{\partial x_{ij}} &= \frac{1}{\lambda}(\lambda(x_i\beta + \sigma\Phi^{-1}(p)) + 1)^{\frac{1}{\lambda}-1} \cdot \lambda\beta_j = (\lambda(x_i\beta + \sigma\Phi^{-1}(p)) + 1)^{\frac{1}{\lambda}-1}\beta_j \end{aligned}$$

This could then be used to generate a confidence interval. Note that models for expectations are less convenient here since  $E(h(y)) \neq h(Ey)$ .

### *Transformations for Proportions*

Often we are interested in estimating models of proportions, for example, Engel Curves for proportions of expenditure, unemployment rates, etc. Two simple alternatives are logit:  $h(y) = \log(y/(1-y))$  or more generally  $h(y, \lambda) = y^\lambda - (1-y)^\lambda$  folded power transformation. Note  $\lim_{\lambda \rightarrow 0} h(y, \lambda) = \log(y/(1-y))$  We will have more to say about these cases later in the term.

## 1. Orthogonal Projection

A very brief review of least squares as orthogonal projection may be useful. Given the classical Gaussian linear model,

$$y = X\beta + u, \quad u \sim \mathcal{N}(0, \sigma^2 I_n),$$

the least squares estimator,  $\hat{\beta}$  is the mle, and takes the form,

$$\hat{\beta} = \operatorname{argmin}_\beta \|y - X\beta\|^2 = (X^\top X)^{-1} X^\top y.$$

This leads to the Pythagorean decomposition,

$$\|y\|^2 = \|\hat{y}\|^2 + \|\hat{r}\|^2 = \|P_X y\|^2 + \|M_X y\|^2$$

where

$$\hat{y} = X\hat{\beta} = X(X^\top X)^{-1} X^\top y \equiv P_X y$$

and

$$\hat{r} = y - \hat{y} = (I - P_X)y \equiv M_X y$$

The matrix  $P_X$  is idempotent, i.e.  $P_X P_X = P_X$  and symmetric, and therefore represents an orthogonal projection. Least squares finds the  $\hat{y}$  in the column space of  $X$ , denoted  $\mathcal{C}(X)$ , that is closest to  $y$  in Euclidean distance.

The matrix  $P_X$  is special in many ways. One way is its eigenstructure. Suppose that  $\xi$  is an eigenvector of  $P_X$  with associated eigenvalue,  $\lambda$ , so  $P_X \xi = \lambda \xi$ . Then idempotency of  $P_X$  implies that  $P_X \xi = \lambda P_X \xi$ . This is possible only if  $\lambda = 1$ , or if  $\lambda = 0$  and  $P_X \xi = 0$ . Thus we can conclude that  $P_X$  has eigenvalues that are either 1 or 0: if  $\xi \in \mathcal{C}(X)$  then  $\lambda = 1$ , and if  $\xi \perp \mathcal{C}(X)$  then  $\lambda = 0$ .

A very special example of the foregoing is the case that  $X = \mathbf{1}_n$ , an  $n$ -vector of ones. (This is the case in which the ‘‘regression’’ has an intercept, but *only* an intercept. Then,

$$P_X = P_1 = \mathbf{1}(\mathbf{1}^\top \mathbf{1})^{-1} \mathbf{1}^\top = n^{-1} J,$$

where  $J$  is an  $n$  by  $n$  matrix of ones. In this case  $\hat{y}$  as defined above is simply an  $n$  vector consisting of  $n$  coordinates all equal to  $\bar{y}$ . We will encounter this special case a few times later in the course.

### *References*

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