Practical R: Joining datasets

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Goals

- Learn how to join data sets (merging)

Data

This data set is taken from a breast cancer proteome database available here and modified for this exercise.

- Clinical data: data/BreastCancer_Clinical.xlsx
- Proteome data: data/BreastCancer_Expression.xlsx

> These data are available in the class Canvas page and the expectation is that you will save them to the `data` folder of your project.

Joins

Putting data sets together

- Quite often, data on individuals lie in different tables
    - Clinical, demographic and bioinformatic data
    - Drug, procedure, and payment data (think Medicare)
    - Personal health data across different healthcare entities

Joining data sets

The simplest case is when we just need to add more data to existing data

- New patients in study, with same protocol (add rows)
- Adding pathology, imaging data for existing patients (add columns)

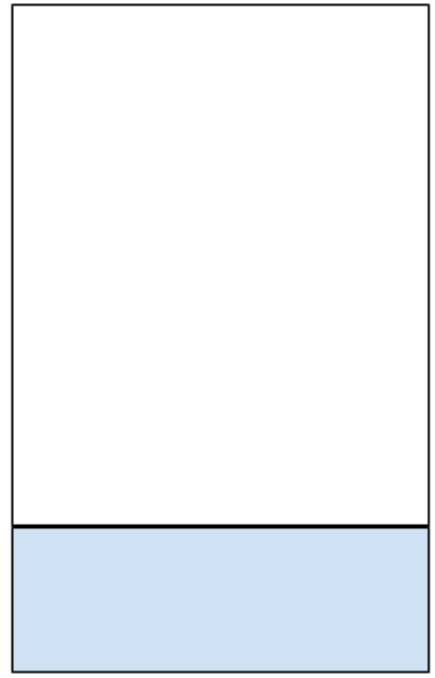
Joining data sets

`cbind(x,y)`

Add columns

Data sets have same subjects/observations, but new variables

`rbind(x,y)`



Add rows

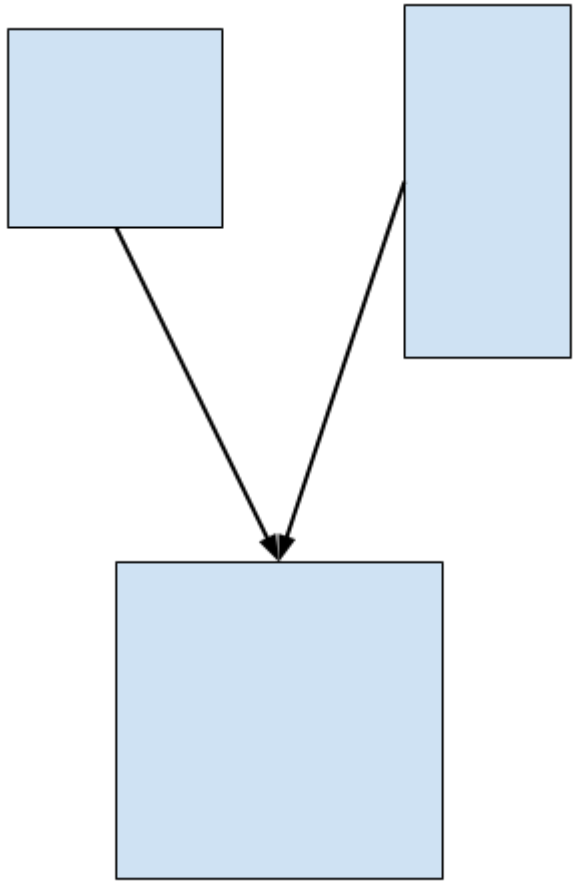
Data sets have same variables, but new subjects

Joining data sets

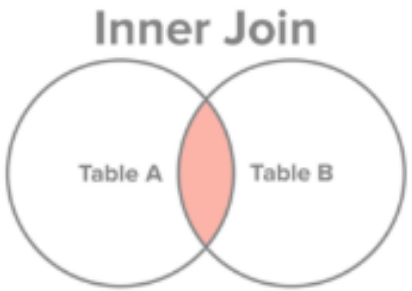
We will talk about more general ways of joining two datasets

We will assume:

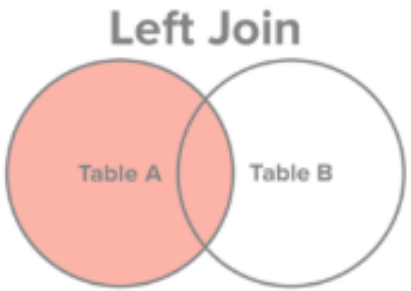
1. We have two rectangular data sets (so `data.frame` or `tibble`)
2. There is at least one variable (column) in common, even if they have different names
    - Patient ID number
    - SSN (Social Security number)
    - Identifiable information



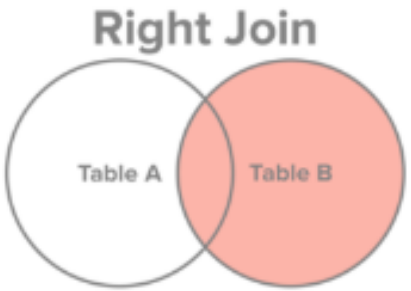
Joining data sets



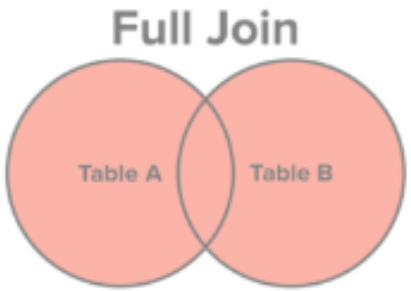
Select all records from Table A and Table B, where the join condition is met.



Select all records from Table A, along with records from Table B for which the join condition is met (if at all).



Select all records from Table B, along with records from Table A for which the join condition is met (if at all).



Select all records from Table A and Table B, regardless of whether the join condition is met or not.

inner_join	left_join	right_join	outer_join

The "join condition" are the common variables in the two datasets, i.e. rows are selected if the values of the common variables in the left dataset matches the values of the common variables in the right dataset

These functions are available in the dplyr package.

A breast cancer example

```
library(readxl)
clinical <- read_excel('data/BreastCancer_Clinical.xlsx',
                       .name_repair = 'universal') # See ?tibble::tibble
proteome <- read_excel('data/BreastCancer_Expression.xlsx',
                       .name_repair = 'universal')
```

```
clinical
```

```
# A tibble: 105 × 30
   Complete.TCGA.ID Gender Age.at.Initial.… ER.Statu
   <chr>            <chr>              <dbl> <chr>
 1 TCGA-A2-A0T2     FEMALE                66 Negative
 2 TCGA-A2-A0CM     FEMALE                40 Negative
 3 TCGA-BH-A18V     FEMALE                48 Negative
 4 TCGA-BH-A18Q     FEMALE                56 Negative
 5 TCGA-BH-A0E0     FEMALE                38 Negative
 6 TCGA-A7-A0CE     FEMALE                57 Negative
 7 TCGA-D8-A142     FEMALE                74 Negative
 8 TCGA-A2-A0D0     FEMALE                60 Negative
 9 TCGA-AO-A0J6     FEMALE                61 Negative
10 TCGA-A2-A0YM     FEMALE                67 Negative
# … with 95 more rows, and 24 more variables: Tumor
#   Tumor..T1.Coded <chr>, Node <chr>, Node.Coded <c
#   Metastasis.Coded <chr>, AJCC.Stage <chr>, Conver
#   Survival.Data.Form <chr>, Vital.Status <chr>,
#   Days.to.Date.of.Last.Contact <dbl>, Days.to.date
#   OS.event <dbl>, OS.Time <dbl>, PAM50.mRNA <chr>,
```

```
proteome
```

```
# A tibble: 83 × 11
   TCGA_ID NP_958782 NP_958785 NP_958786 NP_000436 N
   <chr>       <dbl>     <dbl>     <dbl>     <dbl>
 1 TCGA-A…     1.10      1.11      1.11      1.11
 2 TCGA-C…     2.61      2.65      2.65      2.65
 3 TCGA-A…    -0.660    -0.649    -0.654    -0.632
 4 TCGA-B…     0.195     0.215     0.215     0.205
 5 TCGA-C…    -0.494    -0.504    -0.501    -0.510
 6 TCGA-C…     2.77      2.78      2.78      2.80
 7 TCGA-E…     0.863     0.870     0.870     0.866
 8 TCGA-C…     1.41      1.41      1.41      1.41
 9 TCGA-A…     1.19      1.19      1.19      1.19
10 TCGA-A…     1.10      1.10      1.10      1.10
# … with 73 more rows, and 3 more variables: NP_9587
#   NP_001611 <dbl>
```

A breast cancer example

```
library(readxl)
clinical <- read_excel('data/BreastCancer_Clinical.xlsx',
                       .name_repair = 'universal')
proteome <- read_excel('data/BreastCancer_Expression.xlsx',
                       .name_repair = 'universal')
```

```
clinical[,1:2]
```

```
# A tibble: 105 × 2
   Complete.TCGA.ID Gender
   <chr>            <chr>
 1 TCGA-A2-A0T2     FEMALE
 2 TCGA-A2-A0CM     FEMALE
 3 TCGA-BH-A18V     FEMALE
 4 TCGA-BH-A18Q     FEMALE
 5 TCGA-BH-A0E0     FEMALE
 6 TCGA-A7-A0CE     FEMALE
 7 TCGA-D8-A142     FEMALE
 8 TCGA-A2-A0D0     FEMALE
 9 TCGA-AO-A0J6     FEMALE
10 TCGA-A2-A0YM     FEMALE
# … with 95 more rows
```

```
proteome[,1:2]
```

```
# A tibble: 83 × 2
   TCGA_ID      NP_958782
   <chr>            <dbl>
 1 TCGA-AO-A12D     1.10
 2 TCGA-C8-A131     2.61
 3 TCGA-AO-A12B    -0.660
 4 TCGA-BH-A18Q     0.195
 5 TCGA-C8-A130    -0.494
 6 TCGA-C8-A138     2.77
 7 TCGA-E2-A154     0.863
 8 TCGA-C8-A12L     1.41
 9 TCGA-A2-A0EX     1.19
10 TCGA-AO-A12D     1.10
# … with 73 more rows
```

We see that both have the same ID variable, but with different names and different orders

A breast cancer example

Let's make sure that the ID's are truly IDs, i.e. each row has a unique value

```
length(unique(clinical$Complete.TCGA.ID)) == nrow(clinical)
```

```
[1] TRUE
```

```
length(unique(proteome$TCGA_ID)) == nrow(proteome)
```

```
[1] FALSE
```

Data example

For convenience we'll keep the first instance for each ID in the `proteome` data

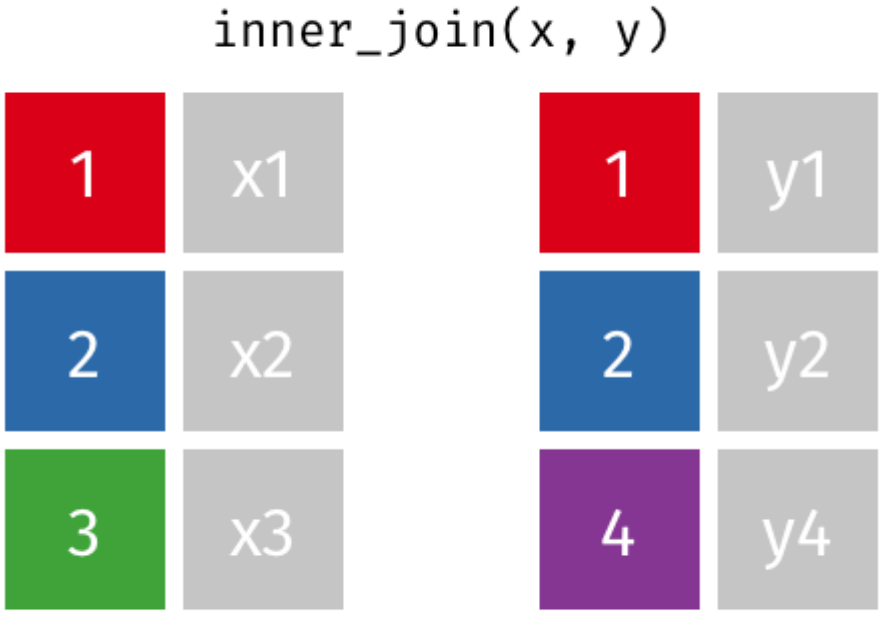
```
proteome <- proteome %>% filter(!duplicated(TCGA_ID))
```

> `duplicated` = TRUE if a previous row contains the same value

```
length(unique(proteome$TCGA_ID)) == nrow(proteome)
```

```
[1] TRUE
```

Inner join



- Keep only rows that have common ids between the two data, and add columns
- The joined data will have no more rows than either data, but more columns than each

Inner join

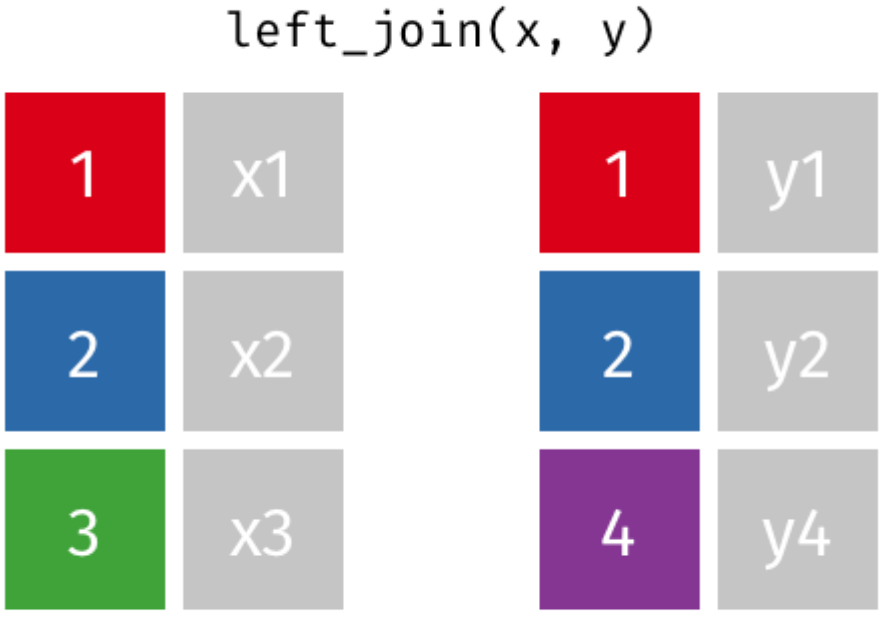
```
common_rows <- inner_join(clinical[,1:6], proteome,
                          by=c('Complete.TCGA.ID'='TCGA_ID'))
```

```
# A tibble: 77 × 16
   Complete.TCGA.ID Gender Age.at.Initial.… ER.Status PR.Status HER2.Final.Stat…
   <chr>            <chr>             <dbl> <chr>     <chr>     <chr>
 1 TCGA-A2-A0CM     FEMALE               40 Negative  Negative  Negative
 2 TCGA-BH-A18Q     FEMALE               56 Negative  Negative  Negative
 3 TCGA-A7-A0CE     FEMALE               57 Negative  Negative  Negative
 4 TCGA-D8-A142     FEMALE               74 Negative  Negative  Negative
 5 TCGA-AO-A0J6     FEMALE               61 Negative  Negative  Negative
 6 TCGA-A2-A0YM     FEMALE               67 Negative  Negative  Negative
 7 TCGA-A2-A0D2     FEMALE               45 Negative  Negative  Negative
 8 TCGA-A2-A0SX     FEMALE               48 Negative  Negative  Negative
 9 TCGA-AO-A0JL     FEMALE               59 Negative  Negative  Negative
10 TCGA-AO-A12F     FEMALE               36 Negative  Negative  Negative
# … with 67 more rows, and 10 more variables: NP_958782 <dbl>, NP_958785 <dbl>,
#   NP_958786 <dbl>, NP_000436 <dbl>, NP_958781 <dbl>, NP_958780 <dbl>,
#   NP_958783 <dbl>, NP_958784 <dbl>, NP_112598 <dbl>, NP_001611 <dbl>
```

Note that we have all the columns from both datasets, but only the common set of IDs from the two datasets

> Without the by option, R will attempt to join on all column names that are common between the data sets. If the ID columns have different names, you **must** use by. Even if they have the same names, it's good practice to be explicity

Left join



- Keep all rows of left data, add columns from right data only for rows with matching IDs
- If a row in left data has no corresponding row in the right data, the corresponding entries in the joined data are replaced by `NA`
- Joined data has same number of rows as left data, but more columns.

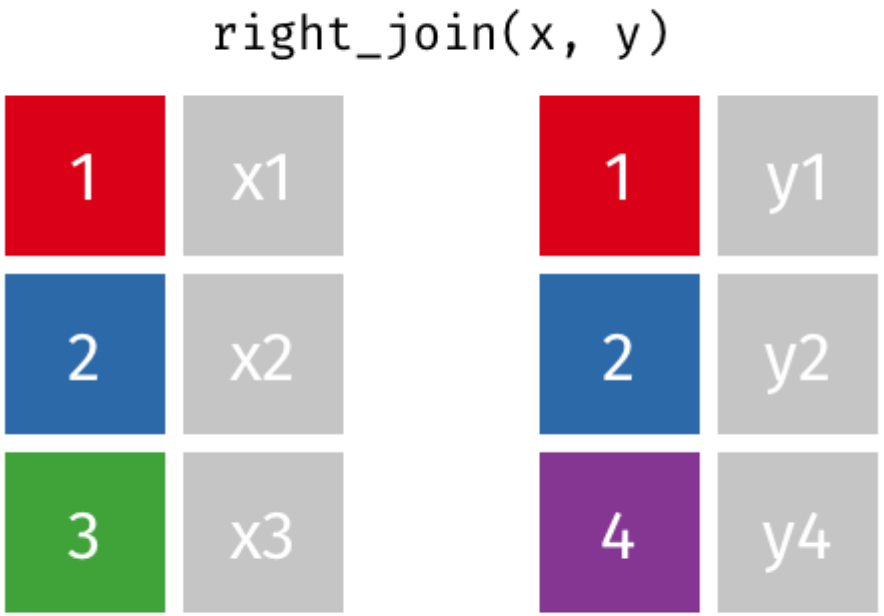
Left join

```
left_rows <- left_join(clinical[,1:6], proteome, by=c('Complete.TCGA.ID'='TCGA_ID'))
```

```
# A tibble: 105 × 16
  Complete.TCGA.ID Gender Age.at.Initial.Pathologic.Diagnosis ER.Status
  <chr>            <chr>                                <dbl> <chr>
1 TCGA-A2-A0T2     FEMALE                                  66 Negative
2 TCGA-A2-A0CM     FEMALE                                  40 Negative
3 TCGA-BH-A18V     FEMALE                                  48 Negative
  PR.Status HER2.Final.Status NP_958782 NP_958785 NP_958786 NP_000436 NP_958781
  <chr>     <chr>                 <dbl>     <dbl>     <dbl>     <dbl>     <dbl>
1 Negative  Negative             NA        NA        NA        NA        NA
2 Negative  Negative              0.683     0.694     0.698     0.687     0.687
3 Negative  Negative             NA        NA        NA        NA        NA
  NP_958780 NP_958783 NP_958784 NP_112598 NP_001611
      <dbl>     <dbl>     <dbl>     <dbl>     <dbl>
1    NA        NA        NA         NA       NA
2     0.698     0.698     0.698     -2.65    -0.984
3    NA        NA        NA         NA       NA
# … with 102 more rows
```

We get 105 rows, which is all the rows of `clinical`, combined with the rows of `proteome` with common IDs. The rest of the rows get `NA` for the proteome columns.

Right join



- Keep all the rows of the *right* data, add corresponding rows of left data *on the left*
- Once again, if there are rows of right data that do not have corresponding rows in left data, the entries are filled with `NA`
- The joined data has the same number of rows as the right data, but more columns (attached to its left). The order of the columns is the columns of the left data followed by the columns of the right data

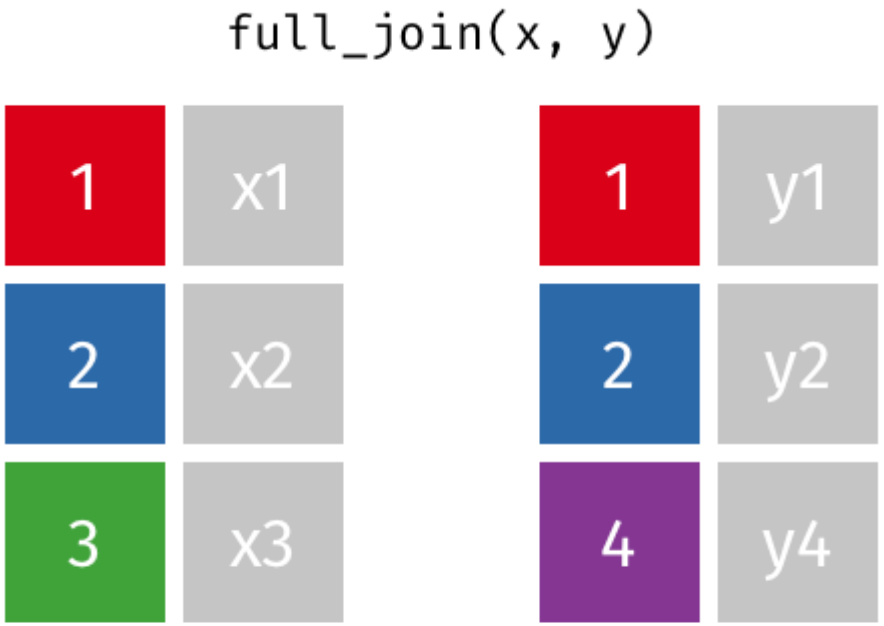
Right join

```
right_rows <- right_join(clinical[,1:6], proteome, by=c('Complete.TCGA.ID'='TCGA_ID'))
```

```
# A tibble: 80 × 16
  Complete.TCGA.ID Gender Age.at.Initial.Pathologic.Diagnosis ER.Status
  <chr>            <chr>                                <dbl> <chr>
1 TCGA-A2-A0CM     FEMALE                                  40 Negative
2 TCGA-BH-A18Q     FEMALE                                  56 Negative
3 TCGA-A7-A0CE     FEMALE                                  57 Negative
  PR.Status HER2.Final.Status NP_958782 NP_958785 NP_958786 NP_000436 NP_958781
  <chr>     <chr>                 <dbl>     <dbl>     <dbl>     <dbl>     <dbl>
1 Negative  Negative              0.683     0.694     0.698     0.687     0.687
2 Negative  Negative              0.195     0.215     0.215     0.205     0.215
3 Negative  Negative             -1.12     -1.12     -1.12     -1.13     -1.13
  NP_958780 NP_958783 NP_958784 NP_112598 NP_001611
      <dbl>     <dbl>     <dbl>     <dbl>     <dbl>
1     0.698     0.698     0.698     -2.65    -0.984
2     0.215     0.215     0.215     -1.04    -0.517
3    -1.12     -1.12     -1.12       2.24    -2.58
# … with 77 more rows
```

Here we get 80 rows, which is all the rows of `proteome`, along with the rows of `clinical` with common IDs, but with the columns of `clinical` appearing first.

Outer/Full Join



This is the *kitchen sink* join

- All rows of the left and right data are included
- Non-corresponding entries are filled with `NA`
- The joined data set has at least as many rows as the larger of the two data, and more columns than either data.

Outer/Full Join

```
full_rows <- full_join(clinical[,1:6], proteome, by=c('Complete.TCGA.ID'='TCGA_ID'))
```

```
# A tibble: 108 × 16
  Complete.TCGA.ID Gender Age.at.Initial.Pathologic.Diagnosis ER.Status
  <chr>            <chr>                                <dbl> <chr>
1 TCGA-A2-A0T2     FEMALE                                  66 Negative
2 TCGA-A2-A0CM     FEMALE                                  40 Negative
3 TCGA-BH-A18V     FEMALE                                  48 Negative
  PR.Status HER2.Final.Status NP_958782 NP_958785 NP_958786 NP_000436 NP_958781
  <chr>     <chr>                 <dbl>     <dbl>     <dbl>     <dbl>     <dbl>
1 Negative  Negative             NA        NA        NA        NA        NA
2 Negative  Negative              0.683     0.694     0.698     0.687     0.687
3 Negative  Negative             NA        NA        NA        NA        NA
  NP_958780 NP_958783 NP_958784 NP_112598 NP_001611
      <dbl>     <dbl>     <dbl>     <dbl>     <dbl>
1    NA        NA        NA         NA       NA
2     0.698     0.698     0.698     -2.65    -0.984
3    NA        NA        NA         NA       NA
# … with 105 more rows
```

Here we obtain 108 rows and 16 columns. So we've expanded the data in both rows and columns, putting missing values in where needed.

Joins

In each of `inner_join`, `left_join`, `right_join` and `full_join`, the number of columns always increases

There are also two joins where the number of columns don't increase. They aren't really "joins" in that sense, but really fancy filters on a dataset

Join	Use	Description
semi_join	semi_join(A,B)	Keep rows in A where ID matches some ID value in B
anti_join	anti_join(A,B)	Keep rows in A where ID does NOT match any ID value in B

These just filter the rows of `A` without adding any columns of `B`. These can be faster than `dplyr::filter` when dealing with large data sets

Putting it in a pipe

```
final_data <- clinical %>%
  inner_join(proteome, by=c("Complete.TCGA.ID"="TCGA_ID")) %>%
  filter(Gender =='FEMALE') %>%
  select(Complete.TCGA.ID, Age.at.Initial.Pathologic.Diagnosis, ER.Status,
         starts_with("NP")) # grabs all the protein data
```

```
# A tibble: 75 × 13
  Complete.TCGA.ID Age.at.Initial.Pathologic.Diagnosis ER.Status NP_958782
  <chr>                                          <dbl> <chr>         <dbl>
1 TCGA-A2-A0CM                                      40 Negative      0.683
2 TCGA-BH-A18Q                                      56 Negative      0.195
3 TCGA-A7-A0CE                                      57 Negative     -1.12
  NP_958785 NP_958786 NP_000436 NP_958781 NP_958780 NP_958783 NP_958784
      <dbl>     <dbl>     <dbl>     <dbl>     <dbl>     <dbl>     <dbl>
1     0.694     0.698     0.687     0.687     0.698     0.698     0.698
2     0.215     0.215     0.205     0.215     0.215     0.215     0.215
3    -1.12     -1.12     -1.13     -1.13     -1.12     -1.12     -1.12
  NP_112598 NP_001611
      <dbl>     <dbl>
1     -2.65    -0.984
2     -1.04    -0.517
3      2.24    -2.58
# … with 72 more rows
```

Some notes

- Joins are very much in the spirit of using SQL in databases
- In SAS, if you use `MERGE` in the `DATA` step to create merged variables, you need to sort the data by the common variables
  - This is a very expensive operation computationally
  - In SAS, you can avoid this by using `PROC SQL`
  - In R, this sorting is not necessary
- Learning to join data sets efficiently is one of the coolest skills of a data scientist, and makes life infinitely easier

Example code: Joining many datasets together

Requirement: Pull together over 200 datasets of variant alleles and expressions (1 per subject/cell line)

```
library(dplyr)

fnames <- dir('~/Desktop/Sreya', full.names = TRUE) # Grab and store the paths to the individual files
ids <- stringr::str_extract(fnames, '[:alnum:]+') # The file names have the subject ids in them
                                                  # as first bit of the string

## Data ingestion
data_corpus <- purrr::map(fnames, read_delim, delim='\t') # Creates a list of raw datasets

## Data munging
for (i in 1:length(data_corpus)){
  data_corpus[[i]] <- data_corpus[[i]] %>% # Note [[]] since I'm manipulating lists
    select(`Variant Allele`, HF) %>% # Keep only allele name and expression
    set_names("variant_allele", ids[i]) %>% # change column names to `variant_allele` and subject ID
    mutate(variant_allele = str_trim(variant_allele)) # Getting rid of extra spaces
}

## Data joining
data_merged <- Reduce(full_join, data_corpus) # Here is the join. This works since
                                              # all the data sets have only `variant_allele` in common
```

> We haven't seen two functions here: `purrr::map` and `Reduce`. I won't go into details here, but see the short version on next slide. Also notice that the number of files to be joined is never specified in the code. This could work for any number of files

Example code: Joining many datasets together

- The `map` function acts on a list (first argument) and applies a function (2nd argument) to each element, storing the result in a list the same size as the first argument. You could replace the map function with a for loop, but map is provably more efficient computationally. It is worth thinking about map like a for loop, though. Nice tutorial
- `Reduce` is a very powerful function that is one of the functional programming functions in R, i.e., it is a function that acts on functions. It takes as inputs a function (in our case, `full_join`), and a list (in our case, data_corpus). The input function should take two arguments of the same type, as `full_join` does, and Reduce goes through the list, applying the function to the first two elements of the list, then to the result and the 3rd element, then to the result and 4th element,and so on.