

1 Supplementary Information
2 *MonoPhy*: A simple R package to find
3 and visualize monophyly issues -
4 Commands for Examples

5
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10
11
12 Below you find the commands used to run the two example cases from the paper.
13 We included comments and outputs, except where outputs are too large to be
14 displayed in this word file, in which case the separate file will be referred to. For a
15 more general treatment of usage and applications of the package, one should refer
16 to the tutorial vignette (`vignette("MonoPhyVignette")`), which contains stepwise
17 instructions for the different functions and their options. For further package details
18 consult the help files (`help("MonoPhy")`).

19 **Example 1 – Ericaceae**

20 For the first demonstration, we use the example files contained in the package. The
21 phylogeny is of the plant family Ericaceae, as published in Schwery *et al.* (2015)
22 pruned down to 77 taxa (original data see Schwery *et al.* (2014). Two taxon files
23 assign tribes or tribes and subfamilies to the tips (in both files, errors in the taxon
24 assignment have been introduced for the sake of demonstrating the functionality of
25 the package).

26 First we load the package:

27 `> library(MonoPhy)`

28

29 Next, we load the example files with the tree and the taxonomy table:

30 `> data(Ericactree)`

31 `> data(Ericactribes)`

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32 Now we can run the main analysis command. In order to access the output later,
33 we should save it to an object. We will run one analysis without taxonomy table,
34 assessing the monophyly of the genera (`solutionG`), and one with the table
35 assessing monophyly of the tribes (`solutionT`):

```
36 > solutionG <- AssessMonophyly(Ericactree)  
37 > solutionT <- AssessMonophyly(Ericactree, Ericactribes)
```

38

39 Running these steps took around 0.045 and 0.093 seconds respectively on a
40 MacBook Pro with 2.4 GHz Intel Core i5 and 8GB Ram. Now we can get a first
41 impression of the monophyly in our tree. Note that 'Taxa' refers to higher order
42 taxa:

```
43 > GetSummaryMonophyly(solutionG)  
44 $Taxlevel_1
```

	Taxa	Tips
Total	32	77
Monophyletic	9	25
Non-Monophyletic	6	35
Monotypic	17	17
Intruder	7	11
Outlier	1	2

52

```
53 > GetSummaryMonophyly(solutionT)  
54 $Taxlevel_1
```

	Taxa	Tips
Total	10	77
Monophyletic	7	44
Non-Monophyletic	2	32
Monotypic	1	1
Intruder	1	2
Outlier	1	1

62

63 We can see that on both taxonomic levels monophyly issues exist to different
64 extents. For more detailed information, we can now look at the results tables for
65 genera (**Table 1**) and tribes (**Table 2**).

```
66 > GetResultMonophyly(solutionG)  
67 > GetResultMonophyly(solutionT)
```

68

69 We can see that the genera *Dimorphantha*, *Erica*, *Paphia*, *Phyllodoce*, *Pyrola* and
70 *Vaccinium* are not monophyletic as well as the tribes Vaccinieae and Andromedaeae.
71 If we want to know which other taxa particularly cause the above to be non-
72 monophyletic, we can list them:

```

73 > GetIntruderTaxa(solutionG)
74 $Taxlevel_1
75 $Taxlevel_1$Dimorphanthera
76 [1] "Paphia"
77
78 $Taxlevel_1$Erica
79 [1] "Bruckenthalia"
80
81 $Taxlevel_1$Paphia
82 [1] "Dimorphanthera"
83
84 $Taxlevel_1$Phyllodoce
85 [1] "Kalmiopsis"
86
87 $Taxlevel_1$Pyrola
88 [1] "Orthilia"
89
90 $Taxlevel_1$Vaccinium
91 [1] "Gaylussacia" "Agapetes"
92
93 > GetIntruderTaxa(solutionT)
94 $Taxlevel_1
95 $Taxlevel_1$Vaccinieae
96 [1] "Andromedaeae"
97

```

98 If we want to figure out which species exactly are the intruders, we can extract
 99 this information as well, *e.g.* for the genus *Vaccinium* alone and for both of the non-
 100 monophyletic tribes:

```

101 > GetIntruderTips(solutionG, taxa="Vaccinium")
102 $Taxlevel_1
103 $Taxlevel_1$Vaccinium
104 [1] "Gaylussacia_dumosa" "Agapetes_hosseana" "Agapetes_serpens"
105 "Agapetes_buxifolia"
106
107 > GetIntruderTips(solutionT)
108 $Taxlevel_1
109 $Taxlevel_1$Vaccinieae
110 [1] "Andromeda_polifolia" "Vaccinium_vitis_idaea"
111

```

112 A look at the intentional errors in the taxonomy table would make clear why
 113 these two species are intruders of the tribe Vaccinieae: the labels of *Vaccinium vitis-*
 114 *idaea* (a member of Vaccinieae) and *Zenobia pulverulenta* (an actual Andromedaeae)

115 were swapped, which makes it appear like *V. vitis-ideae* and the remaining actual
116 Andromedae – *Andromeda polifolia* – would intrude the Vaccinieae clade.

117 Under the default cutoff (0.5), the genus *Vaccinium* has outliers. Analogous to the
118 intruders, we can display the involved taxa (which we already know in this case of
119 course) and the specific species:

```
120 > GetOutlierTaxa(solutionG)
121 $Taxlevel_1
122 [1] "Vaccinium"
123
124 > GetOutlierTips(solutionG)
125 $Taxlevel_1
126 $Taxlevel_1$Vaccinium
127 [1] "Vaccinium_poasanum"    "Vaccinium_uginosum"
128
```

129 Note that in this case, without a cutoff, all tips ‘in between’ these two outliers and
130 the remaining *Vaccinium* species would have been considered ‘intruders’ of
131 *Vaccinium*.

132 For the purpose of orientation on the tree, plotting or any other further
133 operations, we can display the MRCA nodes of any taxon desired, e.g. *Vaccinium*
134 again:

```
135 > GetAncNodes(solutionG, taxa="Vaccinium")
136 $Taxlevel_1
137           MRCA
138 Vaccinium  93
139
```

140 Finally, we can visualize the results using the plot function. The following
141 command will produce the basic monophyly plot, which is displayed in **Fig. S1**.

```
142 > PlotMonophyly(solutionG, Ericactree, plot.type="monophyly")
143
```

144 Example 2 – Embriophyta

145 For the second example, we demonstrate the package’s performance on a tree with
146 several thousand tips. We therefore run the analysis on a tree of 31,749 species of
147 Embriophyta, as published by Zanne *et al.* (2014) (data see Zanne *et al.* (2013)), this
148 times with a higher outlier-cutoff:

```
149 > library(MonoPhy)
150 > tree <- read.tree(file="~/.../Vascular_Plants_rooted.dated.tre")
151 > solution <- AssessMonophyly(tree, outlierlevel=0.9)
152
```

153 On the same computer as in the previous example, this analysis completed after
154 1.78 hours. Again, we get a first impression by looking at the summary and results
155 tables (due to its size, the result table can be found in **Tab. S1**, see separate file).

```
156 > GetSummaryMonophyly(solution)
157 $Taxlevel_1
158             Taxa  Tips
159 Total          8179 31749
160 Monophyletic   1954 10841
161 Non-Monophyletic 1813 16496
162 Monotypic      4412  4412
163 Intruder        335   498
164 Outlier         1703  5275
165
166 > GetResultMonophyly(solution)
167
```

168 Just as before, we could extract more detailed information from the output. Due
169 to the size of the phylogeny, it would not be convenient to inspect the plot in an R
170 plot window. Therefore, we choose to save the plot directly as a PDF, which will
171 make it easier to view. Additionally, we can limit the complexity of the plot, by
172 collapsing all clades for monophyletic taxa to one remaining branch. We create the
173 standard monophyly plot with and without collapsing the monophyletic groups
174 (**Fig. S2** and **Fig. S3** respectively), and the intruder plot without collapsing (**Fig. S4**),
175 colour-coding the intruders and outliers according to the taxa that they are assigned
176 to.

```
177 > PlotMonophyly(solution, tree, plot.type='monophyly', monocoll=TRUE,
178   label.offset=1, type="fan", cex=0.05, edge.width=1.5, PDF=TRUE,
179   PDF_filename='MEE_Fig2.pdf')
180 > PlotMonophyly(solution, tree, plot.type='monophyly',
181   monocoll=FALSE, label.offset=0.75, type="fan", cex=0.05,
182   edge.width=1.5, PDF=TRUE, PDF_filename='SuppFig1.pdf')
183 > PlotMonophyly(solution, tree, plot.type='intruders',
184   monocoll=FALSE, label.offset=0.75, type="fan", cex=0.05,
185   edge.width=1.5, PDF=TRUE, PDF_filename='SuppFig2.pdf')
```

186 Note that plotting such big trees can take as long as or longer than running the
187 analysis itself. Here, **Fig. S2** took 1.22 hours, **Fig. S3** 2.39 hours and **Fig. S4** 4.53
188 hours.

189 **References**

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208 Repository.
- 209

210 Tables

211 **Table 1:** *MonoPhy* result table for the genera of Ericaceae.

	Monophyly	MRCA	#Tips	Delta-Tips	#Intruders	Intruders	#Outliers	Outliers
Agapetes	Yes	114	3	0	0			NA
Allotropa	Monotypic	NA	1	NA	NA			NA
Andromeda	Monotypic	NA	1	NA	NA			NA
Bruckenthalia	Monotypic	NA	1	NA	NA			NA
Bryanthus	Monotypic	NA	1	NA	NA			NA
Calluna	Monotypic	NA	1	NA	NA			NA
Cassiope	Yes	146	5	0	0			NA
Chimaphila	Yes	88	2	0	0			NA
Costera	Monotypic	NA	1	NA	NA			NA
Daboecia	Yes	126	2	0	0			NA
Dimorphantha	No	96	3	2	1	Paphia		0
Enkianthus	Yes	150	5	0	0			NA
Epigaea	Monotypic	NA	1	NA	NA			NA
Erica	No	128	9	1	1	Bruckenthalia		0
Gaylussacia	Monotypic	NA	1	NA	NA			NA
Gonocalyx	Yes	120	2	0	0			NA
Kalmiopsis	Yes	142	2	0	0			NA
Ledothamnus	Yes	138	2	0	0			NA
Moneses	Monotypic	NA	1	NA	NA			NA
Monotropa	Monotypic	NA	1	NA	NA			NA
Notopora	Monotypic	NA	1	NA	NA			NA
Orthaea	Yes	101	2	0	0			NA
Orthilia	Monotypic	NA	1	NA	NA			NA
Oxydendrum	Monotypic	NA	1	NA	NA			NA
Paphia	No	97	2	1	1	Dimorphantha		0
Phyllodoce	No	140	4	2	1	Kalmiopsis		0
Pyrola	No	83	4	1	1	Orthilia		0
Rhodothamnus	Monotypic	NA	1	NA	NA			NA
Sympisia	Monotypic	NA	1	NA	NA			NA
Utleya	Monotypic	NA	1	NA	NA			NA
Vaccinium	No	93	13	17	2	Gaylussacia, Agapetes	2	Vaccinium_poasanum, Vaccinium_uginosum
Zenobia	Monotypic	NA	1	NA	NA			NA

212

213 **Table 2:** *MonoPhy* result table for the tribes of Ericaceae.

	Monophly	MRCA	#Tips	Delta-Tips	#Intruders	Intruders	#Outliers	Outliers
Vaccinieae	No	91	30	2	1	Andromedae	0	
Monotropeae	Yes	81	2	0	0		NA	
Andromedae	No	91	2	30	0		1	<i>Vaccinium_vitis_idaea</i>
Ericae	Yes	125	13	0	0		NA	
Bryanthae	Yes	137	3	0	0		NA	
Cassiopoideae	Yes	146	5	0	0		NA	
Pyroleae	Yes	82	8	0	0		NA	
Enkianthoideae	Yes	150	5	0	0		NA	
Phyllodoceae	Yes	139	8	0	0		NA	
Oxydendreae	Monotypic	NA	1	NA	NA		NA	

214