

UNIVERSIDADE FEDERAL DA PARAÍBA
CENTRO DE CIÊNCIAS EXATAS E DA NATUREZA
DEPARTAMENTO DE ESTATÍSTICA

Análise Multivariada II, 2012.2, Prof. Marcelo Ferreira

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Atividade: Avaliação 4

Análise de Agrupamentos

• **Introdução**

Segundo Bruce e Bruce (2019), os métodos de agrupamentos podem ser usados para identificar grupos de dados significativos. Por exemplo, usando os cliques da web e dados demográficos de usuários em um site, podemos ser capaz de agrupar diferentes tipos de usuários. O site poderia, então, ser personalizado para esses diferentes tipos.

Nesse trabalho iremos propor e escolher o(s) melhor(es) modelo(s) de agrupamentos para o conjunto de dados de Water Quality (Drinking water portability, water_potability {datasets}) disponível em: <https://www.kaggle.com/datasets/adityakadiwal/water-potability>

• **Objetivo**

Reduzir a dimensão dos dados para um conjunto mais gerenciável de variáveis;

Obter uma melhor percepção interna do conjunto de dados e de como as diferentes variáveis se relacionam umas com as outras;

Filtrar e analisar as variáveis e descobrir relacionamentos.

ANÁLISE EXPLORATÓRIA

> head(df)

```
      ph Hardness  Solids Chloramines  Sulfate
1    NA 204.8905 20791.32   7.300212 368.5164
2 3.716080 129.4229 18630.06   6.635246    NA
3 8.099124 224.2363 19909.54   9.275884    NA
4 8.316766 214.3734 22018.42   8.059332 356.8861
5 9.092223 181.1015 17978.99   6.546600 310.1357
6 5.584087 188.3133 28748.69   7.544869 326.6784
      Conductivity Organic_carbon Trihalomethanes Turbidity
```

1	564.3087	10.379783	86.99097	2.963135
2	592.8854	15.180013	56.32908	4.500656
3	418.6062	16.868637	66.42009	3.055934
4	363.2665	18.436524	100.34167	4.628771
5	398.4108	11.558279	31.99799	4.075075
6	280.4679	8.399735	54.91786	2.559708

Potability

1	0
2	0
3	0
4	0
5	0
6	0

> skim(df)

— Data Summary —

Name	Values	df
Number of rows		3276
Number of columns		10

Column type frequency:

numeric	10
---------	----

Group variables None

— Variable type: numeric —

skim_variable	n_missing	complete_rate	mean	sd
1 ph	491	0.850	7.08	1.59
2 Hardness	0	1	196.	32.9
3 Solids	0	1	22014.	8769.
4 Chloramines	0	1	7.12	1.58
5 Sulfate	781	0.762	334.	41.4











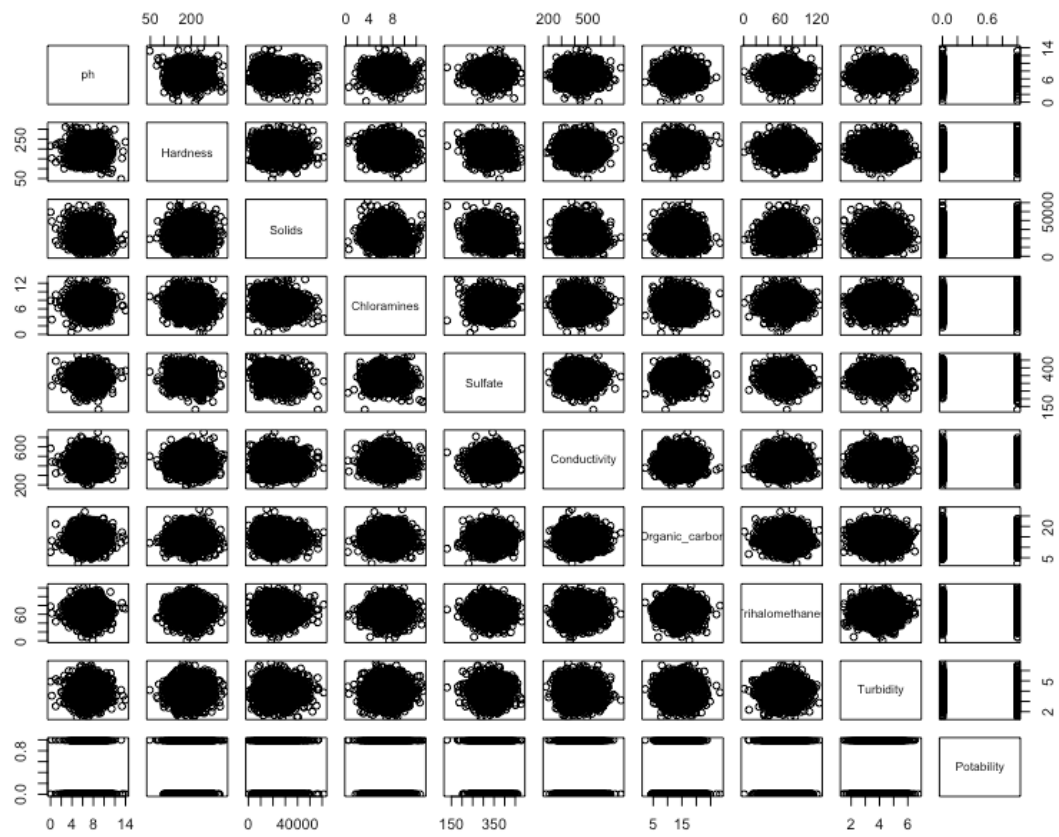
6 Conductivity	0	1	426.	80.8	
7 Organic_carbon	0	1	14.3	3.31	
8 Trihalomethanes	162		0.951	66.4	16.2
9 Turbidity	0	1	3.97	0.780	
10 Potability	0	1	0.390	0.488	
	p0	p25	p50	p75	p100 hist
1	0	6.09	7.04	8.06	14 
2	47.4	177.	197.	217.	323. 
3	321.	15667.	20928.	27333.	61227. 
4	0.352	6.13	7.13	8.11	13.1 
5	129	308.	333.	360.	481. 
6	181.	366.	422.	482.	753. 
7	2.20	12.1	14.2	16.6	28.3 
8	0.738	55.8	66.6	77.3	124 
9	1.45	3.44	3.96	4.50	6.74 
10	0	0	0	1	1 

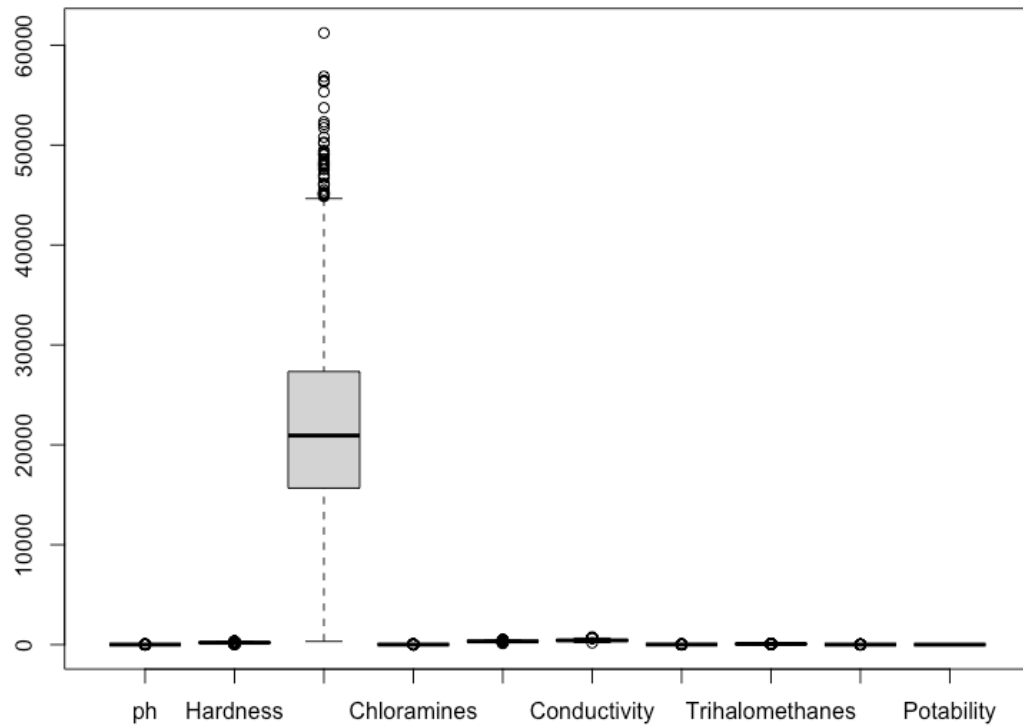
Gráfico 1



A análise inicial demonstra que o banco é composto por 3276 observações e 1º variáveis. Observamos também a presença de NaNs, que serão tratadas posteriormente.

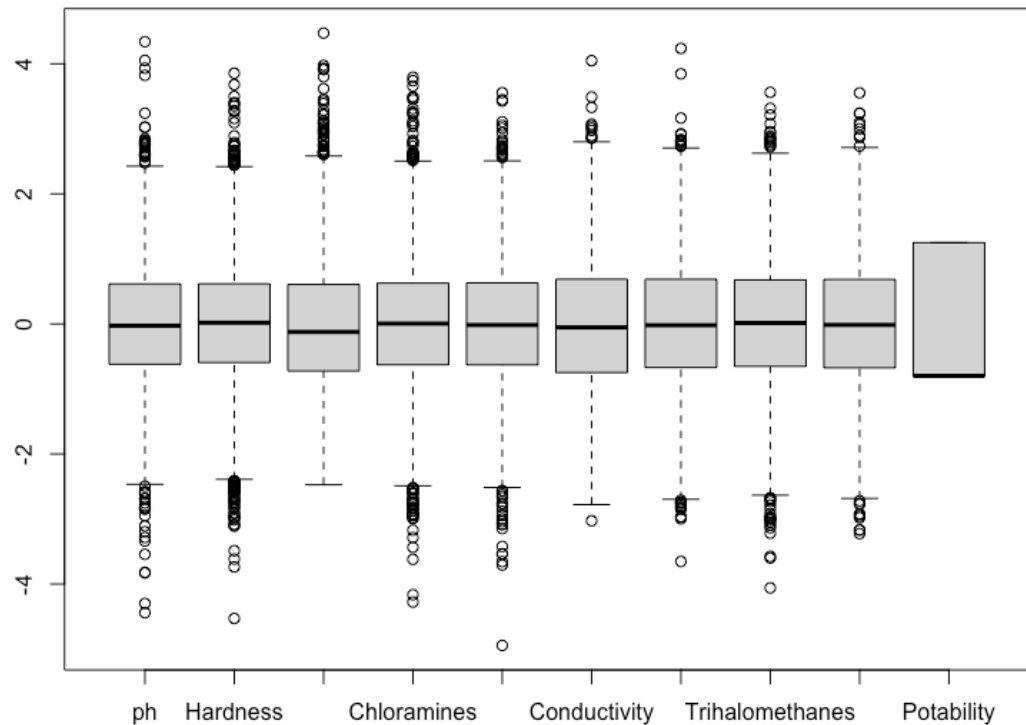
Verificando se os dados estão padronizados

Gráfico 2



O gráfico de boxplot (gráfico 2), mostra que os dados não estão padronizados, apresentando a variável Solids se destacando em relação as demais variáveis, portanto, iremos realizar a padronização do banco de dados utilizando a função `scale()`.

Gráfico 3

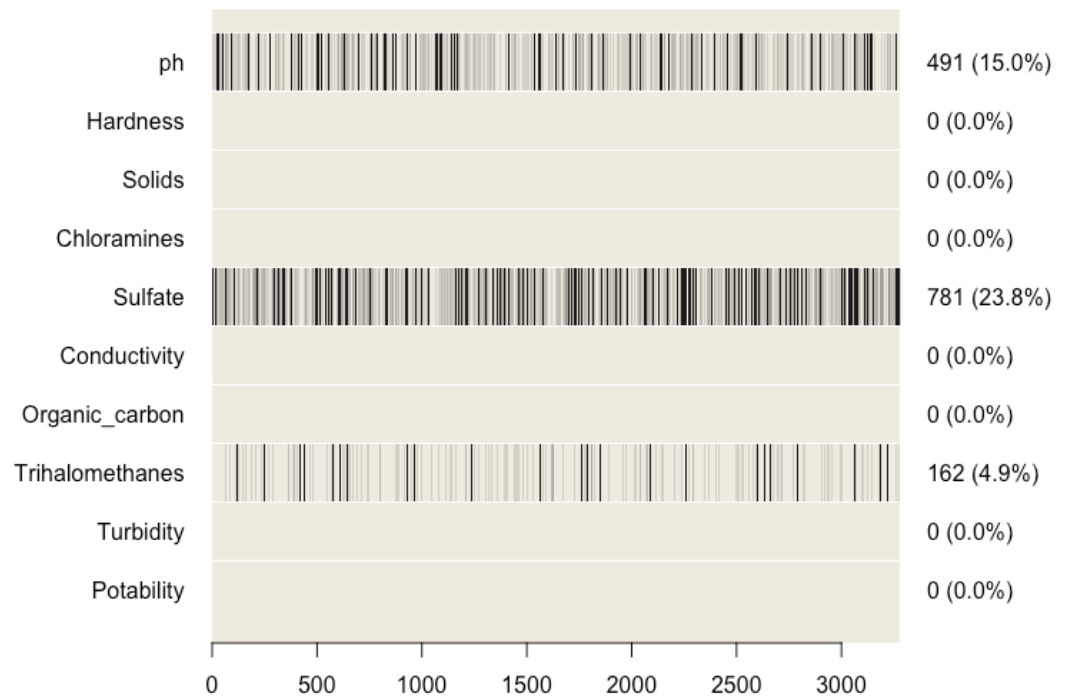


O gráfico de boxplot (gráfico 3) mostra que os dados foram padronizados após a aplicação da função `scale()`.

Dados faltantes

Vamos analisar nossa base de dados com observações faltantes. A primeira pergunta que devemos fazer é: como estão distribuídos os dados faltantes?

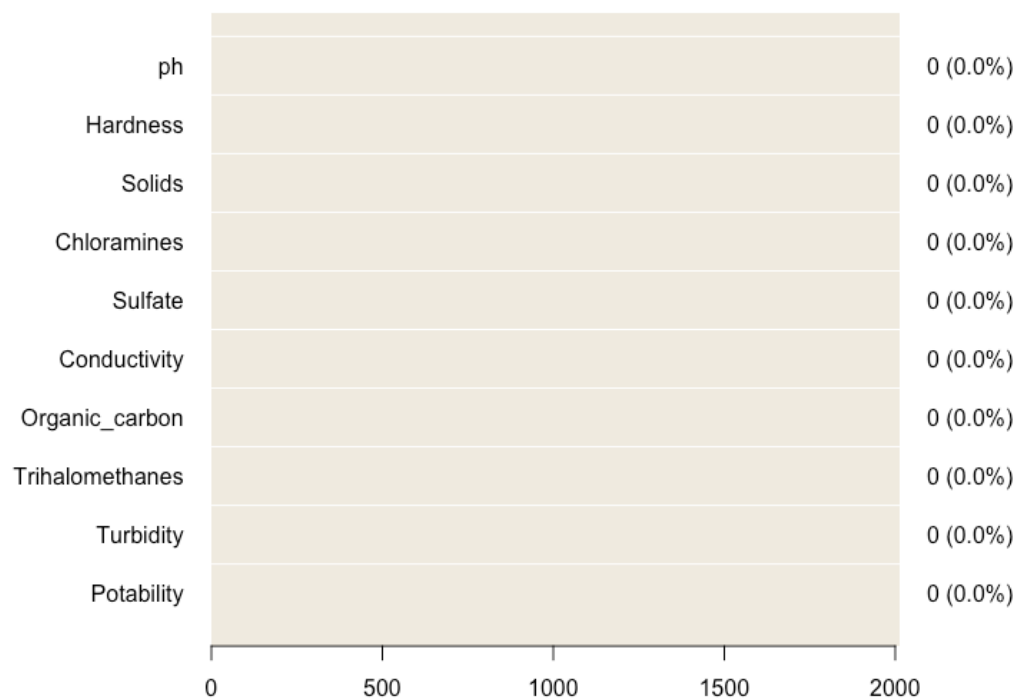
Gráfico 4



/2022-06-15

Observamos no (gráfico 4) a presença de NaNs e como eles estão distribuídos nas variáveis. Iremos proceder a limpeza dos dados faltantes utilizando a função `omit.na()`.

Gráfico 5



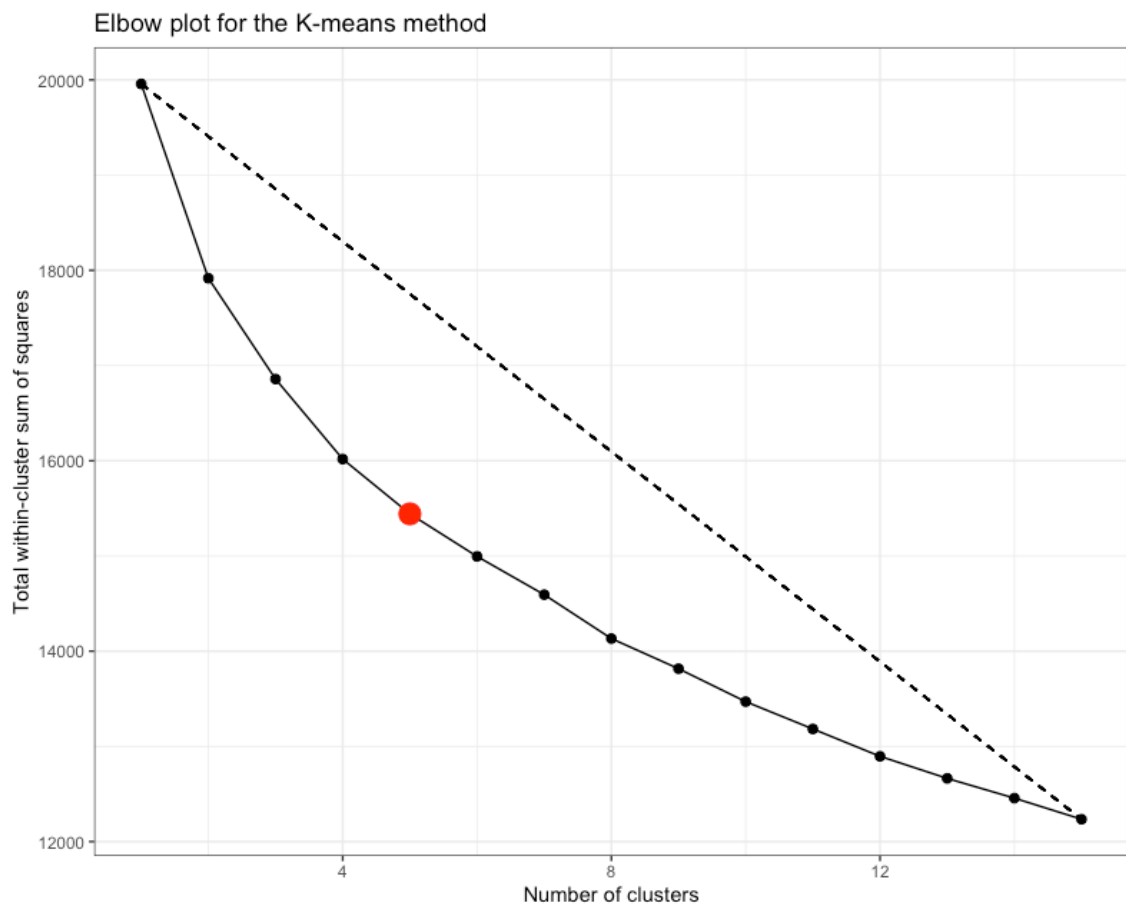
O (gráfico 5) mostra que os NaNs foram todos retirados do nosso banco de dados.

K-Means

O método de clusterização K-means classifica os objetos dentro de múltiplos grupos, de forma que a variação intra-cluster seja minimizada pela soma dos quadrados das distâncias Euclidianas entre os itens e seus centroides.

Encontrando o número ótimo de grupos para o K-means:

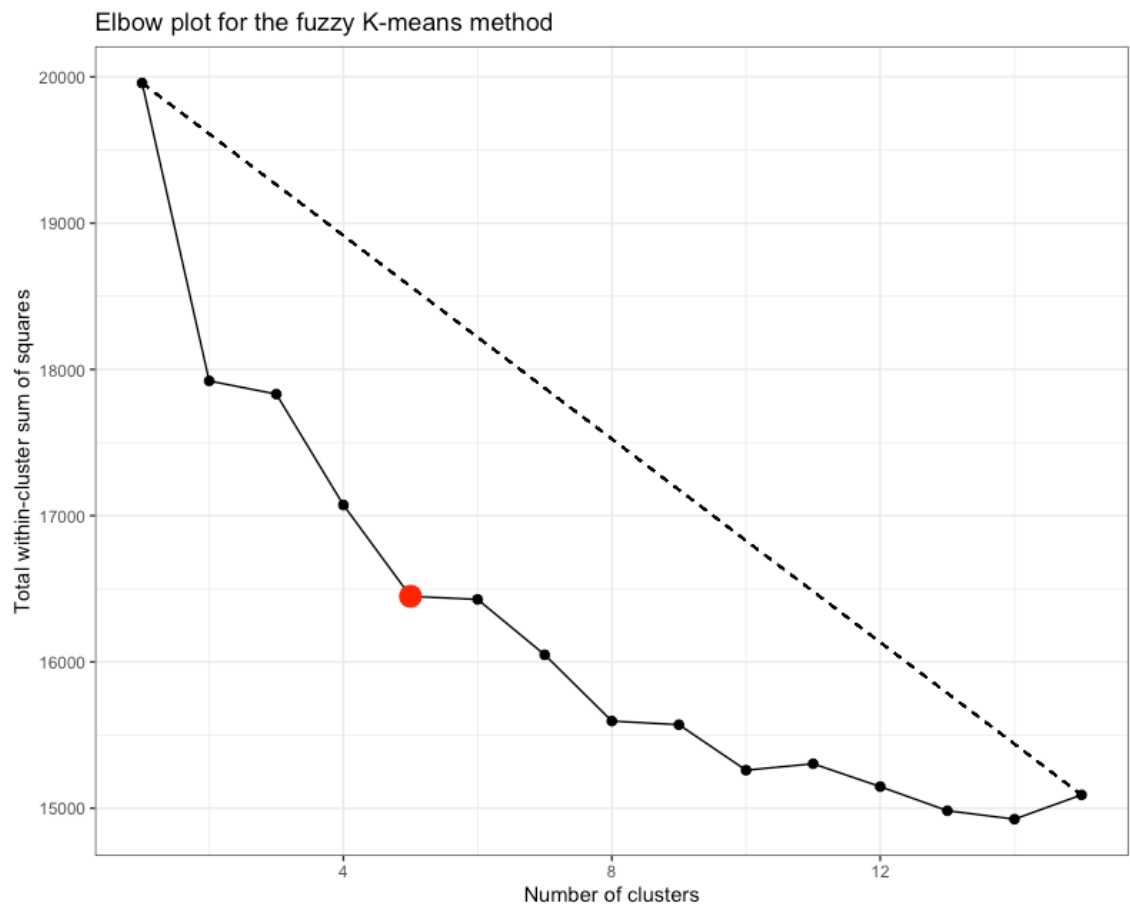
Gráfico 6



O (gráfico 6) mostra que o K "ótimo" é igual a 5 para o nosso banco de dados.

Encontrando agora o número ótimo de grupos para o Fuzzy K-means

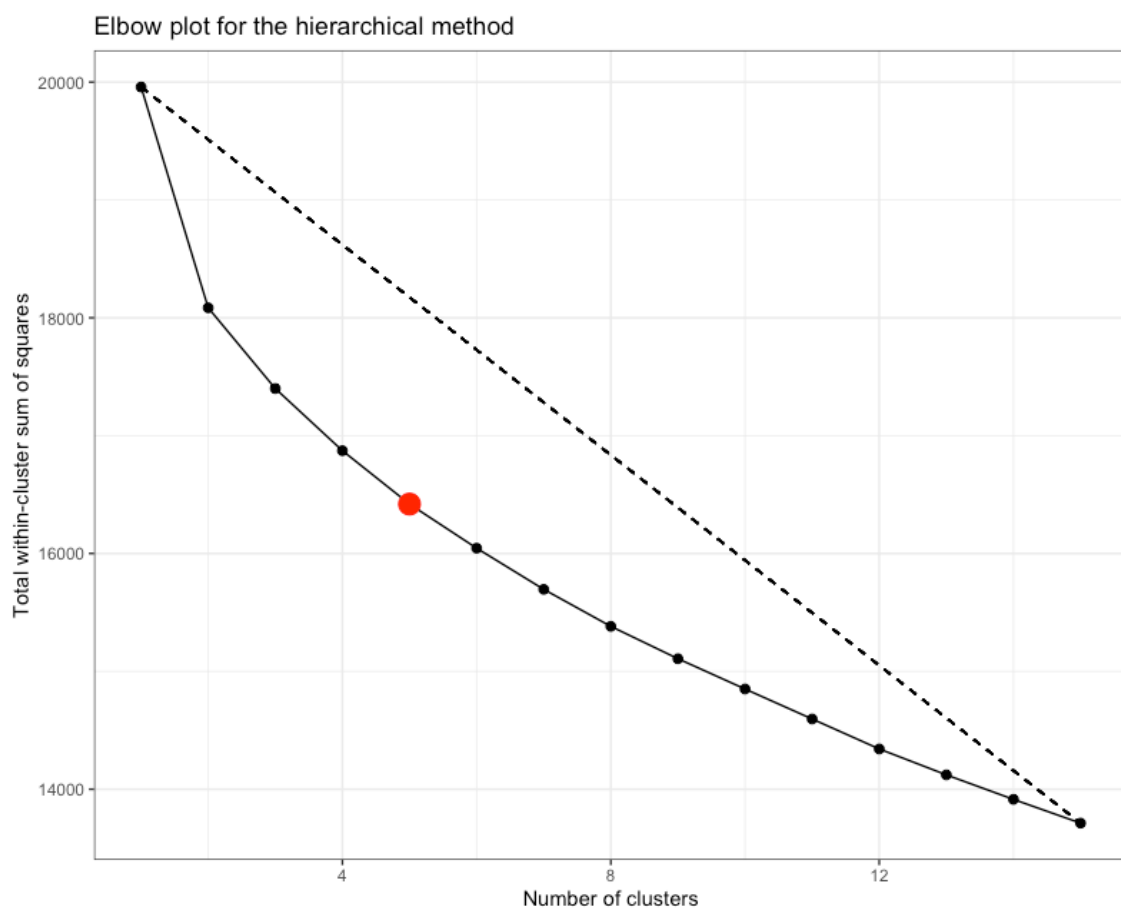
Gráfico 7



O (gráfico 7) nos mostra que o K "ótimo" também é igual a 5 através do método Fuzzy K-means.

Encontrando o número ótimo de grupos para o método hierárquico

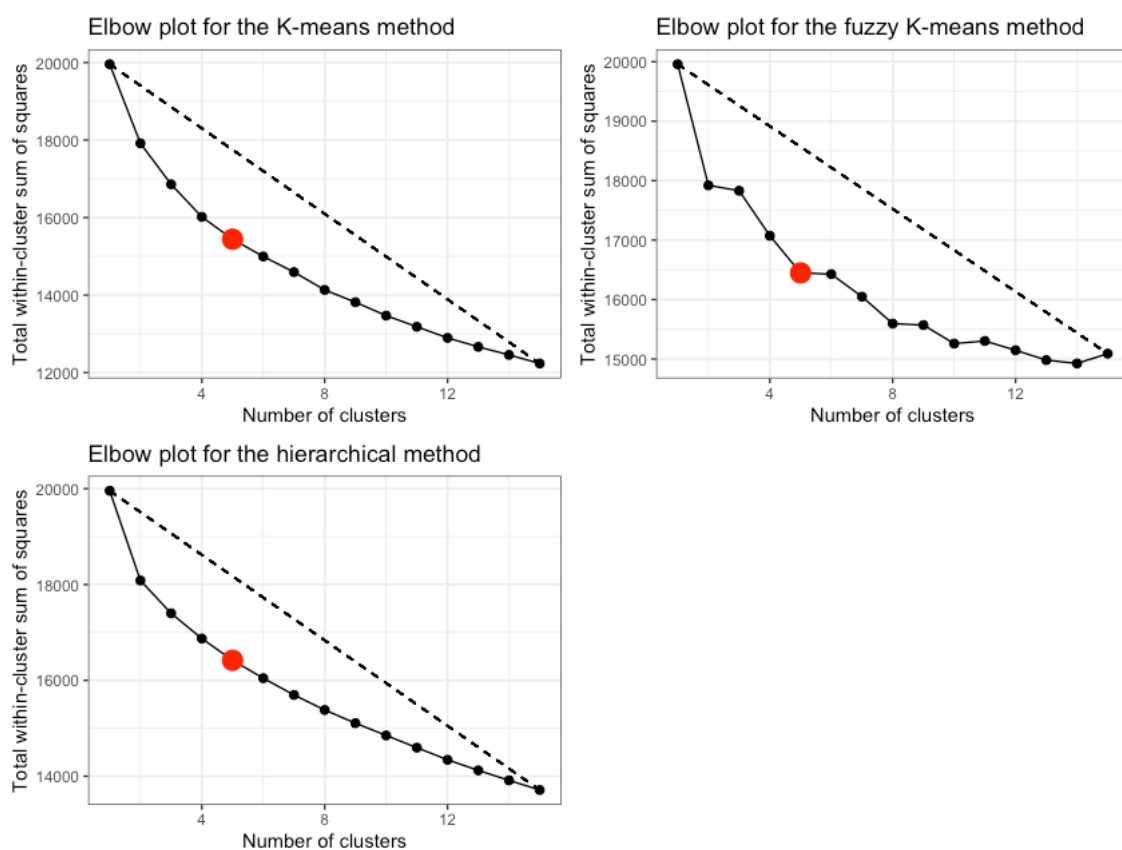
Gráfico 8



Assim como os métodos anteriores, o (gráfico 8) mostra que o K "ótimo" também é igual a 5 através do método hierárquico.

Portanto, nosso $nclust = c(5,5,5)$ conforme é demonstrado pelo (gráfico 9)..

Gráfico 9



Agrupamento usando o K-means

K-means clustering with 5 clusters of sizes 342, 438, 449, 443, 339

Cluster means:

	ph	Hardness	Solids	Chloramines	Sulfate
1	0.4523146	-0.14368862	0.5857378	0.21014697	-0.95242877

2 0.6987339 0.18649100 -0.4859894 -0.19355669 0.20715838
 3 -0.3055112 0.07540519 -0.3756107 -0.08447741 0.67564369
 4 -0.8794434 -0.33853850 0.5279489 0.27616911 -0.16523622
 5 0.2141124 0.17410636 -0.2208180 -0.16573173 -0.06468456

Conductivity Organic_carbon Trihalomethanes Turbidity

1 -0.11013143 -0.1672606 0.16456456 0.07016385
 2 0.11405998 -0.1387859 0.55610610 -0.43436076
 3 0.05630854 0.1190917 -0.07685825 0.03741296
 4 0.02706308 -0.1798285 0.16445455 0.20518053
 5 -0.12262689 0.5557541 -0.99596410 0.19511377

Potability

1 1.2381740
 2 -0.7622131
 3 1.2455959
 4 -0.7765171
 5 -0.7391862

Clustering vector:

[1] 2 5 4 2 2 2 4 2 4 2 2 4 4 4 2 2 5 4 4 5 4 4 5 2 2 5 2 4 5
 [31] 5 5 4 4 5 4 5 2 4 4 4 4 5 4 2 2 4 4 2 2 5 2 2 5 2 4 4 2 4 5
 [61] 5 2 4 5 2 5 4 2 2 4 2 2 4 5 5 4 5 5 5 4 2 2 5 4 2 5 2 5 2
 [91] 2 4 4 4 2 5 2 4 5 2 5 2 2 2 4 2 4 4 5 4 4 5 4 4 4 2 5 2 5
 [121] 2 4 5 2 5 5 2 4 4 4 2 2 5 4 2 2 5 4 2 2 5 4 5 2 4 4 5 5 2 5
 [151] 5 2 4 4 1 1 1 1 3 1 1 3 3 3 3 3 3 1 3 1 1 1 1 1 5 1 3 1 1
 [181] 1 1 1 1 3 3 1 3 1 1 1 3 3 3 3 3 1 1 1 1 1 3 1 1 1 3 3 1 1 3
 [211] 1 3 3 3 3 1 1 1 1 3 3 3 3 3 3 3 3 1 1 1 3 1 3 1 1 1 1 3 1
 [241] 3 1 3 1 3 1 3 3 1 3 3 1 3 3 3 3 5 4 4 4 4 2 4 5 2 2 4 4 4 2
 [271] 2 2 2 5 5 2 4 4 2 4 2 5 2 5 5 2 2 4 2 2 2 2 5 2 4 2 5 4 5 4
 [301] 2 5 2 5 4 4 2 2 4 4 2 4 5 2 4 5 2 4 4 4 4 4 5 2 4 4 4 4 4 5
 [331] 5 2 4 2 5 4 2 4 4 4 4 4 5 2 2 4 2 4 5 5 2 2 2 4 5 5 4 5 4 2
 [361] 2 2 2 4 2 4 2 5 4 5 5 4 5 2 4 2 5 2 2 2 4 2 2 5 4 4 4 4 4 2
 [391] 5 4 2 4 5 2 4 4 2 4 5 5 2 2 2 4 3 1 2 3 1 3 3 3 1 1 1 3 3 1

```

[421] 1 1 1 1 1 4 3 1 3 3 1 1 1 3 1 1 3 1 3 3 1 4 3 1 4 3 1 1 1 3
[451] 1 3 3 3 3 3 3 3 1 3 3 1 1 3 1 1 1 1 3 3 1 3 3 1 1 5 3 1 2 3
[481] 1 3 3 3 3 1 2 1 1 1 1 3 1 1 1 2 3 1 3 3 1 1 3 3 3 4 4 5 2 5
[511] 4 4 4 2 2 4 2 4 2 4 2 2 2 4 4 2 5 5 5 2 2 2 5 5 4 2 2 4 2 4
[541] 4 4 2 4 2 2 4 2 5 4 2 4 4 4 5 2 5 5 4 5 5 5 2 4 5 2 5 4 5 2
[571] 5 4 2 5 4 5 4 2 2 5 2 4 4 4 2 4 2 4 2 4 2 4 4 2 5 2 5 5 4 4
[601] 2 4 4 2 2 5 5 5 5 5 4 4 4 5 4 2 5 2 4 5 5 5 2 4 2 5 2 4 2 2
[631] 4 4 2 5 2 5 2 2 2 2 4 4 2 4 2 4 5 4 4 5 2 2 5 2 2 5 2 4 5 2
[661] 2 2 5 2 5 2 5 4 3 1 3 1 1 3 1 3 1 3 3 3 3 3 1 1 3 3 1 1 3
[691] 3 3 1 1 3 1 3 1 3 5 1 3 3 3 1 3 1 3 1 3 1 3 1 1 3 3 3 1 1 1
[721] 1 1 3 3 3 1 1 3 1 3 3 1 1 3 3 3 3 1 3 1 1 1 3 3 3 3 1 1 3 1
[751] 1 3 3 3 3 3 1 3 3 3 1 4 4 2 4 4 4 5 4 5 4 2 4 4 2 5 2 4 2 4
[781] 2 4 5 2 5 4 4 4 2 2 2 5 2 2 4 4 2 2 4 4 4 4 2 2 5 2 4 2 2 5
[811] 4 4 5 2 2 5 2 2 5 4 4 2 5 5 4 5 2 4 4 5 5 2 2 4 2 5 2 5 5 4
[841] 4 2 2 4 5 5 2 5 5 5 2 4 5 4 2 2 4 5 4 5 2 2 4 2 4 2 5 4 4 2
[871] 4 2 5 5 2 2 2 2 5 2 2 5 2 4 2 2 5 2 4 2 4 4 2 2 2 5 2 2 4 4
[901] 4 4 4 4 4 5 4 4 4 3 3 3 1 1 3 2 3 3 3 3 3 1 1 3 3 1 1 3 1 3
[931] 3 3 1 1 3 1 3 1 3 3 1 3 3 1 3 1 1 1 3 1 3 1 1 1 3 1 3 3 1 1
[961] 3 1 3 3 3 3 1 3 3 3 3 1 3 1 1 1 3 3 3 1 1 1 3 1 3 1 3 3 3 3
[991] 1 3 1 3 1 3 3 3 3 1
[ reached getOption("max.print") -- omitted 1011 entries ]

```

Within cluster sum of squares by cluster:

```

[1] 3005.709 3228.914 3575.035 3289.782 2342.790
(between_SS / total_SS = 22.6 %)

```

Available components:

```

[1] "cluster"    "centers"    "totss"      "withinss"
[5] "tot.withinss" "betweenss"  "size"       "iter"
[9] "ifault"

```

Agrupamento usando o Fuzzy K-means

Fuzzy c-means clustering with 5 clusters

Cluster centers:

	ph	Hardness	Solids	Chloramines	Sulfate
1	0.003309876	-0.01217055	-0.01101303	0.007647791	-0.01331860
2	0.003219246	-0.01223407	-0.01103082	0.007620648	-0.01330774
3	0.003297004	-0.01218615	-0.01102080	0.007621521	-0.01330940
4	0.003179042	-0.01228230	-0.01102310	0.007646414	-0.01327141
5	0.003288098	-0.01217124	-0.01102451	0.007558935	-0.01332433

	Conductivity	Organic_carbon	Trihalomethanes	Turbidity
1	0.003902742	0.02196240	0.0003139698	0.003792758
2	0.004011753	0.02196099	0.0002991695	0.003802998
3	0.003967437	0.02203686	0.0003188474	0.003757085
4	0.003979881	0.02196812	0.0002652721	0.003760499
5	0.004014568	0.02201057	0.0002143065	0.003740428

	Potability
1	0.02742239
2	0.02673830
3	0.02723825
4	0.02677277
5	0.02682970

Memberships:

	1	2	3	4	5
[1,]	0.1999929	0.2000073	0.1999990	0.2000021	0.1999987
[2,]	0.1999846	0.2000076	0.1999870	0.2000067	0.2000142
[3,]	0.1999913	0.2000053	0.1999901	0.2000108	0.2000026
[4,]	0.1999986	0.1999999	0.1999996	0.1999992	0.2000027
[5,]	0.1999788	0.2000136	0.1999878	0.2000022	0.2000176
[6,]	0.1999932	0.2000033	0.1999992	0.1999996	0.2000046

[7,] 0.1999651 0.2000214 0.1999843 0.2000228 0.2000064
[8,] 0.1999863 0.2000069 0.1999943 0.2000054 0.2000070
[9,] 0.1999874 0.2000111 0.1999910 0.2000113 0.1999992
[10,] 0.1999922 0.2000055 0.1999961 0.1999985 0.2000077
[11,] 0.1999783 0.2000080 0.1999903 0.2000061 0.2000172
[12,] 0.1999694 0.2000156 0.1999906 0.2000126 0.2000118
[13,] 0.1999845 0.2000137 0.1999871 0.2000167 0.1999981
[14,] 0.1999790 0.2000226 0.1999852 0.2000154 0.1999978
[15,] 0.1999871 0.2000070 0.1999904 0.2000117 0.2000038
[16,] 0.1999914 0.2000122 0.1999874 0.2000067 0.2000022
[17,] 0.1999926 0.2000072 0.1999939 0.2000054 0.2000009
[18,] 0.1999868 0.2000056 0.1999894 0.2000074 0.2000108
[19,] 0.1999634 0.2000226 0.1999731 0.2000246 0.2000163
[20,] 0.1999832 0.2000125 0.1999878 0.2000125 0.2000040
[21,] 0.1999845 0.2000047 0.1999911 0.2000032 0.2000165
[22,] 0.1999818 0.2000178 0.1999794 0.2000196 0.2000013
[23,] 0.1999929 0.2000088 0.1999902 0.2000054 0.2000027
[24,] 0.1999945 0.2000017 0.2000006 0.1999989 0.2000044
[25,] 0.1999844 0.2000094 0.1999931 0.2000045 0.2000086
[26,] 0.1999954 0.2000051 0.1999948 0.2000006 0.2000041
[27,] 0.1999747 0.2000096 0.1999856 0.2000051 0.2000250
[28,] 0.1999908 0.2000050 0.1999955 0.2000047 0.2000040
[29,] 0.1999783 0.2000142 0.1999881 0.2000112 0.2000082
[30,] 0.1999788 0.2000073 0.1999937 0.2000030 0.2000171
[31,] 0.1999856 0.2000041 0.1999934 0.2000029 0.2000140
[32,] 0.1999927 0.2000053 0.1999916 0.2000043 0.2000061
[33,] 0.1999898 0.2000138 0.1999897 0.2000111 0.1999957
[34,] 0.1999930 0.2000066 0.1999908 0.2000089 0.2000008
[35,] 0.1999858 0.2000049 0.1999894 0.2000068 0.2000131
[36,] 0.1999903 0.2000079 0.1999951 0.2000050 0.2000017
[37,] 0.1999552 0.2000174 0.1999827 0.2000185 0.2000262
[38,] 0.1999902 0.2000084 0.1999937 0.2000032 0.2000044

[39,] 0.1999857 0.2000101 0.1999887 0.2000125 0.2000030
[40,] 0.1999812 0.2000139 0.1999889 0.2000121 0.2000039
[41,] 0.1999899 0.2000098 0.1999901 0.2000125 0.1999978
[42,] 0.1999794 0.2000109 0.1999880 0.2000159 0.2000058
[43,] 0.1999728 0.2000088 0.1999902 0.2000125 0.2000156
[44,] 0.1999902 0.2000090 0.1999900 0.2000103 0.2000005
[45,] 0.1999742 0.2000194 0.1999863 0.2000092 0.2000109
[46,] 0.1999865 0.2000081 0.1999938 0.2000061 0.2000054
[47,] 0.1999884 0.2000099 0.1999936 0.2000064 0.2000017
[48,] 0.1999719 0.2000227 0.1999810 0.2000131 0.2000113
[49,] 0.1999750 0.2000083 0.1999911 0.2000029 0.2000226
[50,] 0.1999973 0.2000031 0.1999973 0.1999977 0.2000045
[51,] 0.1999823 0.2000046 0.1999922 0.2000061 0.2000148
[52,] 0.1999894 0.2000020 0.1999981 0.2000004 0.2000101
[53,] 0.1999784 0.2000133 0.1999865 0.2000080 0.2000138
[54,] 0.1999792 0.2000130 0.1999879 0.2000102 0.2000097
[55,] 0.1999916 0.2000128 0.1999900 0.2000056 0.1999999
[56,] 0.1999861 0.2000137 0.1999914 0.2000123 0.1999964
[57,] 0.1999775 0.2000134 0.1999868 0.2000160 0.2000064
[58,] 0.1999811 0.2000115 0.1999863 0.2000121 0.2000091
[59,] 0.1999768 0.2000147 0.1999824 0.2000218 0.2000043
[60,] 0.1999859 0.2000067 0.1999959 0.2000036 0.2000079
[61,] 0.1999601 0.2000186 0.1999844 0.2000163 0.2000206
[62,] 0.1999991 0.2000055 0.1999951 0.1999999 0.2000003
[63,] 0.1999873 0.2000092 0.1999893 0.2000131 0.2000011
[64,] 0.1999790 0.2000078 0.1999920 0.2000033 0.2000179
[65,] 0.1999894 0.2000112 0.1999875 0.2000061 0.2000057
[66,] 0.1999940 0.2000017 0.1999973 0.2000032 0.2000038
[67,] 0.1999875 0.2000064 0.1999952 0.2000109 0.2000000
[68,] 0.1999967 0.2000042 0.1999977 0.2000013 0.2000000
[69,] 0.1999886 0.2000025 0.1999969 0.1999971 0.2000149
[70,] 0.1999832 0.2000099 0.1999934 0.2000130 0.2000006

[71,] 0.1999782 0.2000109 0.1999925 0.2000052 0.2000132
[72,] 0.1999965 0.2000034 0.1999939 0.2000028 0.2000034
[73,] 0.1999862 0.2000153 0.1999842 0.2000158 0.1999985
[74,] 0.1999534 0.2000186 0.1999795 0.2000186 0.2000299
[75,] 0.1999859 0.2000075 0.1999934 0.2000050 0.2000081
[76,] 0.1999757 0.2000109 0.1999909 0.2000155 0.2000070
[77,] 0.1999811 0.2000057 0.1999939 0.2000073 0.2000119
[78,] 0.1999924 0.2000028 0.1999939 0.2000044 0.2000064
[79,] 0.1999864 0.2000047 0.1999934 0.2000097 0.2000058
[80,] 0.1999628 0.2000194 0.1999853 0.2000173 0.2000152
[81,] 0.1999776 0.2000161 0.1999825 0.2000218 0.2000020
[82,] 0.1999788 0.2000130 0.1999914 0.2000150 0.2000019
[83,] 0.1999751 0.2000122 0.1999885 0.2000025 0.2000217
[84,] 0.1999553 0.2000252 0.1999825 0.2000141 0.2000230
[85,] 0.1999879 0.2000052 0.1999920 0.2000086 0.2000063
[86,] 0.1999647 0.2000258 0.1999874 0.2000136 0.2000085
[87,] 0.1999722 0.2000108 0.1999877 0.2000130 0.2000164
[88,] 0.1999560 0.2000223 0.1999806 0.2000187 0.2000225
[89,] 0.1999961 0.2000025 0.1999966 0.1999983 0.2000064
[90,] 0.1999888 0.2000099 0.1999959 0.2000045 0.2000009
[91,] 0.1999928 0.2000075 0.1999954 0.2000073 0.1999970
[92,] 0.1999884 0.2000136 0.1999886 0.2000129 0.1999966
[93,] 0.1999939 0.2000074 0.1999916 0.2000043 0.2000028
[94,] 0.1999785 0.2000159 0.1999871 0.2000151 0.2000034
[95,] 0.1999878 0.2000054 0.1999905 0.2000088 0.2000074
[96,] 0.1999741 0.2000095 0.1999858 0.2000064 0.2000243
[97,] 0.1999942 0.2000090 0.1999920 0.2000024 0.2000024
[98,] 0.1999561 0.2000301 0.1999743 0.2000332 0.2000063
[99,] 0.1999815 0.2000117 0.1999889 0.2000130 0.2000049
[100,] 0.1999890 0.2000051 0.1999962 0.2000020 0.2000078
[101,] 0.1999912 0.2000073 0.1999943 0.2000033 0.2000040
[102,] 0.1999890 0.2000072 0.1999952 0.2000056 0.2000030

[103,] 0.1999791 0.2000121 0.1999920 0.2000062 0.2000107
[104,] 0.1999834 0.2000118 0.1999940 0.2000025 0.2000083
[105,] 0.1999814 0.2000124 0.1999896 0.2000169 0.1999998
[106,] 0.1999613 0.2000213 0.1999823 0.2000170 0.2000181
[107,] 0.1999594 0.2000261 0.1999752 0.2000200 0.2000193
[108,] 0.1999913 0.2000133 0.1999872 0.2000132 0.1999950
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[reached getOption("max.print") -- omitted 1811 rows]

Closest hard clustering:

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[181] 1
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[991] 1 1 1 1 1 1 1 1 1 1 1
[ reached getOption("max.print") -- omitted 1011 entries ]

```

Available components:

```

[1] "centers" "size" "cluster" "membership"
[5] "iter" "withinerror" "call"

```

Agrupamento usando o método hierárquico

Call:

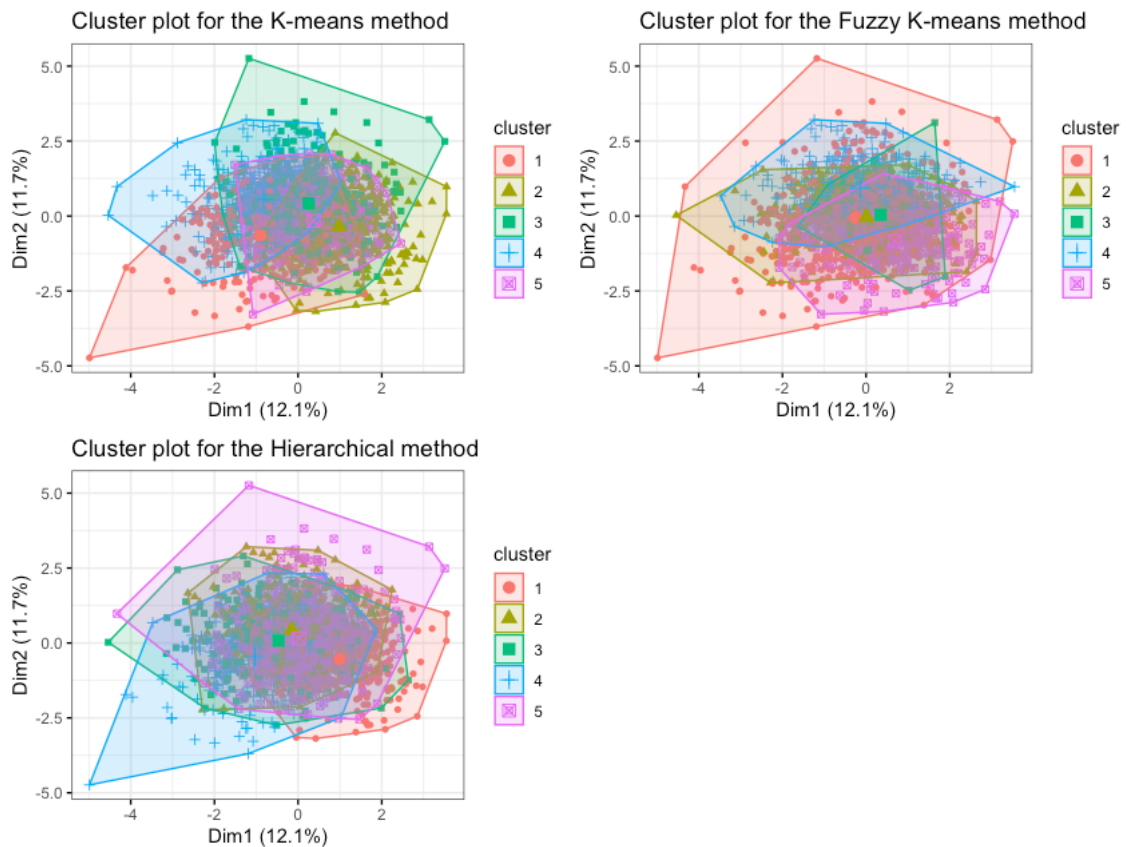
```
stats::hclust(d = x, method = hc_method)
```

Cluster method : ward.D2

Distance : euclidean

Number of objects: 2011

Gráfico 10



O (gráfico 10) mostra os três gráficos juntos (agrupamento usando o K-means, agrupamento usando o Fuzzy K-means e o agrupamento usando o método hierárquico).

Medidas de qualidade

Conectividade: varia de zero a infinito e deve ser minimizado:

c1

[1] 1228.178

c2

[1] 1005.103

> c3

[1] 1148.206

Dunn: varia de zero a infinito e deve ser maximizado:

d1

[1] 0.07689555


```
> d2
```

```
[1] 0.06866552
```

```
> d3
```

```
[1] 0.09785363
```

Silhueta: varia de -1 a 1. Quanto mais próximo de 1, melhor:

```
s.kmeans
```

	cluster	neighbor	sil_width
[1,]	2	4	1.831844e-01
[2,]	5	2	2.896842e-01
[3,]	4	5	1.687673e-01
[4,]	2	5	2.604730e-01
[5,]	2	5	3.784808e-02
[6,]	2	5	1.035331e-01
[7,]	4	2	1.626542e-01
[8,]	2	5	7.739257e-02
[9,]	4	2	3.263218e-01
[10,]	2	5	1.317764e-01
[11,]	2	5	1.447563e-01
[12,]	4	2	1.435883e-01
[13,]	4	5	2.354495e-01
[14,]	4	5	1.942720e-01
[15,]	4	5	9.349498e-02
[16,]	2	4	5.998300e-02
[17,]	2	5	-7.622350e-03
[18,]	5	2	7.017586e-02
[19,]	4	5	4.581699e-02
[20,]	4	2	3.093371e-01
[21,]	5	2	4.252714e-01
[22,]	4	5	1.563988e-01
[23,]	4	5	-1.563359e-03
[24,]	5	2	1.109723e-01
[25,]	2	5	3.095824e-01

[26,]	2	5	2.564220e-01
[27,]	5	2	1.815873e-01
[28,]	2	4	8.433189e-02
[29,]	4	2	3.702329e-02
[30,]	5	2	1.895317e-01
[31,]	5	2	2.836354e-01
[32,]	5	2	2.472065e-02
[33,]	4	2	2.350210e-01
[34,]	4	5	2.415453e-01
[35,]	5	4	3.746885e-01
[36,]	4	2	2.201505e-01
[37,]	5	2	2.529225e-01
[38,]	2	4	2.287303e-01
[39,]	4	5	2.556186e-01
[40,]	4	5	1.018729e-01
[41,]	4	2	3.509787e-01
[42,]	4	5	2.916135e-01
[43,]	5	2	3.237393e-02
[44,]	4	2	6.588044e-02
[45,]	2	4	3.200135e-01
[46,]	2	4	9.260463e-02
[47,]	4	2	1.012709e-01
[48,]	4	5	2.317469e-02
[49,]	2	5	2.476426e-02
[50,]	2	5	1.370838e-01
[51,]	5	2	3.685490e-02
[52,]	2	5	1.215756e-01
[53,]	2	5	7.068125e-02
[54,]	5	4	1.157344e-01
[55,]	2	4	4.201757e-02
[56,]	4	2	3.305081e-01
[57,]	4	5	1.124248e-01

[58,]	2	5	2.029458e-01
[59,]	4	5	2.378853e-01
[60,]	5	2	3.108515e-01
[61,]	5	2	8.935437e-02
[62,]	2	5	1.408178e-01
[63,]	4	5	1.203607e-01
[64,]	5	2	2.245238e-01
[65,]	2	5	1.825010e-01
[66,]	5	2	9.250533e-02
[67,]	4	2	1.936065e-01
[68,]	2	5	2.400548e-02
[69,]	2	5	9.301668e-02
[70,]	4	5	1.600393e-01
[71,]	2	5	1.114412e-01
[72,]	2	5	1.882876e-01
[73,]	4	2	1.046156e-01
[74,]	5	2	3.230883e-01
[75,]	5	2	6.896017e-02
[76,]	4	5	2.256980e-01
[77,]	5	2	1.244587e-01
[78,]	5	4	1.869642e-01
[79,]	5	4	1.466898e-01
[80,]	5	4	7.841933e-02
[81,]	4	2	1.015138e-01
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[87,]	5	4	1.644451e-01
[88,]	2	5	-3.417609e-02
[89,]	5	2	1.024634e-01

[90,]	2	5	1.635345e-01
[91,]	2	4	2.255233e-01
[92,]	4	2	2.883143e-01
[93,]	4	2	1.032701e-02
[94,]	4	5	1.948573e-01
[95,]	2	5	1.743417e-01
[96,]	5	2	3.293729e-01
[97,]	2	5	1.843015e-01
[98,]	4	5	1.378780e-01
[99,]	5	4	1.250863e-01
[100,]	2	5	4.628649e-02
[101,]	5	2	1.843438e-01
[102,]	2	4	2.103636e-01
[103,]	2	4	7.446782e-02
[104,]	2	5	1.695568e-01
[105,]	4	5	3.046943e-01
[106,]	2	4	4.959727e-02
[107,]	4	2	8.031656e-02
[108,]	4	2	2.923128e-01
[109,]	5	2	4.153338e-02
[110,]	4	5	1.168788e-01
[111,]	4	5	1.673807e-01
[112,]	5	4	2.001149e-01
[113,]	4	2	1.135556e-01
[114,]	4	2	1.683044e-01
[115,]	4	2	2.034093e-01
[116,]	4	5	1.787513e-01
[117,]	2	4	1.066148e-01
[118,]	5	2	1.572794e-01
[119,]	2	5	1.805401e-01
[120,]	5	4	1.485314e-01
[121,]	2	5	5.518096e-02

[122,]	4	5	1.621677e-01
[123,]	5	4	2.689460e-01
[124,]	2	4	3.822342e-01
[125,]	5	2	1.197814e-01
[126,]	5	2	5.105419e-02
[127,]	2	5	-8.376638e-04
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[129,]	4	2	1.580580e-01
[130,]	4	5	2.013258e-01
[131,]	2	5	3.283301e-02
[132,]	2	5	8.116167e-02
[133,]	5	2	1.410017e-01
[134,]	4	2	2.216038e-01
[135,]	2	5	4.018762e-02
[136,]	2	5	2.555946e-03
[137,]	5	2	2.701674e-01
[138,]	4	5	-8.506338e-04
[139,]	2	5	2.122364e-01
[140,]	2	5	2.279841e-02
[141,]	5	2	6.312962e-02
[142,]	4	5	1.636501e-02
[143,]	5	4	5.657555e-02
[144,]	2	5	7.327758e-03
[145,]	4	5	1.863949e-01
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[147,]	5	2	6.892592e-02
[148,]	5	4	3.946993e-02
[149,]	2	5	3.444881e-01
[150,]	5	2	1.042631e-01
[151,]	5	2	2.815286e-01
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[201,]	1	4	2.353030e-01
[202,]	3	5	1.299993e-01
[203,]	1	4	2.338930e-01
[204,]	1	3	1.063594e-02
[205,]	1	3	1.230400e-01
[206,]	3	1	1.048622e-01
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[208,]	1	3	1.453771e-01
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[1,]     1      2 0.1050899565
[2,]     2      1 0.0533908487
[3,]     3      2 0.2961344762
[4,]     1      3 0.1476883081
[5,]     2      1 -0.0228558836
[6,]     1      2 0.2354852149
[7,]     3      2 -0.0183307159
[8,]     2      1 0.0729061190
[9,]     3      2 0.0125521246
[10,]    1      2 0.2243088195
[11,]    1      3 0.0477483918

```

[12,]	1	2	-0.1385166982
[13,]	2	3	0.2058253022
[14,]	2	1	0.2537237133
[15,]	3	2	0.0856016555
[16,]	2	1	0.1914169243
[17,]	4	2	-0.1768972017
[18,]	1	3	-0.1204657370
[19,]	2	3	0.1036891936
[20,]	3	2	0.0584828165
[21,]	1	2	0.0306750141
[22,]	2	3	0.0748913269
[23,]	2	1	0.1236851897
[24,]	1	2	0.1893132641
[25,]	2	1	-0.1172985852
[26,]	1	2	0.0738960311
[27,]	1	2	0.0925431812
[28,]	2	1	0.0732470142
[29,]	2	3	0.2223600525
[30,]	1	2	0.2516364688
[31,]	1	2	0.1369910212
[32,]	1	3	-0.0177364904
[33,]	2	3	0.0724081853
[34,]	3	2	0.2032057890
[35,]	2	3	0.0464948306
[36,]	1	2	-0.1370421121
[37,]	2	1	0.0373710086
[38,]	2	1	0.0578977576
[39,]	2	3	0.1100621693
[40,]	2	1	0.3541488913
[41,]	3	2	0.0725046032
[42,]	3	2	0.0860005156
[43,]	1	3	-0.1012001946

[44,]	3	2	0.1783660315
[45,]	1	2	0.0496459557
[46,]	1	3	-0.0505028974
[47,]	2	3	0.1979655311
[48,]	1	2	-0.1501466227
[49,]	1	2	0.2875228214
[50,]	1	2	0.1868440292
[51,]	1	3	0.1112676480
[52,]	1	3	0.1977423657
[53,]	2	1	0.0544145933
[54,]	2	1	0.2673800347
[55,]	2	1	0.1232597630
[56,]	2	3	0.2536916489
[57,]	2	3	0.1707432211
[58,]	3	1	-0.0540681634
[59,]	3	2	0.0843396394
[60,]	2	1	0.0139348288
[61,]	1	2	0.1718134756
[62,]	1	2	0.0168995272
[63,]	3	2	0.0378307334
[64,]	1	2	0.0640159803
[65,]	1	2	-0.0278934914
[66,]	1	3	0.0088398952
[67,]	3	2	0.2277915100
[68,]	1	2	0.1238883406
[69,]	1	2	0.3679012025
[70,]	2	3	0.0888515791
[71,]	1	3	0.2269737617
[72,]	1	3	0.0345169826
[73,]	2	3	0.0182916807
[74,]	1	2	-0.0070836574
[75,]	2	1	0.1365332645

[76,]	3	2	0.0658401845
[77,]	1	2	0.0045611044
[78,]	1	3	-0.0552915707
[79,]	2	3	-0.0318901897
[80,]	2	3	0.1908565778
[81,]	2	3	0.0020810518
[82,]	3	1	0.0314805064
[83,]	1	2	0.2476234321
[84,]	1	2	0.0126698021
[85,]	3	2	0.2109470655
[86,]	1	2	0.0509649902
[87,]	1	3	-0.1647222849
[88,]	2	1	0.0529680563
[89,]	1	2	0.2331972177
[90,]	2	1	0.0594660916
[91,]	1	3	-0.0035277061
[92,]	2	3	0.1648438513
[93,]	2	3	0.1367548540
[94,]	2	3	0.1943732789
[95,]	3	1	0.1855117425
[96,]	2	1	-0.1155193215
[97,]	2	1	-0.1028620327
[98,]	2	3	0.2942869591
[99,]	2	1	0.2774159826
[100,]	1	3	0.2534057441
[101,]	2	1	0.0569083583
[102,]	2	1	0.0261155966
[103,]	1	2	0.0534798167
[104,]	2	1	-0.0012496155
[105,]	3	2	-0.0798804456
[106,]	2	1	-0.0064726965
[107,]	2	3	0.1851856389

[108,]	2	3	-0.0208349774
[109,]	1	3	0.0739873604
[110,]	2	3	0.2564943904
[111,]	1	3	-0.2273462697
[112,]	2	1	0.1960761973
[113,]	2	3	0.2645959837
[114,]	3	2	0.1257334020
[115,]	2	3	0.2384947891
[116,]	2	3	0.1374100646
[117,]	2	1	0.1710365823
[118,]	2	1	0.1232800898
[119,]	2	1	0.0855889253
[120,]	3	1	0.1714399239
[121,]	1	2	0.2622772674
[122,]	2	3	0.2200645277
[123,]	2	1	0.1953822977
[124,]	1	2	0.1006192402
[125,]	2	1	0.1042958562
[126,]	1	3	0.0666771492
[127,]	1	2	0.3072554173
[128,]	2	3	-0.0502005554
[129,]	2	1	0.2273973225
[130,]	2	3	0.2175522028
[131,]	2	1	-0.0059493407
[132,]	1	3	0.2693824855
[133,]	1	2	0.1556785637
[134,]	2	3	0.0260029117
[135,]	1	2	0.0645641832
[136,]	1	2	0.2201973636
[137,]	1	2	-0.0067481120
[138,]	1	3	-0.0332940744
[139,]	1	2	0.1520990703

[140,]	2	1	0.0489636242
[141,]	2	1	-0.0132142766
[142,]	1	3	-0.2087842761
[143,]	2	1	0.2644725620
[144,]	1	3	0.0397070535
[145,]	3	2	0.1613054752
[146,]	2	3	0.2112685633
[147,]	2	1	-0.0727427620
[148,]	3	2	0.0107724115
[149,]	1	2	0.2174347337
[150,]	2	1	0.0105958873
[151,]	1	3	0.1327782811
[152,]	2	1	0.1545198025
[153,]	1	3	-0.0516549574
[154,]	2	1	0.1138884107
[155,]	4	5	0.0296881839
[156,]	4	5	0.1157480070
[157,]	4	3	0.1321387628
[158,]	5	4	0.0529693860
[159,]	5	1	0.0776484216
[160,]	5	4	0.0206808951
[161,]	4	5	0.0970668076
[162,]	4	5	-0.2802617597
[163,]	5	3	0.1261539451
[164,]	5	2	0.1494028333
[165,]	5	1	0.1242009787
[166,]	5	1	0.2186289437
[167,]	5	1	0.1944857462
[168,]	5	2	0.2550809146
[169,]	5	4	0.1067119924
[170,]	4	5	-0.1750287844
[171,]	4	2	0.1615769756

[172,]	4	5	-0.0171170528
[173,]	4	3	0.1090364677
[174,]	5	4	-0.0016195044
[175,]	4	3	0.0021197230
[176,]	5	2	0.1560423040
[177,]	4	2	0.1567141599
[178,]	5	1	0.1305244962
[179,]	4	5	0.1529874722
[180,]	4	5	0.1418123438
[181,]	4	5	0.1901674234
[182,]	5	4	-0.1568819253
[183,]	5	4	-0.1310531679
[184,]	5	4	-0.2321297401
[185,]	5	1	0.1284892597
[186,]	5	1	0.1340304939
[187,]	1	4	-0.1174762401
[188,]	4	5	-0.1347107540
[189,]	5	4	0.0944095350
[190,]	4	3	0.0971719911
[191,]	4	5	0.0349324319
[192,]	5	3	0.1687386862
[193,]	4	5	-0.2381065243
[194,]	4	5	-0.0604343966
[195,]	5	1	0.1620870520
[196,]	5	2	0.0656087204
[197,]	5	4	-0.2206177216
[198,]	4	5	-0.0650379611
[199,]	4	5	0.1687061907
[200,]	4	2	0.0832968586
[201,]	5	4	-0.1384101564
[202,]	5	3	0.1057815260
[203,]	4	3	0.1370120358

[204,]	4	5	-0.0559059230
[205,]	5	4	0.1273774977
[206,]	5	2	0.1425172802
[207,]	5	1	0.2225751107
[208,]	4	5	0.0009916807
[209,]	4	5	0.0020182408
[210,]	5	3	0.2533488487
[211,]	4	5	0.0314256834
[212,]	5	2	0.1013774726
[213,]	5	1	0.0607634673
[214,]	2	5	-0.1250901817
[215,]	5	3	0.2039800515
[216,]	5	4	0.0170783725
[217,]	5	4	0.0719413307
[218,]	5	4	0.0552112229
[219,]	4	3	0.1918053496
[220,]	1	5	-0.1575213536
[221,]	5	1	0.1709393898
[222,]	5	1	0.2041127979
[223,]	5	1	0.1131454393
[224,]	5	3	0.1160061617
[225,]	5	1	0.1288113491
[226,]	5	2	0.1309411745
[227,]	5	2	0.1639196680
[228,]	5	1	0.1039967783
[229,]	4	3	-0.0291977359
[230,]	5	4	0.1613422001
[231,]	5	4	0.1005674581
[232,]	5	2	0.1888635943
[233,]	5	3	-0.1045970079
[234,]	5	2	0.1332608501
[235,]	4	5	0.1663061945

[236,]	5	3	-0.0757560863
[237,]	4	5	0.1096574436
[238,]	4	5	0.1306369468
[239,]	5	2	0.1524132226
[240,]	4	2	0.0184400598
[241,]	4	5	-0.2260214894
[242,]	5	4	-0.0606311656
[243,]	5	1	0.1365602191
[244,]	5	3	0.0385481579
[245,]	5	1	0.1433870655
[246,]	5	4	0.1123460474
[247,]	5	2	0.2075552403
[248,]	5	3	0.1645954095
[249,]	4	3	0.1233820174
[250,]	5	1	0.1926716299
[251,]	5	2	0.1160678048
[252,]	4	5	-0.0022547708
[253,]	5	1	0.1997382385
[254,]	5	1	0.0706140858
[255,]	5	2	0.1276569656
[256,]	5	2	0.1099494540
[257,]	2	1	0.0844556449
[258,]	2	3	-0.0520779958
[259,]	2	3	0.2824797256
[260,]	3	2	0.0251814384
[261,]	1	2	-0.0841106863
[262,]	1	2	0.1810469403
[263,]	3	2	0.0489319340
[264,]	1	3	0.0662790806
[265,]	1	2	-0.0124201480
[266,]	3	1	0.1494413690
[267,]	2	3	0.0553750815

[268,]	1	3	-0.2191232217
[269,]	2	1	0.3042345090
[270,]	1	2	0.2885795419
[271,]	2	1	0.1719383432
[272,]	1	2	0.0406401432
[273,]	1	2	0.2276799201
[274,]	1	2	-0.0215600894
[275,]	2	1	0.1703579012
[276,]	1	3	0.2178437094
[277,]	3	2	0.1558766090
[278,]	3	2	0.1073745971
[279,]	1	2	0.2582896141
[280,]	2	3	0.1929657144
[281,]	3	1	0.0781269241
[282,]	2	3	0.1010598893
[283,]	2	1	-0.1316808301
[284,]	2	1	-0.0225607763
[285,]	1	2	-0.0399575719
[286,]	1	2	0.0776323141
[287,]	2	1	0.0572007657
[288,]	2	3	0.0456760466
[289,]	1	3	0.2025620474
[290,]	1	2	0.1139724009
[291,]	1	2	0.0563852539
[292,]	3	1	-0.1419401508
[293,]	2	1	-0.0347602441
[294,]	2	1	0.0656321630
[295,]	3	1	0.1742154935
[296,]	1	3	0.0376707267
[297,]	3	2	0.2265316566
[298,]	3	2	0.0980389199
[299,]	2	1	0.1819498117

[300,]	3	2	-0.0773427087
[301,]	1	2	0.2586957822
[302,]	2	1	0.2889090798
[303,]	1	2	0.1338165281
[304,]	1	2	-0.0864805491
[305,]	2	3	0.2349853409
[306,]	2	3	0.1710793769
[307,]	2	1	0.1190019765
[308,]	3	1	0.0151321985
[309,]	3	2	-0.0588941011
[310,]	2	3	0.2247649730
[311,]	1	2	0.0647540958
[312,]	2	1	0.0220975967
[313,]	1	2	-0.1166346234
[314,]	1	3	-0.1438039737
[315,]	3	1	0.1940859787
[316,]	2	3	0.2598533437
[317,]	2	1	0.1785265808
[318,]	2	1	0.3299422623
[319,]	2	3	0.1243248425
[320,]	2	1	0.2688291533
[321,]	3	2	0.1759776787
[322,]	3	2	0.2479225273
[323,]	1	2	0.1720639309
[324,]	1	2	0.0932389927
[325,]	1	2	-0.1867724695
[326,]	2	3	0.2232767809
[327,]	3	1	0.0553978581
[328,]	3	2	0.1031224961
[329,]	3	2	0.0279776787
[330,]	2	1	0.2655880289
[331,]	2	3	0.1917995044

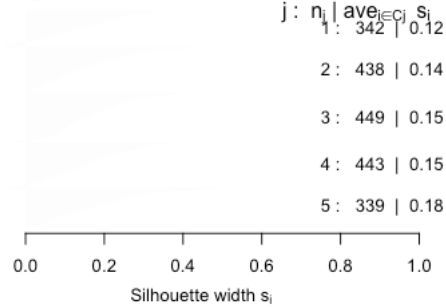

```

[332,]    1    2 0.1390786351
[333,]    3    2 0.1476567081
[ reached getOption("max.print") -- omitted 1678 rows ]
attr("Ordered")
[1] FALSE
attr("call")
silhouette.default(x = fit.hclust$cluster, dist = dist(df)^2)
attr("class")
[1] "silhouette"

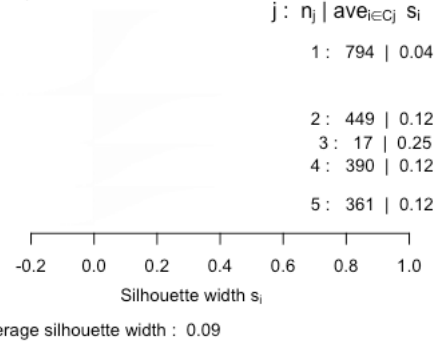
```

Tabela 1

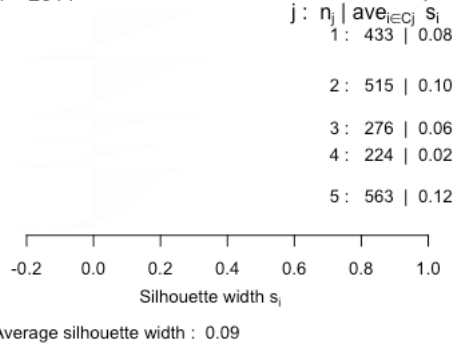
Silhouette plot of (x = fit.kmeans\$cluster, dist =
n = 2011



Silhouette plot of (x = fit.cmeans\$cluster, dist =
n = 2011



Silhouette plot of (x = fit.hclust\$cluster, dist = d
n = 2011



A avaliação de modelos de agrupamentos não tem como levar em consideração uma informação de valores observados de uma variável alvo (ground truth).

Portanto, costuma-se usar métricas (tabela 1) que comparam os elementos dos grupos como os centroides (critério J) ou o quão similar os elementos de um grupo são entre si (coesão) em comparação aos outros clusters (separação), como é o caso da medida de silhueta (silhouette).

Resultados

> results

	Connectivity	Dunn	Silhouette
K-means (K = 5)	1228.178	0.07689555	0.14777435
Fuzzy K-means (K = 5)	1005.103	0.06866552	0.09128905
Hierarchical (K = 5)	1148.206	0.09785363	0.08706726

Conclusão: O método Fuzzy "vence" em 2 medidas (Connectivity e Dunn), dessa forma, utilizaremos o agrupamento fornecido por esse método.

Análise exploratória do agrupamento utilizando o método Fuzzy

```
> head(df)
```

	ph	Hardness	Solids	Chloramines	Sulfate
1	0.7752344	0.5475678	0.0004932291	0.5919175	0.5579943
2	1.2616222	-0.4643582	-0.4601783194	-0.3636424	-0.5707833
3	-0.9387754	-0.2450192	0.7680379557	0.2669421	-0.1713654
4	1.9714164	1.5724639	0.7681552843	0.2470693	1.4459727
5	0.9753717	0.2126544	-0.9513523841	-1.6166335	-0.7355946
6	2.5713102	0.9386313	0.3957789739	1.2348821	1.6965528

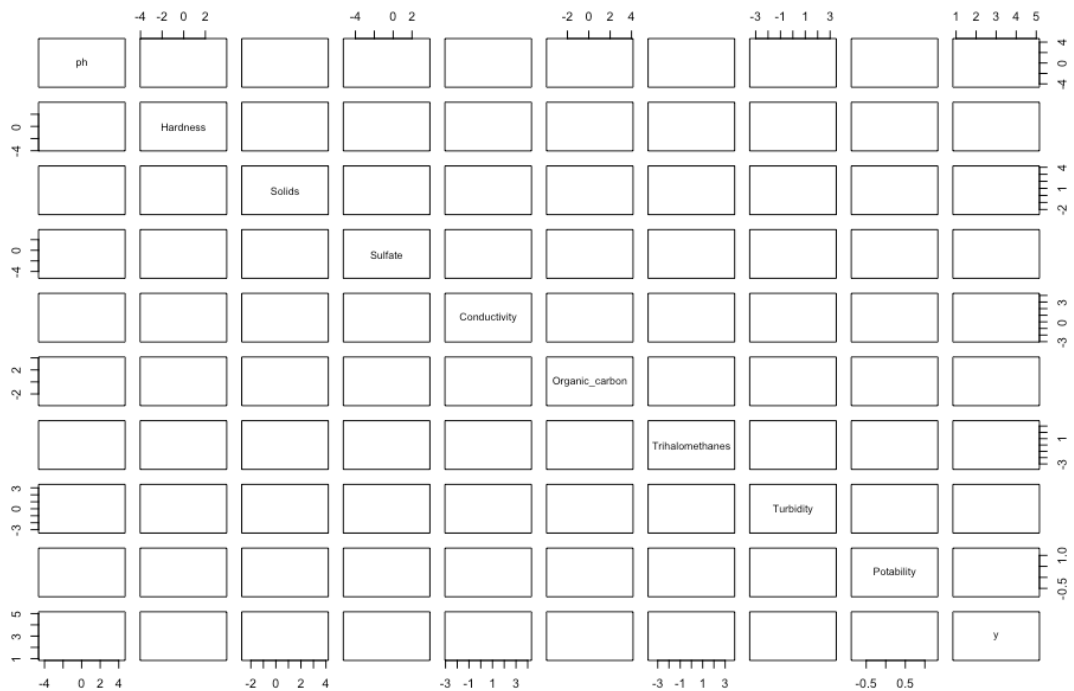
Conductivity Organic_carbon Trihalomethanes Turbidity

1	-0.7787111	1.2549429	2.0986315	0.8482820
2	-0.3438864	-0.8242313	-2.1266326	0.1387643
3	-1.8031411	-1.7790047	-0.7096399	-1.8030621
4	-1.7637504	-0.1497130	1.1256417	-1.6579018
5	0.5988629	-0.5807314	-0.2224409	0.5569558
6	1.7034577	1.1011662	0.3449957	0.5174076

Potability

1	-0.7996527
2	-0.7996527
3	-0.7996527
4	-0.7996527
5	-0.7996527
6	-0.7996527

Gráfico 11



```
Desc(fit.cmeans$cluster, digits = 2, plotit = F )
```

```
-----
fit.cmeans$cluster (integer)
```

```
length    n  NAs unique   0s mean meanCI'
2'011  2'011    0    5    0 2.54  2.47
      100.0% 0.0%    0.0%    2.61
```

```
.05  .10  .25 median .75 .90  .95
1.00  1.00  1.00  2.00 4.00 5.00  5.00
```

```
range    sd vcoef   mad  IQR skew  kurt
4.00  1.58  0.62  1.48 3.00 0.45 -1.45
```

```
level freq  perc cumfreq cumperc
1     1  794 39.5%   794  39.5%
2     2  449 22.3%  1'243  61.8%
```

3	3	17	0.8%	1'260	62.7%
4	4	390	19.4%	1'650	82.0%
5	5	361	18.0%	2'011	100.0%

' 95%-CI (classic)

Gráfico 12

Silhouette plot of (x = fit.cmeans\$cluster, dist = dist(df)^2)

n = 2011

5 clusters C_j
 $j : n_j \mid \text{ave}_{i \in C_j} s_i$

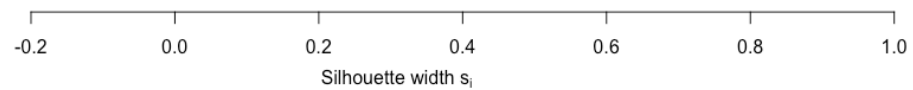
1 : 794 | 0.04

2 : 449 | 0.12

3 : 17 | 0.25

4 : 390 | 0.12

5 : 361 | 0.12



Average silhouette width : 0.09

Referência

BRUCE, Peter; BRUCE, Andrew. **Estatística Prática para Cientistas de Dados**: 50 conceitos essenciais. Rio de Janeiro: Alta Books, 2019. 320 p. Luciana Ferraz

Anexo

Código R

```
library(tidyverse) # Gráficos, manipulação e transformação dos dados
library(cluster) # Avaliação dos grupos
library(clValid) # Avaliação dos grupos
library(e1071) # Fuzzy K-médias
library(factoextra) # Visualização de grupos
library(skimr) # Análise exploratória de dados
library(gridExtra) # Ferramentas gráficas
library(ggforce) # Ferramentas gráficas
library(DescTools)
library(mice)
```

```
#####
```

```
# #
```

```
#---- Análise de Agrupamentos ----#
```

```
# #
```

```
#####
```

```
# Função que obtém o WSS para o método hierárquico
```

```
# NÃO MUDAR!
```

```
get_wss <- function(d, cluster){
```

```
  d <- stats::as.dist(d)
```

```
  cn <- max(cluster)
```

```
  clusterf <- as.factor(cluster)
```

```
  clusterl <- levels(clusterf)
```

```

cnn <- length(clusterl)

if (cn != cnn) {
  warning("cluster renumbered because maximum != number of clusters")
  for (i in 1:cnn) cluster[clusterf == clusterl[[i]] <- i
  cn <- cnn
}
cwn <- cn
# Compute total within sum of square
dmat <- as.matrix(d)
within.cluster.ss <- 0
for (i in 1:cn) {
  cluster.size <- sum(cluster == i)
  di <- as.dist(dmat[cluster == i, cluster == i])
  within.cluster.ss <- within.cluster.ss + sum(di^2)/cluster.size
}
within.cluster.ss
}

# Função que contrói o "gráfico do cotovelo" e aponta o K ótimo
# NÃO MUDAR!
elbow.plot <- function(x, kmax = 15, alg = "kmeans") {
  # alg = c("kmeans", "cmeans", "hclust")
  wss <- c()
  if (alg == "kmeans") {
    for (i in 1:kmax) {
      set.seed(13)
      tmp <- kmeans(x, i)
      # wss[i] <- get_wss(dist(x), tmp$cluster)
      wss[i] <- tmp$tot.withinss
    }
    tmp <- data.frame(k = 1:kmax, wss)
  }
}

```

```

max_k <- max(tmp$k)
max_k_wss <- tmp$wss[which.max(tmp$k)]
max_wss <- max(tmp$wss)
max_wss_k <- tmp$k[which.max(tmp$wss)]
max_df <- data.frame(x = c(max_wss_k, max_k), y = c(max_wss, max_k_wss))
tmp_lm <- lm(max_df$y ~ max_df$x)
d <- c()
for(i in 1:kmax) {
  d <- c(d, abs(coef(tmp_lm)[2]*i - tmp$wss[i] + coef(tmp_lm)[1]) /
    sqrt(coef(tmp_lm)[2]^2 + 1^2))
}
tmp$d <- d
ggplot(data = tmp, aes(k, wss)) +
  geom_line() +
  geom_segment(aes(x = k[1], y = wss[1],
    xend = max(k), yend = wss[which.max(k)]),
    linetype = "dashed") +
  geom_point(aes(size = (d == max(d)), color = (d == max(d))),
    show.legend = FALSE) +
  scale_size_manual(values = c(2,5)) +
  scale_color_manual(values = c("black", "red")) +
  labs(x = "Number of clusters",
    y = "Total within-cluster sum of squares",
    title = "Elbow plot for the K-means method") +
  theme_bw()
}
else if (alg == "cmeans") {
  for (i in 1:kmax) {
    if (i == 1) {
      wss[i] <- get_wss(dist(x), rep(1, nrow(x)))
    }
  }
  else {

```



```

set.seed(13)

tmp <- cmeans(x, i)
wss[i] <- get_wss(dist(x), tmp$cluster)
# wss[i] <- tmp$sumsqrs$tot.within.ss
}
}

tmp <- data.frame(k = 1:kmax, wss)
max_k <- max(tmp$k)
max_k_wss <- tmp$wss[which.max(tmp$k)]
max_wss <- max(tmp$wss)
max_wss_k <- tmp$k[which.max(tmp$wss)]
max_df <- data.frame(x = c(max_wss_k, max_k), y = c(max_wss, max_k_wss))
tmp_lm <- lm(max_df$y ~ max_df$x)
d <- c()
for(i in 1:kmax) {
  d <- c(d, abs(coef(tmp_lm)[2]*i - tmp$wss[i] + coef(tmp_lm)[1]) /
    sqrt(coef(tmp_lm)[2]^2 + 1^2))
}
tmp$d <- d
ggplot(data = tmp, aes(k, wss)) +
  geom_line() +
  geom_segment(aes(x = k[1], y = wss[1],
    xend = max(k), yend = wss[which.max(k)]),
    linetype = "dashed") +
  geom_point(aes(size = (d == max(d)), color = (d == max(d))),
    show.legend = FALSE) +
  scale_size_manual(values = c(2,5)) +
  scale_color_manual(values = c("black", "red")) +
  labs(x = "Number of clusters",
    y = "Total within-cluster sum of squares",
    title = "Elbow plot for the fuzzy K-means method") +
  theme_bw()

```

```

}
else if (alg == "hclust") {
  for (i in 1:kmax) {
    set.seed(13)
    tmp <- hcut(x, i)
    wss[i] <- get_wss(dist(x), tmp$cluster)
  }
  tmp <- data.frame(k = 1:kmax, wss)
  max_k <- max(tmp$k)
  max_k_wss <- tmp$wss[which.max(tmp$k)]
  max_wss <- max(tmp$wss)
  max_wss_k <- tmp$k[which.max(tmp$wss)]
  max_df <- data.frame(x = c(max_wss_k, max_k), y = c(max_wss, max_k_wss))
  tmp_lm <- lm(max_df$y ~ max_df$x)
  d <- c()
  for(i in 1:kmax) {
    d <- c(d, abs(coef(tmp_lm)[2]*i - tmp$wss[i] + coef(tmp_lm)[1]) /
      sqrt(coef(tmp_lm)[2]^2 + 1^2))
  }
  tmp$d <- d
  ggplot(data = tmp, aes(k, wss)) +
    geom_line() +
    geom_segment(aes(x = k[1], y = wss[1],
      xend = max(k), yend = wss[which.max(k)]),
      linetype = "dashed") +
    geom_point(aes(size = (d == max(d)), color = (d == max(d))),
      show.legend = FALSE) +
    scale_size_manual(values = c(2,5)) +
    scale_color_manual(values = c("black", "red")) +
    labs(x = "Number of clusters",
      y = "Total within-cluster sum of squares",
      title = "Elbow plot for the hierarchical method") +

```

```

    theme_bw()
  }
}

# Função visualização dos grupos
# NÃO MUDAR!
cluster_viz <- function(data, clusters,
                        axes = c(1, 2), geom = c("point", "text"), repel = TRUE,
                        show.clust.cent = TRUE, ellipse = TRUE, ellipse.type = "convex",
                        ellipse.level = 0.95, ellipse.alpha = 0.2, shape = NULL,
                        pointsize = 1.5, labelsiz = 12, main = "Cluster plot",
                        ggtheme = theme_bw()) {
  require(factoextra)
  data <- scale(data)
  pca <- stats::prcomp(data, scale = FALSE, center = FALSE)
  ind <- facto_summarize(pca, element = "ind", result = "coord", axes = axes)
  eig <- get_eigenvalue(pca)[axes, 2]
  xlab <- paste0("Dim", axes[1], " (", round(eig[1], 1), "%)")
  ylab <- paste0("Dim", axes[2], " (", round(eig[2], 1), "%)")
  colnames(ind)[2:3] <- c("x", "y")
  label_coord <- ind
  lab <- NULL
  if ("text" %in% geom)
    lab <- "name"
  if (is.null(shape))
    shape <- "cluster"
  plot.data <- cbind.data.frame(ind, cluster = clusters, stringsAsFactors = TRUE)
  label_coord <- cbind.data.frame(label_coord, cluster = clusters, stringsAsFactors = TRUE)
  p <- ggpubr::ggscatter(plot.data, "x", "y", color = "cluster",
                        shape = shape, size = pointsize, point = "point" %in% geom,
                        label = lab, font.label = labelsiz, repel = repel,

```

```

        mean.point = show.clust.cent, ellipse = ellipse, ellipse.type =
ellipse.type,
        ellipse.alpha = ellipse.alpha, ellipse.level = ellipse.level,
        main = main, xlab = xlab, ylab = ylab, ggtheme = ggtheme)

p
}

# Mudar diretório de acordo com o endereço de onde o dataset foi salvo
# no seu computador
# onde <- "C:\\Users\\marce\\Dropbox\\DE-UFPB\\disciplinas\\2021-1\\AM\\Aulas"
onde <- "/Users/user/Documents/ESTATÍSTICA/MULTIVARIADA 2/PROVA
4/PROVA_4"
setwd(onde)

# Mudar nome do arquivo de acordo com o dataset
df <- read.csv("water_potability.csv")
df

# Exploração inicial
head(df)
skim(df)
pairs(df)

# Padronização dos dados
boxplot(df)
df <- scale(df)

#Dados faltantes
PlotMiss(df, col = colorRampPalette(c( "gray10", "gray90"))(1))
#df <- complete(mice(df, printFlag=F))
df <- na.omit(df)
df <- as.data.frame(df)

# Encontrar número ótimo de grupos para o K-means

```

```

set.seed(13)
p1 <- elbow.plot(df)
p1
# K "ótimo" é igual a 5. Mudar de acordo com o seu resultado

# Encontrar número ótimo de grupos para o Fuzzy K-means
set.seed(13)
p2 <- elbow.plot(df, alg = "cmeans")
p2
# K "ótimo" é igual a 5. Mudar de acordo com o seu resultado

# Encontrar número ótimo de grupos para o método hierárquico
set.seed(13)
p3 <- elbow.plot(df, alg = "hclust")
p3
# K "ótimo" é igual a 5. Mudar de acordo com o seu resultado

grid.arrange(p1, p2, p3, nrow = 2) # Os três gráficos juntos
nclust = c(5,5,5) # Número de grupos de acordo com os gráficos

# Agrupamento usando o K-means
set.seed(13)
fit.kmeans <- kmeans(df, nclust[1]) # Ajustar K de acordo com o gráfico
fit.kmeans
g1 <- cluster_viz(df, as.factor(fit.kmeans$cluster), geom = "point",
                  main = "Cluster plot for the K-means method")

# Agrupamento usando o Fuzzy K-means
set.seed(13)
fit.cmeans <- cmeans(df, nclust[2]) # Ajustar K de acordo com o gráfico
fit.cmeans
g2 <- cluster_viz(df, as.factor(fit.cmeans$cluster), geom = "point",

```

```

    main = "Cluster plot for the Fuzzy K-means method")

# Agrupamento usando o método hierárquico
set.seed(13)
fit.hclust <- hcut(df, nclust[3]) # Ajustar K de acordo com o gráfico
fit.hclust
g3 <- cluster_viz(df, as.factor(fit.hclust$cluster), geom = "point",
    main = "Cluster plot for the Hierarchical method")

grid.arrange(g1, g2, g3, nrow = 2) # Os três gráficos juntos

#####
# Medidas de qualidade #
#####

# Conectividade: varia de zero a infinito
# e deve ser minimizado
c1 <- connectivity(clusters = fit.kmeans$cluster, Data = df)
c2 <- connectivity(clusters = fit.cmeans$cluster, Data = df)
c3 <- connectivity(clusters = fit.hclust$cluster, Data = df)

# Dunn: varia de zero a infinito
# e deve ser maximizado
d1 <- dunn(clusters = fit.kmeans$cluster, Data = df)
d2 <- dunn(clusters = fit.cmeans$cluster, Data = df)
d3 <- dunn(clusters = fit.hclust$cluster, Data = df)

# Silhueta: varia de -1 a 1
# Quanto mais próximo de 1, melhor
s.kmeans <- silhouette(fit.kmeans$cluster, dist = dist(df)^2)
s.cmeans <- silhouette(fit.cmeans$cluster, dist = dist(df)^2)
s.hclust <- silhouette(fit.hclust$cluster, dist = dist(df)^2)

```

```

par(mfrow = c(2,2))
plot(s.kmeans)
plot(s.cmeans)
plot(s.hclust)

s1 <- summary(s.kmeans)$avg.width
s2 <- summary(s.cmeans)$avg.width
s3 <- summary(s.hclust)$avg.width

results <- matrix(c(c1, c2, c3, d1, d2, d3, s1, s2, s3), nrow = 3)
colnames(results) <- c("Connectivity", "Dunn", "Silhouette")
row.names(results) <- c(paste0("K-means (K = ", nclust[1], ")"),
                        paste0("Fuzzy K-means (K = ", nclust[2], ")"),
                        paste0("Hierarchical (K = ", nclust[3], ")"))

results

# O método Fuzzy "vence" em 2 medidas (Connectivity e Dunn),
# dessa forma, utilizaremos o agrupamento fornecido por esse método
# MUDAR ESSA CONCLUSÃO DE ACORDO COM OS SEUS RESULTADOS!

head(df)
df$y <- factor(as.numeric(fit.cmeans$cluster))
pairs(df[,-4], col = df[,0])

#Fim

Desc(fit.cmeans, digits = 2, plotit = F)

```