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# WEIGHTED-AVERAGE LEAST SQUARES (WALS): A SURVEY

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**Abstract.** Model averaging has become a popular method of estimation, following increasing evidence that model selection and estimation should be treated as one joint procedure. Weighted-average least squares (WALS) is a recent model-average approach, which takes an intermediate position between frequentist and Bayesian methods, allows a credible treatment of ignorance, and is extremely fast to compute. We review the theory of WALS and discuss extensions and applications.

Keywords. Computing time; Frequentist versus Bayesian; Least squares; Model averaging; Priors

# 1. Introduction

Our story begins with the *t*-ratio. Let us consider the model

$$y_j = \beta_0 + \beta_1 x_{1,j} + \beta_2 x_{2,j} + \epsilon_j$$
  $(j = 1, ..., n)$ 

We obtain estimators  $\hat{\beta}_0$ ,  $\hat{\beta}_1$ , and  $\hat{\beta}_2$ , and their estimated variances  $\hat{\sigma}_0^2$ ,  $\hat{\sigma}_1^2$  and  $\hat{\sigma}_2^2$ . Next, we consider the *t*-ratio  $t_2 = \hat{\beta}_2/\hat{\sigma}_2$ . This *t*-ratio can be viewed in two ways. We could be interested in testing the hypothesis that  $\beta_2 = 0$ . In that case  $t_2$  can be fruitfully employed, because under certain assumptions (such as normality) the *t*-ratio follows a Student distribution under the null hypothesis and if we fix the significance level of the test (say at 5%) then we can reject or not reject the hypothesis.

But the *t*-ratio is also commonly employed in a different way. Suppose we are primarily interested in the value of  $\beta_1$ . Then  $t_2$  is often used as a diagnostic, rather than as a test statistic, in order to decide whether we wish to keep  $x_2$  in the model or not. In this situation the 5% level is also typically used, although we could equally well argue in favor of the 95% or the 50% level or any other percentage. The two situations are different because in the first case we are interested in  $\beta_2$  while in the second case we are interested in  $\beta_1$ . In the first case we ask: Is it true that  $\beta_2 = 0$ ? In the second case: Does inclusion of  $x_2$  improve the estimator of  $\beta_1$ ? Two different questions requiring two different approaches.

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Let us consider the second situation, where  $t_2$  is used as a diagnostic, in more detail. We have three estimators of  $\beta_1$ , namely the estimator from the unrestricted model,  $\hat{\beta}_{1u}$ ; the estimator from the restricted model (where  $\beta_2 = 0$ ),  $\hat{\beta}_{1r}$ ; and the estimator after the preliminary test,

$$b_1 = w\hat{\beta}_{1u} + (1-w)\hat{\beta}_{1r}, \qquad w = \begin{cases} 1 & \text{if } |t_2| > c, \\ 0 & \text{if } |t_2| \le c, \end{cases}$$

for some c > 0, such as c = 1.96 corresponding to the 5% level. This is the pretest estimator. The pretest estimator is "kinked," which has both theoretical and practical consequences (Judge and Bock, 1978; Giles and Giles, 1993). A theoretical drawback is that the estimator is inadmissible, because any estimator which is not differentiable (worse still, discontinuous) is inadmissible (Magnus, 1999). A related practical problem—familiar to all empirical economists—is the property that for  $t_2 = 1.95$  we choose one estimator and for  $t_2 = 1.97$  another, while in fact there is little difference between 1.95 and 1.97. These considerations lead us to reconsider the estimator  $b_1 = w\hat{\beta}_{1u} + (1 - w)\hat{\beta}_{1r}$  by allowing w to be a smoothly increasing function of  $|t_2|$ . This is model averaging in its simplest form, and we see that it is just the continuous counterpart to pretesting.

To bring out the difference between pretesting and model averaging, suppose a king has 12 advisors. He wishes to forecast next year's inflation and calls each of the advisors in for consultation. He knows his advisors and obviously has more faith in some than in others. All 12 deliver their forecast, and the king is left with 12 numbers. How to choose from these 12 numbers? Let us consider two possibilities (there are more). The king could argue: which advisor do I trust most, whom do I believe is most competent? Then I take his or her advice. The king could also argue: all advisors have something useful to say, although not in the same degree. Some are cleverer and more informed than others and their forecast should get a higher weight. Which way of thinking is better? Intuitively most people prefer the second method (model averaging), where all pieces of advice are taken into account. In standard econometrics, however, it is the first method (pretesting) which dominates.

In practice, econometricians use not one or two, but many models. If we use diagnostic tests to search for the best-fitting model, then we need to take into account not only the uncertainty of the estimates in the selected model, but also the fact that we have used the data to select a model. In other words, model selection and estimation should be seen as a combined effort, not as two separate efforts, and failure to do so may lead to misleadingly precise estimates.

In pretesting one typically reports the properties of the estimator as if estimation had not been preceded by model selection. Standard statistical theory is therefore not directly applicable, since the properties of pretest estimators depend not only on the stochastic nature of the selected model, but also on the way the model has been selected. Problems associated with inference after model selection have been investigated in Magnus (1999, 2002), Danilov and Magnus (2004a, b), Leeb and Pötscher (2003, 2005, 2006, 2008), and others. All these studies conclude that ignoring the uncertainty associated with the model selection step can lead to seriously misleading inference. Another major drawback of ignoring the noise produced by model selection is that small perturbations of the data may result in very different models being selected (Yang, 2001).

In model averaging one does not select a single model out of the available set of models—in fact, the question "which is the correct model" is not answered, because model selection is thought of as an intermediate step, not a goal in itself. Each model contributes information on the parameters of interest, and all these pieces of information are combined into an unconditional estimate using a weighted average of the conditional estimates across all possible models. The theory of model averaging thus incorporates the uncertainty arising from estimation and model selection jointly. (Model averaging is not the only method which combines estimation uncertainty and model selection uncertainty—penalized regression is also widely used (see the discussion in Kumar and Magnus (2013, p. 221))).

One can estimate the parameters from either a frequentist or a Bayesian perspective. Also, one can choose the weights from a frequentist or a Bayesian perspective. This gives rise to four different types

of model averaging. The method presented here, called weighted-average least squares (WALS), is a Bayesian combination of frequentist estimators, and it has advantages over other model-average methods that will be discussed later.

The theory and application of WALS was developed in a large number of papers. In many of these papers we did not immediately find the shortest proofs (this is true in particular for the equivalence theorem) or the most suitable prior (Laplace, Weibull), there are some ambiguities and misunderstandings that need to be put right (for example about the semiorthogonal transformation, originally introduced as an assumption—which it is not), and the notation is not consistent across papers. In this review, we attempt to present one consistent theory of WALS. This review paper is, however, rather more than a summary of past results. For example, much attention is given to the underlying assumptions and where and why precisely they are needed, and a new improved prior is introduced for the weight function.

The paper is organized as follows. In Sections 2 and 3, we present the framework and the constrained least-squares estimators. WALS and the equivalence theorem are introduced in Section 4. After an interlude on the question whether weights should necessarily lie between zero and one (Section 5), we discuss preliminary scaling, the semiorthogonal transformation, and its consequences (Sections 6 and 7). Then we turn to the weights by providing a frequentist weight function in Section 8 and a Bayesian weight function in Section 9. We prefer the latter because it allows us to obtain an admissible estimator which also has a credible interpretation in terms of ignorance. The analysis so far has assumed that the error variance in the regression model is known. This is clearly unrealistic and Section 10 discusses how to deal with this additional problem. Section 11 puts it all together and provides a 7-step outline of the procedure.

Next we discuss extensions (Section 12), some of which have already been analyzed in the WALS literature, while some are suggestions for future research. We also highlight some empirical applications of the WALS method. In Section 13, we compare WALS with other model-average estimators and in Section 14 we discuss user-friendly software for WALS, both in MATLAB and Stata.

# 2. Framework and Preliminaries

Our data are assumed to be generated by the linear process

$$y = X_1 \beta_1 + X_2 \beta_2 + \epsilon, \tag{1}$$

where y ( $n \times 1$ ) is the vector of observations on the outcome of interest,  $X_1$  ( $n \times k_1$ ) and  $X_2$  ( $n \times k_2$ ) are matrices of nonrandom regressors,  $\epsilon$  is a random vector of unobservable disturbances, and  $\beta_1$  and  $\beta_2$  are unknown nonrandom parameter vectors. We assume that  $k_1 \ge 1$ ,  $k_2 \ge 1$ ,  $k = k_1 + k_2 \le n - 1$ , that  $X = (X_1 : X_2)$  has full column-rank k, and that the disturbances  $\epsilon_1, \epsilon_2, \ldots, \epsilon_n$  are independent and identically distributed (i.i.d.) and normal, so that  $\epsilon \sim N(0, \sigma^2 I_n)$ .

This is the classical setup of the linear model (including fixed regressors and normality), except that we distinguish between two types of regressors:  $X_1$  and  $X_2$ . The reason for distinguishing between  $X_1$  and  $X_2$  is that  $X_1$  contains explanatory variables which we want to be present in each model on theoretical or other grounds (irrespective of the observed *t*-values of the  $\beta_1$ -parameters), while  $X_2$  contains additional explanatory variables of which we are less certain. This setup is more general than the conventional case where typically all regressors are auxiliary except the constant term. The new setup thus allows the investigator to keep a regressor in the model even when diagnostic tests suggest to remove it. The columns of  $X_1$  are called "focus" regressors and the columns of  $X_2$  "auxiliary" regressors. Similarly, the components of  $\beta_1$  are called "focus" parameters, and the components of  $\beta_2$  "auxiliary" parameters.

In the context of estimation (we shall also consider prediction), our interest is in the estimation of  $\beta_1$ , and the only role for  $X_2$  is to "improve" the estimator of  $\beta_1$ . However, if the investigator is interested in both  $\beta_1$  and  $\beta_2$ , then the analysis and the model-average properties do not change. This is the key

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message of Proposition 4.2 (the equivalence theorem), and we shall expand on this surprising result in Section 4.

The data-generation process (DGP) described in (1) is of course not known to the investigator, and hence the model or models used by him or her will in general deviate from it. We shall only consider models that are *smaller* than (or equal to) the DGP, so that the model space  $\mathcal{M}$  consists of all submodels  $\mathcal{M}_i$  of (1) that contain *all* focus regressors and *some* of the auxiliary regressors. In practice, the DGP and the largest model will not coincide. There may be a set of regressors, say  $X_3$ , such that the DGP is given by

$$y = X_1\beta_1 + X_2\beta_2 + X_3\beta_3 + \epsilon,$$

where  $X_1$  is always in the model,  $X_2$  may or may not be in the model and  $X_3$  is never in the model. This is more general and more realistic than (1). The regressors in  $X_3$  may not be known to us, or we may know them in theory but lack the data, or we may know them in theory and have the relevant data but believe *a priori* that the associated  $\beta_3$ -parameter is so "small" that the increase in misspecification bias is outweighed by the decrease in estimated standard errors. In the first two cases we cannot include  $X_3$  in the DGP, but in the third case we can and we should so that  $X_3$  would belong to the DGP but not to the model space. In what follows we shall not follow this route and make the simplifying assumption that (1) is the DGP, so that the largest model and the DGP coincide. Model uncertainty is thus restricted to a well-defined class of models which is known in advance, the so-called  $\mathcal{M}$ -closed perspective (Hoeting *et al.*, 1999).

When  $k_2 = 1$  (one auxiliary regressor), we have two models: the unrestricted and the restricted (where  $\beta_2 = 0$ ). When  $k_2 = 2$  (two auxiliary regressors), there are four possible models: the unrestricted model, two partially restricted models (one of the two components of  $\beta_2$  is zero) and the fully restricted model (both components of  $\beta_2$  are zero). In general, there are  $2^{k_2}$  models to consider. The *i*th model  $\mathcal{M}_i$  is characterized by a  $k_2 \times r_i$  selection matrix  $S_i$  with rank  $0 \le r_i \le k_2$ , so that  $S'_i = (I_{r_i} : 0)$  or a column-permutation thereof. In other words,  $\mathcal{M}_i$  is defined as the linear model (1) under the restriction  $S'_i\beta_2 = 0$ . The number  $r_i$  denotes the number of excluded auxiliary variables and the matrix  $S_i$  specifies which  $r_i$  variables are excluded. For given  $r_i$ , there are  $\binom{k_i}{r_i}$  different possible choices for the selection matrix  $S_i$ , in total

$$\sum_{r_i=0}^{k_2} \binom{k_2}{r_i} = 2^{k_2}$$

It will be useful to define

$$M_1 = I_n - X_1 (X_1' X_1)^{-1} X_1', \qquad Q = (X_1' X_1)^{-1} X_1' X_2 (X_2' M_1 X_2)^{-1/2}.$$
 (2)

Our first interest is in the constrained least-squares (LS) estimators of  $\beta_1$  and  $\beta_2$  in model  $\mathcal{M}_i$ . As a preliminary to the general results presented in Section 3, we first consider the two extremes: the (fully) restricted model and the unrestricted model. In the restricted model (where  $\beta_2 = 0$ ) we find

$$\hat{\beta}_{1r} = (X_1' X_1)^{-1} X_1' y, \tag{3}$$

while in the unrestricted model we have

$$\hat{\beta}_{1u} = \hat{\beta}_{1r} - (X_1'X_1)^{-1}X_1'X_2\hat{\beta}_{2u}, \qquad \hat{\beta}_{2u} = (X_2'M_1X_2)^{-1}X_2'M_1y.$$
(4)

The subscripts "u" and "r" denote "unrestricted" and "restricted" (with  $\beta_2 = 0$ ), respectively. It is easy to see that  $\hat{\beta}_{1r}$  and  $\hat{\beta}_{1u}$  are always correlated, and that  $\hat{\beta}_{1u}$  and  $\hat{\beta}_{2u}$  are only uncorrelated when  $X'_1X_2 = 0$ . In contrast,  $\hat{\beta}_{1r}$  and  $\hat{\beta}_{2u}$  are always uncorrelated.

**Proposition 2.1.** The two least-squares estimators  $\hat{\beta}_{1r}$  and  $\hat{\beta}_{2u}$  are independent.

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*Proof.* Since  $M_1X_1 = 0$  we have  $cov(X'_1y, X'_2M_1y) = \sigma^2 X'_1M_1X_2 = 0$ , and the result follows.

This simple fact will play an important role in the sequel. We introduce

$$\hat{\theta} = (X_2' M_1 X_2)^{-1/2} X_2' M_1 y, \qquad \theta = (X_2' M_1 X_2)^{1/2} \beta_2, \tag{5}$$

and note that  $\hat{\theta} \sim N(\theta, \sigma^2 I_{k_2})$ , so that the components of  $\hat{\theta}$  are independent. The estimators in (4) now simplify to

$$\hat{\beta}_{1u} = \hat{\beta}_{1r} - Q\hat{\theta}, \qquad \hat{\beta}_{2u} = (X'_2 M_1 X_2)^{-1/2} \hat{\theta}, \tag{6}$$

and Proposition 2.1 tells us that  $\hat{\beta}_{1r}$  and  $\hat{\theta}$  are independent. These two vectors are independent because of the normality of y and the fact that  $X'_1 y$  and  $X'_2 M_1 y$  are uncorrelated. In fact, even if the observations  $y_1, \ldots, y_n$  are not normal and the data-generating process is unknown,  $\hat{\beta}_{1r}$  and  $\hat{\theta}$  will still be uncorrelated, as long as  $y_1, y_2, \ldots, y_n$  are uncorrelated with constant variance (Leeb and Pötscher, 2003, lemma A.1).

### 3. Constrained Least Squares

Let us now consider the general case, that is, the constrained LS estimation of  $\beta_1$  and  $\beta_2$  in model  $\mathcal{M}_i$ under the constraint  $S'_i\beta_2 = 0$ .

**Proposition 3.1.** The LS estimators of  $\beta_1$  and  $\beta_2$  in model  $\mathcal{M}_i$  are given by

$$\hat{\beta}_{1(i)} = \hat{\beta}_{1r} - QW_i\hat{\theta}, \qquad \hat{\beta}_{2(i)} = (X'_2M_1X_2)^{-1/2}W_i\hat{\theta}, \tag{7}$$

where Q is given in (2),  $W_i = I_{k_2} - P_i$ , and

$$P_{i} = (X_{2}'M_{1}X_{2})^{-1/2}S_{i} \left(S_{i}'(X_{2}'M_{1}X_{2})^{-1}S_{i}\right)^{-1}S_{i}'(X_{2}'M_{1}X_{2})^{-1/2}$$
(8)

is a symmetric idempotent  $k_2 \times k_2$  matrix of rank  $r_i$ .

Proof. This follows from Lemma A1 in Danilov and Magnus (2004a).

In the special case where  $r_i = k_2$ , we have  $P_i = I_{k_2}$  and  $W_i = 0$ : the restricted case. In the other extreme where  $r_i = 0$ , we have  $P_i = 0$  and  $W_i = I_{k_2}$ : the unrestricted case. The subscript *i* always refers to the *i*th model ( $i = 1, ..., 2^{k_2}$ ). We write (*i*) instead of *i* when the object is a random variable or a random vector.

We saw in (6) that the unrestricted estimator  $\hat{\beta}_{1u}$  is a linear function of  $\hat{\beta}_{1r}$  and  $\hat{\theta}$ . Proposition 3.1 shows that this remains true, more generally, for each  $\hat{\beta}_{1(i)}$ . The estimator  $\hat{\beta}_{2(i)}$  is a linear function of  $\hat{\theta}$  only and hence independent of  $\hat{\beta}_{1r}$ .

The distribution of the two estimators and the vector of residuals are given in the next two propositions.

**Proposition 3.2.** The distribution of  $\hat{\beta}_{1(i)}$  in model  $\mathcal{M}_i$  is given by

$$\hat{\beta}_{1(i)} \sim \mathrm{N}\left(\beta_1 + QP_i\theta, \ \sigma^2\left((X_1'X_1)^{-1} + QW_iQ'\right)\right),$$

*the distribution of*  $\hat{\beta}_{2(i)}$  *by* 

$$\hat{\beta}_{2(i)} \sim \mathrm{N}\left( (X'_2 M_1 X_2)^{-1/2} W_i \theta, \ \sigma^2 \left( (X'_2 M_1 X_2)^{-1/2} W_i (X'_2 M_1 X_2)^{-1/2} \right) \right),$$

and the covariance of  $\hat{\beta}_{1(i)}$  and  $\hat{\beta}_{2(i)}$  is

$$cov(\hat{\beta}_{1(i)}, \hat{\beta}_{2(i)}) = -\sigma^2 Q W_i (X'_2 M_1 X_2)^{-1/2}$$

*Proof.* This follows from Proposition 3.1 and the fact that

$$\hat{\beta}_{1r} \sim \mathrm{N}(\beta_1 + Q\theta, \ \sigma^2(X_1'X_1)^{-1}), \qquad \hat{\theta} \sim \mathrm{N}(\theta, \ \sigma^2 I_{k_2}),$$

and  $\hat{\beta}_{1r}$  and  $\hat{\theta}$  are independent.

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**Proposition 3.3.** *The residual vector in model*  $M_i$  *is* 

$$e_{(i)} = y - X_1 \hat{\beta}_{1(i)} - X_2 \hat{\beta}_{2(i)} = D_i y,$$

where

$$D_i = M_1 - M_1 X_2 (X'_2 M_1 X_2)^{-1/2} W_i (X'_2 M_1 X_2)^{-1/2} X'_2 M_1$$

is a symmetric idempotent matrix of rank  $n - k + r_i$ , and the distribution of  $s_{(i)}^2 = e'_{(i)}e_{(i)}/(n - k + r_i)$  is given by

$$\frac{(n-k+r_i)s_{(i)}^2}{\sigma^2} \sim \chi^2 \left(n-k+r_i, \frac{\theta' P_i \theta}{\sigma^2}\right).$$

*Proof.* This also follows from Proposition 3.1.

We note that in each model  $\mathcal{M}_i$  the residual vector  $e_{(i)}$  is a linear function of  $e_r = M_1 y$ , the residual vector in the restricted model. This is because  $e_{(i)} = D_i y = D_i M_1 y$ . All residuals (irrespective from which model) are therefore independent of  $\hat{\beta}_{1r}$ , the restricted estimator of  $\beta_1$ .

Finally, we present the covariances between the estimators from two competing models  $\mathcal{M}_i$  and  $\mathcal{M}_j$ .

**Proposition 3.4.** The estimators from models  $M_i$  and  $M_j$  are correlated with each other according to

$$\begin{aligned} & cov(\hat{\beta}_{1(i)}, \hat{\beta}_{1(j)}) = \sigma^2 \left( (X_1'X_1)^{-1} + QW_iW_jQ' \right), \\ & cov(\hat{\beta}_{2(i)}, \hat{\beta}_{2(j)}) = \sigma^2 (X_2'M_1X_2)^{-1/2} W_iW_j(X_2'M_1X_2)^{-1/2}, \\ & cov(\hat{\beta}_{1(i)}, \hat{\beta}_{2(j)}) = -\sigma^2 QW_iW_j(X_2'M_1X_2)^{-1/2}. \end{aligned}$$

Proof. Again, this follows from Proposition 3.1.

As a consequence of Proposition 3.4 and assuming that  $X'_1 X_2 \neq 0$ , we see that  $\hat{\beta}_{2(j)}$  will be correlated with both  $\hat{\beta}_{1(i)}$  and  $\hat{\beta}_{2(i)}$ , unless  $W_i W_i = 0$ .

# 4. WALS and the Equivalence Theorem

In the previous section, we derived the LS estimators for  $\beta_1$  and  $\beta_2$  in model  $\mathcal{M}_i$ , where  $\beta_2$  is restricted by  $S'_i\beta_2 = 0$ . Since there are  $2^{k_2}$  models, there are also  $2^{k_2}$  different sets of estimators  $\hat{\beta}_{1(i)}$  and  $\hat{\beta}_{2(i)}$ . The WALS estimators of  $\beta_1$  and  $\beta_2$  are, as the name suggests, weighted averages of the estimators of  $\beta_1$  and  $\beta_2$  over all models.

**Definition 4.1.** *The WALS estimators of*  $\beta_1$  *and*  $\beta_2$  *are* 

$$b_1 = \sum_{i=1}^{2^{k_2}} \lambda_{(i)} \hat{\beta}_{1(i)}, \qquad b_2 = \sum_{i=1}^{2^{k_2}} \lambda_{(i)} \hat{\beta}_{2(i)},$$

where the sum is taken over all  $2^{k_2}$  different models  $\mathcal{M}_i$  obtained by setting a subset of the  $\beta_2$ 's equal to zero.

The key question, of course, is how to define the model weights  $\lambda_{(i)}$ . (Here and in what follows we refer to the  $\lambda_{(i)}$  as "model" weights to distinguish them from the "WALS" weights  $w_h$  to be defined later.) We shall impose the following restrictions.

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**Assumption 4.1.** The model weights  $\lambda_{(i)}$  satisfy the following three regularity conditions:

(*R1*)  $0 \le \lambda_{(i)} \le 1$ ; (*R2*)  $\sum_{i} \lambda_{(i)} = 1$ ; and (*R3*)  $\lambda_{(i)} = \lambda_{(i)}(M_1 y)$ .

The first two conditions simply state that the  $\lambda_{(i)}$  are weights. Condition (R3), however, requires some justification. If  $\sigma^2$  is known, then most or all pretest procedures will use statistics (such as *t*- and *F*-statistics) which depend on  $\hat{\beta}_{2u}$  (that is, on  $X'_2 M_1 y$ ) only. If  $\sigma^2$  is not known and is estimated by  $s_u^2$  (the estimator of  $\sigma^2$  in the unrestricted model), then all *t*- and *F*-statistics will depend on  $(\hat{\beta}_{2u}, s_u^2)$ . Now, since  $s_u^2$  is a function of  $M_1 y$ , the pretest procedures will use statistics that depend on  $M_1 y$  only. Finally, if  $\sigma^2$  is not known and estimated by  $s_{(i)}^2$  (the estimator of  $\sigma^2$  in model  $\mathcal{M}_i$ ), then it is no longer true that all *t*- and *F*-statistics depend only on  $(\hat{\beta}_{2u}, s_u^2)$ . However, they still depend only on  $M_1 y$ , because Propositions 3.1 and 3.3 imply that both  $\hat{\beta}_{2(i)}$  and the residuals  $e_{(i)}$  from model  $\mathcal{M}_i$  are linear functions of  $M_1 y$ .

If we think of the model weights  $\lambda_{(i)}$  as a measure of 'importance' of model  $\mathcal{M}_i$  based on some diagnostic (say a *t*-statistic), then condition (R3) is satisfied. The regularity conditions on  $\lambda_{(i)}$  thus appear to be reasonable and mild. They allow not only all standard pretest procedures, but also inequality-constrained least squares. Thus, Proposition 4.2 below explains the "surprising symmetry" found by Thomson and Schmidt (1982, p. 176).

**Proposition 4.1.** Under regularity condition (R2), the WALS estimators take the form

$$b_1 = \hat{\beta}_{1r} - QW\hat{\theta}, \qquad b_2 = (X'_2M_1X_2)^{-1/2}W\hat{\theta},$$
(9)

where  $W = \sum_{i} \lambda_{(i)} W_i$  is a symmetric random matrix (because the  $\lambda_{(i)}$  are random) even though the  $W_i$  are nonrandom.

*Proof.* This follows by summing the expressions for  $\hat{\beta}_{1(i)}$  and  $\hat{\beta}_{2(i)}$  in (7) over all  $i = 1, ..., 2^{k_2}$ . Condition (R2) ensures that  $\sum_i \lambda_{(i)} \hat{\beta}_{1r} = \hat{\beta}_{1r}$ .

We note that only condition (R2) is needed to obtain the WALS estimators. We also note that the dependence of the WALS estimators  $b_1$  and  $b_2$  on *i* is completely captured by the symmetric  $k_2 \times k_2$  matrix *W*, which contains  $k_2(k_2 + 1)/2$  essential elements, rather less than the  $2^{k_2}$  different  $\lambda_{(i)}$ 's. As a consequence, in order to obtain the WALS estimates, we don't need to determine all the  $\lambda_{(i)}$ 's—it is sufficient to determine *W*. If *W* were diagonal, this would reduce our task even further, and this is precisely the purpose of the transformation introduced in Section 6.

Let us rewrite (9) as

$$b_1 - \beta_1 = (X'_1 X_1)^{-1} (X'_1 \epsilon) - Q(W\hat{\theta} - \theta),$$
  

$$b_2 - \beta_2 = (X'_2 M_1 X_2)^{-1/2} (W\hat{\theta} - \theta).$$
(10)

Suppose now that, in addition to (R2), regularity condition (R3) also holds, so that the  $\lambda_{(i)}$  depend only on  $M_1 y$ . Then W will also depend only on  $M_1 y$ . Since  $\hat{\theta}$  depends only on  $M_1 y$  as well, condition (R3) guarantees that  $W\hat{\theta}$  depends only on  $M_1 y$  and is therefore independent of  $X'_1 \epsilon$ . Based on these considerations, we prove the following key result.

**Proposition 4.2.** (EQUIVALENCE THEOREM) If regularity conditions (R2) and (R3) on  $\lambda_{(i)}$  are satisfied, then

$$E(b_1) = \beta_1 - QE(W\hat{\theta} - \theta), \quad var(b_1) = \sigma^2 (X'_1 X_1)^{-1} + Qvar(W\hat{\theta})Q',$$

and hence

$$MSE(b_1) = \sigma^2 (X'_1 X_1)^{-1} + QMSE(W\hat{\theta})Q'.$$

*Proof.* This follows from the expressions in (10). Alternatively we have, since  $\hat{\beta}_{1r}$  and  $M_1y$  are independent,

$$E(\hat{\beta}_{1r} \mid M_1 y) = E(\hat{\beta}_{1r}), \quad var(\hat{\beta}_{1r} \mid M_1 y) = var(\hat{\beta}_{1r}),$$

so that

$$E(b_1 \mid M_1 y) = E(\hat{\beta}_{1r} \mid M_1 y) - QE(W\hat{\theta} \mid M_1 y)$$
$$= E(\hat{\beta}_{1r}) - QW\hat{\theta} = \beta_1 - Q(W\hat{\theta} - \theta)$$

and

$$var(b_1 | M_1 y) = var(\hat{\beta}_{1r} | M_1 y) = var(\hat{\beta}_{1r}) = \sigma^2 (X'X)^{-1}.$$

The unconditional mean and variance of  $b_1$  and hence its mean squared error (MSE) follow.

We shall assess the relative performance of estimators by comparing MSEs, that is, by assuming squared error loss. The properties of the complicated WALS estimator  $b_1$  of  $\beta_1$  thus depend critically on the properties of the less complicated estimator  $W\hat{\theta}$  of  $\theta$ . In particular,  $MSE(b_1)$  is small whenever  $MSE(W\hat{\theta})$  is small. Notice that neither the bias, nor the variance or the mean squared error of  $b_1$  depend on  $\beta_1$ . They do, however, depend on  $\beta_2$  or, more accurately, on  $\theta$ .

We can also interpret Proposition 4.2 in terms of  $\beta_1$  and  $\beta_2$ . It follows from (10) that  $MSE(b_1, b_2)$  can be written in the same form as  $MSE(b_1)$ , namely as  $A + BMSE(W\hat{\theta})B'$  for some positive semidefinite matrix A and some matrix B, and hence the question how "good"  $b_1$  and  $b_2$  are as estimators of  $\beta_1$  and  $\beta_2$ depends completely on the question how 'good'  $W\hat{\theta}$  is as an estimator of  $\theta$ . This point is also emphasized by Clarke (2008).

Proposition 4.2 provides a nontrivial generalization of Theorem 2 in Magnus and Durbin (1999), using a simpler proof than in Magnus and Durbin (1999) and Danilov and Magnus (2004a). Extensions to cover, respectively, the cases of large-sample nonnormal errors and uncertainty about linear restrictions of the parameters  $\beta_1$  and  $\beta_2$  are provided in Zou *et al.* (2007) and Clarke (2008).

### 5. Interlude: Should Weights Lie between Zero and One?

Our results so far have not used condition (R1), requiring that the  $\lambda_{(i)}$  lie between zero and one. Although we shall make this assumption later, this condition is not as obvious as it may appear at first. Following Magnus and Vasnev (2008), suppose we have two unbiased estimators of an unknown parameter  $\mu$ :

$$\hat{\mu}_1 = \mu + \epsilon_1, \quad \hat{\mu}_2 = \mu + \epsilon_2,$$

where  $(\epsilon_1, \epsilon_2)$  follows a bivariate normal distribution with mean zero and known variance

$$var\begin{pmatrix}\epsilon_1\\\epsilon_2\end{pmatrix} = \begin{pmatrix}\sigma_1^2 & \sigma_{12}\\\sigma_{12} & \sigma_2^2\end{pmatrix}.$$

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If  $\epsilon_1$  and  $\epsilon_2$  are uncorrelated ( $\sigma_{12} = 0$ ) and the two variances are equal, then we estimate  $\mu$  by the unbiased minimum-variance estimator  $\hat{\mu} = (\hat{\mu}_1 + \hat{\mu}_2)/2$ . If  $\epsilon_1$  and  $\epsilon_2$  are uncorrelated and the two variances are not equal, then the unbiased minimum-variance estimator of  $\mu$  is

$$\hat{\mu} = \lambda \hat{\mu}_1 + (1 - \lambda)\hat{\mu}_2, \quad \lambda = \frac{\sigma_2^2}{\sigma_1^2 + \sigma_2^2},$$

which is a weighted average of  $\hat{\mu}_1$  and  $\hat{\mu}_2$ , where the weight  $\lambda$  lies between zero and one.

Next consider the case where  $\epsilon_1$  and  $\epsilon_2$  are correlated. Then we also obtain  $\hat{\mu} = \lambda \hat{\mu}_1 + (1 - \lambda)\hat{\mu}_2$ , but now with

$$\lambda = \frac{\sigma_2^2 - \sigma_{12}}{\sigma_1^2 + \sigma_2^2 - 2\sigma_{12}}.$$

We see that  $\lambda$  does *not* necessarily lie between zero and one. In particular,  $\lambda < 0$  if and only if  $\sigma_{12} > \sigma_2^2$ , and  $\lambda > 1$  if and only if  $\sigma_{12} > \sigma_1^2$ .

At first glance this may seem puzzling and unsatisfactory. At second glance, however, it becomes clear that this is the correct solution, and that we should not force our estimator to lie in-between the two underlying estimators.

To gain further insight let us consider two cases. First, the situation where the correlation is one  $(\sigma_{12} = \sigma_1 \sigma_2)$  and  $\sigma_1 \neq \sigma_2$ . Then we have  $\hat{\mu}_1 = \mu + \sigma_1 \epsilon^*$  and  $\hat{\mu}_2 = \mu + \sigma_2 \epsilon^*$ , where the common noise  $\epsilon^*$  satisfies  $\epsilon^* \sim N(0, 1)$ . In this case,  $\hat{\mu}$  must lie outside the interval  $(\hat{\mu}_1, \hat{\mu}_2)$ . We simply solve the two equations in two unknowns ( $\mu$  and  $\epsilon^*$ ) and find  $\hat{\mu} = \lambda \hat{\mu}_1 + (1 - \lambda) \hat{\mu}_2$  with

$$\lambda = \frac{\sigma_2}{\sigma_2 - \sigma_1},$$

The "weight"  $\lambda$  in this case is either larger than one (if  $\sigma_1 < \sigma_2$ ) or smaller than zero (if  $\sigma_1 > \sigma_2$ ).

Second, the situation where

$$\hat{\mu}_1 \sim N(\mu, \sigma_1^2), \quad \hat{\mu}_2 = \hat{\mu}_1 + \epsilon_2$$

where  $\epsilon_2$  has mean zero and is distributed independently of  $\hat{\mu}_1$ . In this case  $cov(\hat{\mu}_1, \hat{\mu}_2) = \sigma_1^2$  and  $\hat{\mu} = \hat{\mu}_1$ . The estimator  $\hat{\mu}_1$  is a sufficient statistic for  $\mu$  and the information contained in  $\hat{\mu}_2$  is superfluous.

We conclude that – in the presence of correlation—"weights" may lie outside the (0, 1) interval. This result is not new, but it is little known because it is somewhat disturbing. Suppose the same king as in the Introduction now has two advisors, and that he consults both of them about next year's inflation. One predicts 2%, the other 4%. The first prediction has variance 1, the second has variance 4. If the two advisors were uncorrelated (they do not know each other and they base their forecasts on different data sets), then the king would weigh the two estimates, giving a higher weight to the first advisor because she is more accurate (has a lower variance). The answer then is 2.5%, which is in-between 2% and 4%, but closer to two than to four, as expected. But it is more likely that the advisors are correlated, that they do talk together, and that they use the same or similar data sets. If their correlation is 3/4 (which is not that high), then

$$\lambda = \frac{\sigma_2^2 - \sigma_{12}}{\sigma_1^2 + \sigma_2^2 - 2\sigma_{12}} = \frac{4 - 1.5}{1 + 4 - 2 \times 1.5} = 1.25,$$

and the king should therefore estimate next year's inflation by  $1.25 \times 2\% - 0.25 \times 4\% = 1.5\%$ , which lies outside the range indicated by the two advisors (2% and 4%). Now the king has a problem. He has a prediction which makes mathematical and statistical sense, but if he goes outside the range indicated by his advisors he will surely be heavily criticized. In practice, therefore, policy recommendations typically obey the boundaries specified by the advisors, and weights lie between zero and one. In accordance with all moving average techniques, we too submit to this practice.

# 6. A Semiorthogonal Transformation

The WALS procedure relies on a preliminary orthogonal transformation of the auxiliary regressors which greatly reduces the computational burden of the model-average estimator and has other advantages as well which will be discussed later.

We first scale the focus regressors  $X_1$  by defining

$$Z_1 = X_1 \Delta_1, \qquad \gamma_1 = \Delta_1^{-1} \beta_1, \tag{11}$$

where  $\Delta_1$  is a diagonal  $k_1 \times k_1$  matrix with positive diagonal elements such that the diagonal elements of  $Z'_1Z_1$  are all one. Notice that  $Z_1\gamma_1 = X_1\beta_1$  and that

$$I_n - Z_1 (Z_1' Z_1)^{-1} Z_1' = I_n - X_1 \Delta_1 (\Delta_1 X_1' X_1 \Delta_1)^{-1} \Delta_1 X_1' = M_1.$$

Hence, scaling  $X_1$  is completely harmless, and  $\beta_1$  can always be recovered from  $\gamma_1$  by  $\beta_1 = \Delta_1 \gamma_1$ .

We next scale the auxiliary regressors  $X_2$  by introducing a diagonal  $k_2 \times k_2$  matrix  $\Delta_2$  with positive diagonal elements such that all diagonal elements of  $\Delta_2 X'_2 M_1 X_2 \Delta_2$  are one. As a result, the original regressors  $X_1$  and  $X_2$  are scaled such that all diagonal elements of

$$(X_1\Delta_1)'(X_1\Delta_1)$$
 and  $(X_2\Delta_2)'M_1(X_2\Delta_2)$ 

equal one. These scaling procedures were first proposed in De Luca and Magnus (2011) and stabilize both matrices so that inversion and eigenvalue routines become numerically more accurate.

For the auxiliary regressors we not only scale but also transform. Since the matrix  $\Delta_2 X'_2 M_1 X_2 \Delta_2$  is positive definite, its eigenvalues are all positive and its eigenvectors are linearly independent. Defining the orthogonal  $k_2 \times k_2$  matrix T (whose columns are the eigenvectors) and the diagonal  $k_2 \times k_2$  matrix  $\Xi$  (containing the eigenvalues on the diagonal), we have

$$T'\Delta_2 X'_2 M_1 X_2 \Delta_2 T = \Xi.$$

We then define

$$Z_2 = X_2 \Delta_2 T \Xi^{-1/2}, \qquad \gamma_2 = \Xi^{1/2} T' \Delta_2^{-1} \beta_2, \tag{12}$$

so that  $Z_2 \gamma_2 = X_2 \beta_2$  and

$$Z_{2}'M_{1}Z_{2} = \Xi^{-1/2}T'\Delta_{2}X_{2}'M_{1}X_{2}\Delta_{2}T\Xi^{-1/2} = I_{k_{2}}.$$

The effect of the scaling in  $X_1$  is only for numerical stability; it has no effect on the WALS estimates. But the scaling in  $X_2$  has two effects: numerical stability and scale-independence. This is because of the semiorthogonalization. Without preliminary scaling the WALS estimates would depend on the scaling of the auxiliary variables (unless  $k_2 = 1$ ), because the orthogonal matrix T and the diagonal matrix  $\Xi$  depend on the scaling in a nontrivial (nonlinear) fashion. This dependence vanishes after preliminary scaling, which is obviously important in the interpretation of the WALS estimates. As with  $\beta_1$ , we can recover  $\beta_2$  by  $\beta_2 = \Delta_2 T \Xi^{-1/2} \gamma_2$ .

Since  $X_1\beta_1 = Z_1\gamma_1$  and  $X_2\beta_2 = Z_2\gamma_2$ , the DGP given in (1) can also be written as

$$y = Z_1 \gamma_1 + Z_2 \gamma_2 + \epsilon. \tag{13}$$

The important difference between (1) and (13) is that  $X'_2M_1X_2$  is positive definite but without any known structure, while  $Z'_2M_1Z_2$  is constructed in such a way that it equals the identity matrix  $I_{k_2}$ .

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# 7. Consequences of the Transformation

The fact that the matrix  $M_1Z_2$  is semiorthogonal so that  $Z'_2M_1Z_2 = I_{k_2}$  leads to important simplifications, which we list explicitly below. The matrices  $M_1$  and Q become

$$M_1 = I_n - Z_1 (Z'_1 Z_1)^{-1} Z'_1, \qquad Q = (Z'_1 Z_1)^{-1} Z'_1 Z_2,$$

and the LS estimators of  $\gamma_1$  and  $\gamma_2$  under the constraint  $S'_i \gamma_2 = 0$  are now given by

$$\hat{\gamma}_{1(i)} = \hat{\gamma}_{1r} - Q W_i \hat{\gamma}_{2u}, \qquad \hat{\gamma}_{2(i)} = W_i \hat{\gamma}_{2u}, \tag{14}$$

where

$$\hat{\gamma}_{1r} = (Z'_1 Z_1)^{-1} Z'_1 y, \qquad \hat{\gamma}_{2u} = Z'_2 M_1 y.$$
 (15)

The idempotent matrix  $P_i$  reduces to

$$P_i = S_i (S'_i S_i)^{-1} S'_i = S_i S'_i,$$

because  $S'_i$  is a selection matrix of the form  $(I_{r_i}: 0)$  or a column-permutation thereof, so that  $S'_i S_i = I_{r_i}$ . Hence,  $P_i$  is a *diagonal* matrix with  $r_i$  ones and  $k_2 - r_i$  zeros on the diagonal, and

$$W_i = I_{k_2} - S_i S_i$$

is a *diagonal* matrix with  $k_2 - r_i$  ones and  $r_i$  zeros on the diagonal.

The diagonality of  $W_i$  implies that the *h*th diagonal element of  $W_i$  is 0 if  $\gamma_{2,h}$  (the *h*th component of  $\gamma_2$ ) is constrained to be zero, and 1 otherwise. All models that include the *h*th column of  $Z_2$  as a regressor will therefore have the *same* estimator of  $\gamma_{2,h}$ , irrespective which other  $\gamma_2$ 's are estimated, namely the *h*th component of  $\hat{\gamma}_{2u}$ . Moreover,

$$\hat{\gamma}_{2u} \sim \mathrm{N}(\gamma_2, \sigma^2 I_{k_2}),$$

so that the  $k_2$  components of  $\hat{\gamma}_{2u}$  are independent.

The joint distribution of  $\hat{\gamma}_{1(i)}$  and  $\hat{\gamma}_{2(i)}$  is given by

$$\begin{pmatrix} \hat{\gamma}_{1(i)} \\ \hat{\gamma}_{2(i)} \end{pmatrix} \sim \mathbf{N} \left( \begin{pmatrix} \gamma_1 + \mathcal{Q} S_i S_i' \gamma_2 \\ W_i \gamma_2 \end{pmatrix}, \ \sigma^2 \begin{pmatrix} (Z_1' Z_1)^{-1} + \mathcal{Q} W_i \mathcal{Q}' - \mathcal{Q} W_i \\ -W_i \mathcal{Q}' & W_i \end{pmatrix} \right),$$

and the residual vector is  $e_{(i)} = y - Z_1 \hat{\gamma}_{1(i)} - Z_2 \hat{\gamma}_{2(i)} = D_i y$ , where

$$D_i = M_1 - M_1 Z_2 W_i Z_2' M_1$$

is a symmetric idempotent matrix of rank  $n - k + r_i$ . The distribution of

$$s_{(i)}^{2} = \frac{e_{(i)}^{\prime}e_{(i)}}{n-k+r_{i}} = \frac{y^{\prime}M_{1}\left(I_{n}-Z_{2}W_{i}Z_{2}^{\prime}\right)M_{1}y}{n-k+r_{i}}$$
(16)

is therefore given by

$$\frac{(n-k+r_i)s_{(i)}^2}{\sigma^2} \sim \chi^2\left(n-k+r_i, \frac{\gamma'_2S_iS'_i\gamma_2}{\sigma^2}\right),$$

The WALS estimators of  $\gamma_1$  and  $\gamma_2$  are

$$c_1 = \sum_{i=1}^{2^{k_2}} \lambda_{(i)} \hat{\gamma}_{1(i)} = \hat{\gamma}_{1r} - QW \hat{\gamma}_{2u}, \qquad c_2 = \sum_{i=1}^{2^{k_2}} \lambda_{(i)} \hat{\gamma}_{2(i)} = W \hat{\gamma}_{2u}, \tag{17}$$

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where

$$W = \sum_{i=1}^{2^{k_2}} \lambda_{(i)} W_i$$

and the equivalence theorem implies that

$$MSE(c_1) = \sigma^2 (Z_1' Z_1)^{-1} + QMSE(W \hat{\gamma}_{2u})Q',$$
(18)

where W is a  $k_2 \times k_2$  diagonal random matrix (random, because the  $\lambda_{(i)}$  are random). Although the model space contains  $2^{k_2}$  models, the computational burden of WALS is of the order  $k_2$ , because we need only consider the diagonal elements  $w_1, \ldots, w_{k_2}$  of W, which are linear combinations of the model weights  $\lambda_{(i)}$ . We do not need to know these linear combinations explicitly, only the resulting WALS weights  $w_h$  $(h = 1, \ldots, k_2)$ .

It follows from the equivalence theorem (18) that the WALS estimator  $c_1$  will be a "good" estimator of  $\gamma_1$  (in the mean squared error sense) if and only if  $W\hat{\gamma}_{2u}$  is a "good" estimator of  $\gamma_2$ . Now, W is diagonal and the elements of  $\hat{\gamma}_{2u}$  are independent with  $\hat{\gamma}_{2u,h} \sim N(\gamma_{2,h}, \sigma^2)$ . We want the diagonal elements  $w_h$  of W to lie between zero and one, so that the components of  $W\hat{\gamma}_{2u}$  are shrinkage estimators. It is only at this stage that we require condition (R1) of Assumption 4.1, and in fact the condition is stronger than necessary. Some of the  $\lambda_{(i)}$  may fall outside the (0, 1) interval as long as the  $k_2$  required linear combinations (that is, the diagonal elements of  $\sum_i \lambda_{(i)} W_i$ ) are all inside the (0, 1) interval. Thus, under semiorthogonalization and the full force of Assumption 4.1, it suffices to find the diagonal elements of W such that the shrinkage estimator  $W\hat{\gamma}_{2u}$  is an "optimal" estimator of  $\gamma_2$ . Once we have found these elements, *the same* estimator will provide the optimal WALS estimator  $c_1$  of  $\gamma_1$  using (17).

Suppose that  $\sigma^2$  is known (we discuss the unknown  $\sigma^2$  case later). Then the relevant pretest procedures, and hence the  $\lambda_{(i)}$ , depend only on  $Z'_2M_1y$  as argued under Assumption 4.1. In that case we may strengthen condition (R3) that the  $\lambda_{(i)}$  depend only on  $M_1y$  to the condition that they depend only on  $Z'_2M_1y$ , that is, on  $\hat{\gamma}_{2u}$ . This is formalized in the following assumption.

**Assumption 7.1.** The WALS weights  $w_h$  satisfy  $w_h = w_h(\hat{\gamma}_{2u,h})$  for  $h = 1, \ldots, k_2$ .

Not only does this seem reasonable, but is also has great practical advantages. In particular, since the  $\{\hat{\gamma}_{2u,h}\}$  are independent, so are the  $\{w_h \hat{\gamma}_{2u,h}\}$ . Our  $k_2$ -dimensional problem thus reduces to  $k_2$  (identical) one-dimensional problems: only using the information that  $\hat{\gamma}_{2u,h} \sim N(\gamma_{2,h}, \sigma^2)$  and assuming that  $\sigma^2$  is known, find the best estimator of  $\gamma_{2,h}$ .

### 8. Estimating the Mean of a Univariate Normal Distribution from One Observation

Thus, motivated we address the seemingly trivial problem of estimating one parameter, say  $\gamma$ , given one observation, say x, generated by the normal N( $\gamma$ ,  $\sigma^2$ ) distribution. Since we assume that the variance  $\sigma^2$  is known, at least for the moment, there is no loss in generality by setting it equal to one.

We write our estimator as m(x) = w(x)x. The most obvious estimator of  $\gamma$  is m(x) = x where  $w(x) \equiv 1$ . This estimator is unbiased, admissible, and minimax and its risk (which equals the mean squared error under squared error loss) is constant:

$$risk = E(x - \gamma)^2 = 1.$$

We call this the "usual" estimator. Another estimator is m(x) = 0 with  $w(x) \equiv 0$ . We call this the "silly" estimator. Its risk is

$$risk = E(0 - \gamma)^2 = \gamma^2.$$

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If  $|\gamma| < 1$  then the silly estimator has smaller risk, if  $|\gamma| > 1$  then the usual estimator has smaller risk, and if  $|\gamma| = 1$  then the two estimators have the same risk.

The equivalence theorem (Proposition 4.2) implies that associated with any estimator of  $\gamma$  in the above N( $\gamma$ , 1) problem there exists a unique estimator of  $\beta_1$  in the regression problem defined in Section 2. For example, the unrestricted estimator  $\hat{\beta}_{1u}$  corresponds to the usual estimator m(x) = x of  $\gamma$  and the restricted estimator  $\hat{\beta}_{1r}$  corresponds to the silly estimator m(x) = 0. Now, the usual estimator may make a lot of sense in the N( $\gamma$ , 1) context, but the unrestricted estimator  $\hat{\beta}_{1u}$  makes less sense in the regression context, because it implies choosing  $\hat{\beta}_{1u}$  whatever the values of the diagnostics associated with the auxiliary variables. The equivalence theorem thus shows that we have to reconsider the usefulness of the usual estimator also in the N( $\gamma$ , 1) context, and try and find an alternative to it.

There is no need for w to be constant. We can think of our estimator as a weighted average between the usual and the silly estimator, because

$$m(x) = w(x)x = w(x)x + (1 - w(x))0.$$

The larger is |x| the larger should be w, so that more weight will be put on the usual estimator relative to the silly estimator. In fact, we impose the following regularity conditions on w.

**Assumption 8.1.** The weight w is a real-valued function defined on  $\mathbb{R}$  and satisfies:

A.  $0 \le w(x) \le 1$ ;

B. w(-x) = w(x);

- *C. w* is nondecreasing on  $[0, \infty)$ ;
- D. w is continuous except possibly on a set of measure zero.

Given these regularity conditions we obtain a lower bound for the risk.

**Proposition 8.1.** If  $x \sim N(\gamma, 1)$  and the weight w satisfies Assumption 8.1, then the risk  $E(w(x)x - \gamma)^2$  has lower bound  $\gamma^2/(1 + \gamma^2)$ .

Proof. This is proved in Magnus (2002, Theorem A.7).

In search of a suitable w-function, we notice that any w satisfying Assumption 8.1 for which w(0) = 0and  $w(\infty) = 1$  can be viewed as a distribution function on  $[0, \infty)$ . Let us therefore consider a flexible three-parameter class of distribution functions, namely the reflected Burr class (Burr, 1942):

$$w(x) = 1 - (1 + (|x|/c)^{\alpha})^{-\delta} \qquad (c > 0, \ \alpha > 0, \ \delta > 0),$$
(19)

defined for  $-\infty < x < \infty$ . Given the reflected Burr class we minimize maximum regret, where regret is defined as

$$regret(\gamma; c, \alpha, \delta) = risk(\gamma; c, \alpha, \delta) - \inf_{c,\delta,\alpha} risk(\gamma; c, \alpha, \delta)$$
$$= risk(\gamma; c, \alpha, \delta) - \frac{\gamma^2}{1+\gamma^2}.$$

Extensive optimization searches reveal that the minimax regret estimator is obtained along the path  $\alpha \delta = 1$  when  $\alpha \to \infty$ . This gives

$$w(x) = \begin{cases} 0 & \text{if } |x| \le c \\ 1 - c/|x| & \text{if } |x| > c \end{cases}$$

and hence

$$m(x) = w(x)x = \begin{cases} x + c & \text{if } x < -c \\ 0 & \text{if } -c \le x \le c \\ x - c & \text{if } x > c. \end{cases}$$
(20)

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This is the Burr estimator. The minimax regret solution is obtained for c = 0.545 with maximum regret equal to 0.3850. It seems therefore that we have solved the problem of finding the diagonal elements of W such that the shrinkage estimator  $W \hat{\gamma}_{2u}$  is an "optimal" estimator of  $\gamma_2$ .

# 9. Enter Bayes: Neutrality and Robustness

We could stop here in our search for the "optimal" estimator of  $\gamma$  in the N( $\gamma$ , 1) problem. The Burr estimator, however, is not completely satisfactory. For example, it is "kinked," hence not differentiable and therefore inadmissible. Let us follow a different path, now along Bayesian lines. Our analysis so far has been strictly frequentist, but this section introduces a Bayesian element. The final product will thus contain both Bayesian and frequentist elements. The Bayesian solution will be close to the frequentist Burr solution, but it will be admissible and be based on a proper treatment of ignorance.

We start with the data,

$$x|\gamma \sim N(\gamma, 1),$$

which we combine with information from a prior  $\pi(\gamma)$ . This gives a posterior density  $p(\gamma|x)$  of the form

$$p(\gamma|x) = \frac{\phi(x-\gamma)\pi(\gamma)}{\int_{-\infty}^{\infty} \phi(x-\gamma)\pi(\gamma) \, d\gamma}$$

where  $\phi$  denotes the standard-normal density. The mean and variance of  $\gamma$  in the posterior distribution are denoted as m(x) and v(x), respectively.

If the prior is normal, then so is the posterior. In particular, if the prior distribution of  $\gamma$  is N(0,  $\tau^2$ ), then the mean and variance of  $\gamma$  in the posterior distribution are m(x) = wx and v(x) = w, where  $w = \tau^2/(\tau^2 + 1)$  is a constant. The normal prior, although convenient, is often considered inappropriate because the discrepancy between m(x) and x does not vanish when x becomes large, but rather increases linearly without bound. In other words, the normal prior is not discounted when confronted with an observation with which it drastically disagrees. The normal prior is therefore not "robust" for the normal location problem.

We impose the following restrictions on the prior density.

# **Assumption 9.1.** The prior $\pi$ is

- 1. symmetric around zero:  $\pi(-\gamma) = \pi(\gamma)$  for all  $\gamma > 0$ ;
- 2. positive and nonincreasing on  $(0, \infty)$ ;
- *3. differentiable, except possibly at 0; and*
- 4.  $\omega(\gamma) = -\pi'(\gamma)/\pi(\gamma)$  has a limit (possibly  $\infty$ ) as  $\gamma \to \infty$ .

Assumptions (B1)–(B3) characterize the prior, allowing a nondifferentiable peak at zero. Assumption (B4) is a technical condition required in the proof of Proposition 9.1.

Robustness is formally defined as follows.

**Definition 9.1.** A prior  $\pi(\gamma)$  is said to be robust if the mean m(x) in the posterior distribution based on this prior satisfies  $x - m(x) \to 0$  as  $x \to \infty$ .

To find out whether or not a prior is robust is not trivial, but the following proposition makes it easy.

**Proposition 9.1.** Under Assumption 9.1, a prior  $\pi$  is robust if and only if  $\omega(\gamma) \to 0$  as  $\gamma \to \infty$ .

*Proof.* This is the main result of Kumar and Magnus (2013), and appears there as Theorem 1.

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For example, if the prior  $\pi$  follows a Student(*k*) distribution, then

$$\omega_k(\gamma) = \frac{-d\log \pi(\gamma)}{d\gamma} = \frac{(k+1)\gamma}{\gamma^2 + k}$$

We have  $\lim_{\gamma \to \infty} \omega_k(\gamma) = 0$ , but  $\lim_{\gamma \to \infty} \lim_{k \to \infty} \omega_k(\gamma) = \infty$ , because the sequence of functions  $\{\omega_k\}$  (k = 1, 2, ...) is not uniformly convergent. This explains why the normal prior is not robust, while the Student prior is.

Let us consider a flexible three-parameter class of priors, namely the reflected generalized gamma distribution with density

$$\pi(\gamma) = \frac{qc^{\delta}}{2\Gamma(\delta)} |\gamma|^{-\alpha} e^{-c|\gamma|^{q}},$$
(21)

where  $-\infty < \gamma < \infty$ , c > 0, q > 0,  $0 \le \alpha < 1$  and  $\delta = (1 - \alpha)/q$ . Special cases of (21) include the normal ( $\alpha = 0$ , q = 2 and  $c = (2\sigma^2)^{-1}$ ), the Laplace ( $\alpha = 0$  and q = 1), the reflected Weibull ( $q = 1 - \alpha$ ), and the Subbotin ( $\alpha = 0$ ) distributions, among others. The  $\omega$ -function takes the form

$$\omega(\gamma) = \frac{-d\log \pi(\gamma)}{d\gamma} = -\frac{\alpha}{\gamma} - cq\gamma^{q-1},$$

and hence robustness occurs if and only if 0 < q < 1. We therefore restrict the parameter space to

$$c > 0, \quad 0 < q < 1, \quad 0 \le \alpha < 1.$$
 (22)

In order to restrict the parameter space further we introduce the concept of neutrality.

**Definition 9.2.** A prior  $\pi(\gamma)$  is said to be neutral if the prior median of  $\gamma$  is zero and the prior median of  $|\gamma|$  is one.

The concept of neutrality attempts to capture the vague notion of ignorance in an explicit and applicable form. A prior is neutral when we are ignorant about the fact whether  $\gamma$  is positive or negative, and also about the fact whether  $|\gamma|$  is larger or smaller than one. In other words, we require

$$\Pr(\gamma \le -1) = \Pr(-1 < \gamma \le 0) = \Pr(0 < \gamma \le 1) = \Pr(\gamma > 1) = 1/4.$$

The condition  $Pr(|\gamma| < 1) = Pr(|\gamma| > 1) = 1/2$  corresponds precisely to ignorance about whether the usual or the silly estimator is better (has lower risk), and thus also ignorance about whether or not it is advisable to include the associated additional regressor.

For the reflected generalized gamma distribution defined in (21), neutrality occurs if and only if

$$\int_0^1 \gamma^{-\alpha} e^{-c\gamma^q} \, d\gamma = \frac{\Gamma(\delta)}{2qc^\delta}$$

If we define the (lower) incomplete gamma function as

$$\Gamma(s,z) = \frac{1}{\Gamma(s)} \int_0^z t^{s-1} e^{-t} dt$$

and notice that

$$\int_0^1 \gamma^{-\alpha} e^{-c\gamma^q} d\gamma = \frac{1}{qc^{\delta}} \int_0^c t^{\delta-1} e^{-t} dt = \frac{\Gamma(\delta, c)\Gamma(\delta)}{qc^{\delta}},$$

then an equivalent representation of the neutrality condition is

$$\Gamma(\delta, c) = 1/2. \tag{23}$$

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Prior	α	q	δ	С	γ	Regret
Gamma	0.2076	1	0.7924	0.4942	3.4410	0.4399
Weibull	0.1124	0.8876	1	0.6931	3.5620	0.4546
Subbotin	0	0.7995	1.2508	0.9377	3.6912	0.4697
Laplace	0	1	1	0.6931	4.9320	0.5127

 
 Table 1. Minimax Regret Solutions for the Reflected Generalized Gamma, Reflected Weibull, Subbotin, and Laplace Priors

In the case of the normal distribution we have  $\delta = 1/2$  and  $c = (2\sigma^2)^{-1}$ , so that (23) holds for  $\sigma^2 = 2.1981$ . In the case of the Laplace and reflected Weibull distributions we have  $\delta = 1$ , and hence the neutrality condition becomes

$$\int_0^c e^{-t} dt = 1/2,$$

which leads to  $c = \log 2$ . More generally, the neutrality condition places a restriction on our class of priors by reducing the number of free parameters by one.

The minimax regret for our class of neutral and robust priors can then be written as

$$\inf_{c,q,\alpha} \sup_{\gamma} regret(\gamma; c, q, \alpha)$$
  
subject to  $\Gamma(\delta, c) = 1/2$ ,

with the prior parameters satisfying the inequalities in (22).

Our minimax regret results are presented in Table 1. The Laplace prior is a special case of both the reflected Weibull and the Subbotin priors and is obtained by setting q = 1. It is neutral but not robust, and is included here as a benchmark. The reflected Weibull and Subbotin priors outperform the Laplace prior not only because they are robust while the Laplace prior is not but also because they have lower minimax regret. The reflected generalized gamma prior has a minimax solution on the boundary (q = 1) and this solution is not robust.

In Figure 1 we present the deviations x - m(x) for the four minimax regret solutions. For the Laplace prior the deviation converges to  $\log 2 = 0.6931$  and for the reflected generalized gamma it converges to 1/2. Neither converges to zero in accordance to Proposition 9.1. For the reflected Weibull and Subbotin priors we see that x - m(x) does converge to zero, confirming their robustness, also in accordance to Proposition 9.1.

The risk profiles of the reflected Weibull, Subbotin, and Burr estimators are presented in Figure 2 together with the minimum risk  $\gamma^2/(1 + \gamma^2)$ . The figure shows that the reflected Weibull and Subbotin estimators behave very similarly. Within the family of reflected generalized gamma distributions, as given in (21), the optimal neutral prior is obtained when q = 1, which is on the boundary and therefore not robust, because robustness requires that 0 < q < 1. The optimal neutral *and* robust prior will therefore be obtained for q very close but not equal to one. Such a prior will then be robust but convergence of x - m(x) to zero will be slow. This implies that we should choose q close but not too close to one.

Each of the three estimators in Figure 2 has its advantages and disadvantages. The Subbotin prior (q = 0.80) is "more robust" (x - m(x) converges faster to zero) than the reflected Weibull (q = 0.89), but the reflected Weibull has lower minimax regret. The Burr estimator derived in the previous section has lower regret (0.3850) than any of the Bayesian estimators in the current section. However, it is



Figure 1. Deviations x - m(x) for the Minimax Regret Solutions of the Reflected Generalized Gamma, Reflected Weibull, Subbotin, and Laplace Priors.



Figure 2. Risk of the Posterior Mean of the Reflected Weibull and Subbotin Priors, Compared to the Risk of the Burr Estimator.

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inadmissible and does not have an interpretation in terms of ignorance. In our view the reflected Weibull prior,

$$\pi(\gamma) = \frac{qc}{2} |\gamma|^{-(1-q)} e^{-c|\gamma|^q} \qquad (c = \log 2, \ q = 0.8876), \tag{24}$$

offers the best compromise and we present it as our preferred prior. When we define

$$A_j(x) = \int_{-\infty}^{\infty} (x - \gamma)^j \phi(x - \gamma) \pi(\gamma) \, d\gamma \qquad (j = 0, 1, 2),$$
(25)

then the mean and variance in the posterior distribution are given by

$$m(x) = -\frac{A_1(x)}{A_0(x)} + x, \qquad v(x) = \frac{A_2(x)}{A_0(x)} - \left(\frac{A_1(x)}{A_0(x)}\right)^2.$$
 (26)

# 10. The Effect of Estimating $\sigma^2$

So far we have assumed that the disturbance term in our linear model (1) is normally distributed with mean zero and variance  $\sigma^2 I_n$ , and that  $\sigma^2$  is known. In fact,  $\sigma^2$  is not known and we have to estimate it. The problem can be phrased in terms of the simple model of Section 8 and especially Section 9. There we considered the estimation of  $\gamma$  when we have one observation *x* from the univariate N( $\gamma$ ,  $\sigma^2$ ) distribution, assuming that  $\sigma^2$  is known.

Suppose now that  $\sigma^2$  is not known, but that we have an estimator  $s^2$  of  $\sigma^2$  which is distributed independently of x, such that  $vs^2/\sigma^2$  follows a  $\chi^2(v)$ -distribution. This captures the essence of our problem. In Section 9 we obtained a weight function w such that m(x) = w(x)x is an "optimal" estimator of  $\gamma$ , based on the reflected Weibull prior (24). This weight function was derived under the assumption that  $\sigma^2$  is known. If  $\sigma^2$  is not known we can ask two questions. First, how can we generalize the prior  $\pi(\gamma, \sigma^2)$ , thus obtaining a different posterior distribution than before, implying a different mean (and variance) in this distribution, and hence a different estimator of  $\gamma$  and a different risk profile? Second, if we use the same estimator as before (thus based on the known  $\sigma^2$  situation), then what is the difference in risk when we replace  $\sigma^2$  by  $s^2$  and take the additional randomness of  $s^2$  properly into account?

Both questions were analyzed in Danilov (2005), see also Yüksell *et al.* (2010), but in the context of the Laplace prior rather than the reflected Weibull. We conclude from Danilov's analysis that there is rapid convergence of the risk profiles to the known  $\sigma^2$  case (where  $\nu = \infty$ ) as we let  $\nu$  approach  $\infty$ . For  $\nu > 20$  the risk profiles practically coincide and even for small  $\nu$  the difference is negligible.

We repeat one aspect of Danilov's analysis for the generalized Weibull. In Figure 3, we plot two risk functions. The first is the same risk function as the generalized Weibull in Figure 2, while the second uses the same formula but replaces  $\sigma^2$  by  $s^2$ , thus allowing for the additional randomness caused by estimating  $\sigma^2$ . The risk now depends on the degrees of freedom  $\nu$  and we choose a small value of  $\nu$  ( $\nu = 5$ , as in Danilov (2005, figure 4)) in order to give randomness every chance to reveal itself. The figure shows that, even with such a small value of  $\nu$ , the difference between the known and unknown  $\sigma^2$  case is remarkably small, in fact negligible in practice. This result is not trivial or obvious. For example, when we draw the risk profiles of the pretest estimator, as in Danilov (2005, figure 3), we find large dependence on  $\nu$ .

This concludes our discussion of the known versus unknown  $\sigma^2$  case. The more general situation where the variance of the disturbances is not given by  $\sigma^2 I_n$  but by  $\sigma^2 \Omega$ , where  $\Omega$  depends on some unknown parameters, is more complex and we shall discuss it when we discuss nonspherical disturbances in Section 12.1.



Figure 3. Risk of the Reflected Weibull Estimator: Known versus Unknown  $\sigma^2$ .

# 11. Putting It All Together

We summarize the WALS procedure in seven steps, as follows.

Step 1 (focus versus auxiliary). In the unrestricted model  $y = X\beta + \epsilon$ , determine which are the  $k_1$  focus regressors  $(X_1)$  and which are the  $k_2$  auxiliary regressors  $(X_2)$ . This leads to (1):

$$y = X_1\beta_1 + X_2\beta_2 + \epsilon.$$

Step 2 (scaling). Define the diagonal  $k_1 \times k_1$  matrix  $\Delta_1$  whose *j*th diagonal element is given by

$$(\Delta_1)_{jj} = \frac{1}{\sqrt{(X'_1 X_1)_{jj}}}.$$

Compute  $M_1 = I_n - X_1(X'_1X_1)^{-1}X'_1$  and define the diagonal  $k_2 \times k_2$  matrix  $\Delta_2$  whose *h*th diagonal element is given by

$$(\Delta_2)_{hh} = \frac{1}{\sqrt{(X'_2 M_1 X_2)_{hh}}}$$

As a result, all diagonal elements of

$$(X_1\Delta_1)'(X_1\Delta_1)$$
 and  $(X_2\Delta_2)'M_1(X_2\Delta_2)$ 

are equal to one.

Step 3 (semiorthogonalization). Define

$$Z_1 = X_1 \Delta_1, \qquad \gamma_1 = \Delta_1^{-1} \beta_1,$$

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as in (11), so that  $Z_1\gamma_1 = X_1\beta_1$ . Next compute the orthogonal  $k_2 \times k_2$  matrix T and the diagonal  $k_2 \times k_2$  matrix  $\Xi$  such that

$$T'\Delta_2 X'_2 M_1 X_2 \Delta_2 T = \Xi,$$

and define

$$Z_2 = X_2 \Delta_2 T \, \Xi^{-1/2}, \qquad \gamma_2 = \Xi^{1/2} T' \Delta_2^{-1} \beta_2,$$

as in (12), so that  $Z_2 \gamma_2 = X_2 \beta_2$  and  $Z'_2 M_1 Z_2 = I_{k_2}$ .

Step 4 (estimate  $\gamma_2$  and  $\sigma^2$  in the unrestricted model). Since  $X_1\beta_1 = Z_1\gamma_1$  and  $X_2\beta_2 = Z_2\gamma_2$ , the DGP can also be written as

$$y = Z_1 \gamma_1 + Z_2 \gamma_2 + \epsilon,$$

as in (13). In this (unrestricted) model, compute the estimate of  $\gamma_2$  as

$$\hat{\gamma}_{2u}=Z_2'M_1y,$$

as in (15), and the estimate of  $\sigma^2$  as

$$s_u^2 = \frac{y' M_1 (I_n - Z_2 Z_2') M_1 y}{n - k},$$

as in (16) with  $r_i = 0$  and  $W_i = I_{k_2}$ . Set up the inputs for the Bayesian step by computing the vector of *t*-ratios

$$x = \frac{\hat{\gamma}_{2u}}{s_u} = \frac{\sqrt{n - k} Z'_2 M_1 y}{\sqrt{y' M_1 (I_{k_2} - Z_2 Z'_2) M_1 y}}$$

Step 5 (compute the mean and variance in posterior distribution). Let  $\phi$  denote the standard-normal density and define the reflected Weibull prior,

$$\pi(\gamma) = \frac{qc}{2} |\gamma|^{-(1-q)} e^{-c|\gamma|^q} \qquad (c = \log 2, \ q = 0.8876),$$

as in (24). For each of the  $k_2$  components  $x_h$  of x compute

$$A_j(x_h) = \int_{-\infty}^{\infty} (x_h - \gamma)^j \phi(x_h - \gamma) \pi(\gamma) d\gamma \qquad (j = 0, 1, 2),$$

as in (25), and then the mean and variance in the posterior distribution:

$$m_h = m(x_h) = -\frac{A_1(x_h)}{A_0(x_h)} + x_h, \qquad v_h = v(x_h) = \frac{A_2(x_h)}{A_0(x_h)} - \left(\frac{A_1(x_h)}{A_0(x_h)}\right)^2,$$

as in (26). Compute  $m = (m_1, ..., m_{k_2})'$  and  $V = diag(v_1, ..., v_{k_2})$ .

Step 6 (WALS estimates). Compute the WALS estimates of  $\gamma_1$  and  $\gamma_2$  as

$$c_1 = (Z'_1 Z_1)^{-1} Z'_1 (y - Z_2 c_2), \qquad c_2 = s_u m.$$

The WALS estimates of the original parameters  $\beta_1$  and  $\beta_2$  are then given by

$$b_1 = \Delta_1 c_1, \qquad b_2 = \Delta_2 T \Xi^{-1/2} c_2.$$

Step 7 (WALS precisions). Letting  $Q = (Z'_1 Z_1)^{-1} Z'_1 Z_2$ , compute the variances of  $c_1$  and  $c_2$  as

$$var(c_1) = s_u^2 (Z'_1 Z_1)^{-1} + Qvar(c_2)Q', \quad var(c_2) = s_u^2 V,$$

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and the covariance as  $cov(c_1, c_2) = -Qvar(c_2)$ . The variances of  $b_1$  and  $b_2$  can then be computed as

$$var(b_1) = \Delta_1 var(c_1)\Delta_1, \quad var(b_2) = \Delta_2 T \Xi^{-1/2} var(c_2) \Xi^{-1/2} T' \Delta_2$$

and the covariance as  $cov(b_1, b_2) = \Delta_1 cov(c_1, c_2) \Xi^{-1/2} T' \Delta_2$ .

# 12. Extensions and Applications

The WALS procedure developed so far is designed for the estimation of linear regression models with i.i.d. disturbances, enabling the investigator to allow for both model uncertainty and estimation uncertainty in one joint procedure. Recent contributions have allowed extensions of this method, and in Section 12.1 we present the key ideas of four of these extensions. In Section 12.2, we discuss possible future extensions, and in Section 12.3 some applications. An important conclusion from the extensions is that the  $k_2$ -dimensional reduction, which occurs in the simple linear setting, continues to hold in most extensions by a method of transformation or linearization.

### 12.1 Current Eextensions

(a) *Nonspherical disturbances*. One constraint in the setup of WALS is that the disturbances are assumed to be independent and identically distributed with mean zero and variance  $\sigma^2$ . A more general setup would assume

$$\epsilon \sim \mathrm{N}(0, \sigma^2 \Omega(\theta)),$$

where  $\Omega(\theta)$  is a positive definite  $n \times n$  matrix whose elements are functions of an *m*-dimensional unknown parameter vector  $\theta = (\theta_1, \ldots, \theta_m)$  under the normalizing constraint  $tr(\Omega(\theta)) = n$ . This idea was developed in Magnus *et al.* (2011), mimicking the case where only  $\sigma^2$  needs to be estimated.

If  $\Omega$  were known we would transform model (1) to

$$\Omega^{-1/2} y = \Omega^{-1/2} X_1 \beta_1 + \Omega^{-1/2} X_2 \beta_2 + \Omega^{-1/2} \epsilon$$

and apply WALS to the transformed variables. Since  $\Omega$  is not known, we estimate its parameters from the unrestricted model. This leads to the maximum likelihood (ML) estimator  $\hat{\theta}$  of  $\theta$ , through which we also obtain an estimator  $\hat{\Omega} = \Omega(\hat{\theta})$ . We then act as if  $\hat{\Omega}$  is in fact the true rather than the estimated value of  $\Omega$ , that is, we ignore the randomness in the estimation of the  $\theta$  parameters.

The procedure can be justified by the analysis and results in Section 10, although there is one possibly important difference between estimating only  $\sigma^2$  and estimating both  $\sigma^2$  and  $\theta$ . If  $var(\epsilon) = \sigma^2 I_n$  then the estimators of  $\beta_1$  and  $\beta_2$  do not depend on  $\sigma^2$ , but if  $var(\epsilon) = \sigma^2 \Omega$  then the estimators of  $\beta_1$  and  $\beta_2$  do not depend on  $\sigma^2$ , but if  $var(\epsilon) = \sigma^2 \Omega$  then the estimators of  $\beta_1$  and  $\beta_2$  do not depend on  $\sigma^2$ , but if  $var(\epsilon) = \sigma^2 \Omega$  then the estimators of  $\beta_1$  and  $\beta_2$  do append on  $\Omega$ . The influence of the neglected randomness is therefore more complex, and so far it has not yet been explored.

(b) Hierarchical WALS. In practice the investigator has to decide not only which variables to include in the model, but also how to measure them. For example, one may wish to include "education" or "inflation" in the model, but then one has to decide as well how education and inflation are to be measured. This gives rise to two sources of model uncertainty: uncertainty about "groups" (such as eduction or inflation) and uncertainty about "variables" (different measurements of the group concept). This situation was recently analyzed by Magnus and Wang (2014) and is of interest, not only for its own sake, but also as an example where the number of regressors could exceed the number of observations, while estimation is still possible.

(c) WALS estimation of generalized linear models. A natural extension to the WALS methodology is to move away from the linearity assumption. Attempts to extend WALS to the wider class of generalized linear models (GLMs) were undertaken by Heumann and Grenke (2010) and De Luca *et al.* (2013). This class of models includes a variety of nonlinear models typically employed for discrete or categorical outcomes, such as logit, probit, and Poisson regression models.

In these models the dependence of the outcome on the regressors is modeled through a continuously differentiable and invertible function  $h(\cdot)$ , sometimes called the inverse link, such that  $E(y|X) = h(X_1\beta_1 + X_2\beta_2)$ . Because of model uncertainty about the  $k_2$  columns of  $X_2$ , we consider  $2^{k_2}$  possible models where the *i*th model  $\mathcal{M}_i$  is again defined by a constraint of the form  $S'_i\beta_2 = 0$ . De Luca *et al.* (2013) show that, if we choose the unrestricted ML estimator  $(\hat{\beta}_{1u}, \hat{\beta}_{2u})$  as the initial value, then a first-order approximation to the ML estimator of  $\beta_1$  and  $\beta_2$  under model  $\mathcal{M}_i$  can be obtained. Moreover, after preliminary transformations of the outcome and the regressors, this (one-step) ML estimator closely resembles the constrained LS estimator of  $\beta_1$  and  $\beta_2$  discussed in Section 3.

(d) WALS prediction. Prediction model averaging with WALS is based on the linear DGP

$$\begin{pmatrix} y \\ y_f \end{pmatrix} = \begin{pmatrix} X_1 & X_2 \\ X_{1f} & X_{2f} \end{pmatrix} \begin{pmatrix} \beta_1 \\ \beta_2 \end{pmatrix} + \begin{pmatrix} \epsilon \\ \epsilon_f \end{pmatrix},$$
(27)

where y and  $y_f$  are vectors of observations on the outcome,  $X_1$  and  $X_{1f}$  are matrices of observations on the focus regressors,  $X_2$  and  $X_{2f}$  are matrices of observations on the auxiliary regressors,  $\beta_1$  and  $\beta_2$  are vectors of focus and auxiliary parameters, and  $\epsilon$  and  $\epsilon_f$  are random vectors of unobservable disturbances. Observations are allowed to be correlated and we assume that

$$\begin{pmatrix} \epsilon \\ \epsilon_f \end{pmatrix} \sim \mathbf{N} \left( \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} \Omega & C'_f \\ C_f & \Omega_f \end{pmatrix} \right), \tag{28}$$

where the variance of  $(\epsilon, \epsilon_f)$  is a positive definite matrix whose component blocks  $\Omega$ ,  $C_f$ , and  $\Omega_f$  are functions of a finite-dimensional unknown parameter vector  $\theta$ .

After estimating  $\beta_1$  and  $\beta_2$  from the sample  $(y, X_1, X_2)$ , we wish to predict the  $n_f$  (possibly future) values of  $y_f$  associated with the values of the regressors  $X_{1f}$  and  $X_{2f}$ . Because of model uncertainty, each of the  $k_2$  columns of  $X_2$  and  $X_{2f}$  can either be included or not included in the model and this gives rise to  $2^{k_2}$  possible models. Unlike traditional prediction methods, model-average prediction procedures give predictors of  $y_f$  that take explicit account of both model and error uncertainty. The additional theory required for WALS prediction was recently developed in Magnus *et al.* (2014).

# 12.2 Possible Future Extensions

In addition to the four extensions discussed in the previous subsection, there are many other possible extensions of WALS, and much work is still required to fill these gaps. Below we list five extensions that seem most important to us, but it is easy to think of more extensions, for example panel data, big data  $(k \gg n)$ , or semi- or nonparametric settings.

- (a) Endogeneity. The standard setup requires that the regressors are (weakly) exogenous. If we allow endogenous regressors then we need a WALS version of instrumental variables or two-stage least squares.
- (b) Role of normality. The normality assumption plays an important role in the development of WALS, which goes beyond the specification of the first two moments. At several points in the development we need the fact that if two random variables are uncorrelated, then functions of these random variables are also uncorrelated. This is generally not true, but under normality it is. An extension

to nonnormal errors is therefore far from trivial. Zou *et al.* (2007) provide an extension of the equivalence theorem for large-sample nonnormal errors and De Luca *et al.* (2013) generalize WALS to GLMs where the density of y is assumed to belong to the linear exponential family of density functions. While these extensions are useful, they do not yet provide a full generalization to nonnormality.

- (c) Multivariate models. Extensions from univariate to multivariate models should be feasible within the WALS framework, but so far this has not been investigated. These extensions would open the way to a larger variety of models, such as seemingly unrelated regression equations (SURE), and ordered, multinomial, and conditional logit and probit models.
- (d) *Excluding subsets of parameters.* In the standard WALS setup we allow all  $2^{k_2}$  models to play a part, where the *i*th model is identified by a linear restriction of the form  $S'_i\beta_2 = 0$ . It can happen that if one model is excluded then another model is automatically excluded as well or if one auxiliary regressor appears then this excludes a subset of other auxiliary regressors. The hierarchical procedure in Section 12.1 is an example of the latter situation. A general theory of subset selection allowing for linkage between restrictions would be of great practical importance.
- (e) Nonnested models. Our models are all nested within one (the largest) model, which is also the DGP. A general theory of model selection should allow for the fact that models may not be nested.

# 12.3 Applications

Model averaging techniques are typically applied to growth empirics, where the large number of growth determinants and the limited number of observations available at the national level expose the regressions to a high degree of model uncertainty. The standard WALS procedure, introduced by Magnus *et al.* (2010), also contains an application to growth empirics. The WALS estimates obtained in Magnus *et al.* (2010) are compared to traditional pretest estimates, Bayesian model-average (BMA) estimates, and Bayesian averaging of classical estimates, using the data set analyzed by Sala-i-Martin *et al.* (2004).

The hierarchical WALS estimator discussed in Section 12.1 was applied to growth empirics by Magnus and Wang (2014) in order to take explicit account of the uncertainty due to the choice of the growth determinants (that is, concepts or groups of variables such as education) and the choice of the explanatory variables that can be employed as alternative proxy measures of the same growth determinant (that is, precisely defined variables such as enrollment rate, school years, and share of public education spending). Poghosyan and Magnus (2012) applied WALS to estimate and forecast factor-based dynamic models of real GDP growth and inflation in the Armenian economy. Additional comparisons between WALS, standard BMA, and a modified version of the Mallows model-average (MMA) estimator of Hansen (2007) are provided by Amini and Parmeter (2012) using data from three earlier studies on growth empirics. Similar comparisons between WALS and other frequentist-based model-average estimators can be found in Liu (2014).

The WALS procedure has also been successfully applied in other fields, outside growth empirics. Among these, Wan and Zhang (2009) applied WALS to study the effect of recreation and tourism development on a range of socioeconomic indicators in rural U.S. counties. Liski *et al.* (2010) used WALS to investigate medical care costs of hip fracture treatments in hospital districts of Finland. Magnus *et al.* (2011) provided an application of WALS in the context of a hedonic housing price model with heteroskedastic disturbances using data from the Hong Kong real estate market; Seya and Tsutsumi (2012) extended this analysis to WALS estimation of a hedonic land price model with spatially dependent data from the Tokyo metropolitan area; and Seya *et al.* (2014) provided Monte Carlo simulations on the combined use of WALS and principal components to jointly address problems of model uncertainty and multicollinearity in spatial lag-error models.

Dardanoni *et al.* (2011, 2012) exploited WALS for handling the bias-precision trade-off that arises in the estimation of linear regression models with missing covariate values replaced by imputations. Osterloh (2012) applied WALS to assess the robustness of political environment as determinant of the economic performance in OECD countries. Finally, Cook *et al.* (2013) used WALS to study the determinants of various capital structure measures in US corporations between 1980 and 2007. In contrast to the growth empirics literature, where the number of regressors is large, some of the above studies show that WALS can be used as a general method of estimation, also when the number of regressors is small.

# 13. WALS Compared to other Model-Average Estimators

The method of WALS surveyed in this paper is one of several methods of model averaging (more accurately, estimator averaging). In this section we provide a brief overview of this rapidly expanding literature, emphasizing the advantages and weaknesses of WALS relative to these alternative model-average procedures.

# 13.1 Bayesian Model Averaging

BMA estimators compute weighted averages of the conditional estimates over all possible models using posterior model probabilities as weights in order to reflect the confidence in each model based on prior beliefs and the observed data. By Bayes theorem, the posterior probability of model  $M_i$  is obtained as

$$\lambda_{(i)} = p(\mathcal{M}_i \mid \mathbf{y}) = \frac{p(\mathcal{M}_i) \, p(\mathbf{y} \mid \mathcal{M}_i)}{\sum_i \, p(\mathcal{M}_i) \, p(\mathbf{y} \mid \mathcal{M}_i)} \qquad (i = 1, \dots, 2^{k_2}),\tag{29}$$

where  $p(\mathcal{M}_i)$  is the prior probability that  $\mathcal{M}_i$  is the true model,

$$p(y \mid \mathcal{M}_i) = \int p(y \mid \theta_i, \mathcal{M}_i) \, p(\theta_i \mid \mathcal{M}_i) \, d\theta_i$$
(30)

is the marginal likelihood of model  $\mathcal{M}_i$ ,  $\theta_i$  the vector of its parameters,  $p(y | \theta_i, \mathcal{M}_i)$  its likelihood, and  $p(\theta_i | \mathcal{M}_i)$  the prior density of  $\theta_i$  under model  $\mathcal{M}_i$ . Thus, contrary to WALS which uses priors only on the vector of *t*-ratios  $x = \hat{\gamma}_{2u}/s_u^2$ , BMA estimators require two types of priors: on the model space and on the parameters of each model.

As discussed in the reviews by Hoeting *et al.* (1999), Clyde and George (2004), and Moral-Benito (2013), the choice of uninformative priors is one of the most challenging aspects of BMA. For the prior on the model space, the bulk of the BMA literature uses a uniform prior which assigns equal probability to each model. Although this is a reasonable choice when there is little prior information about the relative plausibility of the models considered, the uniform prior has been criticized because of the implicit assumption that the probability that one regressor appears in the model is independent of the inclusion of others, whereas, in fact, regressors are typically correlated; see, for example, Durlauf *et al.* (2008). For the prior on the parameter space, the major problem is that improper priors on all parameters would result in ill-defined Bayes factors. A widely used strategy to deal with this issue consists of using a hierarchical prior structure that involves improper priors on the parameters that are common to all models and proper priors on the remaining parameters. For the latter, most BMA estimators rely on Zellner's (1986) *g*-prior, which is a normal prior with mean zero and variance

$$var(\beta_2 \mid \mathcal{M}_i) = \frac{\sigma^2}{g} S_i (S'_i X'_2 M_1 X_2 S_i)^{-1} S'_i,$$
(31)

where g > 0 is a scalar hyperparameter that reflects how much importance is given to prior beliefs. This prior structure is attractive since it only requires the elicitation of the scalar parameter g and, in linear

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regression setups, leads to closed-form expressions of the posterior model probabilities. For the choice of the hyperparameter g, various options are available including the unit information prior g = 1/n (Kass and Wasserman, 1995), the risk inflation criterion  $g = 1/k_2^2$  (Foster and George, 1994), and the benchmark prior  $g = 1/\max(n, k_2^2)$  (Fernández *et al.*, 2001). For additional references and recent developments on the choice of priors in BMA, the reader is referred to Eicher *et al.* (2011) and Ley and Steel (2009, 2012).

Another well-known practical issue that plagues standard BMA procedures is how to handle model spaces of large dimensions. A widely used empirical strategy consists of using approximate estimates that consider only a suitable subset of models supported by the data. The subset of models to be investigated can be identified either by deterministic search methods such as Occam's window (Madigan and Raftery, 1994) and the leaps and bounds algorithm (Furnival and Wilson, 1974), or by stochastic search methods based on Markov chain Monte Carlo (MCMC) techniques; see Garcia-Donato and Martinez-Beneito (2013) for a recent review.

Several BMA estimators have been developed in the context of the linear regression model, but extensions to more general regression setups are also available. For example, BMA estimation of GLMs has been considered in Raftery (1996), Clyde (2000), and Czado and Raftery (2006). More recently, Jordan and Lenkoski (2012) and Eicher *et al.* (2012) focused on BMA estimation of models for truncated and censored data; Crespo Cuaresma and Feldkircher (2012) applied BMA in the presence of spatial autocorrelation using spatial filtering; Koop *et al.* (2012), Karl and Lenkoski (2012), and Lenkoski *et al.* (2013) developed BMA methodologies to jointly address model uncertainty and endogeneity; and Chen *et al.* (2009), Moral-Benito (2012), and McCormick *et al.* (2012) proposed BMA estimators for panel data models. Notice that, outside the classical linear regression model with conjugate priors, the marginal likelihoods in (30) do not usually have analytic closed-form expressions. Approximations to either the marginal likelihoods or the posterior model probabilities are therefore needed. Such approximations can be obtained through the Laplace method for integrals (Tierney and Kadane, 1986), the output of some MCMC method (Han and Carlin, 2001; Ghosh and Clyde, 2011), or a suitable combination of these two methods (DiCiccio *et al.*, 1997; Lewis and Raftery, 1997).

# 13.2 Frequentist Model Averaging

Frequentist model averaging (FMA) differs from BMA and WALS in that it avoids the need of priors elicitation, because FMA uses model weights that are totally determined by the data on the basis of some diagnostic criterion. Useful overviews of this approach can be found in Claeskens and Hjort (2008) and Wang *et al.* (2009). The frequentist perspective to model averaging is more recent than the Bayesian perspective, and significant progress has recently been made in developing optimal data-driven weighting schemes and investigating the properties of the resulting estimators. For example, Buckland *et al.* (1997) suggested mixing models with weights based on smoothed Akaike information criterion or Bayesian information criterion scores; Yang (2001, 2003) proposed a frequentist-based adaptive regression mixing method that allows the combination of estimators from different estimation procedures; Hjort and Claeskens (2003) introduced a likelihood-based local misspecification framework to analyze the asymptotic distribution of model-average estimators; Hansen (2007) and Wan *et al.* (2010) developed least-squares model-average estimators with weights selected by minimizing the Mallows criterion; and Liang *et al.* (2011) proposed a weighting procedure which minimizes an unbiased estimator of the mean squared error of the FMA estimator in finite samples.

Most of the available distributional results of FMA estimators are based on large-sample approximations and they are typically established under the assumptions of the local misspecification framework (Hjort and Claeskens, 2003). The work of Pötscher (2006), who investigated the finite-sample and asymptotic distributions of a special case of the FMA estimator discussed in Leung and Barron (2006), provides a helpful guide for further research on these topics.

As for BMA, exact FMA estimation can be computationally very demanding when the model space is large. This issue is typically addressed through a preliminary model-screening step that removes the poorest-performing models before combining the conditional estimates into an unconditional FMA estimate. Applications of this preliminary model screening step can be found in Yuan and Yang (2005), Claeskens *et al.* (2006), Wan *et al.* (2014), and Zhang *et al.* (2013a), among others. The computation of exact FMA estimates in growth applications with large model spaces was first attempted in Amini and Parmeter (2012) by introducing an operational version of the model-average estimator of Hansen (2007), using the same semiorthogonal transformations as adopted in WALS.

Extensions of FMA estimators to more general regression setups cover a variety of models such as logistic regression models (Claeskens *et al.*, 2006); models for survival analysis (Hjort and Claeskens, 2006); generalized additive partial linear models (Zhang and Liang, 2011); Tobit models (Zhang *et al.*, 2012); multinomial and ordered logit models (Wan *et al.*, 2014); and linear mixed-effects models (Zhang *et al.*, 2014). For linear models with nonsperical disturbances, Hansen and Racine (2012) and Zhang *et al.* (2013b) developed jackknife model-average estimators which are asymptotically optimal under heteroskedastic and serially correlated errors, while Liu and Okui (2013) and Liu *et al.* (2013) extended the MMA estimator of Hansen (2007) to models with heteroskedastic errors. In the context of prediction, Hansen (2008) extended the idea of Mallows model averaging to forecast combinations, while Yang (2004), Zou and Yang (2004), and Zhang *et al.* (2013a) developed combining forecasting procedures for time-series models. Finally, Schomaker *et al.* (2010) examined the properties of various FMA estimators in the presence of missing data and Kuersteiner and Okui (2010) used the MMA estimator of Hansen (2007) to construct optimal instruments in the context of linear models with endogenous regressors.

# 13.3 Intermediate Position of WALS

The WALS procedure surveyed in this paper is a Bayesian combination of frequentist estimators. The parameters of each model are estimated by constrained least squares, hence frequentist. However, after implementing a semiorthogonal transformation to the auxiliary regressors, the weighting scheme is developed on the basis of a Bayesian approach in order to obtain desirable theoretical properties such as admissibility and a proper treatment of ignorance. The final result is a model-average estimator that assumes an intermediate position between strict BMA and strict FMA estimators.

WALS is closely related to the FMA estimator proposed by Liang *et al.* (2011). The model setup, the assumptions, and the estimator are the same, but Liang *et al.* choose the weights to minimize an unbiased estimator of the mean squared error of the FMA (or WALS) estimator rather than of the mean squared error itself.

WALS is conceptually also close to BMA. The assumption that the data are normally distributed is the same, and the treatment of noninformative priors on the model space, the focus parameters  $\beta_1$  and the error variance  $\sigma^2$  is essentially the same. The main difference between the two model-average procedures lies in the prior treatment of the auxiliary parameters  $\beta_2$ . In WALS we write  $\beta_2$  as  $\beta_2 = \sigma \Delta_2 T \Xi^{-1/2} \gamma$ , where  $\gamma = \gamma_2/\sigma$ , and assume that the  $k_2$  components of  $\gamma$  are i.i.d. according to a reflected Weibull distribution

$$\pi(\gamma_h) = \frac{qc}{2} |\gamma_h|^{-(1-q)} \exp(-c|\gamma_h|^q)$$

with  $c = \log 2$  and q = 0.8876. This implies that each  $\gamma_h$  is symmetrically distributed around zero, that the median of  $\gamma_h^2$  is one, and that the variance of  $\gamma_h$  is  $\sigma_{\gamma}^2 = \Gamma((q+2)/q)/c^2$ . As argued in Section 9, this choice of prior moments is based on the concept of neutrality which attempts to formalize the vague notion of ignorance in an explicit and applicable form, and on other theoretical considerations related to robustness and optimality in the minimax regret sense.

#### WEIGHTED-AVERAGE LEAST SQUARES

The resulting prior mean of  $\beta_2$  is zero and its prior variance is given by

$$var(\beta_2) = \sigma^2 \sigma_{\gamma}^2 \Delta_2 T \Xi^{-1} T' \Delta_2 = \frac{\sigma^2}{c^2 / \Gamma((q+2)/q)} (X'_2 M_1 X_2)^{-1}.$$
 (32)

A comparison of (31) and (32) shows that the prior moments adopted in BMA and WALS are in fact closely related, and suggests in addition a new value for g in BMA applications, namely  $g = c^2 / \Gamma((q+2)/q) = 0.1878$ .

A key feature of WALS is that the choice of prior is not *ad hoc* (like in BMA) but theoretically based. A second key feature of WALS provides a practical rather than a theoretical advantage over both BMA and FMA, namely that, even though there are  $2^{k_2}$  possible models to consider, the computational burden of this model-average estimator is reduced to the order  $k_2$  by the semiorthogonal transformation of the auxiliary regressors discussed in Section 6. Thus, while standard BMA and FMA estimators require sophisticated approximation algorithms to explore small subsets of the model space, WALS provides exact model-average estimates of the parameters of interest in negligible computing time. This computational advantage is likely to play an important role in a variety of empirical applications where the estimation of all models is impossible.

Both from a theoretical and a practical viewpoint WALS has many attractive features. Of course, the semiorthogonal transformation—which leads to the simplifications which WALS requires—also has a cost, both theoretically and practically. From a theoretical viewpoint, some of our assumptions are not made directly on the auxiliary parameters  $\beta_2$  but rather on the transformed parameters  $\gamma_2$ , whose components are linear combinations of the components of  $\beta_2$ . For example, the notion of ignorance is defined in terms of  $\gamma_2$ , not in terms of  $\beta_2$ . This can be defended because both sets are auxiliary parameters, and if we are ignorant about one set we are equally ignorant about the other. From a more practical viewpoint, the flexibility of the WALS procedure is bounded, although we do not know yet precisely what the bounds are. Consider, for example, certain forms of model uncertainty that require mixing nonnested models such as the choice of the link function in a GLM setup. While these forms of model uncertainty can be handled by standard model-average procedures (Czado and Raftery, 2006), the generalization of WALS along these directions appears to be difficult.

Finally we emphasize (again) that WALS is a model-average procedure, not a model-selection procedure. At the end we cannot and do not want to answer the question: which model is best? This brings with it certain restrictions. For example, WALS cannot handle jointness (Ley and Steel, 2007; Doppelhofer and Weeks, 2009). The concept of jointness refers to the dependence between explanatory variables in the posterior distribution, and available measures of jointness depend on posterior inclusion probabilities of the explanatory variables, which WALS does not provide.

# 14. Software for WALS

User-friendly packages for WALS estimation of linear regression models with i.i.d. errors are available both in MATLAB and Stata. The latest 2.0 version of both packages—together with documentation, examples, and supplementary material—can be downloaded free of charge from the website http://www.janmagnus.nl/items/WALS.pdf.

Version 2.0 differs from earlier versions of the WALS packages in two important respects. First, we have enlarged the set of priors available for WALS estimation to three possible distributions: Weibull (the default), Subbotin, and Laplace. Parameters of all these prior distributions are always fixed to their minimax regret solutions under the neutrality condition.

Second, because of differences in the integration routines available in MATLAB and Stata, we have implemented two alternative strategies for computing the mean and variance in the posterior distribution. By default, the integrals involved in the computation of these posterior moments are solved numerically

by high-order global adaptive quadrature in the MATLAB package and by Gauss-Laguerre quadrature with 100 data points in the Stata package (Cheney and Kincaid, 2008). Even though these integration routines seem to produce very similar results in our examples, we cannot guarantee that this is true in general. For this reason, we introduced the postmoments option which interpolates m(x) and v(x) between the moments of the nearest x-values contained in precompiled tables of posterior means and variances under the Weibull and Subbotin priors at given x-values in the interval [0, 100] with step 0.01. These tables have been computed in MATLAB using a high degree of accuracy. For x > 100, posterior moments are approximated by m(100) and v(100). For the Laplace prior, the postmoments option is not active since moments of the resulting posterior distribution can be computed accurately in any statistical software.

No user-friendly packages are currently available for generalizations of the WALS procedure to more general regression models. However, as discussed in Section 12, most of these generalizations can be easily implemented either by applying standard WALS estimates to suitable transformations of the data, or by computing simple weighted averages of standard WALS estimates.

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