STAD29: Statistics for the Life and Social Sciences

Lecture notes

Section 1

Multidimensional scaling

Multidimensional Scaling

- Have distances between individuals.
- Want to draw a picture (map) in 2 dimensions showing individuals so that distances (or order of distances) as close together as possible. (Or maybe 3 with `rgl`.)
- If want to preserve actual distances, called *metric multidimensional scaling* (in R, `cmdscale`).
- If only want to preserve order of distances, called *non-metric multidimensional scaling* (in R, `isoMDS` in package `MASS`).
- Metric scaling has solution that can be worked out exactly.
- Non-metric only has iterative solution.
- Assess quality of fit, see whether use of resulting map is reasonable. (Try something obviously 3-dimensional and assess its failure.)

Packages

The usual, plus some new stuff:

```
library(MASS)
library(tidyverse)
library(ggrepel)
library(ggmap)
library(shapes)
```

Metric scaling: European cities

CSV file `europe.csv` contains road distances (in km) between 16 European cities. Can we reproduce a map of Europe from these distances?

Read in data:

```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/europe.csv"
europe <- read_csv(my_url)
```

```
## Parsed with column specification:
## cols(
##   City = col_character(),
##   Amsterdam = col_double(),
##   Athens = col_double(),
##   Barcelona = col_double(),
##   Berlin = col_double(),
##   Cologne = col_double(),
##   Copenhagen = col_double(),
##   Edinburgh = col_double(),
##   Geneva = col_double(),
##   London = col_double(),
##   Madrid = col_double(),
##   Marseille = col_double(),
##   Munich = col_double(),
```

The data

```
## # A tibble: 16 x 17
##    City  Amsterdam Athens Barcelona Berlin Cologne Copenhagen
##    <chr>     <dbl>  <dbl>     <dbl>  <dbl>   <dbl>      <dbl>
##  1 Amst…         0   3082      1639    649     280        904
##  2 Athe…      3082      0      3312   2552    2562       3414
##  3 Barc…      1639   3312         0   1899    1539       2230
##  4 Berl…       649   2552      1899      0     575        743
##  5 Colo…       280   2562      1539    575       0        730
##  6 Cope…       904   3414      2230    743     730          0
##  7 Edin…      1180   3768      2181   1727    1206       1864
##  8 Gene…      1014   2692       758   1141     765       1531
##  9 Lond…       494   3099      1512   1059     538       1196
## 10 Madr…      1782   3940       628   2527    1776       2597
## 11 Mars…      1323   2997       515   1584    1208       1914
## 12 Muni…       875   2210      1349    604     592       1204
## 13 Paris       515   3140      1125   1094     508       1329
## 14 Prag…       973   2198      1679    354     659       1033
## 15 Rome       1835   2551      1471   1573    1586       2352
## 16 Vien…      1196   1886      1989    666     915       1345
## # … with 10 more variables: Edinburgh <dbl>, Geneva <dbl>,
## #   London <dbl>, Madrid <dbl>, Marseille <dbl>, Munich <dbl>,
## #   Paris <dbl>, Prague <dbl>, Rome <dbl>, Vienna <dbl>
```

Multidimensional scaling

- Create distance object first using all but first column of `europe`. `europe` has distances in it already, so make into `dist` with `as.dist`.
- Then run multidimensional scaling and look at result:

```
europe %>% select(-City) %>% as.dist() -> europe.d
europe.scale <- cmdscale(europe.d)
head(europe.scale)
```

```
##                    [,1]      [,2]
## Amsterdam  -348.162277  528.2657
## Athens     2528.610410 -509.5208
## Barcelona  -695.970779 -984.6093
## Berlin      384.178025  634.5239
## Cologne       5.153446  356.7230
## Copenhagen -187.104072 1142.5926
```

- This is a `matrix` of x and y coordinates.

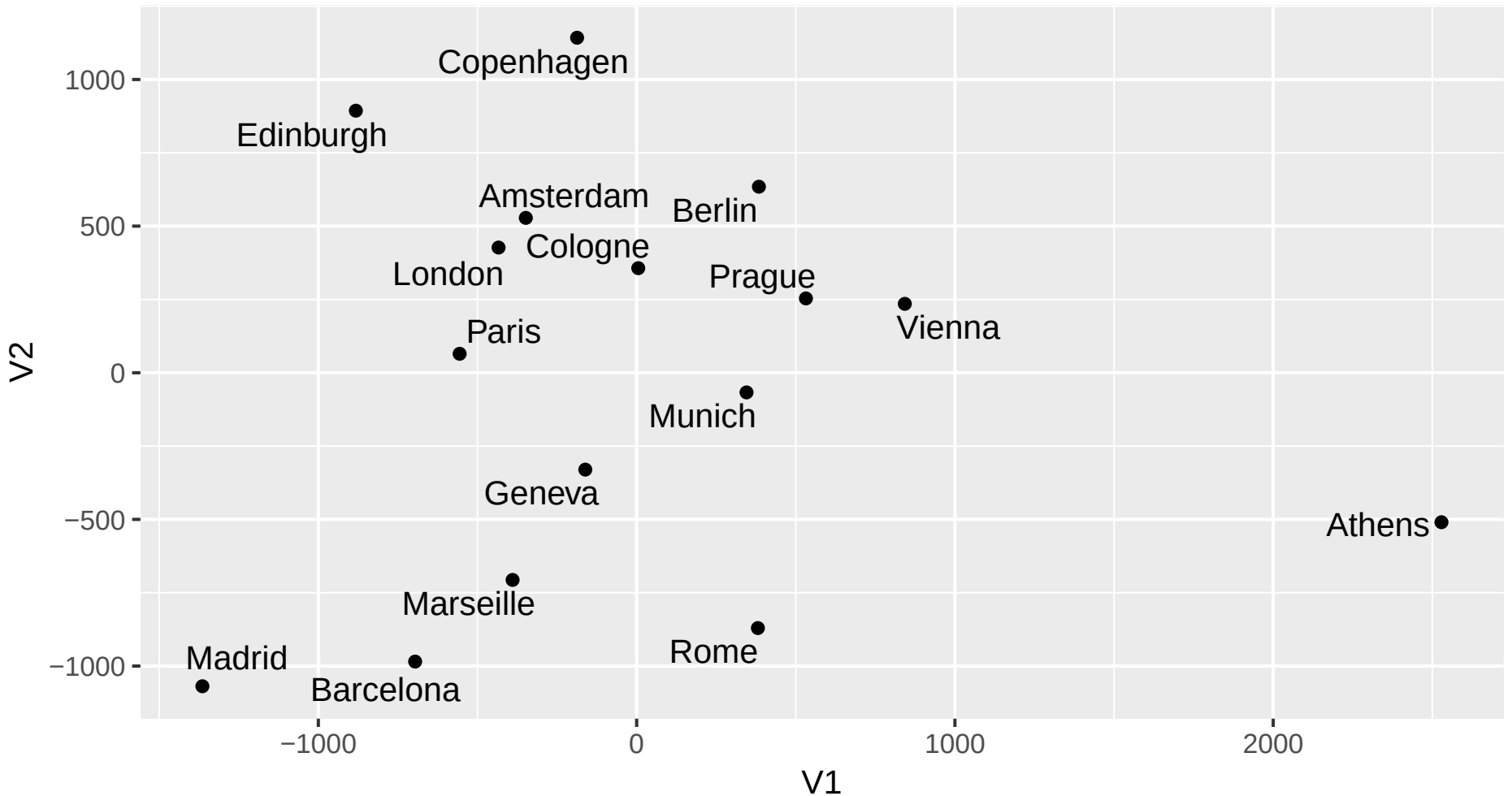
As a data frame; make picture

We know how to plot data frames, so make one first. This gives a warning that you can ignore: xxx

```
europe.scale %>%
  as_tibble() %>%
  mutate(city = europe$City) -> europe_coord
ggplot(europe_coord, aes(x = V1, y = V2, label = city)) +
  geom_point() + geom_text_repel() -> g
```

The map xxx

g


Copenhagen
Edinburgh
Amsterdam
Berlin
Cologne
London
Prague
Vienna
Paris
Munich
Geneva
Athens
Marseille
Madrid
Rome
Barcelona
1000
500
0
−500
−1000
V2
−1000
0
1000
2000
V1

Making a function

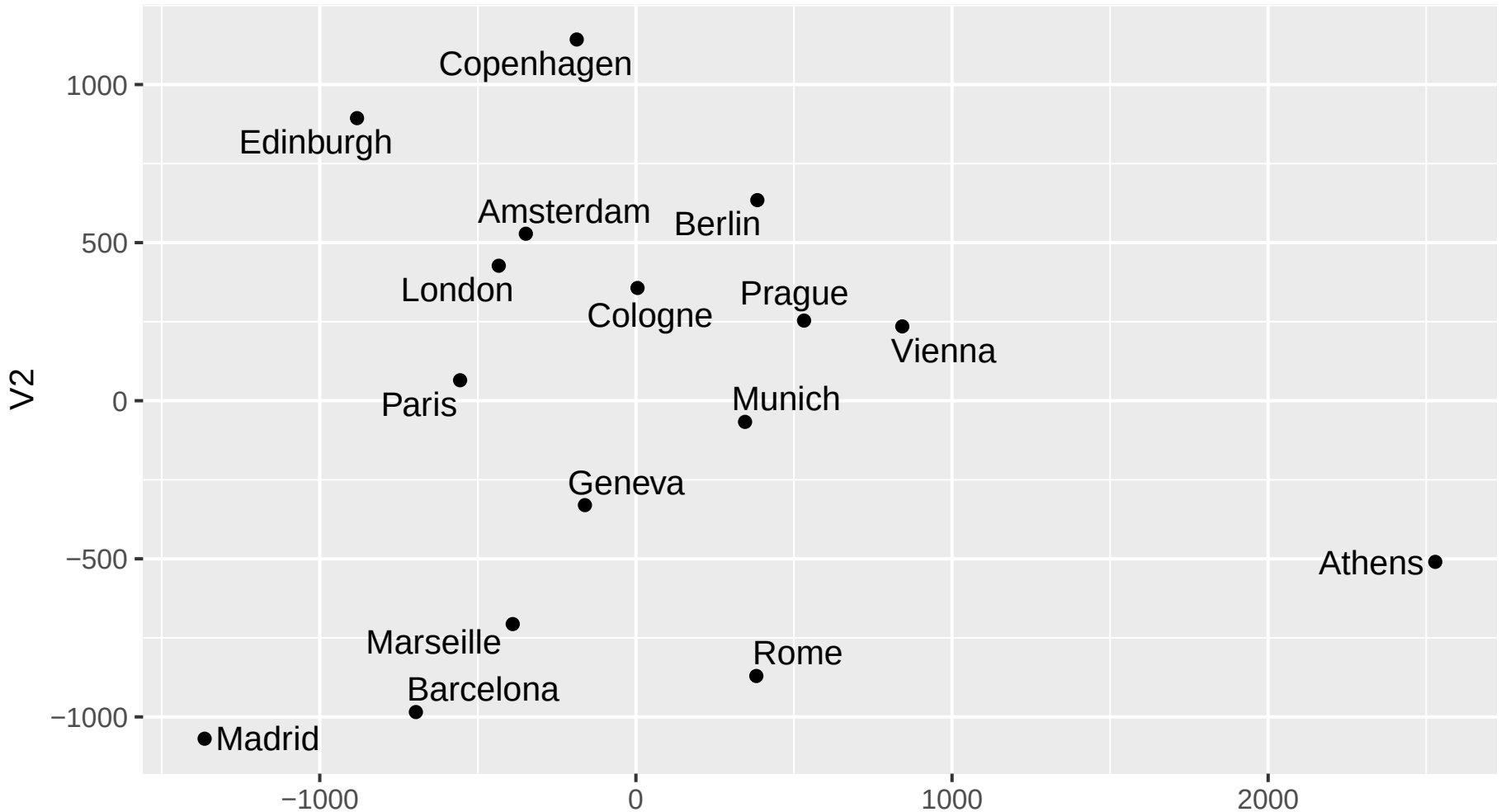
- Idea: given input distance matrix (as stored in a CSV file), output a map (like the one on the previous page). xxx

```
mds_map <- function(filename) {
  x <- read_csv(filename)
  dist <- x %>%
    select_if(is.numeric) %>%
    as.dist()
  x.scale <- cmdscale(dist) # this is a matrix
  x_coord <- x.scale %>%
    as_tibble() %>%
    mutate(place = row.names(x.scale))
  ggplot(x_coord, aes(x = V1, y = V2, label = place)) +
    geom_point() + geom_text_repel() +
    coord_fixed()
}
```

- Use `select_if` to pick out all the numerical columns (no text), whichever they are.
- `x.scale` is matrix with no column headers. Turn into data frame, acquires headers `V1` and `V2`. xxx 1 more

Does it work?

```
mds_map("europe.csv")
```



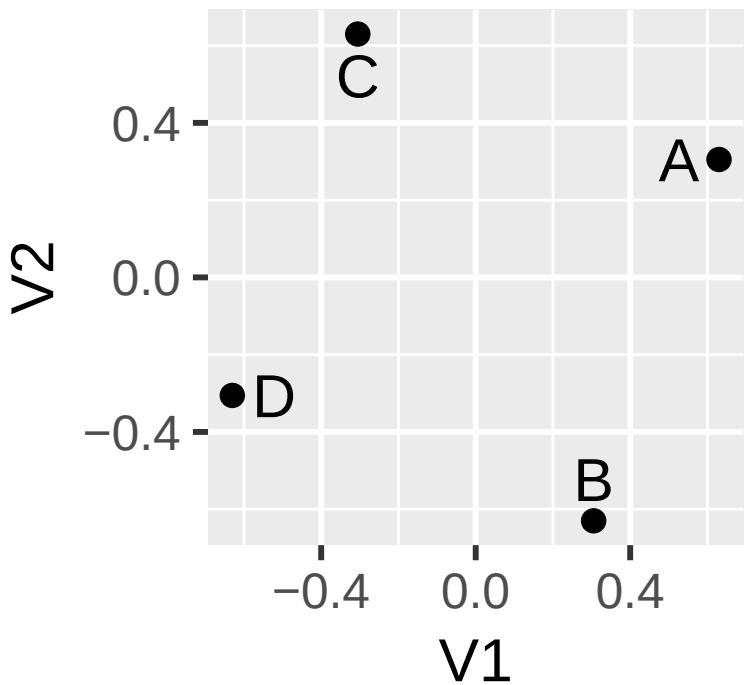
A square xxx

The data, in `square.csv`:

“‘ x,A ,B ,C ,D A,0 ,1 ,1 ,1.4 B,1 ,0 ,1.4,1 C,1 ,1.4,0 ,1 D,1.4,1 ,1 ,0 “‘

- The map: xxx

```
mds_map("square.csv")
```



Drawing a map of the real Europe

- Works with package ggmap.
- First find latitudes and longitudes of our cities, called *geocoding*:

```
latlong <- geocode(europe$City)
latlong <- bind_cols(city = europe$City, latlong)
latlong %>% slice(1:6)
```

```
## # A tibble: 6 x 3
##   city         lon   lat
##   <chr>      <dbl> <dbl>
## 1 Amsterdam   4.90  52.4
## 2 Athens     23.7   38.0
## 3 Barcelona   2.17  41.4
## 4 Berlin     13.4   52.5
## 5 Cologne     6.96  50.9
## 6 Copenhagen 12.6   55.7
```

- Just so you know, there is a limit of 2500 queries per day (it queries

Making the map

- Get a map of Europe from Google Maps (specify what you want a map of any way you can in Google Maps). This one centres the map on the city shown and zooms it so all the cities appear (I had to experiment):

```
map <- get_map("Memmingen DE", zoom = 5)
```

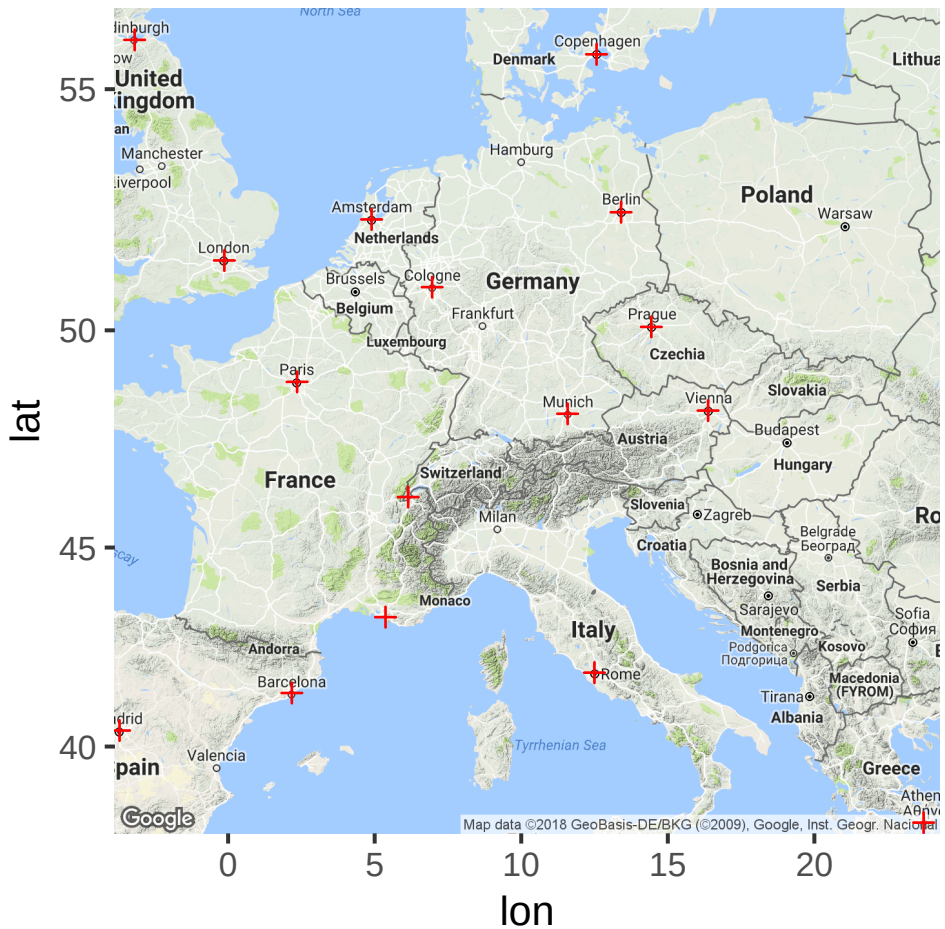
- Plot the map with ggmap. This is ggplot, so add anything to it that you would add to a ggplot, such as cities we want to show:

```
g2 <- ggmap(map) +
  geom_point(
    data = latlong, aes(x = lon, y = lat),
    shape = 3, colour = "red"
  )
```

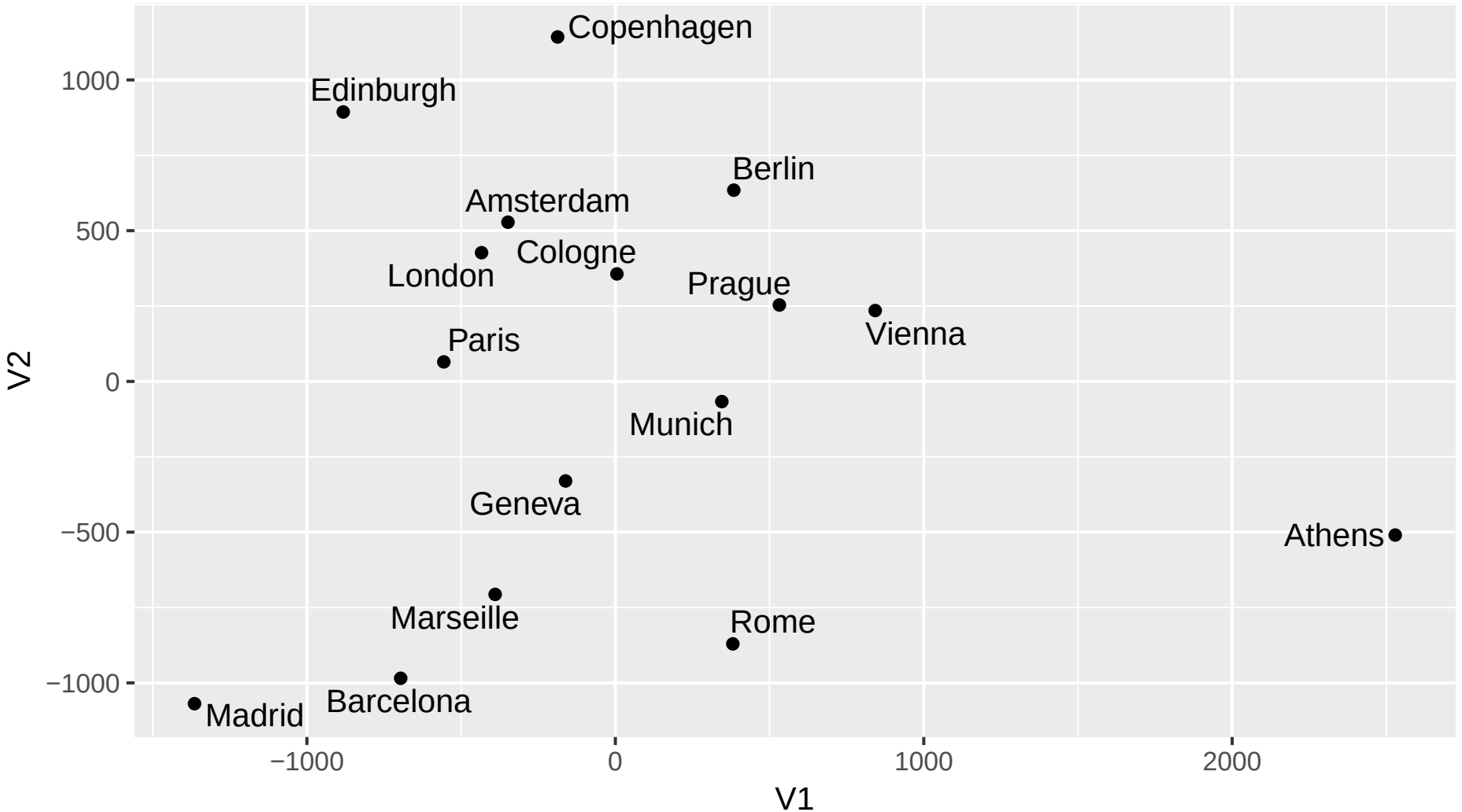
- We don't have a default data frame or aes for our geom_point, so have to specify one.

The real Europe with our cities

g2



Compare our scaling map



Comments

- North-south not quite right: Edinburgh and Copenhagen on same latitude, also Amsterdam and Berlin; Athens should be south of Rome.
- Rotating clockwise by about 45 degrees should fix that.
- General point: MDS only uses distances, so answer can be "off" by rotation (as here) or reflection (flipping over, say exchanging west and east while leaving north and south same).

Exploring the map by plotting in 3 dimensions

- Package `rgl` makes 3D plots.
- We have to fake up a 3rd dimension (by setting all its values to 1).
- Try this code:

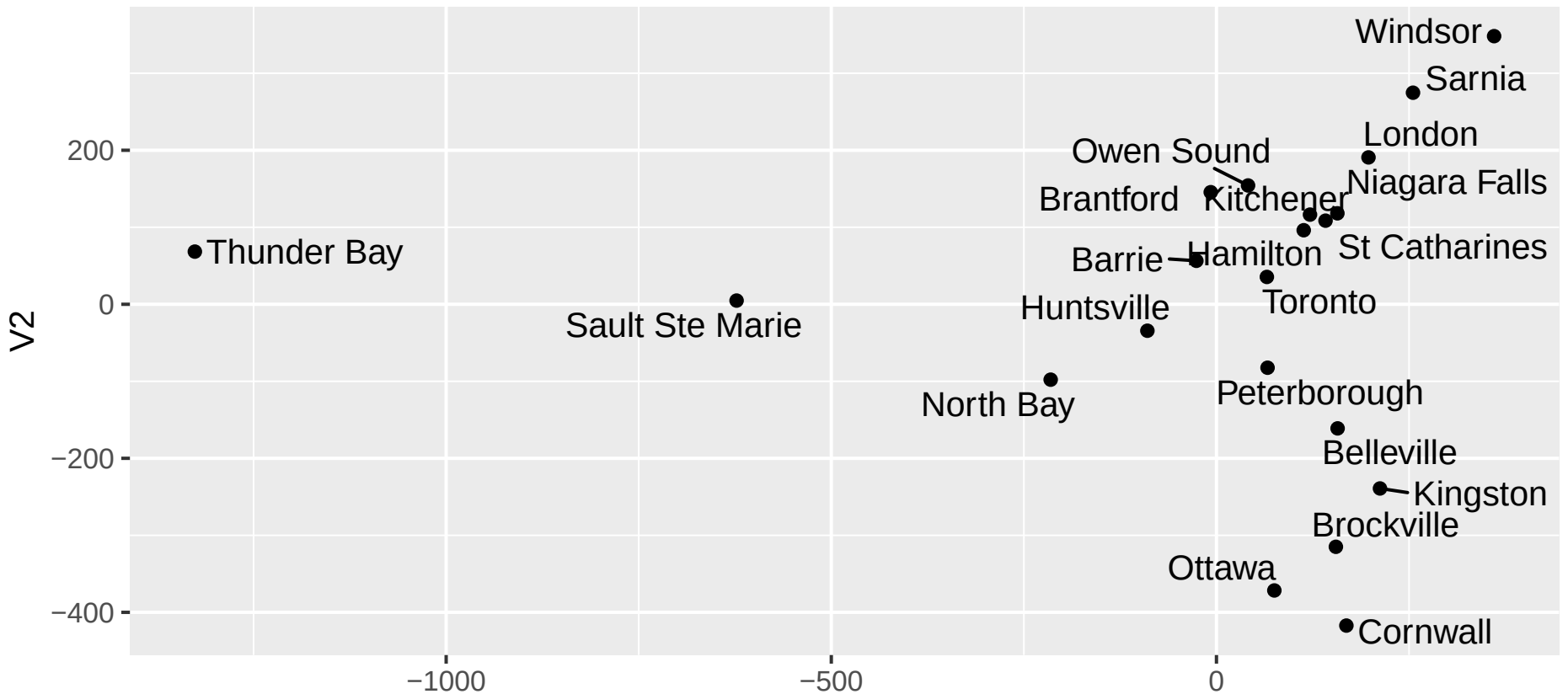
```
library(rgl)
es.2 <- cbind(europe.scale, 1)
plot3d(es.2, zlim = c(-1000, 1000))
text3d(es.2, text = europe$City)
```

- Opens a graphics window with the cities plotted and named.
- Click and hold left mouse button to rotate plot. "Rotate away" 3rd dimension to get a possible map (that preserves distances).

Ontario, the same way

...using our function: xxx

```
url <-
  "http://www.utsc.utoronto.ca/~butler/d29/ontario-road-distances.cs
(g <- mds_map(url))
```



Comment

- Thunder Bay and Sault Ste Marie dominate the picture since they are so far away from everywhere else.
- Remove them and just look at everywhere else.

Removing points

- Messy: have to find which rows and columns contain those cities, then remove just those rows and columns.
- Better:
  - "tidy" the distance matrix
  - then remove rows we don't need
  - then "untidy" it again
  - save into .csv file
- Illustrate with easier data first. xxx

Square data

```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/square.csv"
square <- read_csv(my_url)
square
```

```
## # A tibble: 4 x 5
##   x           A     B     C     D
##   <chr> <dbl> <dbl> <dbl> <dbl>
## 1 A         0     1     1     1.4
## 2 B         1     0     1.4   1
## 3 C         1     1.4   0     1
## 4 D         1.4   1     1     0
```

Make tidy

```
square %>% gather(point, distance, -x)
```

```
## # A tibble: 16 x 3
##    x     point distance
##    <chr> <chr>    <dbl>
##  1 A     A          0
##  2 B     A          1
##  3 C     A          1
##  4 D     A          1.4
##  5 A     B          1
##  6 B     B          0
##  7 C     B          1.4
##  8 D     B          1
##  9 A     C          1
## 10 B     C          1.4
## 11 C     C          0
## 12 D     C          1
## 13 A     D          1.4
## 14 B     D          1
## 15 C     D          1
## 16 D     D          0
```

Remove all references to point C

In column `x` or `point`: xxx

```
square %>%
  gather(point, distance, -1) %>%
  filter(x != "C", point != "C")
```

```
## # A tibble: 9 x 3
##   x     point distance
##   <chr> <chr>    <dbl>
## 1 A     A          0
## 2 B     A          1
## 3 D     A          1.4
## 4 A     B          1
## 5 B     B          0
## 6 D     B          1
## 7 A     D          1.4
## 8 B     D          1
## 9 D     D          0
```

Put back as distance matrix xxx

and save as .csv when we are happy:

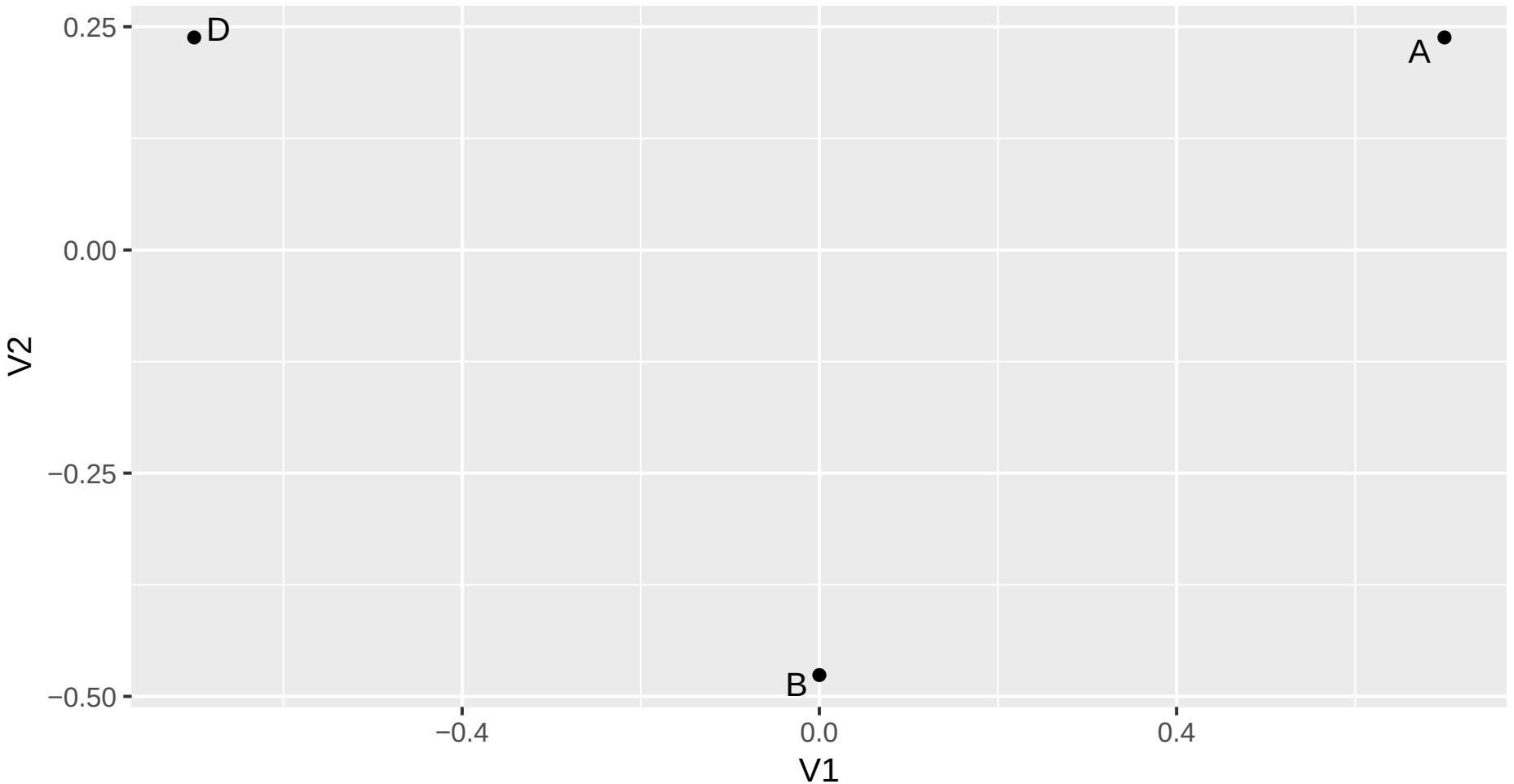
```
square %>%
  gather(point, distance, -1) %>%
  filter(x != "C", point != "C") %>%
  spread(point, distance) -> noc
noc
```

```
## # A tibble: 3 x 4
##   x         A     B     D
##   <chr> <dbl> <dbl> <dbl>
## 1 A         0     1   1.4
## 2 B         1     0   1
## 3 D         1.4   1   0
```

```
noc %>% write_csv("no-c.csv")
```

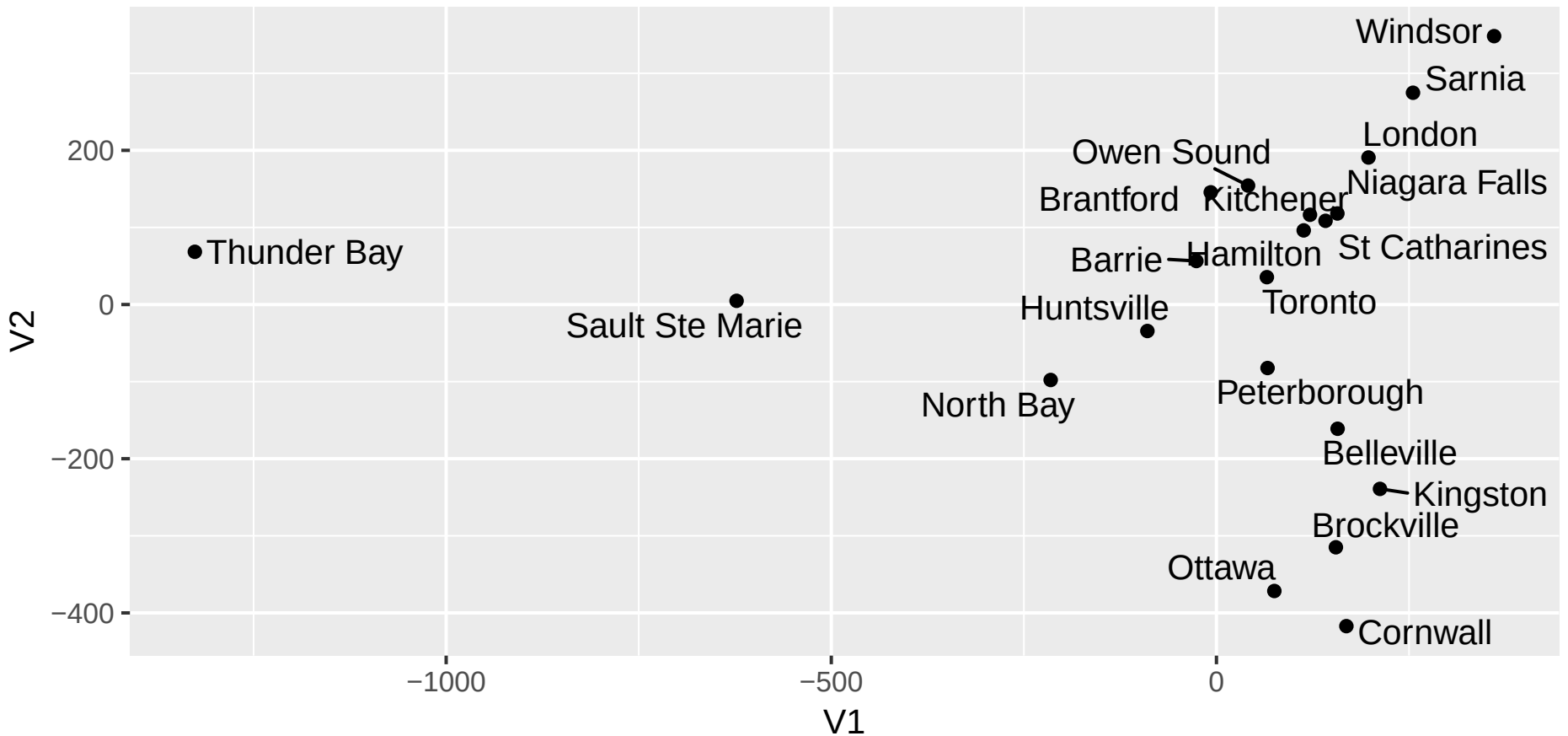
Make map of square-without-C

```
mds_map("no-c.csv")
```



Back to Ontario

```
g
```

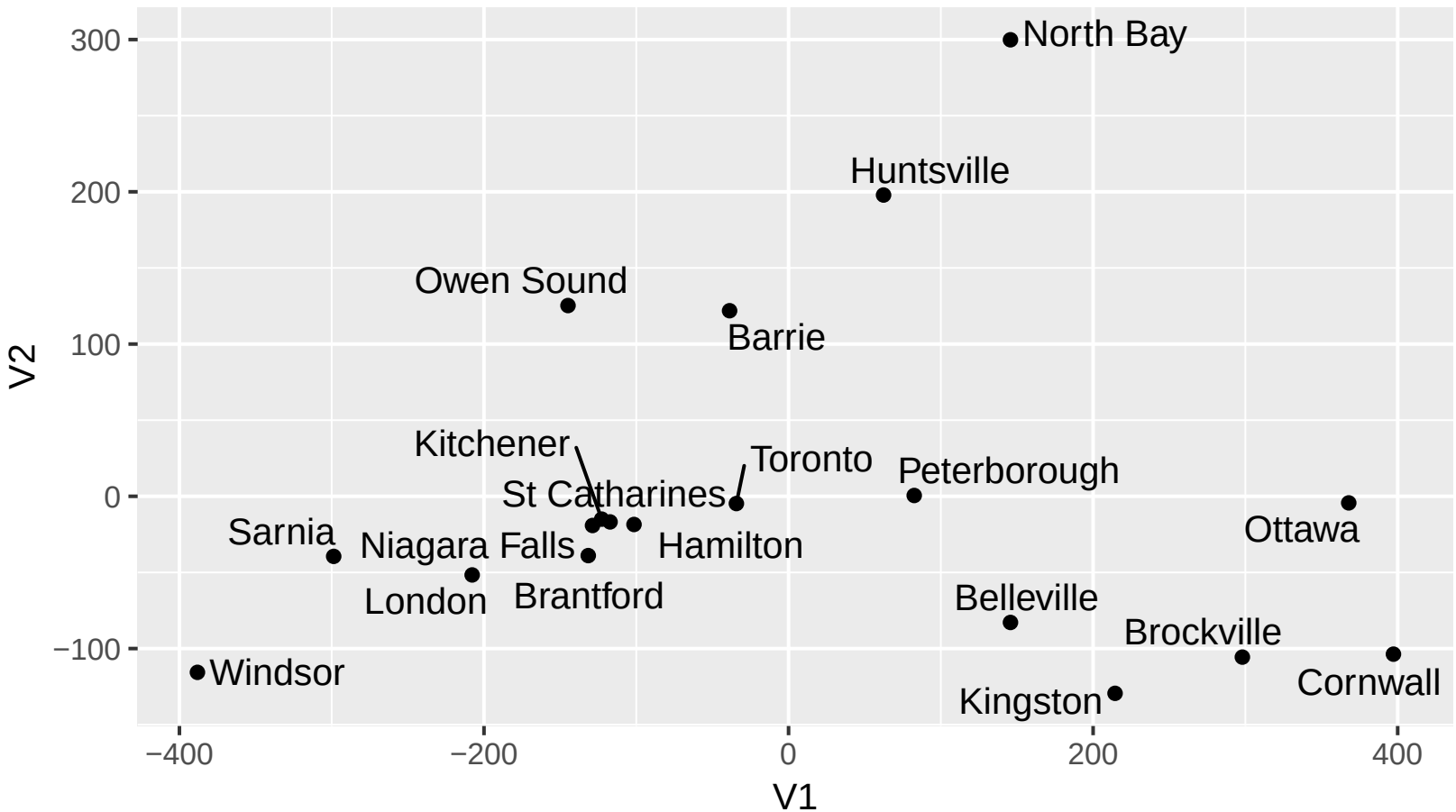


Tidy, remove, untidy xxx

```
my_url <-
  "http://www.utsc.utoronto.ca/~butler/d29/ontario-road-distances.csv"
ontario2 <- read_csv(my_url)
ontario2 %>%
  gather(city, distance, -1) %>%
  filter(
    city != "Thunder Bay",
    place != "Thunder Bay",
    city != "Sault Ste Marie",
    place != "Sault Ste Marie"
  ) %>%
  spread(place, distance) %>%
  write_csv("southern-ontario.csv")
```

Map of Southern Ontario xxx

```
(g <- mds_map("southern-ontario.csv"))
```



What about that cluster of points?

- Plot looks generally good, but what about that cluster of points?
- "Zoom in" on area between -150 and -100 on x axis, -50 to 0 on y axis.
- Code below overrides the `coord_fixed` we had before. xxx

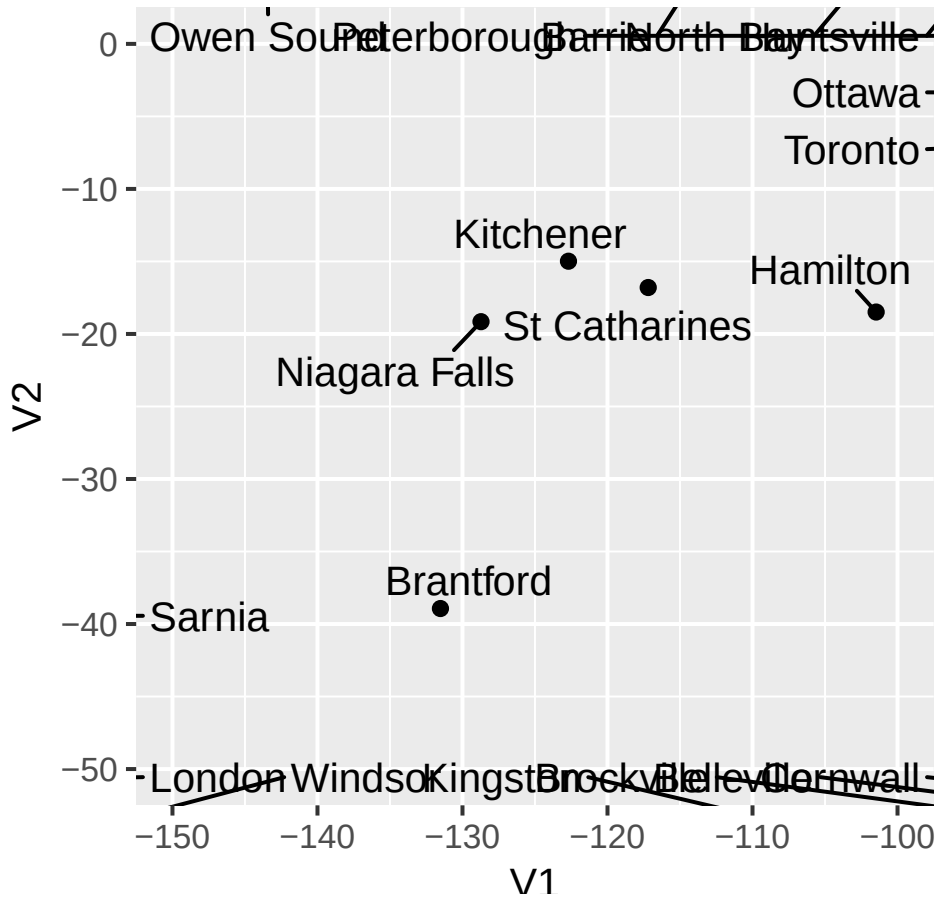
```
g2 <- g + coord_fixed(xlim = c(-150, -100), ylim = c(-50, 0))
```

```
## Coordinate system already present. Adding new coordinate system,
```

Zoomed-in plot

Ignore the arrows to points off the map:

```
g2
```



Does that make sense?

- Get a Google map of the area, with the points labelled.
- First geocode the cities of interest: xxx

```
cities <- c(
  "Kitchener ON", "Hamilton ON", "Niagara Falls ON",
  "St Catharines ON", "Brantford ON"
)
latlong <- geocode(cities)
latlong <- bind_cols(city = cities, latlong) %>% print()
```

```
## # A tibble: 5 x 3
##   city                lon   lat
##   <chr>             <dbl> <dbl>
## 1 Kitchener ON      -80.5  43.5
## 2 Hamilton ON       -79.9  43.3
## 3 Niagara Falls ON -79.1  43.1
## 4 St Catharines ON -79.2  43.2
## 5 Brantford ON      -80.3  43.1
```

Get Google map xxx

- Get a Google map of the area (experiment with zoom):

```
map <- get_map("Hamilton ON", zoom = 8)
```

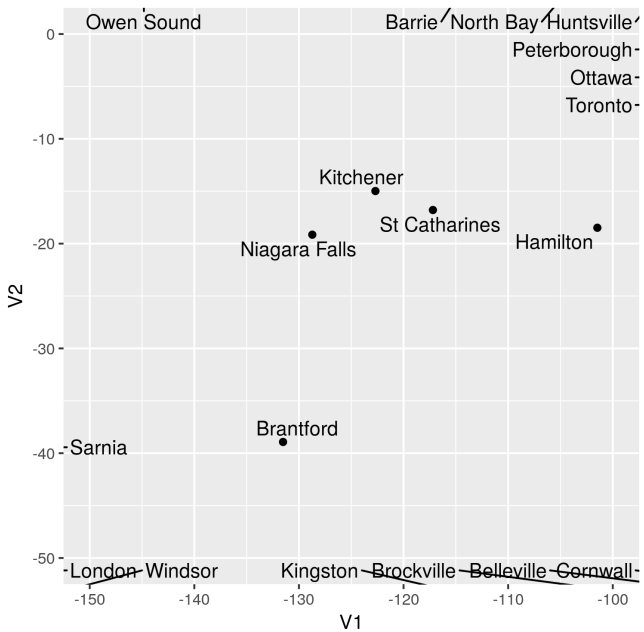
- Plot map with cities marked. xxx

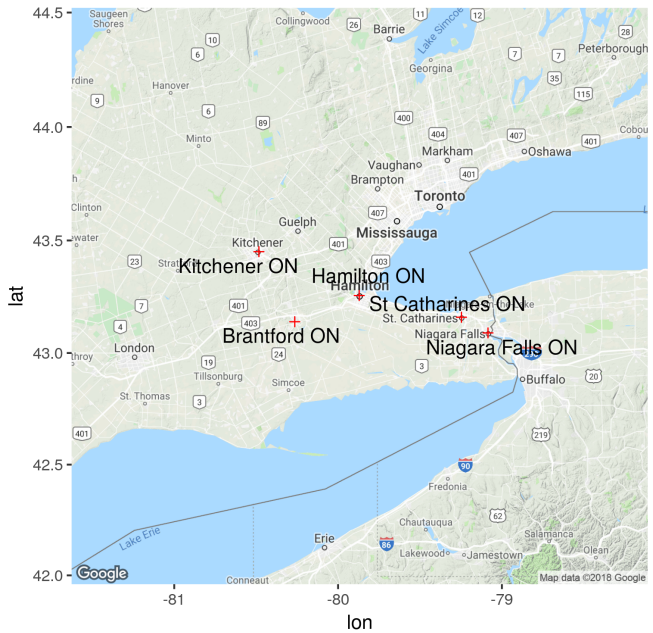
Making the R Google map

Plot the map, plus the cities, plus labels for the cities:

```
ggmap(map) +
  geom_point(
    data = latlong,
    aes(x = lon, y = lat),
    shape = 3, colour = "red"
  ) +
  geom_text_repel(
    data = latlong,
    aes(label = city)
  ) -> gmap
```

MDS and Google map side by side xxx





St Catharines and Niagara Falls should be the *other* side of Hamilton!

Quality of fit

- Read in "southern Ontario" data set from file. Calling `cmdscale` with `eig=T` gives more info: xxx

```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/southern-ontario.csv"
ontario2 <- read_csv(my_url)
ontario2.2 <- ontario2 %>%
  select_if(is.numeric) %>%
  cmdscale(eig = T)
names(ontario2.2)
```

```
## [1] "points" "eig"    "x"      "ac"     "GOF"
```

```
ontario2.2$GOF
```

```
## [1] 0.8381590 0.8914059
```

```
ontario2.3 <- ontario2 %>%
  select_if(is.numeric) %>%
  cmdscale(3, eig = T)
ontario2.3$GOF
```

```
## [1] 0.8852559 0.9414948
```

Comments

- Coordinates now in `points`.
- `GOF` is R-squared-like measure saying how well map distances match real ones. Higher is better.
- For Ontario road distances, `GOF` better for 3 dimensions than 2, presumably to accommodate St Catharines and Niagara Falls?

3-dimensional coordinates, cities attached xxx

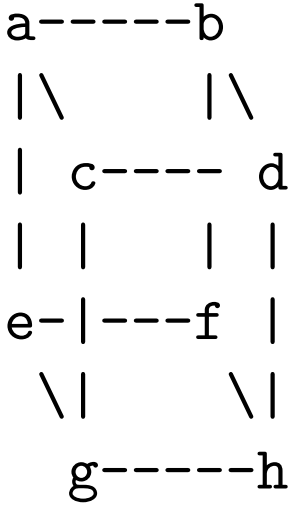
```
ontario2.3$points %>%
  as_tibble() %>%
  mutate(city = ontario2$x)
```

```
## # A tibble: 19 x 4
##        V1       V2      V3 city
##     <dbl>    <dbl>   <dbl> <chr>
##  1  -38.7  122.       4.17 Barrie
##  2  146.   -82.8      1.53 Belleville
##  3 -132.   -38.9     14.1  Brantford
##  4  298.  -106.      -7.74 Brockville
##  5  397.  -104.     -22.0  Cornwall
##  6 -101.   -18.5     30.0  Hamilton
##  7   62.4  198.     -14.0  Huntsville
##  8  214.  -129.      10.8  Kingston
##  9 -123.   -15.0     -6.44 Kitchener
## 10 -208.   -51.6    -36.5  London
## 11 -129.   -19.1    155.   Niagara Falls
## 12  146.   300.     -25.4  North Bay
## 13  368.    -4.30   -47.2  Ottawa
## 14 -145.   125.     -16.0  Owen Sound
## 15   82.5    0.551   -6.92 Peterborough
## 16 -299.   -39.4    -72.5  Sarnia
## 17 -117.   -16.8    123.   St Catharines
## 18  -34.3   -4.75    15.8  Toronto
## 19 -388.  -116.     -99.5  Windsor
```

RGL code for 3 dimensions

```
library(rgl)
plot3d(ontario2.3$points)
text3d(ontario2.3$points, text = ontario2$x)
```

A cube xxx



Cube has side length 1, so distance across diagonal on same face is $\sqrt{2} \simeq 1.4$ and "long" diagonal of cube is $\sqrt{3} \simeq 1.7$.

Try MDS on this obviously 3-dimensional data.

Cube data as distances xxx

```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/cube.txt"
cube <- read_table(my_url)
cube
```

```
## # A tibble: 8 x 9
##   x         a     b     c     d     e     f     g     h
##   <chr> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl>
## 1 a         0    NA    NA    NA    NA    NA    NA    NA
## 2 b         1     0    NA    NA    NA    NA    NA    NA
## 3 c         1     1     0    NA    NA    NA    NA    NA
## 4 d         1.4   1     1     0    NA    NA    NA    NA
## 5 e         1     1.4   1.4   1.7   0    NA    NA    NA
## 6 f         1.4   1     1.7   1.4   1     0    NA    NA
## 7 g         1.4   1.7   1     1.4   1     1.4   0    NA
## 8 h         1.7   1.4   1.4   1     1.4   1     1     0
```

Making dist object

```
cube.d <- cube %>% select(-1) %>% as.dist()
cube.d
```

```
##     a   b   c   d   e   f   g
## b 1.0
## c 1.0 1.0
## d 1.4 1.0 1.0
## e 1.0 1.4 1.4 1.7
## f 1.4 1.0 1.7 1.4 1.0
## g 1.4 1.7 1.0 1.4 1.0 1.4
## h 1.7 1.4 1.4 1.0 1.4 1.0 1.0
```

MDS and plotting commands

- By default in 2 dimensions; save the extra stuff for later:

```
cube.2 <- cube.d %>% cmdscale(eig = T)
```

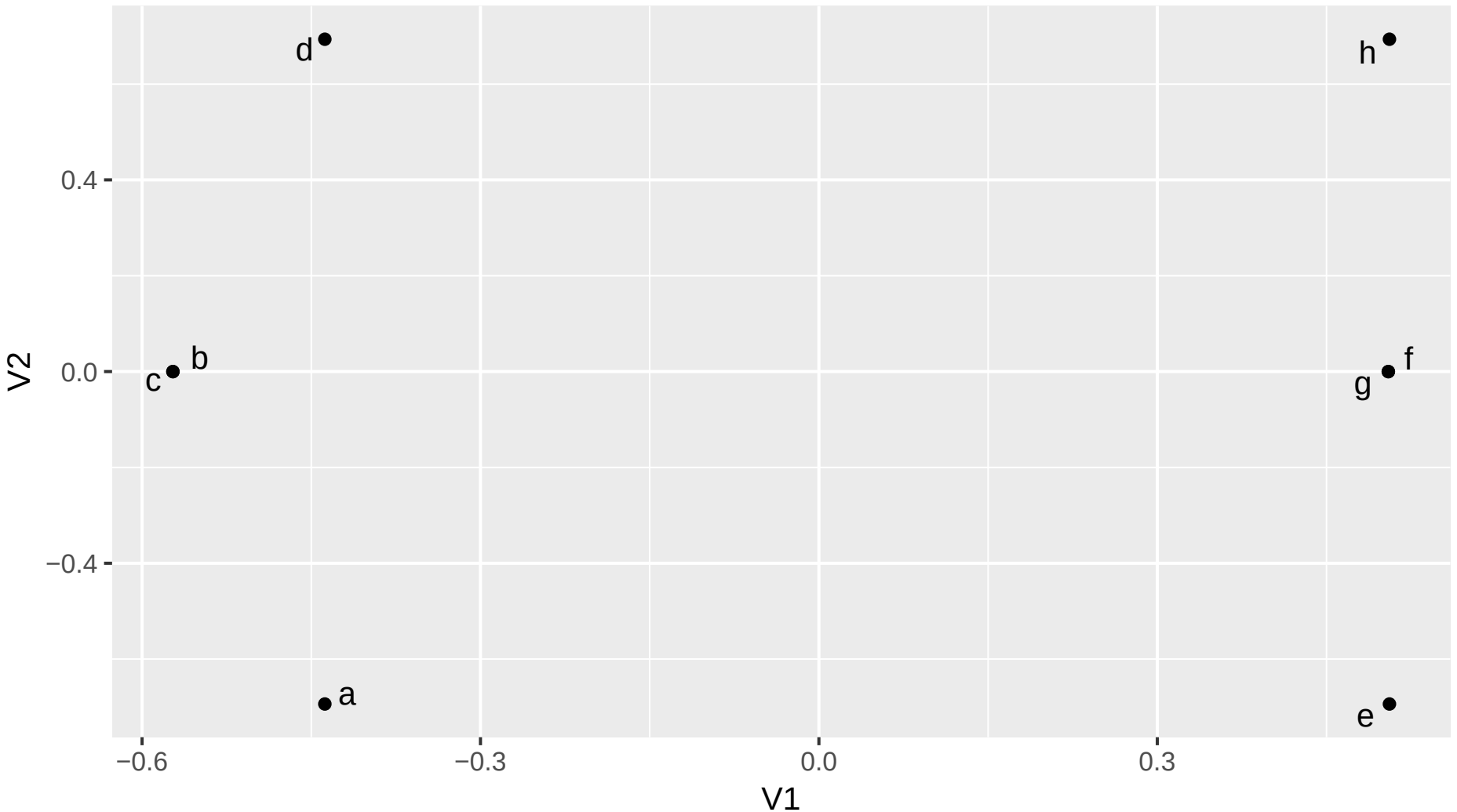
- Make data frame to plot, remembering the points to plot are in `points` now:

```
d <- cube.2$points %>%
  as_tibble() %>%
  mutate(corners = cube$x)
```

- Plot points labelled by our names for the corners:

```
g <- ggplot(d, aes(x = V1, y = V2, label = corners)) +
  geom_point() + geom_text_repel()
```

The "cube"



2 and 3 dimensions

```
cube.3 <- cube.d %>% cmdscale(3, eig = T)
cube.2$GOF
```

```
## [1] 0.639293 0.664332
```

```
cube.3$GOF
```

```
## [1] 0.9143532 0.9501654
```

- Really need 3rd dimension to represent cube.

Non-metric scaling

- Sometimes distances not meaningful *as distances*
- Only order matters: closest should be closest, farthest farthest on map, but how much further doesn't matter.
- Non-metric scaling, aims to minimize **stress**, measure of lack of fit.
- Example: languages. Make map based on "similarity" of number names, without requiring that 1 is "eight times better" than 8.

The languages

- Recall language data (from cluster analysis): 1–10, measure dissimilarity between two languages by how many number names *differ* xxx in first letter:

xxx

```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/languages.txt"
number.d <- read_table(my_url)
number.d
```

```
## # A tibble: 11 x 12
##    la       en    no    dk    nl    de    fr    es
##    <chr> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl>
##  1 en        0     2     2     7     6     6     6
##  2 no        2     0     1     5     4     6     6
##  3 dk        2     1     0     6     5     6     5
##  4 nl        7     5     6     0     5     9     9
##  5 de        6     4     5     5     0     7     7
##  6 fr        6     6     6     9     7     0     2
##  7 es        6     6     5     9     7     2     0
##  8 it        6     6     5     9     7     1     1
##  9 pl        7     7     6    10     8     5     3
## 10 hu        9     8     8     8     9    10    10
```

Non-metric scaling

- Turn language dissimilarities into `dist` object
- Run through `isoMDS` from `MASS` package; works like `cmdscale`.
- Map only reproduces *relative* xxx closeness of languages. xxx

```
d <- number.d %>%
  select_if(is.numeric) %>%
  as.dist()
number.nm <- d %>% isoMDS()
```

```
## initial  value 12.404671
## iter   5 value 5.933653
## iter  10 value 5.300747
## final  value 5.265236
## converged
```

```
names(number.nm)
```

```
## [1] "points" "stress"
```

Results

- Stress is very low (5%, good):

```
number.nm$stress
```

```
## [1] 5.265236
```

$ %$ %$

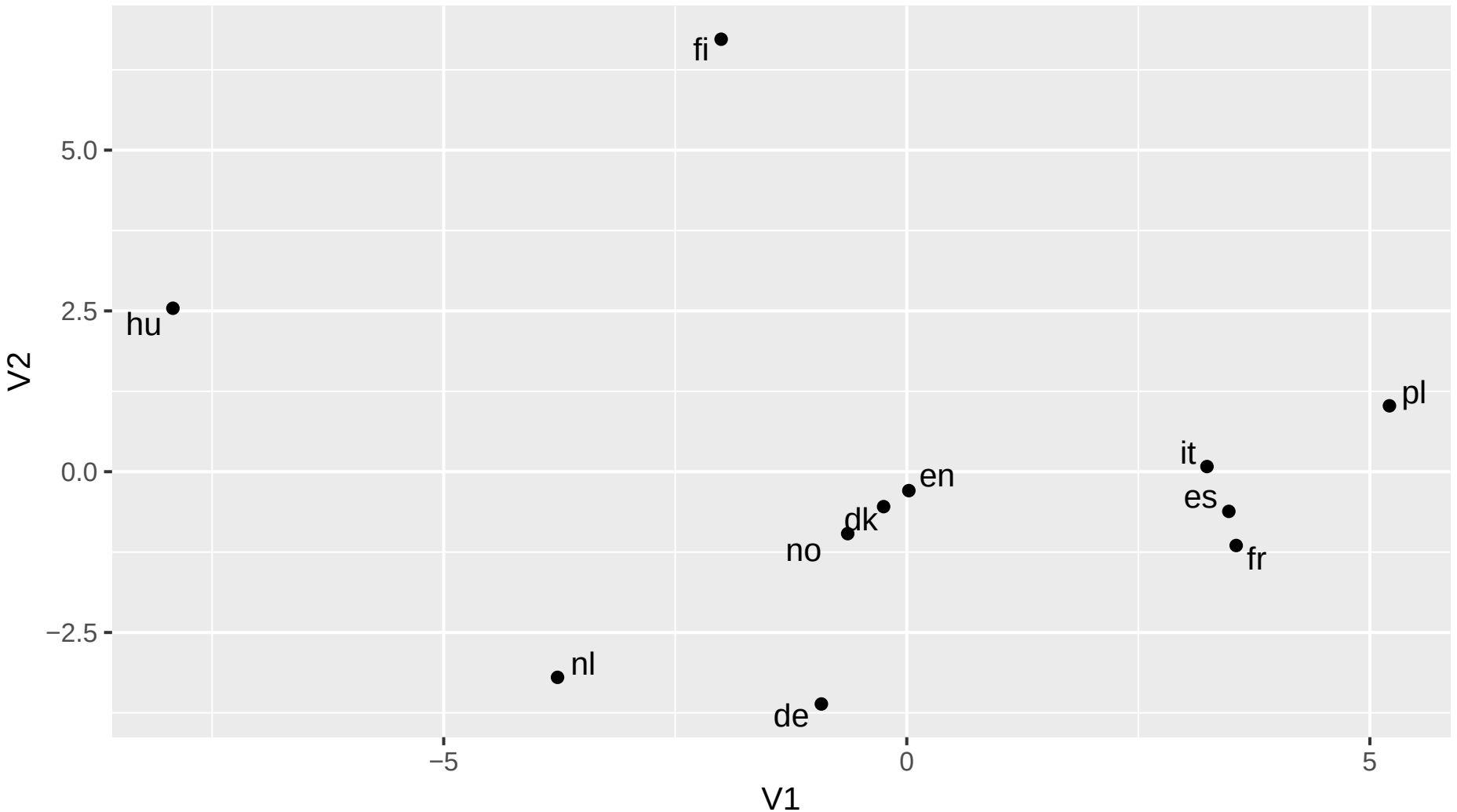
- Familiar process: make a data frame to plot. Use name dd for data frame this time since used d for distance object:

```
dd <- number.nm$points %>%
  as_tibble() %>%
  mutate(lang = number.d$la)
```

- Make plot:

```
g <- ggplot(dd, aes(x = V1, y = V2, label = lang)) +
  geom_point() + geom_text_repel()
```

The languages map



Comments

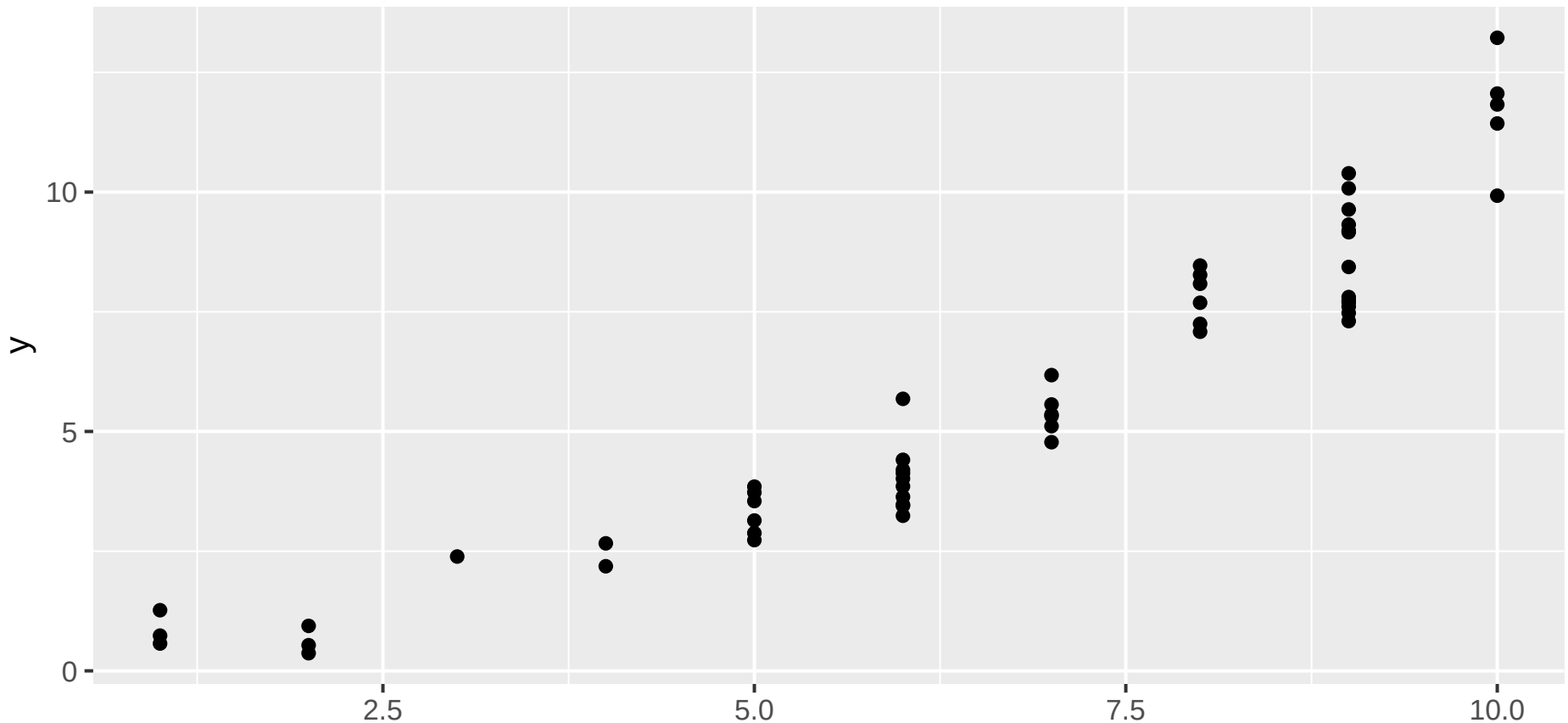
- Tight clusters: Italian-Spanish-French, English-Danish-Norwegian.
- Dutch and German close to English group.
- Polish close to French group.
- Hungarian, Finnish distant from everything else and each other!
- Similar conclusions as from the cluster analysis.

Shepard diagram

- Stress for languages data was 5.3%, very low.
- How do observed dissimilarities and map distances correspond?
- For low stress, expect larger dissimilarity to go with larger map distance, almost all the time.
- Not necessarily a linear trend since non-metric MDS works with *order* of values.
- Actual dissimilarity on x-axis; map distances on y-axis.

Shepard diagram for languages

```
Shepard(d, number.nm$points) %>%
  as_tibble() %>%
  ggplot(aes(x = x, y = y)) + geom_point()
```



Cube, revisited xxx

```
cube.d <- cube %>% select(-x) %>% as.dist(cube)
cube.2 <- isoMDS(cube.d, trace = F)
cube.2$stress
```

```
## [1] 17.97392
```

```
cube.3 <- isoMDS(cube.d, k = 3, trace = F)
cube.3$stress
```

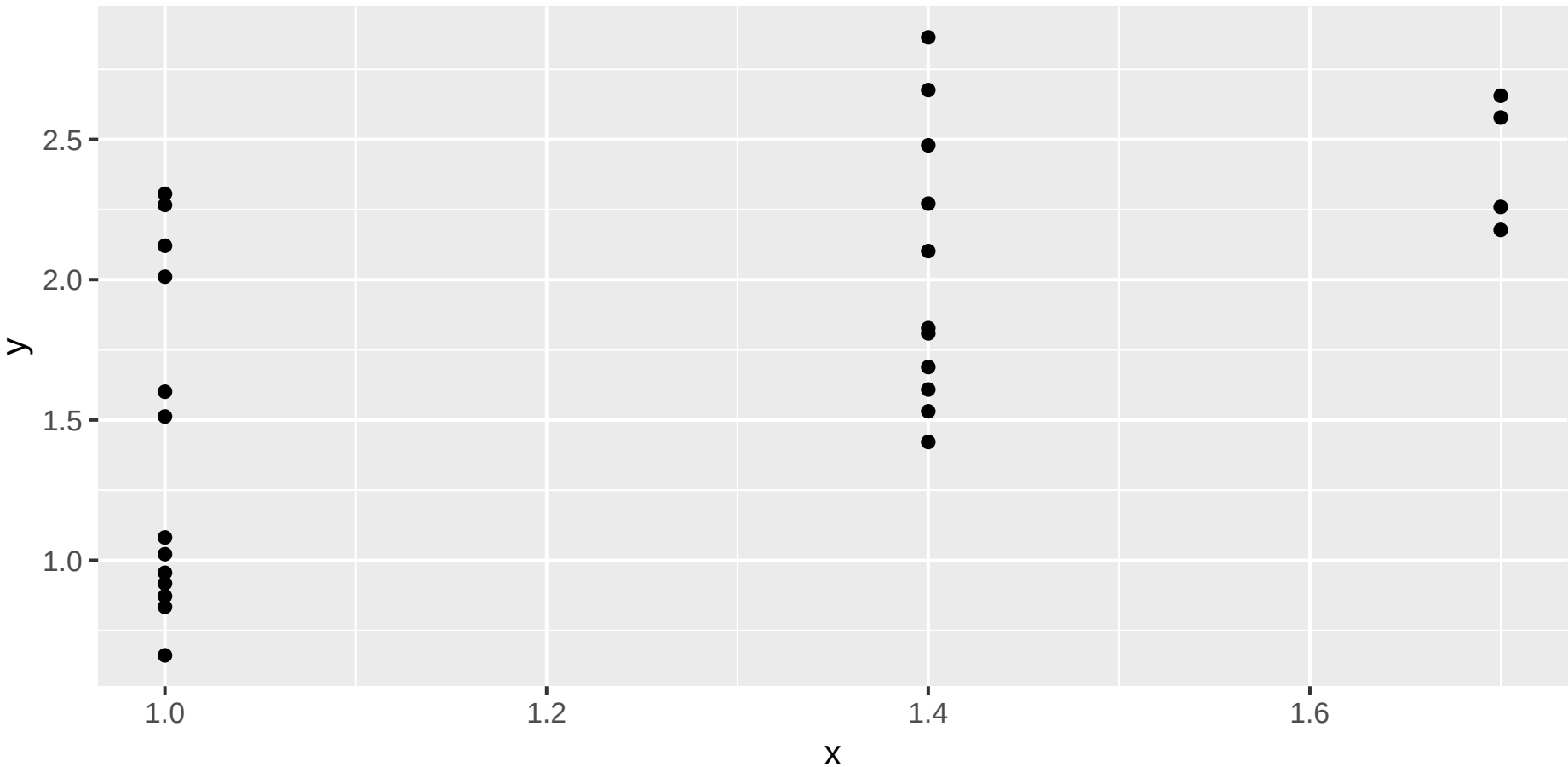
```
## [1] 0.007819523
```

- Stress is 18% for 2 dimensions, basically 0% for 3.
- Three dimensions correct, two dimensions bad.
- Shepard diagrams for these: xxx

```
cube2.sh <- Shepard(cube.d, cube.2$points)
g2 <- ggplot(as.data.frame(cube2.sh), aes(x = x, y = y)) +
  geom_point()
cube3.sh <- Shepard(cube.d, cube.3$points)
g3 <- ggplot(as.data.frame(cube3.sh), aes(x = x, y = y)) +
```

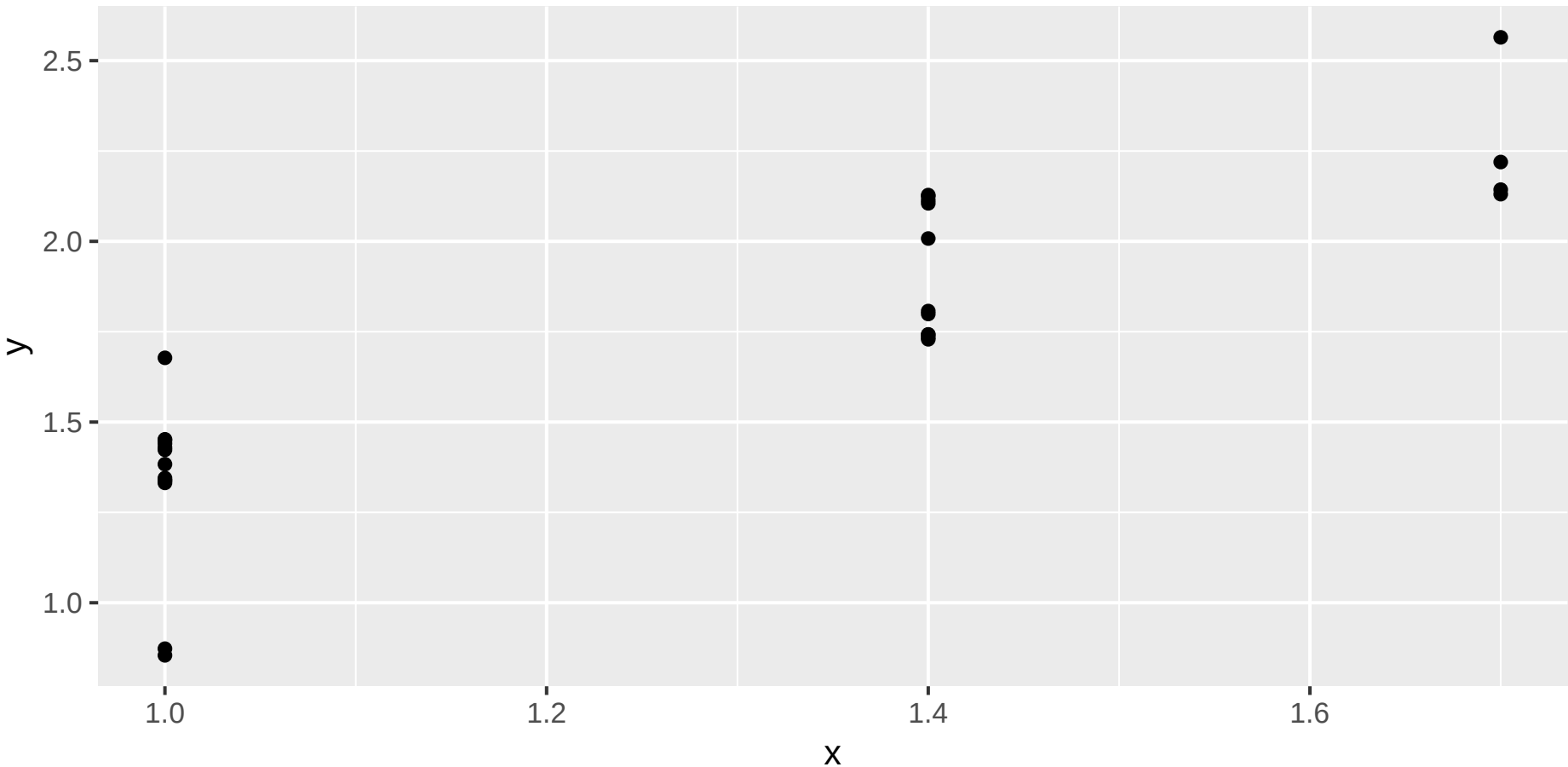
Shepard diagram for 2-dimensional cube

g2



Shepard diagram for 3-dimensional cube

g3



Guidelines for stress values, in %

Smaller is better:

Stress value	Interpretation
Less than 5	Excellent: no prospect of misinterpretation (rarely achieved)
5–10	Good: most distances reproduced well, small prospect of false inferences
10–20	Fair: usable, but some distances misleading.
More than 20	Poor: may be dangerous to interpret

- Languages: stress in "good" range.
- Cube: xxx
  - 2 dimensions "fair", almost "poor";
  - 3 dimensions, "excellent".