

RcppCNPy: Reading and writing NumPy binary files

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This vignette introduces the RcppCNPy package for reading and writing files created by or for the NumPy module for Python.

Motivation

Python¹ is a widely-used and popular programming language. It is deployed in use cases ranging from simple scripting to larger-scale application development. Python is also popular for quantitative and scientific application due to the existence of extension modules such as NumPy² (which is shorthand for Numeric Python) and many other packages for data analysis.

NumPy is used to efficiently represent N -dimensional arrays, and provides an efficient binary storage model for these files. In practice, N is often equal to two, and matrices processed or generated in Python can be stored in this form. As NumPy is popular, many project utilize this file format.

R has no dedicated reading or writing functionality for these type of files. However, Carl Rogers has provided a small Cpp library called `cnpy`³ which is released under the MIT license. Using the 'Rcpp modules' feature in Rcpp (Edebuettel and François, 2011; Edebuettel, 2013; Edebuettel *et al.*, 2018), we provide (some) features of this library to R.

Examples

Data creation in Python. The first code example simply creates two files in Python: a two-dimensional rectangular array as well as a vector.

```
import numpy as np
mat = np.arange(12).reshape(3,4) * 1.1
np.save("fmat.npy", mat)
print(mat)
# [[ 0.  1.1  2.2  3.3]
# [ 4.4  5.5  6.6  7.7]
# [ 8.8  9.9 11. 12.1]]
vec = np.arange(5) * 1.1
np.save("fvec.npy", vec)
print(vec)
# [ 0.  1.1  2.2  3.3  4.4]
```

As illustrated, Python uses the Fortran convention for storing matrices and higher-dimensional arrays: a matrix constructed from a single sequence has its first consecutive elements in its first row—whereas R, following the C convention, has these first few values in its first column. This shows that to go back and forth we need to transpose these matrices (which represented internally as two-dimensional arrays).

Data reading in R. We can read the same data in R using the `npLoad()` function provided by the RcppCNPy package:

```
library(RcppCNPy)
mat <- npLoad("fmat.npy")
mat
#      [,1] [,2] [,3] [,4]
# [1,] 0.0  1.1  2.2  3.3
# [2,] 4.4  5.5  6.6  7.7
# [3,] 8.8  9.9 11.0 12.1
vec <- npLoad("fvec.npy")
vec
# [1] 0.0 1.1 2.2 3.3 4.4
```

The Fortran-order of the matrix is preserved; we obtain the exact same data as we stored.

Reading compressed data in R. A useful extension to the `cnpy` library is the support of `gzip`-compressed data.

```
mat2 <- npLoad("fmat.npy.gz")
mat2
```

Support for writing compressed files has been added in version 0.2.0.

Data writing in R. Matrices and vectors can be written to files using the `npSave()` function.

```
set.seed(42)
m <- matrix(sort(rnorm(6)), 3, 2)
m
#      [,1] [,2]
# [1,] -0.564698 0.404268
# [2,] -0.106125 0.632863
# [3,] 0.363128 1.370958
npSave("randmat.npy", m)
v <- seq(10, 12)
v
# [1] 10 11 12
npSave("simplevec.npy", v)
```

Data reading in Python. Reading the data back in Python is also straightforward as shown in the following example:

```
import numpy as np
m = np.load("randmat.npy")
print(m)
# [[-0.56469817  0.40426832]
# [-0.10612452  0.6328626 ]
# [ 0.36312841  1.37095845]]
v = np.load("simplevec.npy")
print(v)
```

¹<http://www.python.org>

²<http://numpy.scipy.org/>

³<https://github.com/rogersce/cnpy>

```
# [10 11 12]
```

Integer support. Support for integer data types has been conditional on use of either the `-std=c++0x` or the `-std=c++11` compiler extensions. Only these standards support the `long long int` type needed to represent `int64` data on a 32-bit OS. Following the release of R 3.1.0, it has been enabled by default in **RcppCNPY** (whereas it previously required a manual rebuild), and following the release of R 3.3.0 with its updated Windows toolchain, C++11 is now available on all common R platforms. Consequently, support for large integers in **RcppCNPY** is no longer just a compile-time option for some platforms, but generally available on all (current) R installations.

Performance. The R script `timing` in the `demo/` directory of the package **RcppCNPY** provides a simple benchmark. Given two values n and k , a matrix of size $n \times k$ is created with n rows and k columns. It is written to temporary files in i) `ascii` format using `write.table()`; ii) `NumPy` format using `numpySave()`; and iii) `NumPy` format using `numpySave()` with compression via the `zlib` library (used also by `gzip`).

Table 1 shows some timing comparisons for a matrix with five million elements. Reading the `numpy` data is clearly fastest as it required only parsing of the header, followed by a single large binary

Access method	Time in sec.	Relative to best
<code>numpyLoad(pyfile)</code>	0.074	1.000
<code>numpyLoad(pygzfile)</code>	0.190	2.568
<code>read.table(txtfile)</code>	4.189	56.608

Table 1. Performance comparison of data reads using a matrix of size $10^5 \times 50$. File size are 39.7mb for `ascii`, 40.0mb for `numpy` and 10.8mb for `numpy.gz`. Ten replications were performed, and total times are shown. R 3.3.1 was used on a laptop with an SSD disk.

read (and the transpose required to translate the representation used by R). The compressed file requires only one-fourth of the disk space, but takes approximately 2.5 times as long to read as the binary stream has to be transformed. Lastly, the default `ascii` reading mode is clearly by far the slowest.

Limitations

Higher-dimensional arrays. **Rcpp** supports three-dimensional arrays, this could be supported in **RcppCNPY** as well.

npz files. The `cnpy` library supports reading and writing of sets of arrays; this feature could also be exported.

Summary

The **RcppCNPY** package provides simple reading and writing of **NumPy** files, using the `cnpy` library. Reading of compressed files is also supported as an extension, offering more compact storage at the cost of slightly longer read times.

Acknowledgments. This paper can be cited as **Eddelbuettel and Wu (2016)**; see the `citation("RcppCNPY")` command in R for details.

References

- Eddelbuettel D (2013). *Seamless R and C++ Integration with Rcpp*. Use R! Springer, New York. ISBN 978-1-4614-6867-7.
- Eddelbuettel D, François R (2011). "Rcpp: Seamless R and C++ Integration." *Journal of Statistical Software*, **40**(8), 1–18. URL <http://www.jstatsoft.org/v40/i08/>.
- Eddelbuettel D, François R, Allaire J, Ushey K, Kou Q, Russel N, Chambers J, Bates D (2018). *Rcpp: Seamless R and C++ Integration*. R package version 0.12.17, URL `package=Rcpp`.
- Eddelbuettel D, Wu W (2016). "RcppCNPY: Read-Write Support for NumPy Files in R." *Journal of Open Source Software*, **1**. URL <http://dx.doi.org/10.21105/joss.00055>.