A MULTIVARIATE MIXED MODEL SYSTEM FOR WOOD SPECIFIC GRAVITY AND MOISTURE CONTENT OF PLANTED LOBLOLLY PINE STANDS IN THE SOUTHERN UNITED STATES

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ABSTRACT
Specific gravity (SG) and moisture content (MC) both have a strong influence on the quantity and quality of wood fiber. We proposed a multivariate mixed model system to model the two properties simultaneously. Disk SG and MC at different height levels were measured from 3 trees in 135 stands across the natural range of loblolly pine and the stand level values were used for the modeling SG-MC system. Regional variation in mean trend of the properties was incorporated in the model. Contemporaneous correlation between the SG and MC was accounted by defining within stand error structure appropriately. Compared to univariate models, predictions based on the multivariate model were improved by 29 and 26% in root mean square prediction error for disk SG and MC after taking account of the contemporaneous correlation.

INTRODUCTION
A forest is a complex dynamic system with inter-related individual components. Foresters commonly rely on simultaneous modeling systems to explain such inter-dependent systems. One familiar example of such a system to forest biometricians is simultaneous modeling of dominant height, basal area, trees per hectare and volume (Borders 1989; Fang et al. 2001; Hall and Clutter 2004). Two main reasons for the popularity of simultaneous modeling systems in forestry are: 1) compatibility requirement of individual components in the system (Clutter 1963); 2) contemporaneous correlation of error among individual components in the system.

Specific gravity (SG) and moisture content (MC) both have a strong influence on the quantity and quality of wood. SG describes the mass of woody material present in a given volume of wood. It is a unit-less measure and expressed as the ratio of wood basic density (oven dry weight divided by green volume) with the density of water at 4°C (Megraw 1985). SG is considered an important wood property because of its strong correlation with the strength of solid wood products, as well as the yield and quality of pulp produced (Panshin and deZeeuw 1980). Generally the moisture content of wood is expressed as a percentage of the oven dry weight of wood. Moisture content influences the physical and mechanical properties of wood, resistance to biological deterioration and dimensional stability (Haygreen and Bowyer 1996).

SG and MC vary considerably within loblolly pine (Pinus taeda L.) trees. SG follows a decreasing trend with tree height (He 2004; Megraw 1985; Phillips 2002; Zobel and Blair 1976), while MC increases with height (Koch 1972; Phillips 2002). It has been reported that these two variables are highly negatively correlated with high SG associated with low MC and vice-versa (Koch 1972; Zobel and Blair 1976). The primary factor controlling the longitudinal variation in disk SG and MC in a loblolly pine tree is the proportion of juvenile wood (Zobel and Blair 1976; Zobel and vanBuijtenen 1989). In general, the proportion of juvenile wood is higher towards the top of a tree than at the base and juvenile wood has lower SG and higher MC than mature wood.

The objective of this study was to model the longitudinal variation in disk SG and MC as a simultaneous multivariate mixed model system. We will show how contemporaneous correlation between these two variables (disk SG and MC) can be potentially utilized to improve the prediction of disk SG or MC for loblolly pine at any height.

DATA
The Wood Quality Consortium at the University of Georgia and the United States Department of Agriculture (USDA) Forest Service Southern Research station sampled planted loblolly pine across its natural range to study the longitudinal variation in wood SG and MC. Trees were sampled from

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135 stands from six physiographic regions across the southeastern United States. Regions sampled included: 1- southern Atlantic Coastal Plain (R1), 2- northern Atlantic Coastal Plain (R2), 3- Upper Coastal Plain (R3), 4- Piedmont (R4), 5- Gulf Coastal Plain (R5) and 6- Hilly Coastal Plain (R6). A minimum of 12 plantations from each of the six physiographic regions were sampled. The stands selected for sampling included 20- to 25-year-old loblolly pine plantations planted at 1250 or more trees per hectare and having 625 trees per hectare or more after thinning. Only stands that were conventionally managed with no fertilization (except phosphorus at planting on phosphorus deficient sites) and no competition control were sampled. Three trees from each stand were felled and cross sectional disks of 3.8 cm thickness were collected from 0.15, 1.37 m and then 1.52 m intervals along the stem up to a diameter of 50 mm outside bark. The disks were sealed in plastic bags and shipped to the USDA Forest Service laboratory for physical property analysis. Disk SG (based on green volume and oven-dry weight) and disk MC (based on green and oven-dry weights) were determined for each sampling height. Stand averages (at each height) for disk SG and MC were calculated using the three trees sampled per stand. A summary of average stand characteristics for each region is presented in Table 3.1. Plots of stand average disk SG and MC with relative height are presented in Figures 3.1 and 3.2.

**MODEL DEVELOPMENT**

Two response components are considered in this simultaneous model system, disk SG and MC measured at the same heights for 3 trees in a stand. The basic models adopted for these two components are

\[
SG = f_1(x, \beta) = \beta_{0,1} + \beta_{1,1}x + \beta_{2,1}x^2 + \beta_{3,1}(a_{1,1} - x)^2 + \epsilon_{SG} \\
MC = f_2(x, \beta) = \beta_{0,2} + \beta_{1,2}x + \beta_{2,2}(a_{1,2} - x)^2 + \epsilon_{MC}
\]

where \(SG = \text{disk SG}; MC = \text{disk MC}; x = \text{relative height} \ h/H, \ h \text{ is the average height above ground and } H \text{ is the average total height of the stand calculated from the three sampled trees}; \)

\[
[\beta_{0,1}, \beta_{1,1}, \beta_{2,1}, \beta_{0,2}, \beta_{1,2}, \beta_{2,2}, a_{1,1}, a_{2,1}, a_{1,2}, a_{2,1}, a_{1,2}]^T
\]

are parameters to be estimated, with knot parameters \([1 > \alpha_{1,1} > \alpha_{2,1} > 0] \text{ and } [1 > \alpha_{1,2} > 0]\); \(\epsilon_{SG} \text{ and } \epsilon_{MC}\) are error terms for disk SG and MC respectively.

The \((\alpha_j - x)^2\) terms indicates the positive part of the function \(\alpha_j - x\) where “+” sets it to zero for those values of \(x\) where \(\alpha_j - x\) is negative (here \(x > \alpha_j\)). The basic model form for disk SG is equivalent to the standard form of the taper model proposed by Max and Burkhart (1976), which is not constrained to have a value of zero at the tip of the tree.

In order to account for stand-to-stand variability in the data, we used a nonlinear mixed effect model (NLMM). Let \(y_{ijk}\) represent the \(k^{th}\) response \((k = 1, 2)\) variable measured at \(j^{th}\) relative height from \(i^{th}\) stand; the univariate nonlinear mixed model for each property can be represented as

\[
y_{i\cdot k} = \theta_{0,i} + \theta_{1,i}x_i + \theta_{2,i}x^2_i + \theta_{3,i}(a_{1,i} - x_i)^2 + \epsilon_{y_{i\cdot k}} \quad [3]
\]

\[
y_{i\cdot k} = \theta_{0,i} + \theta_{1,i}x_i + \theta_{2,i}(a_{1,i} - x_i)^2 + \epsilon_{y_{i\cdot k}} \quad [4]
\]

The mixed effect parameter \(\theta_{y_{i\cdot k}}\) in the above models takes the form

\[
\theta_{y_{i\cdot k}} = A_{i\cdot k}\beta_{y_{i\cdot k}} + B_{i\cdot k}b_{i\cdot k}\]

where \(b_{i\cdot k}\) is the \(i^{th}\) stand level random effect vector specific to the \(k^{th}\) response variable with \(b_{i\cdot k} \sim N(0, \Psi_{y_{i\cdot k}})\); \(B_{i\cdot k}\) is the associated random effect design matrix; \(A_{i\cdot k}\) is the fixed effect design matrix and \(\beta_{y_{i\cdot k}}\) is the fixed effect parameter vector specific to the \(k^{th}\) response variable.

In order to develop the bivariate model, we first fitted the univariate stand level NLMM’s model for disk SG (Eq. 3) and MC (Eq. 4) separately. Initially we assumed all the parameters in the univariate models were mixed. Final specification of mixed effect parameters in the univariate models were decided based on Akaike’s Information Criteria (AIC), a model selection criterion used for NLMM’s. Parameters \(\beta_{0,j1}, \beta_{1,1}, \beta_{2,j2}, \beta_{0,j2}\) and \(\beta_{1,2}\) were selected as mixed, with random stand level intercepts in these parameters. The regional variation in mean trend for both properties was incorporated by appropriate fixed effect specification (fixed effect design matrix) for all parameters, except the knot parameters, in both univariate modes. The knot parameters were assumed as common for all regions for both properties. Since we had six distinct physiographical regions in the study, we assumed different fixed effect parameters for each region with the southern Atlantic Coastal Plain as the reference region with all other regions having their own parameters which are...
deviations from the reference region. The final fixed effect specifications for each parameter were identified using univariate models for each property and likelihood ratio test between full model and reduced model. The fixed effect specifications corresponds to all parameters used in the bivariate model are presented in Table 3.2.

The variance-covariance structure for \( \text{var}(b_{i,1}) \) and \( \text{var}(b_{i,2}) \) in the univariate models were selected based on the model selection criteria (AIC and Bayesian information criterion (BIC)). We selected a general positive definite form of variance-covariance structure for disk SG and a diagonal form of variance-covariance structure for disk MC. The model information criteria and log likelihood values for the final selected univariate models, called SG1 and MC1 respectively for each response, are presented in Table 3.3.

For fitting the bivariate model, the univariate model equations for two responses were stacked together and can be represented as

\[
y_i = f(x_{ij}, \theta) + \epsilon_{ij}
\]

where \( y_{ij} = (y_{ij1}, y_{ij2}) \). To take account of the correlation between responses measured from the same stand at the same height level, we assumed the within stand variance-covariance matrix as

\[
e_{ij} \sim N(0, \sigma^2 \Lambda)
\]

where \( e_{ij} = (e_{ij1}, e_{ij2}) \). Following Eq. 5, after stacking the fixed effect and random effect vectors and design matrices for two response variables, we can write \( \theta_i = (\theta_{i1}, \theta_{i2}) \) as

\[
\theta_i = A_i \beta + B_i b_i
\]

where \( A_i = \text{diag}(A_{i1}, A_{i2}) \); \( B_i = \text{diag}(B_{i1}, B_{i2}) \);

\[
\beta = (\beta_1^T, \beta_2^T)^T; b_i = (b_{i1}^T, b_{i2}^T)^T
\]

and we assumed that \( b_{i1,2} \sim N(0, \Lambda) \).

All the models were fitted using the nlme package in R, version 2.9.1 (Pinheiro et al. 2009). Initially the two univariate models (Eq. [3] and [4]) were simultaneously fitted, referred to as SGMC1, with a positive definite form of variance-covariance structure for disk SG, a diagonal form of variance-covariance structure for disk MC and unique variance parameter estimate for each response variable. Here, a block-diagonal form was used to define the random effect structure of two responses as follows

\[
\Psi = \begin{pmatrix}
\text{var}(b_{1,1}) & 0 \\
0 & \text{var}(b_{2,1})
\end{pmatrix}
\]

The advantage of multivariate fitting over univariate fitting is that we can incorporate correlation among errors and random effects associated with different response variables in the model by specifying different forms of \( \Lambda \) and \( \Psi \) (Fang et al. 2001; Hall and Clutter 2004). The contemporaneous correlation between responses was incorporated by relaxing the form of \( \tilde{E} \) from an identity matrix to a symmetric positive definite matrix (referred to as SGMC2). We also allowed for correlation among random effects associated with the two models. The final best fitted model (referred to as SGMC3) is represented as follows

\[
y_{ij1} = \left( \beta_{10,1} + b_{10,1} \right) + \left( \beta_{1f,1} + b_{1f,1} \right) x + \left( \beta_{2f,1} + b_{2f,1} \right) x^2 + \beta_{M,1} \left( \alpha_1 - x \right)^2 + \beta_{M,1} \left( \alpha_2 - x \right)^2 + e_{ij1}
\]

\[
y_{ij2} = \left( \beta_{20,2} + b_{20,2} \right) + \left( \beta_{1f,2} + b_{1f,2} \right) x + \beta_{M,2} \left( \alpha_1 - x \right)^2 + \beta_{M,2} \left( \alpha_2 - x \right)^2 + e_{ij2}
\]

where \( \psi = \begin{pmatrix}
\psi_{00,1} & \psi_{01,1} & \psi_{02,1} & \psi_{00,12} & 0 \\
\psi_{10,1} & \psi_{11,1} & \psi_{12,1} & \psi_{10,12} & 0 \\
\psi_{20,1} & \psi_{21,1} & \psi_{22,1} & \psi_{20,12} & 0 \\
0 & 0 & 0 & \psi_{11,2} & 0
\end{pmatrix} \)

\[
(e_{ij1} e_{ij2})^T \sim N(0, R_i)
\]

where

\[
R_i = \sigma^2 G_i^{1/2} (\Gamma(\rho)) G_i^{1/2} (\delta)
\]

\[
G_i(\delta) = \text{diag}(I, \delta I_2)
\]

\[
\Gamma(\rho) = \begin{pmatrix}
1 & \rho \\
\rho & 1
\end{pmatrix}
\]

In [8] the fixed effect \( \beta_{k,1,2} \) indicates parameter \( \beta \) specific to the \( k \) region specified in Table 3.2 for response variable SG (\( k=1 \)) and for response variable MC (\( k=2 \)).

The random effect \( b_{i,k,k} \) indicates the random effect parameter specific to the \( i \) stand for response variable SG (\( k=1 \)) and for response variable MC (\( k=2 \)).

The model information criteria (AIC and BIC) and log likelihood values from simultaneous fitting of the models (SGMC1, SGMC2 and SGMC3) are presented in Table 3.3. The log likelihood and information criteria from SGMC1 were equal to the sum of log likelihood and information
criteria from univariate fitting $SG_1$ and $MC_1$. Incorporation of contemporaneous correlation into the model ($SGMC_2$) significantly improved the model fitting criteria. The final model $SGMC_3$ found to have a significant improvement in model information criteria over $SGMC_2$. The estimated fixed effect parameter from the final simultaneous model is presented in Table 3.4. The estimated random effect variance-covariance matrix $\Psi$ is

$$
\begin{pmatrix}
0.00074 & -0.00100 & 0.00058 & -0.23368 & 0 \\
0.00335 & -0.00257 & 0.32946 & 0 \\
0.00241 & -0.20459 & 0 \\
121.92 & 0 & 0 \\
284.19 & & & & \\
\end{pmatrix}
$$

and the within stand residual parameters are $\delta = 638.68$ and $\rho = -0.779$.

**PREDICTION**

Our primary objective of developing a simultaneous system is to make predictions. The reported advantage of using a multivariate method over univariate method is its improvement in predictive performance (Fang et al. 2001; Hall and Clutter 2004). The information on contemporaneous correlation among response variables can be potentially utilized to improve the prediction of a variable at a particular measurement occasion (here at a particular stand height level) given that the observed value of other response variables at the specified measurement occasion. For example in the proposed multivariate system, information of disk SG at any specific height can be utilized to improve the prediction of disk MC at that height. Similarly, observed disk MC at any specific stand height can be utilized to improve the prediction of disk SG at that height.

There are several situations where we can utilize a multivariate model to make predictions. Fang et al. (2001) dealt with several such prediction scenarios based on their height-basal area-volume simultaneous mixed model system. In the present study, we are primarily interested in prediction from a multivariate model system where observations on one of the correlated response variables are available. For example, we may want to predict disk MC for a stand at different heights when measurements of disk SG are available. To this extent, we can utilize a predictor proposed by Hall and Clutter (2004) for NLMM’s which is based on a linear mixed model (LMM) approximation of NLMM. The proposed predictor is analogous to the empirical best linear unbiased predictor (BLUP) of LMM. It is supposed to perform better than the plug-in-predictor proposed for NLMM by Pinheiro and Bates (2000). The following on the derivation of a predictor was extracted from Hall and Clutter (2004). Generically a NLMM can be represent as

$$
\delta = f(\beta, b, A, B) + \varepsilon
$$

where $\beta$ is $p \times 1$ vector of fixed effect parameters and $A$ is a corresponding fixed effect design matrix; $b$ is $q \times 1$ vector of random effect parameters and $B$ is a corresponding random effect design matrix; and $\varepsilon$ is $N \times 1$ vector of error term with $\varepsilon \sim \mathcal{N}(0, \sigma^2 A)$.

Taking first-order Taylor series linearization of Eq. [9] around the estimates of $(\hat{\beta}, \hat{b})$ gives

$$
\delta \approx f(\hat{\beta}, \hat{b}, A, B) + \hat{A}(\beta-\hat{\beta}) + \hat{B}(b-\hat{b}) + \varepsilon
$$

where $\hat{A} = \frac{\partial f(\beta, b, A, B)}{\partial \beta}$ and $\hat{B} = \frac{\partial f(\beta, b, A, B)}{\partial b}$.

Now the Eq. 10 can be represented as a LMM on $z = y - f(\hat{\beta}, \hat{b}, A, B) + \hat{A}\beta + \hat{B}b + \varepsilon$ as follows

$$
z = \tilde{A} \beta + \tilde{B} b + \varepsilon
$$

Let us decompose the response vector $\delta = (\delta_s^T, \delta_h^T)$, where $\delta_s$ represents the observed component and $\delta_h$ represents the unobserved component. Accordingly, all other model quantities can be divided as

$$
z = \left( \begin{array}{c} z_s \\ z_h \end{array} \right); \quad \tilde{A} = \left( \begin{array}{c} \tilde{A}_s \\ \tilde{A}_h \end{array} \right); \quad \tilde{B} = \left( \begin{array}{c} \tilde{B}_s \\ \tilde{B}_h \end{array} \right);
$$

and

$$
\mathbf{r}(\hat{\beta}, \hat{b}, A, B) = \left( \begin{array}{c} \mathbf{r}_s(\hat{\beta}, \hat{b}, A_s, B_s) \\ \mathbf{r}_h(\hat{\beta}, \hat{b}, A_h, B_h) \end{array} \right)
$$

Then based on LMM [11], the empirical BLUP of $z_h$ based on $Z_s$ is given as

$$
z_h = \tilde{A}_h \hat{\beta} + \tilde{V}_{hs} \tilde{V}_{ss}^{-1} (z_s - \tilde{A}_s \hat{\beta})
$$

where $\tilde{V} = \tilde{B} \tilde{\var{\varepsilon}} + \varepsilon$, the variance-covariance matrix of $z$ based on LMM approximation [11], which can be decomposed into

$$
\tilde{V} = \left( \begin{array}{cc} \tilde{V}_{ss} & \tilde{V}_{sh} \\ \tilde{V}_{hs} & \tilde{V}_{hh} \end{array} \right)
$$
By rearranging [12] using the relation between \( z \) and \( \hat{\delta} \), we will get our predictor for \( \hat{\delta}_h \) as

\[
\hat{y}_h = f_h(\hat{\beta}, \hat{\delta}_h, A_h, B_h) - B_h \hat{\delta}_h + V_{hs}(y - f(\hat{\beta}, \hat{\delta}_h, A_h, B_h) + B \hat{\delta}_h)
\]  

where \( \text{COV}(\hat{\epsilon}_s, \hat{\epsilon}_h) \neq 0 \), the predictor specified in Eq. [13] takes account of this dependence through \( V_{hs} \). However, when \( \text{COV}(\hat{\epsilon}_s, \hat{\epsilon}_h) = 0 \), \( \hat{\delta}_s \) and \( \hat{\delta}_h \) are correlated only through the shared random effects and is best approximated by the plug-in-predictor

\[
y_h = f_h(\hat{\beta}, \hat{\delta}_h, A_h, B_h).
\]

Since we are interested in predicting the value of one response variable using data where another response variable is available or measured at the same height from the same stand, we expect that the predictor [13] performs better than the plug-in-predictor.

In order to evaluate the predictive performance of the fitted multivariate model, we randomly selected data from 25 stands. We created a new data set with data from the 25 selected stands excluded (apart from data measured at relative heights equivalent to heights of 1.37 m and 13.7 m to get the estimate of random effect while fitting) and refitted the final model SGMC3 to this new data. We made predictions based on [13] for both disk SG and MC for the selected 25 stands that were not used for model fitting. Disk SG was predicted for the 25 excluded stands assuming that disk MC measurements were available for all heights and stands. The same assumption was made for disk SG when disk MC was predicted for the excluded stands.

Plots showing the univariate plug-in-prediction, multivariate plug-in-prediction and multivariate improved prediction (based on Eq. [13]) of disk SG and MC for 5 stands randomly selected from the excluded 25 are presented in Figure 3.3 and 3.4. We can see from the figures that additional information for one response variable significantly improved the prediction of the other response variable using Eq. [13] compared to the plug-in-predictors. The curves are closer to their observed values for both disk SG and MC using the Eq. [13] predictor. Table 3.5, presents the root mean square prediction error (RMSPE) for the three prediction methods based on predictions of SG and MC for trees from the 25 excluded stands. Prediction from multivariate approaches, both plug-in-predictor and Eq. [13], was considerably better than those of the univariate approach. Prediction based in Eq. [13] were improved by 29 (SG) and 26 % (MC) (Table 3.5).

**DISCUSSION**

Nonlinear mixed models are an important tool for modeling and predicting growth and wood quality attributes in forestry (Fang 1999; Hall and Bailey 2001; Jordan et al. 2008; Jordan et al. 2006). Univariate mixed models were commonly used in forestry to model different growth and wood properties. Compared to conventional methods univariate mixed models provide improved predictions because of their ability to capture different levels of variability within the data, e.g. variability from stand-to-stand, plot-to-plot and tree-to-tree (Fang et al. 2001) through random effects in the models. In addition to variability observed at different levels of the data, individual components (properties) measured from a forest are usually inter-dependent. The simultaneous modeling technique can take account of the inter-dependency in a system through random effects and the inter-dependency among different components in the system through contemporaneous correlation.

In this article, we proposed a multivariate simultaneous mixed model for stand average disk SG and MC at different tree heights. We observed a high correlation (-0.78) between two components in our system. The inverse relation between SG and MC was identified by Koch (1972), Zobel and Blair (1976) and Zobel and van Buijtenen (1989). Various explanations have been proposed for the inverse relation between SG and MC within trees such as the amount of heartwood, the presence of extractives and the proportion of juvenile wood. According to Zobel and Blair (1976), the dominant factor controlling SG and MC variation within a loblolly pine tree is the proportion of juvenile wood and the proportion of juvenile wood increases longitudinally from stump-to-tip of loblolly pine trees.

The advantage of multivariate simultaneous systems is their improvement in prediction in one component given the other components in the system (Fang et al. 2001; Hall and Clutter 2004). Based on this study, we found a significant improvement in prediction for both properties, approximately 29 and 26 percent reduction in RMSPE for both disk SG and MC respectively, based on the simultaneous system after taking account of the contemporaneous correlation between the components. The multivariate plug-in-predictor improved by 5 and 11 percent in RMSPE compared to univariate approach for both disk SG and MC respectively. This clearly indicates the potential of multivariate model fitting over univariate approach. Operationally, the proposed system can be used to improve the prediction of stand disk SG at different height levels using the measured disk MC using non-destructive sampling methods.

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