Package ‘RMSNumpress’

October 12, 2022

Type Package

Title 'Rcpp' Bindings to Native C++ Implementation of MS Numpress

Version 1.0.1

Date 2021-02-04

Description 'Rcpp' bindings to the native C++ implementation of MS Numpress, that provides two compression schemes for numeric data from mass spectrometers. The library provides implementations of 3 different algorithms, 1 designed to compress first order smooth data like retention time or M/Z arrays, and 2 for compressing non smooth data with lower requirements on precision like ion count arrays. Refer to the publication (Teleman et al., (2014) <doi:10.1074/mcp.O114.037879>) for more details.

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Imports Rcpp (>= 1.0.3)

LinkingTo Rcpp

Suggests testthat

RoxygenNote 7.0.2

NeedsCompilation yes

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Repository CRAN

Date/Publication 2021-02-04 17:20:09 UTC

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RMSNumpress-package

Description

MS Numpress

Implementations of two compression schemes for numeric data from mass spectrometers.

The library provides implementations of 3 different algorithms, 1 designed to compress first order smooth data like retention time or M/Z arrays, and 2 for compressing non smooth data with lower requirements on precision like ion count arrays.

Numpress Pic

MS Numpress positive integer compression

Intended for ion count data, this compression simply rounds values to the nearest integer, and stores these integers in a truncated form which is effective for values relatively close to zero.

Numpress Slof

MS Numpress short logged float compression

Also targeting ion count data, this compression takes the natural logarithm of values, multiplies by a scaling factor and rounds to the nearest integer. For typical ion count dynamic range these values fits into two byte integers, so only the two least significant bytes of the integer are stored.

The scaling factor can be chosen manually, but the library also contains a function for retrieving the optimal Slof scaling factor for a given data array. Since the scaling factor is variable, it is stored as a regular double precision float first in the encoding, and automatically parsed during decoding.

Numpress Lin

MS Numpress linear prediction compression

This compression uses a fixed point representation, achieve by multiplication by a scaling factor and rounding to the nearest integer. To exploit the assumed linearity of the data, linear prediction is then used in the following way.

The first two values are stored without compression as 4 byte integers. For each following value a linear prediction is made from the two previous values:

\[ X_{\text{pred}} = (X(n) - X(n-1)) + X(n) \]

\[ X_{\text{res}} = X_{\text{pred}} - X(n+1) \]
The residual \( \text{Xres} \) is then stored, using the same truncated integer representation as in Numpress Pic.

The scaling factor can be chosen manually, but the library also contains a function for retrieving the optimal Lin scaling factor for a given data array. Since the scaling factor is variable, it is stored as a regular double precision float first in the encoding, and automatically parsed during decoding.

Truncated integer representation

This encoding works on a 4 byte integer, by truncating initial zeros or ones. If the initial (most significant) half byte is 0x0 or 0xf, the number of such halfbytes starting from the most significant is stored in a halfbyte. This initial count is then followed by the rest of the ints halfbytes, in little-endian order. A count halfbyte \( c \) of

- \( 0 \leq c \leq 8 \) is interpreted as an initial \( c \) 0x0 halfbytes
- \( 9 \leq c \leq 15 \) is interpreted as an initial \((c-8)\) 0xf halfbytes

Examples:

```r
int c rest
0 => 0x8
-1 => 0xf 0xf
23 => 0x6 0x7 0x1
```

Author(s)

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References

See: https://github.com/ms-numpress/ms-numpress

See Also

- `encodeLinear`, `decodeLinear`, `encodeSlof`, `decodeSlof`, `encodePic`, `decodePic`, `optimalLinearFixedPoint`, `optimalSlofFixedPoint`, `optimalLinearFixedPointMass`

Examples

```r
## Not run:
# Encode Numpress Linear
## Retention time array
rt_array <- c(4313.0, 4316.4, 4319.8, 4323.2, 4326.6, 4330.1)
## encode retention time array
rt_encoded <- encodeLinear(rt_array, 500)
#> [1] 40 7f 40 00 00 00 00 00 d4 e7 20 00 78 ee 20 00 88 86 23

# Decode Numpress Linear
## Retention time data that is encoded with encodeLinear and is zlib compressed
### NOTE: For the sake of this example, I have broken the raw vector into several parts
### to avoid Rd line widths (>100 characters) issues with CRAN build checks.
rt_raw1 <- c("78", "9c", "73", "50", "61", "00", "83", "aa", "15", "0c", "0c", "73", "80")
```
```r
rt_raw2 <- c("b8", "a3", "5d", "Fe", "47", "07", "84", "28", "fc", "8f", "c4", "40", "e5")
rt_raw3 <- c("61", "51", "84", "a9", "85", "08", "e1", "06", "00", "06", "be", "41", "cf")
## Add all character representation of raw data back together and convert back to hex raw vector
rt_blob <- as.raw(as.hexmode(c(rt_raw1, rt_raw2, rt_raw3 )))
## Decompress blob
rt_blob_uncompressed <- as.raw(Rcompression::uncompress( rt_blob, asText = FALSE ))
## Decode to retention time double values
rt_array <- decodeLinear(rt_blob_uncompressed)
## End(Not run)
```

---

**decodeLinear**

**Description**

Decodes data encoded by `encodeLinear`.

**Usage**

```r
decodeLinear(data)
```

**Arguments**

- `data` pointer to array of bytes to be decoded (need memorycont. repr.)

**Details**

result vector guaranteed to be shorter or equal to (ndata - 8) * 2

Note that this method may throw a const char* if it deems the input data to be corrupt, i.e. that the last encoded int does not use the last byte in the data. In addition the last encoded int need to use either the last halfbyte, or the second last followed by a 0x0 halfbyte.

**Value**

the number of decoded doubles, or -1 if dataSize < 4 or 4 < dataSize < 8

**See Also**

[`encodeLinear`]

**Examples**

```r
## Not run:
## Retention time data that is encoded with encodeLinear and is zlib compressed
### NOTE: For the sake of this example, I have broken the raw vector into several parts
### to avoid Rd line widths (>100 characters) issues with CRAN build checks.
rt_raw1 <- c("78", "9c", "73", "50", "61", "00", "83", "aa", "15", "0c", "0c", "73", "80")
rt_raw2 <- c("b8", "a3", "5d", "Fe", "47", "07", "84", "28", "fc", "8f", "c4", "40", "e5")
```
```r
rt_raw3 <- c("61", "51", "84", "a9", "85", "08", "e1", "06", "06", "be", "41", "cf")
## Add all character representation of raw data back together and convert back to hex raw vector
rt_blob <- as.raw(as.hexmode(c(rt_raw1, rt_raw2, rt_raw3 )))
## Decompress blob
rt_blob_uncompressed <- as.raw(Rcompression:::uncompress( rt_blob, asText = FALSE ))
## Decode to retention time double values
rt_array <- decodeLinear(rt_blob_uncompressed)
## End(Not run)
```

---

**decodePic**

**Description**

Decodes data encoded by encodePic

result vector guaranteed to be shorter of equal to ldatal * 2

**Usage**

```r
dedecodePic(data)
```

**Arguments**

data <- pointer to array of bytes to be decoded (need memorycont. repr.)

**Details**

Note that this method may throw a const char* if it deems the input data to be corrupt, i.e. that the last encoded int does not use the last byte in the data. In addition the last encoded int need to use either the last halfbyte, or the second last followed by a 0x0 halfbyte.

**Value**

the number of decoded doubles

**See Also**

[encodePic]
decodeSlof

Description
Decodes data encoded by encodeSlof
The return will include exactly (|data| - 8) / 2 doubles.

Usage
decodeSlof(data)

Arguments
data pointer to array of bytes to be decoded (need memorycont. repr.)

Details
Note that this method may throw a const char* if it deems the input data to be corrupt.

Value
the number of decoded doubles

See Also
[encodeSlof]

Examples
## Not run:
## Intensity array to encode
### NOTE: For the sake of this example, I have broken the intensity vector into several parts
### to avoid Rd line widths (>100 characters) issues with CRAN build checks.
int_array1 <- c(0.71773432, 0.43443741, 1.71883610, 0.13220307, 0.90664242)
int_array2 <- c(0.00000000, 0.00000000, 0.64213755, 0.43443741, 0.47221479)
## Concatenate into one intensity array
int_array <- c(int_array1, int_array2)
## Encode intensity array using encodeSlof
int_encode <- encodeSlof( int_array, 16 )
## End(Not run)
Description

Encodes the doubles in data by first using a
- lossy conversion to a 4 byte 5 decimal fixed point representation
- storing the residuals from a linear prediction after first two values
- encoding by encodeInt (see above)

The resulting binary is maximally $8 + \text{dataSize} \times 5$ bytes, but much less if the data is reasonably smooth on the first order.

This encoding is suitable for typical m/z or retention time binary arrays. On a test set, the encoding was empirically show to be accurate to at least 0.002 ppm.

Usage

```
encodeLinear(data, fixedPoint)
```

Arguments

- **data**: pointer to array of double to be encoded (need memorycont. repr.)
- **fixedPoint**: the scaling factor used for getting the fixed point repr. This is stored in the binary and automatically extracted on decoding (see optimalLinearFixedPoint or optimalLinearFixedPointMass)

Value

the number of encoded bytes

See Also

[decodeLinear]

Examples

```
## Not run:
## Retention time array
rt_array <- c(4313.0, 4316.4, 4319.8, 4323.2, 4326.6, 4330.1)
## encode retention time array
rt_encoded <- encodeLinear(rt_array, 500)
#> [1] 40 7f 40 00 00 00 00 00 d4 e7 20 00 78 ee 20 00 88 86 23
```

## End(Not run)
**encodePic**

**Description**

Encodes ion counts by simply rounding to the nearest 4 byte integer, and compressing each integer with encodeInt.

**Usage**

`encodePic(data)`

**Arguments**

- **data**
  pointer to array of double to be encoded (need memorycont. repr.)

**Details**

The handleable range is therefore 0 -> 4294967294. The resulting binary is maximally `dataSize * 5` bytes, but much less if the data is close to 0 on average.

**Value**

the number of encoded bytes

**See Also**

[decodePic]

**encodeSlof**

**Description**

Encodes ion counts by taking the natural logarithm, and storing a fixed point representation of this. This is calculated as

```
unsigned short fp = log(d + 1) * fixedPoint + 0.5
```

**Usage**

`encodeSlof(data, fixedPoint)`

**Arguments**

- **data**
  pointer to array of double to be encoded (need memorycont. repr.)
- **fixedPoint**
  fixed point to use for encoding (see optimalSlofFixedPoint)
optimalLinearFixedPoint

Details
the result vector is exactly ldatal * 2 + 8 bytes long

Value
the number of encoded bytes

See Also
[decodeSlof]

optimalLinearFixedPointMass

Description
Compute the maximal linear fixed point that prevents integer overflow.

Usage
optimalLinearFixedPointMass(data, mass_acc)

Arguments
data pointer to array of double to be encoded (need memorycont. repr.)

Value
the linear fixed point safe to use

optimalLinearFixedPointMass

Description
Compute the optimal linear fixed point with a desired m/z accuracy.

Usage
optimalLinearFixedPointMass(data, mass_acc)
Arguments

data pointer to array of double to be encoded (need memorycont. repr.)

mass_acc desired m/z accuracy in Th

Value

the linear fixed point that satisfies the accuracy requirement (or -1 in case of failure).

Note

If the desired accuracy cannot be reached without overflowing 64 bit integers, then a negative value is returned. You need to check for this and in that case abandon numpress or use optimalLinearFixedPoint which returns the largest safe value.

optimalSlofFixedPoint

Description

Compute the maximal natural logarithm fixed point that prevents integer overflow.

Usage

optimalSlofFixedPoint(data)

Arguments

data pointer to array of double to be encoded (need memorycont. repr.)

Value

the slof fixed point safe to use
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