

## NEAR INFRARED SPECTROSCOPY WITH MULTIVARIATE STATISTICAL MODELLING AS A TOOL FOR DIFFERENTIATION OF WOOD FROM TREE SPECIES WITH SIMILAR APPEARANCE\*

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### ABSTRACT

Considerable areas in the northern parts of Norway are afforested with *Picea abies* (L.) H.Karst. (Norway spruce), *Picea × lutzii* Little (Lutz spruce), and *Picea sitchensis* (Bong.) Carrière (Sitka spruce). The species have different machining and wood properties but are similar in visual appearance. We evaluated whether near infrared (NIR) spectroscopy combined with multivariate statistical modelling could be used to identify wood from these three species. In all, 83 wood specimens were available for analyses, 36 of which were used as a test set for model validation. NIR spectra were obtained on the cross-sectional surfaces.

An initial principal component analysis indicated that little information from the first and second components could be used for discrimination, but in score-plots of the third and fourth components the samples from the tree species formed clusters. This showed that the NIR spectra did contain information relevant for tree species identification, and that only a small fraction of the total variance could be used for that purpose.

For classification of the wood specimens, partial least squares discriminant analyses were applied. All 47 specimens in the training set were fitted into the correct group. The test set validated results showed that except for two wood specimens, all specimens were correctly classified. The two misclassified samples were Sitka spruce.

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This study showed that development of well-performing prediction models for differentiation of wood from Norway spruce, Lutz spruce, and Sitka spruce is possible.

**Keywords:** near infrared spectroscopy; discriminant analysis; wood classification; *Picea abies*; *Picea sitchensis*; *Picea × lutzii*.

## INTRODUCTION

For industrial utilisation of wood, knowledge about raw material quality is paramount. Certain raw material properties are needed in order to be able to produce the final product according to specifications. The properties demanded can be stiffness, strength, and visual appearance.

In Norway a considerable afforestation programme started after the Second World War. Plantations of Norway spruce, Sitka spruce, and Lutz spruce were established in western and northern parts of the country. At present the species occur in pure plantations, but as they all prosper in the moist climate they will eventually be found also in mixed stands.

The three species have different properties, such as mechanical and machining properties, and should therefore be treated separately in wood processing as well as for final products. Sandland & Eikenes (1996a) investigated different aspects of lumber manufacturing of Norwegian-grown Sitka spruce. During resawing of lumber with a circular saw, they found that the feeding speed had to be reduced to half the normal speed used for resawing Norway spruce. It was found that the knots in Sitka spruce were harder and that they had a higher density than knots in Norway spruce, and it was concluded that this was why the feeding speed had to be reduced. In an earlier study, Foslie (1985) found that for primary lumber production the power consumption in circular sawing of Sitka spruce was 11.8% higher than Norway spruce. Sandland & Eikenes (1996b) investigated bending strength and density of Sitka spruce lumber from the western part of Norway and found that the strength/density ratio was higher for Sitka spruce than for Norway spruce. Information on properties of wood from Norwegian-grown Lutz spruce is lacking since it has not been tested. However, it is reasonable to expect that this species has properties that differ from the other two.

Differentiation of Norway spruce, Sitka spruce, and Lutz spruce is mostly quite straightforward on standing trees in monoculture plantation forests. The difficulties with species identification increase in mixed forests, and increase further at industrial locations, as logs from different tree species are difficult to identify. For the final product, such as surfaced wood, differentiation of the three tree species can be very difficult because the wood types have similar visual appearance.

NIR spectroscopy is a method that has yielded promising results when used to classify various types of wood. Brunner *et al.* (1996) used NIR spectroscopy to

differentiate wood from 12 tree species, mainly tropicals. Schimleck *et al.* (1996) used NIR spectroscopy and principal component analysis for eucalypt wood classification. Borga *et al.* (1992) found that NIR spectroscopy can be used to classify milled samples from wet-stored timber of *Pinus sylvestris* L. (Scots pine) into heartwood and sapwood. It has been shown that data from NIR spectroscopy measured on solid wood can be successfully used in multivariate statistical models to classify wood specimens of Scots pine into heartwood and sapwood (Flæte & Haartveit 2003). Results have also been presented indicating that NIR spectroscopy may be used to differentiate between wood samples of the same species, but from different origins (Gierlinger *et al.* 2004).

The aim of this study was to evaluate NIR spectroscopy with multivariate statistical modelling as a tool for differentiating wood of three species of spruce which have similar visual appearance.

## MATERIAL AND METHODS

### Sampling of Wood

Sawnwood samples were produced from Norway spruce, Sitka spruce, and Lutz spruce originating from seven locations in northern Norway. Four trees were collected from each location (stand), and a short log section from the lower part of each trunk (1.5–2.5 m above the base) was used to prepare small clear samples (20 × 20-mm cross-sections parallel to the orthogonal planes of the wood matrix). Three specimens were produced from each tree, giving a sample of 12 specimens from each stand (except for Stand 2 where only 11 specimens were available). Descriptive statistics for annual ring width and density for the specimens from the stands are given in Table 1.

TABLE 1—Basic statistics of annual ring width and density of the wood specimens sampled from each of the seven stands.

Stand	Spruce species	n	Annual ring width (mm)				Density, $\rho_{12}$ (kg/m <sup>3</sup> )			
			Mean	Std dev.	Min.	Max.	Mean	Std dev.	Min.	Max.
1	Norway	12	1.6	0.6	1.0	2.7	408	34	352	455
2	Sitka	11	5.6	1.2	3.7	7.4	377	22	339	413
3	Lutz	12	2.0	0.6	1.5	3.6	436	29	394	477
4	Norway	12	1.3	0.4	0.9	2.6	417	30	355	456
5	Lutz	12	2.2	0.5	1.7	3.2	480	32	436	535
6	Norway	12	2.0	0.9	1.2	4.3	410	31	357	453
7	Sitka	12	4.7	0.8	3.6	6.0	380	37	317	431

### NIR Spectroscopy

NIR spectra were collected on one of the cross-sectional faces of each of the 83 air-dry wood specimens. The cross-sectional faces were prepared by circular sawing. There were no visible colour differences between woods from the three different tree species. Scanning of spectra was performed in reflectance mode, in the 700 nm–2500 nm range, in 0.35-nm steps, by a PerkinElmer Spectrum One NTS system equipped with a Near Infrared Reflectance Accessory (NIRA) package (Fig. 1). The specimens were placed directly on the circular sapphire window on top of the Near Infrared Reflectance Accessory. The diameter of the window was 10 mm. For each spectrum 25 scans were collected and averaged. Spectra below 900 nm were discarded because of high levels of noise observed in the region 700–900 nm. Before analyses the wavelength variables were reduced (averaged) by a factor of 6.



FIG. 1—The PerkinElmer Spectrum One NTS system. The wood specimen was placed with a cross-sectional surface on the circular window over the light source.

### Multivariate Data Analyses

The reflectance data expressed as apparent absorbance ( $\log 1/\text{reflectance}$ ) were centred, and to correct for baseline shifts they were transformed to first derivatives.

#### *Principal component analysis*

Principal component analysis, performed to compress the data matrix, is a linear modelling method that projects the original variables on to a smaller set of variables called principal components. By applying principal component analysis to the spectral matrix, the large number of highly correlated variables will be reduced to a few orthogonal (and thereby uncorrelated) principal components.

Principal component scores are the projected locations of each sample on to each principal component. Scores can indicate latent structures and clusters of samples. The loadings express the contribution of each variable (wavelength) to each principal component.

### *Partial least squares regression*

Partial least squares regression is a linear modelling method that compresses the spectral data and projects them on to partial least squares components. The partial least squares 1 method extracts the spectral information with the largest covariance to one dependent variable (Martens & Næs 1989). In the partial least squares 2 method two or more dependent variables are modelled simultaneously. Partial least squares components are created so that they are mutually orthogonal, thus avoiding problems related to co-linearity among the variables in the X-matrix. Compared to traditional statistical modelling based on least squares estimation, independent variables in the X-matrix are not a requirement for the partial least squares method. Partial least squares regression can also handle situations where the number of variables far exceeds the number of samples, which is typical for modelling with NIR data.

### *Partial least squares discriminant analysis*

Partial least squares discriminant analysis involves developing a conventional partial least squares regression model, but instead of a continuous variable the response variable is a binary class indicator variable.

If there are only two classes to separate, the partial least squares model uses one response variable, which codes for class membership as follows: 0 for members of one class, 1 for members of the other one. The partial least squares 1 algorithm is then used. If there are three classes or more, partial least squares 2 is used. Each class is represented by an indicator variable, i.e., a binary variable with value 1 for members of that class, 0 for non-members. By building a partial least squares 2 model with all indicator variables as Y, one can directly predict class membership from the X-variables describing the samples. The model is interpreted by viewing Predicted vs Measured for each class indicator Y-variable:

- $Y_{\text{pred}} > 0.5$  means “member”;
- $Y_{\text{pred}} < 0.5$  means “non-member”.

In this study it was known that each wood specimen was either Norway spruce, Sitka spruce or Lutz spruce. For this reason three binary variables were constructed, one for each tree species. Each wood specimen was assigned to the group for which the model had the highest estimated response.

### *Model evaluation and validation*

The partial least squares discriminant analysis model presented was validated using test-set validation. Although the preferred material for a test set is obtained through conducting a new sampling, a frequently used alternative is to split the obtained data into a training set and a test set. A model that performs well when validated using test sets has a higher chance of performing well when predicting new samples. The

83 samples were divided into a calibration set and a validation set. The validation set consisted of 36 wood specimens (Stands 1, 3, and 7), leaving 47 specimens (Stands 2, 4, 5, and 6) available for model calibration. In all, the test (validation) set consisted of 12 specimens of each species.

The specimens were assigned to a calibration and validation set based on their origin (stand), instead of splitting the data randomly. This is a conservative approach, as it is reasonable to assume that trees from the same origin are somewhat correlated with respect to wood properties. Hence, if trees from the same stand are present in the calibration and the validation set, as would happen with random selection of the data sets, there is a risk of over-estimating the predictive capabilities of the model.

The models were evaluated according to their predictive capabilities measured in terms of the proportion of specimens from the test set that was correctly classified. The models should also preferably fit each wood specimen into the correct group in the calibration.

The statistical analyses were performed in the Unscrambler<sup>®</sup> from Camo Process AS.

## RESULTS

There was no observable colour difference between wood specimens from the different tree species. To identify information useful for classifying wood from the different tree species, an initial principal component analysis was performed on the first derivatives of the spectra from the 83 samples. The optimal number of principal components was four, which described 85% of the original variance in X. A score plot of principal components 1 and 2 is shown in Fig. 2; they explained 64% and 11% of the original variance, respectively. There was no tendency towards clustering of samples from the same species, and little information in the first two principal components could assist in identification of tree species. The score plot of principal components 3 and 4 is shown in Fig. 3. Principal component 3 explained 6% and principal component 4 explained 4% of the original variance in X. There was a tendency for specimens of Sitka spruce and Lutz spruce to be differentiated by principal component 3, while principal component 4 differentiated between Norway spruce and the two other species. It seems that the NIR spectra did contain information relevant for discrimination of the different tree species, but that the information represented only a small fraction of the total variation in the NIR spectra.

For the partial least squares discriminant analysis model the optimal number of partial least squares components was four. The regression coefficients for the partial least squares 2 regression models of Norway spruce, Sitka spruce, and Lutz

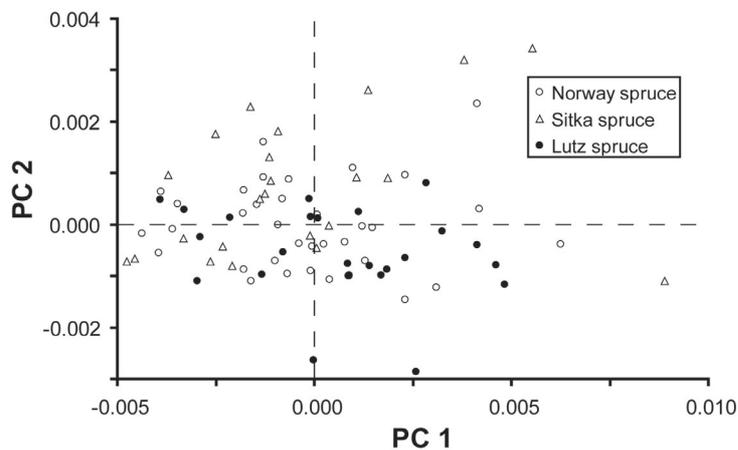


FIG. 2—Principal component analysis score plot of the first and second principal components of the NIR spectra.

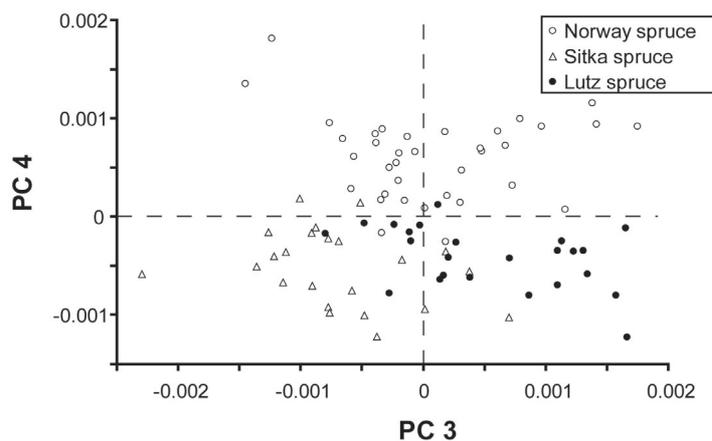


FIG. 3—Principal component analysis score plot of the third and fourth principal components of the NIR spectra.

spruce are given in Fig. 4. The regression coefficients for Norway spruce and Lutz spruce showed a strong inverse relationship. The regression coefficients for Sitka spruce were small for most of the spectral range, except from the areas around 1900 nm and 2500 nm. In these spectral areas, the regression coefficients for Norway spruce and Lutz spruce were close to zero.

A first impression of model performance is given by the fitted values of the response variables. The fitted values based on model calibration are reported in Table 2. The results show that all the 47 specimens had fitted values that classified them to the correct tree species.

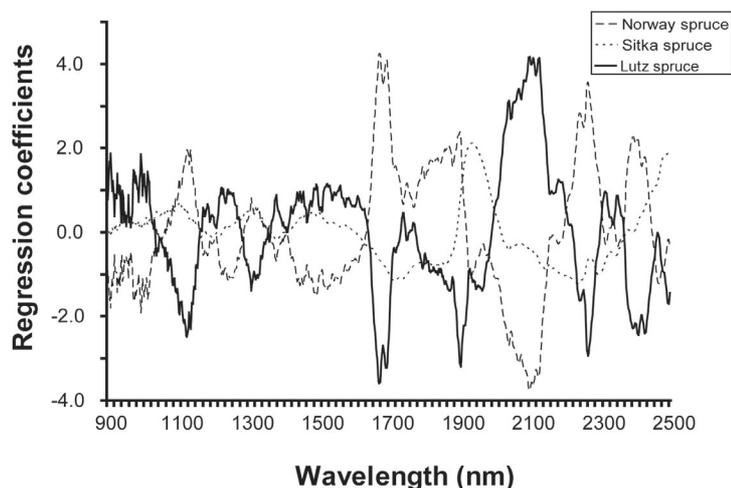


FIG. 4—Regression coefficients from the partial least squares discriminant analysis model for each of the three tree species.

TABLE 2—Results from partial least squares discriminant analysis model calibration. The training set consisted of 47 samples.

Fitted into group	True group		
	Norway spruce	Sitka spruce	Lutz spruce
Norway spruce	24	0	0
Sitka spruce	0	11	0
Lutz spruce	0	0	12
Total number	24	11	12
Number correct	24	11	12
Proportion correct	1.00	1.00	1.00

The partial least squares discriminant analysis model was validated using test set validation as described in the Methods section.

In all, 94% of the wood specimens were correctly classified (Table 3). The wood specimens from Norway spruce and Lutz spruce were all correctly classified. Two Sitka spruce specimens were predicted into wrong groups, one was predicted into the Norway spruce group and the other was predicted into the Lutz spruce group.

Of the 34 correctly classified wood specimens in the test set, three had high predicted values ( $> 0.5$ ) for more than one tree species, and two had low predicted values ( $< 0.5$ ) for all tree species.

TABLE 3—Results from partial least squares discriminant analysis model validation. The test set consisted of 36 samples.

Predicted into group	True group			Total correct
	Norway spruce	Sitka spruce	Lutz spruce	
Norway spruce	12	1	0	12
Sitka spruce	0	10	0	10
Lutz spruce	0	1	12	12
Number correct	12	10	12	34
Total number	12	12	12	36
Proportion correct	1.00	0.83	1.00	0.94

## DISCUSSION

The results presented indicate that NIR spectroscopy can be used successfully to create models for wood classification. The principal component analysis showed that only a small part of the total variance of the NIR spectra contained information relevant for discrimination of these three tree species. This agrees well with the fact that most of the wood matrix of the species included in this study is built up of similar structural elements.

The material we based this study on was small — 83 samples in all, of which 36 samples (43%) belonged to the test set. It is always a difficult trade-off to select the number of observations for model calibration and for model validation, respectively. The validation approach used in this study was conservative as all samples from stands 1, 3, and 7 were placed in the test set. It has been argued that validation using data splitting is of little value (Kozak & Kozak 2003), and that observations should be saved for model calibration. Those authors claimed that validation by data splitting provides little incremental information compared with the information revealed in standard statistical analysis, and that models should always be validated using external data. The requirements for individual sampling are somewhat unclear. In this study the material was sampled by several persons, in several different stands. It could be argued that collecting wood from different stands constitutes an individual sampling. This argument is reinforced if all samples coming from the same forest stand are put into the test set.

Despite the high proportion of correct classifications, some wood specimens had high predicted responses for several tree species, while other wood specimens had small predicted responses for all tree species. This result shows that classification and sorting of tree species are not always straightforward. Still, this study demonstrated that it is possible to classify wood types that are closely related and

have similar visual appearance. The models will steadily improve as more wood specimens are classified, because the classified specimens can be used in calibration sets for new and improved models. NIR spectroscopy is commonly used in this way — for example, for monitoring the quality of different food products.

The partial least squares discriminant analysis resulted in correct classification of all the specimens of Norway spruce and Lutz spruce, while two of the Sitka spruce wood specimens were misclassified. This is not surprising as the regression coefficients for Norway spruce and Lutz spruce showed a strong inverse relationship along the whole spectral range (Fig. 4). Conversely, there were only narrow spectral areas where the partial least squares regression coefficients for Sitka spruce were high and the corresponding regression coefficients for Norway spruce and Lutz spruce were close to zero. Despite the small calibration set and the structure of regression coefficients, the partial least squares discriminant analysis model performed well also for Sitka spruce. This underpins the potential for calibrating partial least squares models with higher classification performance if a large number of calibration samples are used.

The mean values for density were highest for Lutz spruce, lower for Norway spruce, and lowest for Sitka spruce (Table 1). One pitfall when developing models aiming to differentiate between wood species can be that the true response variable in the model is a variable other than the target response variable which does, however, correlate with the response variable of interest. This is a potential problem in the present study, because the densities are somewhat grouped according to species. By developing a model based on density as the response variable, the model would fail when applied on new samples with different wood densities. However, there are no indications of this problem in the present study. Although the mean density of wood specimens from the stands was grouped according to tree species, the values for specimens overlapped in many cases. Additionally, a partial least squares regression model was developed for wood density, and the pattern of the plot of the regression coefficients was different from that shown in Fig. 3.

Brunner *et al.* (1996) used NIR spectroscopy to differentiate 12 species of wood, and found that comparison of test results was possible only when the samples had been prepared identically. It is possible that pre-treatment of the spectral data (e.g., use of transformations) could have handled this problem. However, this aspect has to be considered when calibrating models for applications where the preparation of wood specimens cannot be performed identically.

As differentiating these tree species at an early stage of the production chain will facilitate better utilisation of the raw material, this procedure should also be tested on green timber.

## CONCLUSION

It is possible to develop well-performing prediction models for differentiation of wood from Norway spruce, Lutz spruce, and Sitka spruce based on near infrared spectroscopy.

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