

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

A RNAStringSet 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	Org_name
1 3187	AB015560.1_deep-sea_sediment_clone_BD4-10
2 2816	D14432.1_Rhodovibrio_salinarum_str._NCIMB2243
3 2785	X72908.1_Roseococcus_thiosulfatophilus_str._RB-3_Yurkov_strain_Drews
4 2785	AF173825.1_Antarctic_clone_LB3-94
5 2752	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")
```

	predicted				
actual	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

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

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

```
A DNASTringSet instance of length 20
      width seq                                     names
[1]  1384 TAGTGGCGGACGGGTGAG...TCGAATTTGGGTCAAGT 13652 Root;Bacter...
[2]  1386 ATCTCACCTCTCAATAGC...CGAAGGTGGGGTTGGTG 13655 Root;Bacter...
[3]  1440 ATCTCACCTCTCAATAGC...GCTGGATCACCTCCTTA 13661 Root;Bacter...
[4]  1421 AATAGCGGCGGACGGGTG...ATCGGAAGGTGCGGCTG 13671 Root;Bacter...
[5]  1439 ATCTCACCTCTCAATANC...GGTGGCGGTGGATCACC 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="%s...")

[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: C:\Users\biocbuild\bbs-3.7-bioc\tmpdir\Rtmp8cXMjy\Rbuildf5c4468e1e\rRDP\vignette
```

```
R> testSequences <- readDNASTringSet(
+   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)
```

Acknowledgments

This research is supported by research grant no. R21HG005912 from the National Human Genome Research Institute (NHGRI / NIH).

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