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# Empirical best linear unbiased prediction in cultivar trials using factor-analytic variance-covariance structures

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Abstract Results of multi-environment trials to evaluate new plant cultivars may be displayed in a two-way table of genotypes by environments. Different estimators are available to fill the cells of such tables. It has been shown previously that the predictive accuracy of the simple genotype by environment mean is often lower than that of other estimators, e.g. least-squares estimators based on multiplicative models, such as the additive main effects multiplicative interaction (AMMI) model, or empirical best-linear unbiased predictors (BLUPs) based on a two-way analysis-of-variance (ANOVA) model. This paper proposes a method to obtain BLUPs based on models with multiplicative terms. It is shown by cross-validation using five real data sets (oilseed rape, Brassica napus L.) that the predictive accuracy of BLUPs based on models with multiplicative terms may be better than that of leastsquares estimators based on the same models and also better than BLUPs based on ANOVA models.

**Key words** Genotype by environment interaction • Mixed model • Mean squared error of prediction • *Brassica napus* L. • Cross-validation • Additive main effects multiplicative interaction (AMMI) • Shifted multiplicative model (SHMM) • Restricted maximum likelihood (REML)

## Introduction

An important result of multi-environment trials is a two-way table displaying estimated yields of genotypes

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in the various environments. Such tables are the basis for making recommendations for specific environments and for studying genotype by environment interaction. The most natural and most common estimator used in genotype by environment tables is the simple average across replications for a genotype in an environment. It has been shown, however, that alternative estimators may be predictively more accurate than the simple mean, e.g. leastsquares estimators based models with multiplicative terms such as the additive main effects multiplicative interaction (AMMI) model (Gauch 1992), shrinkage estimators based on multiplicative models (Cornelius et al. 1994, 1996), and best linear unbiased predictions (BLUPs) based on a two-way analysis of variance (ANOVA) model (Cornelius et al. 1994, 1996; Piepho 1994).

The usual BLUP, as considered in Piepho (1994), and Cornelius et al. (1994), assumes that genotype by environment interaction effects are stochastically independent. There are other possible variancecovariance structures to be considered for BLUP. Multiplicative terms, if viewed from a mixed-model perspective, imply correlations among interactions. Mixed models with multiplicative terms are closely related to the so-called factor-analytic variancecovariance structure advocated by Jennrich and Schluchter (1986). Oman (1991), Gogel et al. (1995) and Piepho (1997 a) have shown how to fit models with a factor-analytic variance-covariance structure to genotype by environment data. Subsequently, Piepho (1997 b) suggested how to obtain BLUPs of multiplicative terms in such models and how to construct biplots using these BLUPs. The purpose of the present paper is to investigate whether BLUPs obtained under a factor-analytic variance-covariance structure lead to predictions better than BLUPs based on a two-way ANOVA model (Piepho 1994) and also better than estimators based on least-squares estimates of multiplicative terms.

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#### Theory

For trials laid out as a randomized complete block design, the ANOVA model is given by

$$y_{ijr} = \mu + g_i + \varepsilon_j + u_{ij} + b_{jr} + e_{ijr}, \tag{1}$$

where the various terms are:  $y_{ijr}$  = performance of the *r*-th replicate of the *i*-th genotype in the *j*-th environment (i = 1, ..., G; j = 1 ..., E; r = 1 ..., R),  $\mu$  = general mean,  $g_i$  = effect of the *i*-th genotype,  $\varepsilon_j$  = effect of the *j*-th environment,  $u_{ij}$  = interaction of the *i*-th genotype with the *j*-th environment,  $b_{jr}$  = effect of *r*-th block in the *j*-th environment, and  $e_{ijr}$  = error. The model for means across replications is

$$y_{ij} = \mu + g_i + \varepsilon'_j + u_{ij} + e_{ij}, \tag{2}$$

where  $y_{ij} = \bar{y}_{ij} = \sum_r y_{ijr}/R$ ,  $\varepsilon'_j = \varepsilon_j + \sum_r b_{jr}/R$  and  $e_{ij} = \sum_r e_{ijr}/R$ . The quantity that needs to be estimated to fill a two-way table of genotypes by environments is

$$z_{ij} = \mu + g_i + \varepsilon'_j + u_{ij},\tag{3}$$

i.e. the conditional expectation of  $y_{ijr}$ , given the genotype and the environment. The interaction term  $u_{ij}$  may be modelled by multiplicative terms as follows:

$$u_{ij} = \sum_{k=1}^{K} w_{ik} \lambda_{jk} + v_{ij}, \qquad (4)$$

where  $w_{ik}$  and  $\lambda_{jk}$  are the k-th scores  $[k = 1, ..., K; K \le \max(G - 1, E - 1)]$  corresponding to, respectively, the *i*-th genotype and the *j*-th environment, and  $v_{ij}$  is a residual interaction term. The genotypic scores  $w_{ik}$  can be interpreted as a sensitivity of the *i*-th genotype to a hypothetical unobservable environmental variable  $\lambda_{ik}$ .

Model (2) [in conjunction with the model (4) for the term  $u_{ij}$ ] may be simplified by dropping one of the terms  $\mu$ ,  $g_i$  and  $\varepsilon'_j$ . Following Denis and Gower (1996), we denote the class of models generated by (2) and (4) as B( $\mu$ , g,  $\varepsilon'$ ,  $\pi_K$ ) and enter asterisks to indicate terms dropped from the model. For example B( $\mu$ , g,  $\varepsilon'$ ,  $\pi_1$ ) denotes an AMMI model with one multiplicative term and B( $\mu$ , \*, \*,  $\pi_2$ ) is the shifted multiplicative model (SHMM) of Seyedsadr and Cornelius (1992) with two multiplicative terms. The maximum number of multiplicative terms for the various models is given in Table 1.

When both genotypes and environments are treated as fixed factors, the parameters  $\mu$ ,  $g_i$ ,  $\varepsilon'_j$ ,  $w_{ik}$  and  $\lambda_{jk}$  may be estimated by ordinary least squares (Denis and Gower 1996). The interaction effect is estimated by

$$\hat{u}_{ij} = \sum_{k=1}^{K} \hat{w}_{ik} \hat{\lambda}_{jk}, \tag{5}$$

where  $\hat{w}_{ik}$  and  $\hat{\lambda}_{jk}$  are the least squares estimates of  $w_{ik}$  and  $\lambda_{jk}$ , respectively. Except for  $B(\mu, *, *, \pi_K)$  least-squares estimation amounts to first fitting the grand mean (if  $\mu$  is in the model) and main effects for genotypes (if  $g_i$  is in the model) and environments (if  $\varepsilon'_j$  is in the model) to the data  $y_{ij}$  and then subjecting the matrix of residuals to a singular value decomposition (SVD). For  $B(\mu, *, *, \pi_K)$ , Seyedsadr and Cornelius (1992) proposed a Newton-Raphson algorithm. In this paper, a derivative-free method proposed by Piepho (submitted) is used.

If environments or genotypes are considered random, effects may be estimated by BLUP. A factor is commonly taken as random if the observed levels may reasonably be regarded as a random sample from a population. The assumption of a truly random sample is often debatable for both environments and genotypes. Nevertheless, it is frequently assumed that environments are random, mainly to allow inferences which are not restricted to the observed environments. Hill and Rosenberger (1985) and Stroup and Mulitze (1991)

**Table 1** Maximum number of multiplicative terms and Gollob's *df* for different models with multiplicative terms used to compute the shrinkage estimates of Cornelius et al. (1996)

Model	Maximum number of multiplicative terms (K)	Gollob's <i>df</i> used for shrinking <i>k</i> -th multiplicative term	
$ \begin{array}{l} {\rm B}(\mu,g,\varepsilon',\pi_K) \\ {\rm B}(\mu,g,*,\pi_K) \\ {\rm B}(\mu,*,\varepsilon',\pi_K) \\ {\rm B}(\mu,*,*,\pi_K) \\ {\rm B}(\mu,*,*,\pi_K) \\ {\rm B}(^*,*,*,\pi_K) \end{array} $	min(G - 1, E - 1) min(G, E - 1) min(G - 1, E) min(G, E) min(G, E)	G + E - 2k - 1 G + E - 2k G + E - 2k G + E - 2k + 1	

<sup>a</sup> No shrinkage estimates computed

showed that assuming random genotypes may be preferable in terms of predictive accuracy even when genotypes would be considered fixed by conventional standards. Using five faba bean data-sets, Piepho (1994) showed that the predictive accuracy of BLUPs based on a two-way ANOVA model differed only slightly depending on whether genotypes, environments, or both, were regarded as random and that the most important assumption was that interactions are random.

For the factor-analytic variance-covariance structure considered in this paper, it is necessary that one factor be regarded as fixed, while the other is taken as random. In the real data-sets that are used in this paper, the number of genotypes exceeds that of environments  $(G \ge E)$  and the number of environments is relatively small. Fitting to such data a model for random environments with a factor-analytic variance-covariance structure may cause estimability problems, showing in a failure of the REML algorithm to converge. This is a result of the large number of parameters to be estimated for the variance-covariance structure. For this reason, environments will be taken as fixed and genotypes as random. It is admitted that this model choice is justified by rather pragmatic arguments and that the assumption of random genotypes is made mainly to obtain shrinkage estimates (BLUPs) of interaction terms  $u_{ij}$ .

Taking genotypes as random and environments as fixed in (2) and (4), and assuming that all random effects, i.e.  $g_i$ ,  $w_{ik}$ ,  $v_{ij}$  and  $e_{ijr}$ , are stochastically independent with zero mean, the variance and covariance of the data  $v_{ii}$  are

$$\operatorname{var}(y_{ij}) = \sigma_g^2 + \sum_{k=1}^n \lambda_{jk}^2 \sigma_k^2 + \sigma_v^2 + \sigma_e^2/R$$

and

$$\operatorname{cov}(y_{ij}, y_{ij'}) = \sigma_g^2 + \sum_{k=1}^K \lambda_{jk} \lambda_{j'k} \sigma_k^2, \qquad (6)$$

where  $\sigma_g^2$ ,  $\sigma_k^2$ ,  $\sigma_v^2$  and  $\sigma_e^2$  are the variances of, respectively,  $g_i$ ,  $w_{ik}$ ,  $v_{ij}$  and  $e_{ijr}$ . The terms involving  $\lambda_{jk}$  and  $\sigma_k^2$  are over-parameterized, so restrictions have to be imposed to ensure identifiability. It is convenient to require  $\sigma_k^2 = 1$ , analogous to the fixed-effects model with multiplicative terms. In vector notation

$$E(\mathbf{y}_i) = \boldsymbol{\mu} \text{ and } \operatorname{var}(\mathbf{y}_i) = \boldsymbol{V} = \boldsymbol{11}' \sigma_q^2 + \boldsymbol{\Lambda} \boldsymbol{\Lambda}' + \boldsymbol{I} \sigma_p^2, \tag{7}$$

where  $\mathbf{y}_i = (y_{i1}, y_{i2}, \dots, y_{iE})' \mathbf{\mu} = (\mu_1, \mu_2, \dots, \mu_E)'$  with  $\mu_j = \mathbf{\mu} + \varepsilon'_j$ , *I* is an *E*-vector with all elements equal to 1,  $\mathbf{\Lambda} = \{\lambda_{jk}\}$  is a *E* by *K* matrix of environmental scores (factor loadings), *I* is an identity matrix, and  $\sigma_p^2 = \sigma_v^2 + \sigma_e^2/R$ . Elements of  $\mathbf{\Lambda}$  in the *j*-th row a *k*-th column for k > j are set to zero to cater for identifiability (SAS Institute, 1997). Also, there is an implicit restriction that  $\lambda'_k = (\lambda_{1k}, \dots, \lambda_{Ek}) \propto I'$  is ruled out. Otherwise there would be a correspondence between  $w_{ik}$  and genotypic main effect  $g_i$ . Note that in the mixed-model case, one may drop main effects for genotypes and/or environments, as in the fixed-effects case, so the same set of models can be considered for prediction. To make a distinction from the fixed-effects models, the mixed models will be denoted as B<sup>rg</sup>( $\mu$ , g,  $\varepsilon'$ ,  $\pi_K$ ), where the superscript "rg" stands for "random genotypes". It is stressed that all of these models have the residual interaction variance component  $\sigma_v^2$ . For K = 0, one obtains the BLUPs based on common analysis of variance models with independent interaction effects. Models B<sup>rg</sup>(\*, \*,  $\pi_K$ ) have neither a general mean nor main effects. These models are not considered further, since they imply an expected value of zero for all observations, which does not seem sensible.

The factor-analytic variance-covariance structure may be regarded as an approximation to the completely unstructured variance-covariance matrix. For this reason, I am also considering models with an unstructured variance-covariance matrix. These models can be written as

$$E(\mathbf{y}_i) = \boldsymbol{\mu} \text{ and } \operatorname{var}(\mathbf{y}_i) = \boldsymbol{V} = \{\sigma_{jj'}\} + I\sigma_e^2/R,$$
(8)

where  $\boldsymbol{\mu} = (\mu_1, \mu_2, \dots, \mu_E)'$ . The model (8) with  $\mu_j = \boldsymbol{\mu} + \varepsilon'_j$  is denoted UN( $\mu, \varepsilon'$ ), while that with  $\mu_j = \mu$  is denoted as UN( $\mu, \ast$ ).

There are many derivations of BLUP (Searle et al. 1992). Here, the one based on the multivariate normality assumption will be used for brevity. For prediction of  $z_i = (z_{i1}, ..., z_{iE})'$ , only observations of the *i*-th genotype are informative, provided the variance components are known. So it suffices to consider the joint distribution of  $y_i$  and  $z_i$ . Assuming multivariate normality, we have

$$\begin{pmatrix} \boldsymbol{z}_i \\ \boldsymbol{y}_i \end{pmatrix} \sim N \left[ \begin{pmatrix} \boldsymbol{\mu} \\ \boldsymbol{\mu} \end{pmatrix}, \begin{pmatrix} \boldsymbol{\Gamma} & \boldsymbol{\Gamma} \\ \boldsymbol{\Gamma} & \boldsymbol{V} \end{pmatrix} \right],$$
(9)

where

$$\Gamma = V - I\sigma_e^2/R. \tag{10}$$

The conditional distribution of  $z_i$  for given  $y_i$  is

$$(\mathbf{z}_i|\mathbf{y}_i) \sim N[\boldsymbol{\mu} + \boldsymbol{\Gamma} \boldsymbol{V}^{-1}(\mathbf{y}_i - \boldsymbol{\mu}), \boldsymbol{\Gamma} - \boldsymbol{\Gamma} \boldsymbol{V}^{-1} \boldsymbol{\Gamma}].$$
(11)

The conditional expectation  $\mu + \Gamma V^{-1}(y_i - \mu)$  is the BLUP of  $z_i$ , provided  $\Gamma$ , V and  $\mu$  are known (Searle et al. 1992: 273), and it is also a Bayes estimator under normal priors (Robinson 1991; Searle et al. 1992: 275). In practice, estimates are used in place of unknown parameters. The resulting estimator will be referred to as empirical BLUP, the term 'empirical' indicating that unknown parameters are estimated from the data. The properties of empirical BLUPs are not known, and it should be investigated, e.g. by simulation, whether they perform similarly as BLUPs for known parameters. Estimates of variance components may be obtained by usual procedures for linear mixed models, i.e. by restricted maximum likelihood (REML) or maximum likelihood (ML). In the present paper, the REML method of the MIXED procedure of SAS is used (SAS Institute 1997). For advantages of REML over ML see Searle et al. (1992). The expectation  $\mu$  is estimated by generalized least squares (equivalent to least squares based on models considered in this paper, provided data are balanced).

Cornelius et al. (1996) proposed shrinkage estimators, in which least-squares estimates of multiplicative terms are multiplied by shrinkage factors computed from F-statistics appropriate for testing these same terms. The resulting shrinkage estimators can be expressed in a form analogous to BLUPs based on a two-way ANOVA model with stochastically independent interactions, but they are not equivalent to the BLUPs presented in this paper. Assuming that genotypes and environments are random and that interactions are independent, the BLUP of a cell mean can be written

$$BLUP(z_{ij}) = \bar{y}_{...} + S_G(\bar{y}_{i..} - \bar{y}_{...}) + S_E(\bar{y}_{.j.} - \bar{y}_{...}) + S_{GE}(\bar{y}_{...} - \bar{y}_{i..} - \bar{y}_{.j.} + \bar{y}_{ij.}), \qquad (12)$$

where  $S_G = \max(1 - F_G^{-1}, 0)$ ,  $S_E = \max(1 - F_E^{-1}, 0)$ , and  $S_{GE} = \max(1 - F_{GE}^{-1}, 0)$ , where  $F_G$ ,  $F_E$  and  $F_{GE}$  are the *F*-statistics of genotypic main effects, environmental main effects and interaction, respectively, against the error mean square.  $S_G$ ,  $S_E$  and  $S_{GE}$  are estimators of, respectively,  $(RE\sigma_g^2 + R\sigma_u^2)/(RE\sigma_g^2 + R\sigma_u^2 + \sigma_e^2)$ ,  $(RG\sigma_{e'}^2 + R\sigma_u^2)/(RG\sigma_{e'}^2 + R\sigma_u^2 + \sigma_e^2)$ , and  $R\sigma_u^2/(R\sigma_u^2 + \sigma_e^2)$ , where  $\sigma_g^2, \sigma_e^2, \sigma_u^2$ , and  $\sigma_e^2$  are the variances of  $g_i, \varepsilon'_j, u_{ij}$  and  $e_{ijr}$  in (1) and (2). By analogy, for  $B(\mu, g, \varepsilon', \pi_K)$ ,  $B(\mu, g, *, \pi_K)$ ,  $B(\mu, *, \varepsilon', \pi_K)$  and  $B(*, *, *, \pi_K)$  models, a shrinkage factor for the k-th multiplicative component is defined as

$$S_k = \max(1 - F_k^{-1}, 0) \text{ with } F_k = \frac{R\tilde{\phi}_k^2}{v_k s^2},$$
 (13)

where  $\hat{\phi}_k$  and  $v_k$  are, respectively, the singular value and the degrees of freedom (df) associated with the k-th multiplicative term, and  $s^2$  is the residual error mean square. Note that  $F_k$  has the form of an *F*-statistic for testing the k-th multiplicative term. Cornelius et al. (1996) discuss several ways of obtaining  $v_k$ . The simplest option is to use Gollob's df, which is equal to the number of parameters of a multiplicative term, reduced by the number of constraints on the parameters. More appropriate dfs involve intensive simulations. For simplicity, I am using only Gollob's df to obtain shrinkage factors for least-squares estimates of multiplicative terms (see Table 1). Least-squares estimates of main effects of genotypes and environments are multiplied by the shrinkage factors  $S_G$  and  $S_E$ , respectively, as in (12). I am not considering the shrinkage estimators for B( $\mu$ , \*, \*,  $\pi_K$ ), because they require an iterative scheme and are computationally more demanding (Cornelius et al. 1996).

It may happen that  $S_{k+1} \hat{\phi}_{k+1} > S_k \hat{\phi}_k$  for some k, where  $\hat{\phi}_k$  is the k-th singular value of an SVD of the residuals remaining after fitting the grand mean and main effects, if any, which may be regarded as conflicting with the model constraint that  $\phi_k > \phi_{k+1}$  for all k. If  $S_{k+1}\hat{\phi}_{k+1} > S_k\hat{\phi}_k$ , Cornelius et al. (1996) therefore propose to pool  $\hat{\phi}_{k+1}^2$  and  $\hat{\phi}_k^2$  and re-compute the shrinkage factors  $S_k$  and  $S_{k+1}$ . If after pooling  $S_{k+2}\hat{\phi}_{k+2} > S_{k+1}\hat{\phi}_{k+1}$ , then  $\hat{\phi}_{k+2}^2$ ,  $\hat{\phi}_{k+1}^2$  and  $\hat{\phi}_k^2$  are pooled, and so forth. This approach may be formalized by the following algorithm:

(1) For k = 1 to K set  $v_k =$  Gollob's df and  $\hat{\phi}_k = k$ -th singular value of SVD of residuals after fitting grand mean and main effects, if these are in the model.  $\langle \hat{\phi}_t^2 - v_s s^2/R \rangle$ 

(2) For 
$$k = 1$$
 to  $K$  set  $S_k = \max\left(\frac{\varphi_k - v_k s/R}{\hat{\phi}_k^2}, 0\right)$   
(3) For  $i = 1$  to  $K - 1$  do  
For  $j = i + 1$  to  $K$  do  
If  $S_j \hat{\phi}_j > S_i \hat{\phi}_i$  then do  
For  $m = i$  to  $j$  do  
 $\hat{\phi}_m = \sqrt{\sum_{k=i}^j \hat{\phi}_k^2/(j - i + 1)}$   
 $v_m = \sum_{k=i}^j v_k/(j - i + 1)$   
 $S_m = \max\left(\frac{\hat{\phi}_m^2 - v_m s^2/R}{\hat{\phi}_m^2}, 0\right)$   
End  
End

End

#### **Cross-validation**

To assess the performance of different methods of prediction, I used five oilseed rape (*Brassica napus* L.) data-sets from official variety trials by the Bundessortenamt (Hannover, Germany). The

 Table 2
 Structure of oilseed rape (B. napus L.) data-sets by Bundes-sortenamt (Hannover, Germany). Trials were laid out as random-ized complete block designs

Year	Genotypes	Locations	Replications
1985	32	8	4
1986	35	11	4
1987	35	10	4
1988	42	9	4
1989	41	10	4

trials were laid out as randomized complete block designs. The structure of the data-sets is described in Table 2. The performance was evaluated using a cross-validation procedure based on splitting the data into modelling and validation data (Gauch 1988). For the data-sets used there were four replications per environment (R = 4). For each environment the four complete blocks were randomly split into three blocks for modelling and one block for validation. Keeping blocks intact is preferred to splitting data completely at random, which would introduce added noise to modelling and validation data compared to the complete dataset (Piepho 1994). In yield trials, one is usually mainly interested in predicting differences among genotypes  $\delta_{ii'j} = z_{ij} - z_{i'j} (i' \neq i)$  rather than the genotypic performances  $z_{ij}$  themselves. Thus, an assessment of the predictive accuracy of a model may be based on the discrepancy between observed differences in the validation data  $(y_{ij}^V - y_{i'j}^V)$ , where  $y_{ij}^V$  denotes the validation observation for the ij-th cell, and corresponding differences predicted by the model computed from the modelling data  $(\hat{z}_{ij} - \hat{z}_{i'j})$ . Therefore, I am proposing to assess predictive accuracy by

$$MSEP = \frac{\sum_{j=1}^{E} \sum_{i=1}^{G} \sum_{i \neq i}^{G} (y_{ij}^{V} - y_{i'j}^{V} - (\hat{z}_{ij} - \hat{z}_{i'j}))^{2}}{EG(G-1)} = \frac{2 \sum_{j=1}^{E} \sum_{i=1}^{G} (f_{ij} - \overline{f}_{.j})^{2}}{E(G-1)},$$
(14)

where  $f_{ij} = y_{ij}^V - \hat{z}_{ij}$ . The data splitting and the subsequent cross-validation was replicated 1000 times and the *MSEP* was averaged over the replications.

All computations were done using the SAS System (SAS Institute, Inc.). Estimation of variance components was based on cell means  $y_{ij}$ . The estimates of V and of  $\sigma_p^2$  obtained from the analysis of the cell means of the complete data ( $\hat{V}_C$  and  $\hat{\sigma}_p^2$ ) was stored and used in subsequent computations. An estimate of the variance component  $\sigma_e^2(\hat{\sigma}_e^2)$  was computed from replicate observations using model (1) and treating all effects except  $e_{ijr}$  as fixed. The modeling data had R - 1 replications. Thus, estimates of V and  $\Gamma$  for the modeling data were obtained from  $\hat{V}_C$  as follows:

$$\hat{V} = \hat{V}_C + I(R-1)^{-1} R^{-1} \hat{\sigma}_e^2, \qquad (15)$$

$$\hat{\Gamma} = \hat{V}_C - IR^{-1}\hat{\sigma}_e^2 \quad \text{when} \quad \hat{\sigma}_p^2 > R^{-1}\hat{\sigma}_e^2 \quad \text{and}$$
(16)

$$\hat{\boldsymbol{\Gamma}} = \hat{V}_C - \boldsymbol{I}\hat{\sigma}_p^2$$
 when  $\hat{\sigma}_p^2 \leq R^{-1}\hat{\sigma}_e^2$ 

For the models  $UN(\mu, \varepsilon')$  and  $UN(\mu, *)$ ,  $\Gamma$  was estimated as

$$\hat{\boldsymbol{\Gamma}} = \hat{V}_C - \boldsymbol{I}\boldsymbol{R}^{-1}\,\hat{\sigma}_e^2\,. \tag{17}$$

These estimates were then used to compute BLUPs from the modelling data in each iteration of the cross-validation procedure. Alternatively, one could have estimated variance components in each iteration of the cross-validation procedure. However, REML estimation of the factor-analytic structures turned out to be computationally very demanding, so that repeated estimation on each of 1000 iterations was not feasible. Also, since the computational effort for the estimation of V turned out to increase notably with the number of multiplicative terms, only models with up to K = 7 were considered. This seemed justified because the differences in *MSEP* among models with many multiplicative terms was usually marginal. The residual variance  $s^2$  was estimated from the whole data and stored to compute  $S_k$  by equation (13) in each iteration. In equation (13), R was replaced by (R - 1). Shrinkage factors  $S_G$  and  $S_E$  for the estimates of Cornelius et al. (1996) were also computed from the complete data, stored and used in cross-validations. To take account of the fact that for the complete data there were R replications per environment, while for the modelling data there were (R - 1) observations,  $S_G$  and  $S_E$  for the modelling data were computed as

$$S_G = \max\left(\frac{(MS_G - s^2)(R - 1)/R}{(MS_G - s^2)(R - 1)/R + s^2}, 0\right) \text{ and}$$
(18)

$$S_E = \max\left(\frac{(MS_E - s^2)(R - 1)/R}{(MS_E - s^2)(R - 1)/R + s^2}, 0\right),\tag{19}$$

where  $MS_G$  and  $MS_E$  are the mean squares for, respectively, genotypes and environments of an ANOVA based on the replicate data  $y_{ijr}$ .  $S_G$  and  $S_E$  are estimators of, respectively,  $[(R-1)E\sigma_g^2 + (R-1)\sigma_u^2]/[(R-1)E\sigma_g^2 + (R-1)\sigma_u^2 + \sigma_e^2]$ ,  $[(R-1)G\sigma_{\epsilon'}^2 + (R-1)\sigma_u^2)/[(R-1)G\sigma_{\epsilon'}^2 + (R-1)\sigma_u^2 + \sigma_e^2]$ .

### Results

For all data sets, the estimator with the smallest MSEP was among the BLUPs (Table 3). The shrinkage estimators of Cornelius et al. (1996) (Table 4) were better than the best least-squares estimator based on models with multiplicative terms (Table 5). Among BLUPs, those based on a model without environmental main effects were inferior to those based on a model with environmental main effects. Among BLUPs based on models with environmental main effects, the MSEP differed only slightly, except for the model  $B^{rg}(\mu, *, \varepsilon', *)$ , which had a markedly larger *MSEP* than other models. In case of the 1988 data-set, BLUPs based on UN( $\mu$ ,  $\varepsilon'$ ) had the smallest MSEP, while for the other data-sets the BLUPs with the smallest MSEP were based on a model with multiplicative terms. There were four groups of mixed models given by whether or not main effects for genotypes or environments were included. Within such a group, models with independent interactions were always inferior to at least one of the models with factor-analytic or unstructured variance-covariance matrices. For example, in the 1985 data-set,  $B^{rg}(\mu, g, \varepsilon', *)$ , which has both genotypic and environmental main effects, was inferior to  $B^{rg}(\mu, g, \varepsilon', \pi_k)$  (k = 1, 2, ..., 7). The shrinkage estimators of Cornelius et al. (1996) were often slightly better than BLUPs based on models with independent interactions. This is in reasonable agreement with the findings of Cornelius et al. (1996) for other data-sets.

 Table 3 MSEP (mean square error of prediction; see eq. 14)

 of BLUPs (best linear unbiased predictions) based on different mixed models for oilseed rape (*B. napus* L.) data-sets

Model	1985	1986	1987	1988	1989
$\mathbf{B}^{\mathrm{rg}}(\mu,  g,  \varepsilon',  *)$	33.88	37.96	25.74	21.92	40.94
$\mathbf{B}^{\mathrm{rg}}(\mu, g, \varepsilon', \pi_1)$	33.38	37.58	25.44	21.52	40.92
$\mathbf{B}^{\mathrm{rg}}(\mu, g, \varepsilon', \pi_2)$	33.28	37.86	25.18	21.46	41.50
$\mathbf{B}^{\mathrm{rg}}(\mu, g, \varepsilon', \pi_3)$	33.20	37.70	25.20	21.46	40.94
$\mathbf{B}^{\mathrm{rg}}(\mu, g, \varepsilon', \pi_4)$	33.40	37.70	25.04	21.30	40.70
$\mathbf{B}^{\mathrm{rg}}(\mu, g, \varepsilon', \pi_5)$	33.26	37.92	24.86	21.30	40.42
$\mathbf{B}^{\mathrm{rg}}(\mu, g, \varepsilon', \pi_6)$	33.24	37.88	24.62	21.24	40.16
$\mathbf{B}^{\mathrm{rg}}(\mu, g, \varepsilon', \pi_7)$	33.24	38.20	24.58	21.24	40.44
$\mathrm{B^{rg}}(\mu,^{*},\varepsilon',^{*})$	34.96	40.22	27.00	22.44	42.96
$B^{rg}(\mu, *, \varepsilon', \pi_1)$	33.92	37.68	25.46	21.62	41.94
$\mathrm{B^{rg}}(\mu,^*,\varepsilon',\pi_2)$	33.46	37.92	25.18	21.54	42.66
$B^{rg}(\mu, *, \varepsilon', \pi_3)$	33.42	37.72	25.14	21.42	42.28
$\mathrm{B^{rg}}(\mu, ^*,  \varepsilon',  \pi_4)$	33.60	37.66	25.08	21.38	41.56
$B^{rg}(\mu, *, \varepsilon', \pi_5)$	33.38	37.62	24.96	21.36	41.26
$B^{rg}(\mu, *, \varepsilon', \pi_6)$	33.46	37.92	24.74	21.32	41.02
$\mathbf{B}^{\mathrm{rg}}(\mu,  *,  \varepsilon',  \pi_7)$	33.40	37.96	24.68	21.30	41.20
UN( $\mu$ , $\varepsilon'$ )	33.22	37.96	24.62	21.18	40.78
$B^{rg}(\mu, g, *, *)$	34.88	41.28	27.70	22.68	44.84
$B^{rg}(\mu, g, *, \pi_1)$	33.98	38.26	26.06	22.10	42.86
$B^{rg}(\mu, g, *, \pi_2)$	33.92	38.34	25.76	21.90	41.92
$B^{rg}(\mu, g, *, \pi_3)$	33.84	38.46	25.74	21.88	42.90
$B^{rg}(\mu, g, *, \pi_4)$	33.82	38.02	25.80	21.88	42.20
$B^{rg}(\mu, g, *, \pi_5)$	33.76	38.18	25.34	21.78	41.80
$B^{rg}(\mu, g, *, \pi_6)$	33.82	38.12	25.16	21.74	41.56
$B^{rg}(\mu, g, *, \pi_7)$	33.82	38.30	25.22	21.70	41.66
$B^{rg}(\mu, *, *, *)$	35.52	41.54	27.62	22.76	44.78
$B^{rg}(\mu, *, *, \pi_1)$	34.34	38.46	26.44	22.24	43.04
$B^{rg}(\mu, *, *, \pi_2)$	34.24	38.06	25.40	21.82	41.94
$B^{rg}(\mu, *, *, \pi_3)$	34.18	38.40	25.36	21.76	42.68
$B^{rg}(\mu, *, *, \pi_4)$	34.14	38.12	25.38	21.72	42.22
$B^{rg}(\mu, *, *, \pi_5)$	34.12	38.14	25.24	21.70	41.90
$B^{rg}(\mu, *, *, \pi_6)$	34.14	38.16	25.10	21.66	41.78
$B^{rg}(\mu, *, *, \pi_7)$	34.16	38.18	25.14	21.64	41.58
UN(μ, *)	33.88	38.02	24.86	21.56	41.08

**Table 4** *MSEP* (mean square error of prediction; see eq. 14) of shrinked least squares estimates based on different fixed effects models for oilseed rape (*B. napus* L.) data-sets, using the shrinkage estimators of Cornelius et al. (1996) with Gollob's *df.* Models were estimated by least squares

Model	1985	1986	1987	1988	1989
$     \begin{array}{c}       B(\mu,  g,  \varepsilon',  \pi_K) \\       B(\mu,  *,  \varepsilon',  \pi_K) \\       B(\mu,  g,  *,  \pi_K) \\       B(*,  *,  *,  \pi_K)     \end{array} $	34.84	39.48	26.24	22.30	42.47
	35.05	39.73	26.01	22.26	42.48
	35.15	39.67	26.51	22.42	42.95
	34.87	39.49	25.94	22.30	42.37

# Discussion

This paper has been restricted to the problem of obtaining good estimates of cells in a two-way table, in which observations are available for all cells. The term 'prediction', as used to label estimates of realized values of random effects (BLUPs), is somewhat misleading in this context, since nothing new is predicted. Clearly, the 'predictions' are only for environments under trial, not for 'new' environments. At times, the main interest is in predictions for new environments not under trial. This problem is dealt with by Weber and Westermann (1994) and Piepho et al. (1998).

BLUPs have a clearly understood theoretical basis. They have the smallest mean squared error of prediction among all linear unbiased predictors, provided the assumed model holds and the parameters of the model are known (Searle et al. 1992). If parameters are estimated, this optimality no longer holds, but it can be hoped that the performance of empirical BLUPs is not far from optimal. Since optimality is restricted to the class of linear unbiased predictors, and since one never knows the "true" model in practice, there may other predictors with a smaller mean squared error of prediction. It has been shown previously (Piepho 1994) that empirical BLUPs based on a simple two-way ANOVA model can be predictively more accurate that an AMMI model least-squares estimate of cell means. In Table 5 MSEP (mean squareerror of prediction; see eq. 14) ofleast squares estimates based ondifferent fixed effects models foroilseed rape (B. napus L.)data-sets. Models were estimatedby least squares

Model	1985	1986	1987	1988	1989
$ \begin{array}{c} \mathbf{B}(\mu,  g,  \varepsilon^{\prime},  \ast^{\prime}) \\ \mathbf{B}(\mu,  g,  \varepsilon^{\prime},  \pi_{1}) \\ \mathbf{B}(\mu,  g,  \varepsilon^{\prime},  \pi_{2}) \\ \mathbf{B}(\mu,  g,  \varepsilon^{\prime},  \pi_{2}) \\ \mathbf{B}(\mu,  g,  \varepsilon^{\prime},  \pi_{3}) \\ \mathbf{B}(\mu,  g,  \varepsilon^{\prime},  \pi_{3}) \\ \mathbf{B}(\mu,  g,  \varepsilon^{\prime},  \pi_{5}) \\ \mathbf{B}(\mu,  g,  \varepsilon^{\prime},  \pi_{5}) \\ \mathbf{B}(\mu,  g,  \varepsilon^{\prime},  \pi_{5}) \\ \mathbf{B}(\mu,  g,  \varepsilon^{\prime},  \pi_{7}) \\ \mathbf{B}(\mu,  g,  \varepsilon^{\prime},  \pi_{8}) \\ \mathbf{B}(\mu,  g,  \varepsilon^{\prime},  \pi_{9}) \\ \mathbf{B}(\mu,  g,  \varepsilon^{\prime},  \pi_{10}) \end{array} $	46.70 39.37 38.90 38.98 38.39 37.25 37.09 36.54	42.15 42.04 43.52 43.22 43.08 42.28 42.23 42.48 42.77 42.95 42.95	32.86 30.79 29.21 29.22 28.69 28.44 28.42 28.27 28.21 28.29	31.08 26.01 25.20 24.64 24.07 24.04 23.56 23.70 23.45	47.82 48.37 44.91 44.44 44.83 45.10 45.58 45.69 46.21 46.51
$\begin{array}{l} B(\mu, *, \varepsilon^{\prime}, *)\\ B(\mu, *, \varepsilon^{\prime}, \pi_{1})\\ B(\mu, *, \varepsilon^{\prime}, \pi_{2})\\ B(\mu, *, \varepsilon^{\prime}, \pi_{3})\\ B(\mu, *, \varepsilon^{\prime}, \pi_{4})\\ B(\mu, *, \varepsilon^{\prime}, \pi_{5})\\ B(\mu, *, \varepsilon^{\prime}, \pi_{5})\\ B(\mu, *, \varepsilon^{\prime}, \pi_{7})\\ B(\mu, *, \varepsilon^{\prime}, \pi_{7})\\ B(\mu, *, \varepsilon^{\prime}, \pi_{9})\\ B(\mu, *, \varepsilon^{\prime}, \pi_{10})\\ B(\mu, *, \varepsilon^{\prime}, \pi_{11}) \end{array}$	72.88 44.92 39.05 38.10 38.62 38.22 37.36 36.94 36.54	60.40 41.47 42.66 43.07 43.88 43.58 42.46 42.46 42.46 42.60 42.83 42.97 42.96	56.52 30.83 29.07 29.61 29.35 28.65 27.90 28.10 27.95 28.04 28.29	43.85 26.58 25.81 25.38 24.19 23.97 23.62 23.84 23.73 23.45	$57.14 \\ 47.47 \\ 46.76 \\ 45.13 \\ 44.51 \\ 44.72 \\ 44.84 \\ 45.45 \\ 45.61 \\ 46.24 \\ 46.51 \\ \end{cases}$
$ \begin{array}{l} \mathbf{B}(\mu, g, *, *) \\ \mathbf{B}(\mu, g, *, \pi_1) \\ \mathbf{B}(\mu, g, *, \pi_2) \\ \mathbf{B}(\mu, g, *, \pi_3) \\ \mathbf{B}(\mu, g, *, \pi_3) \\ \mathbf{B}(\mu, g, *, \pi_5) \\ \mathbf{B}(\mu, g, *, \pi_5) \\ \mathbf{B}(\mu, g, *, \pi_7) \\ \mathbf{B}(\mu, g, *, \pi_8) \\ \mathbf{B}(\mu, g, *, \pi_9) \\ \mathbf{B}(\mu, g, *, \pi_{10}) \end{array} $	46.70 43.50 40.07 38.99 38.10 38.21 37.15 36.54	42.15 41.32 42.59 42.90 42.76 41.93 42.23 42.23 42.59 42.62 42.89 42.96	32.86 31.39 29.18 29.65 29.44 28.83 28.56 28.39 28.30 28.29	31.08 30.13 26.22 25.52 24.71 24.14 24.04 23.48 23.45	47.82 48.19 44.86 45.35 44.67 45.09 45.12 45.45 46.19 46.51
$\begin{array}{l} B(\mu,*,*,\pi_{1})\\ B(\mu,*,*,\pi_{1})\\ B(\mu,*,*,\pi_{2})\\ B(\mu,*,*,\pi_{3})\\ B(\mu,*,*,\pi_{3})\\ B(\mu,*,*,\pi_{5})\\ B(\mu,*,*,\pi_{5})\\ B(\mu,*,*,\pi_{7})\\ B(\mu,*,*,\pi_{7})\\ B(\mu,*,*,\pi_{9})\\ B(\mu,*,*,\pi_{10})\\ B(\mu,*,*,\pi_{11}) \end{array}$	72.88 46.23 39.55 39.23 39.08 38.40 37.20 36.94 36.54	60.40 41.78 42.99 43.59 43.24 42.37 42.34 42.55 42.81 42.97 42.96	56.52 31.20 29.09 29.74 29.58 28.79 28.10 28.16 27.94 28.04 28.29	43.85 30.51 25.98 25.24 24.69 24.15 24.18 23.73 23.73 23.73 23.45	57.14 47.65 47.33 44.86 44.28 44.62 44.91 45.47 45.62 46.24 46.51
$B(*, *, *, \pi_1)B(*, *, *, \pi_2)B(*, *, *, \pi_3)B(*, *, *, \pi_4)B(*, *, *, \pi_5)B(*, *, *, \pi_6)B(*, *, *, \pi_7)B(*, *, *, \pi_8)B(*, *, *, \pi_9)B(*, *, *, \pi_{10})B(*, *, *, \pi_{11})$	46.16 39.73 39.24 38.90 38.12 37.07 36.87 36.54	41.62 42.58 42.98 43.42 43.08 42.20 42.17 42.40 42.73 42.93 42.96	31.21 29.15 29.80 29.46 28.53 27.98 28.21 27.94 28.00 28.29	31.63 25.89 25.13 24.58 24.10 24.04 23.51 23.70 23.45	47.36 48.38 44.77 44.21 44.61 44.86 45.50 45.77 46.26 46.51

the present paper it has been shown how to obtain BLUPs based on more complex models, specifically based on models with multiplicative terms such as AMMI and SHMM, which imply factor-analytic variance-covariance structures in a mixed-model framework. It has been demonstrated by cross-validation using real data that the simple variance-covariance structures implied by ANOVA models, which assume that interaction effects are independent, may be predictively inferior to other structures, which imply correlations among interactions. In addition to models with factor-analytic variance-covariance structure, several other variance-covariance structures can be used (Wolfinger 1996; Denis et al. 1997). A comparison with the factor-analytic variance-covariance structure would be rewarding, but is beyond the scope of this paper.

Van Eeuwijk et al. (1995) suggested to obtain a genotype by environment BLUPs based on an ANOVA mixed model and then subject this table to AMMI analysis, using an SVD procedure. This procedure may be seen as an approximation to the more direct approach of computing BLUPs based on a factor-analytic variance-covariance structure. The major approximation lies in the fact that an ANOVA model implies stochastically independent interaction effects, while the AMMI model, if viewed from a mixed-model perspective, implies correlated interactions.

In the data considered in this paper, BLUPs were slightly better than the shrinkage estimators of Cornelius et al. (1996) based on Gollob's *df*. Cornelius et al. (1996) proposed an iterative scheme to obtain shrinkage estimators with a more appropriate *df*, and these may fare better than those based on Gollob's *df*. Also, I have not considered shrinkage estimators based on the B( $\mu$ , \*, \*,  $\pi_k$ ) as of Cornelius et al. (1996), which may perform somewhat better than the shrinkage estimators based on other models. An important advantage of BLUPs compared to shrinkage estimators of Cornelius et al. (1996) is that they are easily obtained for unbalanced data.

My experience with the rapeseed data-sets indicates that fitting models with random main effects (here: genotypic main effects) and a factor-analytic variancecovariance structure on the residuals may be computationally much more demanding than the fitting of models without genotypic main effects. Among models with a factor-analytic variance-covariance structure, the predictive accuracy of models with a random genotypic main effect and the corresponding model without genotypic main effects was small. Thus, if computational resources are limiting, it may be sufficient to consider only models without random main effects for prediction.

Finally, it is remarked that the embedding within a mixed model framework allows models to be selected using likelihood-based criteria (likelihood ratio tests, information criteria) (see Wolfinger 1996; SAS Institute 1997). This may be preferable in practice to the computer-intensive cross-validation. SAS code for fitting mixed models used in this paper is available from the author upon request.

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