Coordinatized Data: A Fluid Data Specification

John Mount and Nina Zumel

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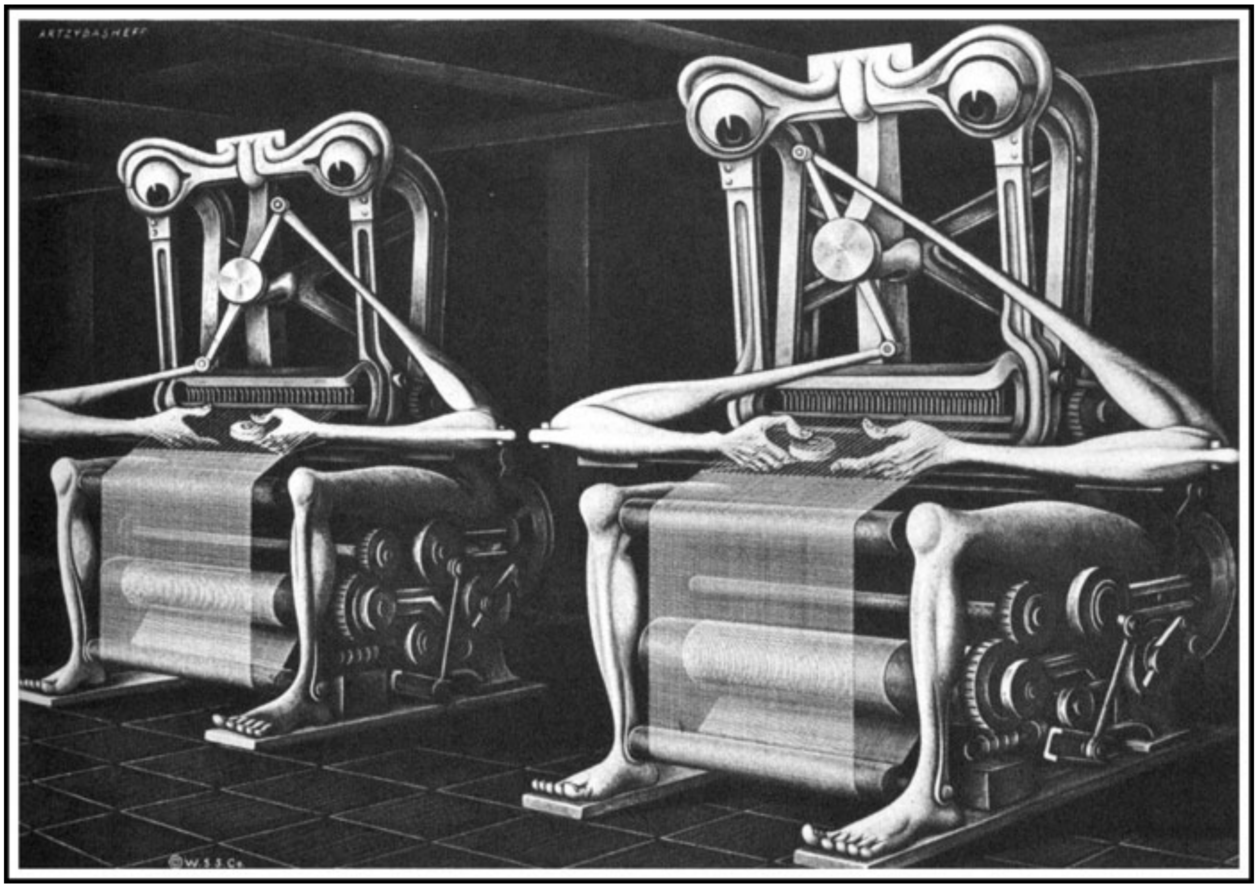
Introduction

It has been our experience when teaching the data wrangling part of data science that students often have difficulty understanding the conversion to and from row-oriented and column-oriented data formats (what is commonly called pivoting and un-pivoting).



http://www.darkroastedblend.com/2014/01/machines-alive-whimsical-art-of-boris.html)][Boris Artzybasheff illustration](http://www.darkroastedblend.com/2014/01/machines-alive-whimsical-art-of-boris.html)
Figure 1: (

Real trust and understanding of this concept doesn't fully form until one realizes that rows and columns are *inessential* implementation details when *reasoning* about your data. Many *algorithms* are sensitive to how data is arranged in rows and columns, so there is a need to convert between representations. However, confusing representation with semantics slows down understanding.

In this article we will try to separate representation from semantics. We will advocate for thinking in terms of *coordinatized data*, and demonstrate advanced data wrangling in `R`.

Example

Consider four data scientists who perform the same set of modeling tasks, but happen to record the data differently.

In each case the data scientist was asked to test two decision tree regression models (*a* and *b*) on two test-sets (*x* and *y*) and record both the model quality on the test sets under two different metrics (`AUC` and `pseudo R-squared`). The two models differ in tree depth (in this case model *a* has depth 5, and model *b* has depth 3), which is also to be recorded.

Data Scientist 1

Data Scientist 1 Data scientist 1 is an experienced modeler, and records their data as follows:

```r
library("tibble")
d1 <- tribble(
  ~model, ~depth, ~testset, ~AUC, ~pR2,
  'a',    5,      'x',      0.4,  0.2,
  'a',    5,      'y',      0.6,  0.3,
  'b',    3,      'x',      0.5,  0.25,
  'b',    3,      'y',      0.5,  0.25
)
knitr::kable(d1)
```

model	depth	testset	AUC	pR2
a	5	x	0.4	0.20
a	5	y	0.6	0.30
b	3	x	0.5	0.25
b	3	y	0.5	0.25

Data Scientist 1 uses what is called a *denormalized form* (we use this term out of respect for the priority of Codd's relational model theory). In this form each row contains all of the facts we want ready to go. If we were thinking about "column roles" (a concept we touched on briefly in Section A.3.5 "How to Think in SQL" of *Practical Data Science with R*, Zumel, Mount; Manning 2014), then we would say the columns `model` and `testset` are *key columns* (together they form a *composite key* that uniquely identifies rows), the `depth` column is derived (it is a function of `model`), and `AUC` and `pR2` are *payload columns* (they contain data).

Denormalized forms are the most ready for tasks that reason across columns, such as training or evaluating machine learning models.

Data Scientist 2

Data Scientist 2 Data Scientist 2 has data warehousing experience and records their data in a normal form:

```
models2 <- tribble(
  ~model, ~depth,
  'a',    5,
  'b',    3
)
knitr::kable(models2)
```

model	depth
a	5
b	3

```
d2 <- tribble(
  ~model, ~testset, ~AUC, ~pR2,
  'a',   'x',      0.4,  0.2,
  'a',   'y',      0.6,  0.3,
  'b',   'x',      0.5,  0.25,
  'b',   'y',      0.5,  0.25
)
knitr::kable(d2)
```

model	testset	AUC	pR2
a	x	0.4	0.20
a	y	0.6	0.30
b	x	0.5	0.25
b	y	0.5	0.25

The idea is: since `depth` is a function of the model name, it should not be recorded as a column unless needed. In a normal form such as above, every item of data is written only one place. This means that we cannot have inconsistencies such as accidentally entering two different depths for a given model. In this example all our columns are either key or payload.

Data Scientist 2 is not concerned about any difficulty that might arise by this format as they know they can convert to Data Scientist 1's format by using a `join` command:

```
suppressPackageStartupMessages(library("dplyr"))

d1_2 <- left_join(d2, models2, by='model') %>%
  select(model, depth, testset, AUC, pR2) %>%
  arrange(model, testset)
knitr::kable(d1_2)
```

model	depth	testset	AUC	pR2
a	5	x	0.4	0.20
a	5	y	0.6	0.30
b	3	x	0.5	0.25
b	3	y	0.5	0.25

```
all.equal(d1, d1_2)
```

```
## [1] TRUE
```

Relational data theory (the science of joins) is the basis of Structured Query Language (`SQL`) and a topic any data scientist *must* master.

Data Scientist 3

Data Scientist 3 Data Scientist 3 has a lot of field experience, and prefers an entity/attribute/value notation. They log each measurement as a separate row:

```
d3 <- tribble(
  ~model, ~depth, ~testset, ~measurement, ~value,
  'a',    5,      'x',      'AUC',        0.4,
  'a',    5,      'x',      'pR2',        0.2,
  'a',    5,      'y',      'AUC',        0.6,
  'a',    5,      'y',      'pR2',        0.3,
  'b',    3,      'x',      'AUC',        0.5,
  'b',    3,      'x',      'pR2',        0.25,
  'b',    3,      'y',      'AUC',        0.5,
  'b',    3,      'y',      'pR2',        0.25
)
knitr::kable(d3)
```

model	depth	testset	measurement	value
a	5	x	AUC	0.40
a	5	x	pR2	0.20
a	5	y	AUC	0.60
a	5	y	pR2	0.30

model	depth	testset	measurement	value
b	3	x	AUC	0.50
b	3	x	pR2	0.25
b	3	y	AUC	0.50
b	3	y	pR2	0.25

In this form `model`, `testset`, and `measurement` are key columns. `depth` is still running around as a derived column and the new `value` column holds the measurements (which could in principle have different types in different rows!).

Data Scientist 3 is not worried about their form causing problems as they know how to convert into Data Scientist 1's format with an `R` command:

```
library("tidyr")

d1_3 <- d3 %>%
  spread('measurement', 'value') %>%
  select(model, depth, testset, AUC, pR2) %>%  # to guarantee column order
  arrange(model, testset)  # to guarantee row order
knitr::kable(d1_3)
```

model	depth	testset	AUC	pR2
a	5	x	0.4	0.20
a	5	y	0.6	0.30
b	3	x	0.5	0.25
b	3	y	0.5	0.25

```
all.equal(d1, d1_3)
```

```
## [1] TRUE
```

You can read a bit on `spread()` here.

We will use the term `pivot_to_rowrecs()` for this operation later. The `spread()` will be replaced with the following.

```
  pivot_to_rowrecs(data = d3,
                   columnToTakeKeysFrom = 'measurement',
                   columnToTakeValuesFrom = 'value',
                   rowKeyColumns = c('model', 'testset'))
```

The above operation is a bit exotic and it (and its inverse) already go under number of different names:

- `pivot` / un-pivot (Microsoft Excel)
- `pivot` / anti-pivot (databases)
- `crosstab` / shred (databases)
- `unstack` / `stack` (R)
- `cast` / `melt` (`reshape`, `reshape2`)
- `spread` / `gather` (`tidyr`)
- "widen" / "narrow" (colloquial)
- `pivot_to_rowrecs()` and `unpivot_to_blocks()` (this writeup, basic "coordinatized data"[1])
- `blocks_to_rowrecs()` and `rowrecs_to_blocks()` (the more genaral "fluid data" operators)

[1] original here

And we are certainly neglecting other namings of the concept. We find none of these particularly evocative (though cheatsheets help), so one purpose of this note will be to teach these concepts in terms of the deliberately verbose ad-hoc terms: `pivot_to_rowrecs()` and `unpivot_to_blocks()`.

Note: often the data re-arrangement operation is only exposed as part of a larger aggregating or tabulating operation. Also `pivot_to_rowrecs()` is considered the harder transform direction (as it has to group rows to work), so it is often supplied in packages, whereas analysts often use ad-hoc methods for the simpler `unpivot_to_blocks()` operation (to be defined next).

Data Scientist 4

Data Scientist 4 Data Scientist 4 picks a form that makes models unique keys, and records the results as:

```
d4 <- tribble(
  ~model, ~depth, ~x_AUC, ~x_pR2, ~y_AUC, ~y_pR2,
  'a',    5,      0.4,    0.2,   0.6,    0.3,
  'b',    3,      0.5,    0.25,  0.5,    0.25
)
```

```
knitr::kable(d4)
```

model	depth	x_AUC	x_pR2	y_AUC	y_pR2
a	5	0.4	0.20	0.6	0.30
b	3	0.5	0.25	0.5	0.25

This is not a problem as it is possible to convert to Data Scientist 3's format.

```
d3_4 <- d4 %>%
  gather('meas', 'value', x_AUC, y_AUC, x_pR2, y_pR2) %>%
  separate(meas, c('testset', 'measurement')) %>%
  select(model, depth, testset, measurement, value) %>%
  arrange(model, testset, measurement)
knitr::kable(d3_4)
```

model	depth	testset	measurement	value
a	5	x	AUC	0.40
a	5	x	pR2	0.20
a	5	y	AUC	0.60
a	5	y	pR2	0.30
b	3	x	AUC	0.50
b	3	x	pR2	0.25
b	3	y	AUC	0.50
b	3	y	pR2	0.25

```
all.equal(d3, d3_4)
```

```
## [1] TRUE
```

We will replace the `gather` operation with `unpivot_to_blocks()` and the call will look like the following.

```
 unpivot_to_blocks(data = d4,
                   nameForNewKeyColumn = 'meas',
                   nameForNewValueColumn = 'value',
                   columnsToTakeFrom = c('x_AUC', 'y_AUC', 'x_pR2', 'y_pR2'))
```

`unpivot_to_blocks()` is (under some restrictions) an inverse of `pivot_to_rowrecs()`.

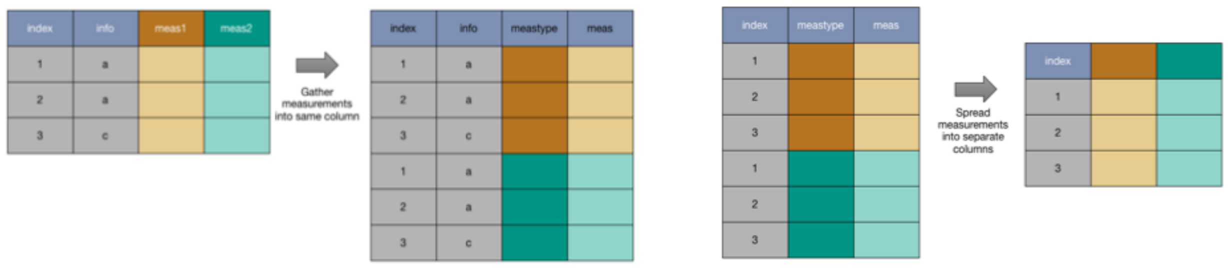

index
info
meas1
meas2
Gather measurements into same column
meastype
meas
Spread measurements into separate columns

Figure 2: Figures we will explain later

We find the more verbose naming (and calling interface) more intuitive. So we encourage you to think directly in terms of `unpivot_to_blocks()` as moving values to different rows (in the same column), and `blocks_to_rowrecs()`

as moving values to different columns (in the same row). It will usually be apparent from your problem which of these operations you want to use.

The Theory of Coordinatized Data

When you are working with transformations you look for invariants to keep your bearings. All of the above data share an invariant property we call being *coordinatized* data. In this case the invariant is so strong that one can think of all of the above examples as being equivalent, and the row/column transformations as merely changes of frame of reference.

Let's define *coordinatized data* by working with our examples. In all the above examples a value carrying (or payload) cell or entry can be uniquely named as follows:

```
c(Table=tableName, (KeyColumn=KeyValue)*, ValueColumn=ValueColumnName)
```

The above notations are the coordinates of the data item (hence "coordinatized data").

For instance: the `AUC` of 0.6 is in a cell that is named as follows for each of our scientists as:

- Data Scientist 1: `c(Table='d1', model='a', testset='y', ValueColumn='AUC')`
- Data Scientist 2: `c(Table='d2', model='a', testset='y', ValueColumn='AUC')`
- Data Scientist 3: `c(Table='d3', model='a', testset='y', measurement='AUC', ValueColumn='value')`
- Data Scientist 4: `c(Table='d4', model='a', ValueColumn= paste('y', 'AUC', sep= '_'))`

From our point of view these keys all name the same data item. We deliberately do not call one form tidy or another form un-tidy (which can be taken as a needlessly pejorative judgement), each has advantages depending on the application.

The fact that we are interpreting one position as a table name and another as a column name is just convention (one can try to take these key-based representations further, as in RDF triples, but this usually leads to awkward data representations). We can even write `R` code that uses these keys on all our scientists' data without performing any reformatting:

```
# take a map from names to scalar conditions and return a value.
# inefficient method; notional only
lookup <- function(key) {
  table <- get(key[['Table']])
  col <- key[['ValueColumn']]
  conditions <- setdiff(names(key),
                        c('Table', 'ValueColumn'))
  for(ci in conditions) {
    table <- table[table[[ci]]==key[[ci]], ,
                   drop= FALSE]
  }
  table[[col]][[1]]
}

k1 <- c(Table='d1', model='a', testset='y',
        ValueColumn='AUC')
k2 <- c(Table='d2', model='a', testset='y',
        ValueColumn='AUC')
k3 <- c(Table='d3', model='a', testset='y',
        measurement='AUC', ValueColumn='value')
k4 = c(Table='d4', model='a',
       ValueColumn= paste('y', 'AUC', sep= '_'))

print(lookup(k1))

## [1] 0.6

print(lookup(k2))

## [1] 0.6

print(lookup(k3))

## [1] 0.6

print(lookup(k4))

## [1] 0.6
```

The `lookup()` procedure was able to treat all these keys and key positions uniformly. This illustrates that what is in tables versus what is in rows versus what is in columns is just an implementation detail. Once we understand that all of these data scientists recorded the same data we should not be surprised we can convert between representations.

The thing to remember: coordinatized data is in cells, and every cell has unique coordinates. We are going to use this invariant as our enforced precondition before any data transform, which will guarantee our data meets this invariant as a postcondition. I.e., if we restrict ourselves to coordinatized data and exclude wild data, the