How to quantify nutrient export: Additive Biomass functions for spruce fit with Nonlinear Seemingly Unrelated Regression

IBS-DR Biometry Workshop, Würzburg

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1. Introduction

2. data

3. methods applied
   • Nonlinear Seemingly Unrelated Regression

4. results
   • NSUR fit
   • comparison

5. Discussion
EnNa: Energywood and sustainability (funded by FNR)

- harvesting removes wood (i.e., C) and also nutrients (Ca, K, Mg, P, . . .)

→ sustainability required regarding C and also Ca, K, Mg, P, . . .

- nutrient balance:

\[
NB = \left( VW + DP - SI \right) - HV \\
\text{soil}
\]

\[
HV = \sum \text{trees} = \sum \text{compartments}
\]

- nutrient concentration differs within different compartments

→ compartment-specific biomass functions required
collected data

- spruce (*Picea abies*)
- 6 data compilations (incl. Wirth et al., 2004)
- homogenisation
- stump/B coarse wood/B small wood needles
- ≈ 1200 trees

(only referenced shown; +CH|DK|B)
## Overview of collected data

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Number of data sets:

- dbh [cm]
- height [m]
- aboveground biomass [kg]
general methodological design

- wanted: biomass functions for all compartments, and the total mass
- maintain additivity (see Parresol, 2001)

1. $BM_{total} = \sum BM_{comp}$
   with $var(\hat{y}_{total}) = \sum_{i=1}^{c} var(\hat{y}_i) + 2 \sum \sum_{i<j} cov(\hat{y}_i, \hat{y}_j)$

2. Nonlinear Seemingly Unrelated Regression (NSUR)
general methodological design

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- Nonlinear Seemingly Unrelated Regression (NSUR)

- NSUR requires rectangular data set (i.e. no NA's)
- but some of the studies contain NA's
  - complete case
  - imputation
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2. Nonlinear Seemingly Unrelated Regression (NSUR)

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linear SUR-Regression, see Zellner (1962):

\[ y_{\text{sur}} = X\beta + \epsilon \quad \text{with} \quad \epsilon \sim N(0, \Sigma_c \otimes I_N) \quad (1) \]

with the stacked column vectors \( y_{\text{sur}} = [y'_1 \ y'_2 \ \cdots \ y'_m]' \), \( \beta = [\beta'_1 \ \beta'_2 \ \cdots \ \beta'_m]' \) and error term \( \epsilon = [\epsilon'_1 \ \epsilon'_2 \ \cdots \ \epsilon'_m]' \).

The design matrix \( X \) now is blockdiagonal:

\[
X = \begin{bmatrix}
X_1 & 0 & \cdots & 0 \\
0 & X_2 & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & X_M
\end{bmatrix}
\]

where \( N=\text{number of Observation} \), \( M=\text{number of equations} \).
the variance-covariance matrix of the errors is:

\[
\Sigma = \Sigma_c \otimes I_N = \begin{bmatrix}
\sigma_{11} & \sigma_{12} & \cdots & \sigma_{1M} \\
\sigma_{21} & \sigma_{22} & \cdots & \sigma_{2M} \\
\vdots & \vdots & \ddots & \vdots \\
\sigma_{M1} & \sigma_{M2} & \cdots & \sigma_{MM}
\end{bmatrix} \otimes I_N
\]

Zellner (1962, S. 350) and Rossi et al. (2005, S. 66):
„In a formal sense, we regard (1) as a single-equation regression model [. . .]“. „Given \( \Sigma \), we can transform (1) into a system with uncorrelated errors“ [. . .] „by a matrix \( H \), so that \( E(H \epsilon \epsilon' H') = H \Sigma H' = I \).“ „This means that, if we premultiply both sides of (1) by \([H]\), the transformed system has uncorrelated errors“.
the resulting model fulfills the LS-assumptions and the LS-estimator is (Zellner, 1962):

\[
\hat{\beta}_{\text{sur}} = (X' H' H X)^{-1} X' H' H y = (X' \Sigma^{-1} X)^{-1} X' \Sigma^{-1} y \quad (3)
\]

where the covariance matrix of the estimator is:

\[
\text{Var}(\beta) = (X' \Sigma^{-1} X)^{-1} \quad (4)
\]

where

\[
\Sigma^{-1} = \Sigma_c^{-1} \otimes I \quad (5)
\]

BUT: \( \Sigma \) is not known and must be estimated from the data.
in the non-linear case, the model is (see Parresol, 2001): 

\[ y_{nsur} = f(X, \beta) + \epsilon \quad \text{mit} \quad \epsilon \sim N(0, \Sigma \otimes I_N) \]  

(6)

with the stacked column vectors 

\[ y_{nsur} = [y'_1 \, y'_2 \ldots y'_m]', \]

\[ f = [f'_1 \, f'_2 \ldots f'_m]', \]

and error term 

\[ \epsilon = [\epsilon'_1 \, \epsilon'_2 \ldots \epsilon'_m]' . \]

if a weighted regression is needed (as in this case):

\[ \Psi(\theta) = \begin{bmatrix} 
\Psi_1(\theta_1) & 0 & \cdots & 0 \\
0 & \Psi_2(\theta_2) & \cdots & 0 \\
\vdots & \vdots & & \vdots \\
0 & 0 & \cdots & \Psi_M(\theta_M) 
\end{bmatrix} \]  

(7)
weighted nonlinear seemingly unrelated regression II

Considering a univariate gnls, the estimated parameter vector minimises the (weighted) sum of squares of the residuals

\[ S(\beta) = \epsilon' \Psi^{-1} \epsilon = [Y - f(X, \beta)]' \Psi^{-1} [Y - f(X, \beta)] \quad (8) \]

with weights-matrix \( \Psi \).

In the NSUR-model, this term is updated to:

\[ S(\beta) = \epsilon' \Delta' (\Sigma^{-1} \otimes I) \Delta \epsilon \]
\[ = [Y - f(X, \beta)]' \Delta' (\Sigma^{-1} \otimes I) \Delta [Y - f(X, \beta)] \quad (9) \]

where \( \Delta = \sqrt{\Psi^{-1}} \) and \( \Sigma \) (still) not known.

Parresol (2001) estimates \( \Sigma \) from the residuals of an univariate gnls-fit \((i, j)\):

\[ \sigma_{ij} = \frac{1}{\sqrt{N - K_i} \sqrt{N - K_j}} \epsilon_i \hat{\Delta}_i' \hat{\Delta}_j \epsilon_j \quad (10) \]
weighted nonlinear seemingly unrelated regression III

to estimate $\beta$, we can use the Gauss-Newton-Minimisation method (Parresol, 2001):

$$
\beta_{n+1} = \beta_n + l_n \cdot [F(\beta_n)' \hat{\Delta}'(\hat{\Sigma}^{-1} \otimes I) \hat{\Delta} F(\beta_n)]^{-1} F(\beta_n)' \hat{\Delta}'(\hat{\Sigma}^{-1} \otimes I) \hat{\Delta} [y - f(X, \beta_n)]
$$

(11)

where $F(\beta_n)$ is the jacobian.

the covariance-matrix of the parameter estimates is:

$$
\hat{\Sigma}_b = [F(\beta_n)' \hat{\Delta}'(\hat{\Sigma}^{-1} \otimes I) \hat{\Delta} F(\beta_n)]^{-1}
$$

(12)

and the NSUR-system-variance is:

$$
\hat{\sigma}^2_{NSUR} = \frac{S(b)}{MN - K}
$$

(13)
wait, what about study-effects?

\[
y_{\text{corr}} = y_{\text{obs}} - (f(A\beta, \nu) - f(A\beta, \nu))
\]

**Methods**

- **Data**
- **Results**
- **Discussion**
- **Literature**

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### Data

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### NLME-Fit

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### Gnls-Fit

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wait, what about study-effects?

**gnls cannot model random effects**

- and hence, the NSUR-code can’t as well
- but we are not interested in these anyway...
wait, what about study-effects?

gnls cannot model random effects

- and hence, the NSUR-code can’t as well
- but we are not interested in these anyway…

\[ y_{corr} = y_{obs} - \left( f(A\beta + Bb, \nu) - f(A\beta, \nu) \right) \]

fixed + random effects \quad fixed effects

raw data  nlme-fit  gnls-fit
effect on biomass data

Comparison of glns-, nlme- and glns/nlme-full-model for coarse wood mass
NSUR step-by-step

**NSUR procedure**

1. fit nlme-model with *Study* as grouping variable
2. remove difference between fixed-effects and random-effects
3. fit an univariate, unweighted nls-model
4. deduce weights for the summary compartment
5. fit weighted gnls-model
6. estimate $\Sigma$ from weighted residuals
7. fit NSUR-model using $\Sigma$ and weights from univariate fits
results for spruce

how the model looks like

- **stump**: \( a_{11} \cdot \text{dbh}^{a_{12}} \cdot \text{stumph}^{a_{13}} \cdot \text{age}^{a_{14}} \cdot \text{hsl}^{a_{15}} \)
- **stumpB**: \( a_{21} + a_{22} \cdot \text{dbh}^{a_{23}} \cdot \text{stumph}^{a_{24}} \cdot \text{height}^{a_{25}} \)
- **cw**: \( a_{31} \cdot \text{dbh}^{a_{32}} \cdot \text{height}^{a_{33}} \cdot D_03^{a_{34}} \cdot \text{age}^{a_{35}} \)
- **cwB**: \( a_{41} \cdot \text{dbh}^{a_{42}} \cdot \text{height}^{a_{43}} \cdot D_03^{a_{44}} \cdot \text{age}^{a_{45}} \cdot \text{hsl}^{a_{46}} \)
- **sw**: \( a_{51} + a_{52} \cdot \text{dbh}^{a_{53}} \cdot \text{height}^{a_{54}} \cdot D_03^{a_{55}} \cdot cl^{a_{56}} \)
- **needles**: \( a_{61} + a_{62} \cdot \text{dbh}^{a_{63}} \cdot \text{height}^{a_{64}} \cdot D_03^{a_{65}} \cdot \text{age}^{a_{66}} \cdot \text{hsl}^{a_{67}} \cdot cl^{a_{68}} \)

**totalBM**: \( \text{stump} + \text{stumpB} + \text{cw} + \text{cwB} + \text{sw} + \text{needles} \)
results for spruce

how the model looks like

\[
\text{stump} \quad a_{11} \cdot \text{dbh}^{a_{12}} \cdot \text{stumph}^{a_{13}} \cdot \text{age}^{a_{14}} \cdot \text{hsl}^{a_{15}}
\]
\[
\text{stumpB} \quad a_{21} + a_{22} \cdot \text{dbh}^{a_{23}} \cdot \text{stumph}^{a_{24}} \cdot \text{height}^{a_{25}}
\]
\[
\text{cw} \quad a_{31} \cdot \text{dbh}^{a_{32}} \cdot \text{height}^{a_{33}} \cdot D_{03}^{a_{34}} \cdot \text{age}^{a_{35}}
\]
\[
\text{cwB} \quad a_{41} \cdot \text{dbh}^{a_{42}} \cdot \text{height}^{a_{43}} \cdot D_{03}^{a_{44}} \cdot \text{age}^{a_{45}} \cdot \text{hsl}^{a_{46}}
\]
\[
\text{sw} \quad a_{51} + a_{52} \cdot \text{dbh}^{a_{53}} \cdot \text{height}^{a_{54}} \cdot D_{03}^{a_{55}} \cdot cl^{a_{56}}
\]
\[
\text{needles} \quad a_{61} + a_{62} \cdot \text{dbh}^{a_{63}} \cdot \text{height}^{a_{64}} \cdot D_{03}^{a_{65}} \cdot \text{age}^{a_{66}} \cdot \text{hsl}^{a_{67}} \cdot cl^{a_{68}}
\]
\[
\text{totalBM} \quad \text{stump} + \text{stumpB} + \text{cw} + \text{cwB} + \text{sw} + \text{needles}
\]

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observed and fitted

- **Stock**
- **Stockrinde**
- **DerbGesamt**
- **DerbGesamtRinde**
- **NichtDerbmitRinde**
- **Nadeln**
- **oiBT**
effect of random-effects-correction
confidence intervals

- Stump
- Stump bark
- Coarse wood
- Coarse wood bark
- Small wood
- Needles
- Total wood
comparison to NFI3
comparison to Wirth et al. 2004

coarse wood + B

each wood + B
dbh

small wood

needles

mfull

Wirth et al. 2004
NSUR-Method

- additivity maintained
- study effect included
- seem to be comparable to NFI-results
- comparability to Wirth et al. (2004) limited
NSUR-Method

- additivity maintained
- study effect included
- seem to be comparable to NFI-results
- comparability to Wirth et al. (2004) limited
- prediction intervals not yet set up
- confidence & prediction intervals for univariate functions
- differences to Wirth still to be evaluated
THANK YOU!
THANK YOU!

- mixed effects correction OK
- NSUR-method sensible
- any other suggestions


