Using make_design to generate experimental designs

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Where are we so far?

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In vignette("gc03_incorporate_designs"), we focused on importing designs from files, since that's the most common way of creating designs. Here, we're going to show how designs can alternatively be generated within R using the gcplyr function make_design.

If you haven't already, load the necessary packages.

library(gcplyr)

Including design elements

As a reminder, gcplyr enables incorporation of design elements in two ways:

- 1. Designs can be imported from files
- 2. Designs can be generated in R using make_design

For generating designs in R, make_design can create:

- block-shaped data.frames with your design information (for saving to files)
- tidy-shaped data.frames with your design information (for saving to files and merging with tidy-shaped data)

An example with a single design

Let's start with a simple design.

Imagine you have a 96 well plate (12 columns and 8 rows) with a different bacterial strain in each row, leaving the first and last rows and columns empty.

Row names	Column 1	Column 2	Column 3	 Column 11	Column 12
Row A Row B Row B	Blank Blank Blank	Blank Strain #1 Strain #2	Blank Strain #1 Strain #2	 Blank Strain #1 Strain #2	Blank Blank Blank
Row G Row H	 Blank Blank Blank	 Strain #5 Strain #6 Blank	 Strain #5 Strain #6 Blank	 Strain #5 Strain #6 Blank	 Blank Blank Blank

Typing a design like this manually into a spreadsheet can be tedious. But generating it with make_design is easier.

make_design first needs some general information, like the nrows and ncols in the plate, and the output_format you'd like (typically blocks or tidy).

Then, for each different design component, make_design needs five different pieces of information:

- a vector containing the possible values
- a vector specifying which rows these values should be applied to
- a vector specifying which columns these values should be applied to
- a string or vector of the pattern of these values
- a Boolean for whether this pattern should be filled byrow (defaults to TRUE)

So for our example above, we can see:

- the possible values are c("Strain 1", "Strain 2", "Strain 3", "Strain 4", "Strain 5", "Strain 6")
- the rows these values should be applied to are 2:7
- the columns these values should be applied to are 2:11
- the pattern these values should be filled in by is "123456"
- and these values should not be filled by row (they should be filled by column)

```
my_design_blk
#> [[1]]
#> [[1]]$data
   1 2
               3
                             5
                                    6
                                           7
                                                   8
                                                                 10
                                                                               12
                      4
#> A NA NA
               NA
                      NA
                             NA
                                    NA
                                           NA
                                                  NA
                                                         NA
                                                                 NA
                                                                        NA
                                                                               NA
#> B NA "Str1" "NA
#> C NA "Str2" NA
#> D NA "Str3" NA
#> E NA "Str4" "NA
#> F NA "Str5" "Str5" "Str5" "Str5" "Str5" "Str5" "Str5" "Str5" "Str5" "NA
#> G NA "Str6" "Str6" "Str6" "Str6" "Str6" "Str6" "Str6" "Str6" "Str6" "NA
#> H NA NA
               NA
                      NA
                             NA
                                    NA
                                           NA
                                                  NA
                                                          NA
#>
#> [[1]]$metadata
#> block_name
#> "Bacteria"
```

This produces a data.frame with Bacteria as the block_name in the metadata. If we save this design to a file or transform it to tidy-shaped, this block_name metadata will come in handy.

A few notes on the pattern

The pattern in make_design is flexible to make it easy to input designs.

The "0" character is reserved for NA values, and can be put into your pattern anywhere you'd like to have the value be NA

```
my_design_blk <- make_design(</pre>
  output format = "blocks",
  nrows = 8, ncols = 12,
  Bacteria = list(c("Str1", "Str2", "Str3",
                     "Str4", "Str5", "Str6"),
                  2:7,
                   2:11,
                   "123056",
                  FALSE)
)
my_design_blk
#> [[1]]
#> [[1]]$data
#>
   1 2
               3
                              5
                                      6
                                             7
                                                     8
                                                                    10
                                                                           11
                                                                                  12
                       4
#> A NA NA
                                                                                  NA
               NA
                       NA
                              NA
                                      NA
                                             NA
                                                    NA
                                                            NA
                                                                   NA
#> B NA "Str1" NA
#> C NA "Str2" NA
```

```
#> D NA "Str3" "NA
#> E NA NA
                                    NA
                      NA
                             NA
                                           NA
                                                  NA
                                                         NA
                                                                NA
#> F NA "Str5" NA
#> G NA "Str6" "Str6" "Str6" "Str6" "Str6" "Str6" "Str6" "Str6" "Str6" "NA
#> H NA NA
              NA
                      NA
                             NA
                                    NA
                                           NA
                                                  NA
                                                         NA
                                                                NA
#>
#> [[1]]$metadata
#> block_name
#> "Bacteria"
```

In the previous examples, I used the numbers 1 through 6 to correspond to our values. If you have more than 9 values, you can use letters too. By default, the order is numbers first, then uppercase letters, then lowercase letters (so "A" is the 10th index). However, if you'd like to only use letters, you can simply specify a different lookup_tbl_start so that make_design knows what letter you're using as the 1 index.

```
my_design_blk <- make_design(
  output_format = "blocks",
  nrows = 8, ncols = 12, lookup_tbl_start = "A",
  Bacteria = list(
    c("Str1", "Str2", "Str3", "Str4", "Str5", "Str6"),
    2:7,
    2:11,
    "ABCDEF",
    FALSE)
)</pre>
```

You can also specify the pattern as a vector rather than a string.

```
my_design_blk <- make_design(
  output_format = "blocks",
  nrows = 8, ncols = 12,
  Bacteria = list(
    c("Str1", "Str2", "Str3", "Str4", "Str5", "Str6"),
    2:7,
    2:11,
    c(1,2,3,4,5,6),
    FALSE)
)</pre>
```

Continuing with the example: multiple designs

Now let's return to our example growth curve experiment. In addition to having a different bacterial strain in each row, we now also have a different media in each column of the plate.

Row names	Column 1	Column 2	Column 3	 Column 11	Column 12
Row A Row B	Blank Blank	Blank Media #1	Blank Media #2	 Blank Media #10	Blank Blank
Row G Row H	 Blank Blank	 Media #1 Blank	 Media #2 Blank	 Media #10 Blank	 Blank Blank

We can generate both designs with make_design:

```
my_design_blk <- make_design(</pre>
  output_format = "blocks",
  nrows = 8, ncols = 12, lookup_tbl_start = "a",
  Bacteria = list(c("Str1", "Str2", "Str3",
                    "Str4", "Str5", "Str6"),
                  2:7,
                  2:11,
                  "abcdef",
                  FALSE),
  Media = list(c("Med1", "Med2", "Med3",
                 "Med4", "Med5", "Med6",
                 "Med7", "Med8", "Med9",
                 "Med10", "Med11", "Med12"),
               2:7,
               2:11,
               "abcdefghij")
  )
my_design_blk
#> [[1]]
#> [[1]]$data
#>
   1 2
               3
                              5
                                     6
                                            7
                                                    8
                                                           9
                                                                  10
                                                                         11
                                                                                 12
                                                           NA
                                                                         NA
               NA
                      NA
                              NA
                                     NA
                                            NA
                                                   NA
                                                                  NA
#> B NA "Str1" NA
#> C NA "Str2" NA
#> D NA "Str3" "NA
#> E NA "Str4" "NA
#> F NA "Str5" NA
#> G NA "Str6" NA
#> H NA NA
               NA
                      NA
                              NA
                                     NA
                                            NA
                                                    NA
                                                           NA
                                                                  NA
#>
#> [[1]]$metadata
#> block_name
#> "Bacteria"
#>
#>
#> [[2]]
#> [[2]]$data
   1 2
               3
                              5
                                     6
                                            7
                                                                  10
                                                                         11
                                                                                  12
#> A NA NA
               NA
                      NA
                             NA
                                     NA
                                            NA
                                                   NA
                                                           NA
                                                                  NA
#> B NA "Med1" "Med2" "Med3" "Med4" "Med5" "Med6" "Med7" "Med8" "Med9" "Med10" NA
#> C NA "Med1" "Med2" "Med3" "Med4" "Med5" "Med6" "Med7" "Med8" "Med9" "Med10" NA
#> D NA "Med1" "Med2" "Med3" "Med4" "Med5" "Med6" "Med7" "Med8" "Med9" "Med10" NA
#> E NA "Med1" "Med2" "Med3" "Med4" "Med5" "Med6" "Med7" "Med8" "Med9" "Med10" NA
#> F NA "Med1" "Med2" "Med3" "Med4" "Med5" "Med6" "Med7" "Med8" "Med9" "Med10" NA
#> G NA "Med1" "Med2" "Med3" "Med4" "Med5" "Med6" "Med7" "Med8" "Med9" "Med10" NA
#> H NA NA
               NA
                      NA
                              NA
                                     NA
                                            NA
                                                   NA
                                                           NA
                                                                  NA
                                                                                 NA
#> [[2]]$metadata
#> block_name
   "Media"
```

However, the real strength of make_design is that it is not limited to simple alternating patterns. make_design can use irregular patterns too, replicating them as needed to fill all the wells.

```
my_design_blk <- make_design(</pre>
  output_format = "blocks",
  nrows = 8, ncols = 12, lookup_tbl_start = "a",
  Bacteria = list(c("Str1", "Str2"),
                  2:7,
                  2:11,
                  "abaaabbbab",
                  FALSE),
 Media = list(c("Med1", "Med2", "Med3"),
               2:7,
               2:11,
               "aabbbc000abc"))
my_design_blk
#> [[1]]
#> [[1]]$data
                                            7
   1 2
               3
                              5
                                     6
                                                                  10
                                                                         11
                                                                                 12
                      4
#> A NA NA
               NA
                             NA
                                     NA
                                            NA
                                                           NA
                                                                  NA
                                                                         NA
                                                                                 NA
                      NA
                                                   NA
#> B NA "Str1" "Str2" "Str1" "Str1" "Str1" "Str1" "Str2" "Str1" "Str1" "Str1" NA
#> C NA "Str2" "Str2" "Str1" "Str2" "Str2" "Str2" "Str2" "Str1" "Str2" "Str2" NA
#> D NA "Str1" "Str1" "Str1" "Str1" "Str2" "Str1" "Str1" "Str1" "Str1" "Str1" "Str2" NA
#> E NA "Str1" "Str2" "Str2" "Str2" "Str1" "Str2" "Str2" "Str2" "Str2" NA
#> F NA "Str1" "Str1" "Str2" "Str1" "Str1" "Str1" "Str1" "Str2" "Str1" "Str1" NA
#> G NA "Str2" "Str2" "Str2" "Str1" "Str2" "Str2" "Str2" "Str2" "Str1" "Str2" NA
#> H NA NA
               NA
                      NA
                             NA
                                     NA
                                            NA
                                                   NA
                                                           NA
                                                                  NA
#>
#> [[1]]$metadata
#> block name
#> "Bacteria"
#>
#>
#> [[2]]
#> [[2]]$data
                                            7
   1 2
               3
                                     6
                                                    8
                                                           9
                                                                  10
                                                                         11
                                                                                 12
#> A NA NA
                             NA
                                     NA
                                            NA
                                                    NA
                                                           NA
                                                                  NA
                                                                         NA
                                                                                 NA
               NA
                      NA
#> B NA "Med1" "Med1" "Med2" "Med2" "Med2" "Med3" NA
                                                           NA
                                                                  NA
                                                                          "Med1" NA
#> C NA "Med2" "Med3" "Med1" "Med1" "Med2" "Med2" "Med2" "Med3" NA
                                                                                 NA
#> D NA NA
               "Med1" "Med2" "Med3" "Med1" "Med1" "Med2" "Med2" "Med2" "Med3" NA
                              "Med1" "Med2" "Med3" "Med1" "Med1" "Med2" "Med2" NA
#> E NA NA
               NA
                      NA
#> F NA "Med2" "Med3" NA
                                             "Med1" "Med2" "Med3" "Med1" "Med1" NA
                                     NA
#> G NA "Med2" "Med2" "Med2" "Med3" NA
                                                           "Med1" "Med2" "Med3" NA
                                            NA
                                                   NA
#> H NA NA
               NA
                      NA
                              NA
                                     NA
                                            NA
                                                   NA
                                                           NA
                                                                  NA
                                                                         NA
#>
#> [[2]]$metadata
#> block_name
#> "Media"
```

There is also an optional helper function called make_designpattern, or mdp for short. make_designpattern just reminds us what arguments are necessary for each design. For example:

```
my_design_blk <- make_design(
  output_format = "blocks",
  nrows = 8, ncols = 12, lookup_tbl_start = "a",</pre>
```

```
Bacteria = mdp(
   values = c("Str1", "Str2", "Str3",
              "Str4", "Str5", "Str6"),
   rows = 2:7, cols = 2:11, pattern = "abc0ef",
   byrow = FALSE),
 Media = mdp(
   values = c("Med1", "Med2", "Med3",
              "Med4", "Med5", "Med6",
              "Med7", "Med8", "Med9",
              "Med10", "Med11", "Med12"),
   rows = 2:7, cols = 2:11, pattern = "abcde0ghij"))
my_design_blk
#> [[1]]
#> [[1]]$data
#> 1 2
              3
                           5
                                   6
                                          7
                                                8
                                                              10
                                                                     11
                                                                            12
#> A NA NA
              NA
                           NA
                                   NA
                                         NA
                                                NA
                                                       NA
                     NA
#> B NA "Str1" "NA
#> C NA "Str2" NA
#> D NA "Str3" "NA
#> E NA NA
                         NA
                                  NA NA
                                              NA NA
              NA
                   NA
                                                              NA NA
#> F NA "Str5" "Str5" "Str5" "Str5" "Str5" "Str5" "Str5" "Str5" "Str5" "NA
#> G NA "Str6" NA
#> H NA NA
             NA
                     NA
                            NA
                                   NA
                                          NA
                                                NA
                                                       NA
                                                              NA
#>
#> [[1]]$metadata
#> block name
#> "Bacteria"
#>
#>
#> [[2]]
#> [[2]]$data
#> 1 2
              3
                            5
                                   6
                                          7 8
                                                    9
                                                          10
                                                                 11
                                                                         12
#> A NA NA
             NA
                     NA
                           NA
                                   NA
                                          NA NA
                                                    NA
#> B NA "Med1" "Med2" "Med3" "Med4" "Med5" NA "Med7" "Med8" "Med9" "Med10" NA
#> C NA "Med1" "Med2" "Med3" "Med4" "Med5" NA "Med7" "Med8" "Med9" "Med10" NA
#> D NA "Med1" "Med2" "Med3" "Med4" "Med5" NA "Med7" "Med8" "Med9" "Med10" NA
#> E NA "Med1" "Med2" "Med3" "Med4" "Med5" NA "Med7" "Med8" "Med9" "Med10" NA
#> F NA "Med1" "Med2" "Med3" "Med4" "Med5" NA "Med7" "Med8" "Med9" "Med10" NA
#> G NA "Med1" "Med2" "Med3" "Med4" "Med5" NA "Med7" "Med8" "Med9" "Med10" NA
#> H NA NA
                                          NA NA
              NA
                     NA
                            NA
                                   NA
                                                    NA
                                                          NA
                                                                 NA
#>
#> [[2]]$metadata
#> block name
#> "Media"
```

For merging our designs with plate reader data, we need it tidy-shaped, so we just need to change the output_format to tidy.

```
my_design_tdy <- make_design(
  output_format = "tidy",
  nrows = 8, ncols = 12, lookup_tbl_start = "a",
  Bacteria = mdp(</pre>
```

```
values = c("Str1", "Str2", "Str3",
              "Str4", "Str5", "Str6"),
   rows = 2:7, cols = 2:11, pattern = "abc0ef",
   byrow = FALSE),
  Media = mdp(
   values = c("Med1", "Med2", "Med3",
              "Med4", "Med5", "Med6",
               "Med7", "Med8", "Med9",
               "Med10", "Med11", "Med12"),
   rows = 2:7, cols = 2:11, pattern = "abcde0ghij"))
#> Inferred 'into' column names as: Bacteria, Media
head(my design tdy, 20)
      Well Bacteria Media
#>
#> 1
        A1
               <NA> <NA>
#> 2
        A2
               <NA> <NA>
#> 3
       A3
               <NA> <NA>
#> 4
               <NA> <NA>
       A4
#> 5
       A5
               <NA> <NA>
#> 6
               <NA> <NA>
       A6
#> 7
       A7
               <NA> <NA>
       A8
#> 8
               <NA> <NA>
#> 9
       A9
               <NA> <NA>
#> 10 A10
               <NA> <NA>
#> 11 A11
               <NA>
                    <NA>
#> 12 A12
               <NA>
                    <NA>
#> 13
               <NA> <NA>
       B1
#> 14
              Str1 Med1
       B2
#> 15
       ВЗ
              Str1 Med2
#> 16
       B4
              Str1 Med3
#> 17
       B5
               Str1 Med4
#> 18
       B6
               Str1 Med5
#> 19
        B7
               Str1
                    <NA>
#> 20
       B8
              Str1 Med7
```

Saving designs to files

If you'd like to save the designs you've created with make_design to files, you just need to decide if you'd like them tidy-shaped or block-shaped. Both formats can easily be read back into R by gcplyr.

Saving tidy-shaped designs

These design files will be less human-readable, but easier to import and merge. Additionally, tidy-shaped files are often better for data repositories, like Dryad. To save tidy-shaped designs, simply use the built-in write.csv function.

Saving block-shaped designs

These design files will be more human-readable but slightly more computationally involved to import and merge. For these, use the gcplyr function write_blocks. Typically, you'll use write_blocks to save files in one of two formats:

- multiple each block will be saved to its own .csv file
- single all the blocks will be saved to a single .csv file, with an empty row in between them

Saving block-shaped designs to multiple files The default setting for write_blocks is output_format = 'multiple'. This creates one csv file for each block. If we set file = NULL, the default is to name the files according to the block names in the metadata.

```
# See the previous section where we created my_design_blk
write_blocks(my_design_blk, file = NULL)
# Let's see what the files look like
print_df(read.csv("Bacteria.csv", header = FALSE, colClasses = "character"))
  1
          3
              4
                5
                     6
                        7
                            8
                                9
                                  10
                                       11 12
#> A
#> B
    #> C
    #> D
    #> E
#> F
    #> G
    #> H
print_df(read.csv("Media.csv", header = FALSE, colClasses = "character"))
                     67
                                10
       2
          3
              4
                 5
                          8
                              9
#> A
#> B
    Med1 Med2 Med3 Med4 Med5
                        Med7 Med8 Med9 Med10
#> C Med1 Med2 Med3 Med4 Med5
                       Med7 Med8 Med9 Med10
#> D
    Med1 Med2 Med3 Med4 Med5
                       Med7 Med8 Med9 Med10
#> E
    Med1 Med2 Med3 Med4 Med5
                        Med7 Med8 Med9 Med10
#> F
    Med1 Med2 Med3 Med4 Med5
                        Med7 Med8 Med9 Med10
#> G
    Med1 Med2 Med3 Med4 Med5
                        Med7 Med8 Med9 Med10
#> H
```

Saving block-shaped designs to a single file The other setting for write_blocks is output_format = 'single'. This creates a single csv file that contains all the blocks, putting metadata like block_names in rows that precede each block.

Let's take a look what the single output format looks like:

```
# See the previous section where we created my_design_blk
write_blocks(my_design_blk, file = "Design.csv", output_format = "single")

# Let's see what the file looks like
print_df(read.csv("Design.csv", header = FALSE, colClasses = "character"))
#> block_name Bacteria
#> 1 2 3 4 5 6 7 8 9 10 11 12
#> A
```

```
#>
              #>
       C
              #>
       D
              E
#>
#>
       F
              #>
       G
#>
       Н
#>
#> block_name
          Media
                2
                   3
                         5
#>
             1
                                         10
                                             11 12
#>
       Α
#>
       В
              Med1 Med2 Med3 Med4 Med5
                                 Med7 Med8 Med9 Med10
#>
       C
              Med1 Med2 Med3 Med4 Med5
                                 Med7 Med8 Med9 Med10
#>
       D
              Med1 Med2 Med3 Med4 Med5
                                 Med7 Med8 Med9 Med10
       E
                                 Med7 Med8 Med9 Med10
#>
              Med1 Med2 Med3 Med4 Med5
       F
#>
              Med1 Med2 Med3 Med4 Med5
                                 Med7 Med8 Med9 Med10
#>
       G
              Med1 Med2 Med3 Med4 Med5
                                 Med7 Med8 Med9 Med10
```

Here we can see all our design information has been saved to a single file, and the metadata has been added in rows before each block.

Merging growth curve data with designs

Once we have both our design and data in R and tidy-shaped, we can merge them just the same way as described in vignette("gc03_incorporate_designs")