Likelihood-based Inference for Mixed Models
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# Branch litter quality and decomposition in drained peatlands predicted by IR spectroscopy.

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**Introduction:**

Branch litter may form a considerable proportion of organic matter inputs to the soil in forest ecosystems. Yet, we still know very little of the behaviour of this component in the carbon cycle. Inputs may be estimated based on stand biomass, but the decomposition rates have to be measured in the field and for organic quality measurements laboured laboratory methods still need to be applied. Recent research has suggested that IR spectroscopy may be a useful tool in decomposition studies, and in this course project, I will examine its applicability for predicting branch litter decomposition in peatland forests.

We have studied the decomposition of branch litter in three drained (meso-) oligotrophic fen sites forming a climatic gradient from central Estonia to northern Finland. At each site dead branches were harvested from four live Scots pines (the dominant tree species) and divided into two size classes: diameter ≤ 1 cm and diameter > 1 cm. For each tree individual and branch size class, decomposition (mass loss) has been measured separately using the litterbag method; we set up a ten-year experiment with 2-5 replicates per site for annual recovery. The initial chemical composition: the amount of soluble compounds, holocellulose, acid insoluble and acid soluble lignin, was analyzed of each tree and size class using a sequential extraction method.

Different methods of Fourier transform infrared (FT-IR) spectroscopy: DRIFT and transmission in mid-infrared region, were used to explore their potential to predict/explain variability in the chemical composition and mass loss values of the branch litter, and their evolution in time. Predictive equations will be established between the IR spectral data of the initial litter materials, their organic quality and the decomposition rates of the first years.

**Hierarchical structure of the dataset:**

1)
- level 4: site (3)
- level 3: tree (12)
- level 2: branch size class (24)
- level 1: litterbag (118)

2)
- level 4: site (2)
- level 3: tree (8)
- level 2: branch size class (16)
- level 1: litterbag (78)

<u>Explanatory variables (</u>*branch size* level):

- initial chemical quality (% of different carbon fractions: total lignin, holocellulose, total extractives)
- IR absorption spectra (863 absorbance per each spectrum)

Response variables (*litterbag* level):

- decomposition rate for 1 (dataset 1) and 1-3 years (expressed as % of mass remaining after 1st, 2nd and 3rd year)

**Hypothesis testing:**

- IR spectroscopy can distinguish to which site, tree and size class each sample belongs.
- Chemical properties, detectable by IR, are correlated with decomposition rates of litters.
- Litter quality characteristics obtained by IR spectroscopy have better predictive value for the mass loss than the ones obtained by analytical methods.
- DRIFT method (the less laboured one) gives similar or better predictive value for the mass loss than the transmission method.

**Data analysis:**

To reduced the amount of predictors obtained by IR spectroscopy (the number of absorbance per each spectrum) I used Principal Component Analysis ( Statistica for Windows).
Principal components 1, 2, 3 and 4 explained 86.5, 6.5, 3.6 and 1.5% of the spectra variation respectively. They were then used in other data analysis as predictors representing variability in IR spectra of different litter types.
For all the other analysis MLwiN was used.

Two-level model with chemical quality (......

$$\text{massrem\%}_{ij} \sim \mathrm{N}(XB, \Omega)$$
$$\text{massrem\%}_{ij} = \beta_{0ij}\text{cons} + 0{,}963(0{,}758)\text{Tot lig\%}_j + 1{,}399(0{,}719)\text{TE\%}_j + 1{,}203(0{,}349)\text{Holl \%}_j$$
$$\beta_{0ij} = -40{,}977(54{,}430) + u_{0j} + e_{0ij}$$
$$\begin{bmatrix} u_{0j} \end{bmatrix} \sim \mathrm{N}(0,\ \Omega_u)\ :\ \Omega_u = \begin{bmatrix} 9{,}018(3{,}540) \end{bmatrix}$$
$$\begin{bmatrix} e_{0ij} \end{bmatrix} \sim \mathrm{N}(0,\ \Omega_e)\ :\ \Omega_e = \begin{bmatrix} 14{,}937(2{,}201) \end{bmatrix}$$

*-2*loglikelihood(IGLS Deviance)* = 675,473(116 of 116 cases in use)

$$\text{massrem\%}_{ij} \sim \mathrm{N}(XB, \Omega)$$
$$\text{massrem\%}_{ij} = \beta_{0ij}\text{cons} + 0{,}853(0{,}455)\text{Tot lig\%}_j + 0{,}550(0{,}091)\text{Holl \%}_j + -2{,}233(1{,}286)\text{site\_id\_2}_j + -7{,}266(1{,}233)\text{site\_id\_3}_j$$
$$\beta_{0ij} = 19{,}521(22{,}346) + u_{0j} + e_{0ij}$$
$$\begin{bmatrix} u_{0j} \end{bmatrix} \sim \mathrm{N}(0,\ \Omega_u)\ :\ \Omega_u = \begin{bmatrix} 2{,}562(1{,}689) \end{bmatrix}$$
$$\begin{bmatrix} e_{0ij} \end{bmatrix} \sim \mathrm{N}(0,\ \Omega_e)\ :\ \Omega_e = \begin{bmatrix} 14{,}916(2{,}199) \end{bmatrix}$$

*-2*loglikelihood(IGLS Deviance)* = 657,133(116 of 116 cases in use)

$$\text{massrem\%}_{ij} \sim \mathrm{N}(XB, \Omega)$$

$$\text{massrem\%}_{ij} = \beta_{0ij}\text{cons} + 0{,}137(0{,}021)\text{AX1\_ST}_j + -0{,}093(0{,}078)\text{AX2\_ST}_j + 0{,}084(0{,}104)\text{AX3\_ST}_j + -0{,}624(0{,}165)\text{AX4\_ST}_j$$

$$\beta_{0ij} = 86{,}351(0{,}567) + u_{0j} + e_{0ij}$$

$$\left[u_{0j}\right] \sim \mathrm{N}(0,\ \Omega_u) \ : \ \Omega_u = \left[4{,}569(2{,}266)\right]$$

$$\left[e_{0ij}\right] \sim \mathrm{N}(0,\ \Omega_e) \ : \ \Omega_e = \left[14{,}992(2{,}210)\right]$$

*-2*loglikelihood(IGLS Deviance)* = 664,905(116 of 116 cases in use)

$$\text{massrem\%}_{ij} \sim \mathrm{N}(XB, \Omega)$$

$$\text{massrem\%}_{ij} = \beta_{0ij}\text{cons} + 0{,}096(0{,}024)\text{AX1\_ST}_j + -0{,}091(0{,}072)\text{AX2\_ST}_j + 0{,}260(0{,}107)\text{AX3\_ST}_j + -0{,}085(0{,}272)\text{AX4\_ST}_j + 1{,}372(1{,}385)\text{site\_id\_2}_j + -5{,}128(2{,}460)\text{site\_id\_3}_j$$

$$\beta_{0ij} = 87{,}593(1{,}199) + u_{0j} + e_{0ij}$$

$$\left[u_{0j}\right] \sim \mathrm{N}(0,\ \Omega_u) \ : \ \Omega_u = \left[2{,}616(1{,}710)\right]$$

$$\left[e_{0ij}\right] \sim \mathrm{N}(0,\ \Omega_e) \ : \ \Omega_e = \left[14{,}905(2{,}195)\right]$$

*-2*loglikelihood(IGLS Deviance)* = 657,279(116 of 116 cases in use)

$$\text{massrem\%}_{ijk} \sim \mathrm{N}(XB, \Omega)$$

$$\text{massrem\%}_{ijk} = \beta_{0ijk}\text{cons} + -6{,}496(1{,}326)\text{durat\_2}_{jk} + -19{,}555(1{,}326)\text{durat\_3}_{jk} + 0{,}033(0{,}044)\text{AX1\_ST}_k + -0{,}380(0{,}133)\text{AX2\_ST}_k + 0{,}310(0{,}159)\text{AX3\_ST}_k + 0{,}302(0{,}461)\text{AX4\_ST}_k$$

$$\beta_{0ijk} = 89{,}574(1{,}642) + v_{0k} + u_{0jk} + e_{0ijk}$$

$$\left[v_{0k}\right] \sim \mathrm{N}(0,\ \Omega_v) \ : \ \Omega_v = \left[7{,}368(4{,}408)\right]$$

$$\left[u_{0jk}\right] \sim \mathrm{N}(0,\ \Omega_u) \ : \ \Omega_u = \left[5{,}260(3{,}618)\right]$$

$$\left[e_{0ijk}\right] \sim \mathrm{N}(0,\ \Omega_e) \ : \ \Omega_e = \left[42{,}730(4{,}431)\right]$$

*-2*loglikelihood(IGLS Deviance)* = 1580,330(234 of 234 cases in use)

$$\text{massrem\%}_{ijk} \sim \mathrm{N}(XB, \Omega)$$

$$\text{massrem\%}_{ijk} = \beta_{0ijk}\text{cons} + -6{,}495(1{,}239)\text{durat\_2}_{jk} + -19{,}576(1{,}239)\text{durat\_3}_{jk} + 0{,}062(0{,}547)\text{Tot lig\%}_{k} + 1{,}171(0{,}726)\text{TE\%}_{k} + 1{,}240(0{,}331)\text{Holl\%}_{k}$$

$$\beta_{0ijk} = -0{,}355(41{,}288) + v_{0k} + u_{0jk} + e_{0ijk}$$

$$\left[v_{0k}\right] \sim \mathrm{N}(0, \Omega_v) : \Omega_v = \left[0{,}000(0{,}000)\right]$$

$$\left[u_{0jk}\right] \sim \mathrm{N}(0, \Omega_u) : \Omega_u = \left[3{,}504(2{,}657)\right]$$

$$\left[e_{0ijk}\right] \sim \mathrm{N}(0, \Omega_e) : \Omega_e = \left[42{,}667(4{,}421)\right]$$

*-2*loglikelihood(IGLS Deviance)* = 1558,504(234 of 234 cases in use)

**Conclusions:**