VIDO BIOINFO Bioinformatics and Systems Biology Lab

Canadian Bioinformatics Hub

Canadian Bioinformatics Workshops

Introduction to R Programming for Bioinformatics

Day 1- Module 1B: Exploring your data in R

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Why Explore Data?

- Understand structure and types of variables
- Detect missing or incorrect values early
- Check for outliers and unusual patterns
- Guide decisions about cleaning and analysis
- Prevent errors in downstream analysis

Key Tools in R for Data Exploration

- **Preview your data**
  - head() → first few rows
  - tail() → last few rows

- **Inspect structure**
  - str() → data type & structure of each column

- **Quick summary**
  - summary() → basic statistics for each variable

- **Check dimensions**
  - dim(), nrow(), ncol()

- **Frequency counts**
  - table() → frequency counts of categorical variables

```
> summary(df)
      age             name               group
 Min.   :25.00   Length:2           Length:2
 1st Qu.:26.25   Class :character   Class :character
 Median :27.50   Mode  :character   Mode  :character
 Mean   :27.50
 3rd Qu.:28.75
 Max.   :30.00
```

Demo: Basic Data Inspections

- **Inspecting real life data of 128 patients of T- and B-cell Acute Lymphocytic Leukemia (ALL)**

RStudio

Go to file/function | Addins

Basic.R | ALL | Main_alignment_app.R | df

Filter

	X	Code	Diagnosis	Sex	Age	BT	Remission	CR	Cyto.normal	Relapse
1	1	1005	5/21/1997	M	53	B2	CR	CR	FALSE	FALSE
2	2	1010	3/29/2000	M	19	B2	CR	CR	FALSE	TRUE
3	3	3002	6/24/1998	F	52	B4	CR	CR	NA	TRUE
4	4	4006	7/17/1997	M	38	B1	CR	CR	FALSE	TRUE
5	5	4007	7/22/1997	M	57	B2	CR	CR	FALSE	TRUE
6	6	4008	7/30/1997	M	17	B1	CR	CR	FALSE	TRUE
7	7	4010	10/30/1997	F	18	B1	CR	CR	FALSE	TRUE
8	8	4016	2/10/2000	M	16	B1	CR	CR	FALSE	TRUE
9	9	6002	3/19/1997	M	15	B2	CR	CR	TRUE	TRUE
10	10	8001	1/15/1997	M	40	B2	CR	CR	FALSE	TRUE
11	11	8011	8/21/1998	M	33	B3	CR	CR	FALSE	FALSE
12	12	8012	10/22/1998	M	55	B3	CR	CR	FALSE	TRUE
13	13	8018	8/27/1999	M	5	B3	CR	CR	NA	TRUE
14	14	8024	7/20/2000	M	18	B2	CR	DEATH IN CR	FALSE	NA
15	15	9008	12/17/1999	M	41	B3	CR	CR	FALSE	FALSE
16	16	9017	2/3/2000	F	27	B	CR	CR	TRUE	TRUE
17	17	11005	6/1/1998	M	27	B2	CR	DEATH IN CR	FALSE	FALSE
18	18	12006	2/20/1997	M	46	B3	REF	REF	FALSE	NA
19	19	12007	3/11/1997	M	37	B2	CR	CR	FALSE	TRUE
20	20	12012	5/21/1997	F	36	B3	REF	REF	FALSE	NA
21	21	12019	9/4/1997	M	53	B2	CR	CR	TRUE	FALSE

Showing 1 to 22 of 128 entries, 10 total columns

Demo: Basic Data Inspections

- **The ALL dataset:**
  - Microarray gene expression data from acute lymphoblastic leukemia (ALL) patients.

- **Metadata includes patient-level information:**
  - Code: patient ID
  - Diagnosis: date of diagnosis
  - Sex, Age: demographics
  - BT: B-cell tumor subtype (e.g., B1, B2, B3, B4)
  - Remission & CR: clinical outcomes (Complete Remission, Death in CR, etc.)
  - Cyto.normal: cytogenetic normality (TRUE/FALSE)
  - Relapse: indicator of relapse

- **Key Learning Point:**
  - Understanding the structure of your dataset is the first step before any analysis.

Summarizing with Statistics

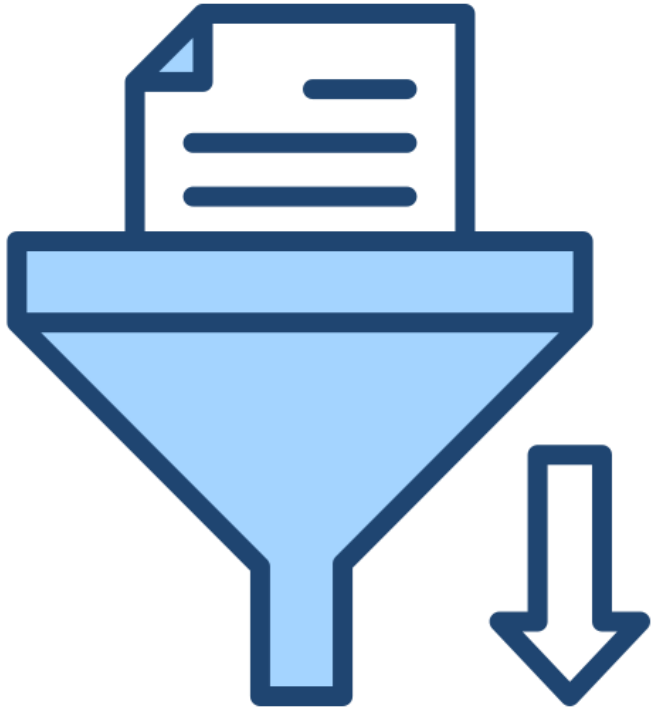
- **Central tendency:**
  - mean()
  - median()
- **Variability:**
  - sd() standard deviation
  - var() variance
- **Extremes:**
  - min()
  - max()
- **Frequency counts:**
  - table() for categorical variables
  - hist() for histogram creation
  - summary () Quick summary

```r
# View patient metadata
data("ALL")
df2 <- pData(ALL)

# Quick summary
summary(pData(ALL)[, c("age", "sex", "BT", "relapse")])

# mean and median age
mn <- mean(df2$age) # this will return NA
md <- median(df2$age) # this will return NA

mn <- mean(df2$age, na.rm = TRUE) # this will work
md <- median(df2$age, na.rm = TRUE) # this will work

# standard deviation and variance
std <- sd(df2$age, na.rm = TRUE)
vr <- var(df2$age, na.rm = TRUE)

# Extremes
mxx <- max(df2$age, na.rm = T)
mnn <- min(df2$age, na.rm = T)

# Table and (Frequency)
age_dit <- table(df2$age)

# Quick summary
summary(df2[, c("age", "sex", "BT", "relapse")])
```

Data Filtering

- **Filtering or Subsetting:**
  - Let us focus on specific patients or conditions of interest
  - Help reduce complexity
  - Prepare data for analysis or visualization

- **Common use cases (in the ALL example):**
  - Select patients above a certain age
  - Select patients by tumor subtype (BT)
  - Identify patients who relapsed



Data Filtering (Combining Conditions)

We can apply multiple filters at once

- **Real data is messy and multi-factorial.**
  - In bioinformatics, we rarely filter by just one variable. For example:
    - You might want patients older than 40 AND with relapse.
    - Or find females OR patients with subtype B2.
- **Supports hypothesis-driven exploration.**
  - Scientists often ask multi-dimensional questions like:
    - Do older male patients relapse more often?
    - Are remission rates different in B2 vs B3 subtypes, but only in females?
- **Use logical operators:**
  - & = AND
  - | = OR
  - ! = NOT

Demo: Data Filtering (Combining Conditions)

- **Subsetting**
  - subset()
- **Indexing with [**
  - df[df$Age > 40,]
  - df[df$Age > 40 & df$Relapse,]
- **Assignment with condition**
  - df <- df[df$Sex == "F",]
- **cleaner syntax: with()**
  - with(df, df[Age > 40 & Relapse == TRUE,])
  - df[which(df$Age > 40),]
- **Matching values**
  - match() / %in%
  - df[df$BT %in% c("B2", "B3"),]
- **Logical indexing directly**
  - df[df$Relapse == TRUE | df$Sex == "F",]

```r
# Subsetting and Filtering
# subset()
subset(df2, Age > 40 & Relapse == TRUE)

# Indexing with [
df2[df2$Age > 40, ]                 # filter rows
df2[df2$Age > 40 & df2$Relapse, ]   # multiple conditions (same as df$Relapse == T)
df2[, c("Age", "BT")]              # select columns
df <- df2[df$Sex == "F", ] # female patients only (#Assignment with condition)

# with()
with(df, df[Age > 40 & Relapse == TRUE, ]) #for cleaner syntax
df[which(df$Age > 40), ] # more cleanr syntax

#match() / %in% (matching values)
  df[df$BT %in% c("B2", "B3"), ]

# Logical indexing directly
  df[df$Relapse == TRUE | df$Sex == "F", ]
```

Hands-on Practice: Subsetting the ALL Metadata

- **Task 1 – Basic Filtering**
  - Extract all patients who are younger than 20 years
- **Task 2 – Single Condition + Column Selection**
  - Get only Age and Sex for patients with BT = "B2"
- **Task 3 – Combining Conditions**
  - Find male patients older than 40
  - Get patients who are female OR had a relapse
- **Mini-Challenge**
  - Find all patients who are male, had relapse, and whose age is greater than 30. How many are there?

THANK YOU

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