7. Storing and retrieving large data

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August 2010, 北京

Large data

“R is well known to be unable to handle large data sets.”

Solutions:

- Get a bigger computer: Linux computer with 16Gb memory for $< \$2500$
- Don’t load all the data at once (methods from the mainframe days).

Storage formats

R has two convenient data formats for large data sets

- For ordinary large data sets, the `RSQLite` package provides storage using the SQLite relational database.

- For very large 'array-structured' data sets such as whole-genome SNP chips, the `ncdf` package provides storage using the netCDF data format.

Large data

netCDF was designed by the NSF-funded UCAR consortium, who also manage the National Center for Atmospheric Research.

Atmospheric data are often array-oriented: eg temperature, humidity, wind speed on a regular grid of (x, y, z, t).

Need to be able to select ‘rectangles’ of data – eg range of (x, y, z) on a particular day t.

Because the data are on a regular grid, the software can work out where to look on disk without reading the whole file: efficient data access.

WGA

Array oriented data (position on genome, sample number) for genotypes, probe intensities.

Potentially very large data sets:

2,000 people × 300,000 = tens of Gb

16,000 people × 1,000,000 SNPs = hundreds of Gb.

Even worse after imputation to 2,500,000 SNPs.

R can't handle a matrix with more than $2^{31} - 1 \approx 2$ billion entries even if your computer has memory for it. Even data for one chromosome may be too big.

Using netCDF data

With the `ncdf` package:

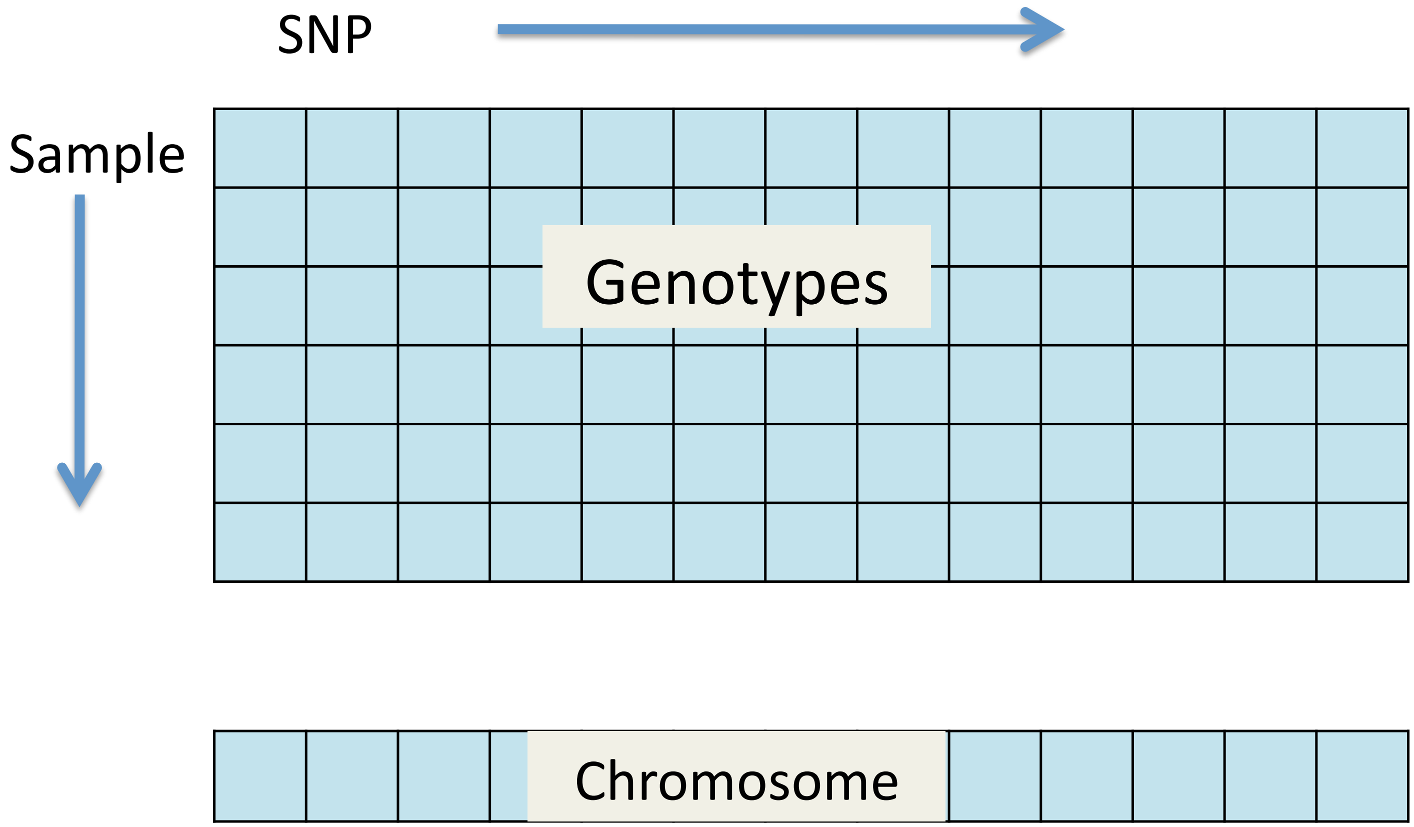
`open.ncdf()` opens a netCDF file and returns a connection to the file (rather than loading the data)

`get.var.ncdf()` retrieves all or part of a variable.

`close.ncdf()` closes the connection to the file.

Dimensions

Variables can use one or more array dimensions of a file



SNP

Sample

Genotypes

Chromosome

Example

Finding long homozygous runs (possible deletions)

```
library("ncdf")
nc <- open.ncdf("hapmap.nc")

## read all of chromosome variable
chromosome <- get.var.ncdf(nc, "chr", start=1, count=-1)
## set up list for results
runs<-vector("list", nsamples)

for(i in 1:nsamples}{
   ## read all genotypes for one person
   genotypes <- get.var.ncdf(nc, "geno", start=c(1,i),count=c(-1,1))
   ## zero for htzygous, chrm number for hmzygous
   hmzygous <- genotypes != 1
   hmzygous <- as.vector(hmzygous*chromosome)
```

Example

```
   ## consecutive runs of same value
   r <- rle(hmzygous)
   begin <- cumsum(r$lengths)
   end <- cumsum(c(1, r$lengths))
   long <- which ( r$lengths > 250 & r$values !=0)
   runs[[i]] <- cbind(begin[long], end[long], r$lengths[long])
}

close.ncdf(nc)
```

Notes

- `chr` uses only the 'SNP' dimension, so `start` and `count` are single numbers
- `geno` uses both SNP and sample dimensions, so `start` and `count` have two entries.
- `rle` compresses runs of the same value to a single entry.

Creating netCDF files

Creating files is more complicated

- Define dimensions
- Define variables and specify which dimensions they use
- Create an empty file
- Write data to the file.

Dimensions

Specify the name of the dimension, the units, and the allowed values in the `dim.def.ncdf` function.

One dimension can be ’unlimited’, allowing expansion of the file in the future. An unlimited dimension is important, otherwise the maximum variable size is 2Gb.

```
snpdim<-dim.def.ncdf("position","bases", positions)
sampledim<-dim.def.ncdf("seqnum","count",1:10, unlim=TRUE)
```

Variables

Variables are defined by name, units, and dimensions

```
varChrm <- var.def.ncdf("chr","count",dim=snpdim,
         missval=-1, prec="byte")
varSNP <- var.def.ncdf("SNP","rs",dim=snpdim,
        missval=-1, prec="integer")
vargeno <- var.def.ncdf("geno","base",dim=list(snpdim, sampledim),
        missval=-1, prec="byte")
vartheta <- var.def.ncdf("theta","deg",dim=list(snpdim, sampledim),
        missval=-1, prec="double")
varr <- var.def.ncdf("r","copies",dim=list(snpdim, sampledim),
       missval=-1, prec="double")
```

Creating the file

The file is created by specifying the file name ad a list of variables.

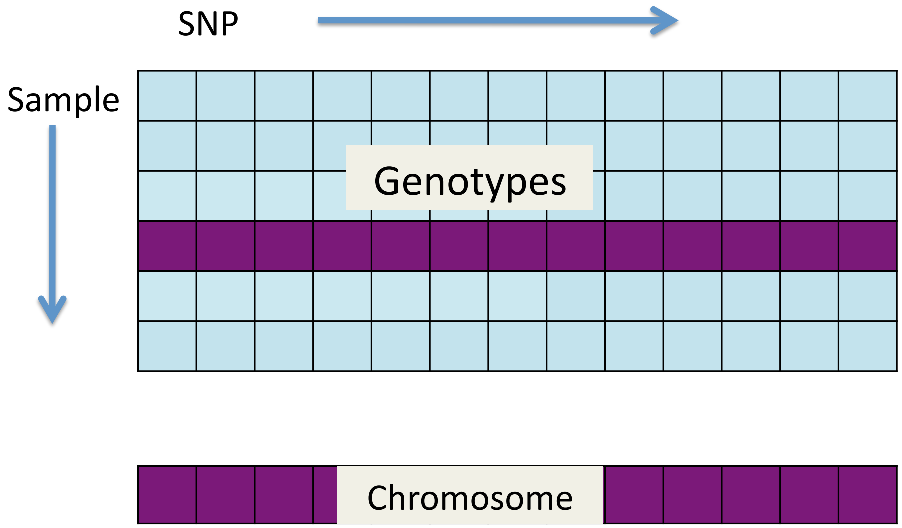
```
genofile<-create.ncdf("hapmap.nc", list(varChrm, varSNP, vargeno,
                      vartheta, varr))
```

The file is empty when it is created. Data can be written using `put.var.ncdf()`. Because the whole data set is too large to read, we might read raw data and save to netCDF for one person at a time.

```
for(i in 1:4000){
    geno<-readRawData(i) ## somehow
    put.var.ncdf(genofile, "geno", genc,
           start=c(1,i), count=c(-1,1))
}
```

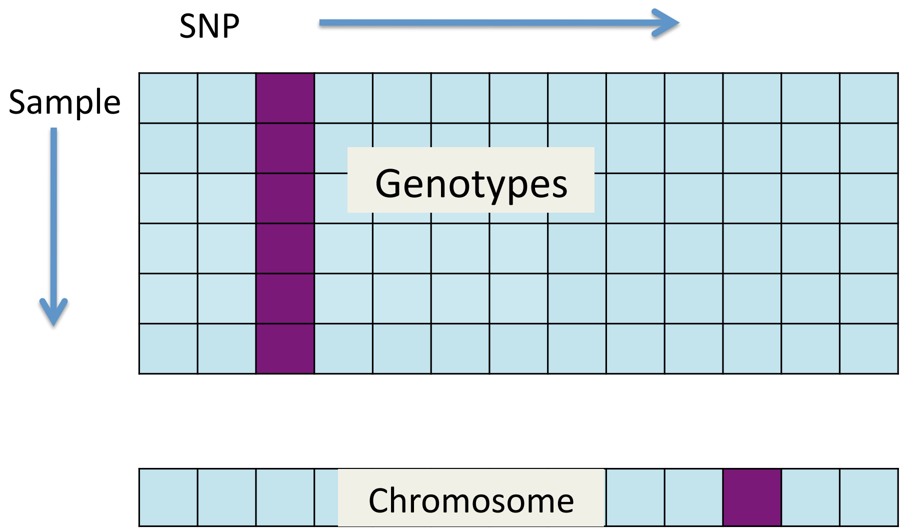
Efficient use of netCDF

Read all SNPs, one sample



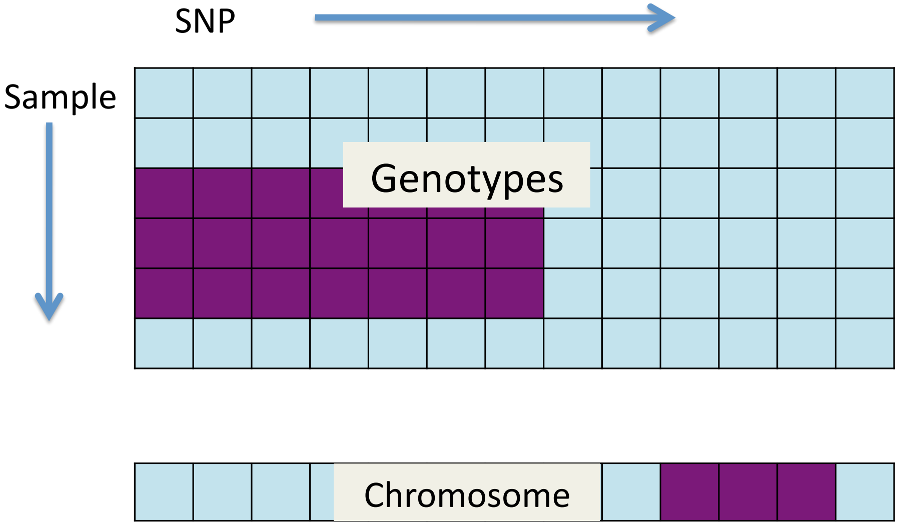
Efficient use of netCDF

Read all samples, one SNP



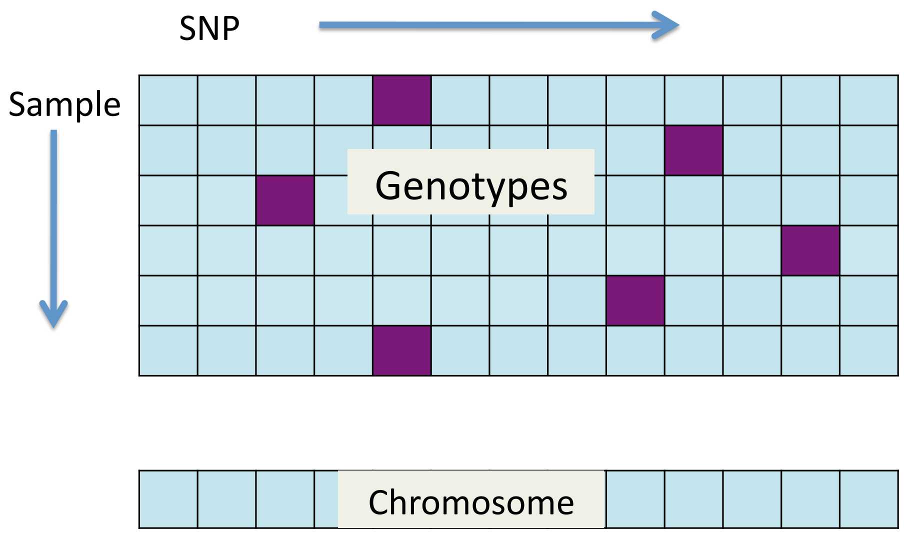
Efficient use of netCDF

Read some samples, some SNPs.



Efficient use of netCDF

Random access is not efficient: eg read probe intensities for all missing genotype calls.



Efficient use of netCDF

- Association testing: read all data for one SNP at a time

- Computing linkage disequilibrium near a SNP: read all data for a contiguous range of SNPs

- QC for aneuploidy: read all data for one individual at a time (and parents or offspring if relevant)

- Population structure and relatedness: read all SNPs for two individuals at a time.