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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what it is about

- EnNa: Energywood and sustainability (funded by FNR)
- havesting removes wood (i. e. C) and also nutrients (Ca, K, Mg, P, ...)

$\rightarrow$ sustainability required regaring C and also Ca, K, Mg, P, ...

- nutrient balance:

$$NB = \underbrace{VW + DP - SI}_{soil} - HV$$

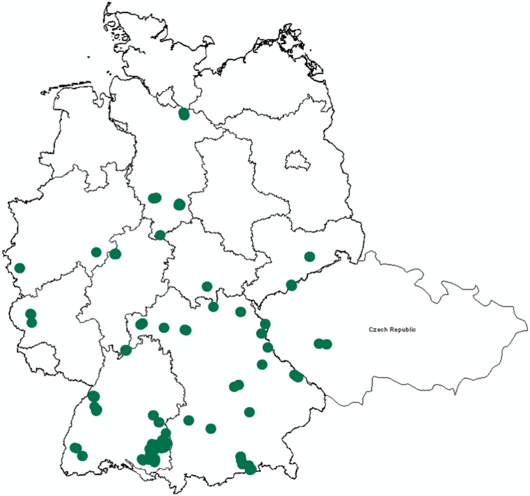
$$HV = \sum trees = \sum compartments$$

- nutrient concentration differs within different compartments

$\rightarrow$ compartment-specific biomass functions required

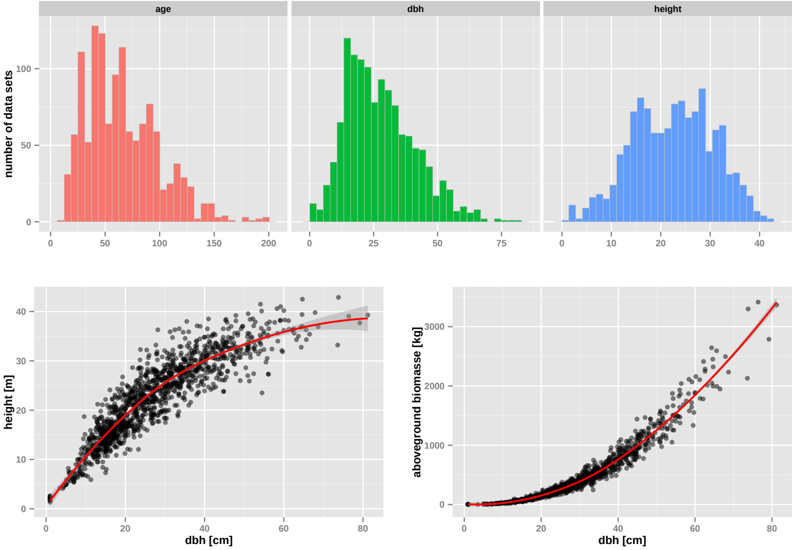
collected data

- 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



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)

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- but some of the studies contain NA's
  - complete case
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SUR: seemingly-unrelated regression I

linear SUR-Regression, see Zellner (1962):

$$\boldsymbol{y_{sur}} = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{\epsilon} \qquad \text{with} \qquad \boldsymbol{\epsilon} \sim N(0, \boldsymbol{\Sigma_c} \otimes \boldsymbol{I}_N) \tag{1}$$

with the stacked column vectors $\boldsymbol{y_{sur}} = [\boldsymbol{y_1' y_2'} \cdots \boldsymbol{y_m'}]'$, $\boldsymbol{\beta} = [\boldsymbol{\beta_1' \beta_2'} \cdots \boldsymbol{\beta_m'}]'$ and error term $\boldsymbol{\epsilon} = [\boldsymbol{\epsilon_1' \epsilon_2'} \cdots \boldsymbol{\epsilon_m'}]'$.
The design matrix $\boldsymbol{X}$ now is blockdiagonal:

$$\boldsymbol{X} = \begin{bmatrix} \boldsymbol{X_1} & 0 & \cdots & 0 \\ 0 & \boldsymbol{X_2} & \cdots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & \boldsymbol{X}_M \end{bmatrix}$$

where N=number of Observation, M=number of equations

SUR: seemingly-unrelated regression II

the variance-covariance matrix of the errors is:

$$\boldsymbol{\Sigma} = \boldsymbol{\Sigma_c} \otimes \boldsymbol{I_N} = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \cdots & \sigma_{1M} \\ \sigma_{21} & \sigma_{22} & \cdots & \sigma_{2M} \\ \vdots & \vdots & & \vdots \\ \sigma_{M1} & \sigma_{M2} & \cdots & \sigma_{MM} \end{bmatrix} \otimes \boldsymbol{I}_N \qquad (2)$$

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 $\boldsymbol{\Sigma}$, we can transform (1) into a system with uncorrelated errors“ [. . .] „by a matrix $\boldsymbol{H}$, so that $E(\boldsymbol{H}\boldsymbol{\epsilon}\boldsymbol{\epsilon}'\boldsymbol{H}') = \boldsymbol{H}\boldsymbol{\Sigma}\boldsymbol{H}' = \boldsymbol{I}$.“ „This means that, if we premultiply both sides of (1) by $[\boldsymbol{H}]$, the transformed system has uncorrelated errors“.

SUR: seemingly-unrelated regression III

the resulting model fulfills the LS-assumptions and the LS-estimator is (Zellner, 1962):

$$\hat{\beta}_{sur} = (\boldsymbol{X}'\boldsymbol{H}'\boldsymbol{H}\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{H}'\boldsymbol{H}\boldsymbol{y} = (\boldsymbol{X}'\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{\Sigma}^{-1}\boldsymbol{y} \tag{3}$$

where the covariance matrix of the estimator is:

$$Var(\boldsymbol{\beta}) = (\boldsymbol{X}'\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1} \tag{4}$$

where

$$\boldsymbol{\Sigma}^{-1} = \boldsymbol{\Sigma}_{\boldsymbol{c}}^{-1} \otimes \boldsymbol{I} \tag{5}$$

BUT: $\boldsymbol{\Sigma}$ is not known and must be estimated from the data.

weighted nonlinear seemingly unrelated regression I

in the non-linear case, the model is (see Parresol, 2001):

$$\boldsymbol{y}_{nsur} = \boldsymbol{f}(\boldsymbol{X}, \boldsymbol{\beta}) + \boldsymbol{\epsilon} \qquad \text{mit} \qquad \boldsymbol{\epsilon} \sim N(0, \boldsymbol{\Sigma} \otimes \boldsymbol{I}_N) \tag{6}$$

with the stacked column vectors $\boldsymbol{y}_{nsur} = [\boldsymbol{y}_1' \boldsymbol{y}_2' \cdots \boldsymbol{y}_m']'$, $\boldsymbol{f} = [\boldsymbol{f}_1' \boldsymbol{f}_2' \cdots \boldsymbol{f}_m']'$ and error term $\boldsymbol{\epsilon} = [\boldsymbol{\epsilon}_1' \boldsymbol{\epsilon}_2' \cdots \boldsymbol{\epsilon}_m']'$.
if a weighted regression is needed (as in this case):

$$\boldsymbol{\Psi}(\boldsymbol{\theta}) = \begin{bmatrix} \boldsymbol{\Psi}_1(\boldsymbol{\theta}_1) & \boldsymbol{0} & \cdots & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{\Psi}_2(\boldsymbol{\theta}_2) & \cdots & \boldsymbol{0} \\ \vdots & \vdots & & \vdots \\ \boldsymbol{0} & \boldsymbol{0} & \cdots & \boldsymbol{\Psi}_M(\boldsymbol{\theta}_M) \end{bmatrix} \tag{7}$$

weighted nonlinear seemingly unrelated regression II

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

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

with weights-matix $\boldsymbol{\Psi}$.
In the NSUR-model, this term is updated to:

$$\begin{aligned} S(\boldsymbol{\beta}) &= \boldsymbol{\epsilon}'\boldsymbol{\Delta}'(\boldsymbol{\Sigma}^{-1} \otimes \boldsymbol{I})\boldsymbol{\Delta}\boldsymbol{\epsilon} \\ &= [\boldsymbol{Y} - \boldsymbol{f}(\boldsymbol{X}, \boldsymbol{\beta})]'\boldsymbol{\Delta}'(\boldsymbol{\Sigma}^{-1} \otimes \boldsymbol{I})\boldsymbol{\Delta}[\boldsymbol{Y} - \boldsymbol{f}(\boldsymbol{X}, \boldsymbol{\beta})] \end{aligned} \tag{9}$$

where $\boldsymbol{\Delta} = \sqrt{\boldsymbol{\Psi}^{-1}}$ and $\boldsymbol{\Sigma}$ (still) not known.
Parresol (2001) estimates $\boldsymbol{\Sigma}$ from the residuals of an univariate gnls-fit (i, j):

$$\sigma_{ij} = \frac{1}{\sqrt{N - K_i}\sqrt{N - K_j}}\boldsymbol{\epsilon}_i\hat{\boldsymbol{\Delta}}_i'\hat{\boldsymbol{\Delta}}_j\boldsymbol{\epsilon}_j \tag{10}$$

weighted nonlinear seemingly unrelated regression III

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

$$\begin{aligned}\boldsymbol{\beta_{n+1}} = \boldsymbol{\beta_n} + l_n \cdot [\boldsymbol{F}(\boldsymbol{\beta_n})'\hat{\boldsymbol{\Delta}}'(\hat{\boldsymbol{\Sigma}}^{\boldsymbol{-1}} \otimes \boldsymbol{I})\hat{\boldsymbol{\Delta}}\boldsymbol{F}(\boldsymbol{\beta_n})]^{-1} \\ \boldsymbol{F}(\boldsymbol{\beta_n})'\hat{\boldsymbol{\Delta}}'(\hat{\boldsymbol{\Sigma}}^{\boldsymbol{-1}} \otimes \boldsymbol{I})\hat{\boldsymbol{\Delta}}[\boldsymbol{y} - \boldsymbol{f}(\boldsymbol{X}, \boldsymbol{\beta_n})]\end{aligned} \tag{11}$$

where $\boldsymbol{F}(\boldsymbol{\beta_n})$ is the jacobian.
the covariance-matrix of the parameter estimates is:

$$\hat{\boldsymbol{\Sigma}}_{\boldsymbol{b}} = [\boldsymbol{F}(\boldsymbol{\beta_n})'\hat{\boldsymbol{\Delta}}'(\hat{\boldsymbol{\Sigma}}^{\boldsymbol{-1}} \otimes \boldsymbol{I})\hat{\boldsymbol{\Delta}}\boldsymbol{F}(\boldsymbol{\beta_n})]^{-1} \tag{12}$$

and the NSUR-system-variance is:

$$\hat{\sigma}^2_{NSUR} = \frac{S(\boldsymbol{b})}{MN - K} \tag{13}$$

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

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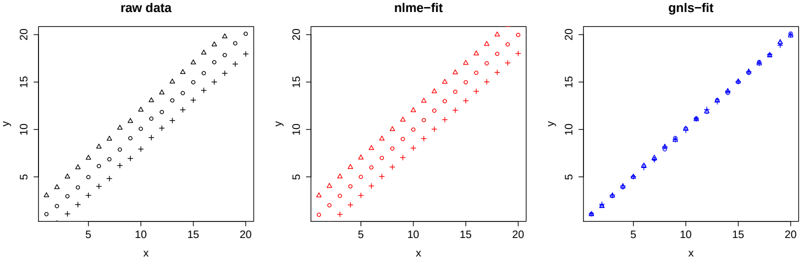
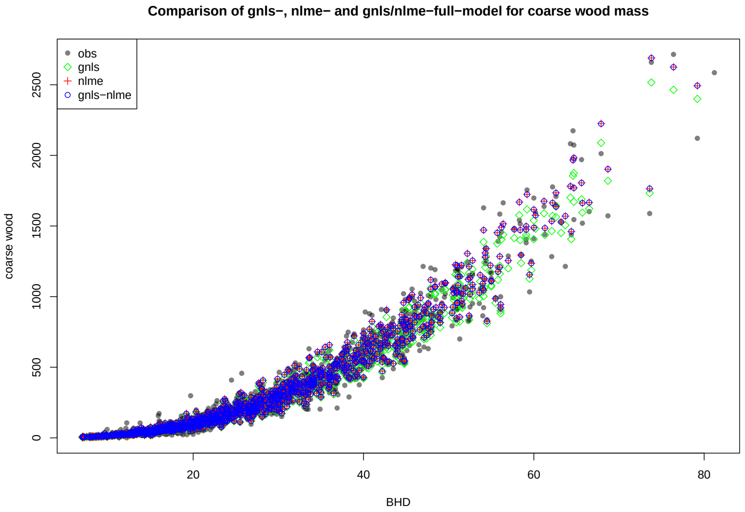
- but we are not interested in these anyway...
- $$y_{corr} = y_{obs} - \big(\underbrace{f(\boldsymbol{A\beta} + \boldsymbol{Bb}, \nu)}_{\text{fixed+random effects}} - \underbrace{f(\boldsymbol{A\beta}, \nu)}_{\text{fixed effects}}\big)$$



effect on biomass data



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 Σ from weighted residuals
7. fit NSUR-model using Σ and weights from univariate fits

results for spruce

how the model looks like

stump	$a11 \cdot dbh^{a12} \cdot stumph^{a13} \cdot age^{a14} \cdot hsl^{a15}$
stumpB	$a21 + a22 \cdot dbh^{a23} \cdot stumph^{a24} \cdot height^{a25}$
cw	$a31 \cdot dbh^{a32} \cdot height^{a33} \cdot D03^{a34} \cdot age^{a35}$
cwB	$a41 \cdot dbh^{a42} \cdot height^{a43} \cdot D03^{a44} \cdot age^{a45} \cdot hsl^{a46}$
sw	$a51 + a52 \cdot dbh^{a53} \cdot height^{a54} \cdot D03^{a55} \cdot cl^{a56}$
needles	$a61 + a62 \cdot dbh^{a63} \cdot height^{a64} \cdot D03^{a65} \cdot age^{a66} \cdot hsl^{a67} \cdot cl^{a68}$
totalBM	$stump + stumpB + cw + cwB + sw + needles$

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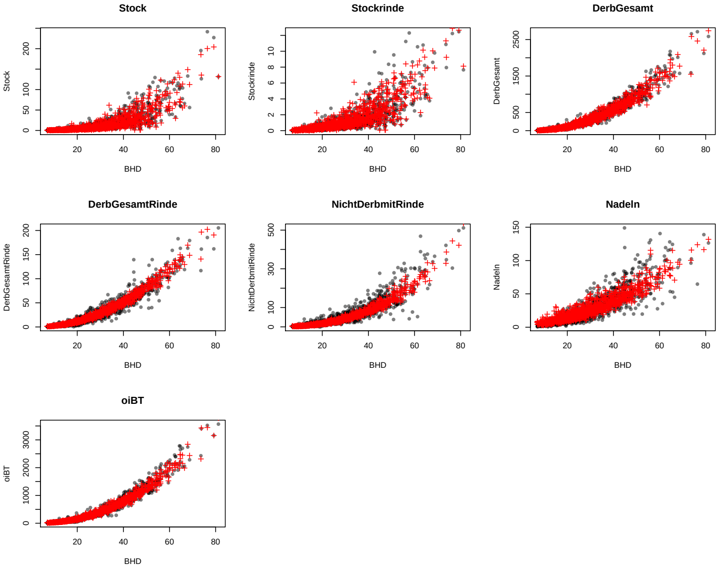
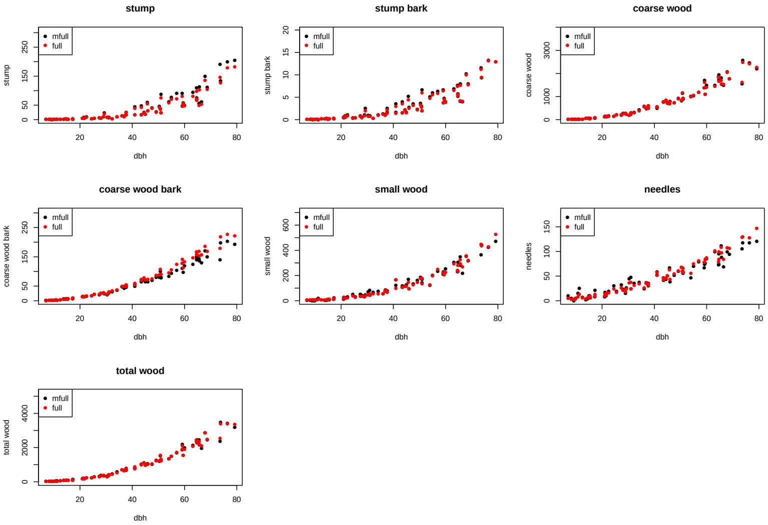
eqn	stump	stumpB	cw	cwB	sw	needles	totalBM
r2	0.919	0.874	0.976	0.948	0.866	0.802	0.977

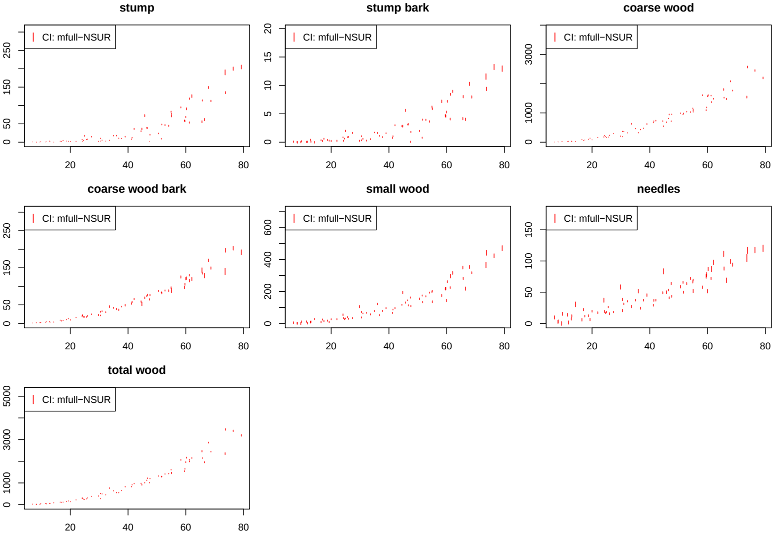
observed and fitted



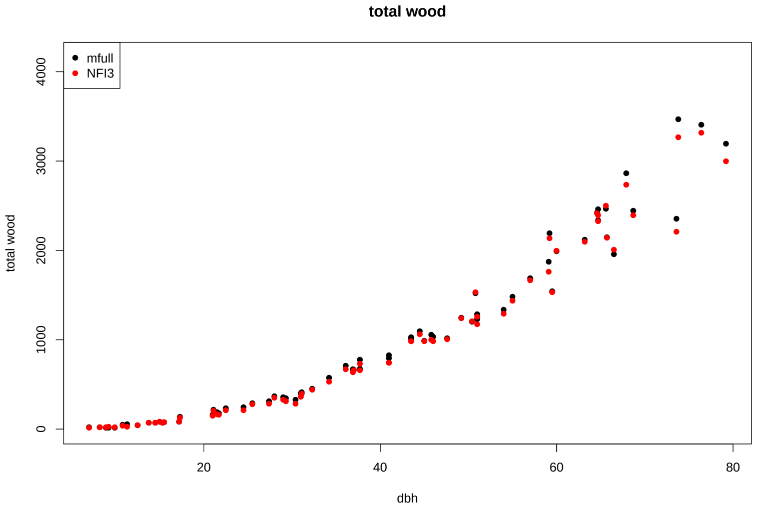
effect of random-effects-correction



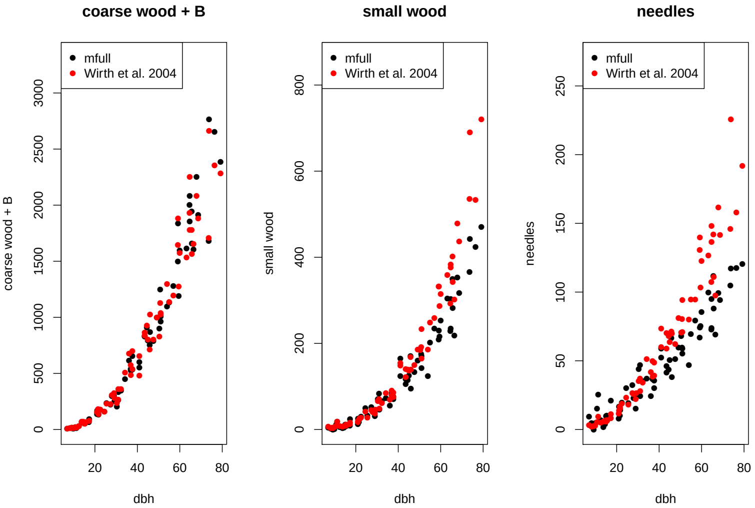
confidence intervals



comparison to NFI3



comparison to 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

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- prediction intervals not yet set up
- confidence & prediction intervals for univariate functions
- differences to Wirth still to be evaluated

THANK YOU!

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

Joosten, R., Schumacher, J., Wirth, C., Schulte, A., 2004. Evaluating tree carbon predictions for beech (Fagus sylvatica L.) in western Germany. Forest Ecology and Management 189 (1-3), 87–96.

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