

rRDP: Interface to the RDP Classifier

Michael Hahsler
Southern Methodist University

Anurag Nagar
Southern Methodist University

Abstract

This package installs and interfaces the naive Bayesian classifier for 16S rRNA sequences developed by the Ribosomal Database Project (RDP). With this package the classifier trained with the standard training set can be used or a custom classifier can be trained.

Keywords: bioinformatics, Bioconductor, Biostrings, sequence classification.

1. Classification with RDP

The RDP classifier was developed by the Ribosomal Database Project which provides various tools and services to the scientific community for data related to 16S rRNA sequences. The classifier uses a Naive Bayesian approach to quickly and accurately classify sequences. The classifier uses 8-mer counts as features [Wang, Garrity, Tiedje, and Cole \(2007\)](#).

1.1. Using the RDP classifier trained with the default training set

RDP is shipped trained with a 16S rRNA training set. The model data is available in the data package **rRDPData**.

For the following example we load some test sequences shipped with the package.

```
R> library(rRDP)
R> seq <- readRNStringSet(system.file("examples/RNA_example.fasta",
+   package="rRDP"))
R> seq

A RNStringSet instance of length 5
  width seq                                     names
[1] 1481 AGAGUUUGAUCCUGGCUC...AGUCGUAACAAGGUAACC 1675 AB015560.1 d...
[2] 1404 GCUGGCGGCAGGCCUAAC...UAAGGUCAGCGACUGGGG 4399 D14432.1 Rho...
[3] 1426 GGAAUGCUNAACAACAU...GGUAGCCGUAGGGGAACC 4403 X72908.1 Ros...
[4] 1362 GCUGGCGGAAUGCUUAAC...UAGGUGUCUAGGCUAACC 4404 AF173825.1 A...
[5] 1458 AGAGUUUGAUUAUGGCUC...UCGUAACAAGGUAACCGU 4411 Y07647.2 Dre...
```

Note that the name contains the annotation from the FASTA file. In this case the annotation contains the actual classification information and is encoded in Greengenes format. For convenience, we replace the annotation with just the sequence id.

```
R> annotation <- names(seq)
R> names(seq) <- sapply(strsplit(names(seq), " "), "[", 1)
R> seq
```

```
A RNAStringSet instance of length 5
  width seq                                     names
[1] 1481 AGAGUUUGAUCCUGGCUC...AGUCGUAACAAGGUAACC 1675
[2] 1404 GCUGGCGGCAGGCCUAAC...UAAGGUCAGCGACUGGGG 4399
[3] 1426 GGAAUGCUNAACACAUGC...GGUAGCCGUAGGGGAACC 4403
[4] 1362 GCUGGCGGAAUGCUUAAC...UAGGUGUCUAGGCUAACC 4404
[5] 1458 AGAGUUUGAUUAUGGCUC...UCGUAACAAGGUAACCGU 4411
```

Next, we apply RDP with the default training set. Note that the data package **rRDPDate** needs to be installed!

```
R> pred <- predict(rdp(), seq)
R> pred
```

```
      rootrank  domain      phylum      class
1675      Root  Bacteria  Proteobacteria  Deltaproteobacteria
4399      Root  Bacteria  Proteobacteria  Alphaproteobacteria
4403      Root  Bacteria  Proteobacteria  Alphaproteobacteria
4404      Root  Bacteria  Proteobacteria  Alphaproteobacteria
4411      Root  Bacteria  Proteobacteria  Alphaproteobacteria
      order      family      genus
1675      <NA>      <NA>      <NA>
4399 Rhodospirillales Rhodospirillaceae Rhodovibrio
4403 Rhodospirillales Acetobacteraceae Roseococcus
4404 Rhodospirillales Acetobacteraceae Roseococcus
4411 Rhodospirillales Acetobacteraceae      <NA>
```

The prediction confidence is supplied as the attribute "confidence".

```
R> attr(pred, "confidence")
```

```
      rootrank  domain  phylum  class  order  family  genus
1675      1      1      0.91  0.91  0.43  0.43  0.42
4399      1      1      1.00  1.00  1.00  1.00  1.00
4403      1      1      1.00  1.00  1.00  1.00  1.00
4404      1      1      1.00  1.00  1.00  1.00  1.00
4411      1      1      1.00  1.00  1.00  1.00  0.39
```

To evaluate the classification accuracy we can compare the known classification with the predictions. The known classification was stored in the FASTA file and encoded in Greengenes format. We can decode the annotation using `decode_Greengenes()`.

```
R> actual <- decode_Greengenes(annotation)
R> actual
```

Kingdom	Phylum	Class	Order
1 Bacteria	Proteobacteria	Deltaproteobacteria	Desulfobacterales
2 Bacteria	Proteobacteria	Alphaproteobacteria	Rhodospirillales
3 Bacteria	Proteobacteria	Alphaproteobacteria	Rhodospirillales
4 Bacteria	Proteobacteria	Alphaproteobacteria	Rhodospirillales
5 Bacteria	Proteobacteria	Alphaproteobacteria	Rhodospirillales

	Family	Genus	Species
1	Nitrospinaceae	Nitrospina	unknown
2	Rhodospirillaceae	Rhodovibrio	Rhodovibrio salinarum
3	Acetobacteraceae	Roseococcus	unknown
4	Acetobacteraceae	Roseococcus	unknown
5	Acetobacteraceae; Unclassified	unknown	unknown

Otu
1 3187
2 2816
3 2785
4 2785
5 2752

	Org_name
1	AB015560.1_deep-sea_sediment_clone_BD4-10
2	D14432.1_Rhodovibrio_salinarum_str._NCIMB2243
3	X72908.1_Roseococcus_thiosulfatophilus_str._RB-3_Yurkov_strain_Drews
4	AF173825.1_Antarctic_clone_LB3-94
5	Y07647.2_Drentse_grassland_soil_clone_vii

Id
1 1675
2 4399
3 4403
4 4404
5 4411

Now we can compare the prediction with the actual classification by creating a confusion table and calculating the classification accuracy. Here we do this at the Genus level.

```
R> confusionTable(actual, pred, rank="genus")
```

actual	predicted				
	Nitrospina	Rhodovibrio	Roseococcus	unknown	<NA>
Nitrospina	0	0	0	0	1
Rhodovibrio	0	1	0	0	0
Roseococcus	0	0	2	0	0
unknown	0	0	0	0	1
<NA>	0	0	0	0	0

```
R> accuracy(actual, pred, rank="genus")
```

```
[1] 0.6
```

1.2. Training a custom RDP classifier

RDP can be trained using `trainRDP()`. We use an example of training data that is shipped with the package.

```
R> trainingSequences <- readDNAStrngSet(
+   system.file("examples/trainingSequences.fasta", package="rRDP")
R> trainingSequences
```

```
A DNAStrngSet instance of length 20
  width seq                      names
[1] 1384 TAGTGGCGGACGGGTGAG...TCGAATTTGGGTCAAGT 13652 Root;Bacter...
[2] 1386 ATCTCACCTCTCAATAGC...CGAAGGTGGGTTGGTG 13655 Root;Bacter...
[3] 1440 ATCTCACCTCTCAATAGC...GCTGGATCACCTCCTTA 13661 Root;Bacter...
[4] 1421 AATAGCGGCGGACGGGTG...ATCGGAAGGTGCGGCTG 13671 Root;Bacter...
[5] 1439 ATCTCACCTCTCAATANC...GGTGGGCTGGATCACC 13677 Root;Bacter...
...
[16] 1478 TGGCTCAGGACGAACGCT...CGTATCGGAAGGTGCGG 13763 Root;Bacter...
[17] 1507 CCTGGCTCAGGACGAACG...TATCGGAAGGTGCGGCT 13781 Root;Bacter...
[18] 1481 TGGAGAGTTTGATCCTGG...GCAAGGATATAGCCGTC 13797 Root;Bacter...
[19] 1463 CGGCGTGCTTGGACCCAC...GGTCCTAAGGTGGGGGC 13799 Root;Bacter...
[20] 1389 CGAGTGGCAAACGGGTGA...GCAAGGATGCAGCCGTC 13800 Root;Bacter...
```

Note that the training data needs to have names in a specific RDP format:

```
"<ID> <Kingdom>;<Phylum>;<Class>;<Order>;<Family>;<Genus>"
```

In the following we show the name for the first sequence. We use here `sprintf` to display only the first 65 characters so the it fits into a single line.

```
R> sprintf(names(trainingSequences[1]), fmt="%0.65s...")

[1] "13652 Root;Bacteria;Firmicutes;Clostridia;Clostridiales;Peptococc..."
```

Now, we can train a the classifier. The model is stored in a directory specified by the parameter `dir`.

```
R> customRDP <- trainRDP(trainingSequences, dir = "myRDP")
R> customRDP
```

```
RDPClassifier
```

```
Location: /tmp/RtmpepCh5Q/Rbuild17016752c34b/rRDP/vignettes/myRDP
```

```
R> testSequences <- readDNAStrngSet(
+   system.file("examples/testSequences.fasta", package="rRDP")
R> pred <- predict(customRDP, testSequences)
R> pred
```

	rootrank	Kingdom	Phylum	Class	Order
13811	Root	Bacteria	Firmicutes	Clostridia	Clostridiales
13813	Root	Bacteria	Firmicutes	Clostridia	Clostridiales
13678	Root	Bacteria	Firmicutes	Clostridia	Clostridiales
13755	Root	Bacteria	Firmicutes	Clostridia	Clostridiales
13661	Root	Bacteria	Firmicutes	Clostridia	Clostridiales
					Family
13811				Veillonellaceae	
13813				Veillonellaceae	
13678				Peptococcaceae	
13755	Thermoanaerobacterales	Family III.	Incertae Sedis		
13661				Peptococcaceae	
					Genus
13811		Selenomonas			
13813		Selenomonas			
13678		Desulfotomaculum			
13755	Thermoanaerobacterium				
13661		Desulfotomaculum			

Since the custom classifier is stored on disc it can be recalled anytime using `rdp()`.

```
R> customRDP <- rdp(dir = "myRDP")
```

To permanently remove the classifier use `removeRDP()`.

```
R> removeRDP(customRDP)
```

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References

Wang Q, Garrity GM, Tiedje JM, Cole JR (2007). "Naive Bayesian classifier for rapid assignment of rRNA sequences into the new bacterial taxonomy." *Applied and environmental microbiology*, **73**(16), 5261–5267.

Affiliation:

Michael Hahsler
Engineering Management, Information, and Systems
Lyle School of Engineering
Southern Methodist University
P.O. Box 750123
Dallas, TX 75275-0123
E-mail: mhahsler@lyle.smu.edu
URL: <http://lyle.smu.edu/~mhahsler>

Anurag Nagar
Computer Science and Engineering
Lyle School of Engineering
Southern Methodist University
P.O. Box 750122
Dallas, TX 75275-0122
E-mail: anagar@smu.edu