pavo: Perceptual Analysis, Visualization and Organization of Color Data in R

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Introduction

pavo is an R package developed with the goal of establishing a flexible and integrated workflow for working with spectral color data. It includes functions that take advantage of new data classes in order to work seamlessly from importing raw data to visualization and analysis.

Although pavo deals largely with spectral reflectance data from bird feathers, it is meant to be applicable for a range of taxa and applications. It provides flexible ways to input spectral data from a variety of equipment manufacturers, process these data, extract variables and produce publication-quality graphics.

pavo was written with the following workflow in mind:

- 1. **Organize** spectral data by inputting files, processing spectra (e.g., to remove noise, negative values, smooth curves, etc.)
- 2. **Analyze** the resulting files, either using typical tristimulus color variables (hue, saturation, brightness) or using visual models based on perceptual data from the taxon of interest.
- 3. Visualize the output, with multiple options provided for exploratory analyses.

Below we will show the main functions in the package in an example workflow.

1 Data Description

The data used in this example is available from github by clicking here. You can download and extract it to follow the vignette.

The data consists of reflectance spectra obtained using Avantes equipment and software from seven bird species: Northern Cardinal (Cardinalis cardinalis), Wattled Jacana (Jacana jacana), Baltimore Oriole (Icterus galbula), Peach-fronted Parakeet (Aratinga aurea), American Robin (Turdus migratorius), and Sayaca Tanager (Thraupis sayaca). Several individuals were measured (sample size varies by species), and 3 spectra were collected from each individual.

The samples do not have the same sample sizes and have additional peculiarities that should emphasize the flexibility pavo offers, as we'll see below.

2 Organizing and Processing Spectral Data

2.1 Importing Data

The first thing we need to do is import the spectral data into R using the funciton <code>getspec()</code>. Since the spectra were obtained using Avantes software, we will need to specify that the files have the ".ttt" extension. Further, the data is organized in subdirectories for each species. <code>getspec</code> does recursive sampling, and may include the names of the subdirectories in the spectra name if desired. A final issue with the data is that it was collected using a computer with international numbering input, which means it uses commas instead of periods as a decimal separator. We can specify that in the function call.

I have downloaded the file and placed it in a directory called "/github/pavo/vignette_data". By default, getspec will search for files in the default folder, but a different one can be specified:

```
> specs <- getspec("~/github/pavo/vignette_data/", ext="ttt", decimal=",",
                    subdir=T, subdir.names=F)
> specs[1:10,1:4]
    wl cardinal.0001 cardinal.0002 cardinal.0003
1
   300
              5.7453
                             8.0612
                                            8.0723
                             8.3926
                                            8.8669
2
   301
              6.0181
   302
              5.9820
                             8.8280
                                            9.0680
3
   303
              6.2916
                             8.7621
                                            8.7877
4
5
   304
              6.6277
                             8.6819
                                            9.3450
6
   305
              6.3347
                             9.6016
                                            9.4834
7
   306
              6.3189
                             9.5712
                                            9.3533
8
   307
              6.7951
                             9.4650
                                            9.9492
   308
              7.0758
                             9.4677
                                            9.8587
9
10 309
              7.2126
                            10.6172
                                           10.5396
```

> dim(specs) #data has 214 spectra, from 300 to 700 nm

[1] 401 214

When pavo imports spectra, it creates an object of class rspec, which inherits attributes from the data.frame class:

> is.rspec(specs)

[1] TRUE

If you already have multiple spectra in a single data frame that you'd like to use with pavo functions, you can use the command as.rspec to convert it to an rspec object. The function will attempt to identify the wavelength variable or, if it doesn't have one, it can be specified in the function call.

2.2 Processing Data

2.3 Averaging Spectra

As previously described, our data constitutes of multiple individuals, and each was measured three times, as is common in order to avoid measurement bias. A good way to visualize the repeatability of our measurements is to plot the spectra of each individual separately. The function explorespec provides an easy way of doing so. You may specify the number of spectra to be plotted in the same panel using the argument specreps, and the function will adjust the number of panels per page accordingly. We will exemplify this function using only the 12 cardinal individuals measured:

```
> explorespec(specs[,1:37], specreps=3)
```

> # 36 spectra plus the first (wl) column

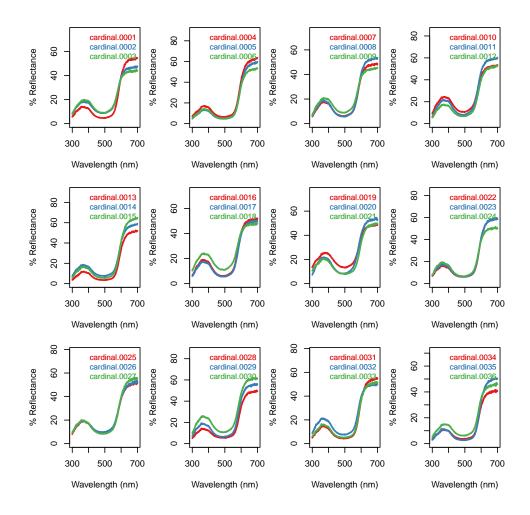


Figure 1: Result from explorespec, showing the three measurements for each individual in separate panels

So our first step would be to take the average of each of these three measurements in order to obtain average individual spectra to be used in further analyses. The function aggspec does this. The by argument can be either a number (specifying how many specs should be averaged for each new sample) or a vector specifying the identities of the spectra to be combined (see below):

```
> mspecs <- aggspec(specs, by=3, FXN=mean)</pre>
> mspecs[1:5, 1:4]
   wl cardinal.0001 cardinal.0004 cardinal.0007
                         5.676700
                                        6.387233
1 300
           7.292933
2 301
           7.759200
                         5.806700
                                        6.698200
3 302
           7.959333
                         5.858467
                                        6.910500
4 303
           7.947133
                         6.130267
                                        7.357567
5 304
           8.218200
                         6.127933
                                        7.195267
```

> dim(mspecs) #data now has 72 spectra, one for each individual

[1] 401 72

Now we'll use the aggspec function again, but this time to take the average spectrum for each species. However, each species has a different number of samples, so we can't use the by argument as before. Instead we will use regular expressions to create a species name vector by removing the numbers that identify individual spectra:

Instead, we are going to use the spp vector we created to tell the aggspec function how to average the spectra in mspec:

```
> sppspec <- aggspec(mspecs, by=spp, FXN=mean)
> sppspec[1:5, ]

wl cardinal jacana oriole parakeet robin
1 300 7.049397 7.334781 3.889693 7.629954 3.981747
2 301 7.254161 7.354033 3.905322 7.746882 3.914297
```

```
3 302 7.444275 7.452556 4.126619 7.886877 4.187073
```

tanager

- 1 9.021043
- 2 9.525854
- 3 9.405980
- 4 10.199843
- 5 9.684522

> explorespec(sppspec, 7)

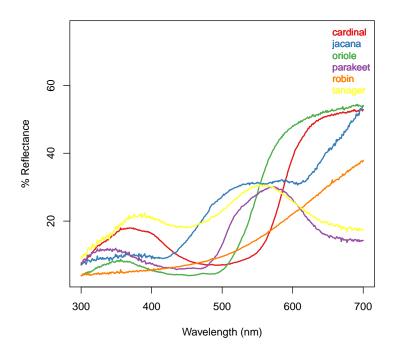


Figure 2: Result from explorespec for species means

^{4 303 7.820686 8.085541 4.390685 8.491367 4.507410}

^{5 304 7.843394 7.714526 4.183637 8.658000 4.068800}

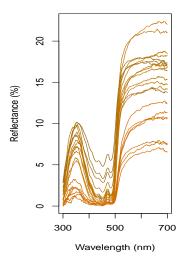


Figure 3: Overlay plot with colors calculated from human color matching functions

3 Visualizing Spectral Data

```
> data(sicalis)
> par(mfrow=c(1,2))
> plot(sicalis, type='o', col=spec2rgb(sicalis))
> plot(procspec(sicalis, opt='smooth'), type='o', col=spec2rgb(sicalis))

processing options applied:
    smoothing spectra with a span of 0.25
> #plot(sicalis, type='s', col=spec2rgb(sicalis))
```

Colors can be mapped to spectra using spec2rgb as shown in Figure 3.

4 Analyzing Spectral Data

4.1 Overview

pavo offers two main approaches for spectral data analysis. First, variables can be calculated based on the shape of the reflectance spectra. By using special R classes for spectra data frame objects, this can easily be done using the summary function in an rspec object (see below). The second function for spectral shape analysis is peakshape, which returns descriptors for peaks in spectral curves, as outlined below.

Second, reflectance spectra can be analyzed accounting for the visual system receiving the color signal, therefore representing reflectance spectra as preceived colors. We have implemented Endler's (REF) segment analysis model, which approximates visual models but does not directly use sensory information; the model of Osorio & Vorobyev (REF), which provides a flexible framework for visual modeling; and the tetrahedral color space (GOLDSMITH, ENDLER, STODDARD) which has been extensively developed to represent colors in the avian vision color space.

4.2 Spectral Shape Analysis

Trichromatic variables

Obtaining trichromatic color variables (related to hue, saturation and value) is pretty straightforward in pavo. Since reflectance spectra is stored in an object of class rspec, the summary function recognizes the object as such and extracts 23 variables, as outlined in MONT-GOMERIE. Though outlined in a book chapter on bird coloration, these variables are broadly applicable to any reflectance data, particularly if the taxon of interest has color vision within the UV-human visible range.

The description and formulas for these variables can be found in Table 1.

> summary(sppspec)

```
B2
                                 ВЗ
                                         S1.UV S1.violet
cardinal 8983.870 22.40367 52.96101 0.16618070 0.19132718
         9668.442 24.11083 53.48957 0.09623268 0.11048401
jacana
         9107.568 22.71214 54.31982 0.07474281 0.08314578
oriole
parakeet 6022.866 15.01962 28.82353 0.16803871 0.18515359
         5741.033 14.31679 37.96515 0.08500350 0.10012432
robin
        8516.756 21.23879 29.76561 0.20342675 0.23931496
tanager
            S1.blue S1.green S1.yellow
                                           S1.red
cardinal 0.11784952 0.1900225 0.2517886 0.5332009
                                                   7.329535
         0.19475522 0.3082406 0.2479744 0.4079294 6.883918
jacana
         0.05721376 0.3256520 0.3630756 0.5491879 12.992914
oriole
```

```
parakeet 0.14334383 0.4252528 0.3397279 0.2717663 4.768352
         0.14429801 \ 0.2675057 \ 0.2668015 \ 0.5099805 \ \ 9.172749
robin
tanager 0.26109724 0.3199401 0.2430633 0.2238215 3.120773
                S3
                           S4
                                    S5
                                             S6
cardinal 0.3682957 0.15813546 4004.193 45.73531 -0.38403228
        0.2469875 0.01690805 3312.697 45.71935 -0.46942827
jacana
         0.3444943 0.06767440 5232.176 50.13910 -0.70982859
oriole
parakeet 0.4467452 0.23727515 1900.192 22.77878 -0.20889035
         0.3031191 0.01271259 2531.901 33.82625 -0.57712488
robin
tanager 0.3341862 0.15240014 1105.252 20.22771 -0.08198454
                           S9
                                     S10 H1 H2 H3
                S8
cardinal 2.0414210 -0.8373693 12.909318 700 425 596
jacana 1.8962165 -0.7357544 112.148743 700 388 504
        2.2075903 -0.9257720 32.620756 700 388 500
oriole
parakeet 1.5166018 -0.5816948
                               6.391743 568 613 502
         2.3626975 -0.8148189 185.854859 700 349 500
robin
tanager 0.9523946 0.0359801 6.249303 557 600 428
                 H4 H5
cardinal 1.54995089 617
jacana
        0.85480076 463
oriole
        1.15606660 538
parakeet 0.59271149 500
         1.15020735 637
robin
tanager 0.04509807 512
```

$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	Color		
B2 $B_1/n_{ m wl}$ Mean brightness. B3 $R_{ m max}$ Intensity. Chroma, spectral purity. S2 $R_{ m max}/R_{ m min}$ Spectral saturation S3 S4 S5 S6 S7 S8 S9 S10 H1 $\lambda_{ m Rmax}$ Hue: wavelength of peak reflectance			Description
B2 $B_1/n_{ m wl}$ Mean brightness. B3 $R_{ m max}$ Intensity. Chroma, spectral purity. S2 $R_{ m max}/R_{ m min}$ Spectral saturation S3 S4 S5 S6 S7 S8 S9 S10 H1 $\lambda_{ m Rmax}$ Hue: wavelength of peak reflectance	B1	$\sum_{\lambda=300}^{700} R_{\lambda}$	Total brightness, total reflectance
S1 Chroma, spectral purity. S2 $R_{\rm max}/R_{\rm min}$ Spectral saturation S3 S4 S5 S6 S7 S8 S9 S10 H1 $\lambda_{\rm Rmax}$ Hue: wavelength of peak reflectance	B2	$\overline{B}_1/n_{\rm wl}$	Mean brightness.
S2 $R_{\rm max}/R_{\rm min}$ Spectral saturation S3 S4 S5 S6 S7 S8 S9 S10 H1 $\lambda_{\rm Rmax}$ Hue: wavelength of peak reflectance H2	В3	$R_{ m max}$	Intensity.
S3 S4 S4 S5 S6 S7 S8 S9 S10 H1 $\lambda_{\rm Rmax}$ Hue: wavelength of peak reflectance H2	S1		Chroma, spectral purity.
S4 S5 S6 S7 S8 S9 S10 H1 $\lambda_{ m Rmax}$ Hue: wavelength of peak reflectance H2	S2	$R_{\rm max}/R_{\rm min}$	Spectral saturation
S5 S6 S7 S8 S9 S10 H1 $\lambda_{ m Rmax}$ Hue: wavelength of peak reflectance H2	S3		
S6 S7 S8 S9 S10 H1 $\lambda_{\rm Rmax}$ Hue: wavelength of peak reflectance H2	S4		
S7 S8 S9 S10 H1 $\lambda_{ m Rmax}$ Hue: wavelength of peak reflectance H2	S5		
S8 S9 S10 Hue: wavelength of peak reflectance H2	S6		
S9 S10 H1 $\lambda_{ m Rmax}$ Hue: wavelength of peak reflectance H2	S7		
S10 H1 $\lambda_{ m Rmax}$ Hue: wavelength of peak reflectance H2	S8		
H1 $\lambda_{ m Rmax}$ Hue: wavelength of peak reflectance	S9		
H2	S10		
	H1	$\lambda_{ m Rmax}$	Hue: wavelength of peak reflectance
Н3	H2		
	Н3		
H4	H4		
Н5	H5		

Table 1: The complete set of tristimulus variables calculated by summary in pavo

$Peak\ shape\ descriptors$

Particularly in cases of reflectance spectra that have a single, discrete peak, it might be useful to obtain variables that describe that peak's properties. The peakshape function identifies the peak location (H1), returns the reflectance at that point (B3), and identifies the wavelengths at which the reflectance is half that at the peak, calculating the wavelength bandwith of that interval (the Full Width at Half Maximum, or FWHM). The function also returns the half widths, which are useful when the peaks are located near the edge of the measurement limit and half maximum reflectance can only be reliably estimated from one of its sides.

If this all sounds too esoteric, fear not: peakshape has the option of returning plots indicating what it's calculating. The vertical continuous red line indicates the peak location, the horizontal continuous red line indicates the half-maximum reflectance, and the distance between the dashed lines is the FWHM:

```
> par(mfrow=c(2,3), mar = c(5, 4, 0.5, 0.5) + 0.1)
> peakshape(sppspec, plot=T)
```

	В3	H1	FWHM	HWHM.1	HWHM.r	status
${\tt cardinal}$	52.89508	687	104	100	4	OK
jacana	53.90258	700	NA	93	NA	OK
oriole	54.40384	692	148	141	7	OK
parakeet	30.05703	575	125	66	59	OK
robin	37.91676	700	NA	107	NA	OK
tanager	30.71021	555	232	142	90	OK

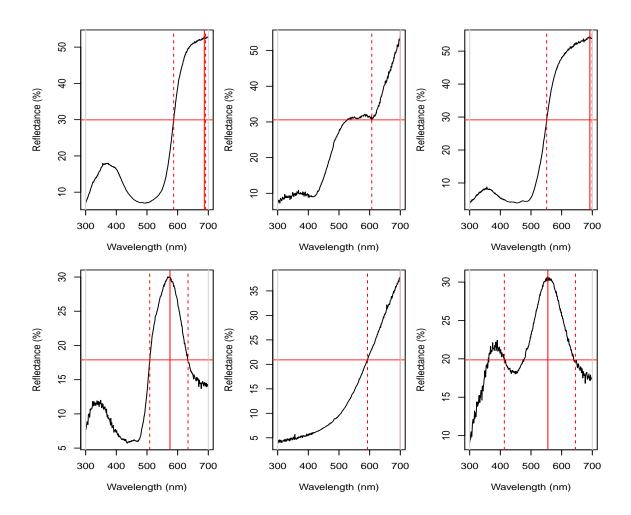


Figure 4: Plots from peakshape

As it can be seen, the variable is meaningless if the curve doesn't have a clear peak. Sometimes, such as in the case of the Cardinal (Figure 4, first panel), there might be a peak which is not the point of maximum reflectance of the entire spectral curve. The half-width can also be erroneously calculated when there are two peaks, as can be seen in the case of the Tanager (Figure 4, last panel). In this case, it's useful to set bounds when calculating the FWHM, using the bounds argument. peakshape also offers a select argument to facilitate subsetting the spectral data frame:

> peakshape(sppspec, select=2, bounds=c(300,500), plot=T)

 $$\rm B3\ H1\ FWHM\ HWHM.1\ HWHM.r\ status}$ cardinal 17.99853 369 100 47 53 OK

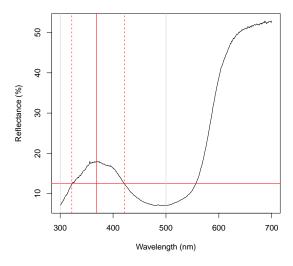


Figure 5: Plot from peakshape, setting the bounds to 300-500nm

Examples

> hist(rnorm(50))

More examples

Some more examples: