Mixed metrics

Comparing heterogeneous objects

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Ascendant hierarchical clustering

Hot points :

- Agregation criteria
  - Centroid criterion
  - Ward's criterion
- Distance between individuals
  - Only quantitative variables → Euclidean, Correlations
  - Only qualitative variables → χ^2 (Benzécri 80)
  - Heterogenous variables (compatibility measures) → Gower (71)
    Gowda i Diday (91)
    Gibert's Mixed (91)
    Ichino i Yaguchi (94)
    Ralambondrainy (95)
    Generalized Gibert's Mixed (13)

Ascendant hierarchical clustering

- Benzécri, J. P. (1980). Pratique de l'analyse des données. vol. 1, analyse des correspondances.
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- Diday, E. and Gowda, K.C. Symbolic clustering using a new similaritiy measure IEEE Trans. on systems, mans,and cybernetics 22(2) 368-378, 1992
- Gibert, K. (1991). *Klass. Estudi d’un sistema d’ajuda al tractament estadıstic de grans bases de dades* (Doctoral dissertation, Master’s thesis, UPC).
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- Ichino, M. and Yaguchi, H. (1990), Generalized Minkowski metrics for mixed features. Electron. Comm. Jpn. Pt. III, 73: 12–20. doi: 10.1002/ecjc.4430730602
- [Ralambondrainy 1995] Ralambondrainy, H A conceptual version of the K-means algorithm Lifetime Learning Publications, Belmont, California, 1995
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Proximity measures

Distance: $d : \mathrm{E}\times\mathrm{E} \longrightarrow \mathrm{R}^{+}$

$$1. \forall x \in E \qquad d(x,x) = 0$$
$$2. \forall x, \forall y \qquad d(x,y) = d(y,x)$$
$$3. \forall x, \forall y, \forall z \quad d(x,z) \leq d(x,y) + d(y,z)$$

Distance index: Verifies 1. and 2., but 3.

Similarity index: $s : \mathrm{E}\times\mathrm{E} \longrightarrow \mathrm{R}^{+}$

$$1. \forall x, \forall y \qquad s(x,y) = s(y,x)$$
$$2. \forall x, \forall y \qquad s(x,x) = s(y,y) > s(y,z)$$

Dissimilarty index:

$$1. \forall x, \forall y \qquad d_s(x,y) = d_s(y,x)$$
$$2. \forall x, \forall y \qquad d_s(x,x) = d_s(y,y) < d_s(y,z)$$

$$d_s(x,y) = s(x,x) - s(x,y)$$

Euclidean

$$d^2(i,i') = \sum_{j=1}^{p} (x_{ij} - x_{i'j})^2$$

Distances

- **Minkowski distances:** $d(i,i') = \sum_{j=1}^{p} (|x_{ij} - x_{i'j}|^{d})^{1/d}$
  - Euclidean (L$_2$): $d^2(i,i') = \sum_{j=1}^{p} (x_{ij} - x_{i'j})^2$
  - Manhattan (L$_1$) (absolute value): $d(i,i') = \sum_{j=1}^{p} |x_{ij} - x_{i'j}|$
  - Chebichev (L$_\infty$): $d(i,i') = \max_j |x_{ij} - x_{i'j}|$
  - Correlation $d^2(x_j, x_{j'}) = 2\left(1 - cor(x_j, x_{j'})\right)$

    (L$_2$ with standardized *variables*)
  - Cosine similarity between individuals $1 - \cos(x_i, x_{i'}) = 1 - \frac{\langle x_i, x_{i'} \rangle}{|x_i||x_{i'}|}$

Distances

- To scale or not to scale
  - Standardization

$$x_{ij} \leftarrow \frac{x_{ij} - \overline{x}_j}{s_j}$$

Better to Scale

  - Max normalization

$$x_{ij} \leftarrow \frac{x_{ij}}{\max(x_j) - \min(x_j)}$$

Context required to scale

Distance correlation

Pearson correlation:

For linear association between two variables

$$\mathrm{cov}(x,y) = \frac{1}{n}\sum_{i=1}^{n}(x_i - \overline{x})(y_i - \overline{y})$$

$$r_{xy} = cor(x,y) = \frac{\mathrm{cov}(x,y)}{\sqrt{\mathrm{cov}(x,x)\cdot \mathrm{cov}(y,y)}}$$

Distance correlation:

For non linear association between two sets of variables (eventually two variables)

(x,y) Let x and y be two random vectors of p and q dimensions

$$a_{kl} = d(x_k, x_l) \quad k,l = 1,\ldots,n$$

$$b_{kl} = d(y_k, y_l) \quad k,l = 1,\ldots,n$$

Let a and b all pair distances between the x and y vectors respectively

$$\overline{\overline{a}}_{kl} = a_{kl} - a_{k\cdot} - a_{\cdot l} + a_{\cdot\cdot}$$

$$\overline{\overline{b}}_{kl} = b_{kl} - b_{k\cdot} - b_{\cdot l} + b_{\cdot\cdot}$$

(double centering of the distance matrices)

Distance covariance

$$dv^2(x,y) = \frac{1}{n^2}\sum_{k=1}^{n}\sum_{l=1}^{n}\overline{\overline{a}}_{kl} \times \overline{\overline{b}}_{kl}$$

Distance standard deviation

$$dv(x,x)$$

Distance correlation

$$\boxed{dc^2(x,y) = \frac{dv^2(x,y)}{dv(x,x)\times dv(y,y)}}$$

Distance
Binary variables (Logical)

$$d(i,i') = f(n_{11}, n_{00}, n_{10}, n_{01})$$

$$\begin{array}{c|cc} & \multicolumn{2}{c}{\textit{Object i}} \\ \hline \textit{Object i'} & n_{11} & n_{10} \\ & n_{01} & n_{00} \end{array}$$

n_{00} ← Uninformative

Jaccard

$$d(i,i') = \frac{n_{10} + n_{01}}{n_{10} + n_{01} + n_{11}}$$

Assymetrical distance

Sokal

$$d(i,i') = \frac{n_{10} + n_{01}}{n}$$

Symetrical distance

Distances
Nominal variables
Simple matching coefficient (Hamming)

$$d(i,i') = \frac{\#\,\text{vars mismatch}}{p}$$

Chi-2 distance

$$X^2 = \sum_{k=1}^{p} \sum_{j=1}^{q} \frac{\left(n_{kj} - {}^{n_k n_j}\!/_{n}\right)^2}{{}^{n_k n_j}\!/_{n}}$$

Distances

Ordinal variables

normalized ranks

$$x_{ij} = \frac{r_{ij} - 1}{R_j - 1} \in [0,1]$$

treat them as numerical

Distances
strings and curves

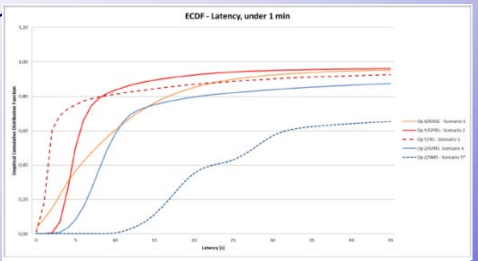
- **Edit distance** between two strings (or DNA sequences)
  Minimum number of operations to transform one string into the other (removals, insertions and substitutions). It verifies the three axioms of a distance. Operations can be weighted inversely to their likelihood.

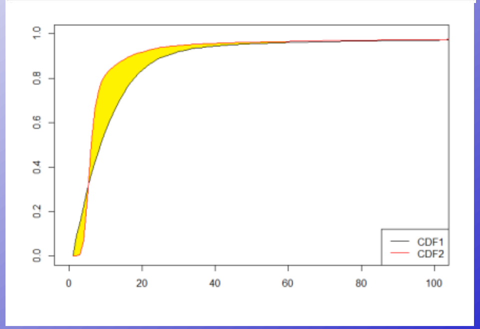
  What is the edit distance between "SEAL" and "ATE"?

Step	Comparison	Edit necessary	Total Editing
1.	“A" to “S"	replace: +1 edit	"STE” in 1 edit
2.	"T"	delete: +1 edit	"SE" in 2 edits
3.	“A"	insertion: +1 edit	"SEA" in 3 edits
4.	“L"	insertion: +1 edit	"SEAL“ in 4 edits

- **Hamming distance** between two strings of the same length
  Counts the minimum number of substitutions to convert one string in the oth

  dist(cats,dogs) = 3/4
  cats => dats (substitute 'd' for 'c')
  dats => dots (substitute 'o' for 'a')
  dots => dogs (substitute 'g' for 't')





- **Vertical distance between curves** $\max | F(x) - G(x) |$

- **Histogram matching distance** $\int | F(x) - G(x) |$

Management of heterogeneous data matrices

Heterogeneous matrices faced. Several approaches [Anderberg 73]:

Variables partitioning

(Ex, naive bayes classifier)

Variables converting

Compatibility measures

Mixed metrics required

Gower [Gow 71]

$$s(i,i') = \frac{\sum_{k=1}^{K} w_k(i,i')\, s_k(i,i')}{\sum_{k=1}^{K} w_k(i,i')};$$

$$d(i,i')=1-s(i,i')$$

$$w_k(i,i') = \begin{cases} 0 & \text{if } (x_{ik} = missing) \text{ or } (x_{i'k} = \text{missing}) \\ 0 & \text{if } (X_k \text{ binary}) \text{ and } (x_{ik} = \text{false}) \text{ i } (x_{i'k} = \text{false}) \\ & \text{and negative absence of } X_k \text{ excluded} \\ 1 & \text{otherwise} \end{cases}$$

$$s_k(i,i') = \begin{cases} 1 - \frac{|\mathrm{x_{ik}} - \mathrm{x_{i'k}}|}{R_k} & \text{if } \mathrm{X}_k \text{ numerical} \\ 1 & \text{if } (\mathrm{X}_k \text{ qualitative}) \text{ and } (\mathrm{x_{ik}} = \mathrm{x_{i'k}}) \\ 0 & \text{if } (\mathrm{X}_k \text{ qualitative}) \text{ and } (\mathrm{x_{ik}} \neq \mathrm{x_{i'k}}) \end{cases}$$

Gowda-Diday [Gow 91]

$$D(i,i') = \sum_{k=1}^{K} D_k(i_k, i'_k) \quad \textbf{with} \quad D_k(i,i') = D_p(i,i') + D_s(i,i') + D_c(i,i')$$

Component Position

$$D_{kp}(i,i') = \begin{cases} \dfrac{|\,\mathrm{x}_{\mathrm{ik}} - \mathrm{x}_{\mathrm{i'k}}\,|}{R_k} & \text{if } (\,\mathrm{X}_k \text{ numerical) and } R_k \text{ is rang of } \mathrm{X}_k \\ 0 & \text{if } (\,\mathrm{X}_k \text{ qualitative)} \end{cases}$$

Component Span

$$D_{ks}(i,i') = \begin{cases} 0 & \text{if } \mathrm{X}_k \text{ numerical} \\ 0 & \text{if } \mathrm{X}_k \text{ qualitative and not nultivalued} \end{cases}$$

Component Content

$$D_{kc}(i,i') = \begin{cases} 0 & \text{if } \mathrm{X}_k \text{ numerical} \\ 0 & \text{if } (\,\mathrm{X}_k \text{ qualitative) and } (\mathrm{x}_{\mathrm{ik}} = \mathrm{x}_{\mathrm{i'k}}) \\ 1 & \text{if } (\,\mathrm{X}_k \text{ qualitative) and } (\mathrm{x}_{\mathrm{ik}} \neq \mathrm{x}_{\mathrm{i'k}}) \end{cases}$$

Mixed Metrics [Gib 91]

$$d^2_{(\alpha,\beta)}(i, i') = \alpha\, d_\varsigma^2(i, i') + \beta\, d_Q^2(i, i')$$

$$d_\varsigma^2(i,i') = \sum_{\forall k \in \varsigma} \frac{(x_{ik} - x_{i'k})^2}{s_k^2}$$

$$d_k^2(i,i') = \begin{cases} 0, & \text{if } x_{ik} = x_{i'k} \\ \dfrac{1}{I_{k^i}} + \dfrac{1}{I_{k^{i'}}}, & \text{otherwise, for compact } i \text{ and } i' \text{ with respect } X_k \\ \dfrac{(f_i^{k_s} - 1)^2}{I^{k_s}} + \sum_{j \neq s}^{n_k} \dfrac{(f_i^{k_j})^2}{I^{k_j}}, & \text{if } x_{ik} = c_s^k \text{, and extended } i' \text{ with respect } X_k \\ \sum_{j=1}^{n_k} \dfrac{(f_i^{k_j} - f_{i'}^{k_j})^2}{I^{k_j}}, & \text{for } i, i' \text{ extended with respect } X_k \end{cases}$$

- **Proposal [Gib 91]:**

$$\alpha = \frac{n_\zeta}{d_\zeta^2 max^*} \qquad \beta = \frac{n_Q}{d_Q^2 max^*}$$

Ralambondrainy [Ral95]

$$d^2(i,i') = \pi_1 d^2_{1/\sigma^2}(i,i') + \pi_2 d^2_{\chi^2}(i,i')$$

- Proposal [Ral 88] :
  - Standardisation by the inertia

$$\pi_1 = \frac{1}{Card(\zeta)} \qquad \pi_2 = \frac{1}{n_k - 1}$$

  - Standardisation by the norm

$$\pi_1 = \frac{1}{\sqrt{\sum\{\rho^2(X_k, X_{k'})/k,k' \in \zeta\}}} \qquad \pi_2 = \sqrt{n_k - 1}$$

Ichino-Yaguchi [Ichi 94]

Generalized Minkowski metrics, p-order (p >= 1)

$$d_p(i,i') = \sqrt[p]{\sum_{k=1}^{K} \left(\frac{\phi(x_{ik}, x_{i'k})}{|U_k|} \right)^p}$$

where $|U_k|$ **Normalizes (with R_k o n_k)**

$\phi(x_{ik}, x_{i'k})$ **Is a function of :**

- **Cartesian Joint** $$|x_{ik} \oplus x_{i'k}| = \begin{cases} |x_{ik} - x_{i'k}|, & \text{if } X_k \text{ numerical} \\ 1, & \text{if } X_k \text{ categorical and } x_{ik} = x_{i'k} \\ 2, & \text{if } X_k \text{ categorical and } x_{ik} \neq x_{i'k} \end{cases}$$
- **Catesian Meet** $$|x_{ik} \oplus x_{i'k}| = \begin{cases} |x_{ik} - x_{i'k}|, & \text{if } X_k \text{ numerical} \\ 1, & \text{if } X_k \text{ categorical and } x_{ik} = x_{i'k} \\ 2, & \text{if } X_k \text{ categorical and } x_{ik} \neq x_{i'k} \end{cases}$$
- **Cardinality of x, $|x_{ik}|$, (0 o 1)**
- **Factor** $\gamma \in [0,0.5]$

Example Michalski data

(Gibert mixed metrics)

	A	B	C	F	J	M	P	R	S	T
A	0	1.2488811	1.2438452	0.8309088	1.1683081	1.2438452	0.8309088	0.63954794	1.4049911	0.90644586
B	1.2488811	0	0.8309088	1.2438452	0.90644586	1.4352059	0.63954794	0.8309088	0.8309088	1.1683081
C	1.2438452	0.8309088	0	1.3999553	1.1330574	1.0474486	1.6920323	1.0474486	1.8229634	0.7201209
F	0.8309088	1.2438452	1.3999553	0	0.7201209	1.2388093	1.5006716	1.2388093	1.2488811	1.1330574
J	1.1683081	0.90644586	1.1330574	0.7201209	0	0.97191143	1.1632721	1.5762087	1.2942033	1.2488811
M	1.2438452	1.4352059	1.0474486	1.2388093	0.97191143	0	1.2488811	1.2085946	2.2661147	1.1632721
P	0.8309088	0.63954794	1.6920323	1.5006716	1.1632721	1.2488811	0	1.2488811	0.63451207	0.97191143
R	0.63954794	0.8309088	1.0474486	1.2388093	1.5762087	1.2085946	1.2488811	0	2.2661147	1.7675694
S	1.4049911	0.8309088	1.8229634	1.2488811	1.2942033	2.2661147	0.63451207	2.2661147	0	0.7201209
T	0.90644586	1.1683081	0.7201209	1.1330574	1.2488811	1.1632721	0.97191143	1.7675694	0.7201209	0

Ralambondrainy normalized by inertia pi1=0.5, pi2=0.2

	A	B	C	F	J	M	P	R	S	T
A	0	1.2560605	0.84210527	1.7314991	0.8254386	0.84210527	1.7314991	0.70877194	4.7996807	1.7481657
B	1.2560605	0	1.7314991	0.84210527	1.7481657	1.8648324	0.70877194	1.7314991	1.7314991	0.8254386
C	0.84210527	1.7314991	0	1.2893938	0.25	2.5017545	3.6244814	2.5017545	4.3242416	1.1393938
F	1.7314991	0.84210527	1.2893938	0	1.1393938	3.5244815	2.6017544	3.5244815	1.2560605	0.25
J	0.8254386	1.7481657	0.25	1.1393938	0	2.4850879	3.507815	2.618421	4.2075753	1.2560605
M	0.84210527	1.8648324	2.5017545	3.5244815	2.4850879	0	1.2560605	0.26666668	6.692663	3.507815
P	1.7314991	0.70877194	3.6244814	2.6017544	3.507815	1.2560605	0	1.2560605	3.391148	2.4850879
R	0.70877194	1.7314991	2.5017545	3.5244815	2.618421	0.26666668	1.2560605	0	6.692663	3.641148
S	4.7996807	1.7314991	4.3242416	1.2560605	4.2075753	6.692663	3.391148	6.692663	0	1.1393938
T	1.7481657	0.8254386	1.1393938	0.25	1.2560605	3.507815	2.4850879	3.641148	1.1393938	0

Ralambondrainy normalized by norm, pi1= 0,617, p2=2,236

	A	B	C	F	J	M	P	R	S	T
A	0	3.8718193	3.5263379	3.298699	3.3399992	3.5263379	3.298699	2.035626	7.0879183	3.4850378
B	3.8718193	0	3.298699	3.5263379	3.4850378	4.7894106	2.035626	3.298699	3.298699	3.3399992
C	3.5263379	3.298699	0	4.2444973	2.795085	4.415724	6.796831	4.415724	7.6610384	2.5674462
F	3.298699	3.5263379	4.2444973	0	2.5674462	5.678797	5.533758	5.678797	3.8718193	2.795085
J	3.3399992	3.4850378	2.795085	2.5674462	0	4.229385	5.492458	5.7200966	6.356665	3.8718193
M	3.5263379	4.7894106	4.415724	5.678797	4.229385	0	3.8718193	2.981424	10.58605	5.492458
P	3.298699	2.035626	6.796831	5.533758	5.492458	3.8718193	0	3.8718193	4.1880846	4.229385
R	2.035626	3.298699	4.415724	5.678797	5.7200966	2.981424	3.8718193	0	10.58605	6.9831696
S	7.0879183	3.298699	7.6610384	3.8718193	6.356665	10.58605	4.1880846	10.58605	0	2.5674462
T	3.4850378	3.3399992	2.5674462	2.795085	3.8718193	5.492458	4.229385	6.9831696	2.5674462	0

Gower

	A	B	C	F	J	M	P	R	S	T
A	0	0.625	0.625	0.5	0.625	0.625	0.5	0.375	0.625	0.5
B	0.625	0	0.5	0.625	0.5	0.75	0.375	0.5	0.5	0.625
C	0.625	0.5	0	0.625	0.5	0.5	0.875	0.5	0.75	0.375
F	0.5	0.625	0.625	0	0.375	0.625	0.75	0.625	0.625	0.5
J	0.625	0.5	0.5	0.375	0	0.5	0.625	0.75	0.5	0.625
M	0.625	0.75	0.5	0.625	0.5	0	0.625	0.5	1.0	0.625
P	0.5	0.375	0.875	0.75	0.625	0.625	0	0.625	0.375	0.5
R	0.375	0.5	0.5	0.625	0.75	0.5	0.625	0	1.0	0.875
S	0.625	0.5	0.75	0.625	0.5	1.0	0.375	1.0	0	0.375
T	0.5	0.625	0.375	0.5	0.625	0.625	0.5	0.875	0.375	0

Example

Michalski data

Gower

	A	B	C	F	J	M	P	R	S	T
A	0	0.625	0.625	0.5	0.625	0.625	0.5	0.375	0.625	0.5
B	0.625	0	0.5	0.625	0.5	0.75	0.375	0.5	0.5	0.625
C	0.625	0.5	0	0.625	0.5	0.5	0.875	0.5	0.75	0.375
F	0.5	0.625	0.625	0	0.375	0.625	0.75	0.625	0.625	0.5
J	0.625	0.5	0.5	0.375	0	0.5	0.625	0.75	0.5	0.625
M	0.625	0.75	0.5	0.625	0.5	0	0.625	0.5	1.0	0.625
P	0.5	0.375	0.875	0.75	0.625	0.625	0	0.625	0.375	0.5
R	0.375	0.5	0.5	0.625	0.75	0.5	0.625	0	1.0	0.875
S	0.625	0.5	0.75	0.625	0.5	1.0	0.375	1.0	0	0.375
T	0.5	0.625	0.375	0.5	0.625	0.625	0.5	0.875	0.375	0

Gibert mixed metrics

	A	B	C	F	J	M	P	R	S	T
A	0	1.2488811	1.2438452	0.8309088	1.1683081	1.2438452	0.8309088	0.63954794	1.4049911	0.90644586
B	1.2488811	0	0.8309088	1.2438452	0.90644586	1.4352059	0.63954794	0.8309088	0.8309088	1.1683081
C	1.2438452	0.8309088	0	1.3999553	1.1330574	1.0474486	1.6920323	1.0474486	1.8229634	0.7201209
F	0.8309088	1.2438452	1.3999553	0	0.7201209	1.2388093	1.5006716	1.2388093	1.2488811	1.1330574
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S	1.4049911	0.8309088	1.8229634	1.2488811	1.2942033	2.2661147	0.63451207	2.2661147	0	0.7201209
T	0.90644586	1.1683081	0.7201209	1.1330574	1.2488811	1.1632721	0.97191143	1.7675694	0.7201209	0

Ralambondrainy, Pi1=0,1, Pi2=0,2

	A	B	C	F	J	M	P	R	S	T
A	0	1.2560605	0.84210527	1.7314991	0.8254386	0.84210527	1.7314991	0.70877194	4.7996807	1.7481657
B	1.2560605	0	1.7314991	0.84210527	1.7481657	1.8648324	0.70877194	1.7314991	1.7314991	0.8254386
C	0.84210527	1.7314991	0	1.2893938	0.25	2.5017545	3.6244814	2.5017545	4.3242416	1.1393938
F	1.7314991	0.84210527	1.2893938	0	1.1393938	3.5244815	2.6017544	3.5244815	1.2560605	0.25
J	0.8254386	1.7481657	0.25	1.1393938	0	2.4850879	3.507815	2.618421	4.2075753	1.2560605
M	0.84210527	1.8648324	2.5017545	3.5244815	2.4850879	0	1.2560605	0.26666668	6.692663	3.507815
P	1.7314991	0.70877194	3.6244814	2.6017544	3.507815	1.2560605	0	1.2560605	3.391148	2.4850879
R	0.70877194	1.7314991	2.5017545	3.5244815	2.618421	0.26666668	1.2560605	0	6.692663	3.641148
S	4.7996807	1.7314991	4.3242416	1.2560605	4.2075753	6.692663	3.391148	6.692663	0	1.1393938
T	1.7481657	0.8254386	1.1393938	0.25	1.2560605	3.507815	2.4850879	3.641148	1.1393938	0

Ralambondrainy, Pi1=0,617, Pi2=0,2236

	A	B	C	F	J	M	P	R	S	T
A	0	3.8718193	3.5263379	3.298699	3.3399992	3.5263379	3.298699	2.035626	7.0879183	3.4850378
B	3.8718193	0	3.298699	3.5263379	3.4850378	4.7894106	2.035626	3.298699	3.298699	3.3399992
C	3.5263379	3.298699	0	4.2444973	2.795085	4.415724	6.796831	4.415724	7.6610384	2.5674462
F	3.298699	3.5263379	4.2444973	0	2.5674462	5.678797	5.533758	5.678797	3.8718193	2.795085
J	3.3399992	3.4850378	2.795085	2.5674462	0	4.229385	5.492458	5.7200966	6.356665	3.8718193
M	3.5263379	4.7894106	4.415724	5.678797	4.229385	0	3.8718193	2.981424	10.58605	5.492458
P	3.298699	2.035626	6.796831	5.533758	5.492458	3.8718193	0	3.8718193	4.1880846	4.229385
R	2.035626	3.298699	4.415724	5.678797	5.7200966	2.981424	3.8718193	0	10.58605	6.9831696
S	7.0879183	3.298699	7.6610384	3.8718193	6.356665	10.58605	4.1880846	10.58605	0	2.5674462
T	3.4850378	3.3399992	2.5674462	2.795085	3.8718193	5.492458	4.229385	6.9831696	2.5674462	0