K-means clustering

Tomáš Vinař

22.11.2018

Formulácia problému

Vstup: n-rozmerné vektory $x_1, x_2, \ldots, x_t$ a počet zhlukov k

Výstup: Rozdelenie vektorov do k zhlukov:

- priradenie vstupných vektorov do zhlukov zapísané ako čísla $c_1, c_2, \ldots, c_t$, kde $c_i \in \{1, 2, \ldots, k\}$ je číslo zhluku pre x_i
- centrum každého zhluku, t.j. n-rozmerné vektory $\mu_1, \mu_2, ..., \mu_k$

Hodnoty $c_1, \ldots, c_t$ a $\mu_1, ..., \mu_k$ volíme tak, aby sme minimalizovali súčet štvorcov vzdialeností od každého vektoru k centru jeho zhluku:

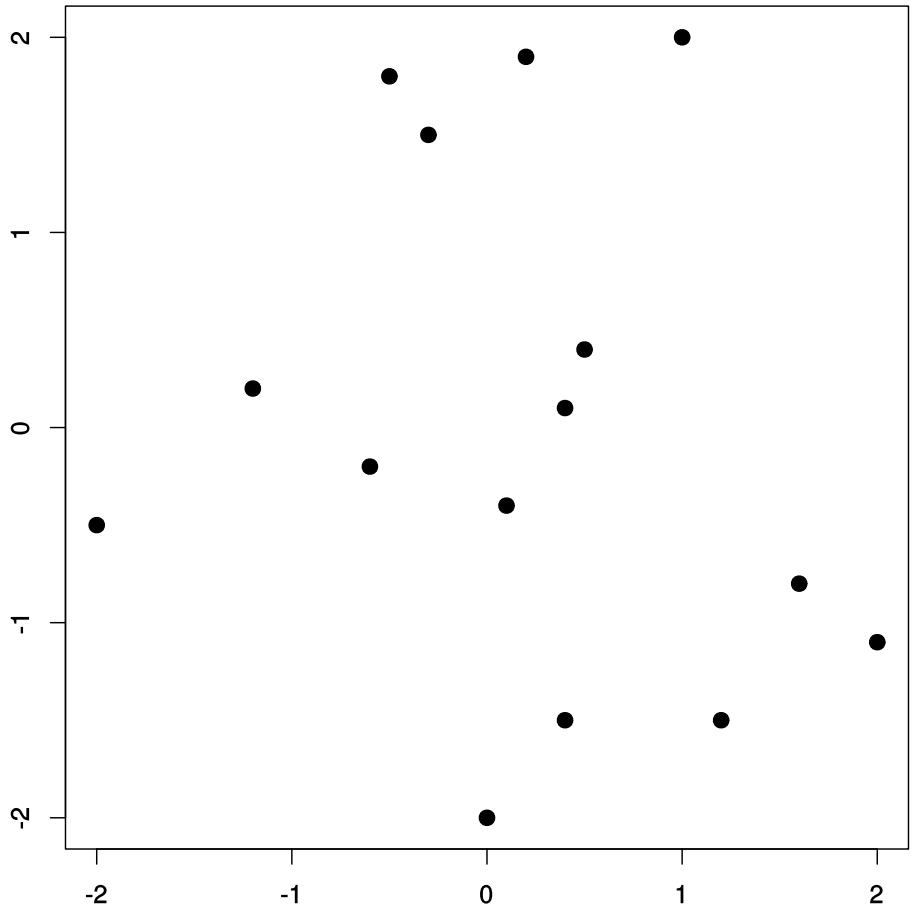
$$\sum_{i=1}^{t} \left\| x_i - \mu_{c_i} \right\|_2^2$$

Pre vektory $a = (a_1, \ldots, a_n)$ a $b = (b_1, \ldots b_n)$ je druhá mocnina vzdialenosti $\left\| a - b \right\|_2^2 = \sum_{i=1}^{n} (a_i - b_i)^2$

Príklad vstupu

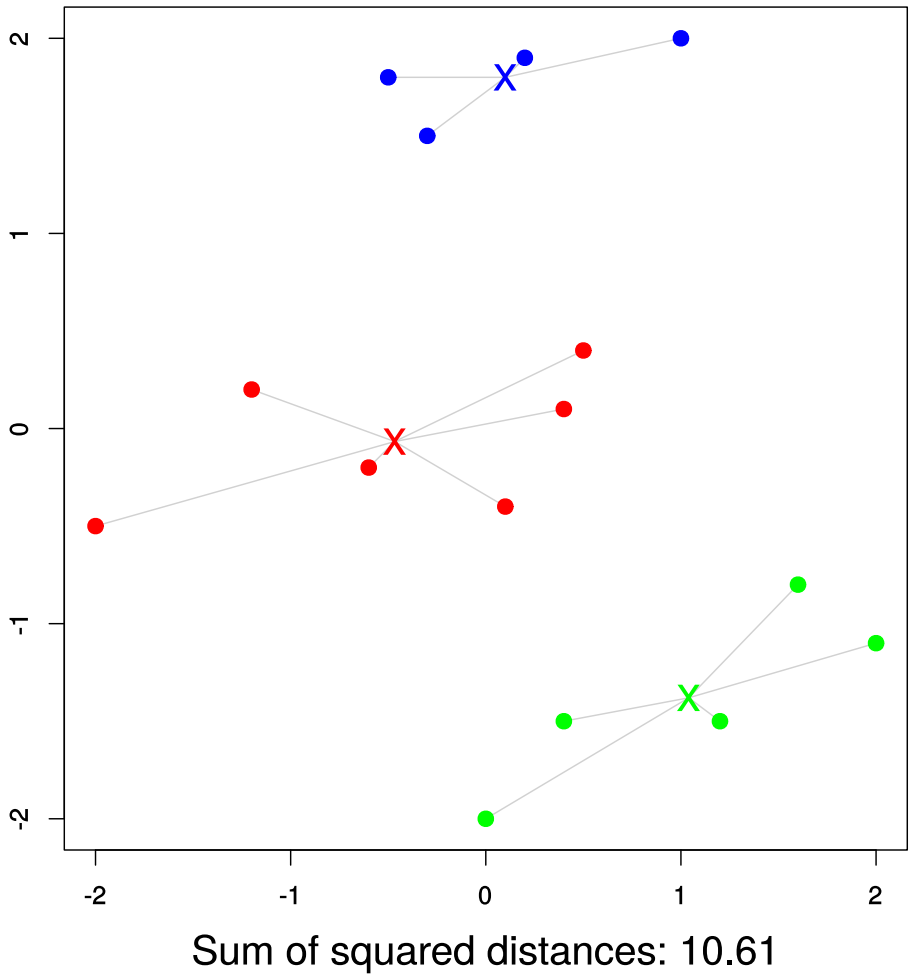
x_1	-2.00	-0.50
x_2	-1.20	0.20
x_3	-0.60	-0.20
x_4	-0.50	1.80
x_5	-0.30	1.50
x_6	0.00	-2.00
x_7	0.10	-0.40
x_8	0.20	1.90
x_9	0.40	0.10
x_{10}	0.40	-1.50
x_{11}	0.50	0.40
x_{12}	1.00	2.00
x_{13}	1.20	-1.50
x_{14}	1.60	-0.80
x_{15}	2.00	-1.10

$k = 3$



Príklad výstupu

x_1	-2.00	-0.50	1
x_2	-1.20	0.20	1
x_3	-0.60	-0.20	1
x_4	-0.50	1.80	3
x_5	-0.30	1.50	3
x_6	0.00	-2.00	2
x_7	0.10	-0.40	1
x_8	0.20	1.90	3
x_9	0.40	0.10	1
x_{10}	0.40	-1.50	2
x_{11}	0.50	0.40	1
x_{12}	1.00	2.00	3
x_{13}	1.20	-1.50	2
x_{14}	1.60	-0.80	2
x_{15}	2.00	-1.10	2
μ_1	**-0.47**	**-0.07**	
μ_2	**1.04**	**-1.38**	
μ_3	**0.10**	**1.80**	



Sum of squared distances: 10.61

Algoritmus

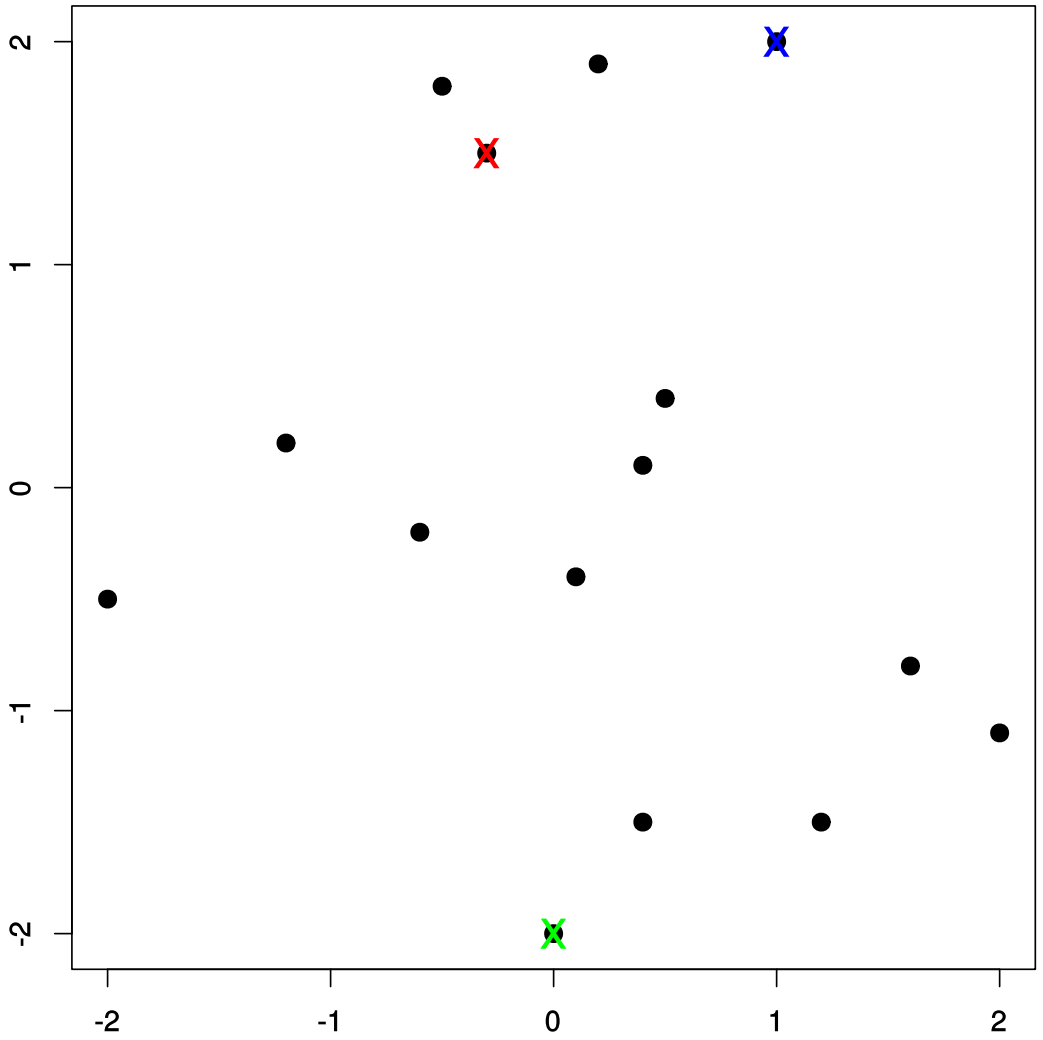
Heuristika, ktorá nenájde vždy najlepšie zhlukovanie.
Začne z nejakého zhlukovania a postupne ho zlepšuje.

Inicializácia:
náhodne vyber k centier $\mu_1, \mu_2, ..., \mu_k$ spomedzi vstupných vektorov

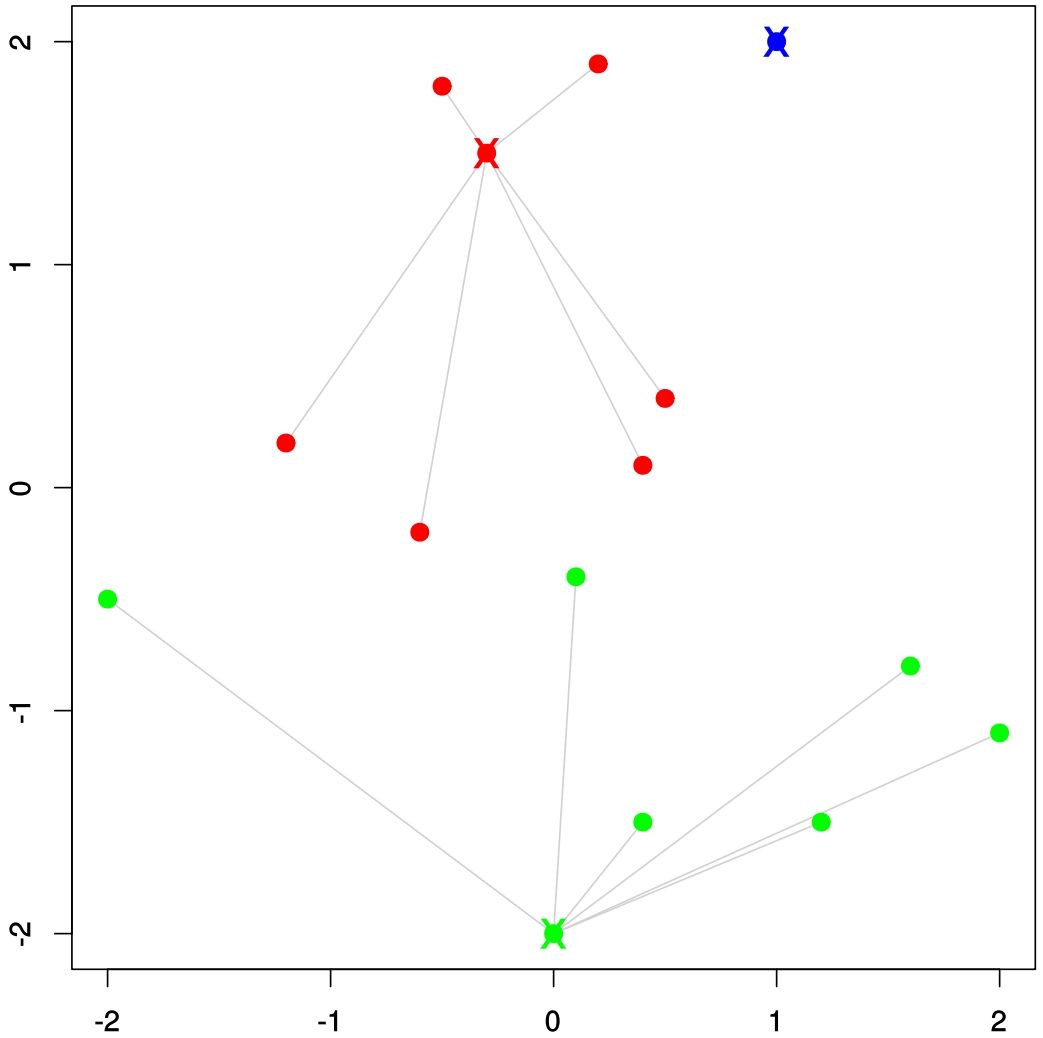
Opakuj, kým sa niečo mení:

- priraď každý bod najbližšiemu centru: $c_i = \arg\min_j \left\|x_i - \mu_j\right\|_2$
- vypočítaj nové centroidy: μ_j bude priemerom (po zložkách) z vektorov x_i, pre ktoré $c_i = j$

Zvolíme náhodné centrá μ_i

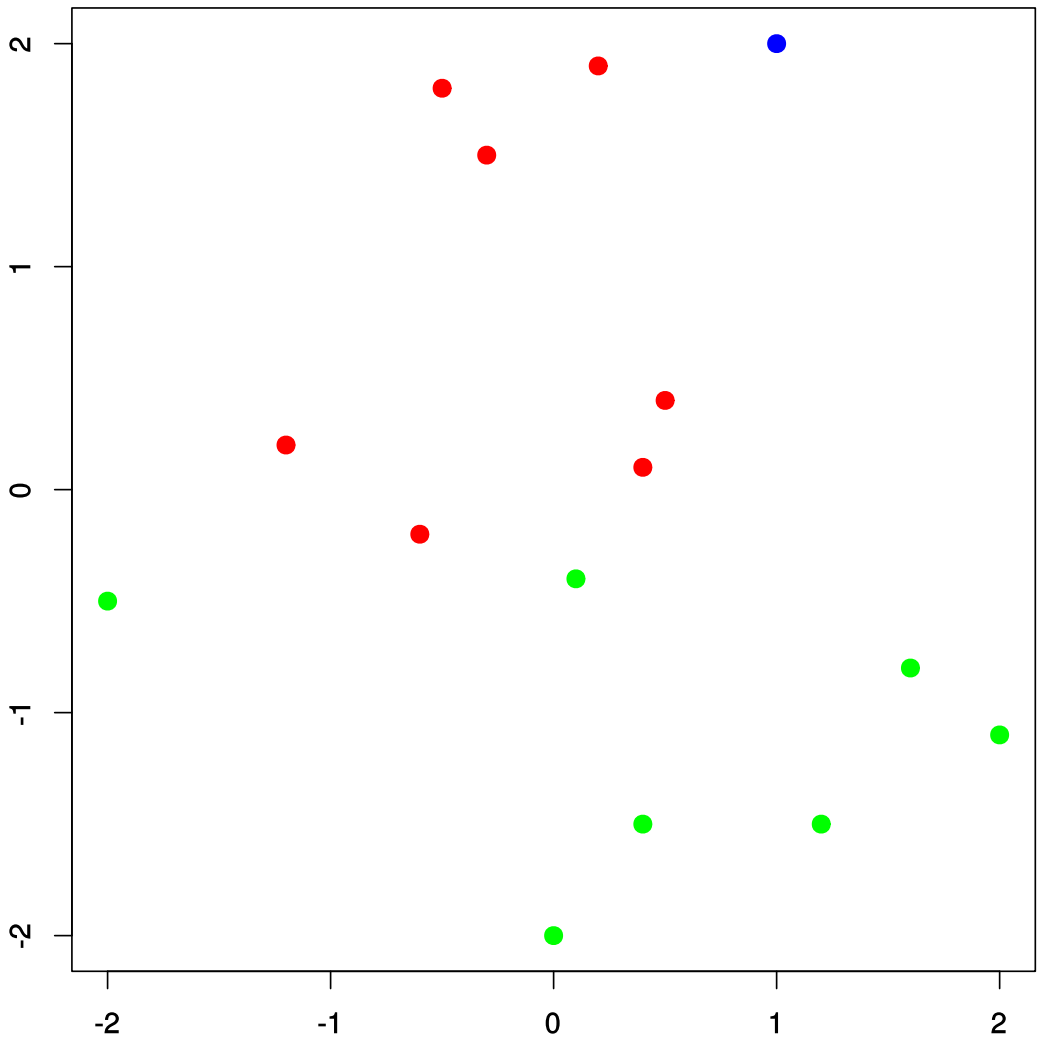


Vektory priradíme do zhlukov (hodnoty c_i)

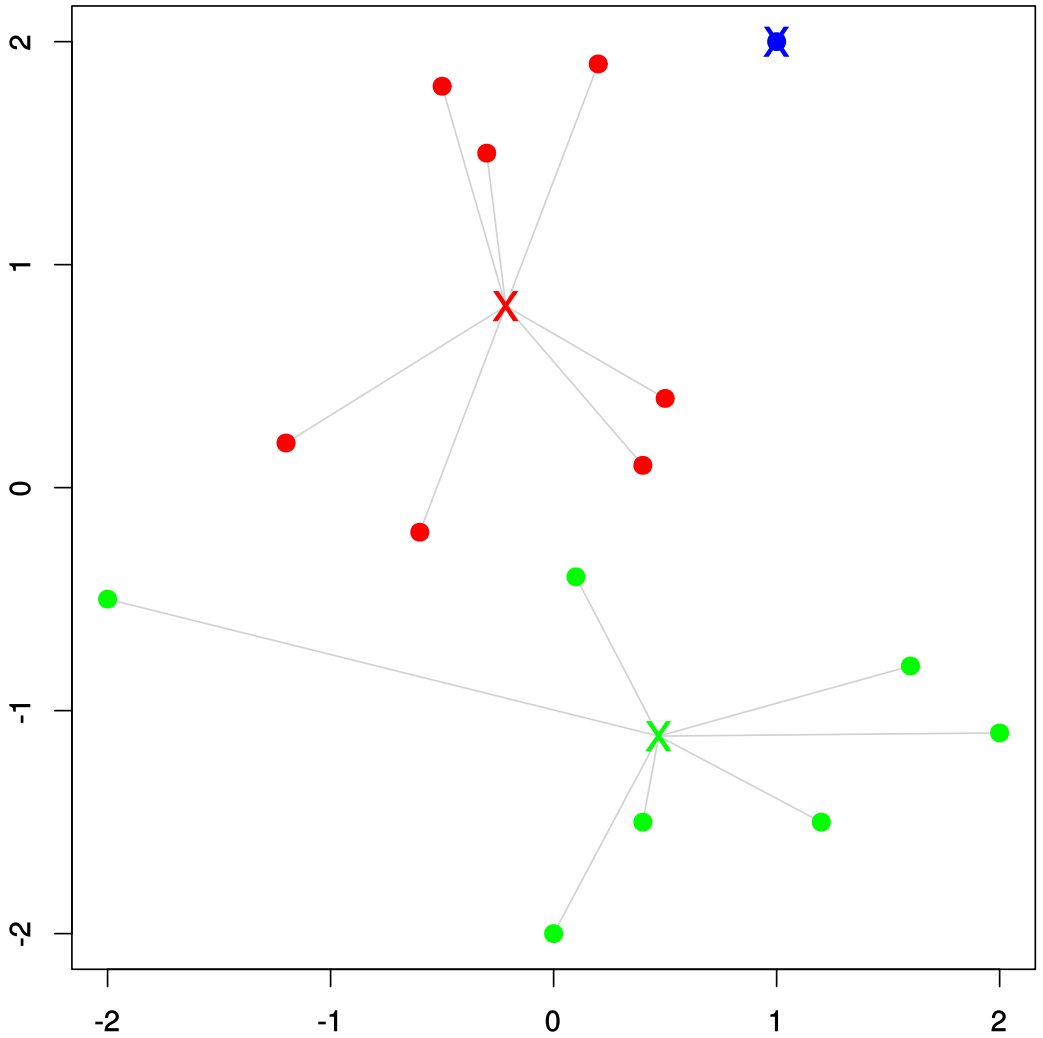


Sum of squared distances: 30.05

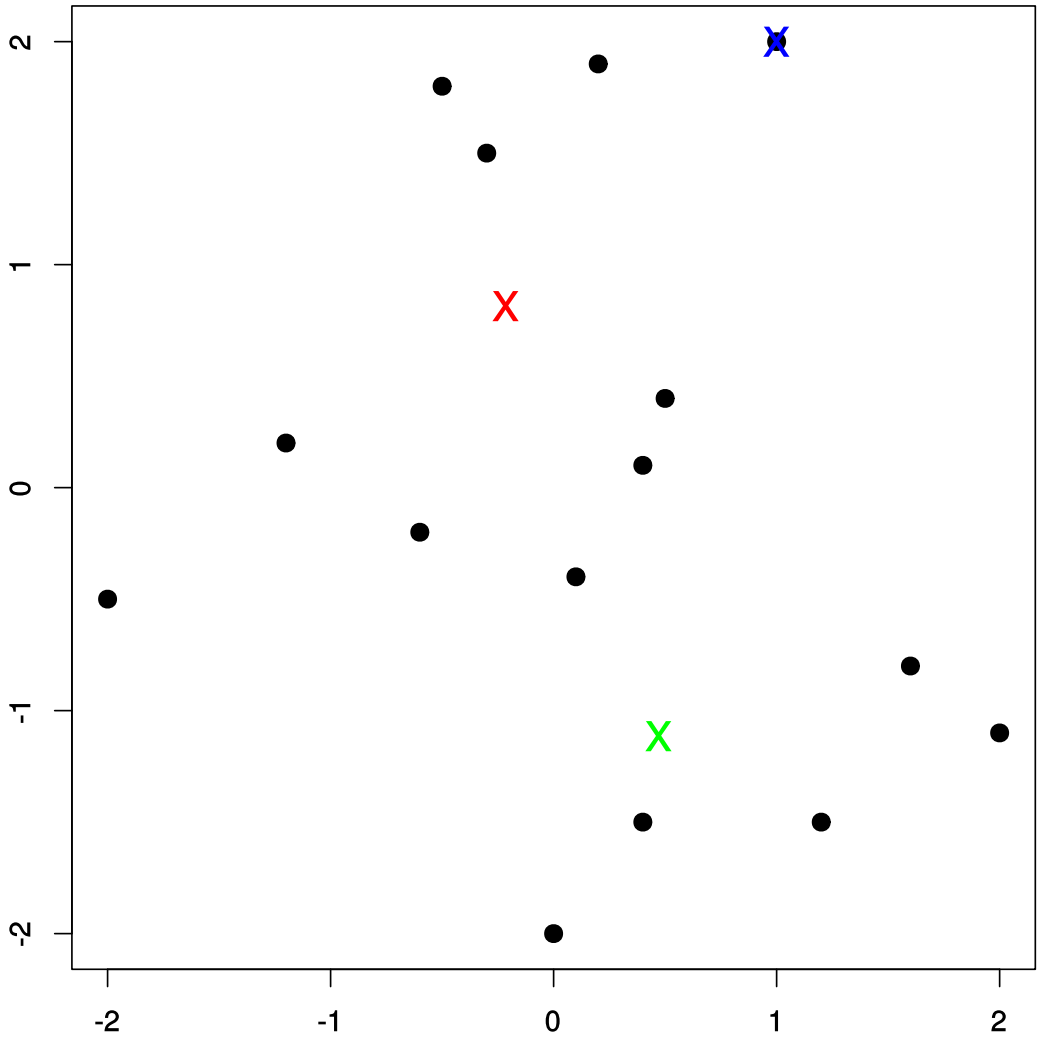
Zabudneme μ_i



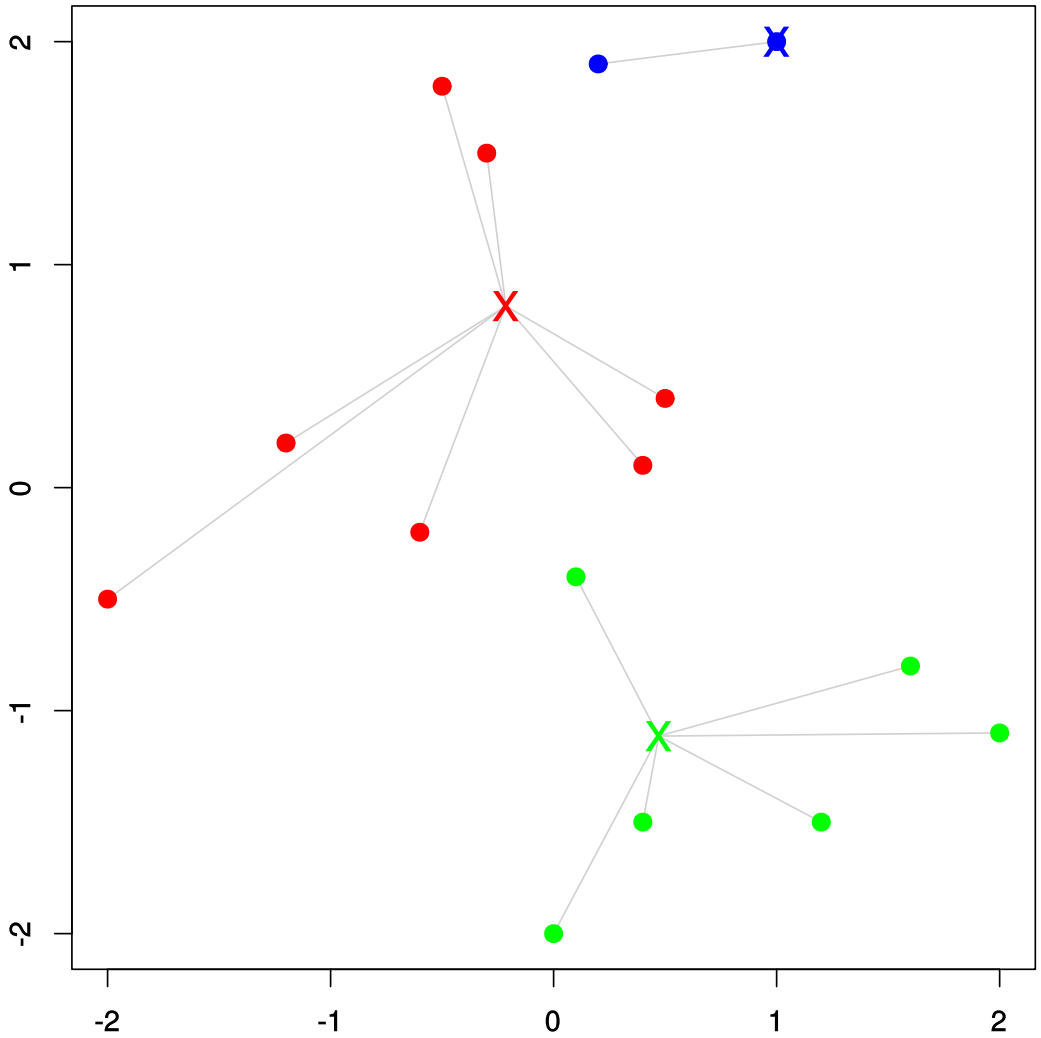
Dopočítame nové μ_i (suma klesla z 30.05 na 19.66)



Zabudneme c_i

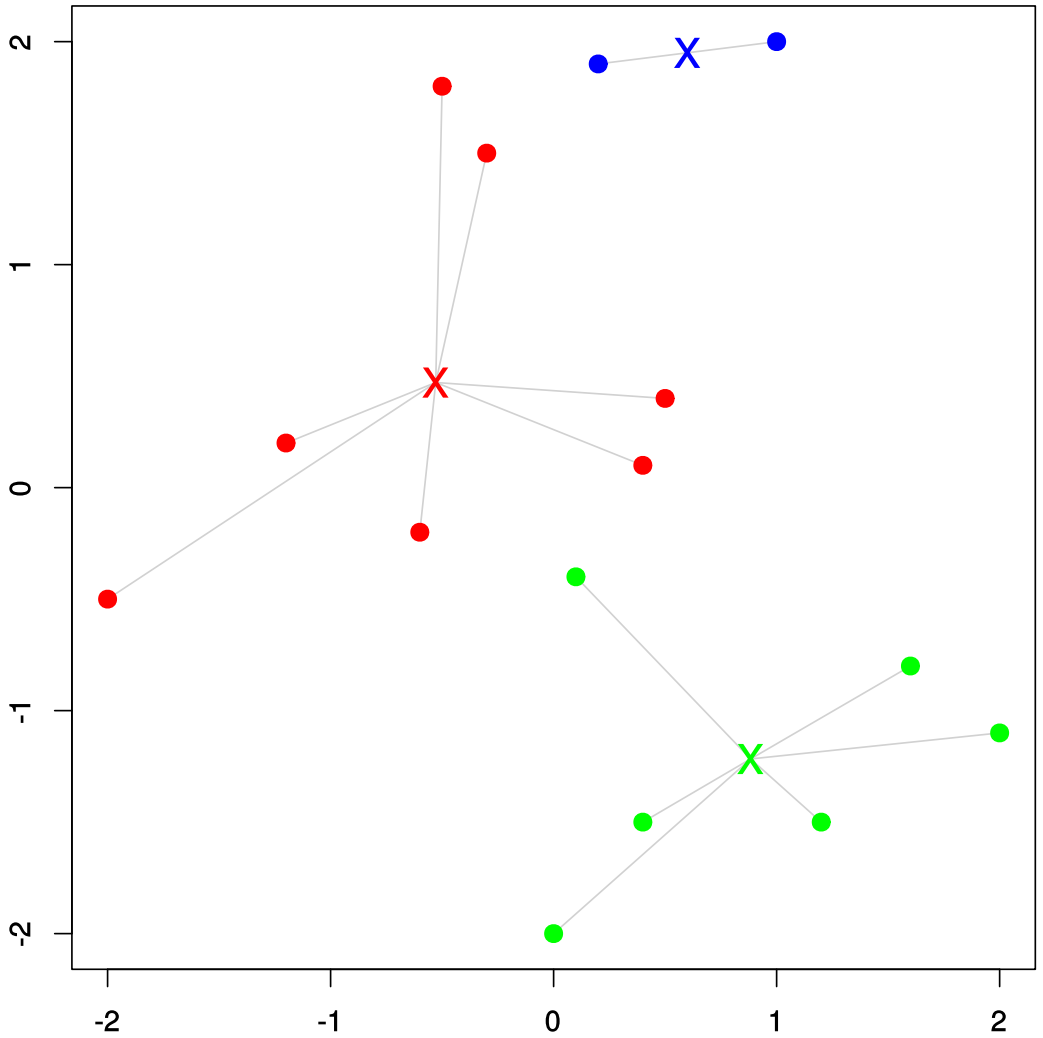


Dopočítame nové c_i (suma klesla z 19.66 na 17.39)



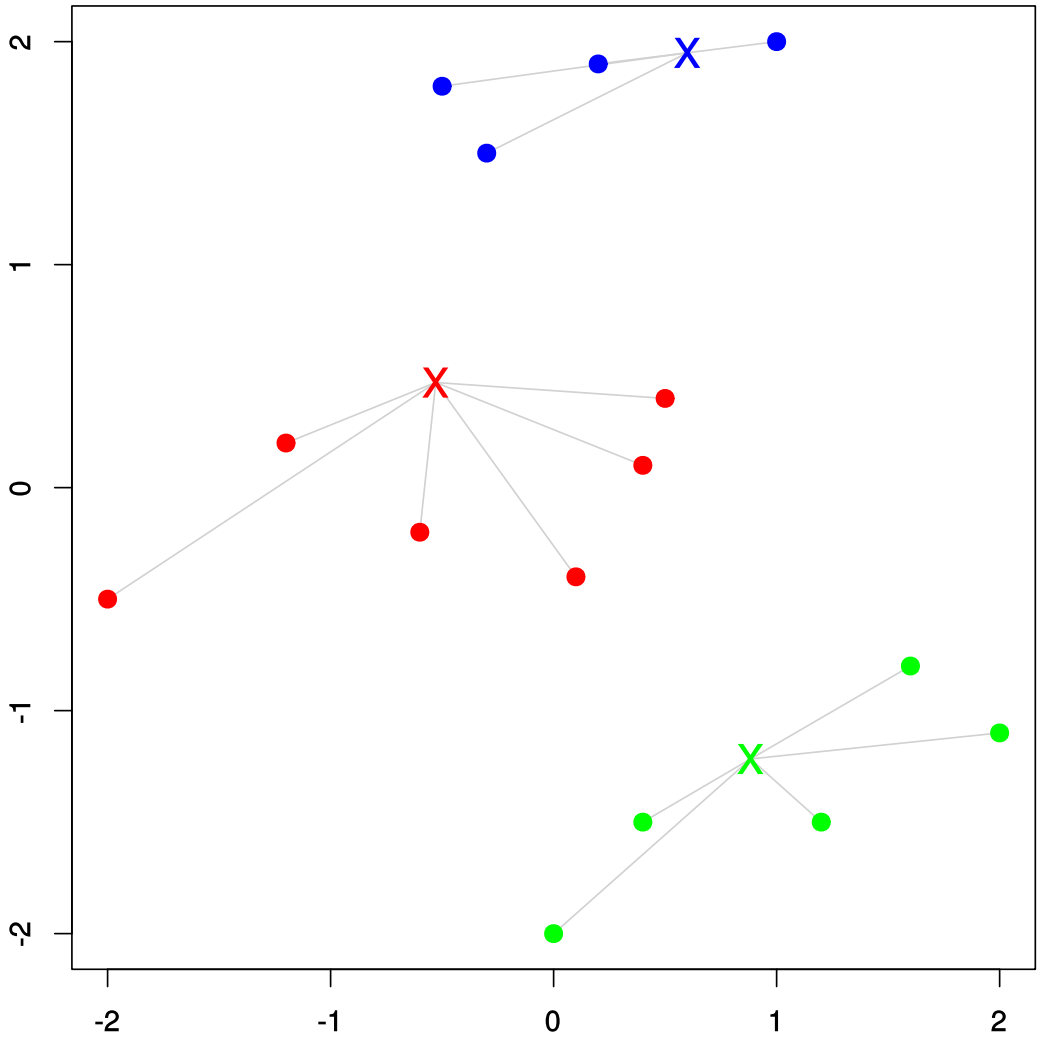
Sum of squared distances: 17.39

Prepočítame μ_i



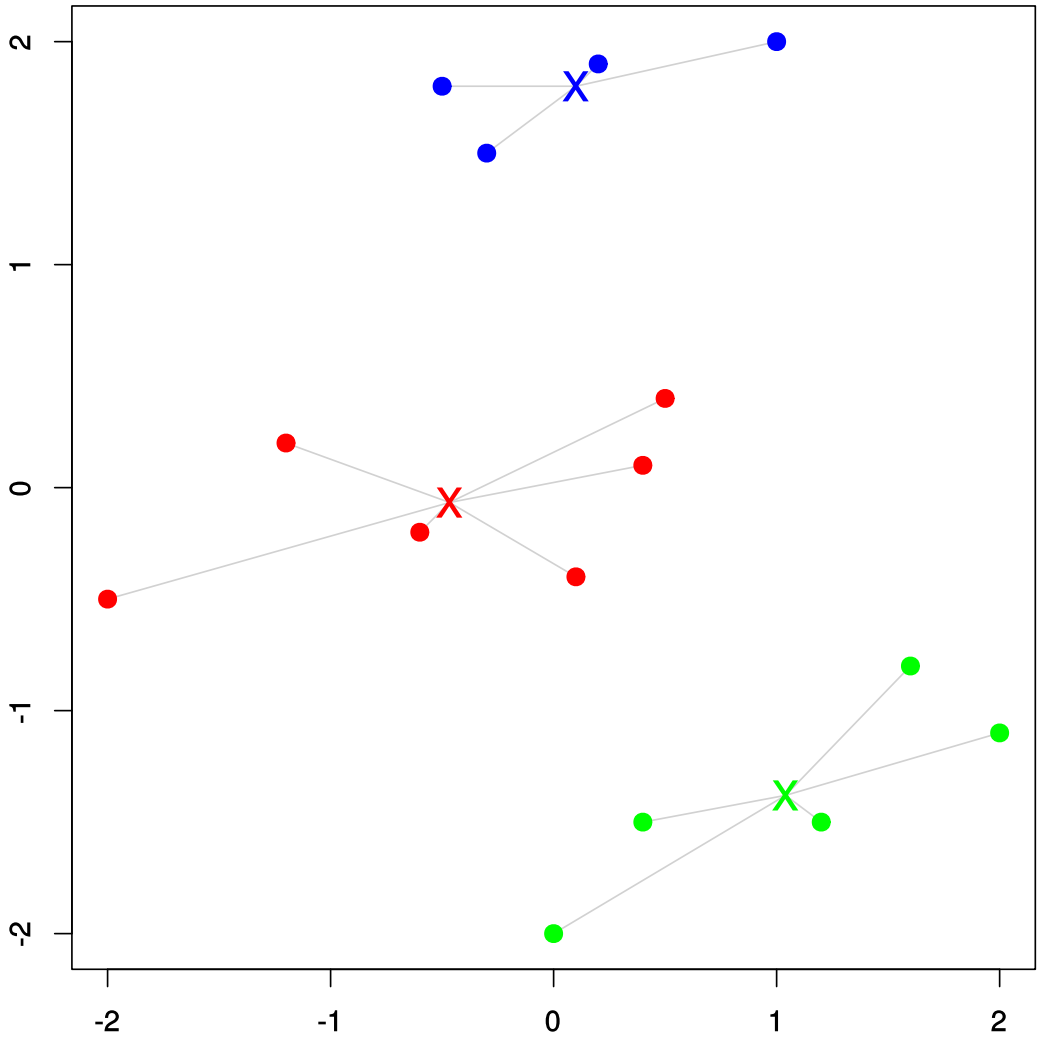
Sum of squared distances: 14.47

Prepočítame c_i

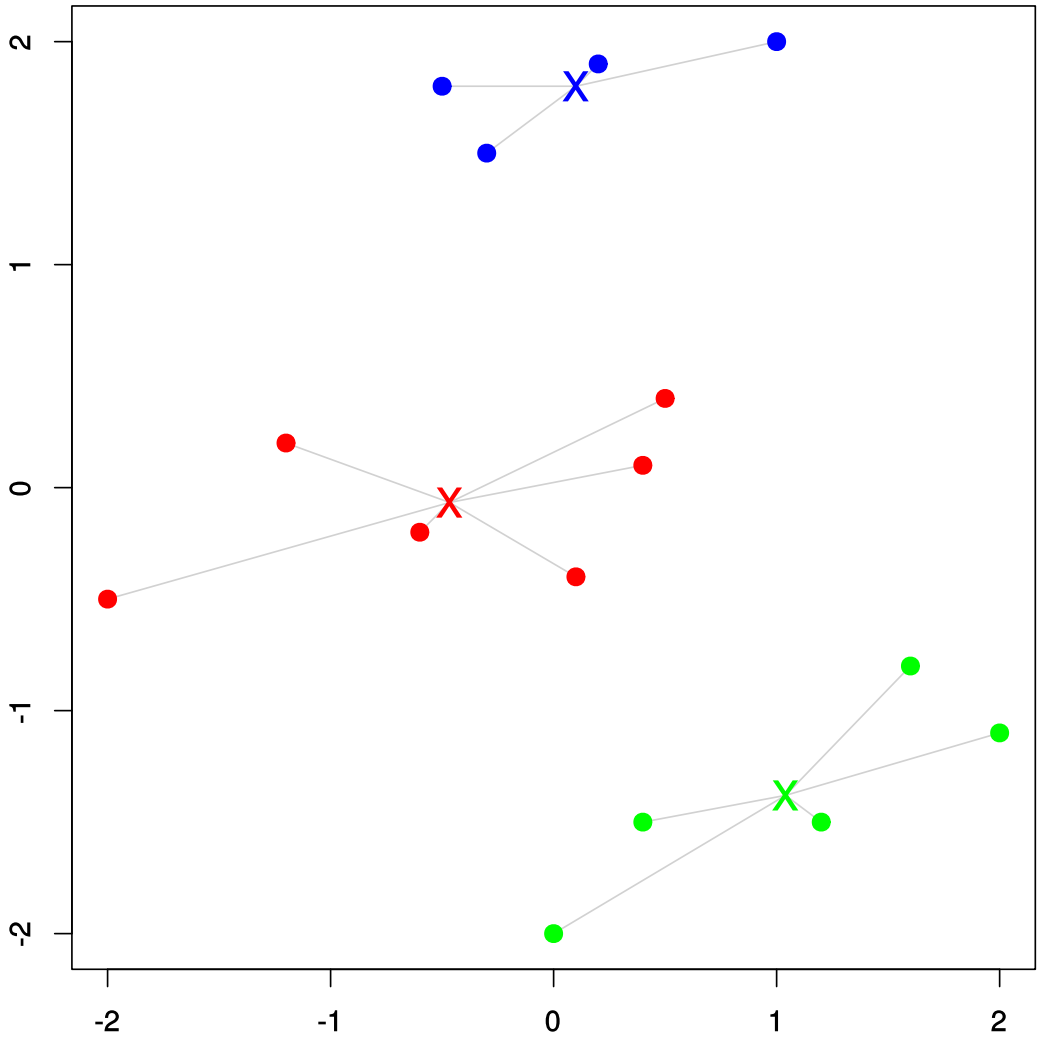


Sum of squared distances: 13.71

Prepočítame μ_i

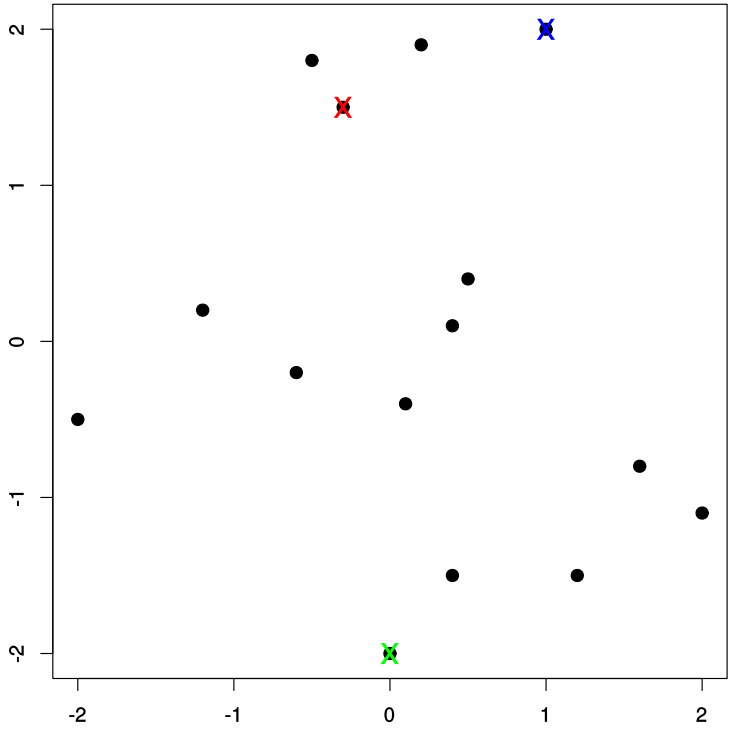


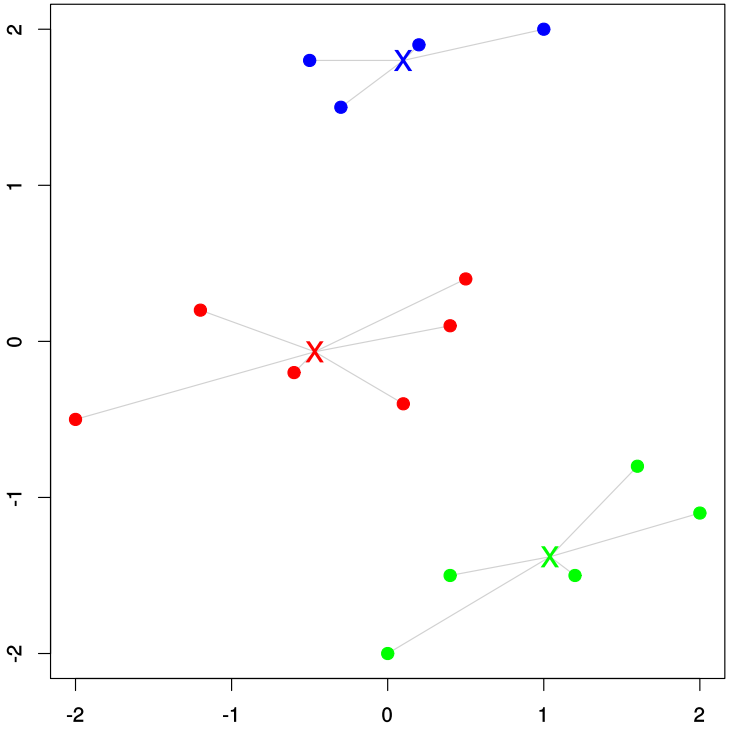
Prepočítame c_i (žiadna zmena, končíme)



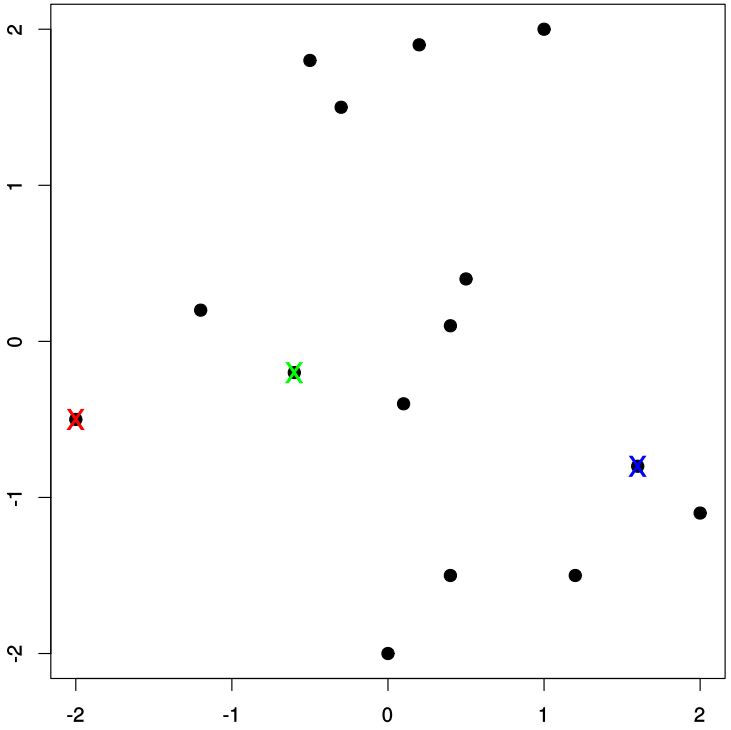
Sum of squared distances: 10.61

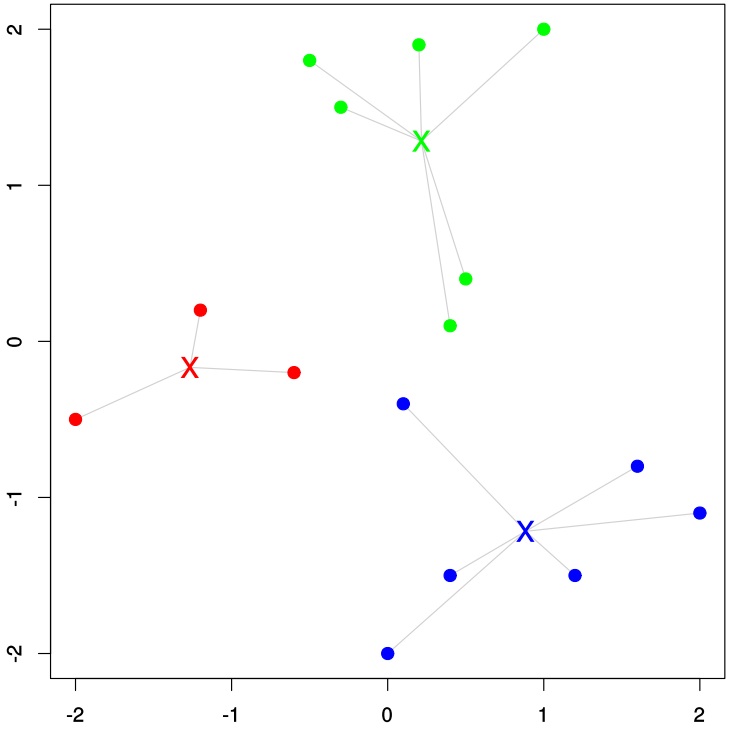
Príklady niekoľkých behov programu





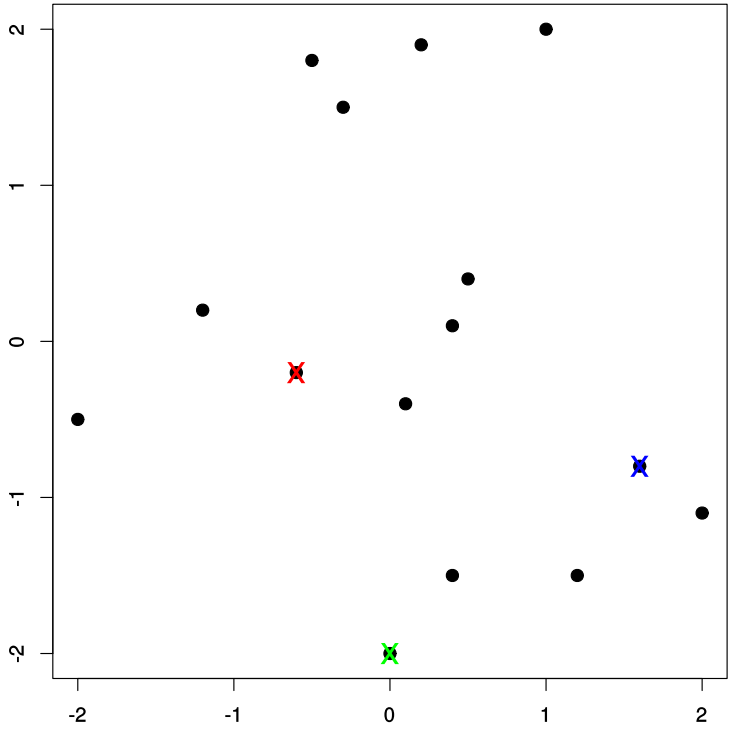
Príklady niekoľkých behov programu

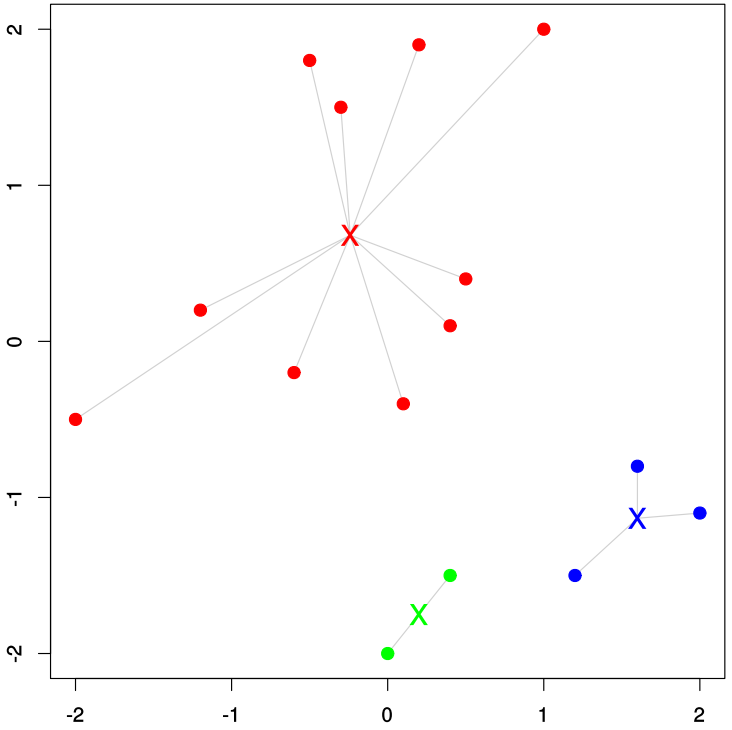




Sum of squared distances: 11.25

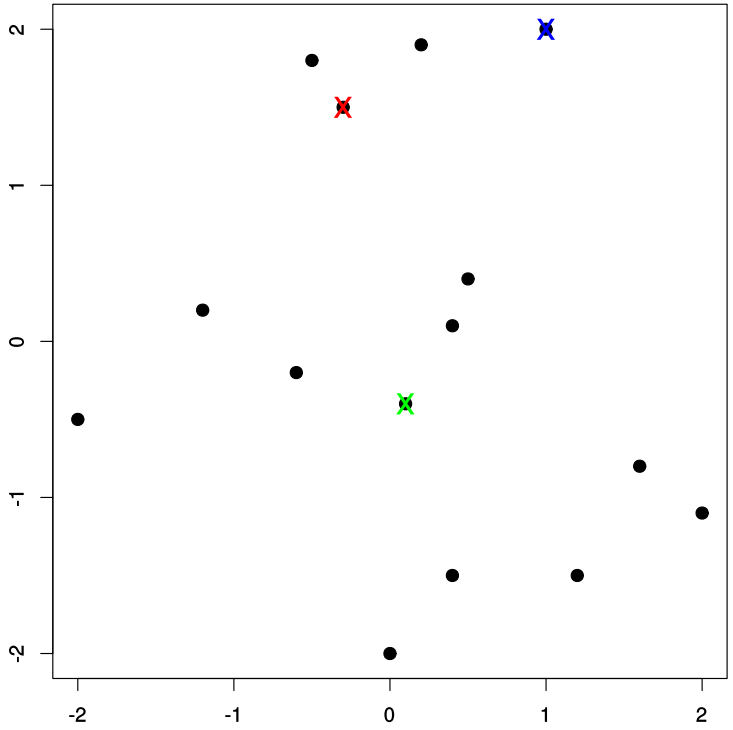
Príklady niekoľkých behov programu

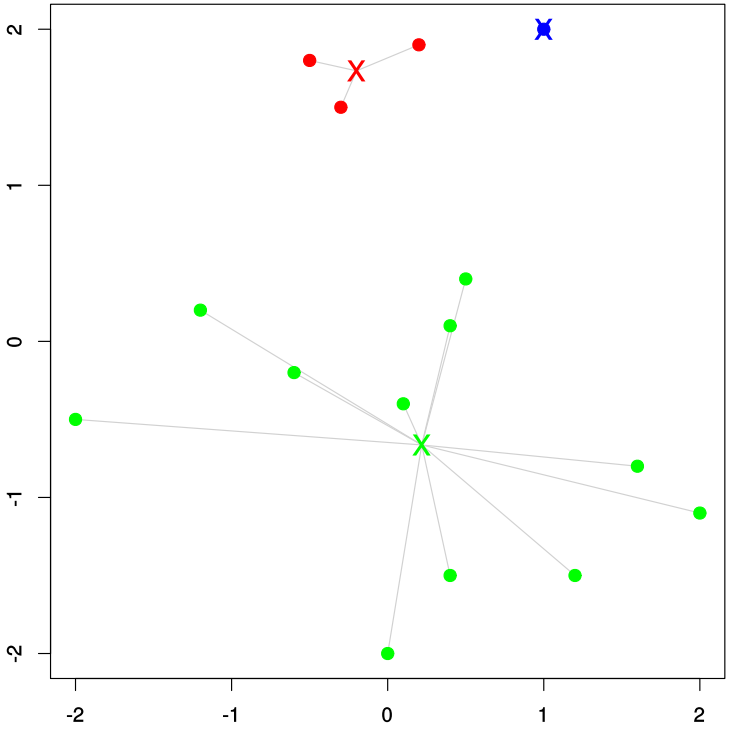




Sum of squared distances: 16.93

Príklady niekoľkých behov programu





Sum of squared distances: 20.37