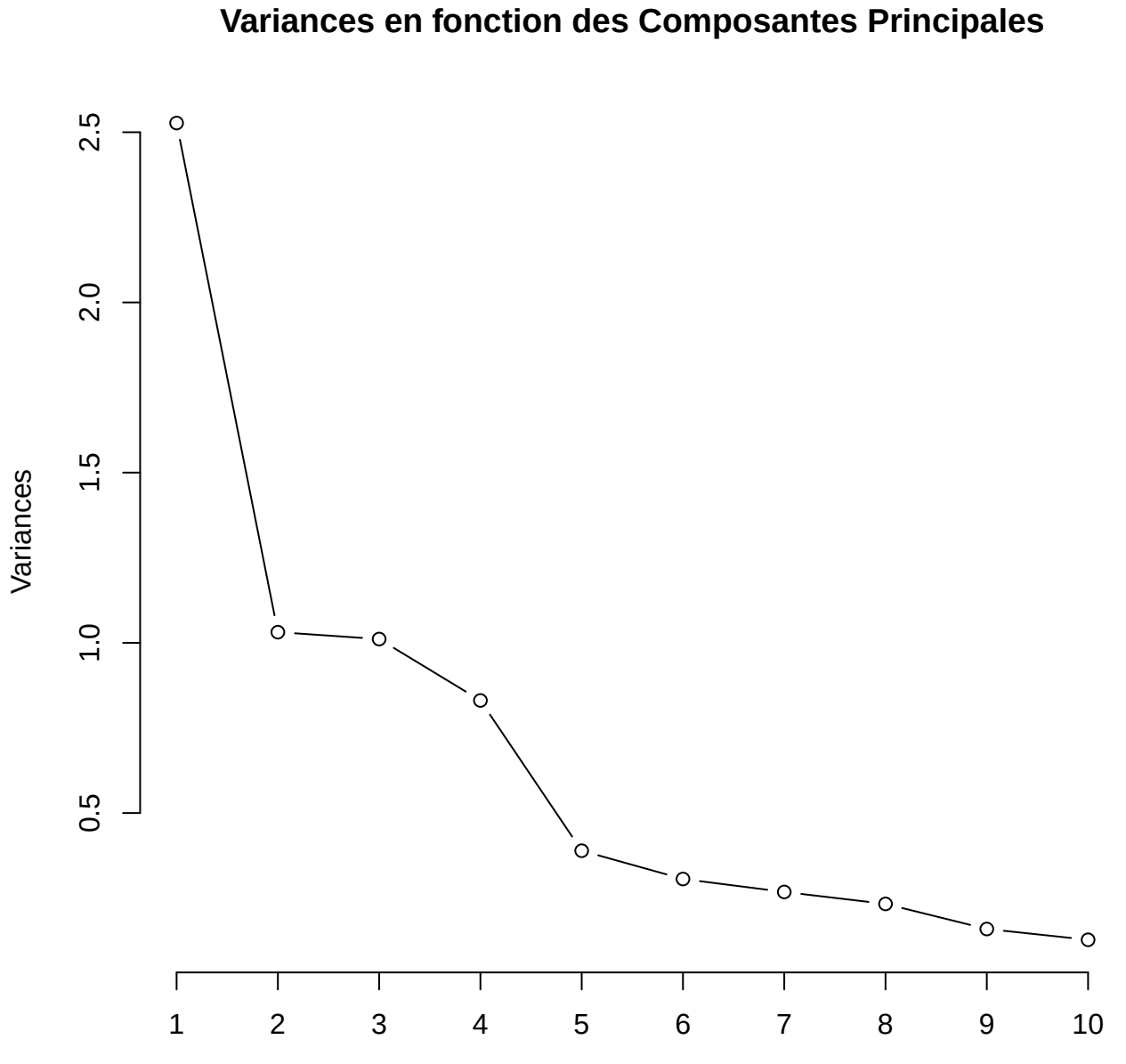
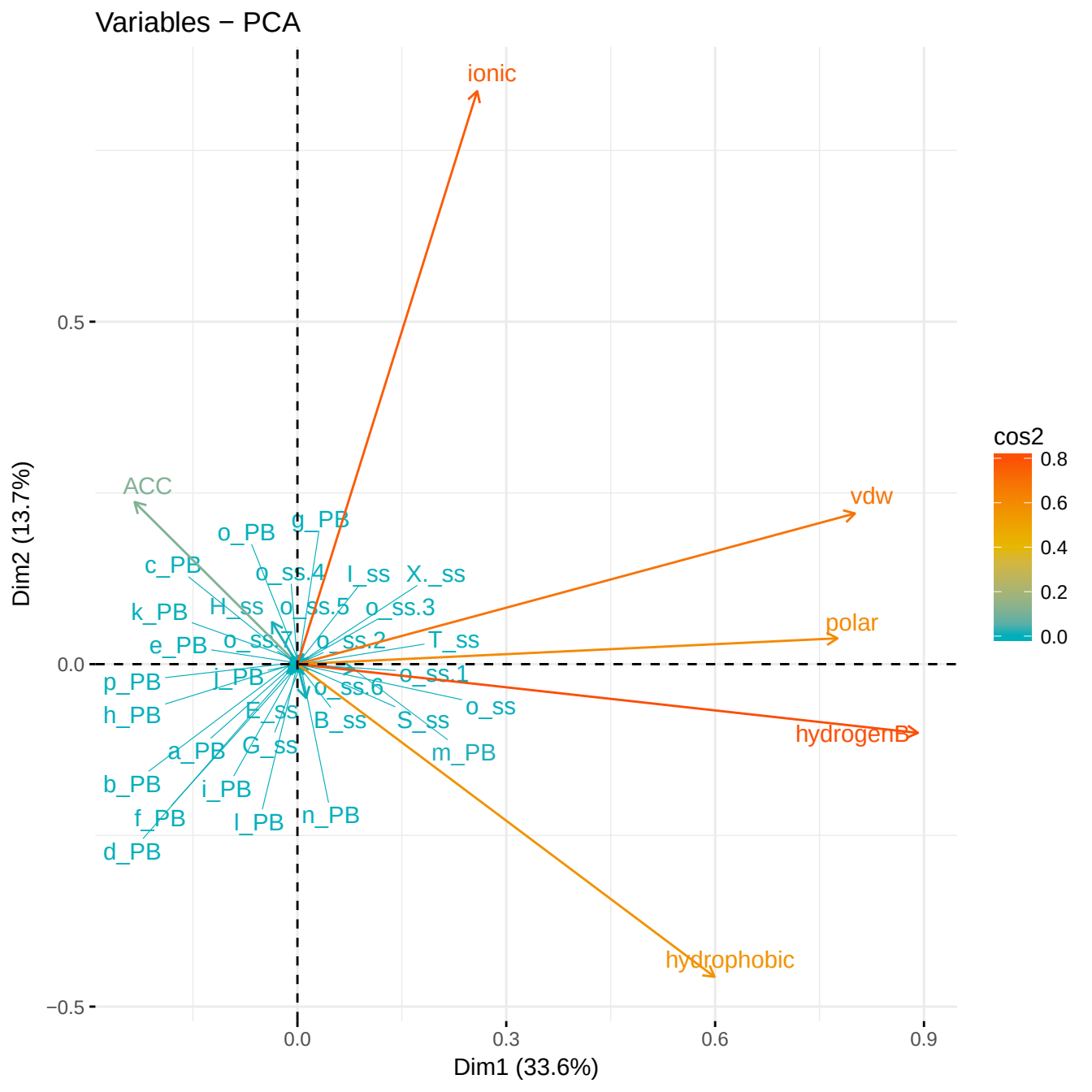
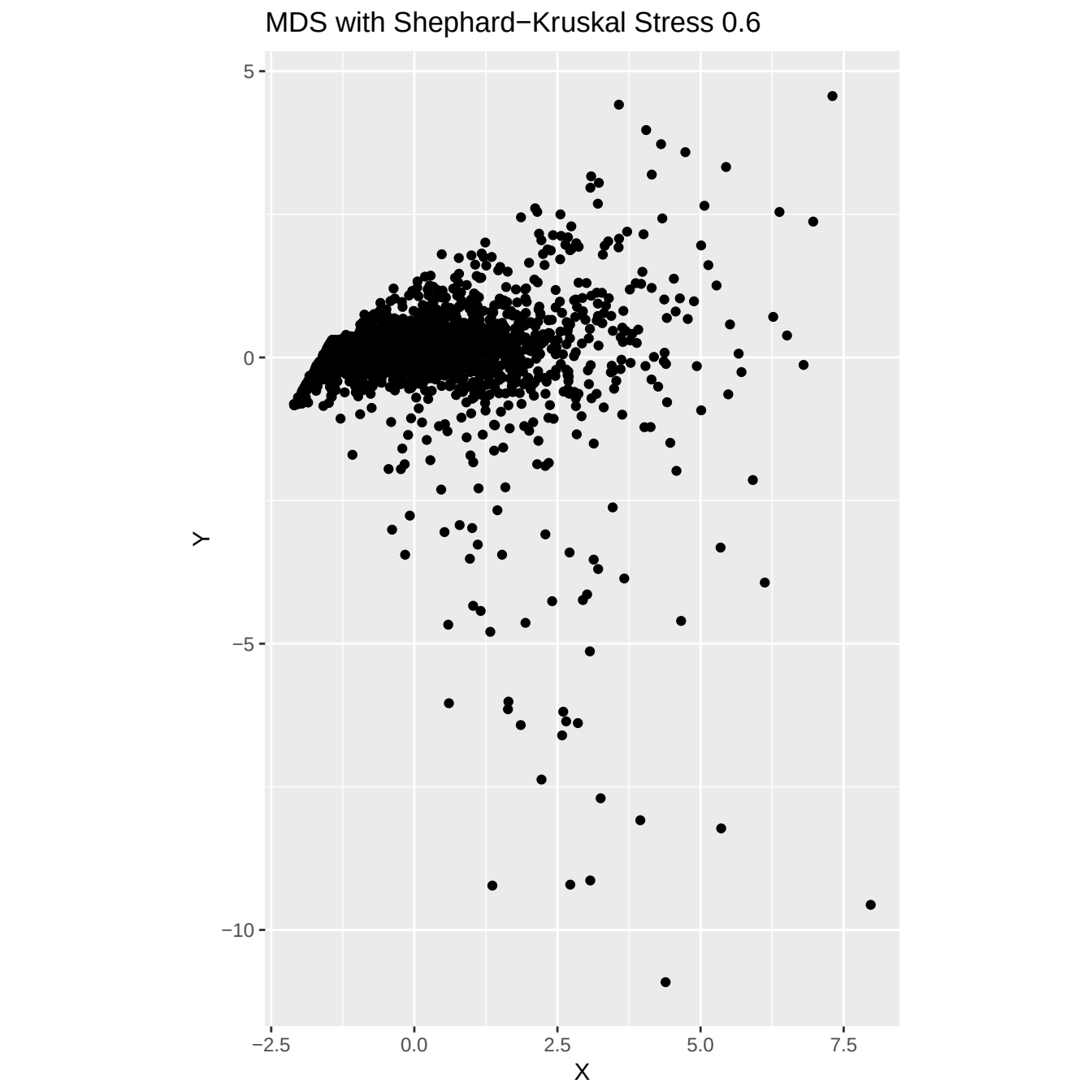
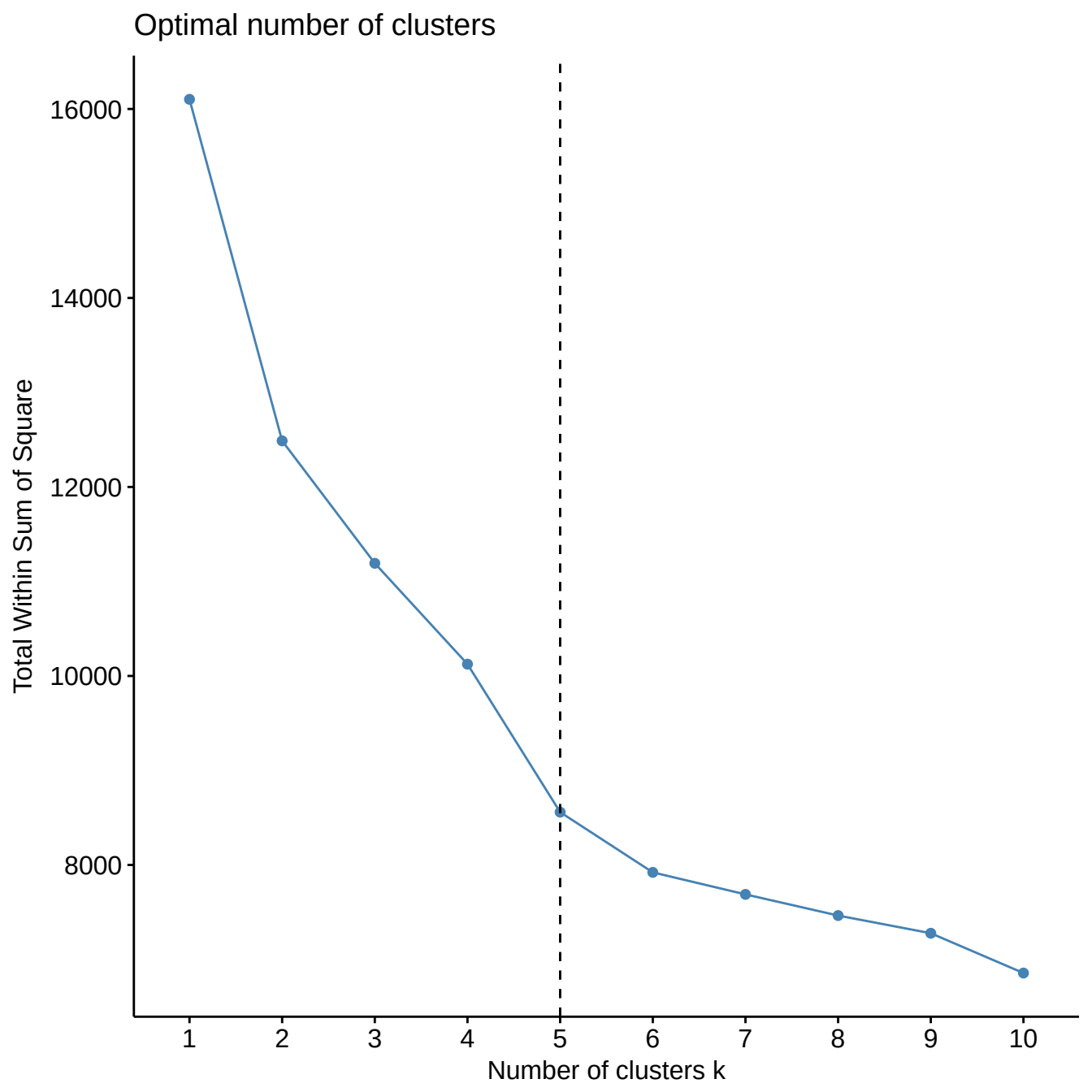
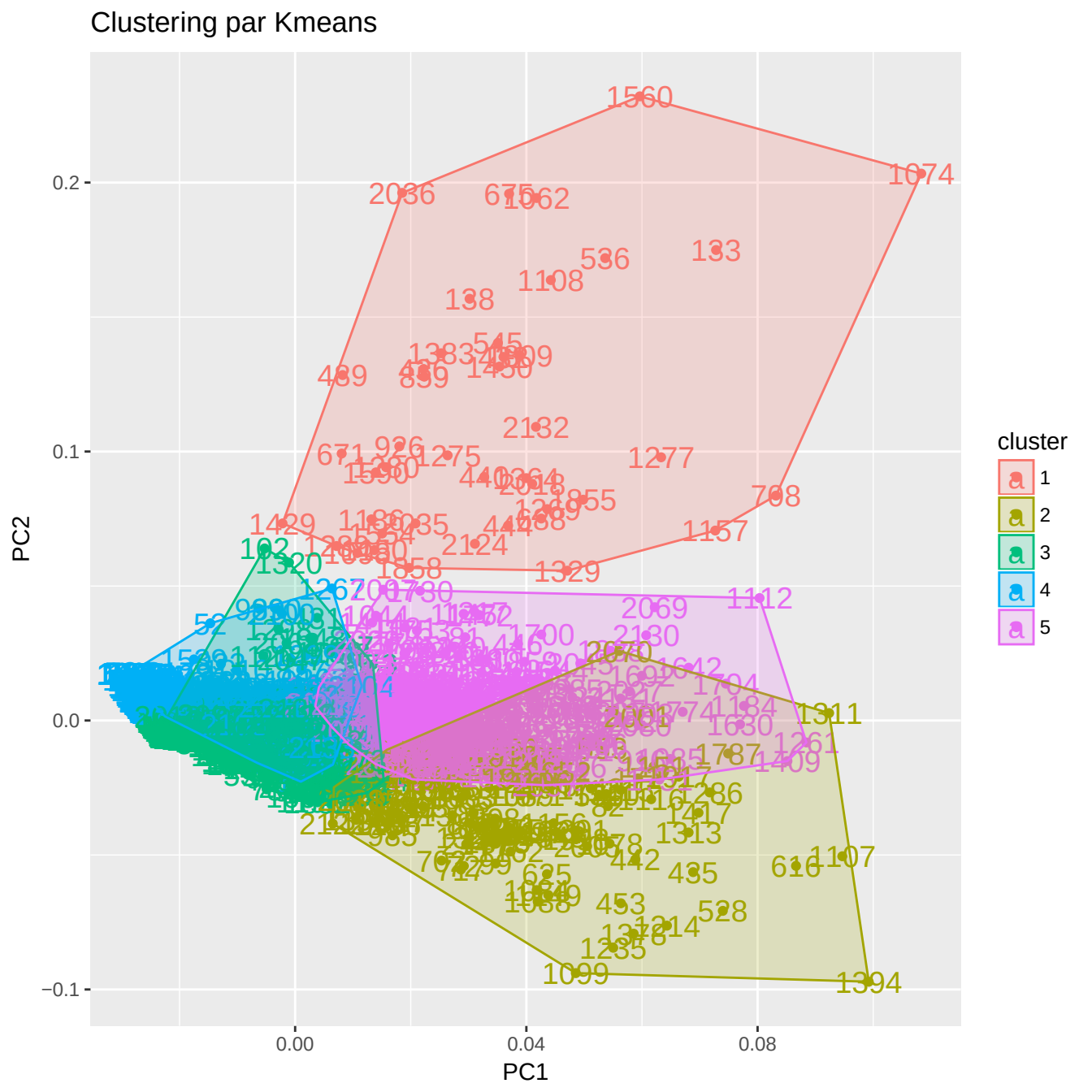
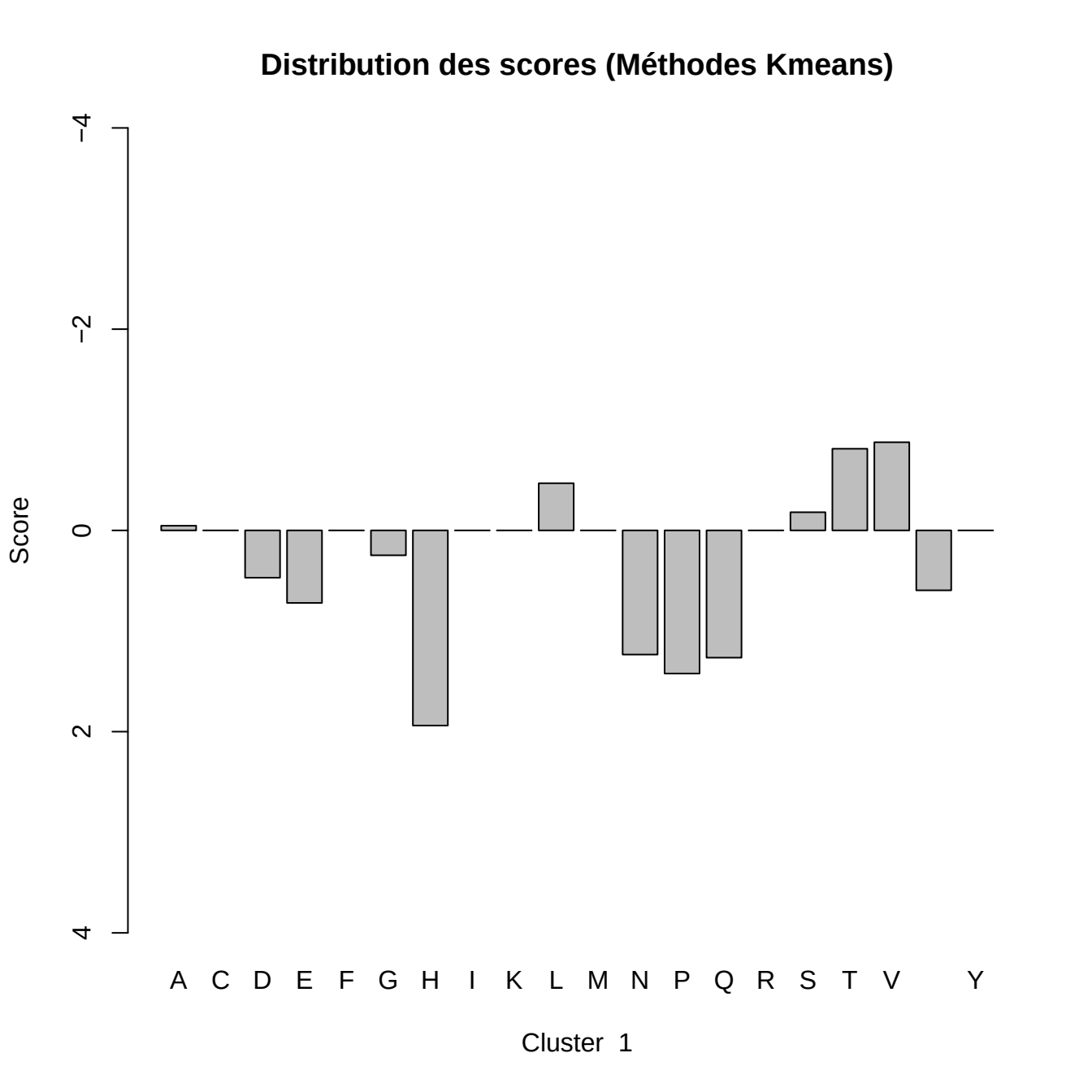

Variances en fonction des Composantes Principales
Variances
0.5
1.0
1.5
2.0
2.5
1
2
3
4
5
6
7
8
9
10

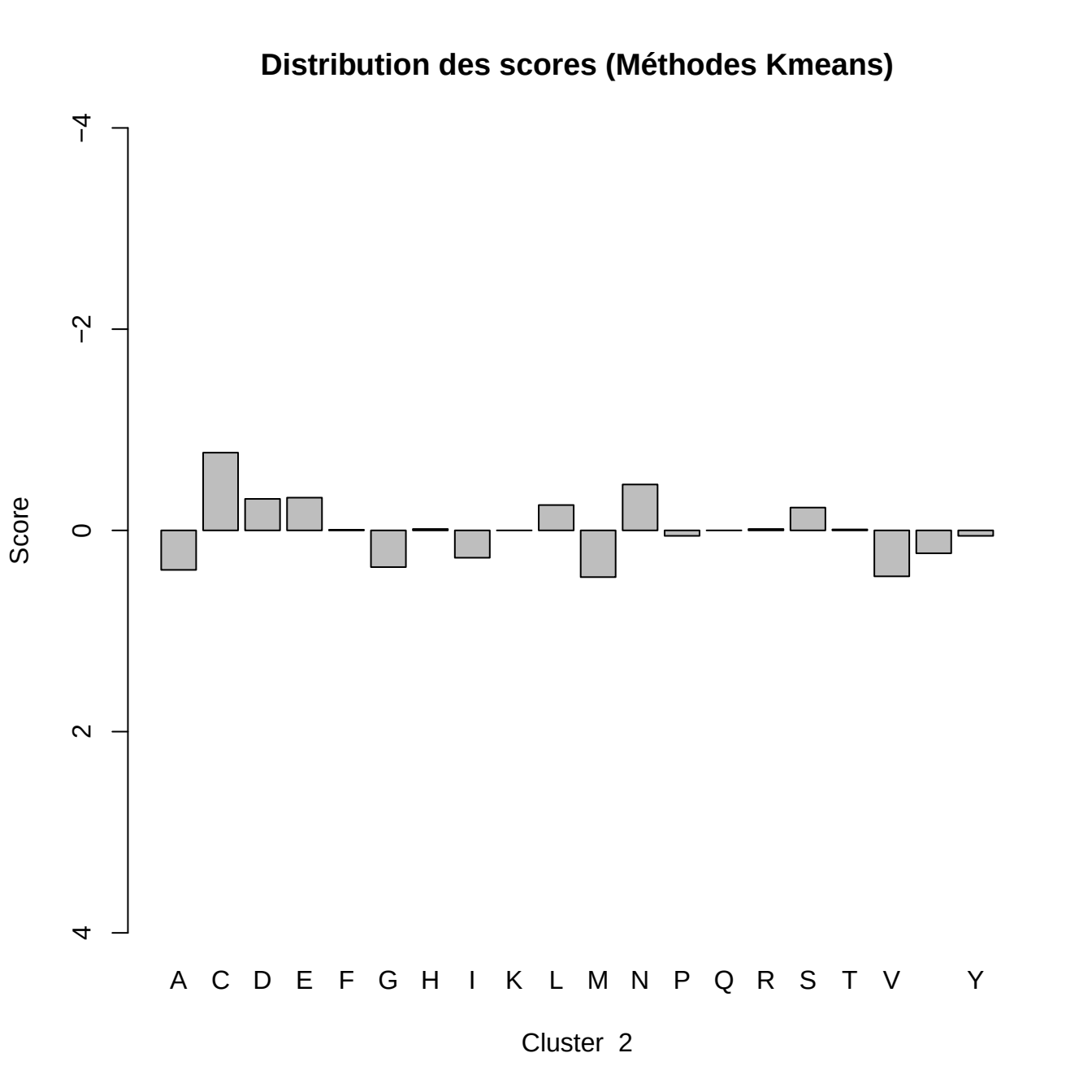

Variables − PCA
ionic
vdw
polar
hydrogenB
hydrophobic
ACC
o_PB
g_PB
c_PB
o_ss.4
l_ss
X._ss
k_PB
H_ss
o_ss.5
o_ss.3
e_PB
o_ss.7
o_ss.2
T_ss
p_PB
l_PB
o_ss.1
o_ss.6
h_PB
E_ss
B_ss
S_ss
o_ss
a_PB
G_ss
m_PB
b_PB
i_PB
f_PB
l_PB
n_PB
d_PB
cos2
0.8
0.6
0.4
0.2
0.0
0.5
0.0
−0.5
Dim2 (13.7%)
0.0
0.3
0.6
0.9
Dim1 (33.6%)

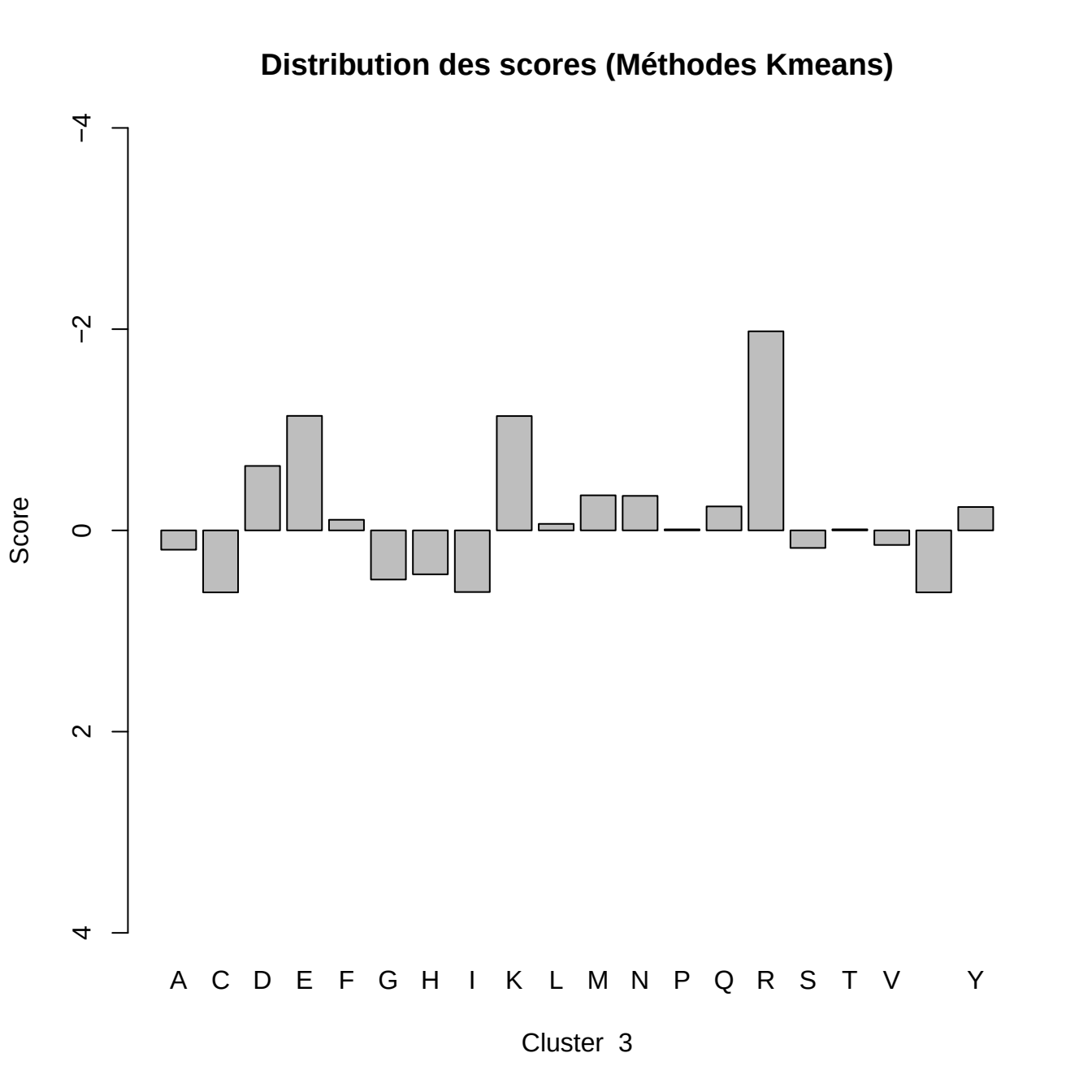

MDS with Shephard−Kruskal Stress 0.6
5
0
−5
−10
Y
−2.5
0.0
2.5
5.0
7.5
X

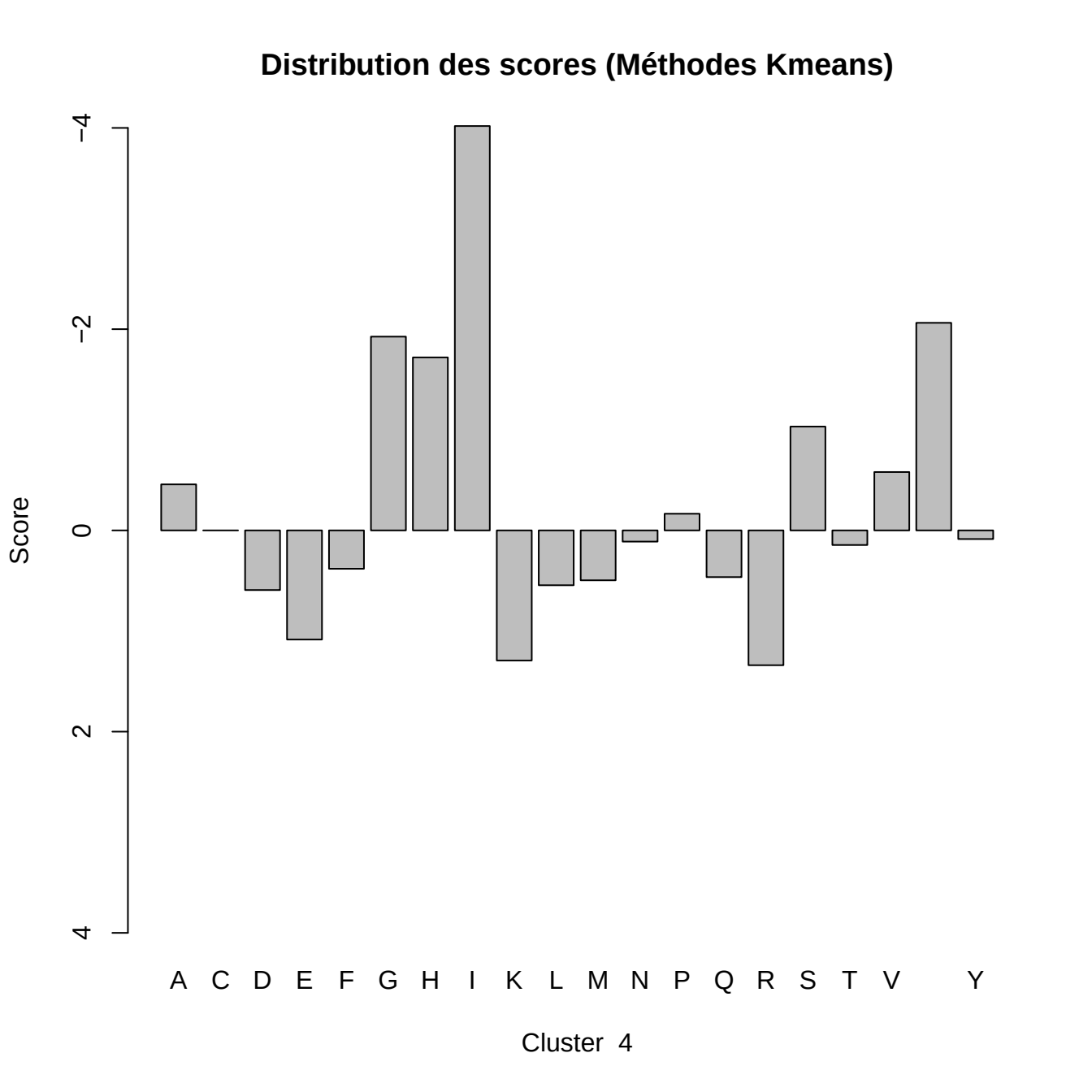

Optimal number of clusters
Total Within Sum of Square
16000
14000
12000
10000
8000
1
2
3
4
5
6
7
8
9
10
Number of clusters k

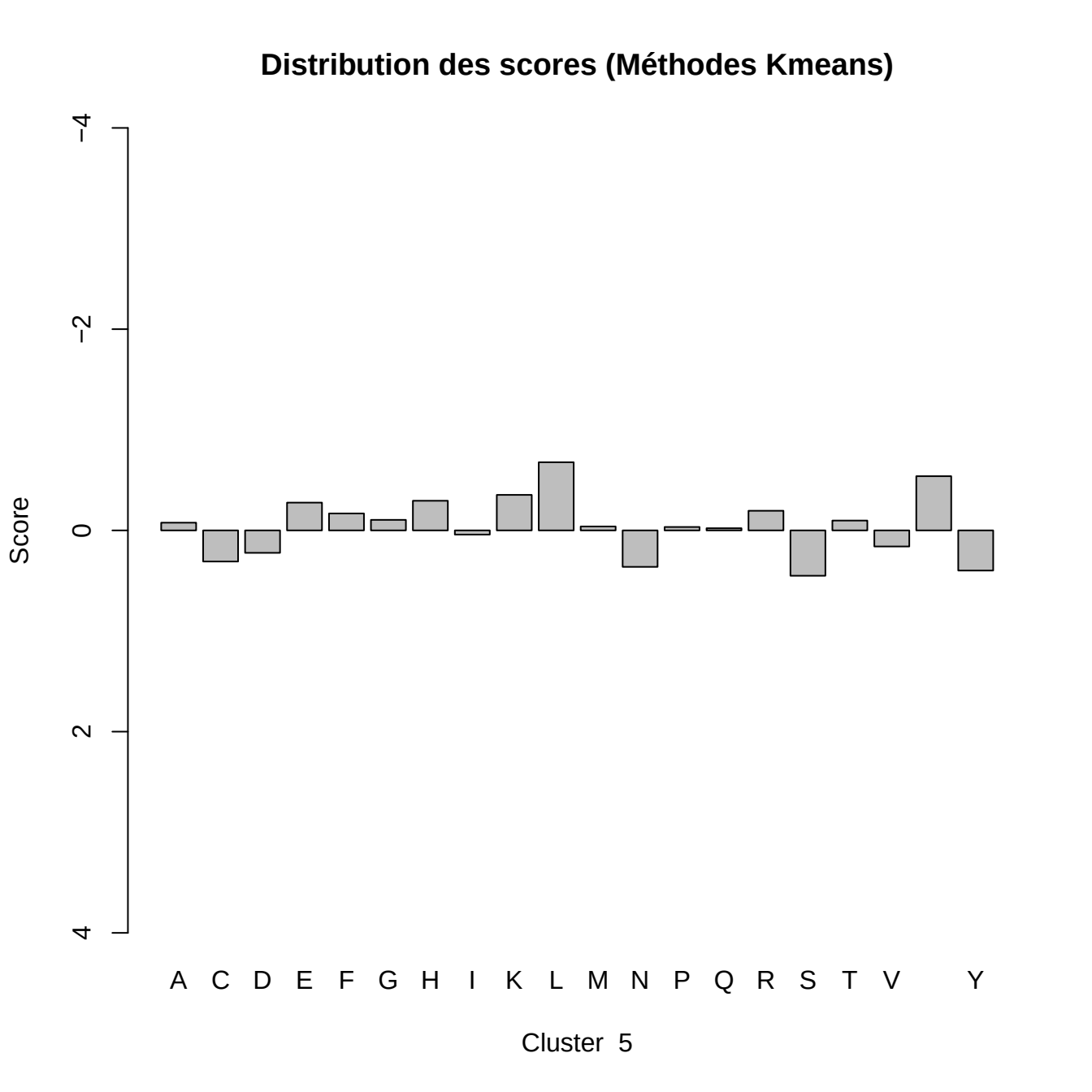

Clustering par Kmeans
PC2
PC1
0.2
0.1
0.0
−0.1
0.00
0.04
0.08
cluster
1
2
3
4
5

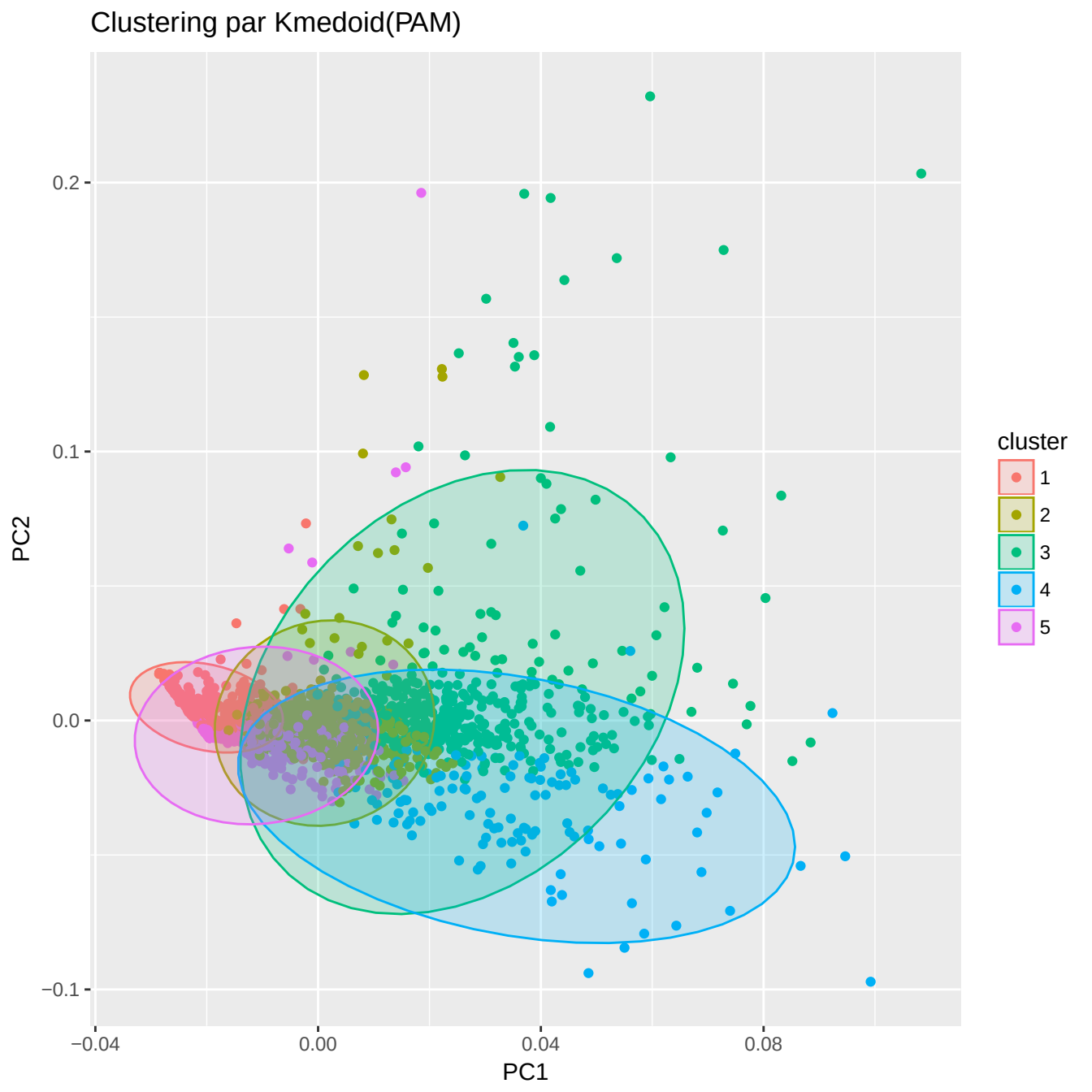

Distribution des scores (Méthodes Kmeans)
Score
−4
−2
0
2
4
A C D E F G H I K L M N P Q R S T V Y
Cluster 1

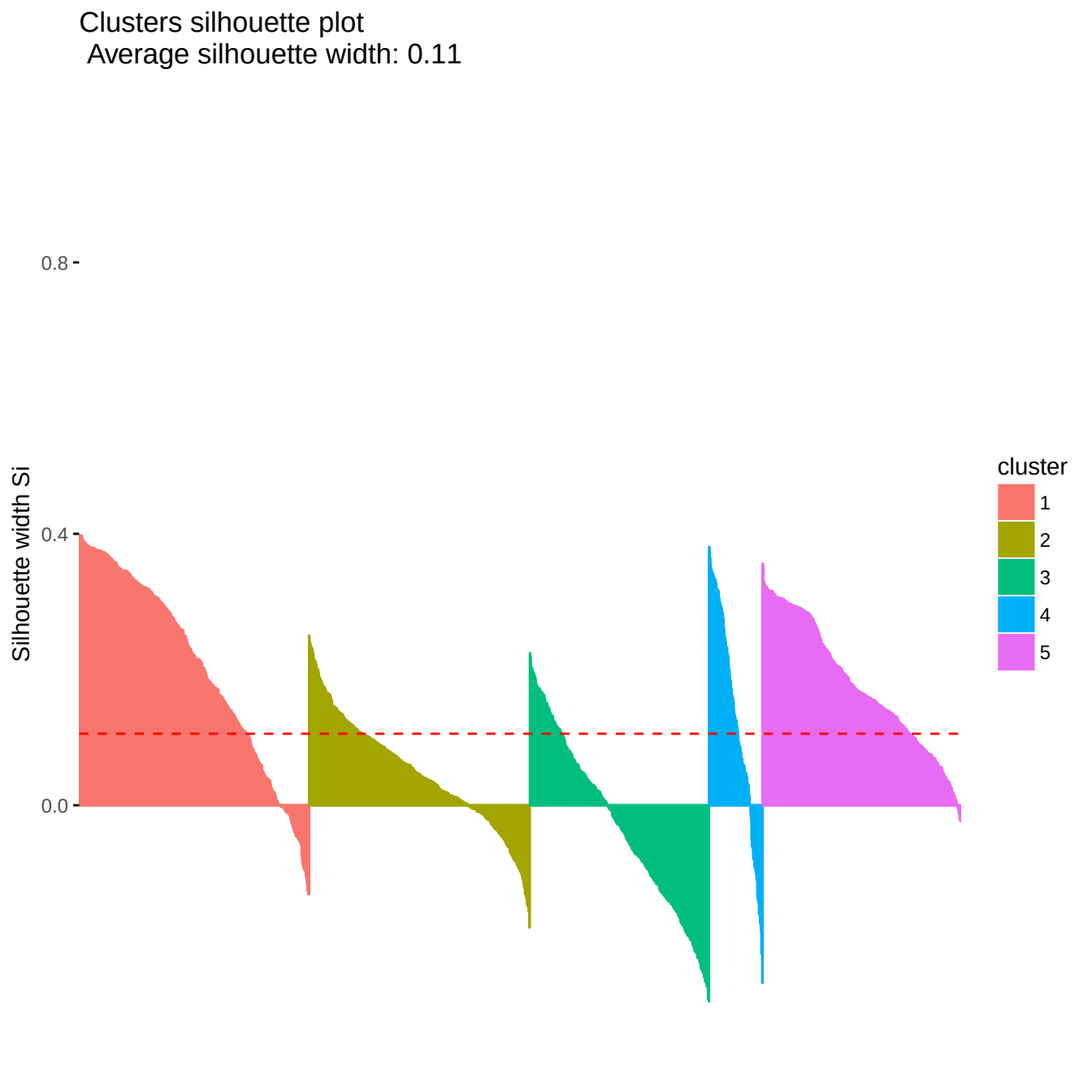

Distribution des scores (Méthodes Kmeans)
Score
−4
−2
0
2
4
A C D E F G H I K L M N P Q R S T V Y
Cluster 2

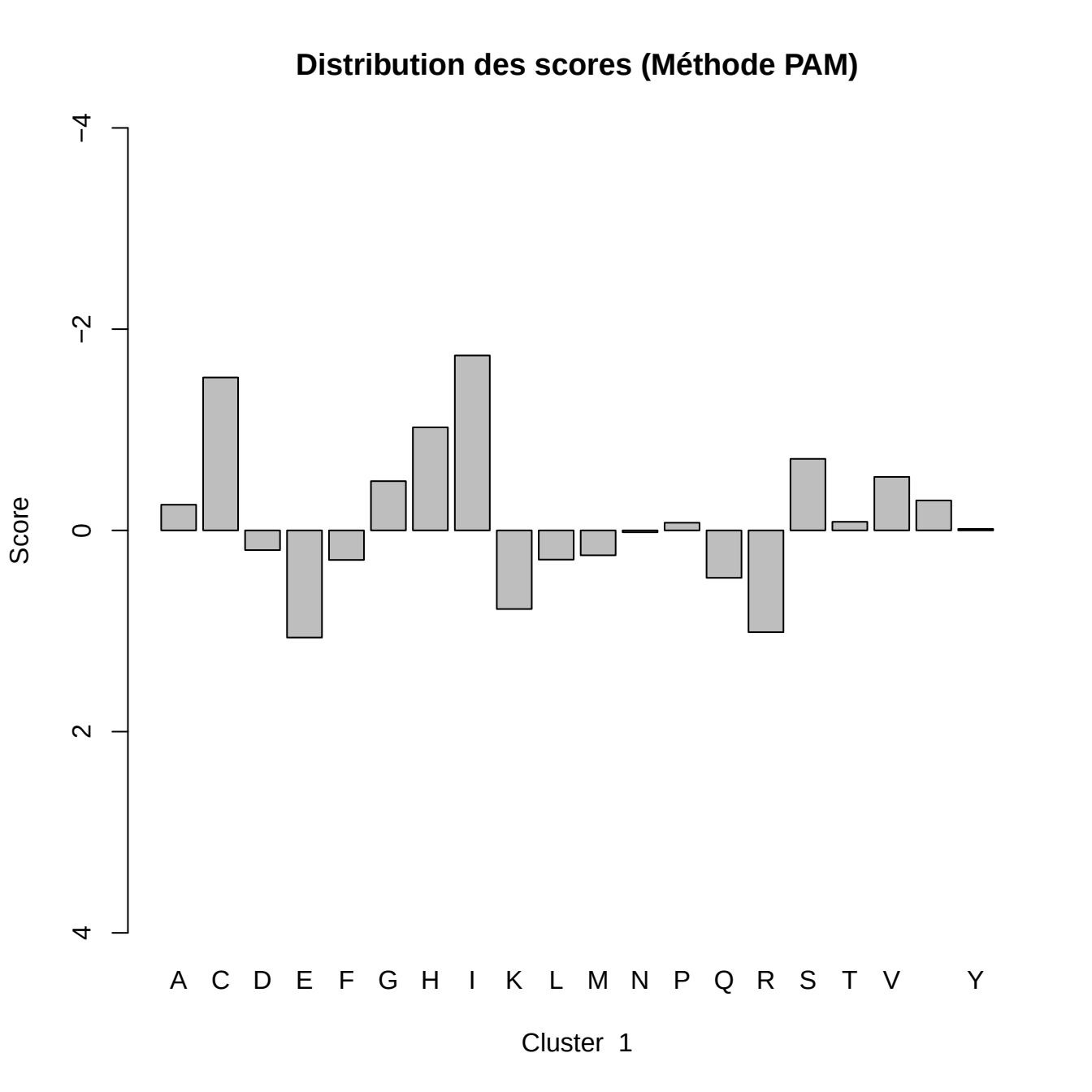

Distribution des scores (Méthodes Kmeans)
Score
−4
−2
0
2
4
A C D E F G H I K L M N P Q R S T V Y
Cluster 3

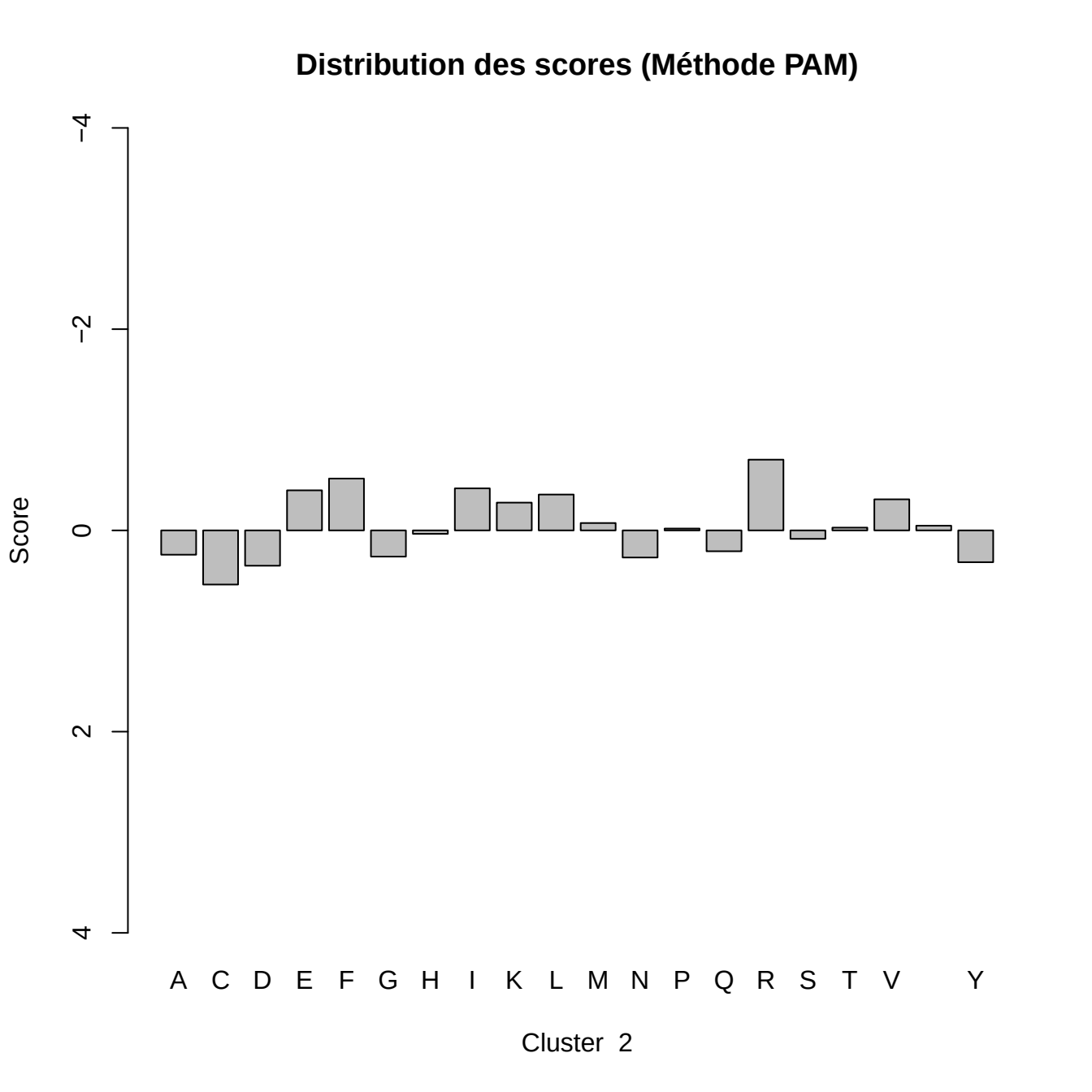

Distribution des scores (Méthodes Kmeans)
Score
−4
−2
0
2
4
A C D E F G H I K L M N P Q R S T V Y
Cluster 4

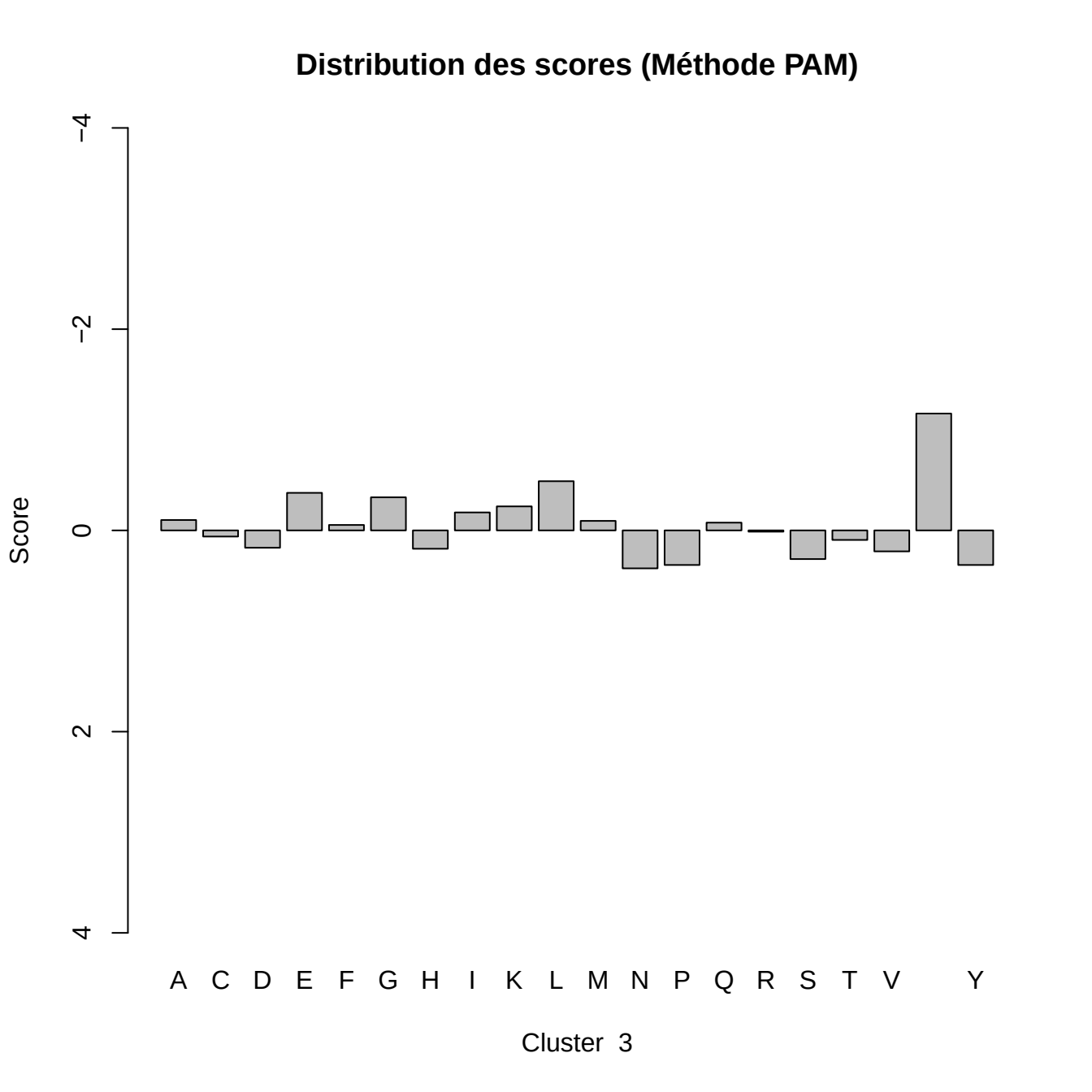

Distribution des scores (Méthodes Kmeans)
Score
−4
−2
0
2
4
A C D E F G H I K L M N P Q R S T V Y
Cluster 5

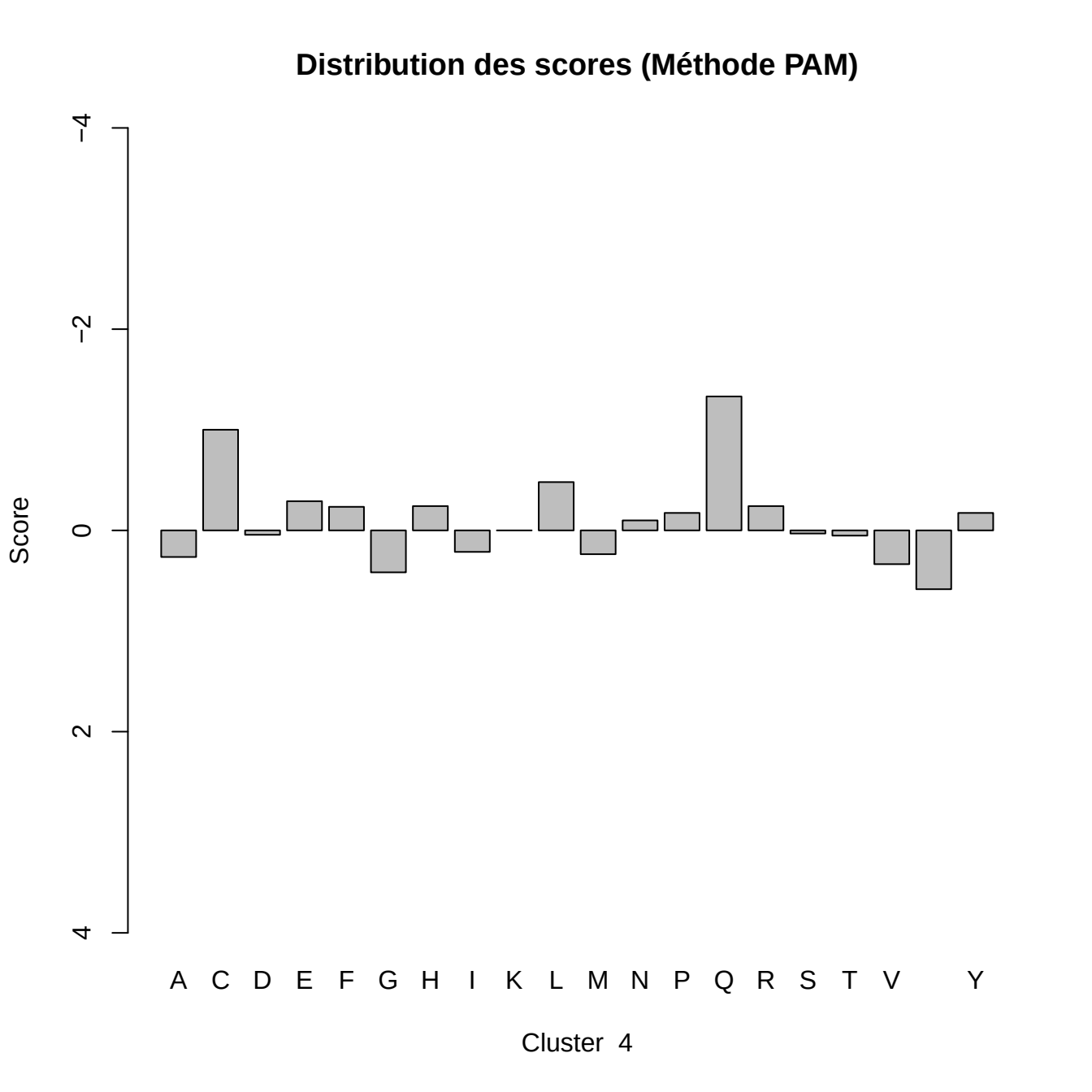

Clustering par Kmedoid(PAM)
PC2
PC1
0.2
0.1
0.0
−0.1
−0.04
0.00
0.04
0.08
cluster
1
2
3
4
5

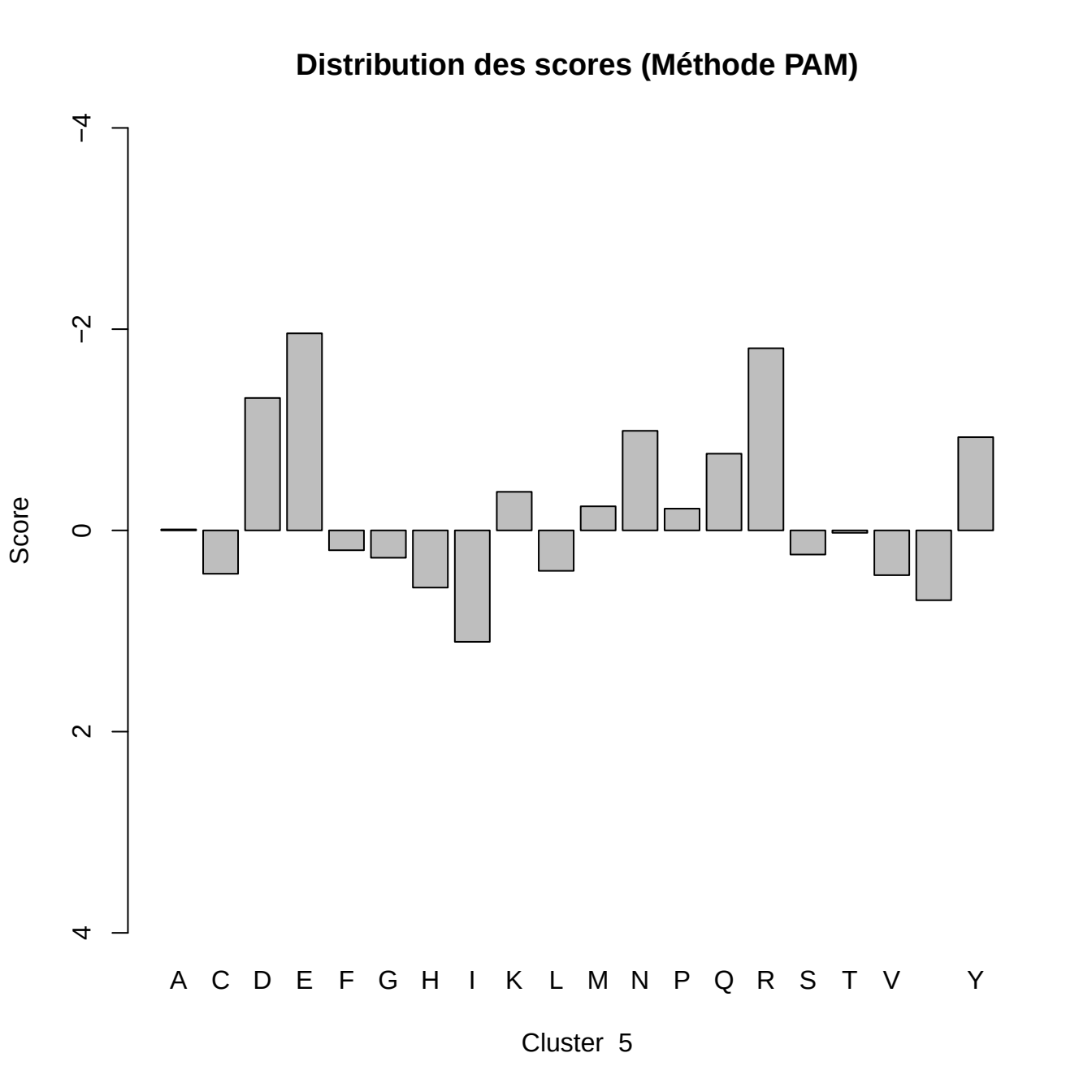

Clusters silhouette plot
Average silhouette width: 0.11
Silhouette width Si
0.8
0.4
0.0
cluster
1
2
3
4
5

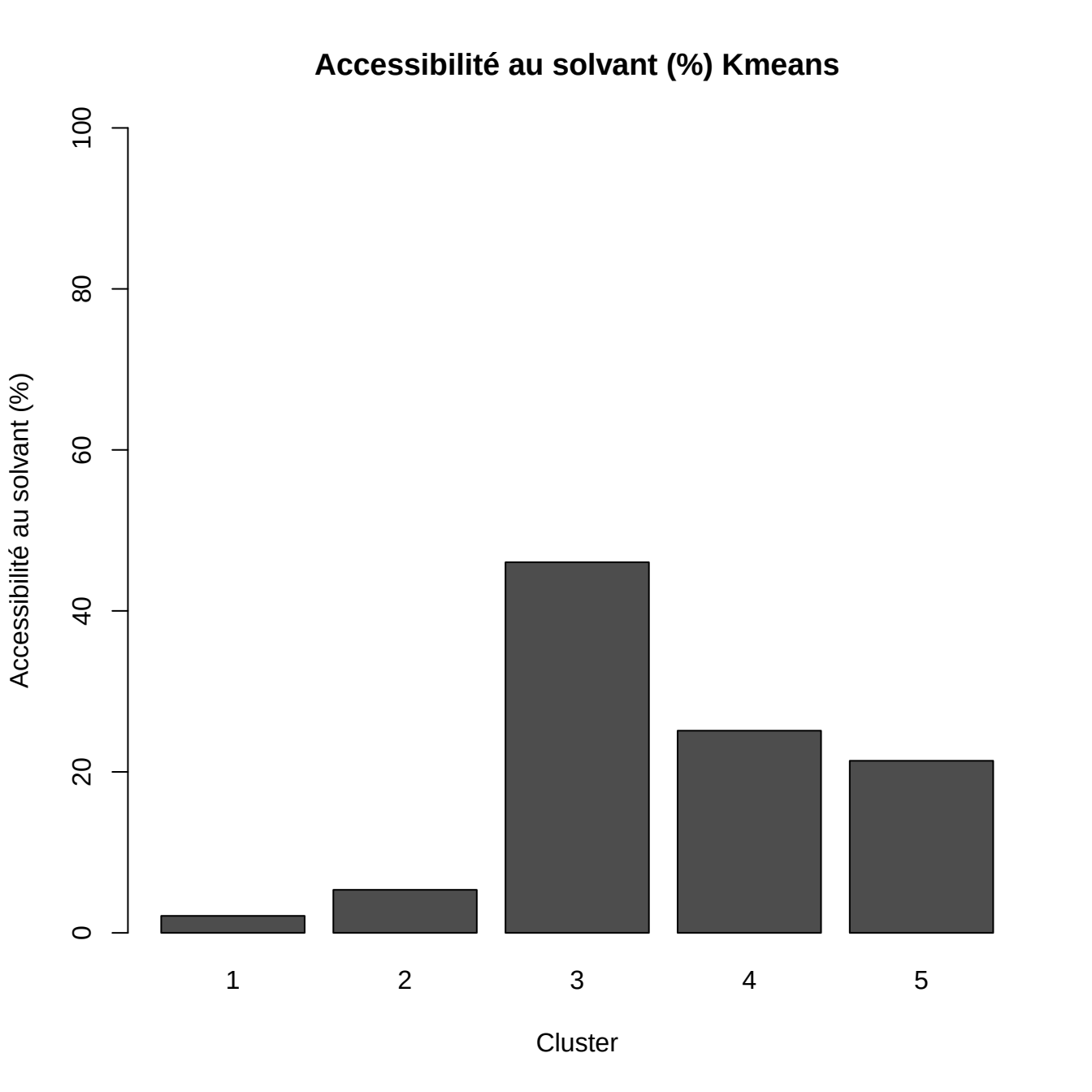

Distribution des scores (Méthode PAM)
Score
−4
−2
0
2
4
A C D E F G H I K L M N P Q R S T V Y
Cluster 1

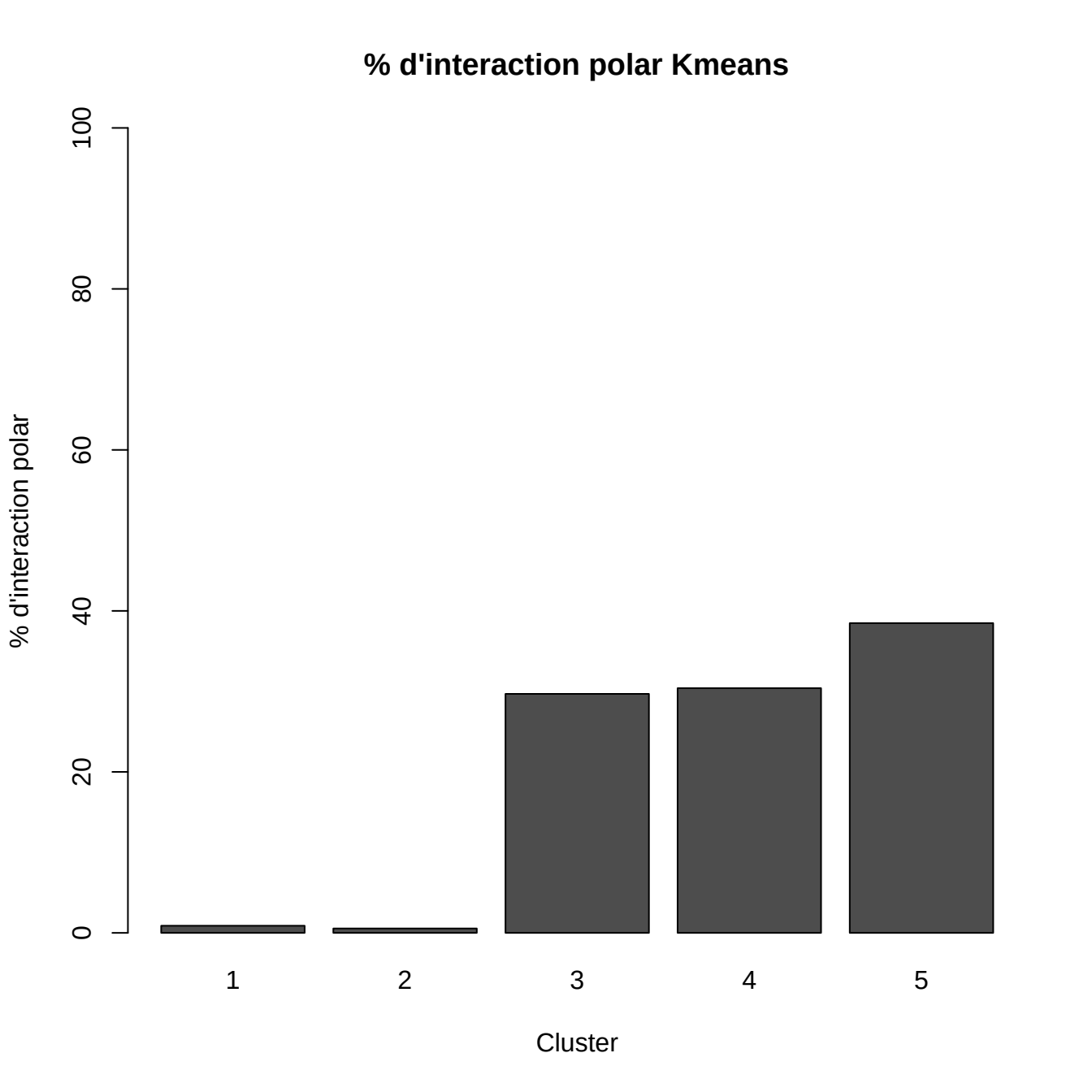

Distribution des scores (Méthode PAM)
Score
−4
−2
0
2
4
A C D E F G H I K L M N P Q R S T V Y
Cluster 2

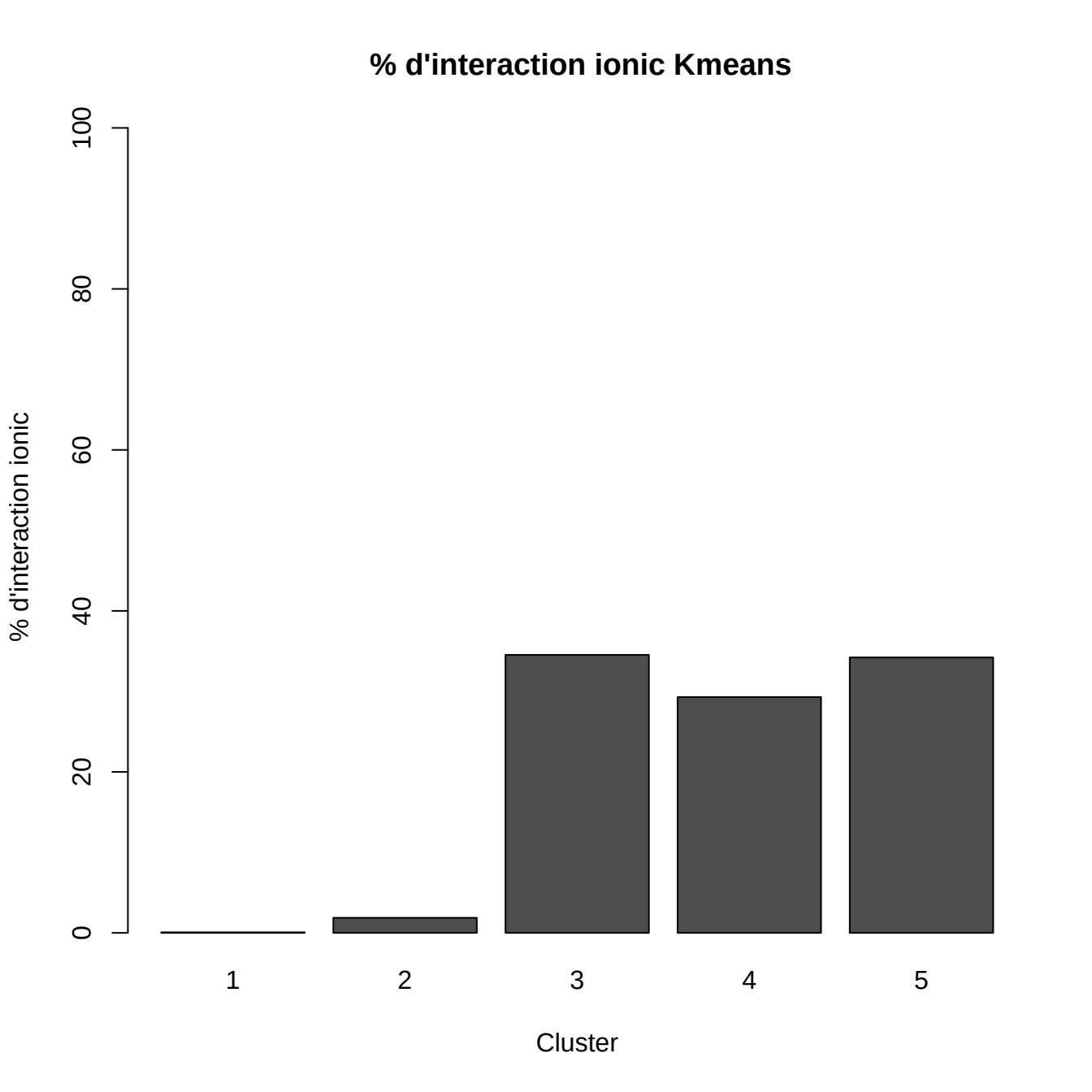

Distribution des scores (Méthode PAM)
Score
−4
−2
0
2
4
A C D E F G H I K L M N P Q R S T V Y
Cluster 3

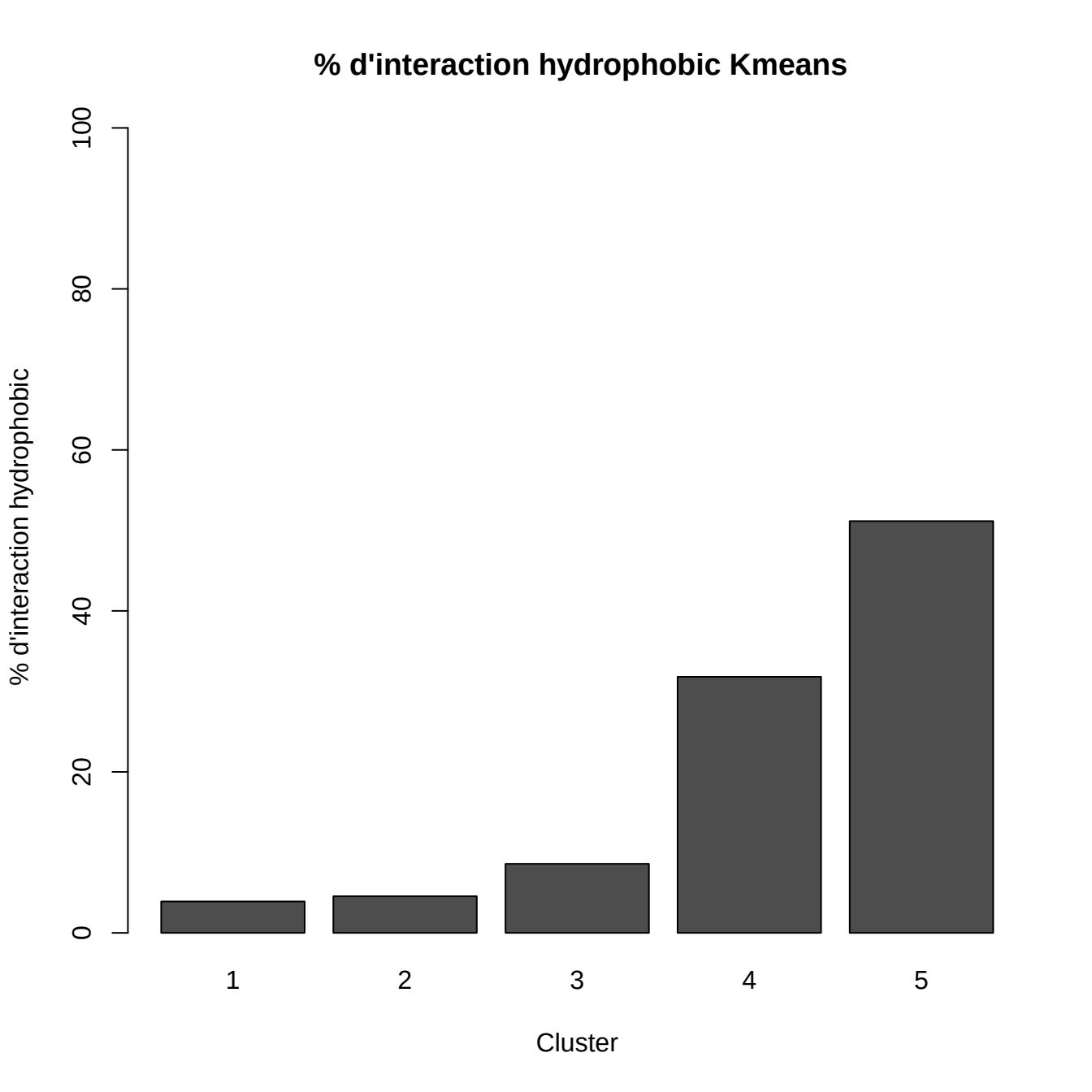

Distribution des scores (Méthode PAM)
Score
−4
−2
0
2
4
A C D E F G H I K L M N P Q R S T V Y
Cluster 4

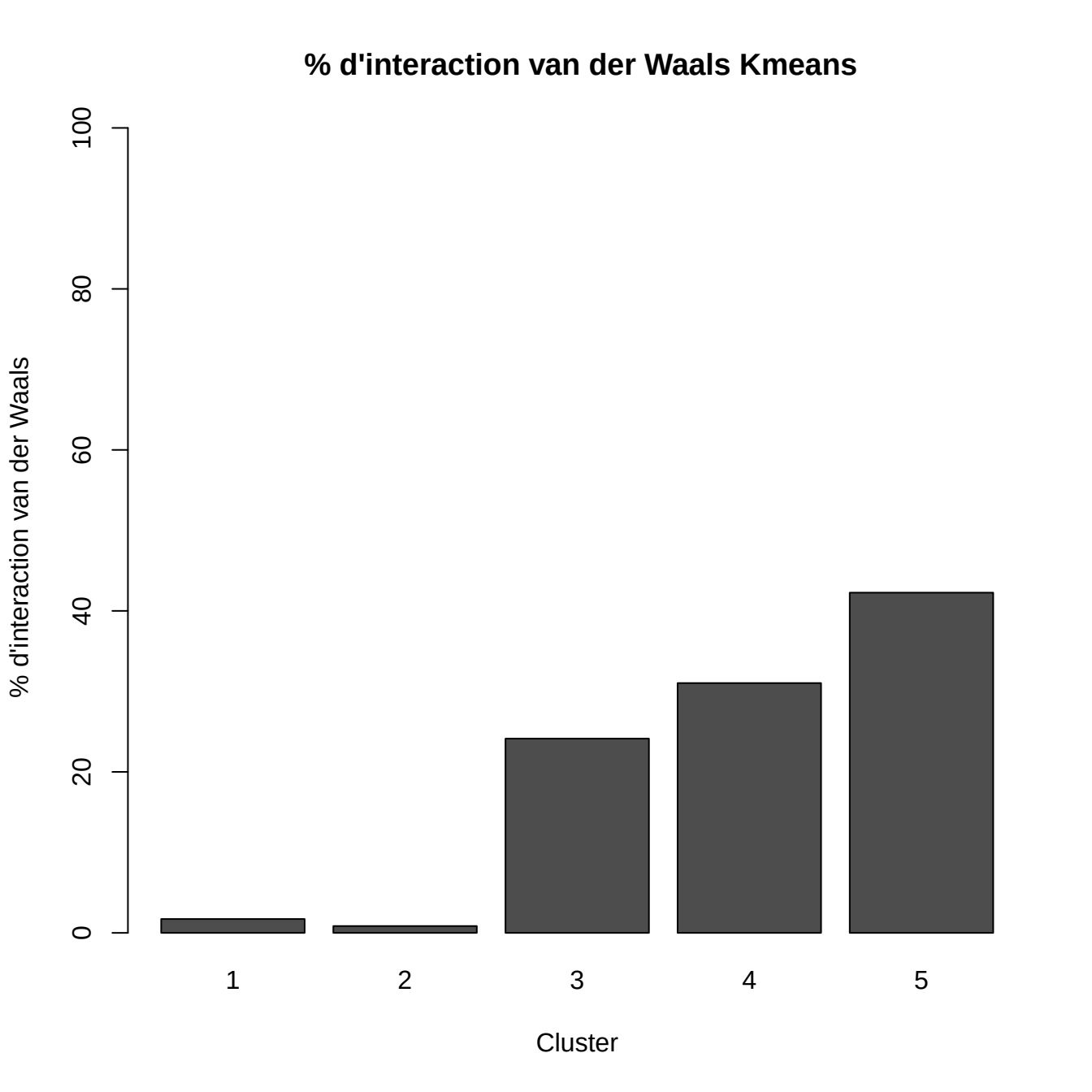

Distribution des scores (Méthode PAM)
Score
−4
−2
0
2
4
A C D E F G H I K L M N P Q R S T V Y
Cluster 5

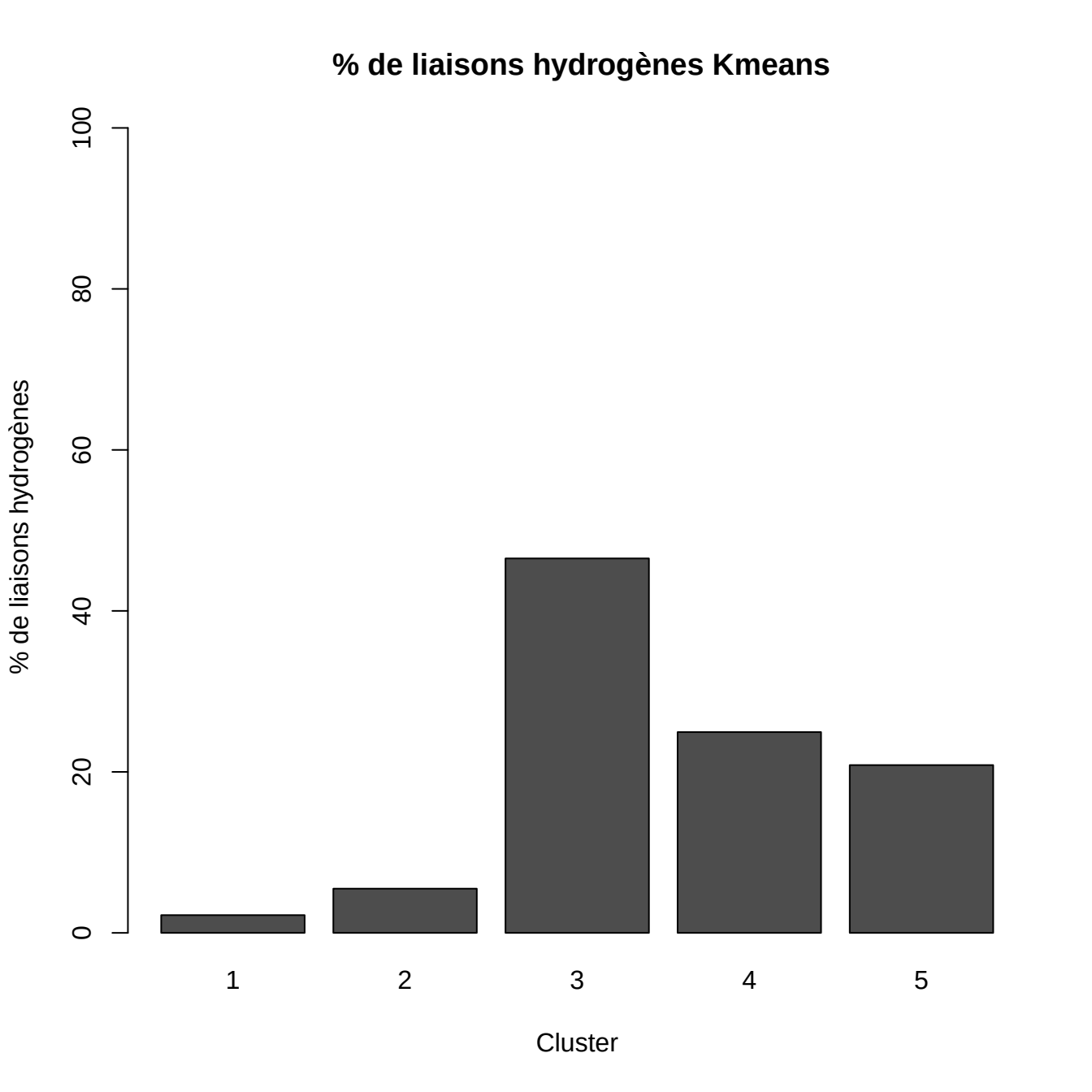

Accessibilité au solvant (%) Kmeans
Accessibilité au solvant (%)
0
20
40
60
80
100
1
2
3
4
5
Cluster

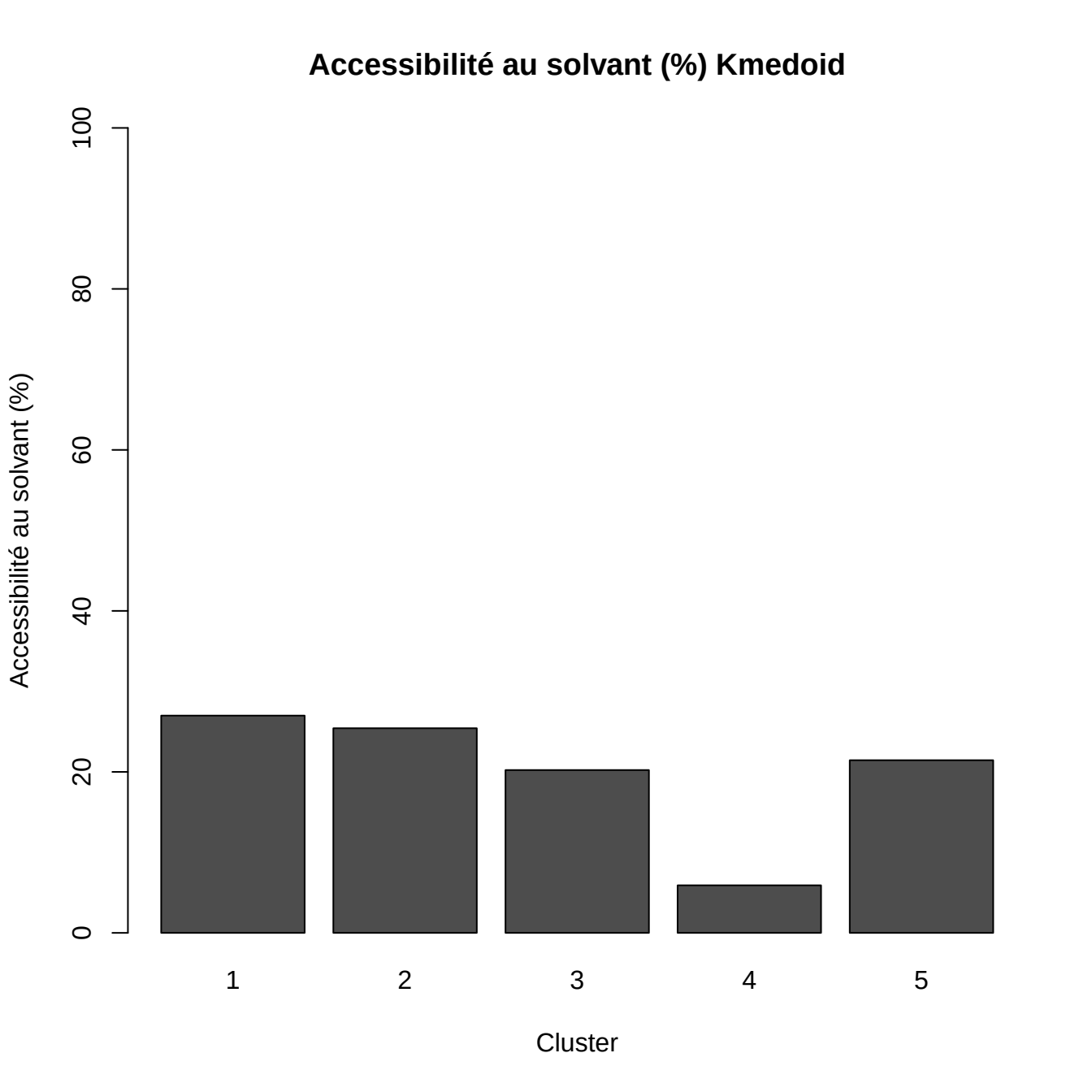

% d'interaction polar Kmeans
% d'interaction polar
0
20
40
60
80
100
1
2
3
4
5
Cluster

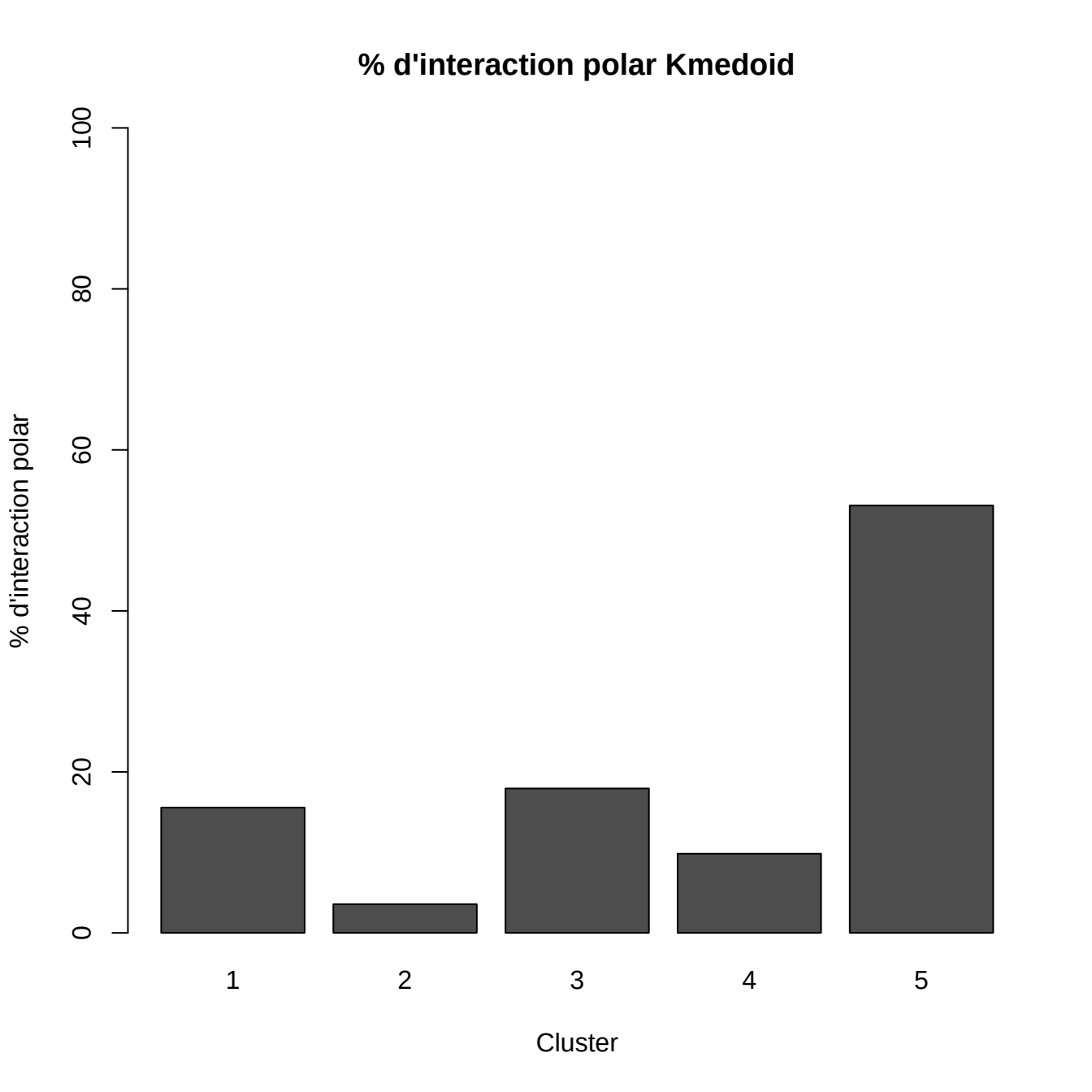

% d'interaction ionic Kmeans
% d'interaction ionic
0
20
40
60
80
100
1
2
3
4
5
Cluster

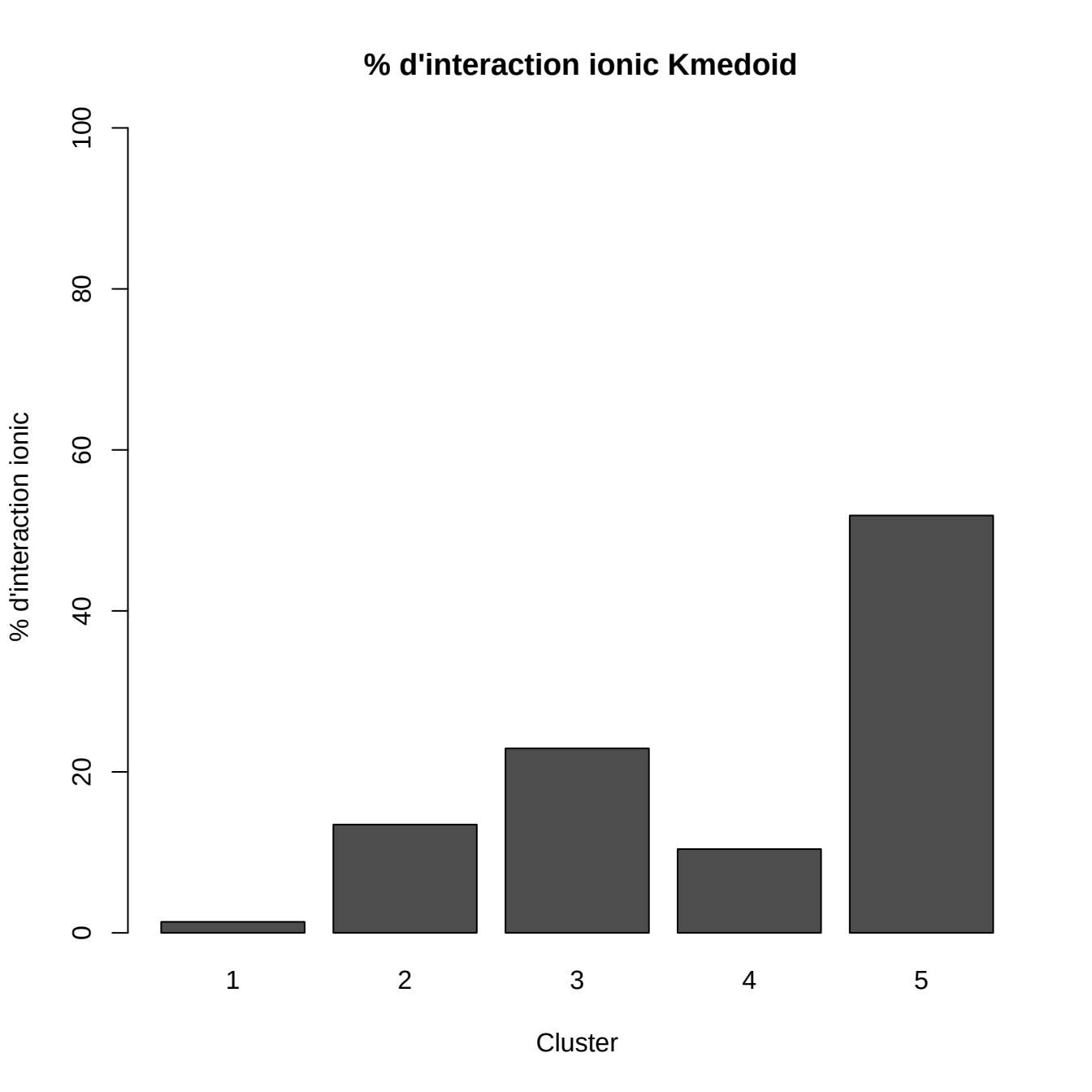

% d'interaction hydrophobic Kmeans
% d'interaction hydrophobic
0
20
40
60
80
100
1
2
3
4
5
Cluster

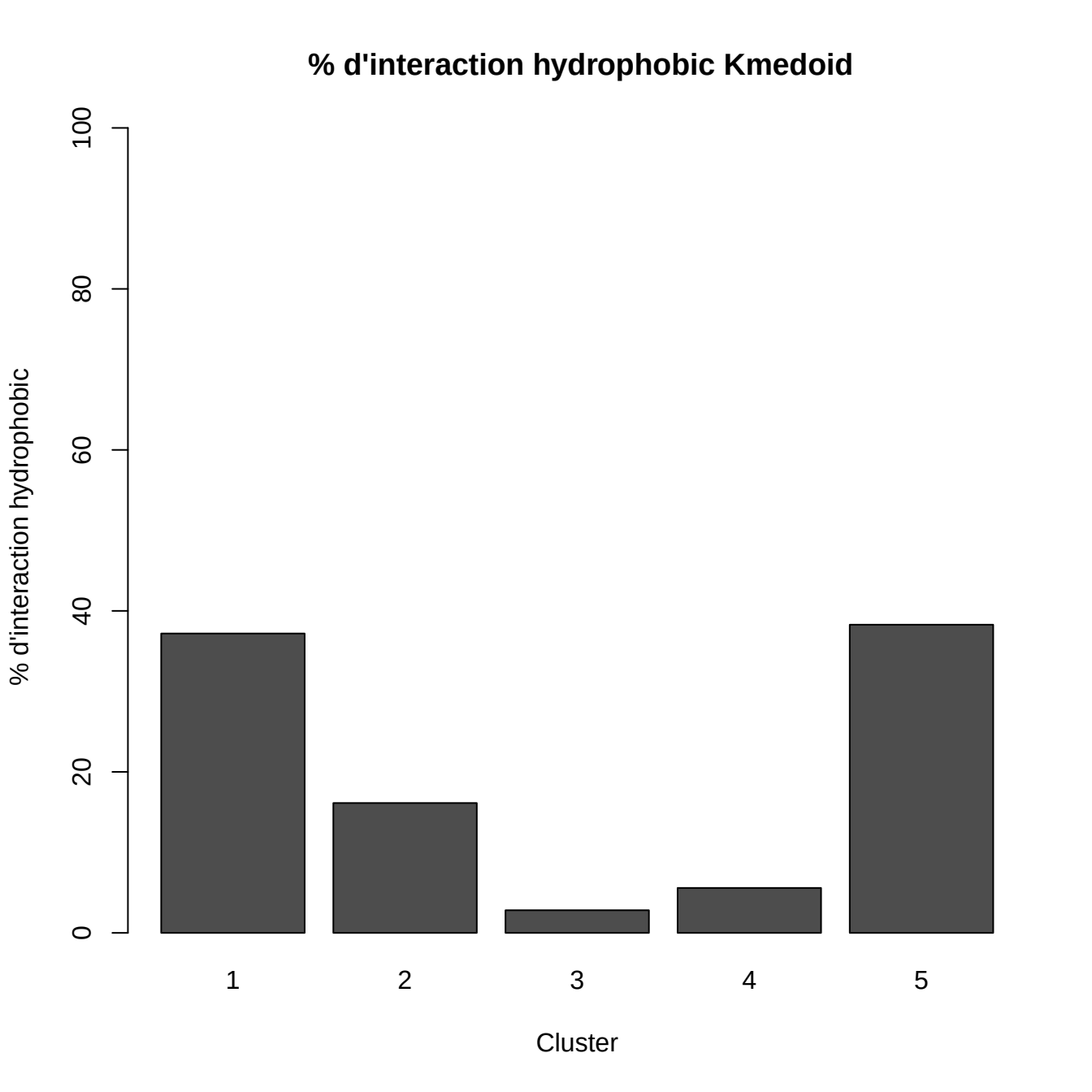

% d'interaction van der Waals Kmeans
% d'interaction van der Waals
0
20
40
60
80
100
1
2
3
4
5
Cluster

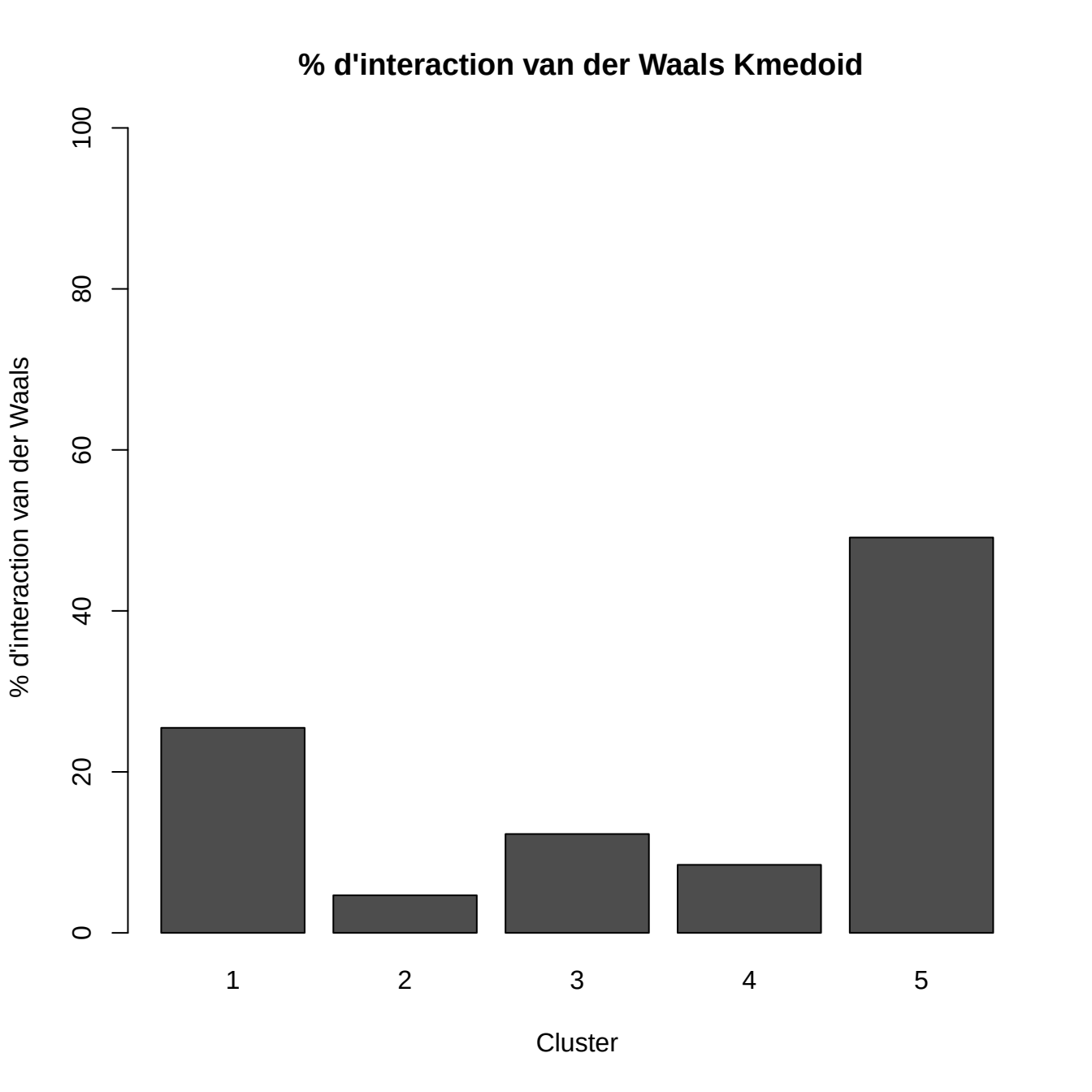

% de liaisons hydrogènes Kmeans
% de liaisons hydrogènes
0
20
40
60
80
100
1
2
3
4
5
Cluster

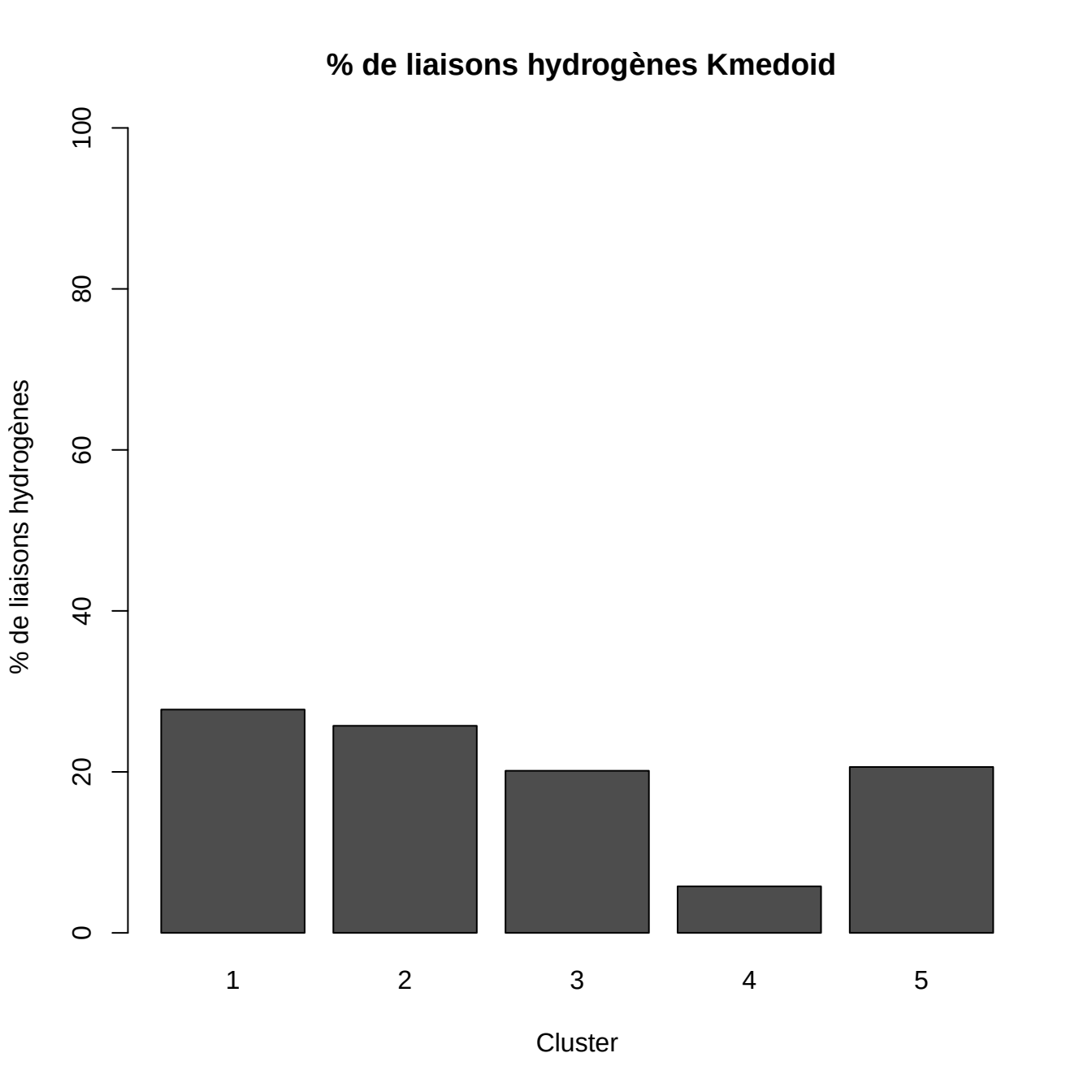

Accessibilité au solvant (%) Kmedoid
Accessibilité au solvant (%)
0
20
40
60
80
100
1
2
3
4
5
Cluster

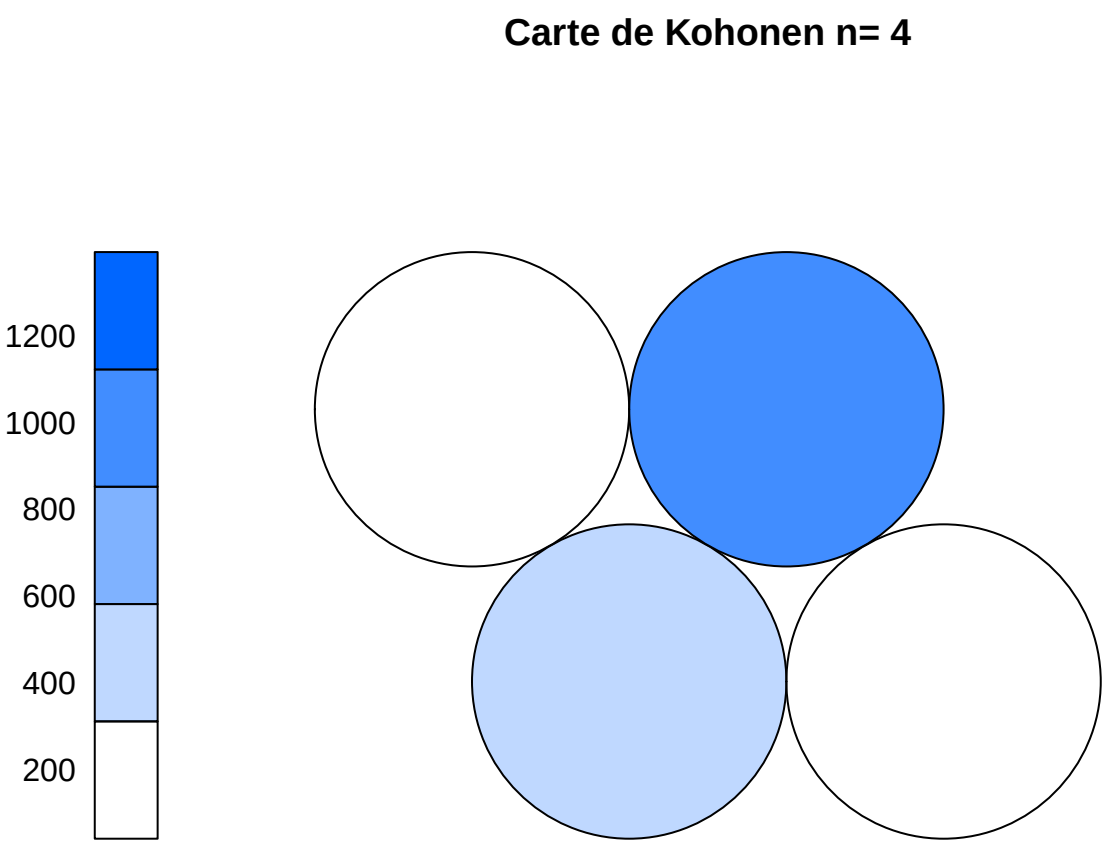

% d'interaction polar Kmedoid
% d'interaction polar
0
20
40
60
80
100
1
2
3
4
5
Cluster

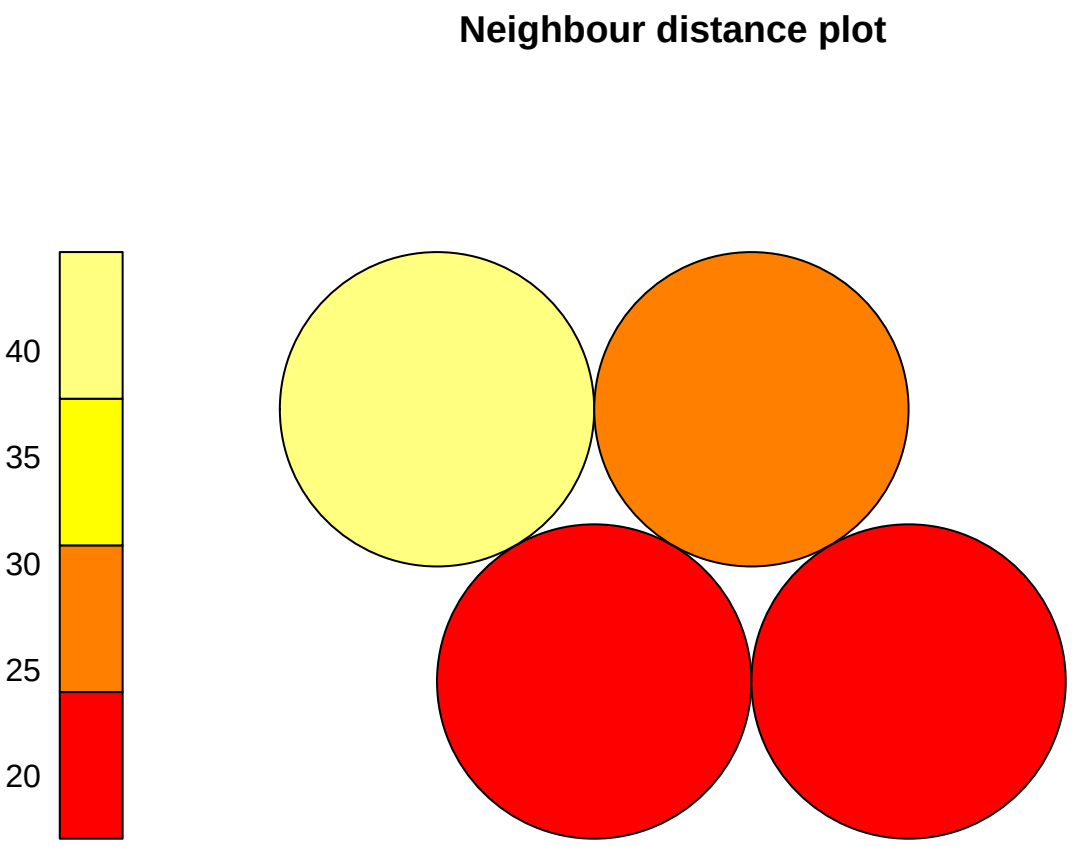

% d'interaction ionic Kmedoid
% d'interaction ionic
0
20
40
60
80
100
1
2
3
4
5
Cluster


% d'interaction hydrophobic Kmedoid
% d'interaction hydrophobic
0
20
40
60
80
100
1
2
3
4
5
Cluster

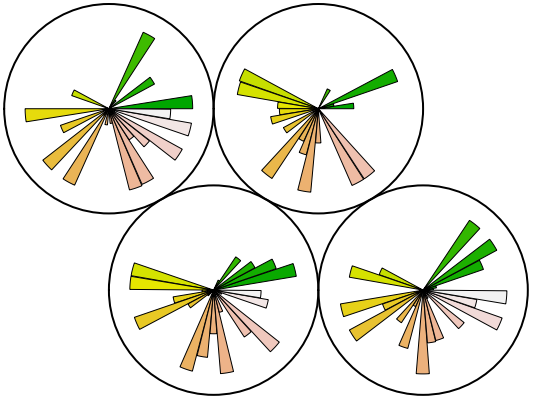

% d'interaction van der Waals Kmedoid
% d'interaction van der Waals
0
20
40
60
80
100
1
2
3
4
5
Cluster

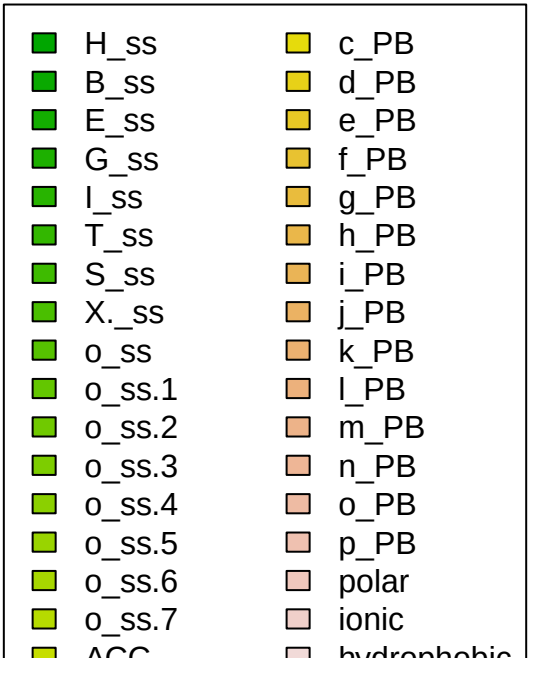

% de liaisons hydrogènes Kmedoid
% de liaisons hydrogènes
0
20
40
60
80
100
1
2
3
4
5
Cluster

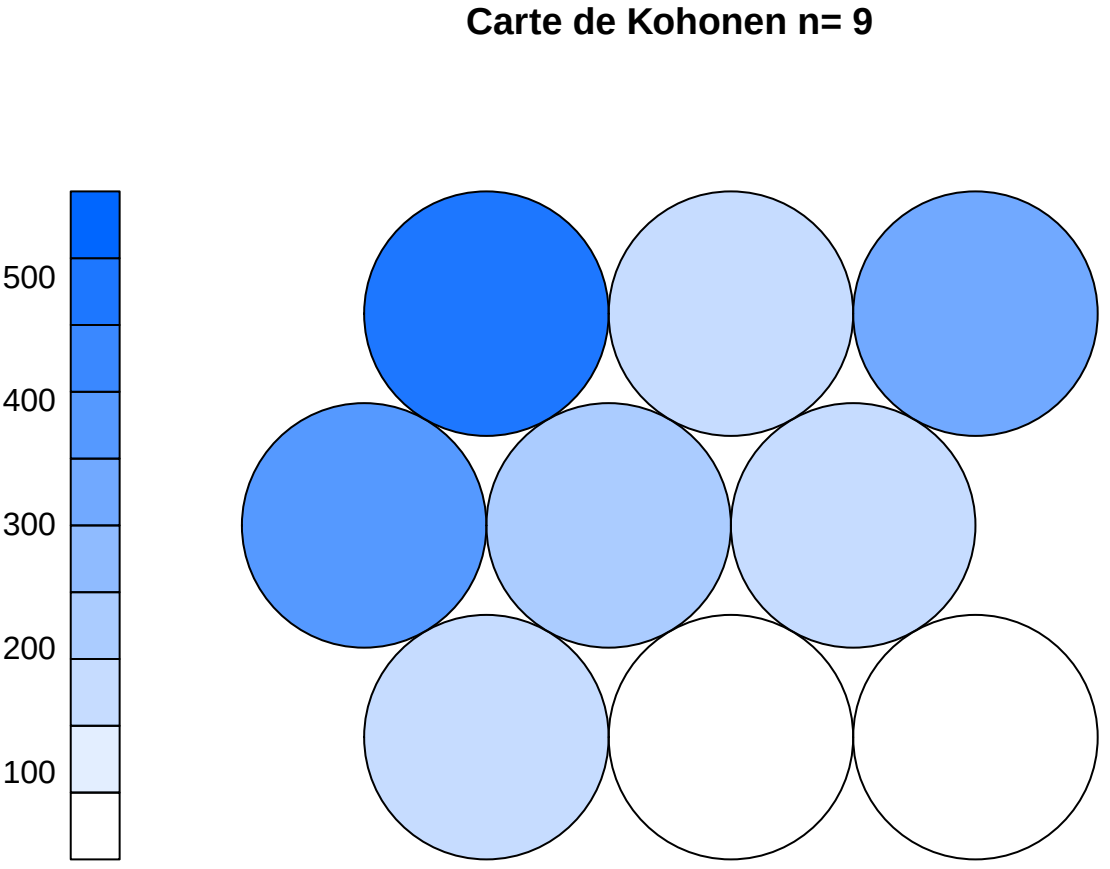

Carte de Kohonen n= 4
1200
1000
800
600
400
200


Neighbour distance plot
40
35
30
25
20

Codes plot



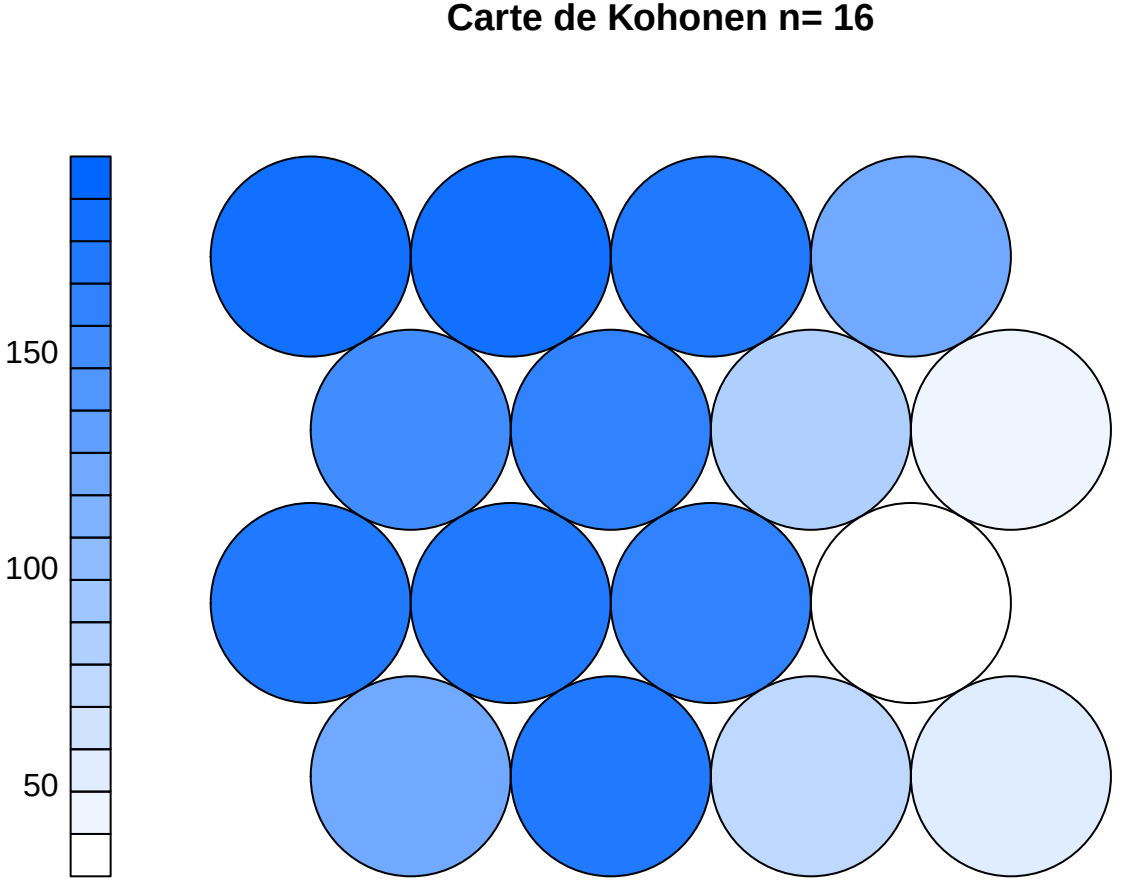

H_ss
B_ss
E_ss
G_ss
I_ss
T_ss
S_ss
X._ss
o_ss
o_ss.1
o_ss.2
o_ss.3
o_ss.4
o_ss.5
o_ss.6
o_ss.7
c_PB
d_PB
e_PB
f_PB
g_PB
h_PB
i_PB
j_PB
k_PB
l_PB
m_PB
n_PB
o_PB
p_PB
polar
ionic

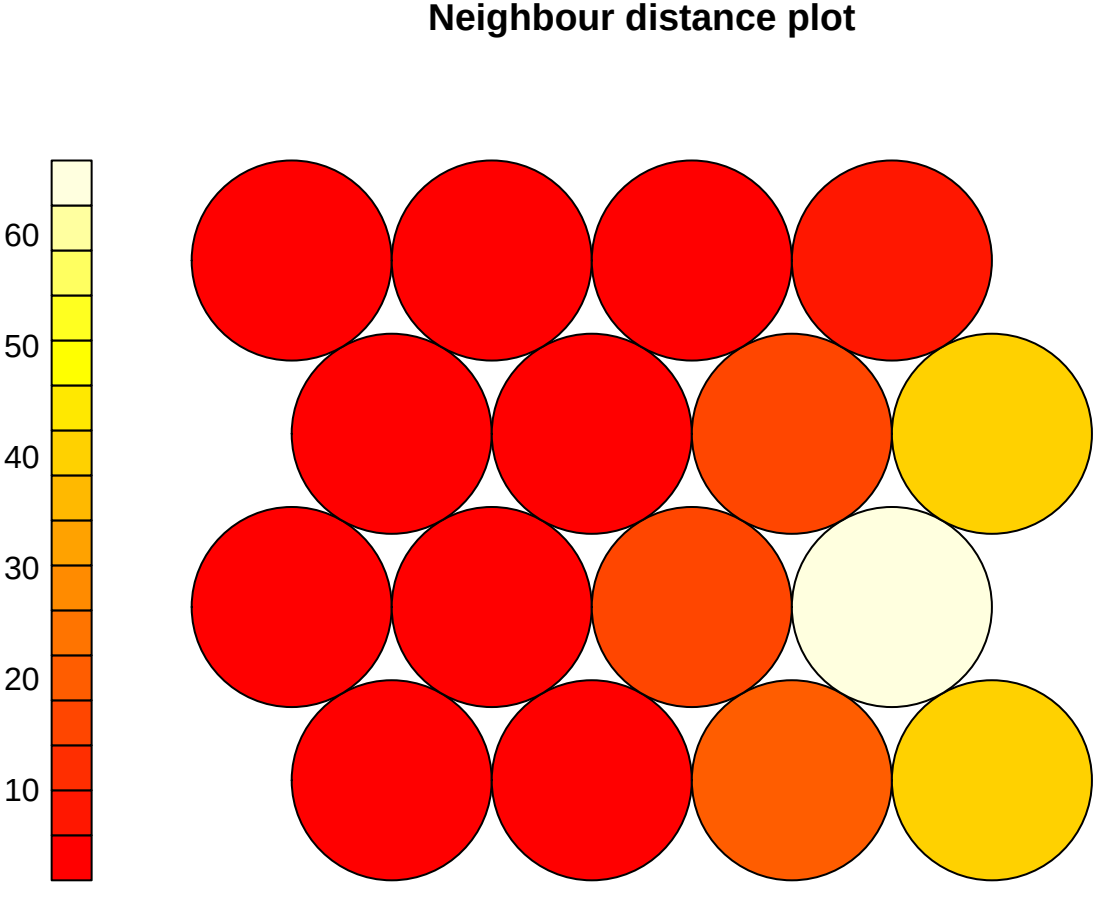

Carte de Kohonen n= 9
500
400
300
200
100


Neighbour distance plot
70
60
50
40
30
20
10

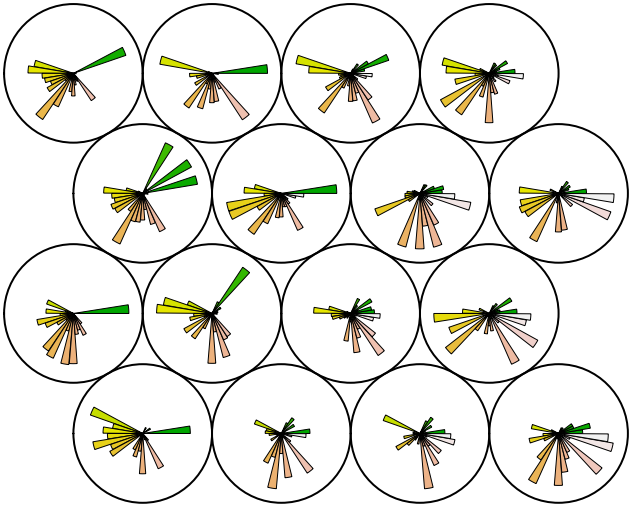
Codes plot

- H_ss
- B_ss
- E_ss
- G_ss
- I_ss
- T_ss
- S_ss
- X._ss
- o_ss
- o_ss.1
- o_ss.2
- o_ss.3
- o_ss.4
- o_ss.5
- o_ss.6
- o_ss.7
- c_PB
- d_PB
- e_PB
- f_PB
- g_PB
- h_PB
- i_PB
- j_PB
- k_PB
- l_PB
- m_PB
- n_PB
- o_PB
- p_PB
- polar
- ionic

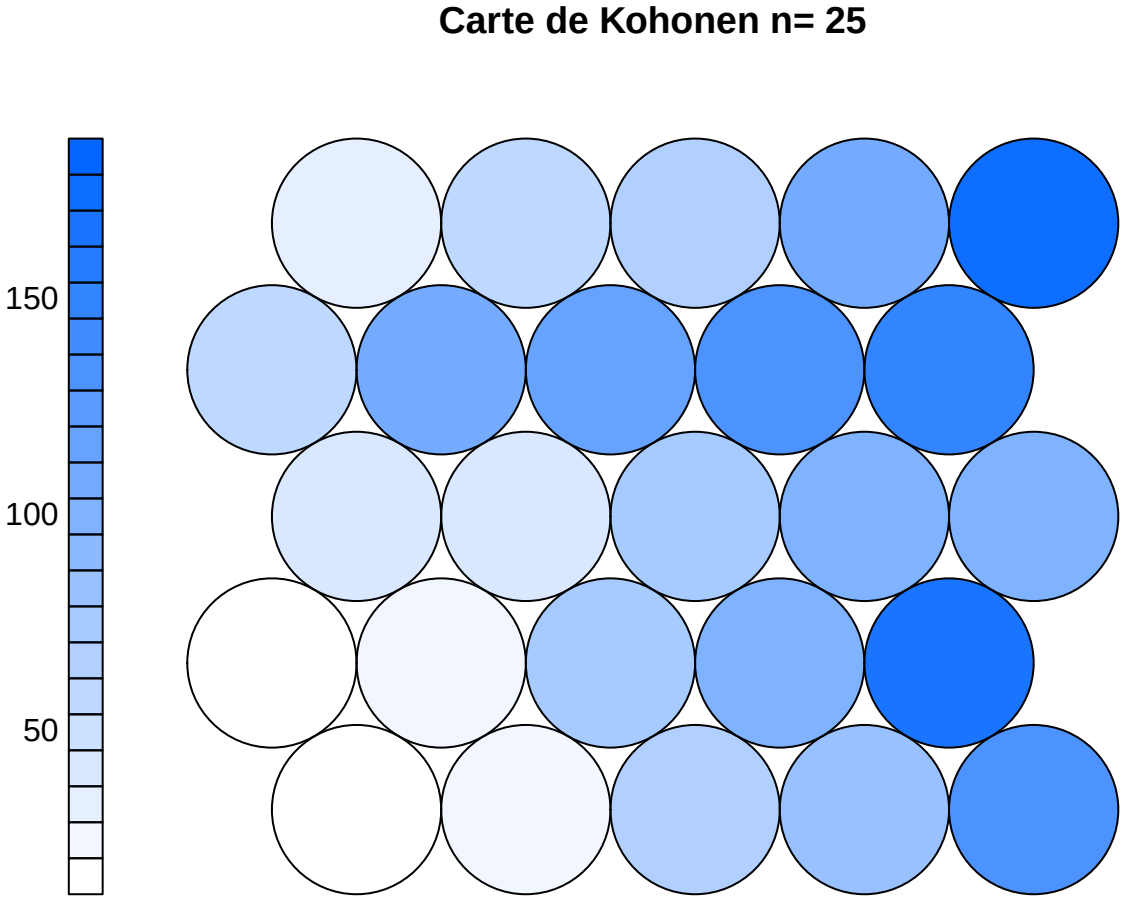

Carte de Kohonen n= 16
150
100
50

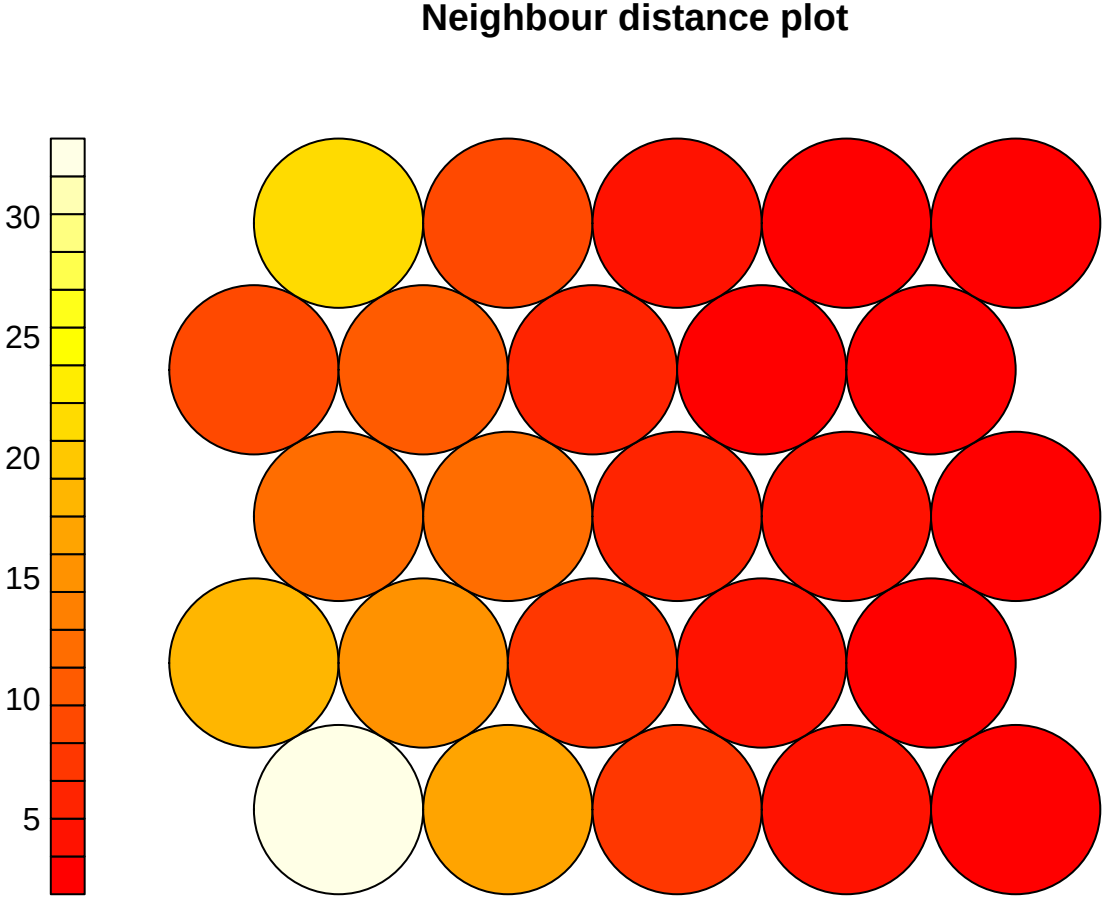

Neighbour distance plot
60
50
40
30
20
10

Codes plot

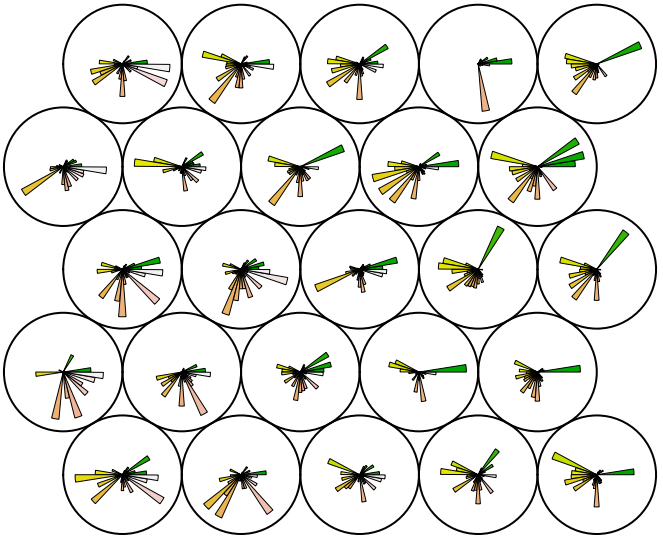


H_ss
B_ss
E_ss
G_ss
I_ss
T_ss
S_ss
X._ss
o_ss
o_ss.1
o_ss.2
o_ss.3
o_ss.4
o_ss.5
o_ss.6
c_PB
d_PB
e_PB
f_PB
g_PB
h_PB
i_PB
j_PB
k_PB
l_PB
m_PB
n_PB
o_PB
p_PB
polar

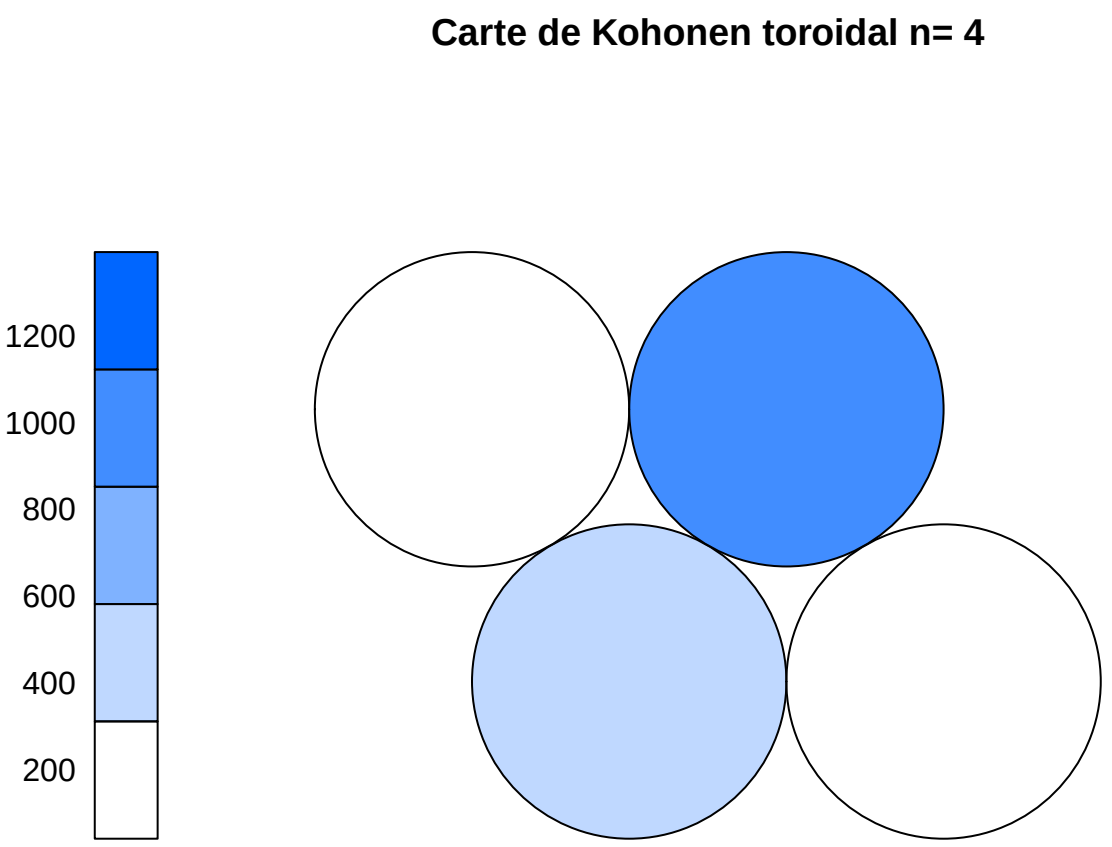

Carte de Kohonen n= 25
150
100
50

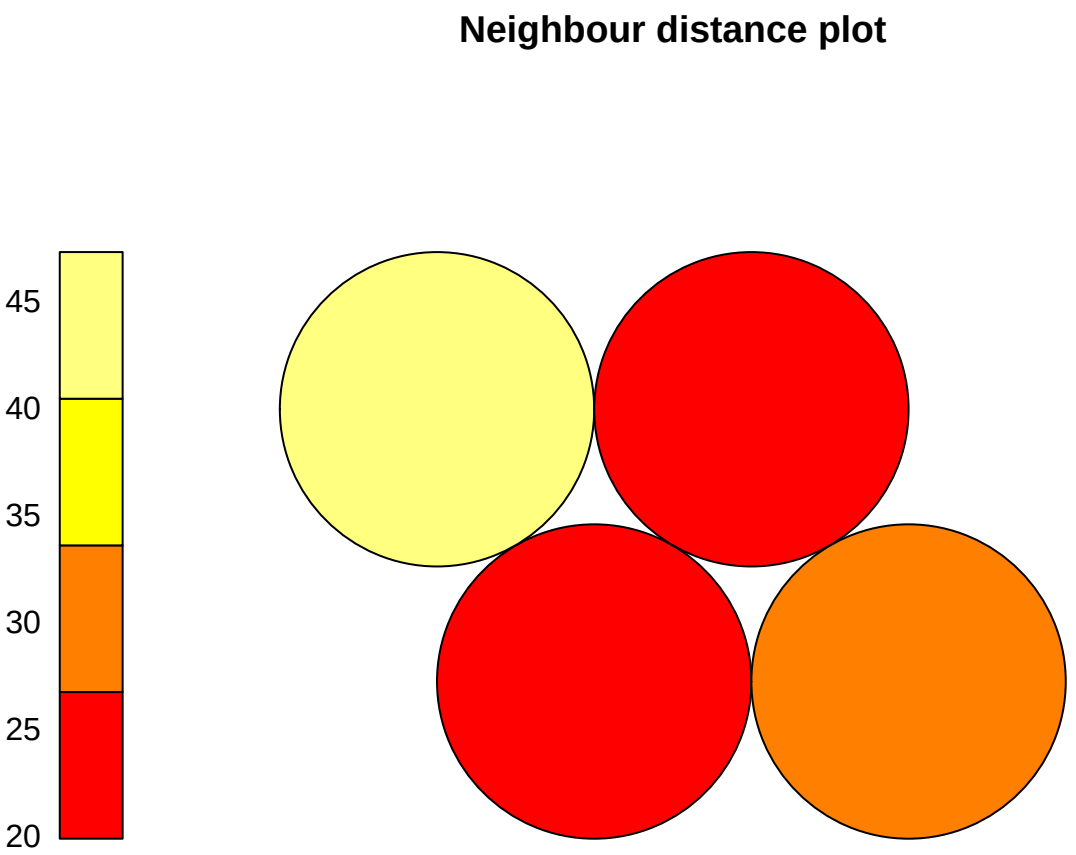

Neighbour distance plot
30
25
20
15
10
5

Codes plot

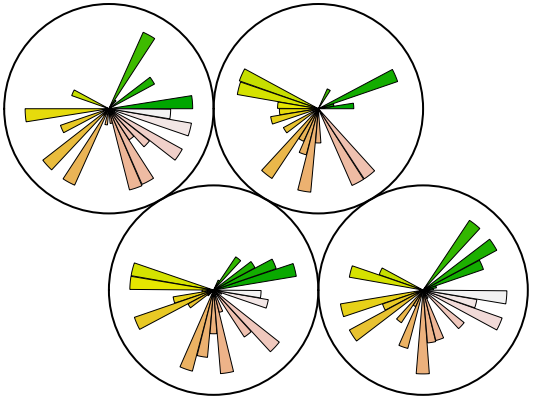


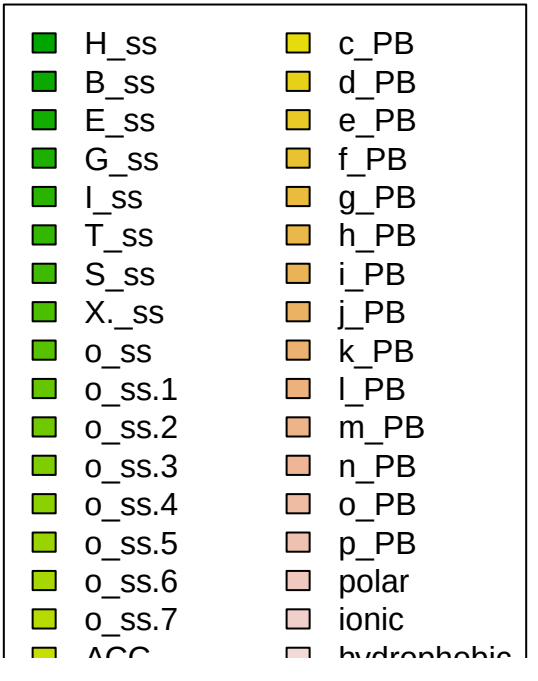
H_ss	c_PB
B_ss	d_PB
E_ss	e_PB
G_ss	f_PB
I_ss	g_PB
T_ss	h_PB
S_ss	i_PB
X._ss	j_PB
o_ss	k_PB
o_ss.1	l_PB
o_ss.2	m_PB
o_ss.3	n_PB
o_ss.4	o_PB
o_ss.5	p_PB
o_ss.6	polar


Carte de Kohonen toroidal n= 4
1200
1000
800
600
400
200


Neighbour distance plot
45
40
35
30
25
20

Codes plot

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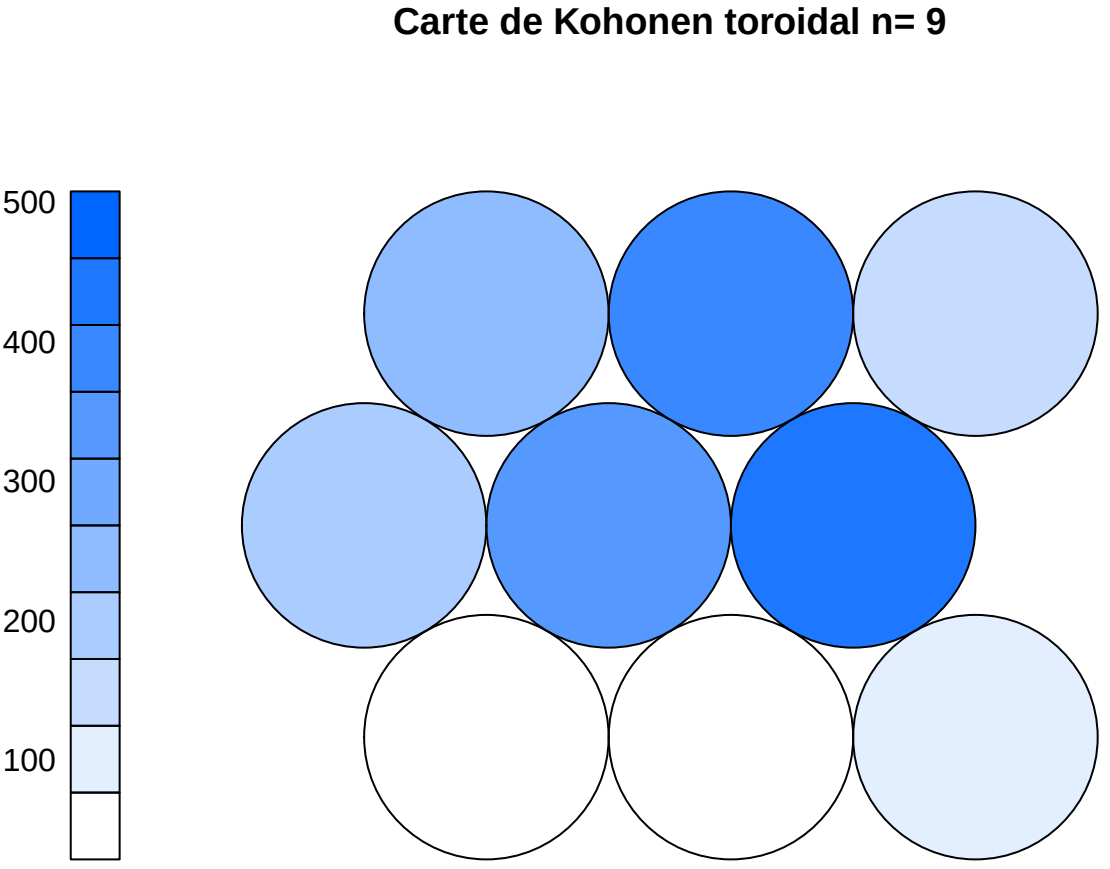
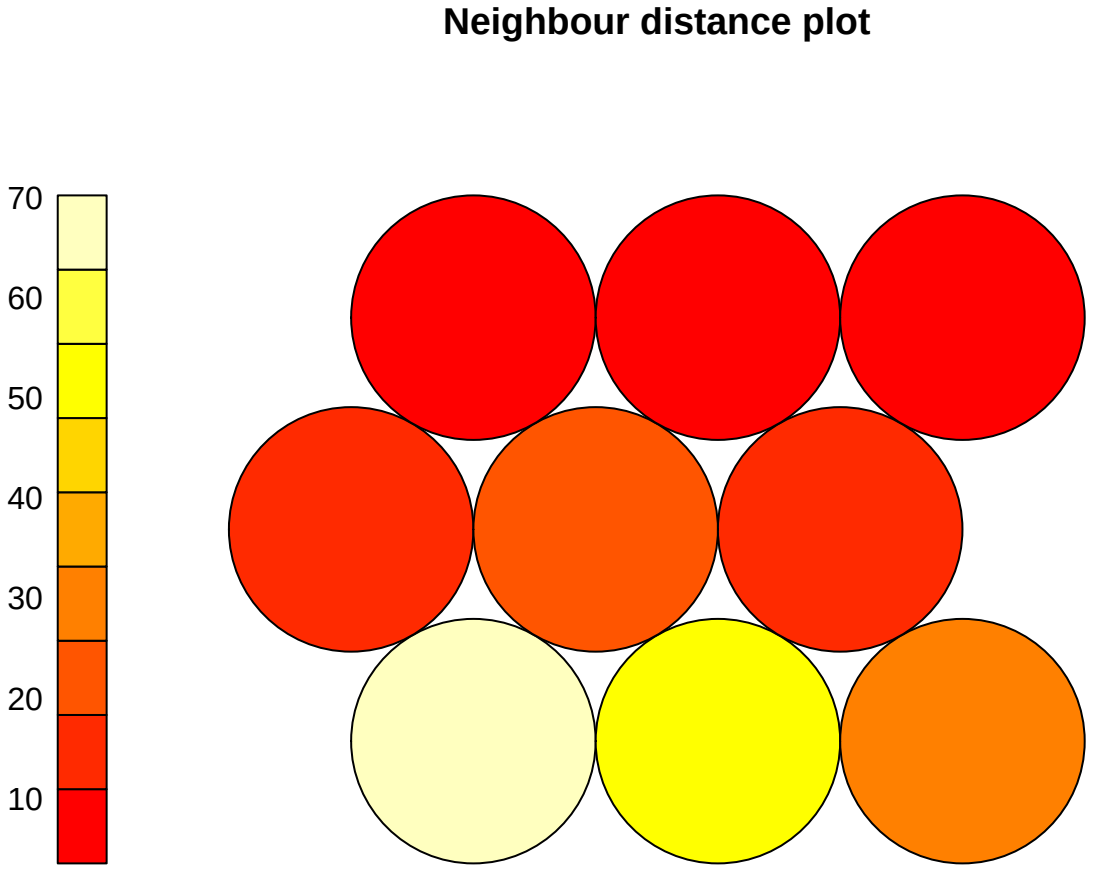
o_PB
p_PB
polar
ionic


Carte de Kohonen toroidal n= 9
500
400
300
200
100


Neighbour distance plot
70
60
50
40
30
20
10

Codes plot

- H_ss
- B_ss
- E_ss
- G_ss
- I_ss
- T_ss
- S_ss
- X._ss
- o_ss
- o_ss.1
- o_ss.2
- o_ss.3
- o_ss.4
- o_ss.5
- o_ss.6
- o_ss.7
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- d_PB
- e_PB
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- g_PB
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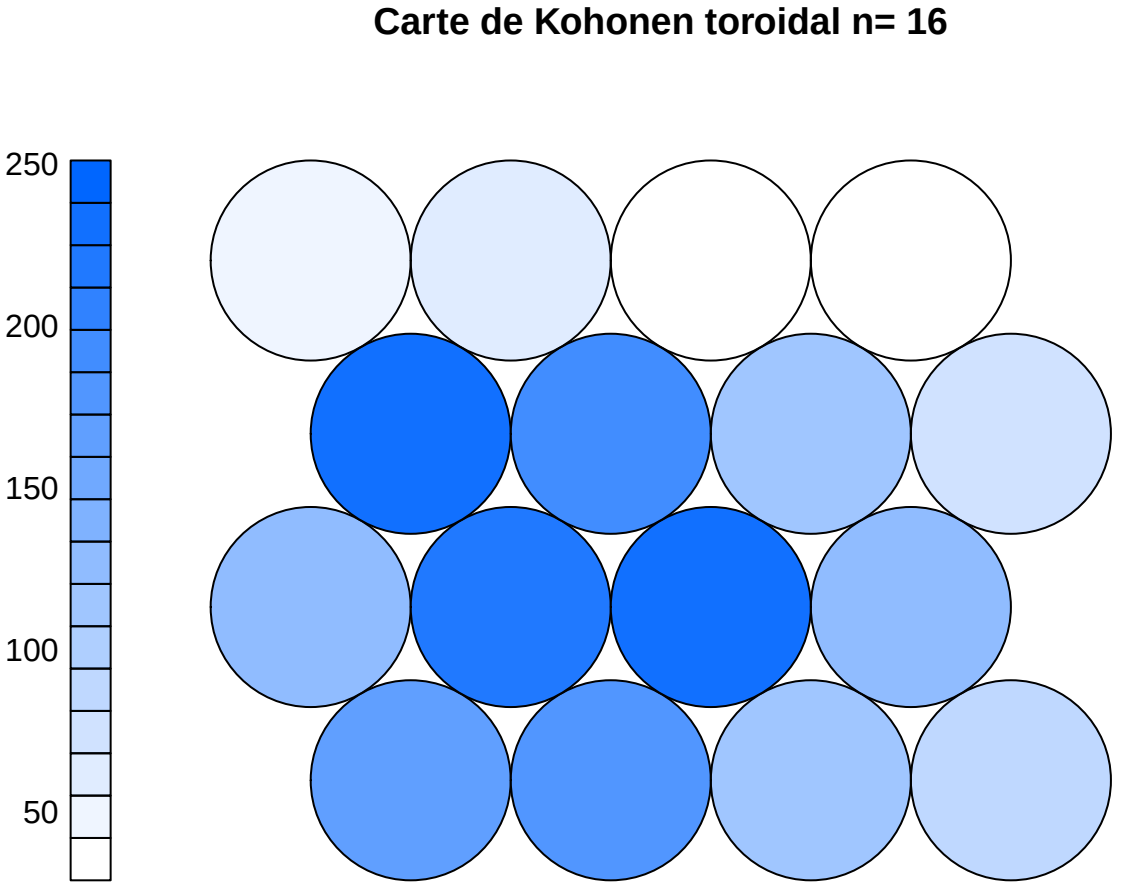
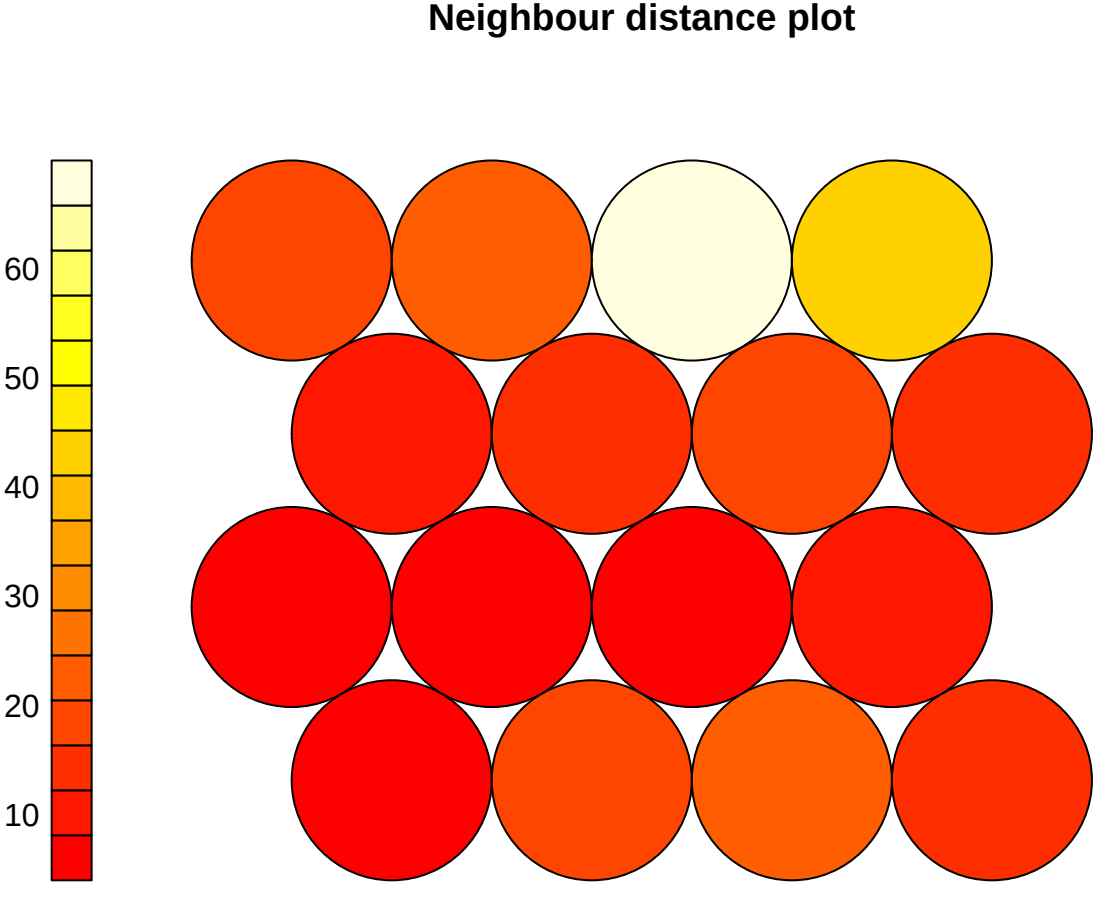
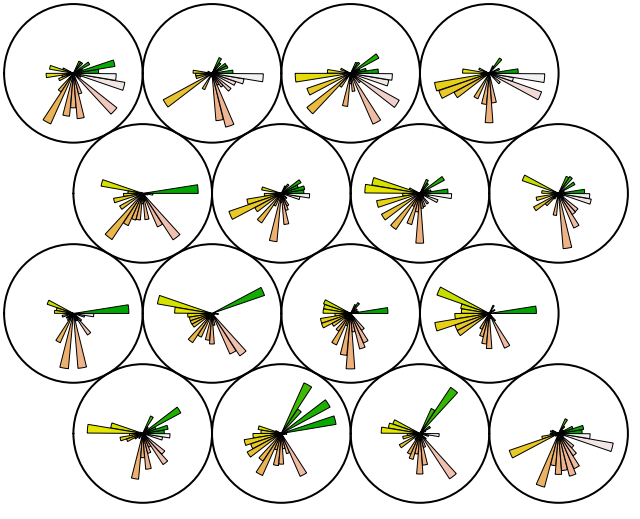
- n_PB
- o_PB
- p_PB
- polar
- ionic


Carte de Kohonen toroidal n= 16
250
200
150
100
50


Neighbour distance plot
60
50
40
30
20
10

Codes plot



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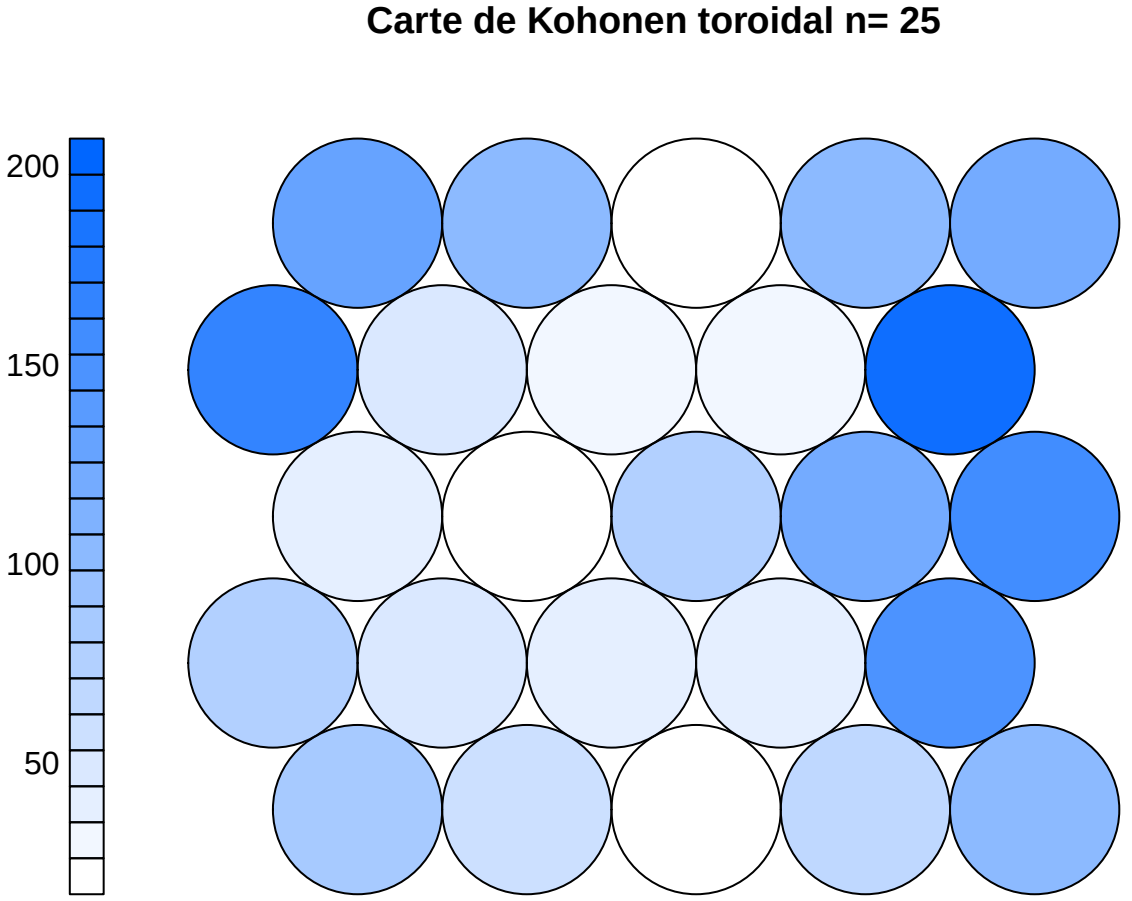
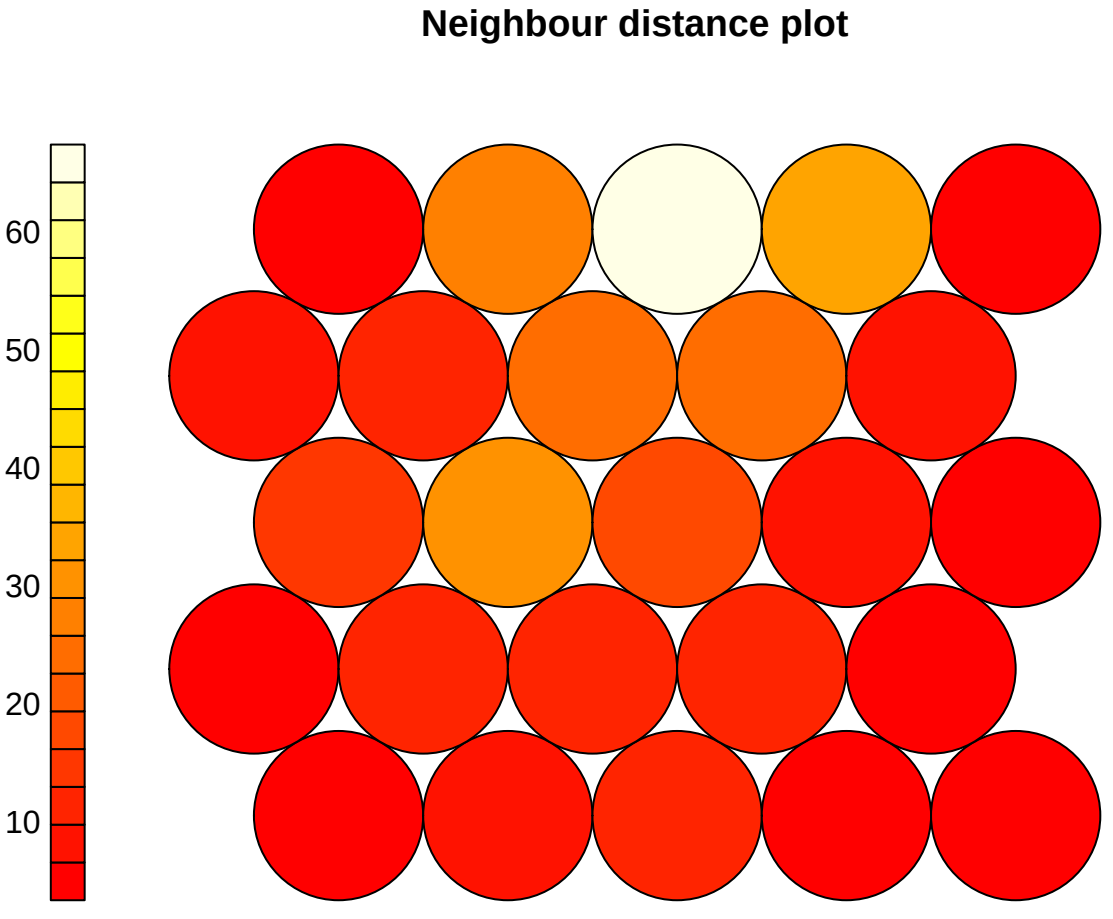
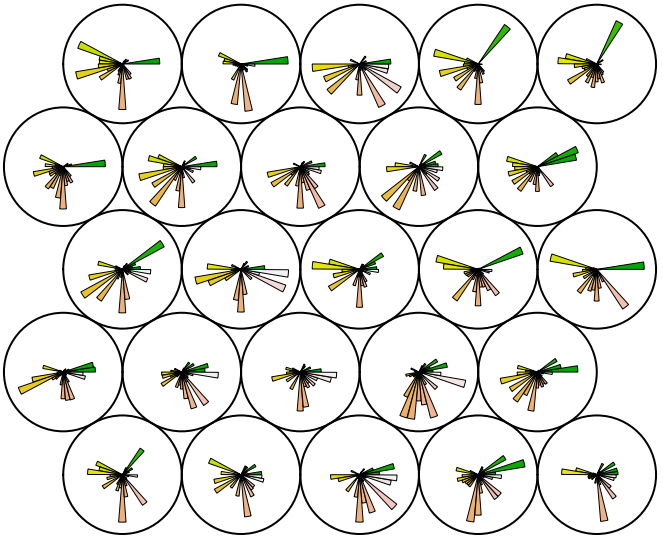
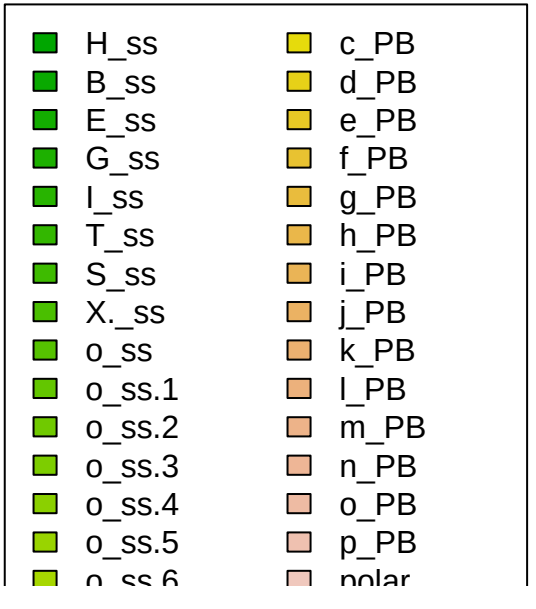

Carte de Kohonen toroidal n= 25
200
150
100
50


Neighbour distance plot
60
50
40
30
20
10

Codes plot

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o_ss.4
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o_ss.6
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polar