Distances and similarity

Distances and similarity

- Distance and similarity are more or less opposite concepts.
- Distance is a **numerical measure** describing how are two objects (defined by certain variables) different (*pairwise distance*).
- Different distance measures exist for different data types.

Distance

- Scale $0 - \infty$
- 0 – Two objects with 0 distance between them.
- ∞ – Two objects with infinite distance.
- In practice, maximum distance is often 1.
- Denoted by D (for distance, or dissimilarity).
- $D = 1 - S$

Similarity

- Scale 0 – 1
- 0 – Two objects completely dissimilar (0%).
- 1 – Two objects competely similar (100%).
- Denoted by S (for similarity).
- $S = 1 - D$

Different distance measures

- Dichotomous variables
  - Symmetrical – Simple matching distance
  - Asymmetrical – Jaccard index (binary distance)

- Categorical variables
    - Hamming distance
- Numeric continuous variables
    - Euclidean distance
    - Mahalanobis distance
- Mixed data sets
    - Gower's distance

Binary distances

- For `TRUE/FALSE`, `1/0`, `presence/absence` (etc.) data

Symmetrical

- Two **presences** as **match**.
- Two **absences** as **match**.

If a trait is present, two objects are more similar. If a trait is absent, two objects are more similar. For example if *biological sex* is encoded in one variable with `0` for *male* and `1` for *female*, it is symmetrical.

- **Simple maching distance**

Asymmetrical

- Two **presences** as **match**.
- Two **absences** as **mismatch**.

If a trait is present, two objects are more similar. If a trait is **absent** in both cases, e.g. **undetermined**, **missing** etc., this does not affect similarity. This is more practical in archaeology.

- **Jaccard index**, i.e. **binary distance**

```
dist(x, method = "binary")
```

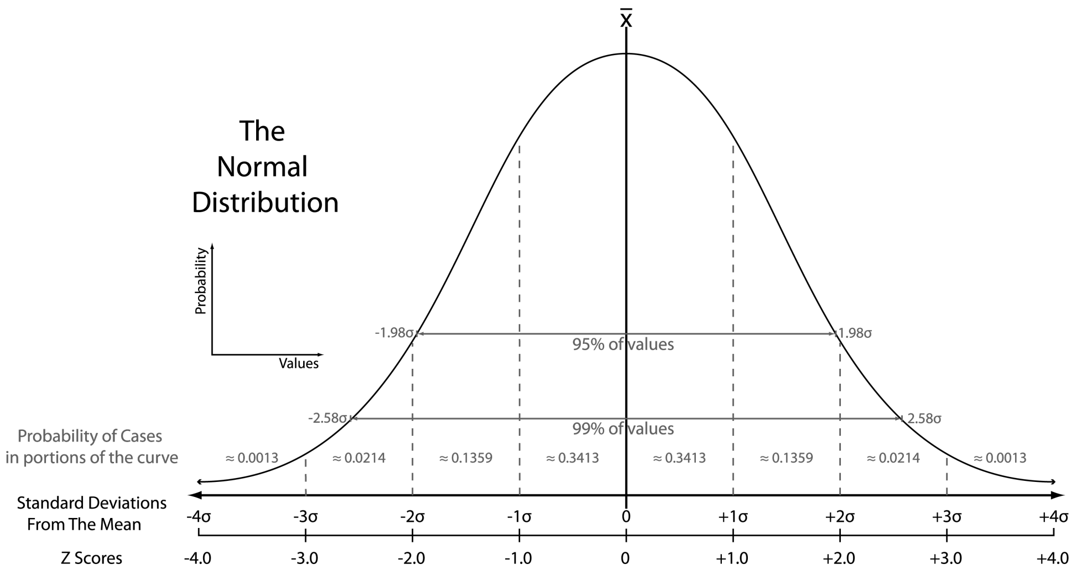
Distance between (continuous) numeric data

- To **remove effects of scale** (different units etc.), variables should be scaled (normalized).

Normalization

- *z-score* or *z-transformation*

$$z = \frac{x - \mu}{\sigma}$$



Euclidean distance

- Defined for a **Cartesian coordinate space**.
- Uses **Pythagorean theorem**.

$$d(p, q) = \sqrt{(q_1 - p_1)^2 + (q_2 - p_2)^2}$$

In R...

Normalization:
`scale(x, center = TRUE, scale = TRUE)`

Euclidean distance:
`dist(x, method = "euclidean")`

Code along

```
library(dplyr)
darts <- read.csv("https://petrpajdla.github.io/stat4arch/lect/w09/data/dartpoints_numeric.cs
```

```
# summary of values
summary(select(darts, Length, Width, Thickness, Weight))
```

```
     Length           Width          Thickness          Weight
 Min.   : 30.60   Min.   :14.50   Min.   : 4.000   Min.   : 2.300
 1st Qu.: 40.85   1st Qu.:18.55   1st Qu.: 6.250   1st Qu.: 4.550
 Median : 47.10   Median :21.10   Median : 7.200   Median : 6.800
 Mean   : 49.33   Mean   :22.08   Mean   : 7.271   Mean   : 7.643
 3rd Qu.: 55.80   3rd Qu.:25.15   3rd Qu.: 8.250   3rd Qu.:10.050
 Max.   :109.50   Max.   :49.30   Max.   :10.700   Max.   :28.800
```

```
# normalization
darts_norm <- darts %>%
  mutate(Length = scale(Length), Width = scale(Width),
         Thickness = scale(Thickness), Weight = scale(Weight))

# or this shorthand can be used
darts_norm <- darts %>%
  mutate(across(all_of(c("Length", "Width", "Thickness", "Weight")), scale))
```

```
# summary of normalized values
summary(select(darts_norm, Length, Width, Thickness, Weight))
```

```
      Length.V1           Width.V1           Thickness.V1
 Min.   :-1.470673   Min.   :-1.469440   Min.   :-2.1363403
 1st Qu.:-0.665879   1st Qu.:-0.683998   1st Qu.:-0.6670233
```

```
 Median :-0.175152   Median :-0.189461   Median :-0.0466450
 Mean   : 0.000000   Mean   : 0.000000   Mean   : 0.0000000
 3rd Qu.: 0.507941   3rd Qu.: 0.595981   3rd Qu.: 0.6390363
 Max.   : 4.724271   Max.   : 5.279540   Max.   : 2.2389592
      Weight.V1
 Min.   :-1.269966
 1st Qu.:-0.735154
 Median :-0.200342
 Mean   : 0.000000
 3rd Qu.: 0.572164
 Max.   : 5.028928
```

Code along

```
# subset of Travis and Darl types of dart points
darts_subset <- filter(darts_norm, Name %in% c("Travis", "Darl"))

# matrix with numerical variables only
darts_mx <- darts_subset %>%
  select(Length, Width, Thickness, Weight) %>%
  as.matrix()

# add row names to the matrix
rownames(darts_mx) <- darts_subset$Name

# count Euclidean distance
darts_d <- dist(darts_mx, method = "euclidean", diag = TRUE)

round(as.matrix(darts_d)[1:6, 1:6], 2)
```

```
     Darl Darl Darl Darl Darl Darl
Darl 0.00 0.42 0.47 0.40 1.57 1.14
Darl 0.42 0.00 0.43 0.43 1.50 1.18
Darl 0.47 0.43 0.00 0.28 1.51 1.36
Darl 0.40 0.43 0.28 0.00 1.74 1.47
Darl 1.57 1.50 1.51 1.74 0.00 0.90
Darl 1.14 1.18 1.36 1.47 0.90 0.00
```

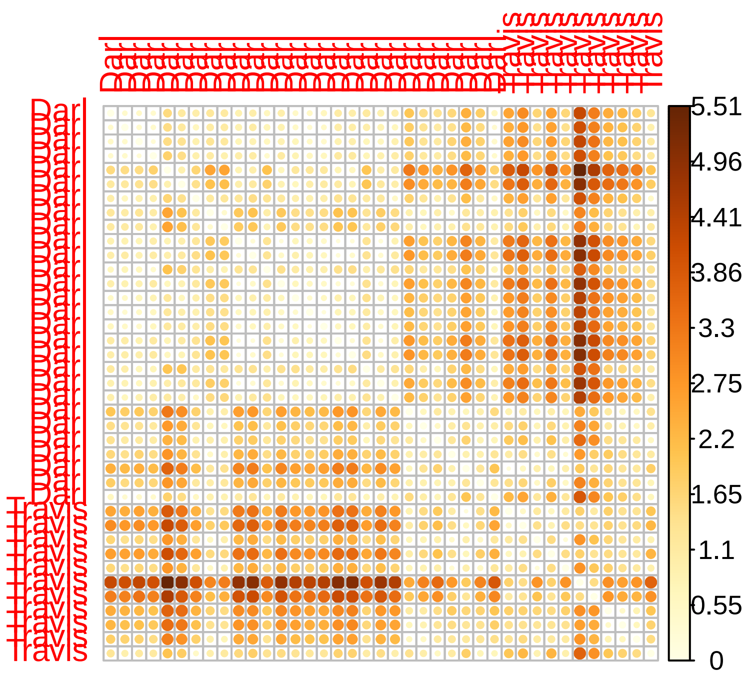
- Result is a **distance matrix**.
- It is **symmetrical**. **Lower triangular** is the same as **upper triangular**.
- On the **diagonal**, there is distance of the given object to itself, i.e. 0.

Visualizing distance matrix

- Package `corrplot` has a nice way of plotting heatmaps.

```r
library(corrplot)

# arg. is.corr set to FALSE, because we are not visualizing correlation matrix
corrplot(as.matrix(darts_d), is.corr = FALSE)
```



Resources

For a much more detailed overview of distance methods, see the tutorial on classification by Schmidt, S. C. et al. DOI: 10.5281/zenodo.6325372 (direct link to a HTML file is here).