prospect: an R package to link leaf optical properties with their chemical and structural properties with the leaf model PROSPECT

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Summary

PROSPECT simulates optical properties for a leaf, based on its content in absorbing constituents, and a structure parameter accounting for light scattering. We present prospect, an R package aiming at providing the most recent versions of the model, along with inversion routines to assess leaf chemistry from optical properties.

Statement of need

The capacity to measure, map and monitor vegetation traits corresponding to biophysical and chemical properties is crucial to better understand ecosystem and agrosystem functions, as well as carbon, water and energy budgets. At leaf scale, these vegetation traits are linked to their optical properties through absorption and scattering mechanisms. Spectroscopic techniques provide rapid, accurate and non-destructive assessment of leaf chemical composition. Physical models aim at simulating optical properties of leaves from their chemical composition. Inversion techniques take advantage of these models to assess leaf chemical composition from optical properties. The model PROSPECT (leaf optical PROperties SPECtra) is currently the most popular physical model for the simulation of leaf optical properties. PROSPECT simulates leaf directional-hemispherical reflectance and transmittance from a combination of chemical constituents and their corresponding specific absorption coefficients. It uses a simplified representation of leaf structure through the generalised plate model (Allen et al., 1970) to account for scattering. PROSPECT can be coupled with canopy reflectance models to analyze Earth observation data. Hence, it is a key component for remote sensing applications dedicated to vegetation monitoring.

Multiple versions have been released since its first version (S. Jacquemoud & Baret, 1990). (J.-B. Féret et al., 2008) introduced carotenoids and (J.-B. Féret et al., 2017) introduced anthocyanins, to simulate leaf optical properties from juvenile to mature and senescent development stages. (J.-B. Féret et al., 2021) introduced PROSPECT-PRO, the latest version separating dry matter constituents into proteins and carbon based constituents. In parallel with updated versions of the model, model inversion strategies have been introduced to improve the assessment of leaf chemical constituents (J.-B. Féret et al., 2019; Spafford et al., 2021).

PROSPECT implementations since (J.-B. Féret et al., 2008) can be found at this webpage. This includes distributions in matlab, R and fortran programming languages. PROSPECT is coupled with vegetation models, including COSINE dedicated to close-range imaging spectroscopy (Jay et al., 2016) and SAIL for canopy reflectance modeling Stéphane Jacquemoud et al. (2009). A version of prospect coupled with SAIL is available in the R package prosail. Note that PROSPECT and PROSAIL are also available in packages written in python, Julia and R.

Overview

PROSPECT simulation in forward mode

In forward mode, PROSPECT simulates leaf directional-hemispherical reflectance and transmittance from a set of chemical constituents and a leaf structure parameter identified as N. N represents the number of homogeneous layers introduced in the generalized plate model.

Two versions of PROSPECT are implemented in prospect: PROSPECT-D (J.-B. Féret et al., 2017) and PROSPECT-PRO (J.-B. Féret et al., 2021). PROSPECT-4 and 5 are deprecated. Table 1 lists the input leaf chemical constituents and structure parameter for versions D and PRO available with the function PROSPECT.

Table 1: Input variables for the two versions of PROSPECT implemented in the prospect package (CHL: chlorophylls; CAR: carotenoids; ANT: anthocyanins; BROWN: brown pigments; EWT: equivalent water thickness; LMA: leaf mass per area; PROT: proteins; CBC: carbon based constituents; N: leaf structure parameter).

Version	D	PRO
CHL	X	X
CAR	X	X
ANT	X	X
BROWN	X	X
EWT	X	X
LMA	X	
PROT		X
CBC		X
N	X	X

PROSPECT is a relatively simple and computationally efficient model. Hence iterative optimization can be considered to invert PROSPECT and assess leaf chemistry and structure from their optical properties. Iterative optimization aims at minimizing a merit function comparing measured and simulated leaf optical properties. This procedure is based on the function fmincon included in the package pracma. It usually takes less than 1 second to perform PROSPECT inversion.

Various inversion strategies using iterative optimization are described in the literature J.-B. Féret et al. (2019). These inversion strategies differ either by the merit function, or by the selection of specific spectral domains used to retrieve one or several leaf biophysical properties, or by the introduction of prior information. The default merit function, Merit_PROSPECT_RMSE, corresponds to the root mean square of the mean quadratic difference between measured and simulated leaf optical properties (reflectance and/or transmittance). Alternative merit functions using the same input and output variables as Merit_PROSPECT_RMSE can be defined. The online documentation provides an example of alternative merit function.

Table 2 details the optimal spectral domains to assess leaf chemical constituents from their optical properties (J.-B. Féret et al., 2019; Spafford et al., 2021).

Table 2: Optimal spectral domains to assess vegetation chemical constituents from leaf optical properties.

Constituent	Optimal spectral domain	Versions
CHL	$700 - 720$	D, PRO
CAR	$520 - 560$	D, PRO
ANT	$400 - 800$	D, PRO
BROWN	NA	NA

Constituent	Optimal spectral domain	Versions
EWT	1700 − 2400	D, PRO
LMA	1700 − 2400	D
PROT	2100 − 2139; 2160 − 2179	PRO
CBC	1480 − 1499; 1560 − 1579; 1760 − 1799; 2040 − 2059; 2120 − 2139; 2160 − 2239; 2260 − 2279; 2340 − 2359; 2380 − 2399	PRO

Example 1: running PROSPECT in forward mode

Input parameters listed in Table 1 are required to simulate leaf optical properties with PROSPECT. Optical constants corresponding to specific absorption coefficients and leaf refractive index are identical for all leaves, and are defined over the spectral domain ranging from 400 nm to 2500 nm. They are accessible through the variable SpecPROSPECT_FullRange, a data frame automatically loaded with the package. Multiple functions in the package prospect expect a variable SpecPROSPECT as input. SpecPROSPECT_FullRange is used as default value for this input variable. Simulated spectral characteristics, including spectral domain, sampling and sensor-specific spectral response can be derived from SpecPROSPECT_FullRange.

The function PROSPECT identifies the version to be used: PROSPECT-D is used if LMA is defined, while PROSPECT-PRO is used if proteins (PROT) and carbon based constituents (CBC) are defined. If LMA, PROT and CBC are defined simultaneously, PROSPECT-PRO is used and LMA is set to 0. Figure 1 compares simulated leaf optical properties. Here, the differences between PROSPECT-D and PROSPECT-PRO are mainly driven by the different value set for the N structure parameter.

```r
# Load prospect package
library(prospect)
# Run PROSPECT-D
LRT_D <- PROSPECT(CHL = 45, CAR = 10, ANT = 0.2,
                  EWT = 0.012, LMA = 0.010, N = 1.3)
# Run PROSPECT-PRO
LRT_PRO <- PROSPECT(CHL = 45, CAR = 10, ANT = 0.2,
                    EWT = 0.012, PROT = 0.001, CBC = 0.009, N = 1.7)
```
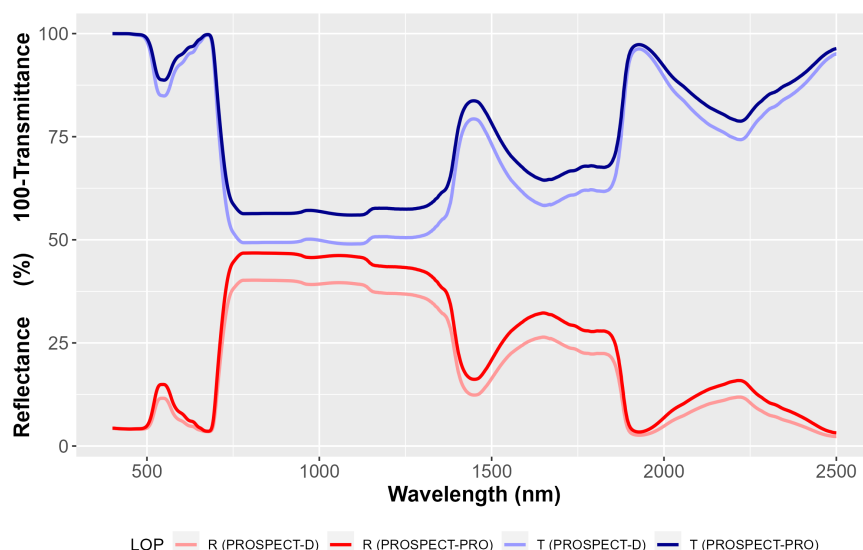
Figure 1: Leaf optical properties simulated with PROSPECT-D and PROSPECT-PRO. Different values of N were set to highlight differences in simulated leaf optics.

The spectral domain covered with PROSPECT simulations can be adjusted with the function `FitSpectralData`, which adjust information from `SpecPROSPECT_FullRange` to a user-defined spectral domain.

```
# define spectral bands for Visible / Near InfraRed (VNIR) simulation
wvlRange_VNIR <- seq(400,1000)
# adjust spectral properties used in PROSPECT to VNIR domain
VNIR <- FitSpectralData(lambda = wvlRange_VNIR)
# Run PROSPECT-D in VNIR domain
LRT_VNIR <- PROSPECT(SpecPROSPECT = VNIR$SpecPROSPECT,
                     N = 1.4, CHL = 30, CAR = 6, EWT = 0.02, LMA = 0.01)
```

Example 2: PROSPECT inversion using iterative optimization

Inversion is illustated with the experimental database **ANGERS**, a publicly available dataset used to calibrate PROSPECT. ANGERS can be downloaded from a gitlab repository with the function `download_LeafDB`.

```
LeafDB <- download_LeafDB(dbName = 'ANGERS')
```

PROSPECT inversion using the full spectral information

The spectral domains covered by `SpecPROSPECT` and the leaf optical properties are expected to match when performing inversion over the full spectral domain covered by the leaf optical properties. The function `FitSpectralData` harmonizes the spectral domain for `SpecPROSPECT` and the leaf optical properties. A vector listing the wavelengths of interest can also be provided with `UserDomain`. The following R code adjusts `SpecPROSPECT` to the spectral domain of the leaf optical properties.

```
# Adjust spectral domain for SpecPROSPECT to fit leaf optical properties
SubData <- FitSpectralData(SpecPROSPECT = SpecPROSPECT_FullRange,
                           Refl = LeafDB$Refl,
                           Tran = LeafDB$Tran,
```

```
                              lambda = LeafDB$lambda,
                              UserDomain = LeafDB$lambda)
```

95 The main inversion procedure is called with the function `Invert_PROSPECT`, which minimizes
96 a merit function defined by `Merit_PROSPECT_RMSE` as default option. Part or all parameters
97 from Table 1 can be assessed. Parameters assessed from PROSPECT inversion are defined
98 with an input list, `Parms2Estimate`. The default parameterization of PROSPECT inversion
99 leads to the assessment of all parameters listed in Table 1 except BROWN. BROWN can be
100 assessed during inversion (if working with senescent leaves) by setting `Est_Brown_Pigments =`
101 `TRUE` as input for `Invert_PROSPECT`. The value of unassessed parameters is set in `InitValues`.

```
# Assess all parameters using PROSPECT inversion applied to full spectral data
res_all_WL <- Invert_PROSPECT(SpecPROSPECT = SubData$SpecPROSPECT,
                              Refl = SubData$Refl,
                              Tran = SubData$Tran)
```

PROSPECT inversion using optimal spectral domains for each constituent

103 The function `Invert_PROSPECT_OPT` performs PROSPECT inversion using optimal spectral
104 domains, specific to each constituent (J.-B. Féret et al., 2019; Spafford et al., 2021). The
105 function automatically adjusts the spectral domain of the leaf optical properties provided as
106 input.

```
# Assess a set of parameters using PROSPECT inversion with optimal spectral domains
Parms2Estimate <- c('CHL', 'CAR', 'EWT', 'LMA')
res_opt_WL <- Invert_PROSPECT_OPT(lambda = LeafDB$lambda,
                                  Refl = LeafDB$Refl,
                                  Tran = LeafDB$Tran
                                  Parms2Estimate = Parms2Estimate)
```

Performances of the two types of inversion: Comparison with ANGERS data

108 Figure 2 compares lab measurements from CHL, CAR, EWT and LMA with values assessed
109 from `Invert_PROSPECT` and `Invert_PROSPECT_OPT` using ANGERS.
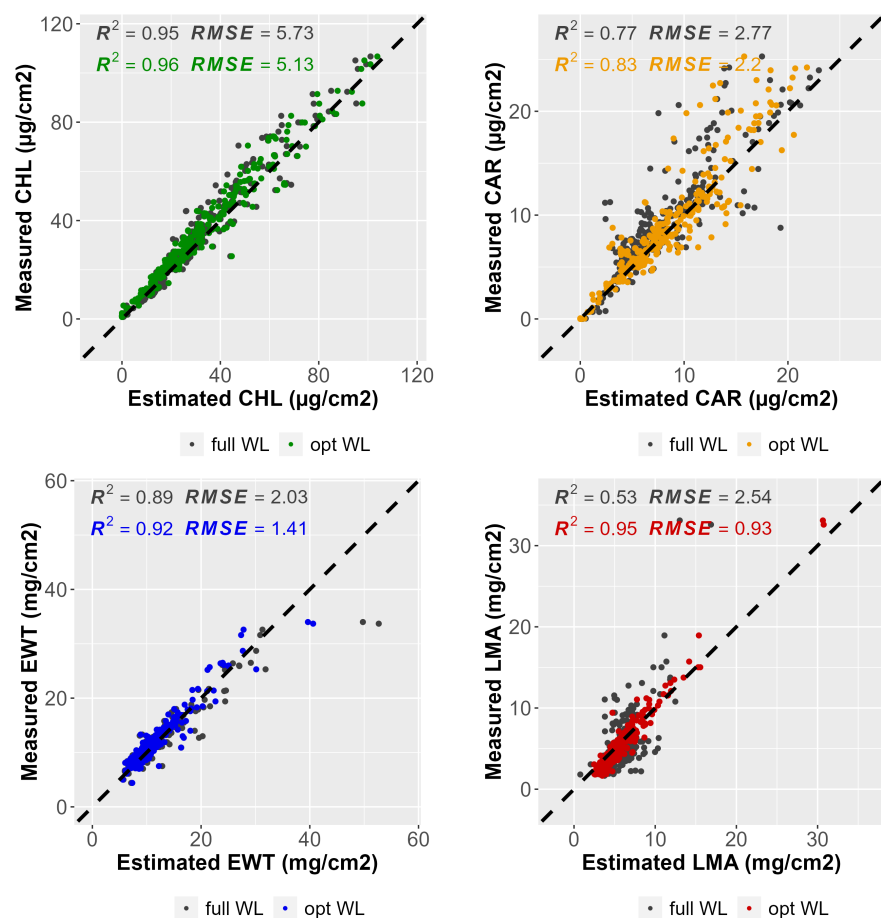
Figure 2: Estimation of chlorophyll content, carotenoid content, EWT and LMA from PROSPECT inversion applied on the ANGERS data set. `full WL` corresponds to the inversion performed with the full spectral information (function `Invert_PROSPECT`); `opt WL` corresponds to the inversion performed with the optimal spectral information (function `Invert_PROSPECT_OPT`).

Conclusion

We introduce `prospect`, an R package dedicated to the PROSPECT leaf model. `prospect` runs various versions of the model in direct mode to simulate directional-hemispherical reflectance and transmittance. It also includes inversion routines to assess leaf structure and chemical constituent content from reflectance and/or transmittance. `prospect` provides latest advances in terms of model version and inversion procedures to the leaf spectroscopy community. `prospect` is coupled with the canopy model SAIL through the R package prosail. prosail is dedicated to applications focusing on Earth observation imagery analysis and allows simulation of canopy reflectance for multispectral and hyperspectral sensors. Hybrid inversions based on physical modeling and machine learning are also implemented in `prosail` to assess vegetation traits at canopy scale from imagery data.

Availability

prospect is an open-source software package made available under the MIT license. Tutorials are available at https://jbferet.gitlab.io/prospect/.

Acknowledgements

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