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cubble: An R Package for Structuring Spatio-temporal Data

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Abstract

The abstract of the article.

Keywords: spatio-temporal data, R.

1. Introduction

Motivation

Many data structures have been proposed for spatial (**sf** by Pebesma (2018)) and temporal (**tsibble** by Wang, Cook, and Hyndman (2020)) data in the R community, while less has been done for spatio-temporal data. The lack of such tools could potentially because analysts usually treat the spatial and temporal dimension of the data separately, without realising the need to create a new data structure. While this approach follows the third tidy data principal (Wickham 2014) (*Each type of observational unit forms a table*), analysts always need to manually join results from different observational units or combining multiple tables into one for downstream analysis. This additional step doesn't add new operations into the data but can be error prone.

Existing packages

Currently, available spatio-temporal data structure in R includes: **spacetime** (Pebesma 2012), which proposes four space-time layouts: Full grid (STF), sparse grid (STS), irregular (STI), and trajectory (STT). The data structure it uses is based on **sp** (Pebesma and Bivand 2005) and **xts** (Ryan and Ulrich 2020), both of which has been replaced by more recent implementations. **spatstat** (Baddeley and Turner 2005) implements a **ppp** class for point pattern data; and more recent, **stars** (Pebesma 2021) implements a spatio-temporal array with the dplyr's data cube structure **cubelyr** (Wickham 2020) as its backend. While these implementations either store spatial and temporal variables all in a single table, hence duplicate the spatial variables for each temporal unit; or split them into two separate tables that has the problem of manually joining, mentioned in the previously. None of these packages enjoy both the benefits of being able to separate manipulation in the two dimensions while also keep the data object as a whole. This create a gap in the software development. The requirement for such a tool is important given the ubiquity of spatio-temporal vector data in the wild: the Ireland wind data from **gstat** is an classic example data that splits variables into spatial (**wind.loc**) and temporal (**wind**) dimension; Bureau of Meteorology (BoM) provides climate observations that are widely applied in agriculture and ecology study; air pollution data.

Our new data structure for spatio-temporal data This paper describes the implementation of a new spatio-temporal data structure: **cubble**. **cubble** implements a relational data structure that uses two forms to manage the switch between spatial and temporal dimension. With this structure, users can manipulate the spatial or temporal dimension separately, while leaves the linking of two dimensions to `\pkg{cubble}\pkg{}`. The software is available from the Comprehensive R Archive Network (CRAN) at [CRAN link].

Section division

The rest of the paper will be divided as follows: [complete when the paper structure is more solid]

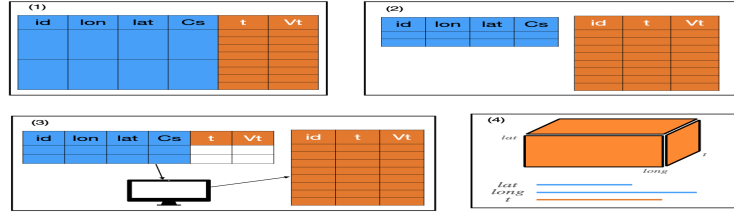


Figure 1: Illustration of incoming data formats for spatio-temporal data. (1) Data comes in as a single table; (2) Separate tables for spatial and temporal variables; (3) A single table with all the parameters used to query the database and a separate table for queried data; and (4) Cubical data in array or NetCDF format.

2. The cubble package

Spatio-temporal data usually come in various forms and Figure 1 shows four examples of this. No matter which form the data is in, these formats share some common components that characterise spatio-temporal data. A spatial identifier (`id` in the diagram) is the unique identifier of each site. The temporal identifier (`t` in the diagram) prescribes the time stamp each site is recorded. Coordinates, comprising of latitude and longitude (`lon` and `lat` in the diagram), locates each site on the map. These identifiers will be the building blocks for the data structure introduced below. Other variables in the data can be categorised into two groups: spatial variables that are invariant at each time stamp for every site, i.e. the name or code of the weather station and temporal variables that varies with time.

In a cubble, there are two forms: nested form and long form, and Figure 2 sketches the two forms along with the associated attributes. The decision on which form to use is output-oriented, meaning analysts need to first think about whether the output of a particular operation is identified only by the spatial identifier, or a combination of spatial and temporal identifier. The nested cubble is suitable for working with operations that are only identified by site and this type of operation can be a pure manipulation of spatial variables, or a summary of temporal variables by site (i.e. the output of counting the number of raining day is only identified by sites and hence should be performed with the nested form). Underneath the nested form, a cubble is built from a row-wise dataframe (`rowwise_df`) where each site forms a separate group. This structure simplifies the calculation that involves temporal variables by avoiding the use of `map` syntax when working with list-column.

For those operations whose output involves both a spatial and temporal dimension, long form should be used. The long form is identified by both the spatial and temporal identifier and adopts a grouped dataframe (`grouped_df`) to forms each site as a group. Spatial variables are stored separately in a **tibble** as an special attribute of the long cubble. This design avoids repeating the spatial variables at each time stamp while not dropping information from spatial variables.

2.1. Create a cubble in the nested form

To use functionalities from cubble, data analysts first need to create a cubble. `as_cubble` create a **cubble** by supplying the three key components: **key** as the spatial identifier; **index**

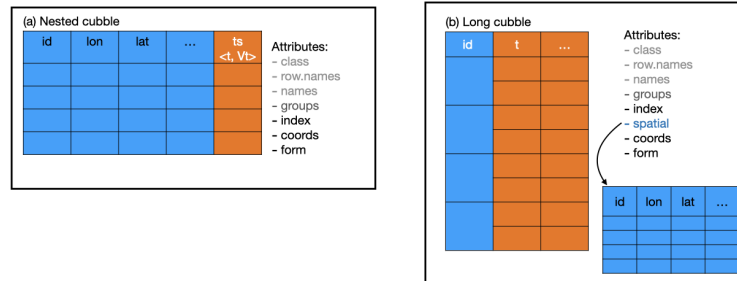


Figure 2: Illustration of nested and long cubble.

as the temporal identifier; and a vector of `coords` in the order of longitude first and then latitude. The naming of `key` and `index` follows the convention in the `tsibble` package. The cubble created by default is in the nested form. Below is an example of creating a cubble:

```
# cubble:   id [5]: nested form
# bbox:     [115.97, -32.94, 133.55, -12.42]- check gap on long and lat
# temporal: date [date], prcp [dbl], tmax [dbl], tmin [dbl]
  id          lat long elev name          wmo_id ts
<chr>        <dbl> <dbl> <dbl> <chr>        <dbl> <list>
1 ASN00009021 -31.9  116.  15.4 perth airport  94610 <tibble [366 x 4]>
2 ASN00010311 -31.9  117.  179  york          94623 <tibble [366 x 4]>
3 ASN00010614 -32.9  117.  338  narrogin       94627 <tibble [366 x 4]>
4 ASN00014015 -12.4  131.  30.4 darwin airport  94120 <tibble [366 x 4]>
5 ASN00015131 -17.6  134.  220  elliot         94236 <tibble [366 x 4]>
```

There are a few information in the **cubble** header: the name of the **key** variable, **bbox**, and also the name of variable nested in the **ts** column. In this example, each site is identifier is **id** and the number in the bracket means there are 5 unique **id** in this dataset. The **bbox** in the second row gives the range of the coordinates. The temporal variables are all nested in the **ts** column, but it could be useful to know the name these variables. The third row in the cubble header shows these names and in this example this includes: precipitation, **prcp**, maximum temperature, **tmax**, and minimum temperature, **tmin**.

2.2. Stretch a nested cubble into the long form

The long cubble is suitable to manipulate the time dimension of the data. The function `stretch()` switches the nested cubble into the long cubble by first extracts all the spatial variables into a separate tibble and store in the `spatial` attribute and then unnests the `ts` column:

```
# cubble:  date, id [5]: long form
# bbox:    [115.97, -32.94, 133.55, -12.42]- check gap on long and lat
# spatial: lat [dbl], long [dbl], elev [dbl], name [chr], wmo_id [dbl]
  id      date      prcp tmax tmin
  <chr>    <date>    <dbl> <dbl> <dbl>
1 ASN00009021 2020-01-01      0  31.9  15.3
2 ASN00009021 2020-01-02      0  24.9  16.4
3 ASN00009021 2020-01-03      6  23.2   13
4 ASN00009021 2020-01-04      0  28.4  12.4
5 ASN00009021 2020-01-05      0  35.3  11.6
6 ASN00009021 2020-01-06      0  34.8  13.1
7 ASN00009021 2020-01-07      0  32.8  15.1
8 ASN00009021 2020-01-08      0  30.4  17.4
9 ASN00009021 2020-01-09      0  28.7  17.3
10 ASN00009021 2020-01-10      0  32.6  15.8
# ... with 1,820 more rows
```

Notice here that the third line in the header now shows the name of spatial variables rather than the temporal variables.

2.3. Tamp a long cubble back to the nested form

Manipulation on the spatial and temporal dimension can be an iterative process. Many times, analysts will need to go back and forth between the nested and long cubble. The `stretch()` function introduced in the previous section switches a nested cubble into a long cubble and function `tamp()` is its inverse function to switch a long cubble back to the nested cubble:

```
# cubble:  id [5]: nested form
# bbox:    [115.97, -32.94, 133.55, -12.42]- check gap on long and lat
# temporal: date [date], prcp [dbl], tmax [dbl], tmin [dbl]
  id      lat long elev name      wmo_id ts
  <chr>    <dbl> <dbl> <dbl> <chr>    <dbl> <list>
1 ASN00009021 -31.9  116.  15.4 perth airport  94610 <tibble [366 x 4]>
2 ASN00010311 -31.9  117.  179  york      94623 <tibble [366 x 4]>
3 ASN00010614 -32.9  117.  338  narrogin  94627 <tibble [366 x 4]>
4 ASN00014015 -12.4  131.  30.4 darwin airport  94120 <tibble [366 x 4]>
5 ASN00015131 -17.6  134.  220  elliot    94236 <tibble [366 x 4]>
```

2.4. Migrate spatial variables to a long cubble

As a final data output for modelling or visualisation, spatio-temporal data is usually expected to be in a single table. Function `migrate()` moves the spatial variables from the `spatial` attribute into the long cubble:

```
# cubble:  date, id [5]: long form
# bbox:    [115.97, -32.94, 133.55, -12.42]- check gap on long and lat
# spatial: lat [dbl], long [dbl], elev [dbl], name [chr], wmo_id [dbl]
  id      date      prcp  tmax  tmin  long  lat
<chr>    <date>    <dbl> <dbl> <dbl> <dbl> <dbl>
1 ASN00009021 2020-01-01    0  31.9  15.3  116. -31.9
2 ASN00009021 2020-01-02    0  24.9  16.4  116. -31.9
3 ASN00009021 2020-01-03    6  23.2  13    116. -31.9
4 ASN00009021 2020-01-04    0  28.4  12.4  116. -31.9
5 ASN00009021 2020-01-05    0  35.3  11.6  116. -31.9
6 ASN00009021 2020-01-06    0  34.8  13.1  116. -31.9
7 ASN00009021 2020-01-07    0  32.8  15.1  116. -31.9
8 ASN00009021 2020-01-08    0  30.4  17.4  116. -31.9
9 ASN00009021 2020-01-09    0  28.7  17.3  116. -31.9
10 ASN00009021 2020-01-10    0  32.6  15.8  116. -31.9
# ... with 1,820 more rows
```

In this workflow described above, data objects come into cubble in the nested form, then various operations on the spatial and temporal dimension can go back and forth between the nested and long form, and finally, the data will come out of cubble in the long form for further modelling or visualisation.

Building from an underlying `tbl_df` structure, it is natural to implement methods available in `dplyr` to cubble. Supported methods in the cubble with `dplyr` generics includes:

basics	mutate, filter, summarise, select, arrange, rename, left_join
grouping	group_by, ungroup
slice family	slice_head, slice_tail, slice_sample, slice_min and slice_max

cubble is also compatible with **tsibble** in the sense that the original list-column can be a `tbl_ts` object. Duplicates and gaps should be first checked before structuring the data into a cubble. If the input data is a **tsibble** object, the long form cubble is also a **tsibble** where users can directly apply time series operations.

3. Advanced features/ considerations

3.1. Hierarchical structure

Imposing a clustering structure can be thought of as building a hierarchical structure where stations are nested within clusters. This can be useful when there's intrinsic nesting structure in the data (i.e. country nested in the continent, county nested in the state) or there's some clustering. When we have access to both level, `switch_key()` is the function to re-structure the data as one cluster per row. Temporal observations from different stations while within the same cluster are bound in the nested column `ts`.

One thing we hope to do with the cluster is to find the coordinates of the centroid. These are variables variant to the station but invariant to the cluster and it would be nice to have

a function that structure each cluster as a row. `switch_key()` is the function that does this: it lets you to specify a new key, say `cluster` and nests all spatial variables variant to `cluster` into a column. Spatial variables are all nested inside a new column `.val`. Temporal observations from different stations while within the same cluster are bound in the nested column `ts`.

This structure makes it easy to compute cluster level variable, for example, the convex hull and the centroid coordinate of each cluster. These can be amended into the nested form with function `get_centroid`.

After we have got `cluster_nested`, spatial and temporal data at both levels can be easily obtained. Figure ?? illustrate the relationship between the long and nested form cubble at both site and cluster level. More description on this. Start with the original `station_nested`, `stretch()` expands the `ts` column with each station (`id`) forming a group and attach variables invariant to `id` as an attribute. `switch_key()` changes the key from `id` to `cluster` and nests all the spatial variables that variant to `cluster`. `stretch()` `cluster_nested` will store variables that are invariant to `cluster` as a tibble in the attribute.

this fit into the remaining data pipeline.

3.2. Data fusion and matching

3.3. Interactive graphics

The cubble structure fits in naturally with the interactive graphic pipeline discussed in the literature (Buja, Asimov, and Hurley 1988; Buja, Cook, and Swayne 1996; Sutherland, Rossini, Lumley, Lewin-Koh, Dickerson, Cox, and Cook 2000; Xie, Hofmann, and Cheng 2014; Cheng, Cook, and Hofmann 2016). Diagram 3 illustrates how linking works with the two forms in a cubble, where a time series plot is created with the long cubble and a map is created with the nested cubble. When a user action is captured from the map, the site will be activated in the nested cubble. Then, the nested cubble will communicate to the long cubble to activate all the observations with the same `id`. The long cubble will then highlight the activated series in the time series plot.

The linking is also available from the time series plot to the map. The selection on the time series is through selecting the point on the time series and once a point is selected, it will be activated in the long cubble. All the observations that share the same `id`, either in the long and nested cubble, are then activated. This includes other points in the same time series in the long cubble and the corresponding observation of site in the nested cubble. These activated observations will then being reflected in the updated plots and Diagram 9 in the Appendix illustrates this process.

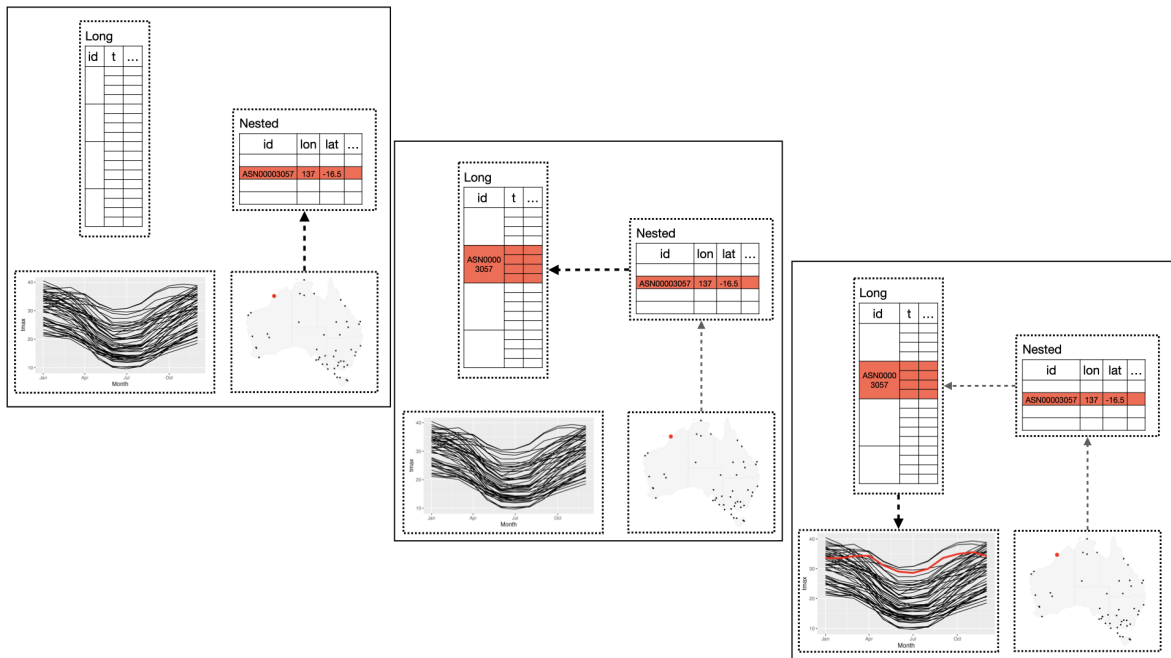


Figure 3: demon interactivity

4. Examples

4.1. Australia precipitation pattern in 2020

Basic manipulation

Bureau of Meteorology (BoM) collects climate variables. This variables can be openly queried via `rnoaa`. `weatherdata` provides a readily available copy of several data. `weatherdata::historical_tmax` provides historical maximum temperature recorded for Australian stations with the earliest dating back to 1859 and this can be used to understand the change of maximum temperature from a past period to nowadays. Figure 4 shows the steps involved from the initial data to the final glyph map in Figure 5.

Aggregation

In figure 5, there are a few stations around Sydney (151E, 34S) and New castle (152E, 33S). Aggregating them into averages or other statistics would give a better picture. This can be done with `cubble` through a hierarchical structure, where the cluster indicator is one level above the individual station.

In Figure 6

The `weatherdata::climate_full` data has daily climate data of 639 Australia stations from 2016 to 2020.

calculate distance matrix As an example to illustrate here, a kmean clustering algorithm based on the distance matrix is used and the number of centres is set to 20. More complex

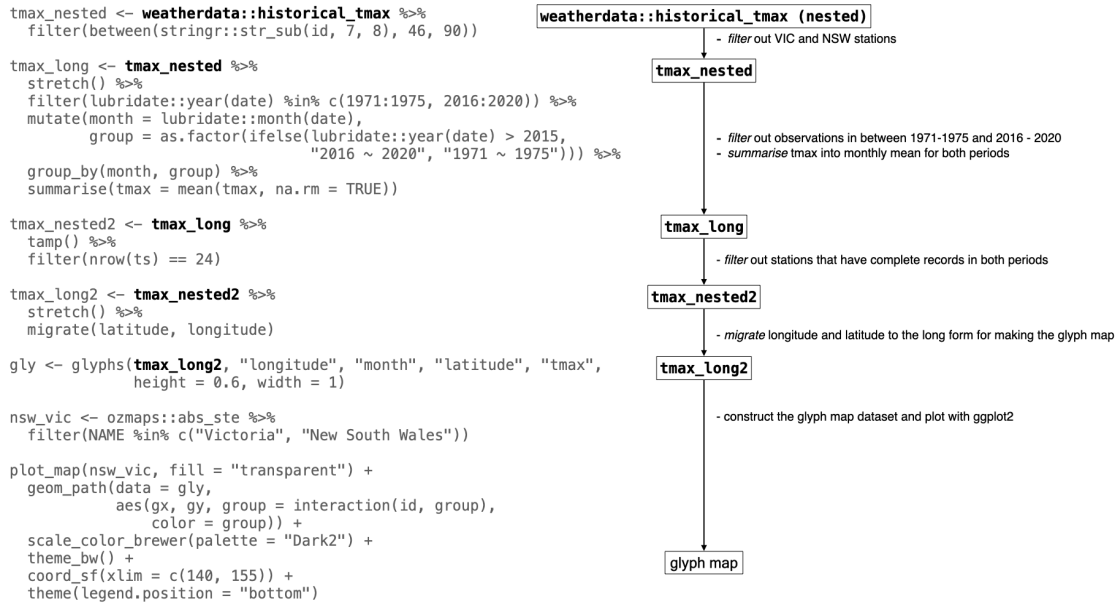


Figure 4: demon code

algorithms can also be used for more complex problem, as long as a mapping from each station id to the cluster id can be constructed.

4.2. River level data in Victoria water gauges

The water level data comes from [Bureau of Meteorology](#) and has a copy in `weatherdata`. Here we extract the water course level and add a column annotate this data of type `river`. For the rainfall data, we will still use the `weatherdata::climate_full`, filtering for Victorian stations in 2020 should be pretty familiar by now. Again, we first look at where these stations are on the map first:

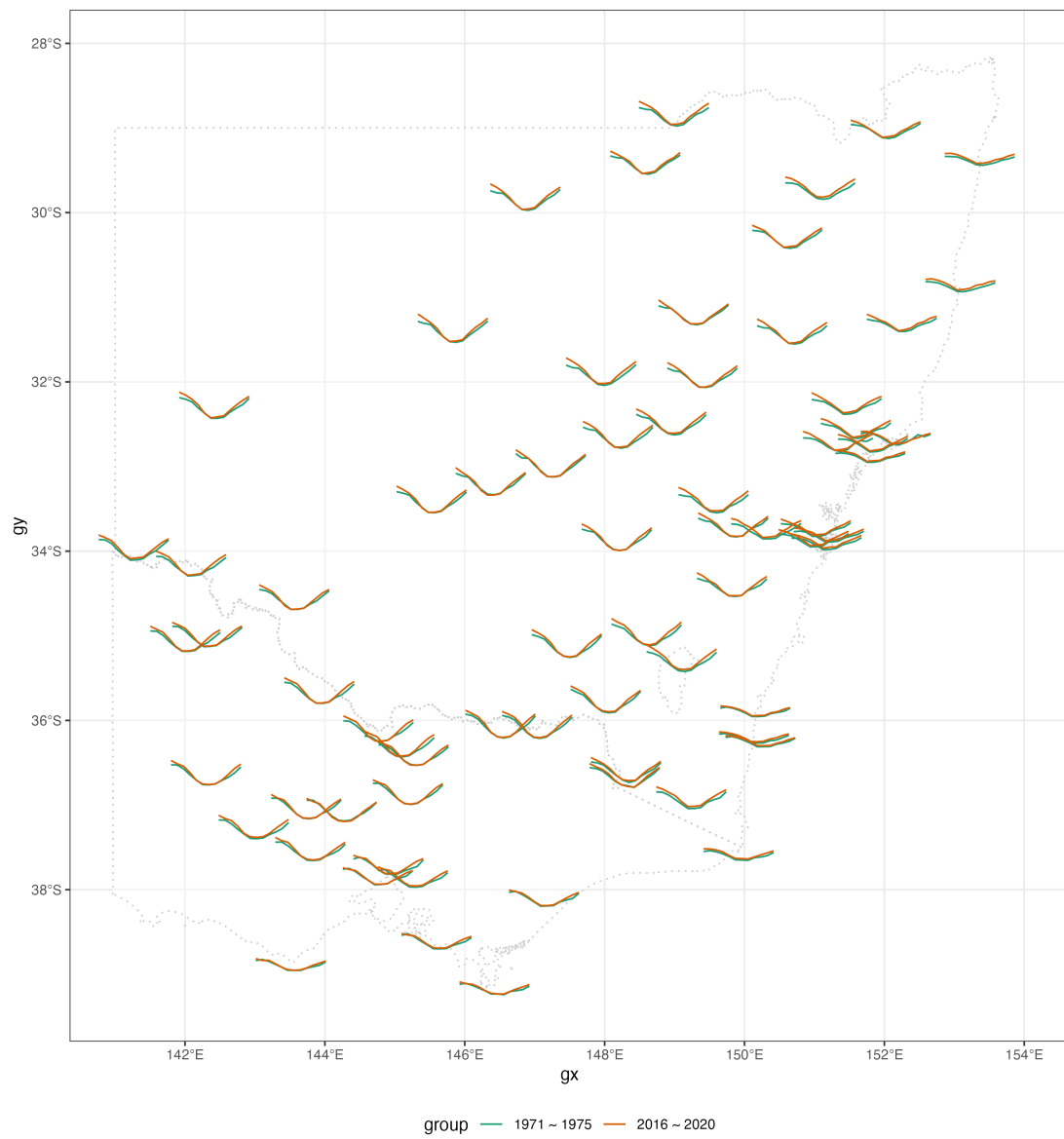
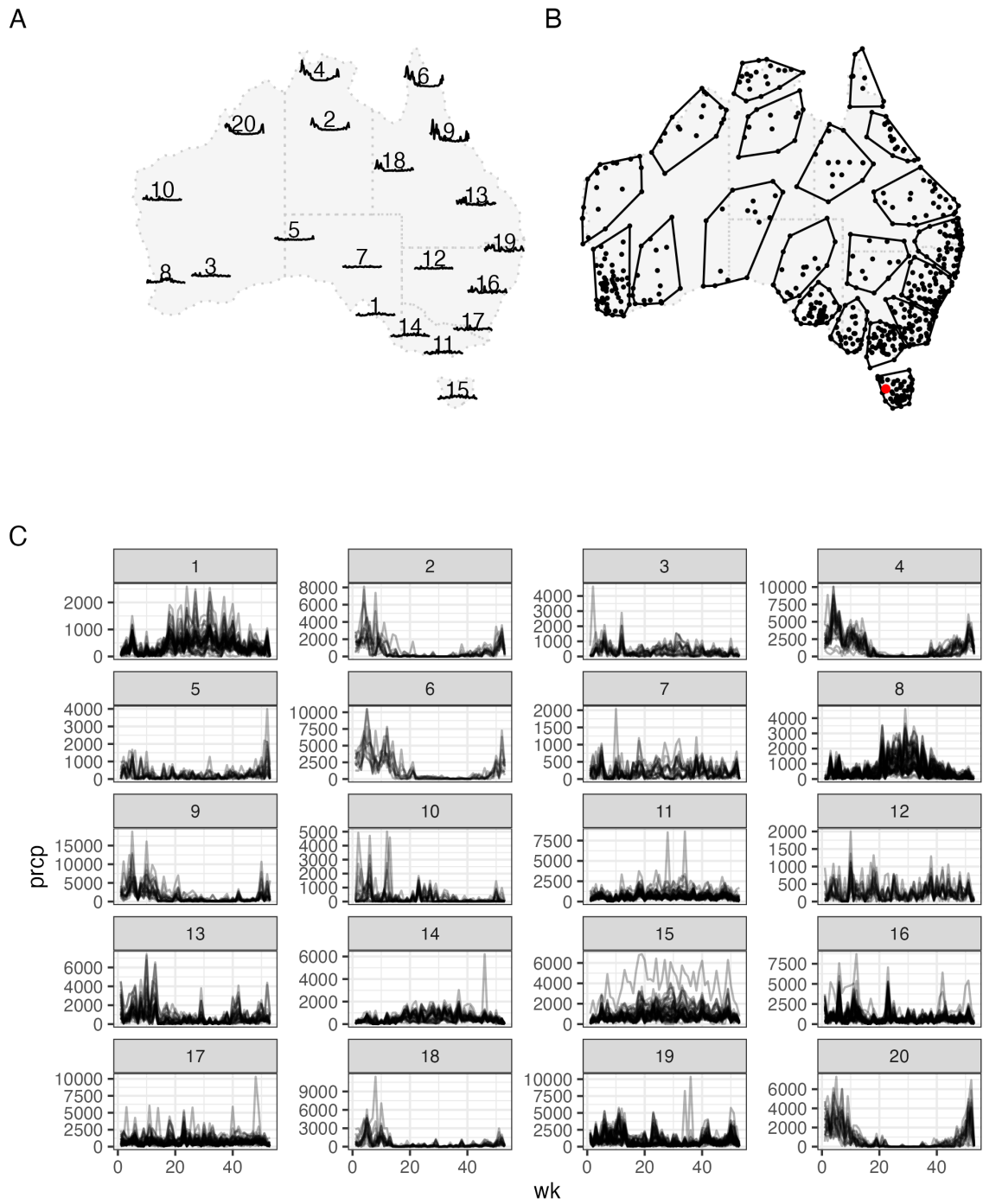


Figure 5: asdfasd



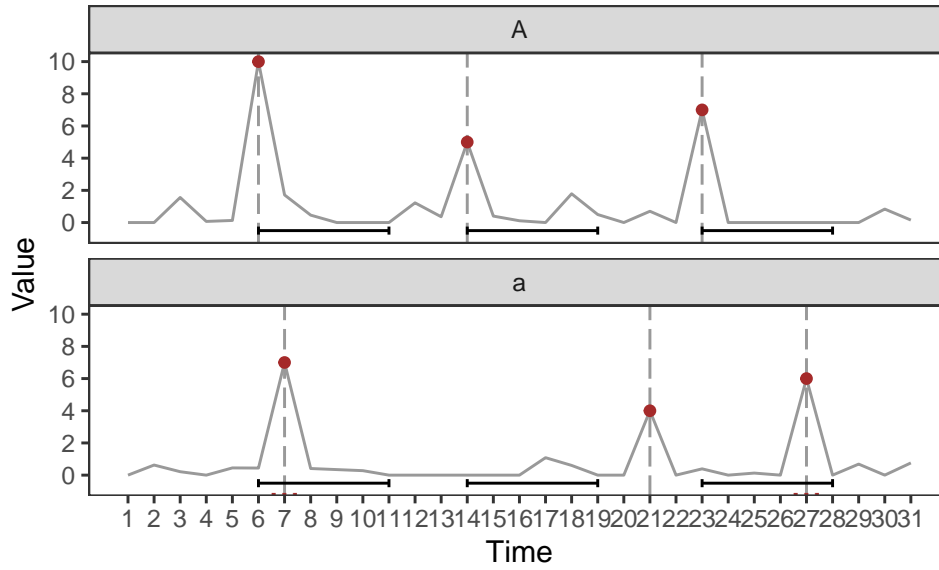
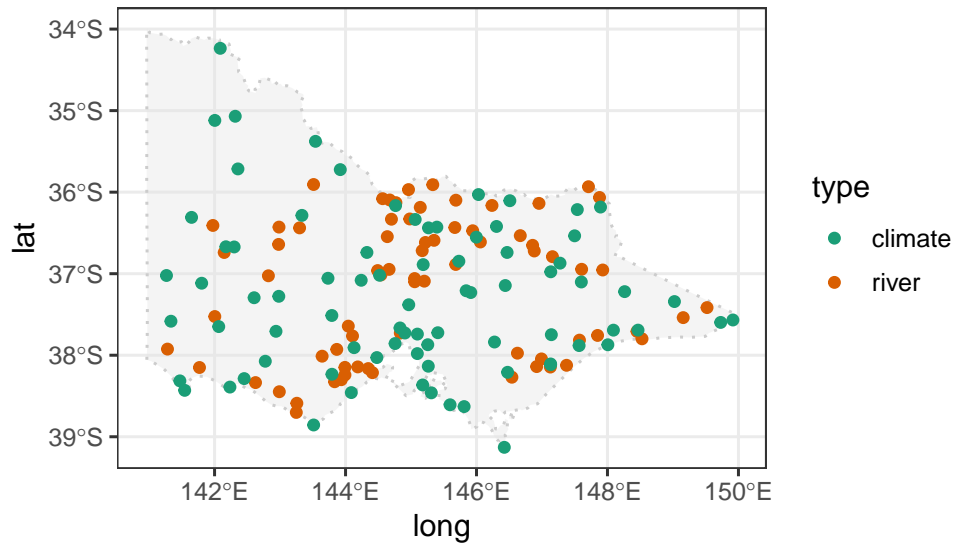


Figure 7: shtishisaasdf



Temporal matching checks how spatially matched pairs align temporally. We use the following chart to illustrate how the temporal matching works:

For each spatially matched pair, say **A** and **a**, we first find the largest **n** points in each series, colored in brown points here. Here we use the largest three but you can tune this number by `temporal_n_highest`. Then we construct the interval of the largest points from one series and see how many points, from the other series, fall into the intervals. The series used to construct the interval is controlled by `temporal_independent` and the window size by `temporal_window` with a default of 5.

In this illustration, we construct the interval based on series **A** and two of the three peaks from **a** falls into this interval at Time 7 and 27.

There's another mandatory argument that hasn't been introduced above: `temporal_var_to_match`.

This argument controls the variable to match and it needs to appear in both the `major` and `minor` set. In the water level matching example, we match the variable `Water_course_level` from `river` to `prcp` from `climate`, hence need to manually rename one of them to match the other, here we rename `Water_course_level` to `prcp` in `river`:

Now we use `match_sites()` to first pair the weather stations with the river gauges spatially and then apply the temporal matching on `prcp`. We will construct the interval based on peaks in `climate` since we would expect a lag effect for precipitation to flow into the river and cause a raise in river level, hence `temporal_independent = climate`. We select the 30 highest peak from the series to construct the match by setting `temporal_n_highest = 30`. This is a tuning parameter and you can start with 10% of the points of one series (here we have daily data for a year, 10% is roughly 30 points). `temporal_min_match` filters out pairs don't have enough match and to return all the pairs, set `temporal_min_match` to 0.

```
# cubble:   id [8]: nested form
# bbox:     [144.52, -37.73, 146.06, -36.55]
# temporal: date [date], prcp [dbl]
```

	id	name	lat	long	type	ts	.dist	.group	n_match
	<chr>	<chr>	<dbl>	<dbl>	<chr>	<list>	<dbl>	<int>	<int>
1	405234	SEVEN CREEKS @ D~	-36.9	146.	river	<tibble ~	6.15	5	21
2	ASN00082042	strathbogie	-36.8	146.	clim~	<tibble ~	6.15	5	21
3	404207	HOLLAND CREEK @ ~	-36.6	146.	river	<tibble ~	8.54	10	21
4	ASN00082170	benalla airport	-36.6	146.	clim~	<tibble ~	8.54	10	21
5	230200	MARIBYRNONG RIVE~	-37.7	145.	river	<tibble ~	6.17	6	19
6	ASN00086038	essendon airport	-37.7	145.	clim~	<tibble ~	6.17	6	19
7	406213	CAMPASPE RIVER @~	-37.0	145.	river	<tibble ~	1.84	1	18
8	ASN00088051	redesdale	-37.0	145.	clim~	<tibble ~	1.84	1	18

The output from temporal matching is also a cubble, with additional column `.dist` and `.group` inherent from spatial matching and `n_match` for the number of matched temporal peaks. Then you can use this output to plot the location of match or to look at the series:

4.3. ERA5: climate reanalysis data

4.4. Interactive graphic with cubble

With a larger dataset, interactive graphics can be helpful to explore these data from multiple perspective. Two examples are presented here to show how interactivity can be used to explore the climate data across Australia.

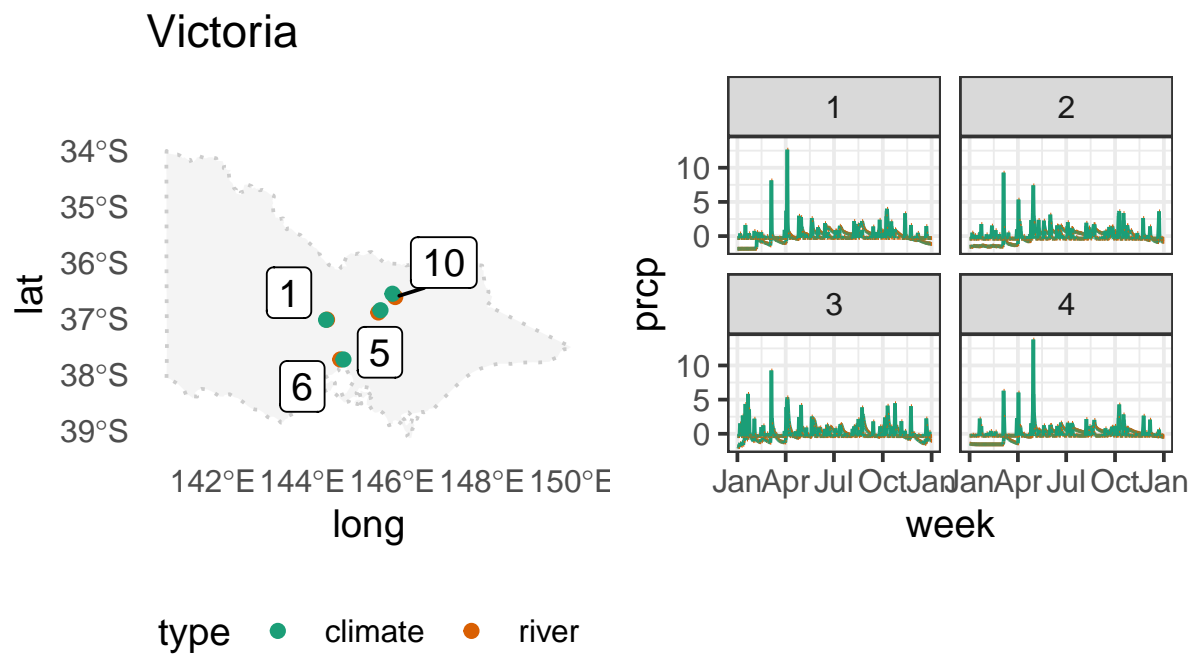
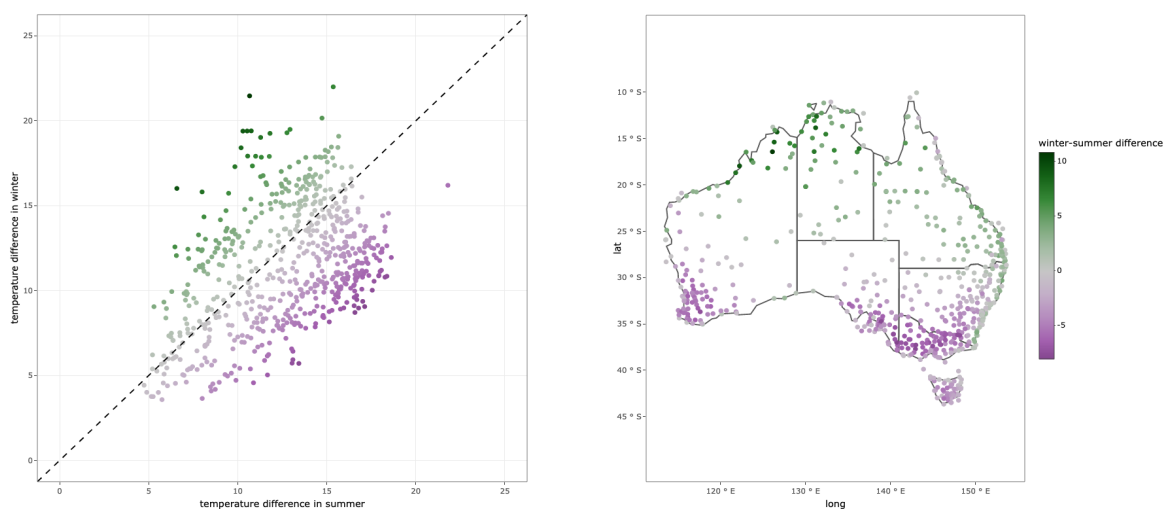


Figure 8: ...



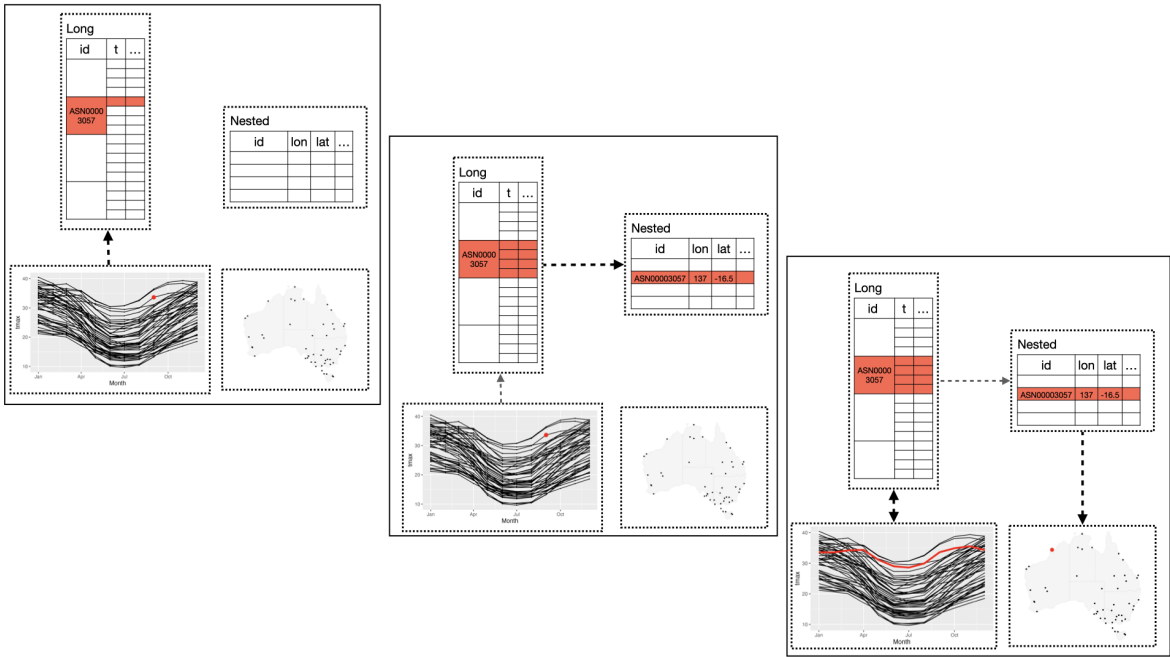
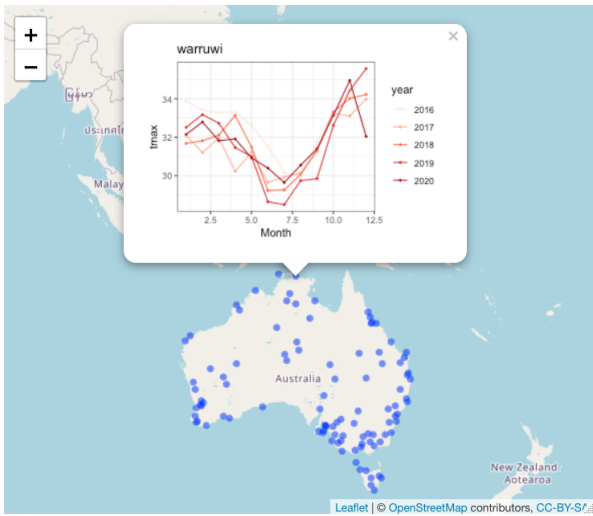


Figure 9: demon interactivity



5. Conclusion

6. Appendix

7. Old stuff

In the temporal aspect, the `tsibble` (?) structure and its tidyverts ecosystem have provided a [...] workflow to work with temporal data. In a `tsibble` structure, temporal data is characterised by `index` and `key` where `index` is the temporal identifier and `key` is the identifier for multiple series, which could be used as a spatio identifier. However, a `tsibble` object, by construction, always requires the `index` in its structure. This makes it less appealing for spatio-temporal data since the output of calculated spatio-specific variables (i.e. features of each series) don't have the time dimension. Analysts will either need to have an additional step to join this output to the original `tsibble` or operate with variables stored in two separate objects. In addition, the long form structure of a `tsibble` object means spatio variables (i.e. longitude, latitude, and features of each series if joined back to the `tsibble`) of each spatio identifier will be repetitively recorded at each timestamp. This repetition is unnecessary and would inflate the object size for long series.

8. Create a cubble

The creation of a `cubble` requires the site identifier (`key`), as well as the spatial (`coords`) and temporal (`index`) identifier. `climate_flat` is already a `tibble` and it uses `id` to identify each station, `date` as the time identifier, and `c(long, lat)` as the spatial identifier. To create a `cubble` for this data, use:

```
# cubble:   id [5]: nested form
# bbox:     [115.97, -32.94, 133.55, -12.42]- check gap on long and lat
# temporal: date [date], prcp [dbl], tmax [dbl], tmin [dbl]
  id      lat long elev name      wmo_id ts
<chr>    <dbl> <dbl> <dbl> <chr>    <dbl> <list>
1 ASN00009021 -31.9 116. 15.4 perth airport  94610 <tibble [366 x 4]>
2 ASN00010311 -31.9 117. 179  york          94623 <tibble [366 x 4]>
3 ASN00010614 -32.9 117. 338  narrogin    94627 <tibble [366 x 4]>
4 ASN00014015 -12.4 131. 30.4 darwin airport 94120 <tibble [366 x 4]>
5 ASN00015131 -17.6 134. 220  elliot     94236 <tibble [366 x 4]>
```

Most of the time, spatio-temporal data doesn't come into this form and analysts need to query the climate variables based on station metadata. **This is also a problem illustrated in Section 3.5 in @tidydata. Here we provide a structured way to query this data based on the row-wise operator and nested list.** For this type of task, one can structure a metadata into a `tibble` and use row-wise operator to query the climate variables into a nested list. As an example here we demonstrate the workflow to find the 5 closest stations to Melbourne. We first create a station data frame with the 5 target stations.

```
# A tibble: 5 x 8
  id      lat long elev name      wmo_id dist city
<chr>    <dbl> <dbl> <dbl> <chr>    <dbl> <dbl> <chr>
1 ASN00086038 -37.7 145. 78.4 essendon airport  95866 10.8 melbourne
2 ASN00086282 -37.7 145. 113. melbourne airport  94866 20.1 melbourne
```



```

3 ASN00086077 -38.0 145. 12.1 moorabbin airport      94870 21.9 melbourne
4 ASN00088162 -37.4 145. 528. wallan (kilmore gap) 94860 48.1 melbourne
5 ASN00087113 -38.0 144. 10.6 avalon airport        94854 48.8 melbourne

```

We can query the climate information into a nested list named `ts` for each station with the `rowwise()` operator. To create a cubble, supply the same identifiers as with the first example.

```

# cubble:   id [5]: nested form
# bbox:     [144.47, -38.03, 145.1, -37.38]
# temporal: date [date], prcp [dbl], tmax [dbl], tmin [dbl]
  id      lat long elev name      wmo_id dist city  ts
  <chr>    <dbl> <dbl> <dbl> <chr>      <dbl> <dbl> <chr>  <list>
1 ASN00086038 -37.7 145. 78.4 essendon airport    95866 10.8 melbo~ <tibbl~
2 ASN00086282 -37.7 145. 113. melbourne airport    94866 20.1 melbo~ <tibbl~
3 ASN00086077 -38.0 145. 12.1 moorabbin airport    94870 21.9 melbo~ <tibbl~
4 ASN00088162 -37.4 145. 528. wallan (kilmore gap) 94860 48.1 melbo~ <tibbl~
5 ASN00087113 -38.0 144. 10.6 avalon airport        94854 48.8 melbo~ <tibbl~

```

Below are the how the nested and long form look like for Australia climate data, which records daily precipitation, maximum and minimum temperature for 55 stations across Australia from 2015- 2020. Notice that each station forms a group in both forms and specifically, the nested and long form have a underlying `rowwise_df` and `grouped_df` respectively.

With a cubic framework on mind, different types of manipulation with cubble can be thought of as slicing the cube in various way. The table below shows how some `dplyr` verbs are mapped into the operation in a cubble. With the existing grouping on the station, additional grouping can be added with `group_by` and removed with `ungrouped`. [talk about why it is useful]

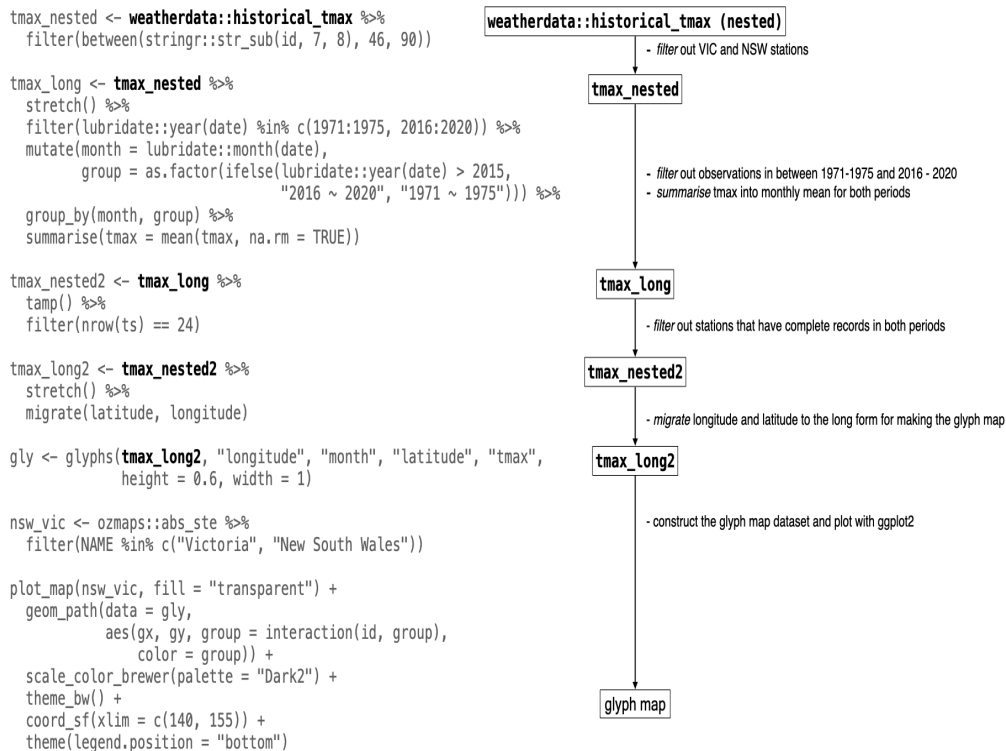


Figure 10: Cubble operations

8.1. Cubble operations

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