

# Nukleární magnetická rezonance (NMR)

Viktor Bartošík

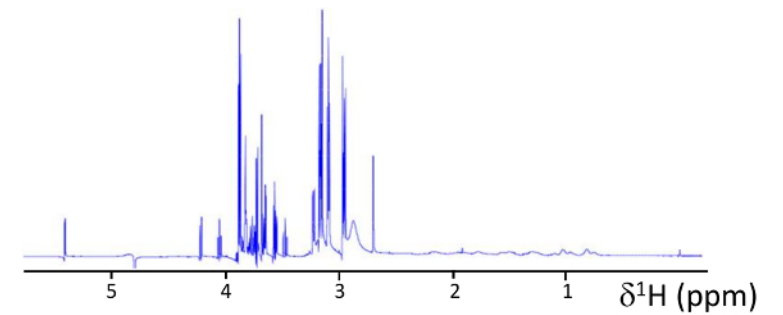
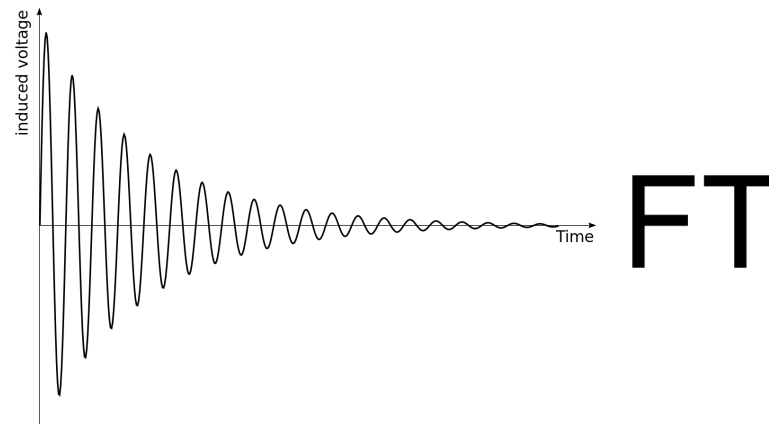
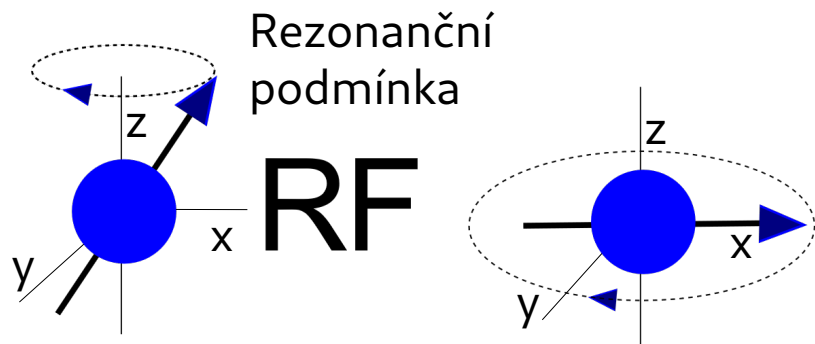
26. 11. 2024

- <https://www.youtube.com/watch?v=t8JIBwLsCGA&t=54s>

# Následující semináře

4./6. 12.	1. seminář NMR: vzdálenosti mezi atomy, tvar molekul
11./13. 12.	2. seminář NMR: přiřazení frekvencí k atomům
18. /20. 12.	NMR test (20.12. taky exkurze)

# Nukleární magnetická rezonance (NMR)



# Efekt magnetického pole

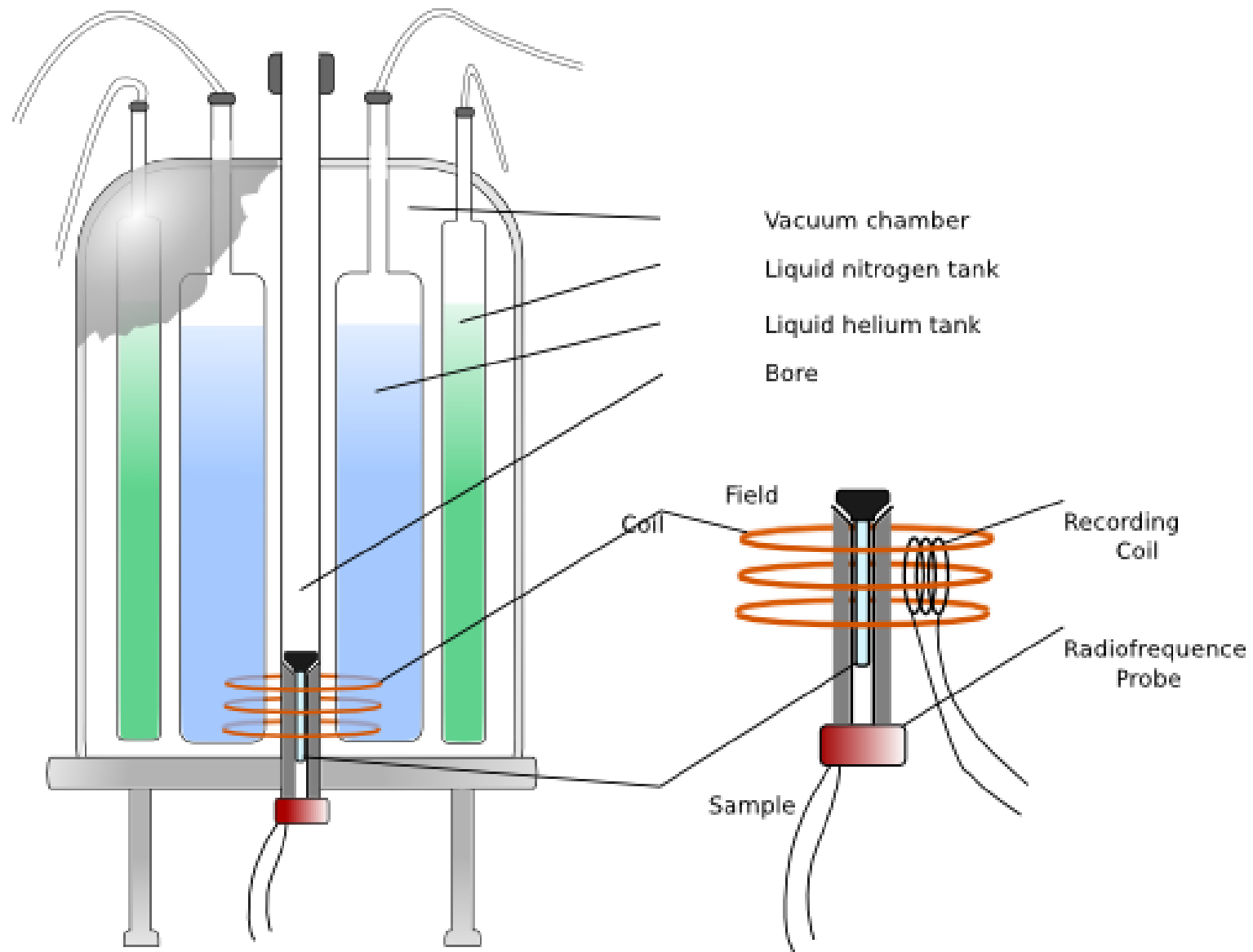
- používáme spiny  $S = 1/2$   
 $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{15}\text{N}$ ,  $^{31}\text{P}$

- Larmorova precesní frekvence:

$$\boldsymbol{\omega} = -\gamma \cdot \mathbf{B}_0$$

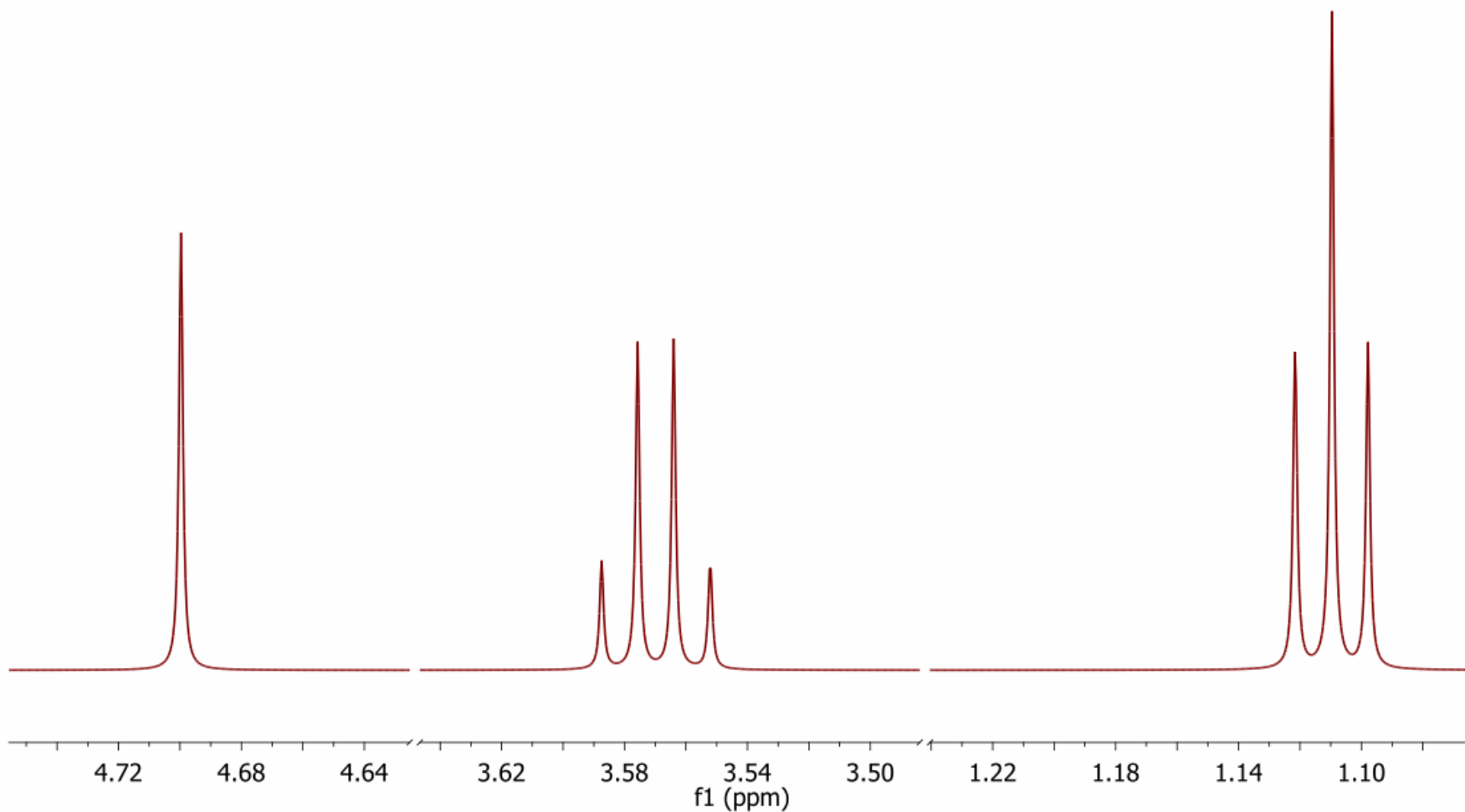
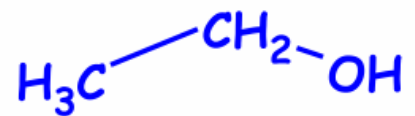
- dána gyromagnetickou konstantou jádra  
 $\gamma$  ( $\text{MHz}\cdot\text{T}^{-1}$ ):  $42.6(^1\text{H})$ ,  $10.7(^{13}\text{C})$ ,  $-4.3(^{15}\text{N})$
- a silou magnetického pole  $\mathbf{B}_0$

# NMR spektrometr



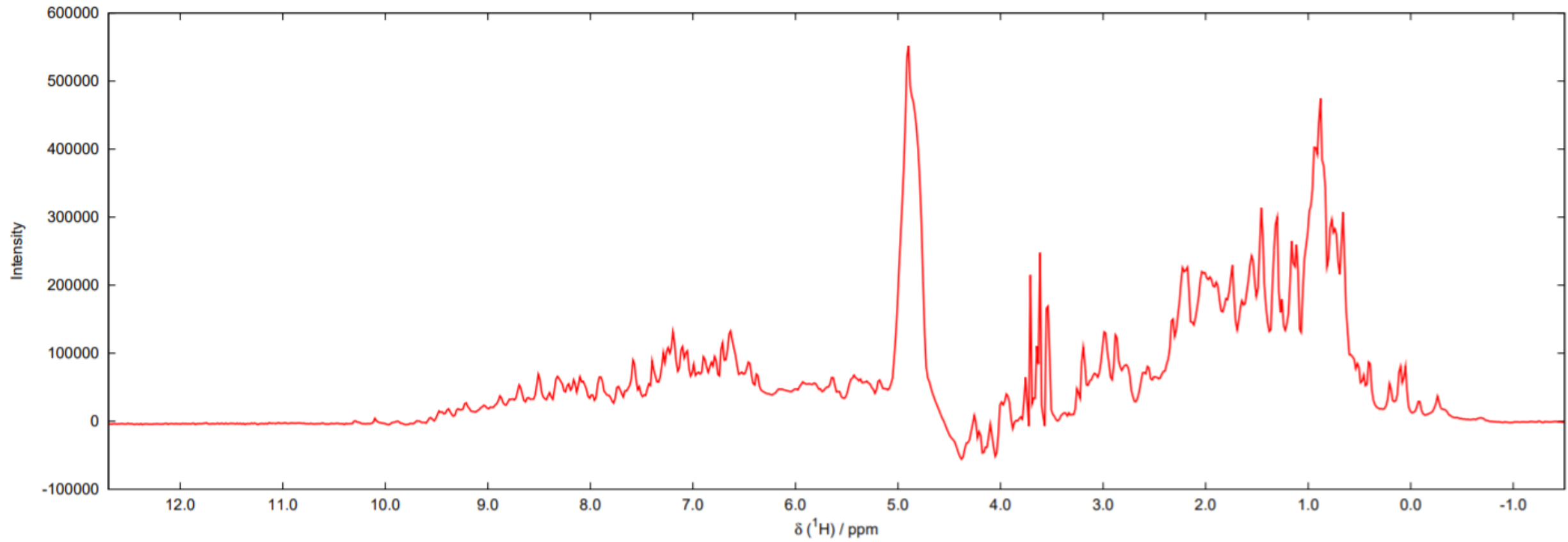


# NMR organických molekul

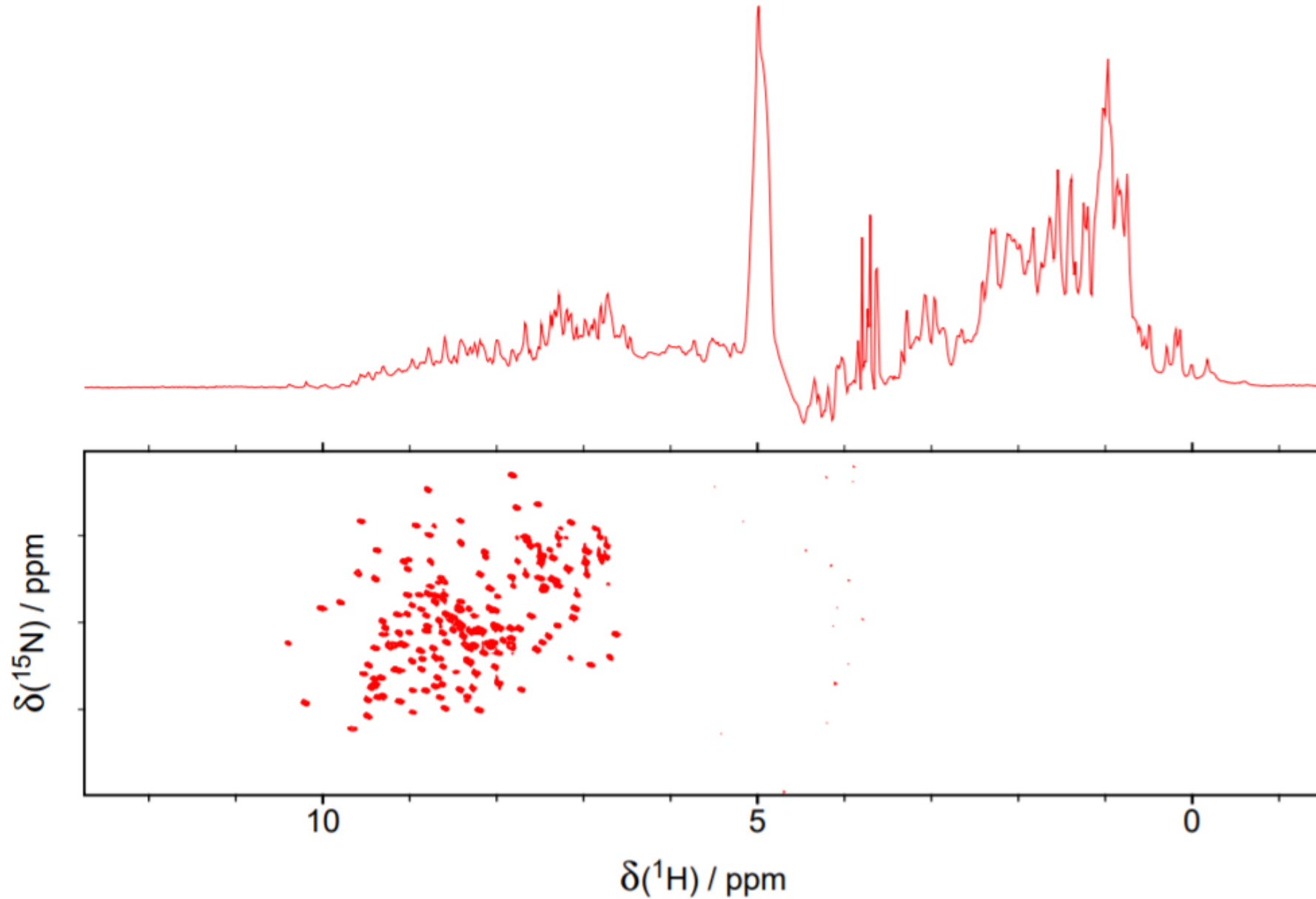




# NMR proteinů 1D



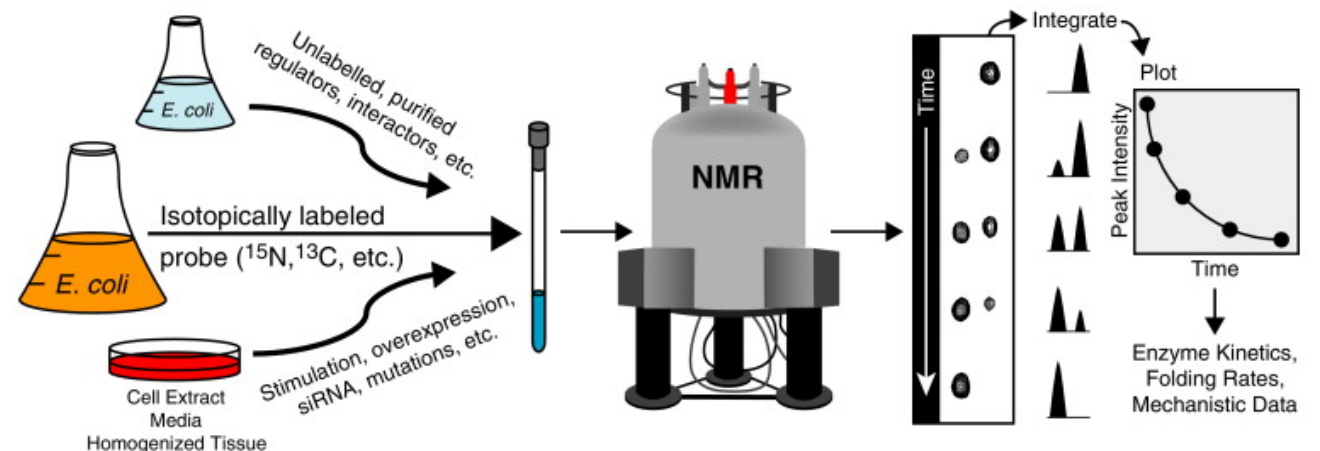
# NMR proteinů 1D, 2D



# NMR proteinů

- 1 dimenze nestačí
- $^1\text{H}$ ,  $^{31}\text{P}$  přirozeně
- $^{13}\text{C}$ ,  $^{15}\text{N}$  isotopické značení (nákladné)  
často  $^{13}\text{C}$  glukóza,  $^{15}\text{NH}_4\text{Cl}$
- vysoké koncentrace (0,2 - 1 mM)
- celkový objem cca 100-600  $\mu\text{l}$
- atomární rozlišení
- struktura a dynamika proteinů (i neuspořádaných!)

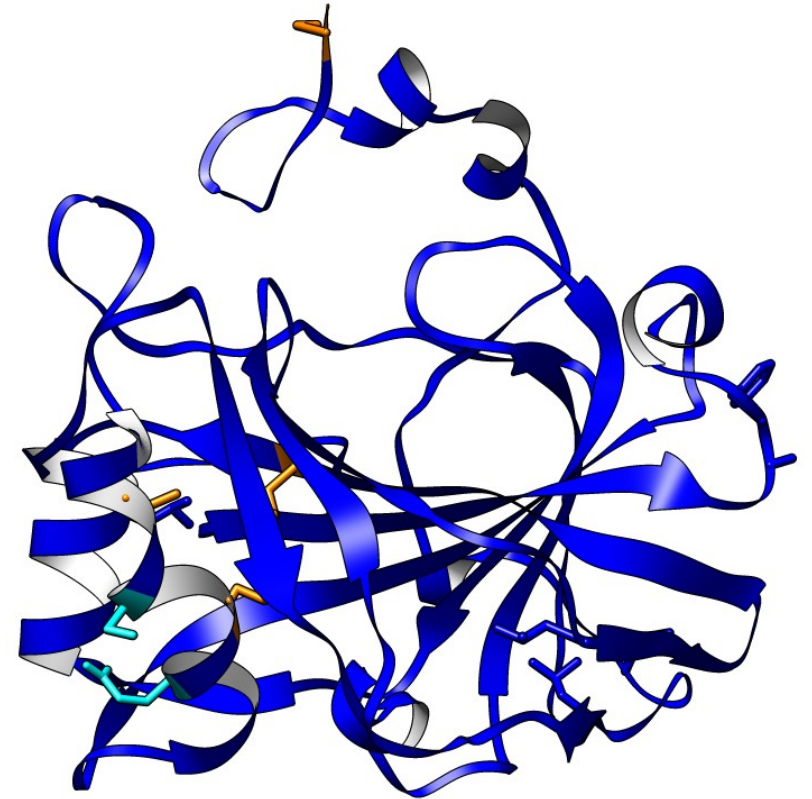
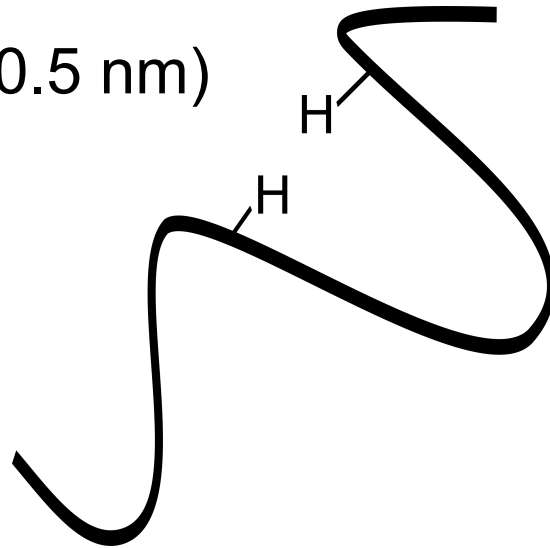
Isotop	Přírodní zastoupení
$^1\text{H}$	99,99 %
$^{13}\text{C}$	1,10 %
$^{15}\text{N}$	0,37 %
$^{19}\text{F}$	100 %
$^{31}\text{P}$	100 %





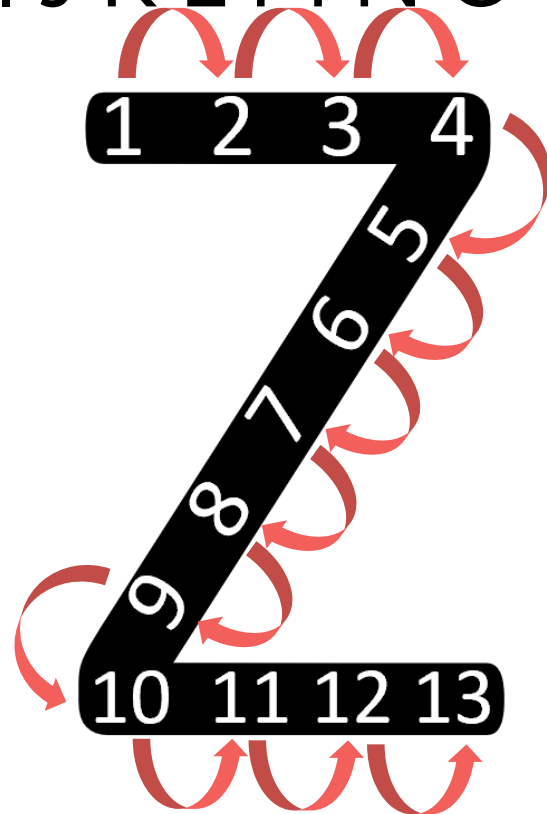
# NOESY (Nuclear Overhauser Effect Spectroscopy)

- přenos polarizace mezi jádry blízkými v prostoru
- 2D metoda
- intenzita signálu klesá s  $r^6$
- maximální dosah cca 5 Å (0.5 nm)
- obvykle mezi atomy  $^1\text{H}$



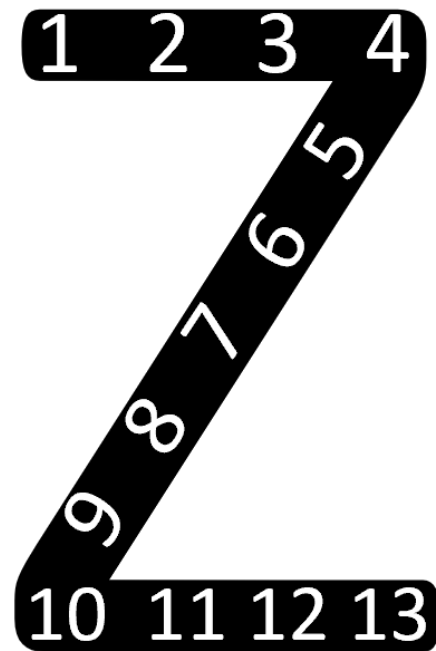
# Zjednodušené cvičení pro přiřazení NOESY – písmeno abecedy

A B C D E F G H I J K L M N O P Q R S T U V W X Y Z



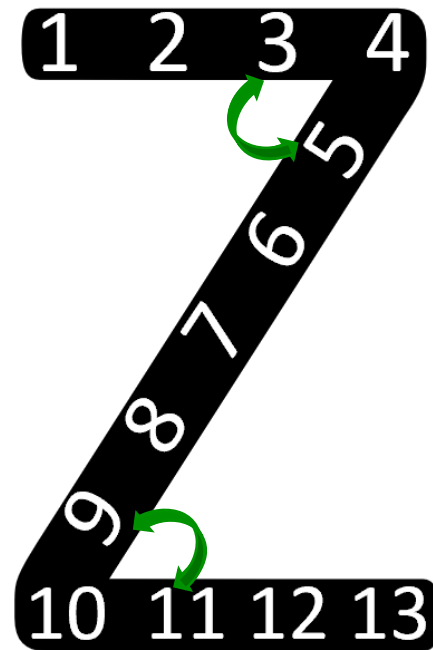
# Zjednodušené cvičení pro přiřazení NOESY – písmeno abecedy

A B C D E F G H I J K L M N O P Q R S T U V W X Y Z



# Zjednodušené cvičení pro přiřazení NOESY – písmeno abecedy

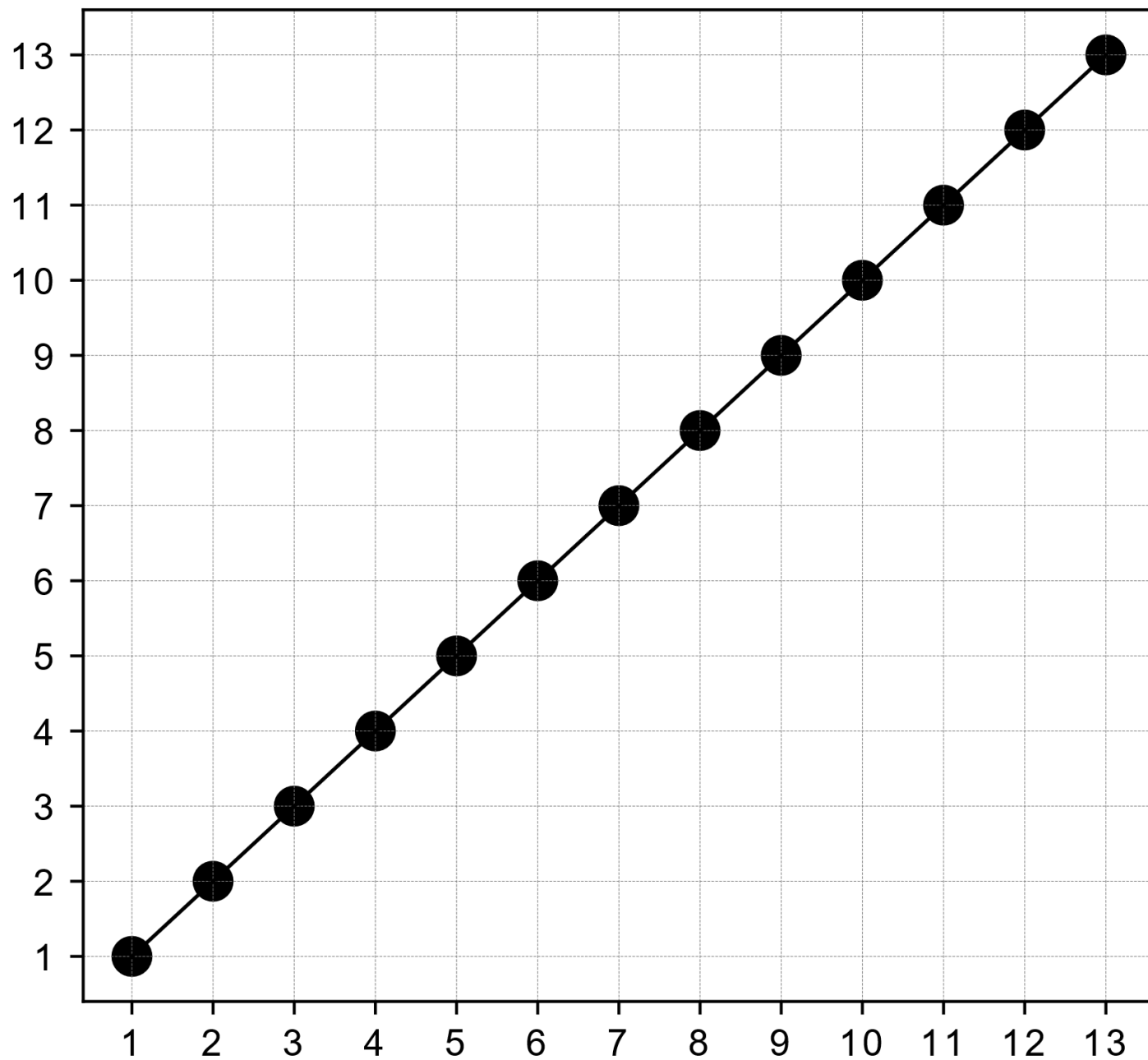
A B C D E F G H I J K L M N O P Q R S T U V W X Y Z



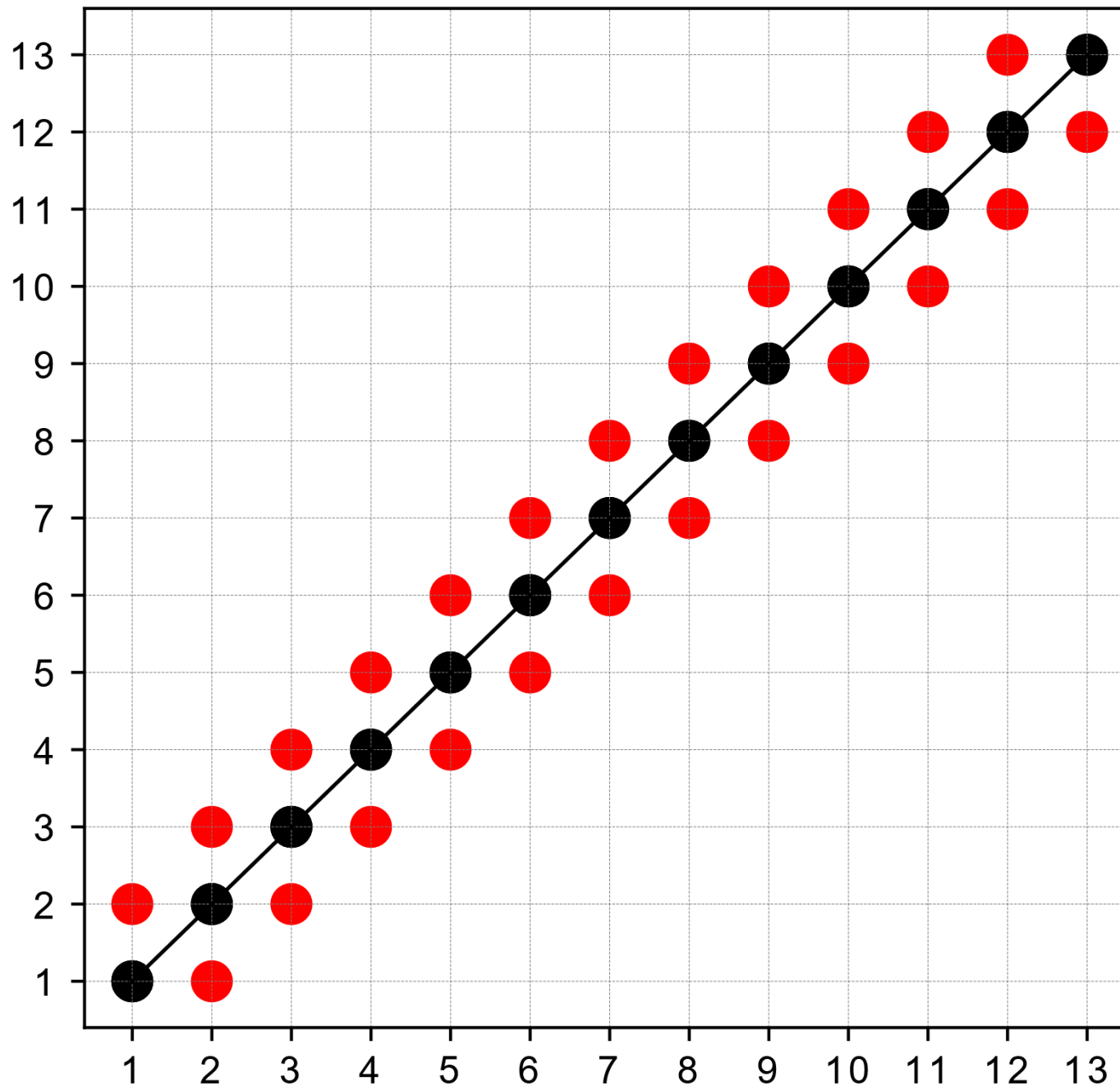


## Symetrie spektra

diagonální peak = vlastní  
(diagonal peak)



# Písmeno č. 1

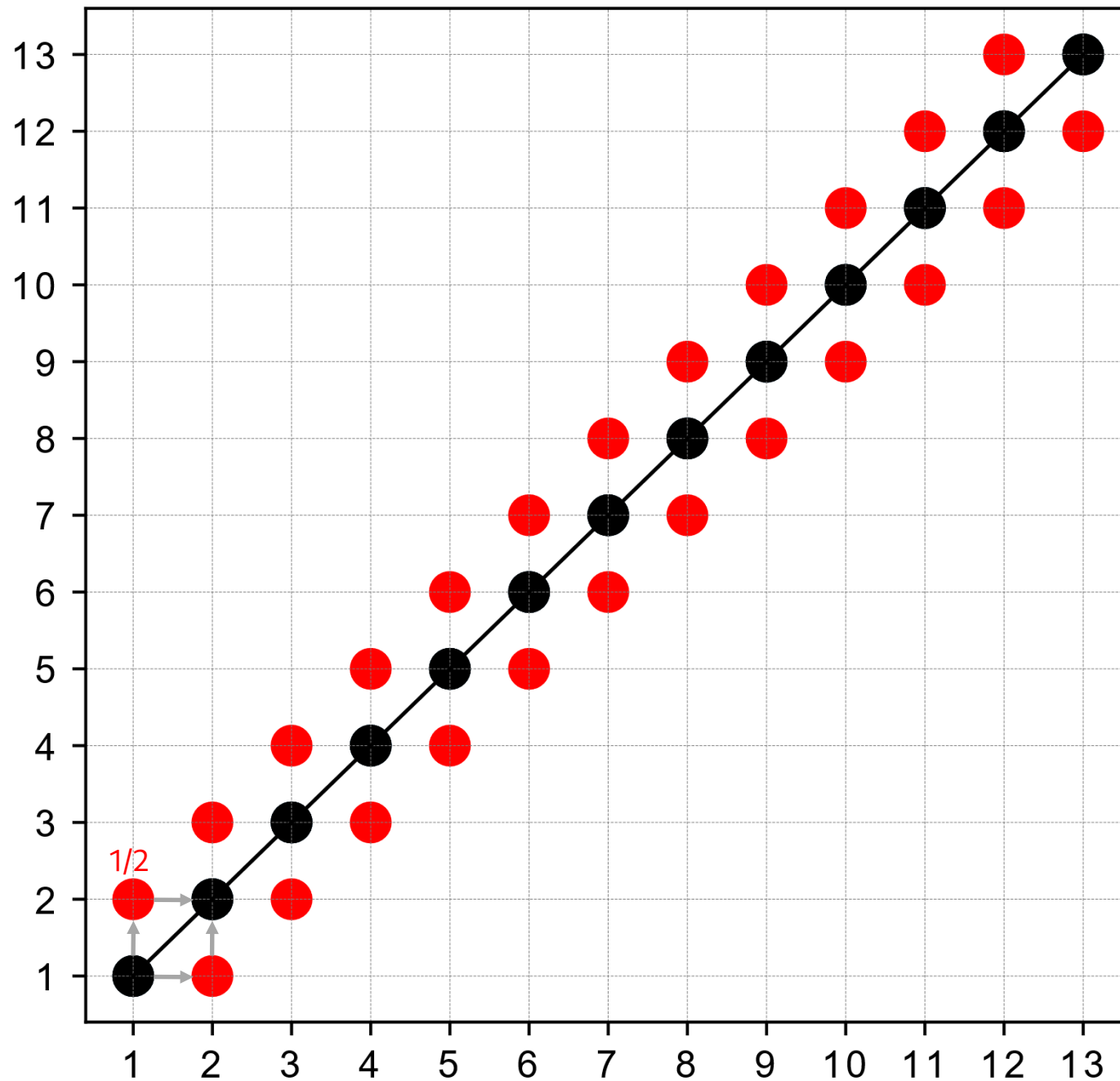


## Symetrie spektra

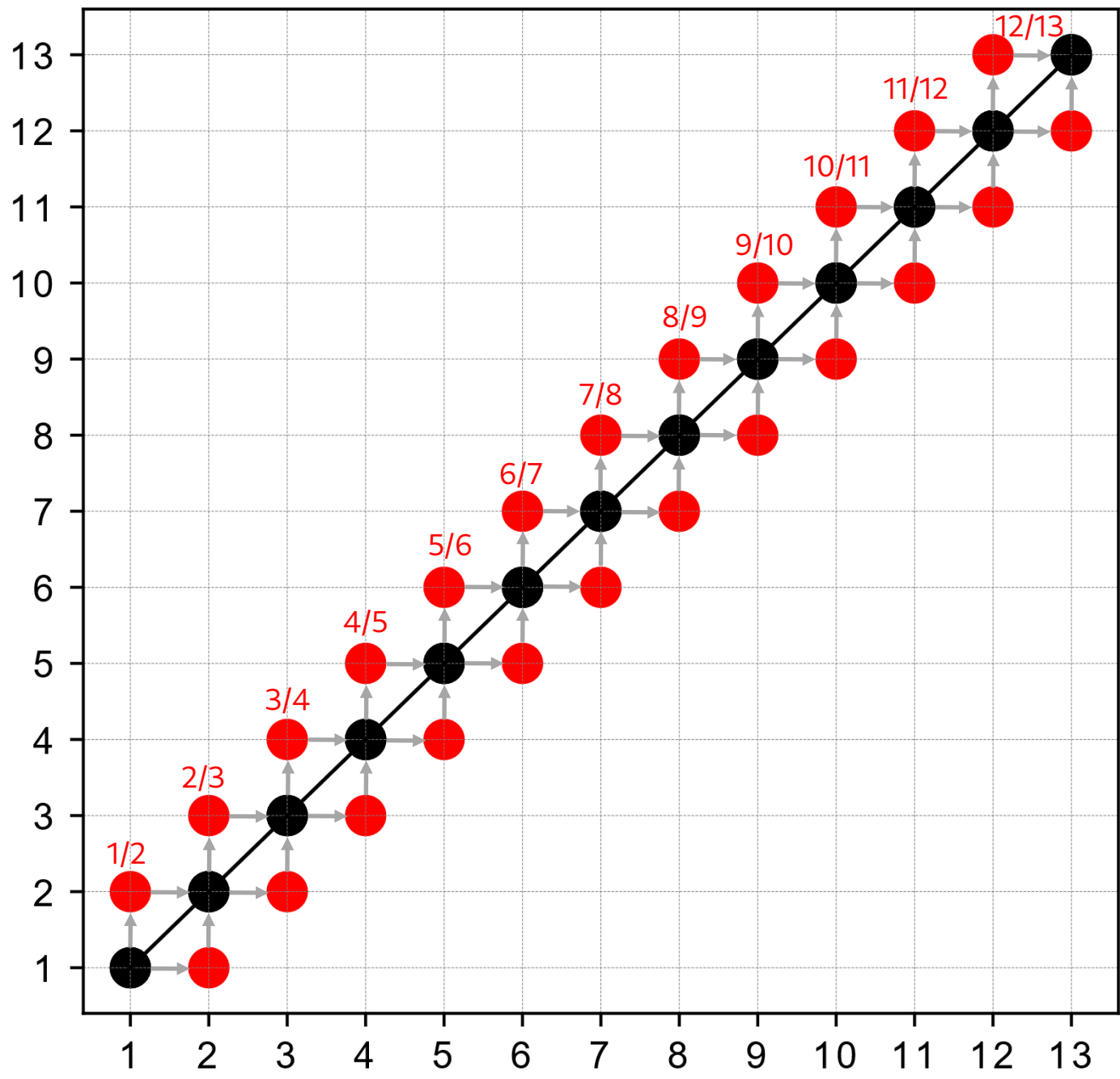
diagonální peak = vlastní  
(diagonal peak)

nediagonální peak = interakce  
(cross-peak)

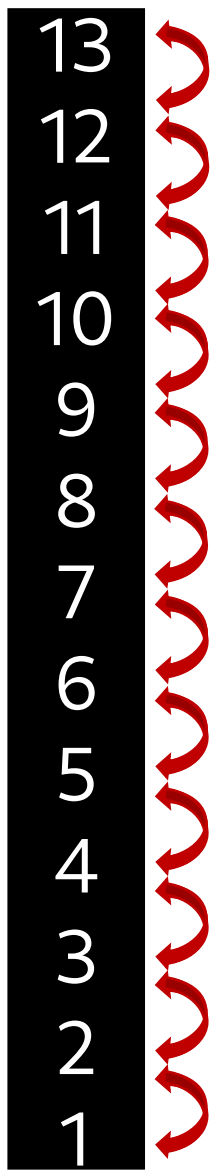
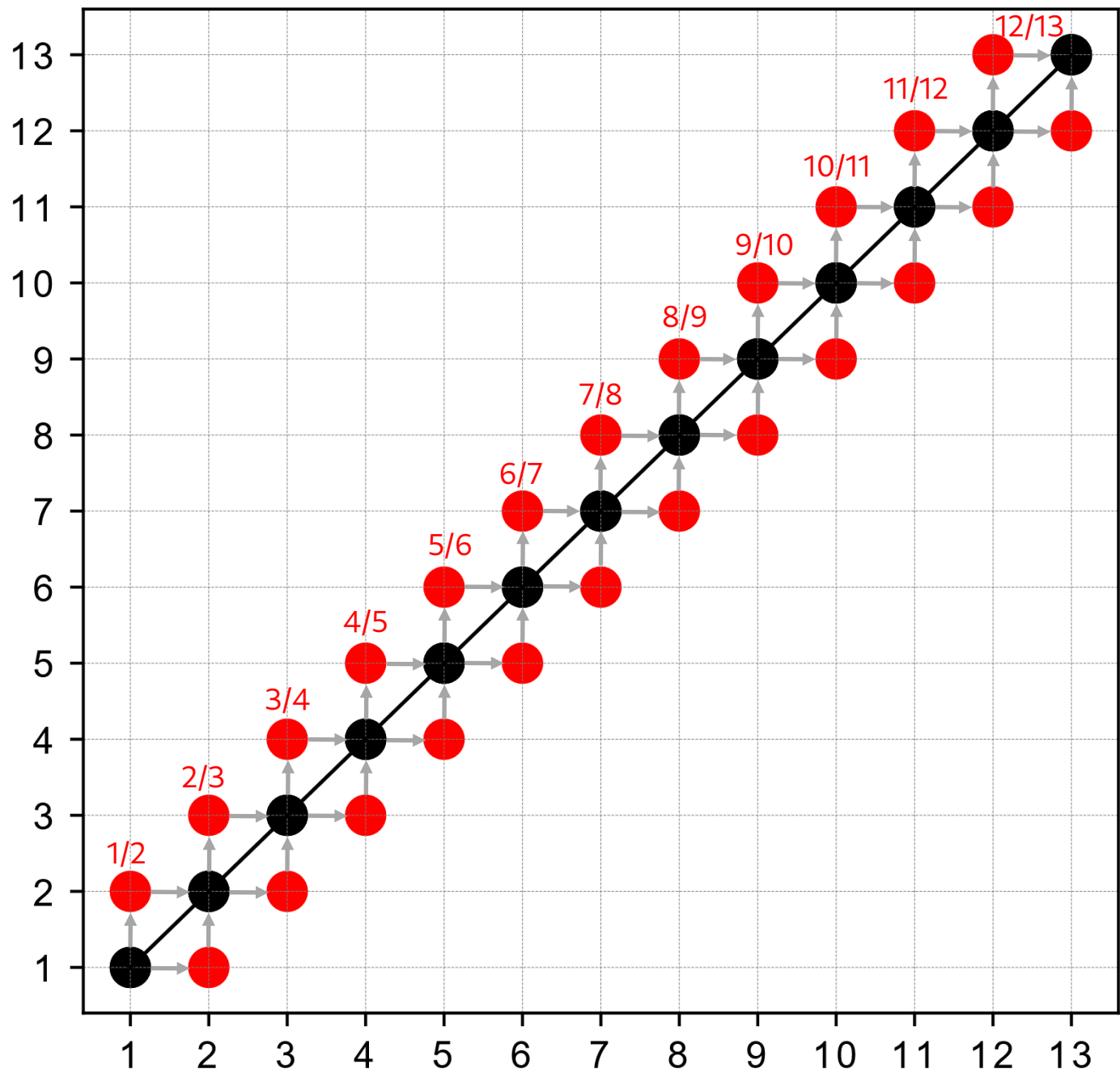
# Písmeno č. 1



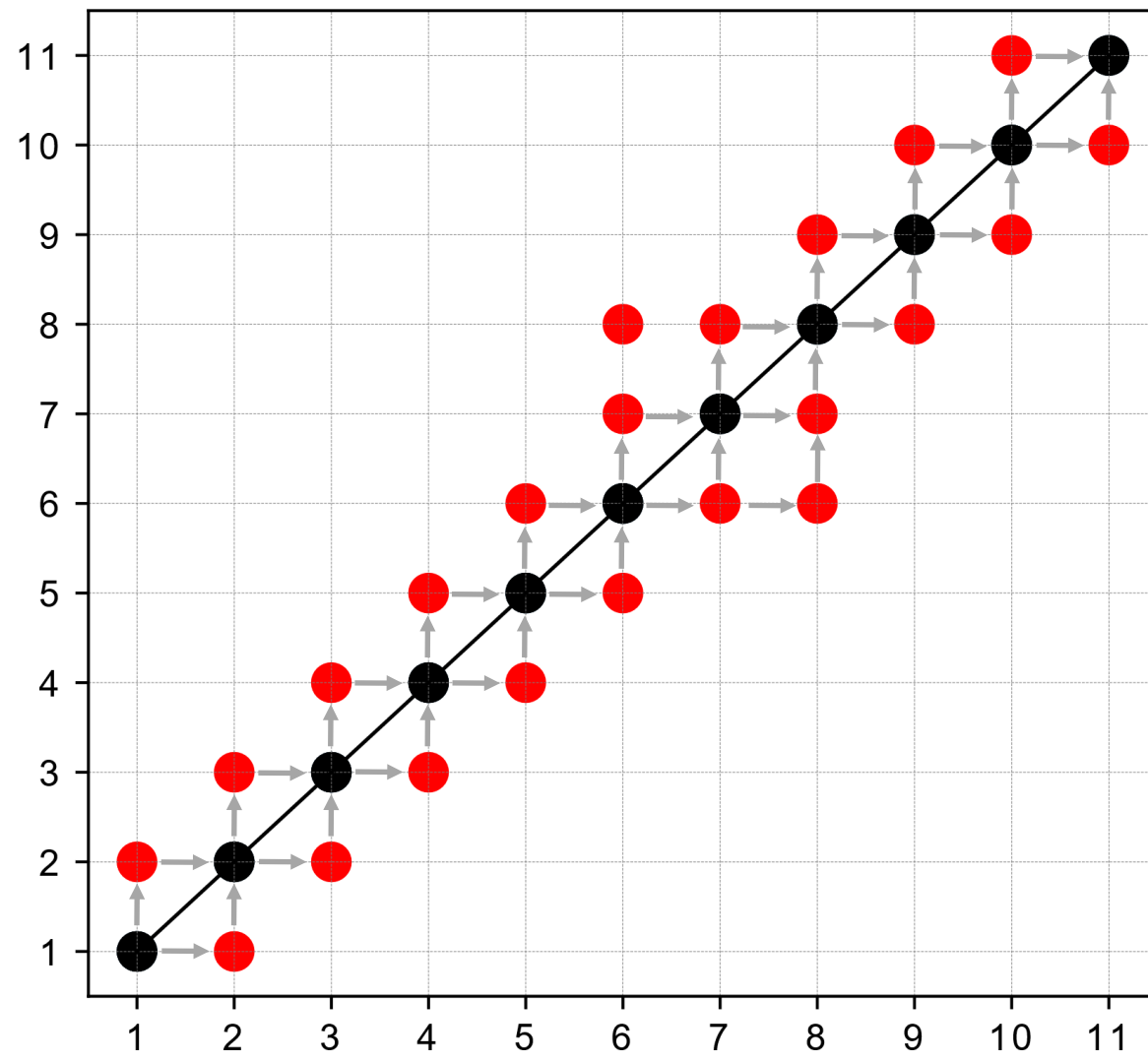
# Písmeno č. 1



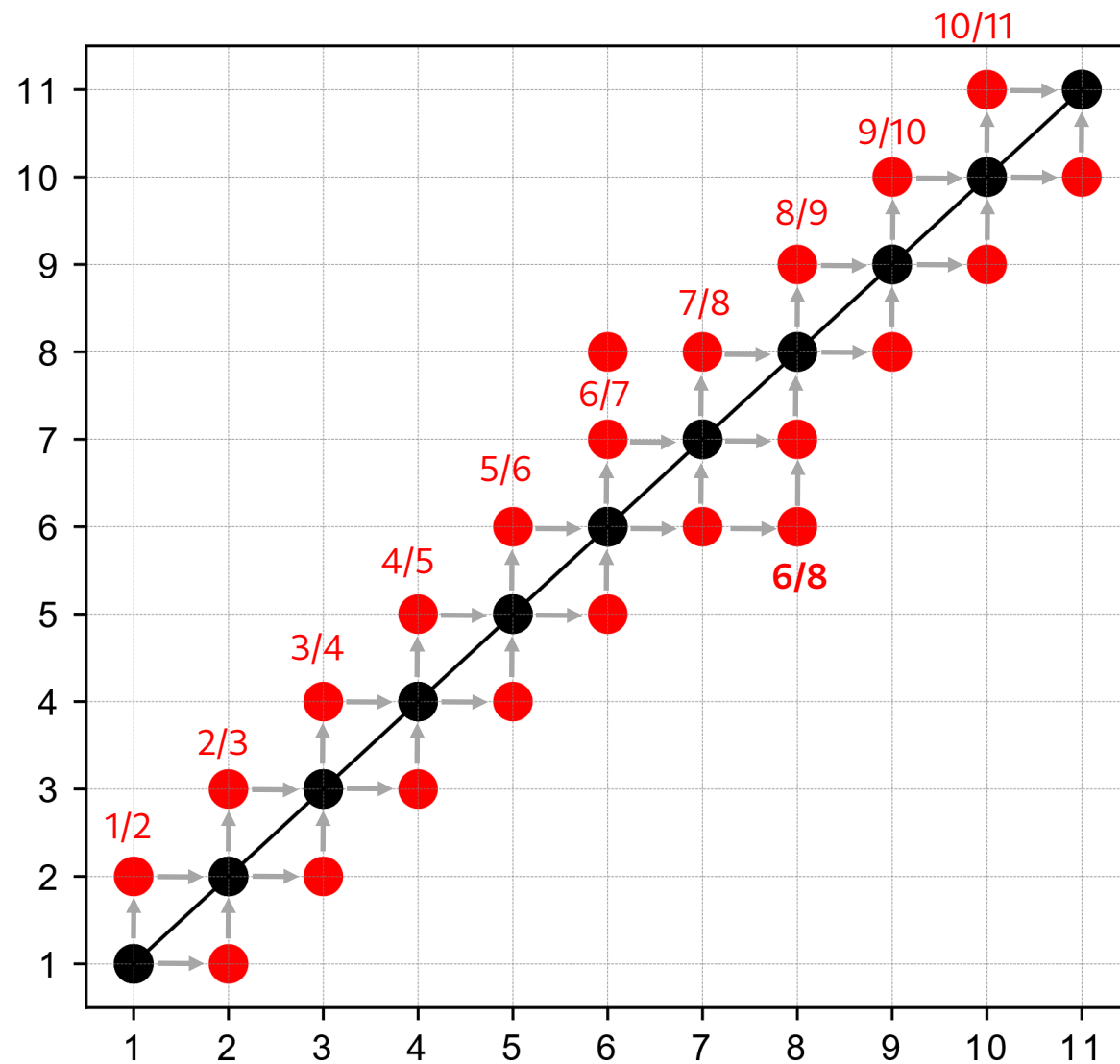
# Písmeno č. 1



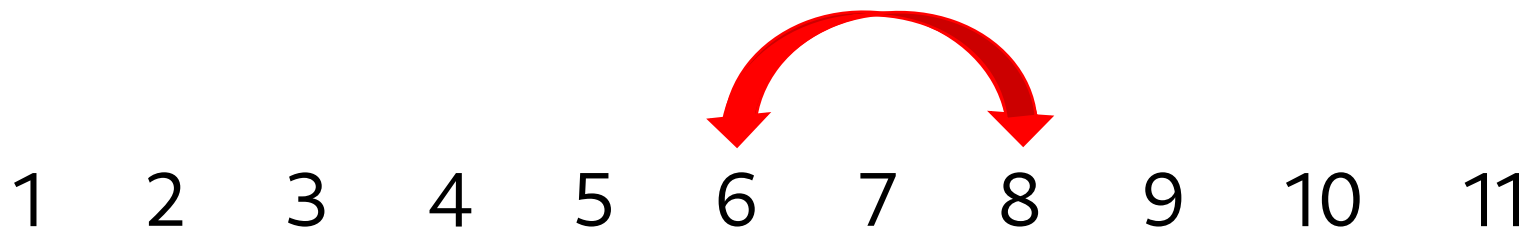
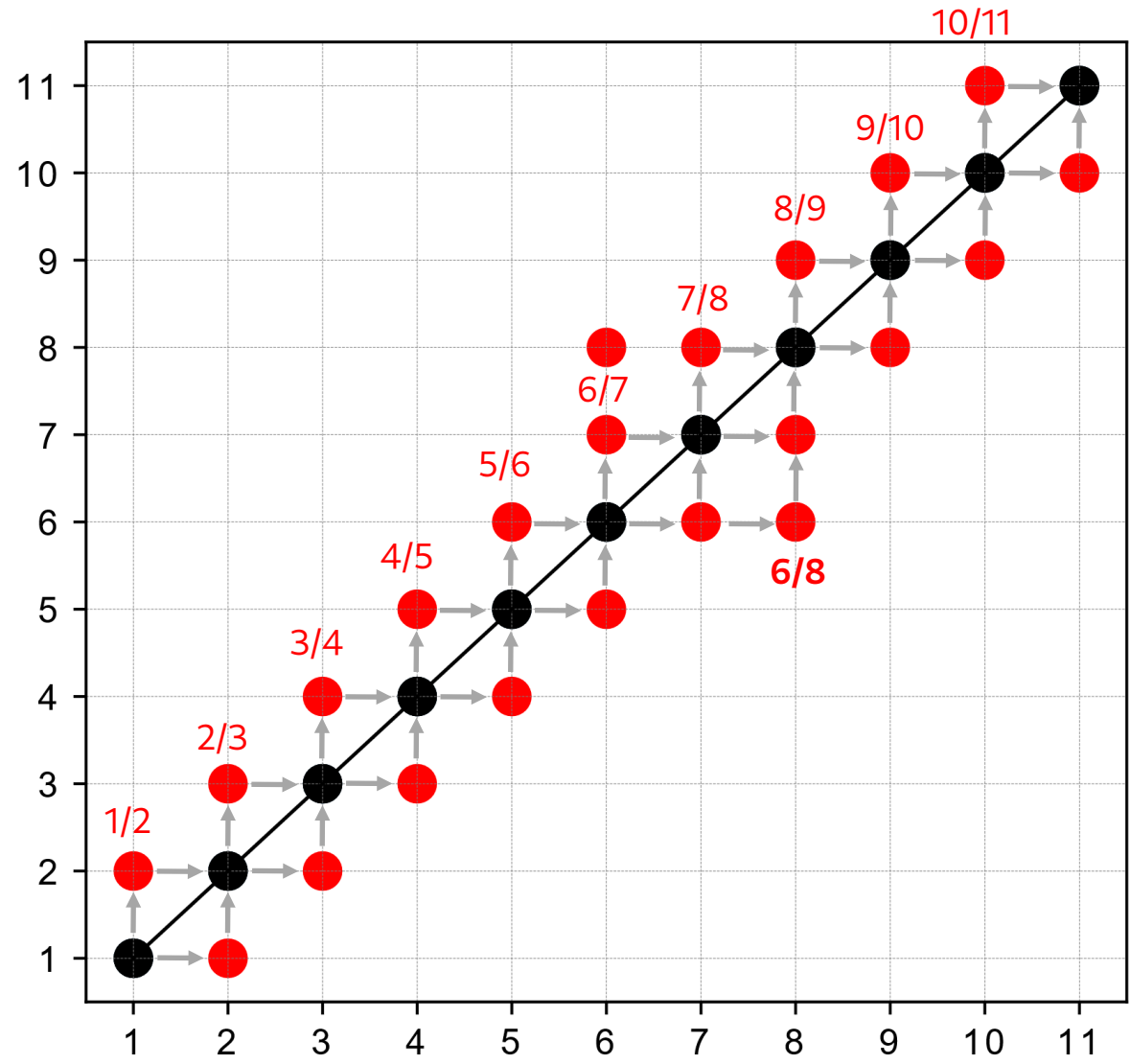
# Písmeno č. 2



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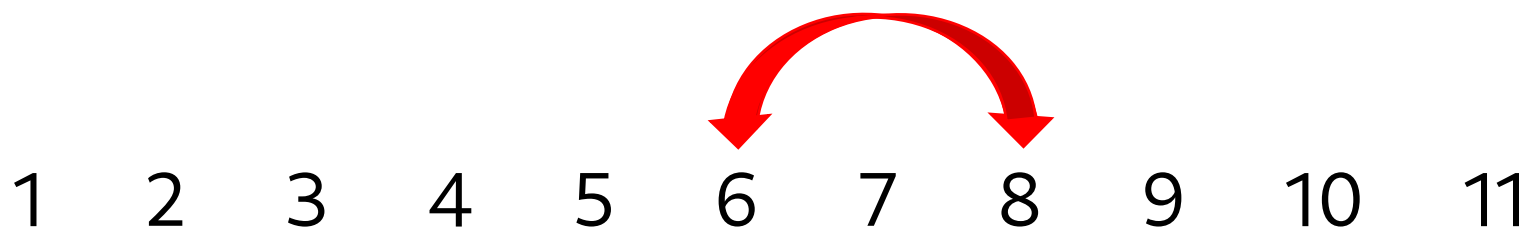
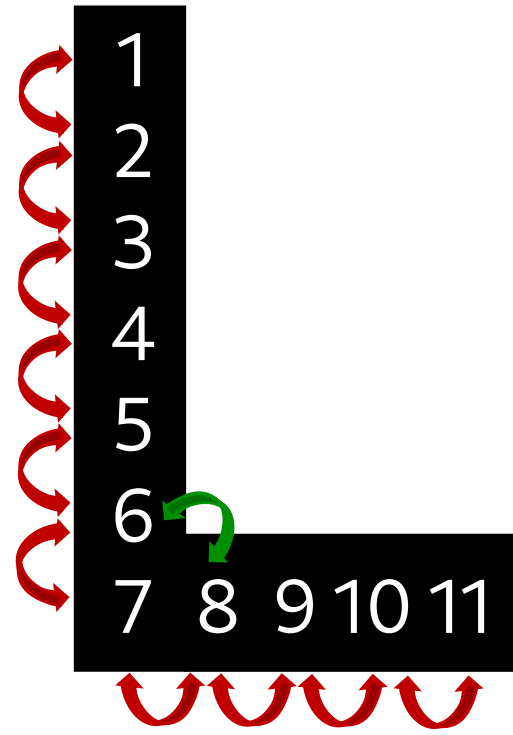
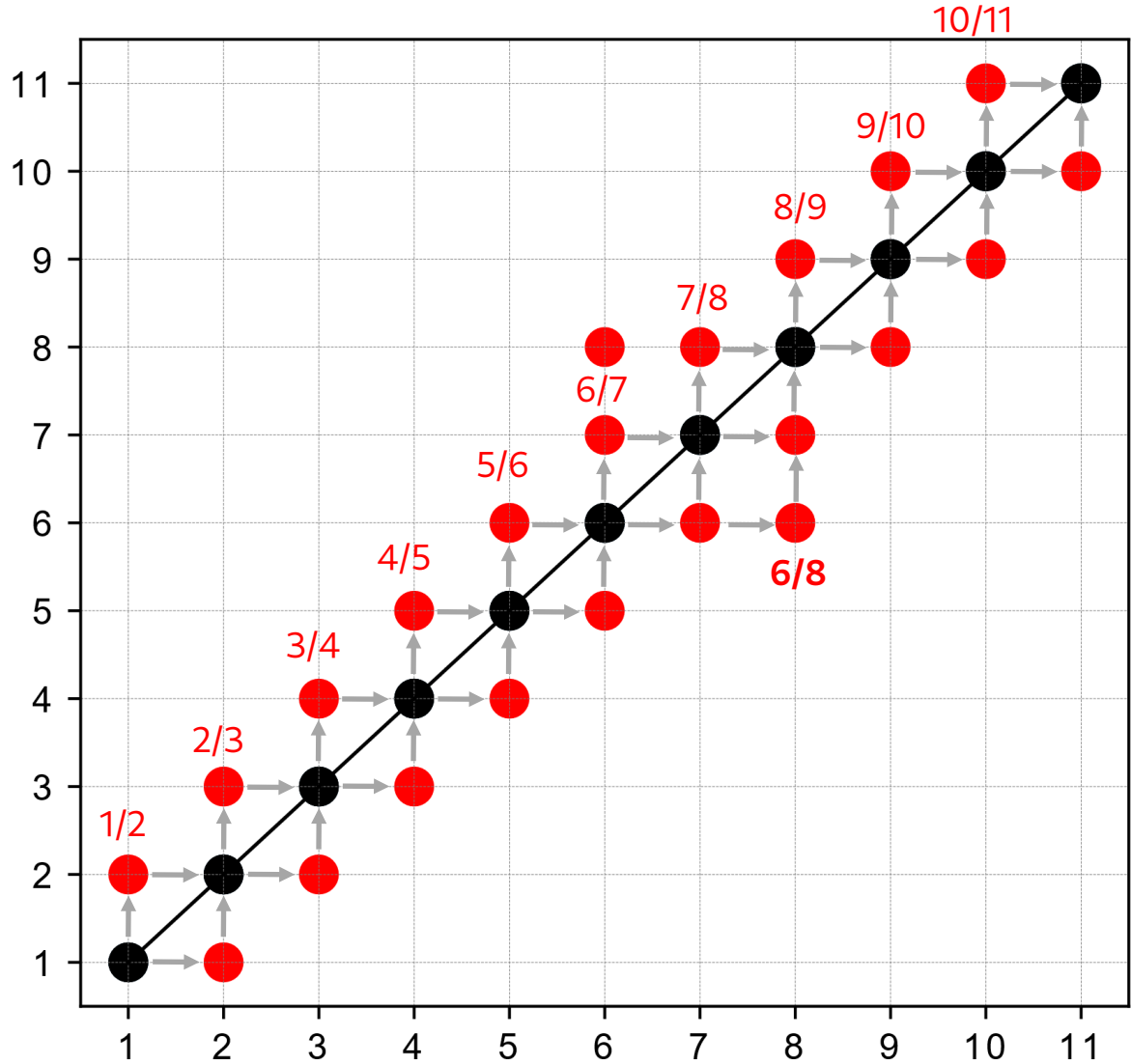


# Písmeno č. 2





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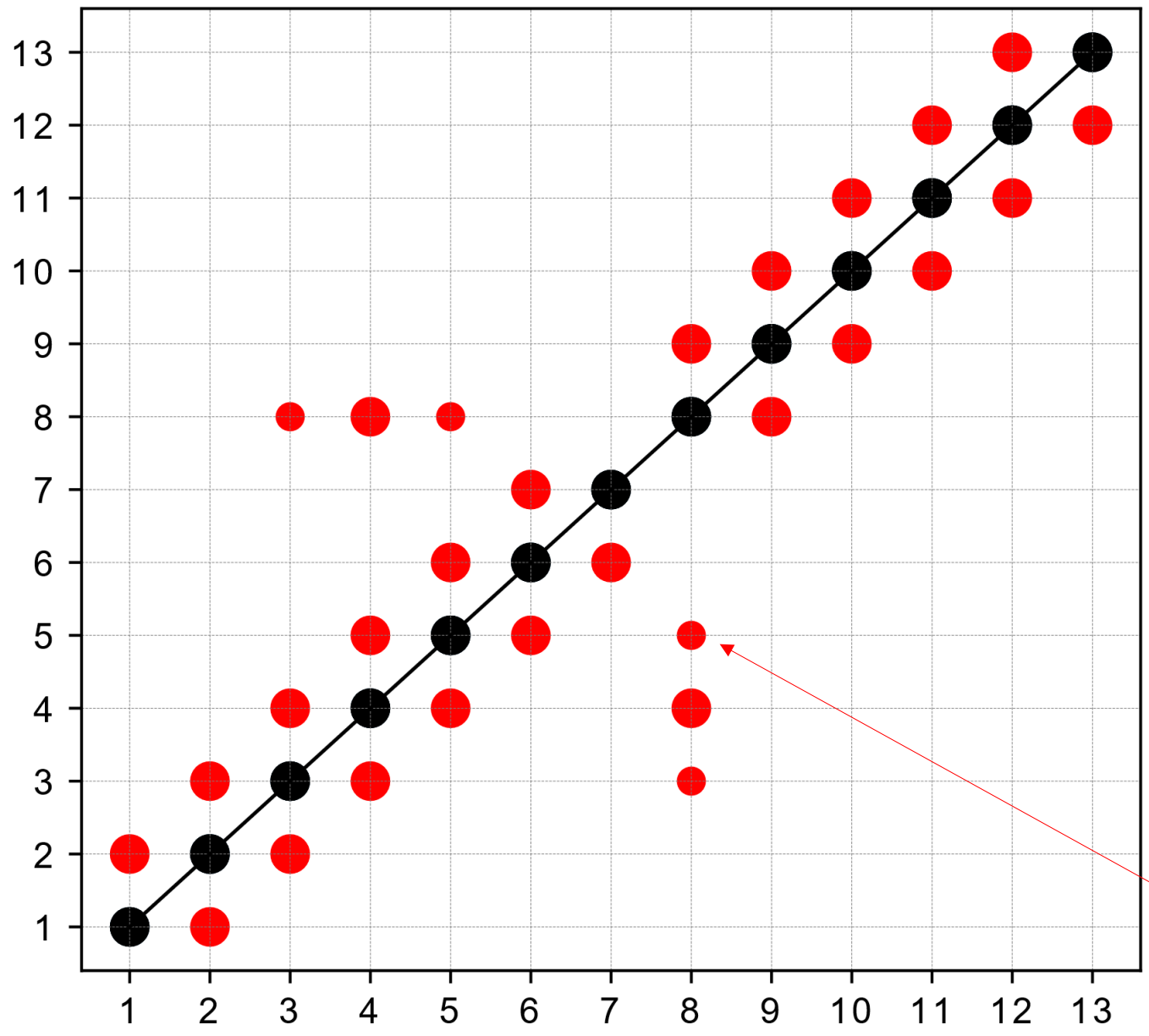


# Písmeno č. 3

## Symetrie spektra

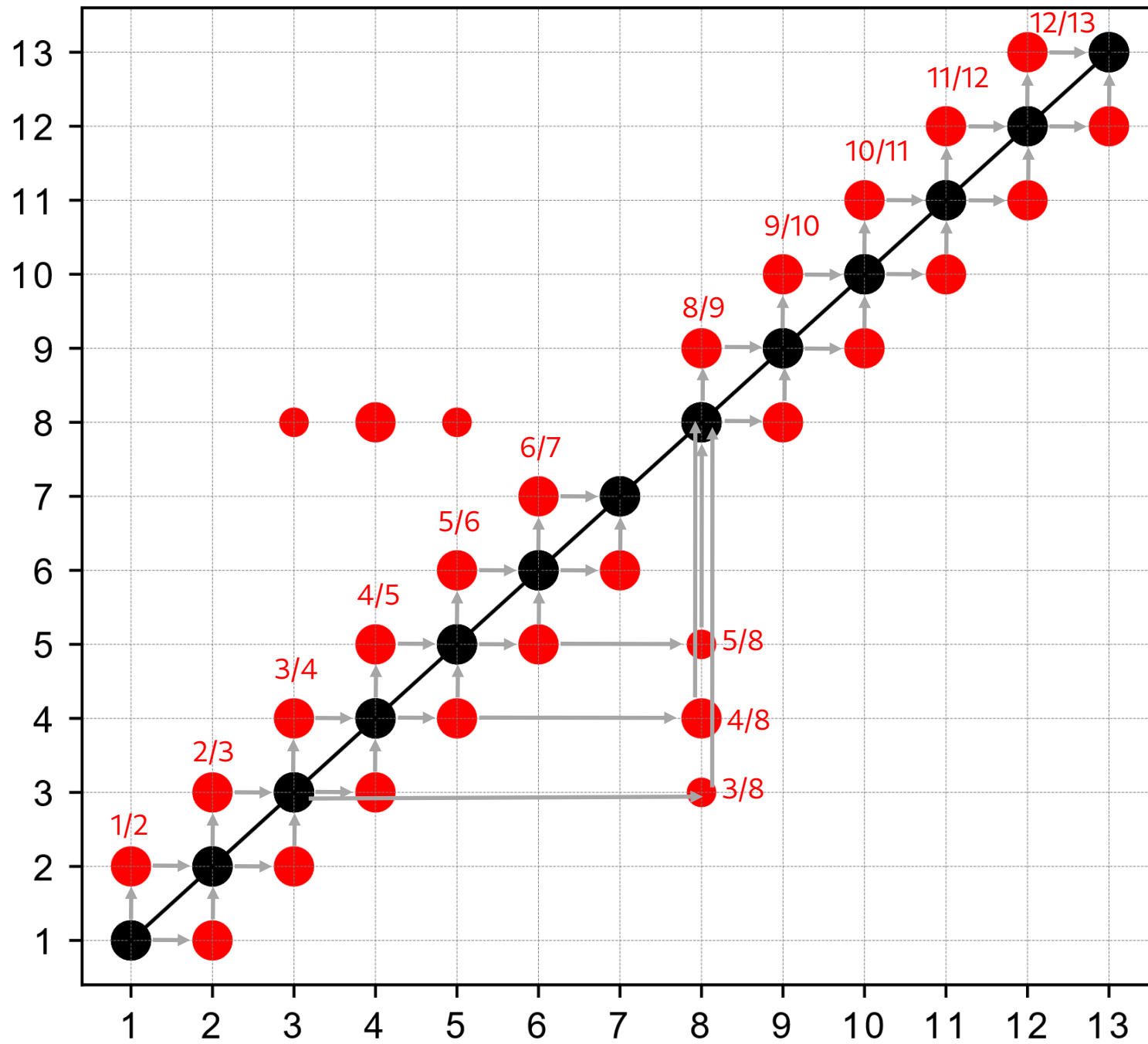
diagonální peak = vlastní (diagonal peak)

nediagonální peak = interakce (cross-peak)

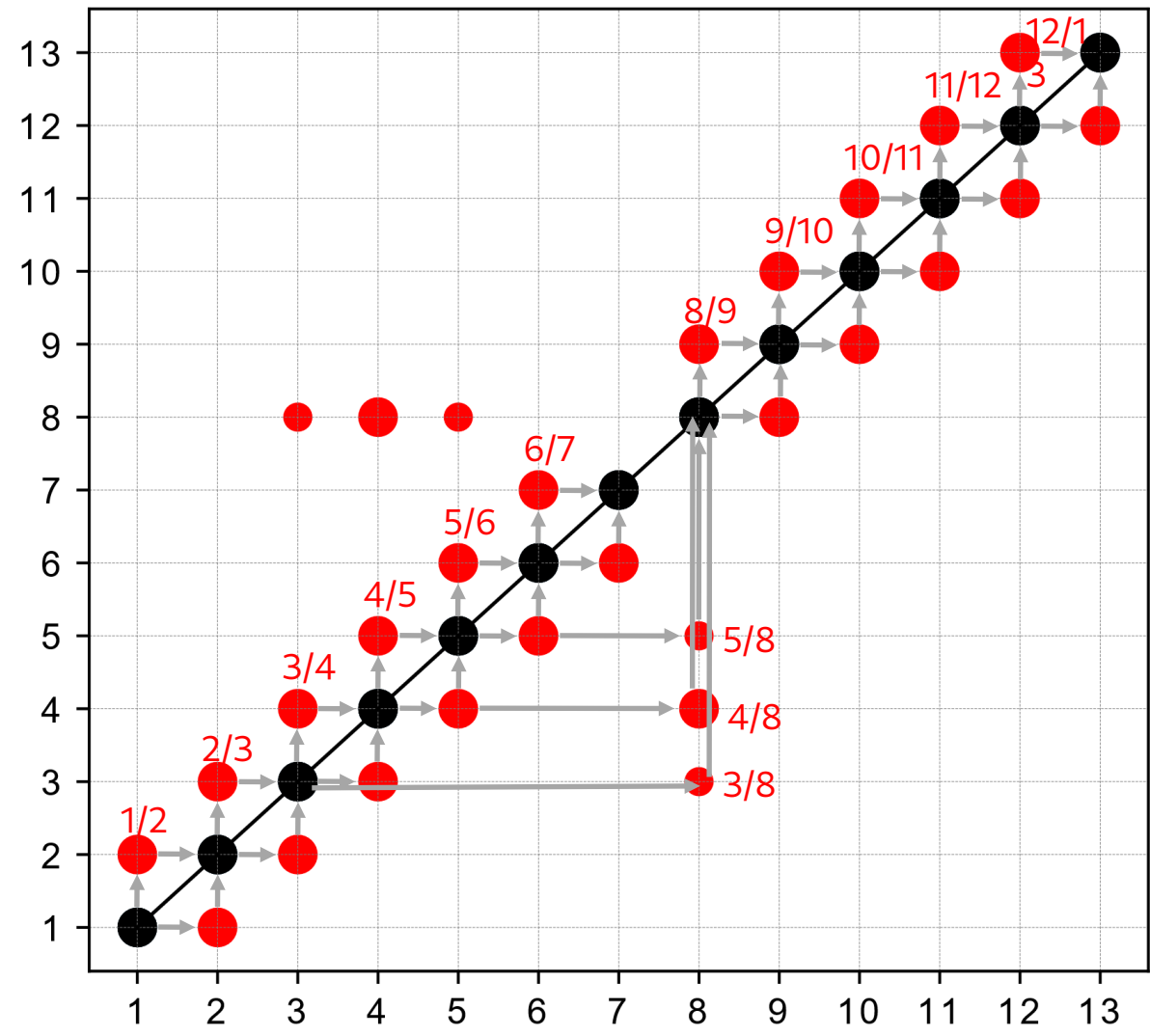


5. menší interakce = jsou od sebe dál

# Písmeno č. 3

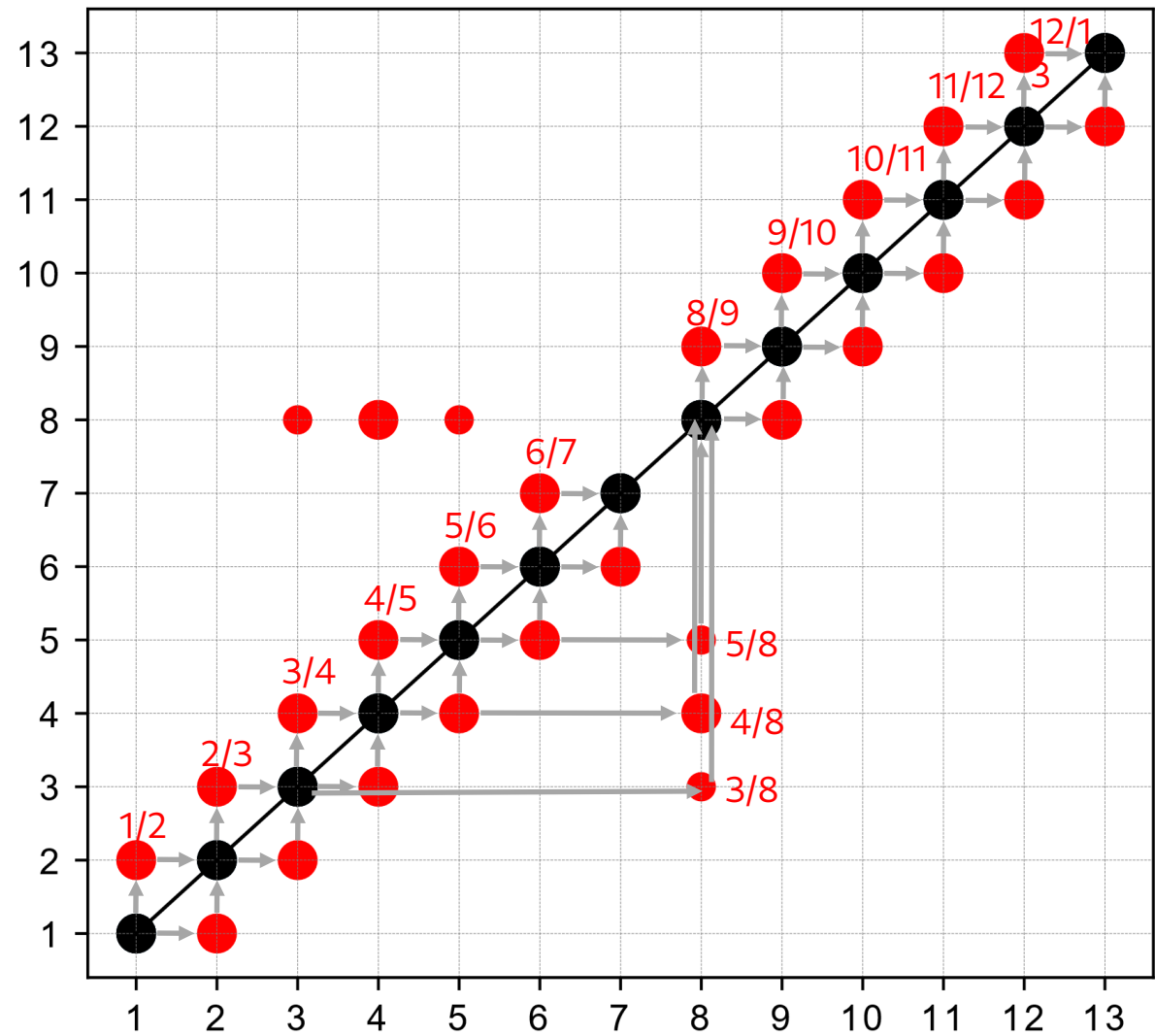


# Písmeno č. 3



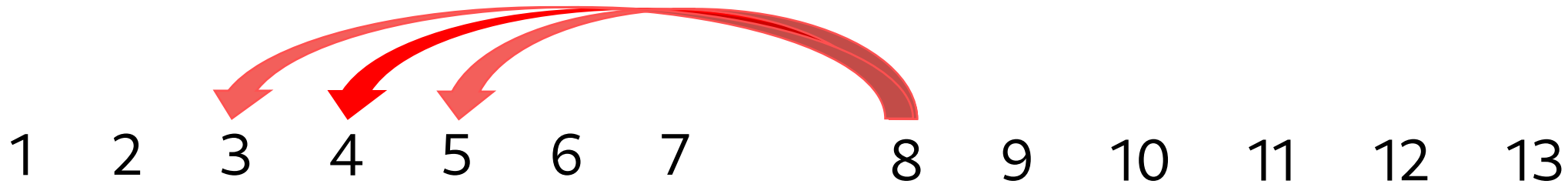
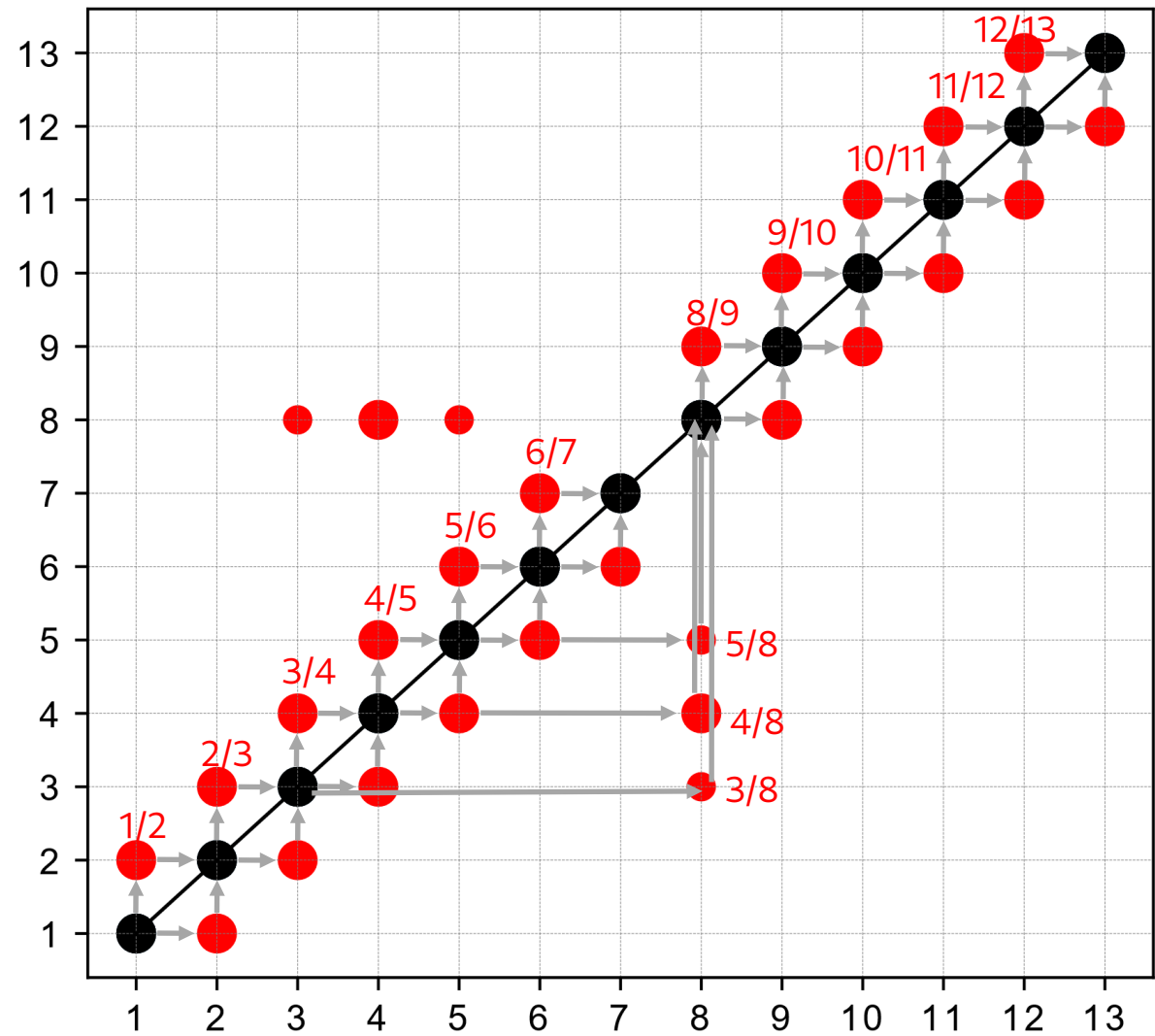
1 2 3 4 5 6 7

# Písmeno č. 3

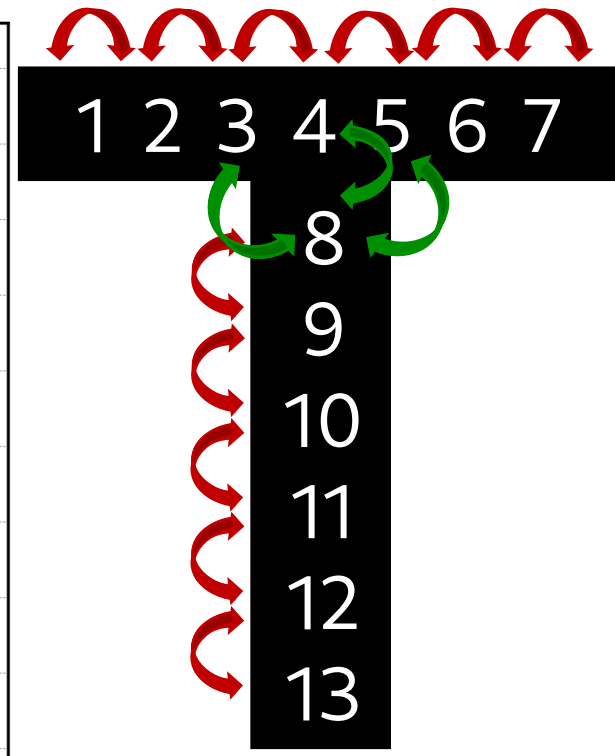
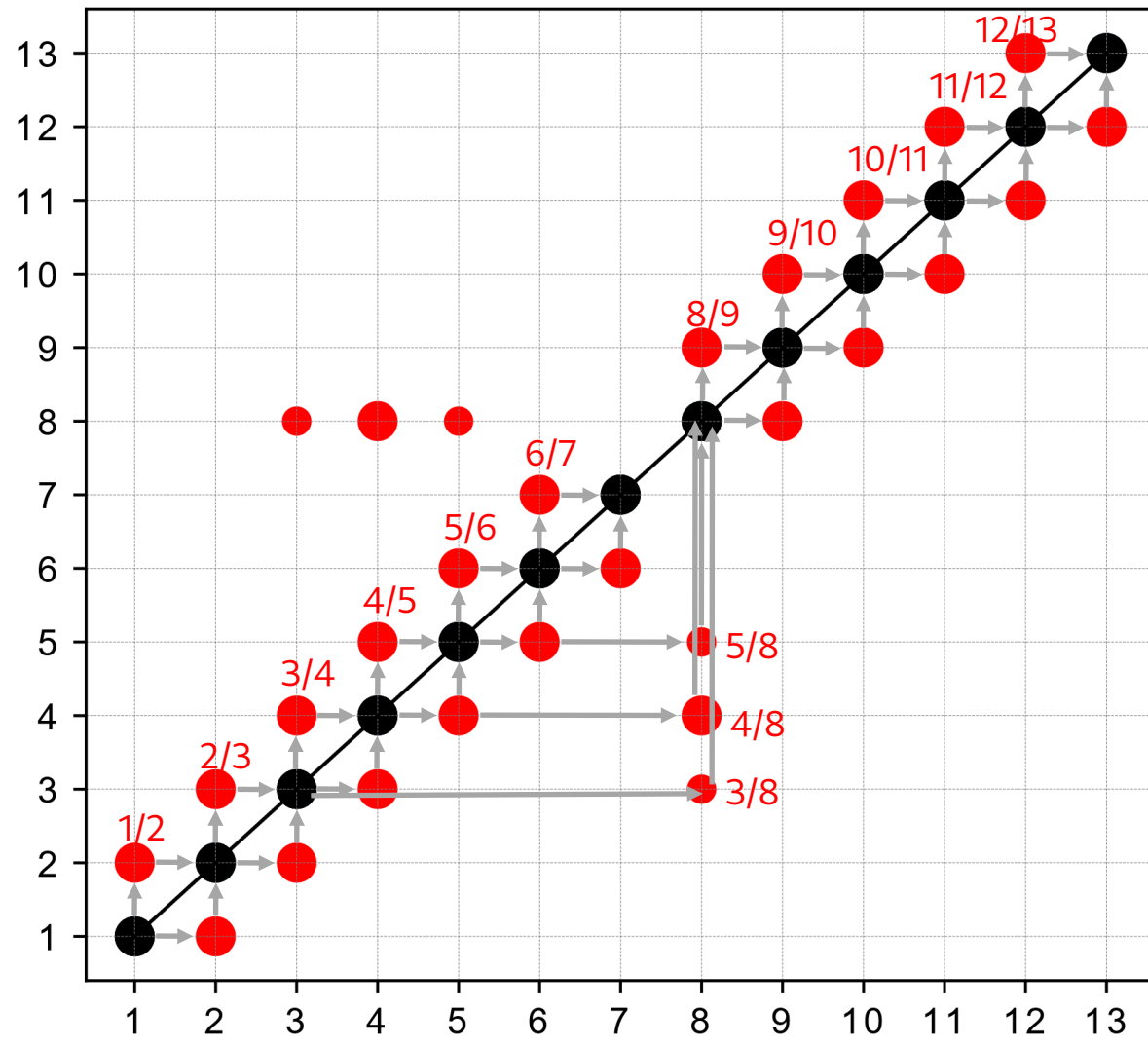


1 2 3 4 5 6 7 8 9 10 11 12 13

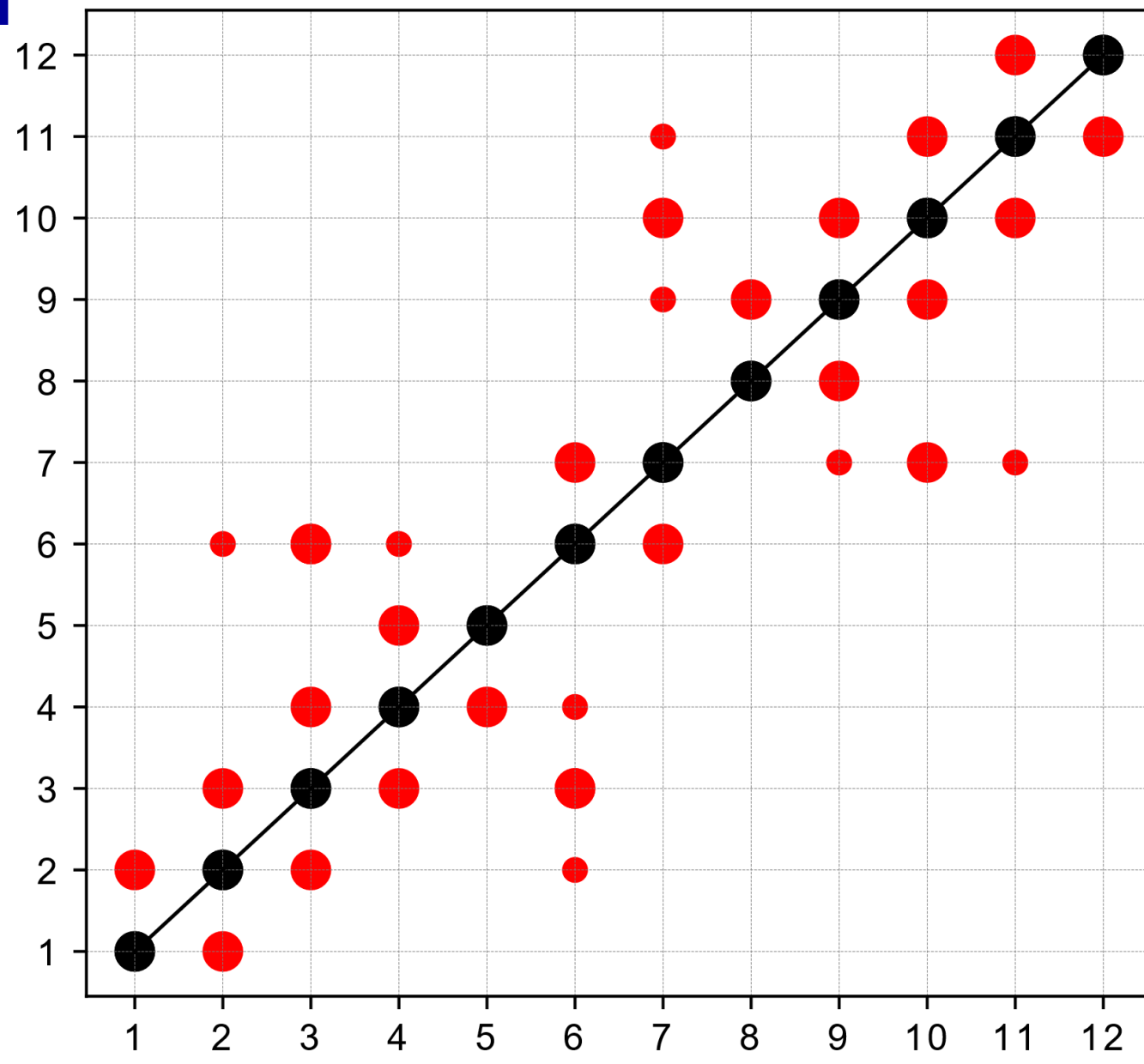
# Písmeno č. 3



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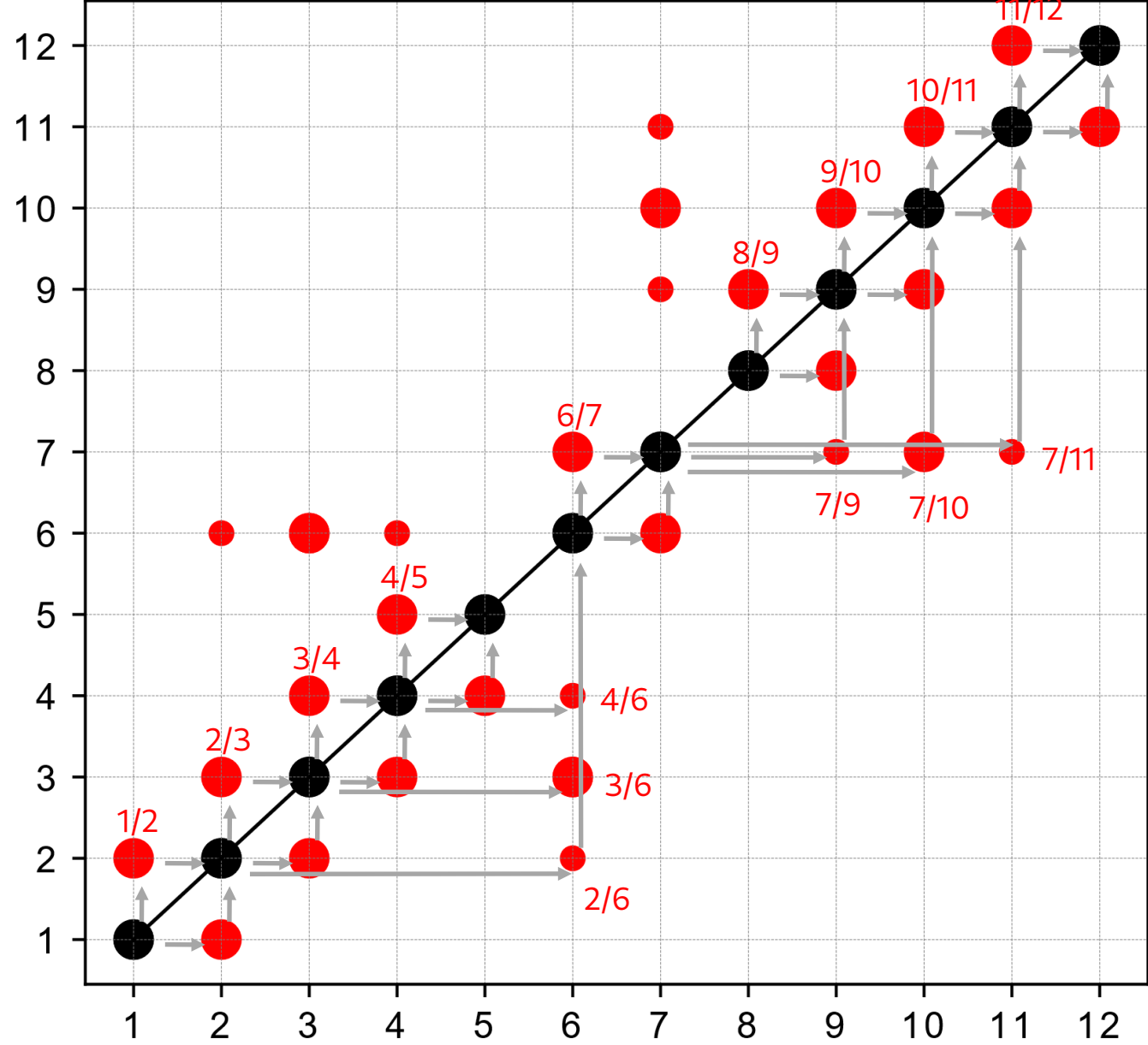


# Písmeno č. 4



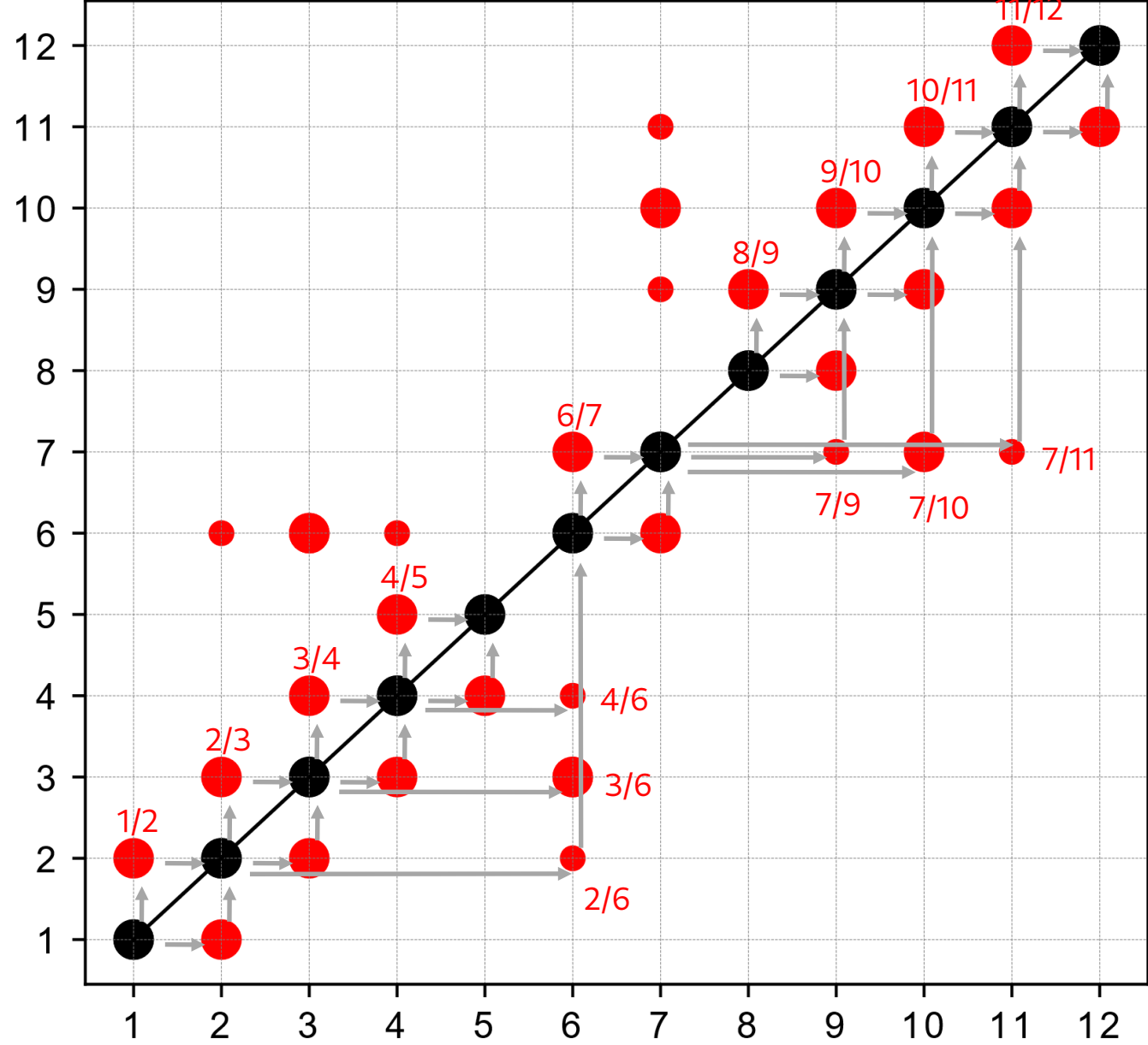


# Písmeno č. 4

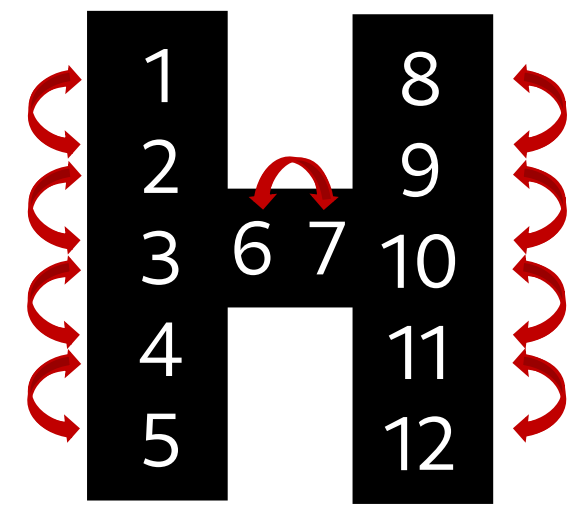
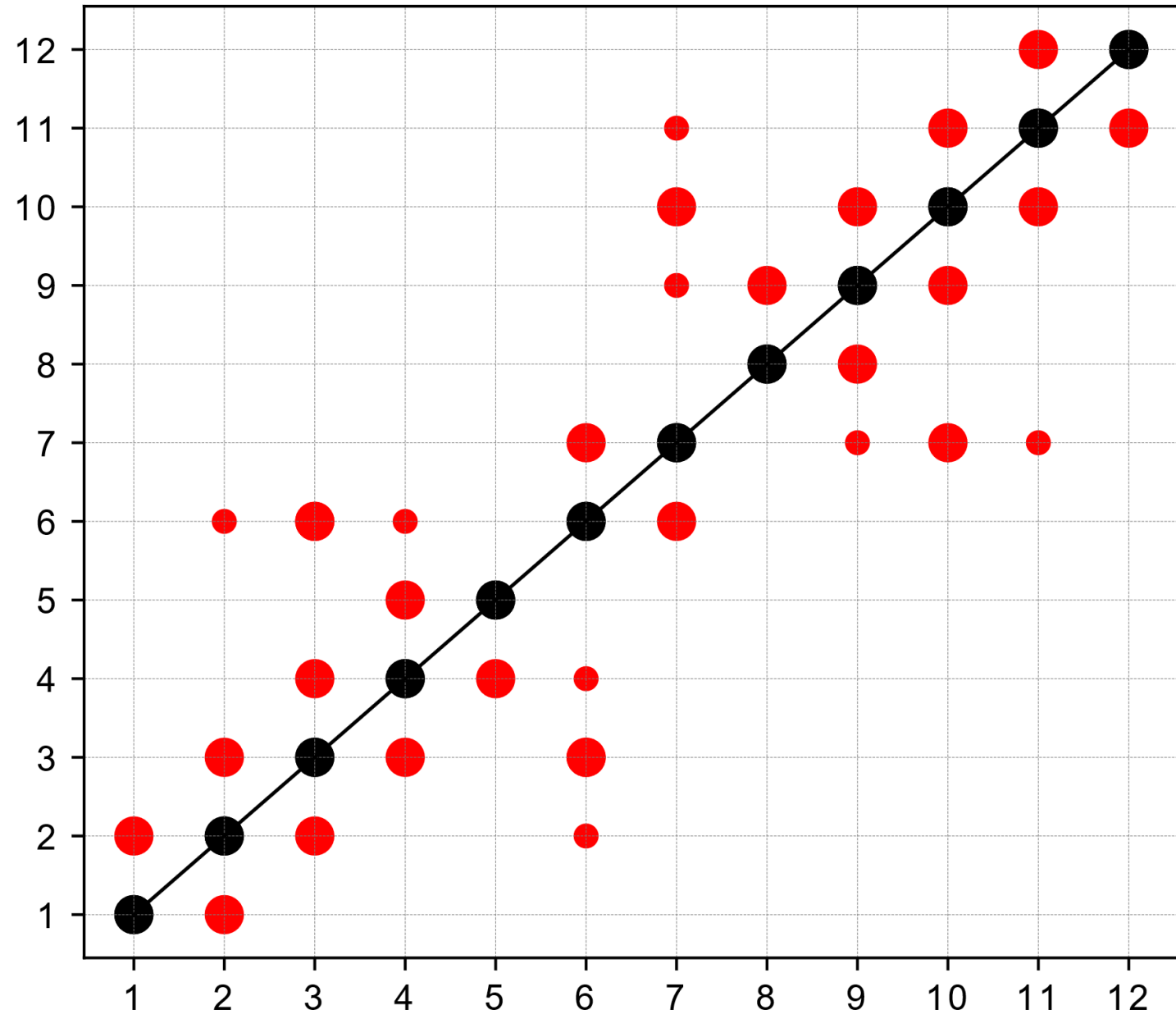


1 2 3 4 5 6 7 8 9 10 11 12

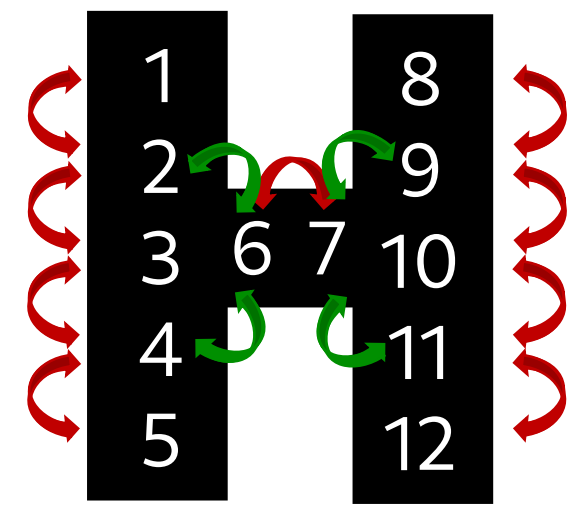
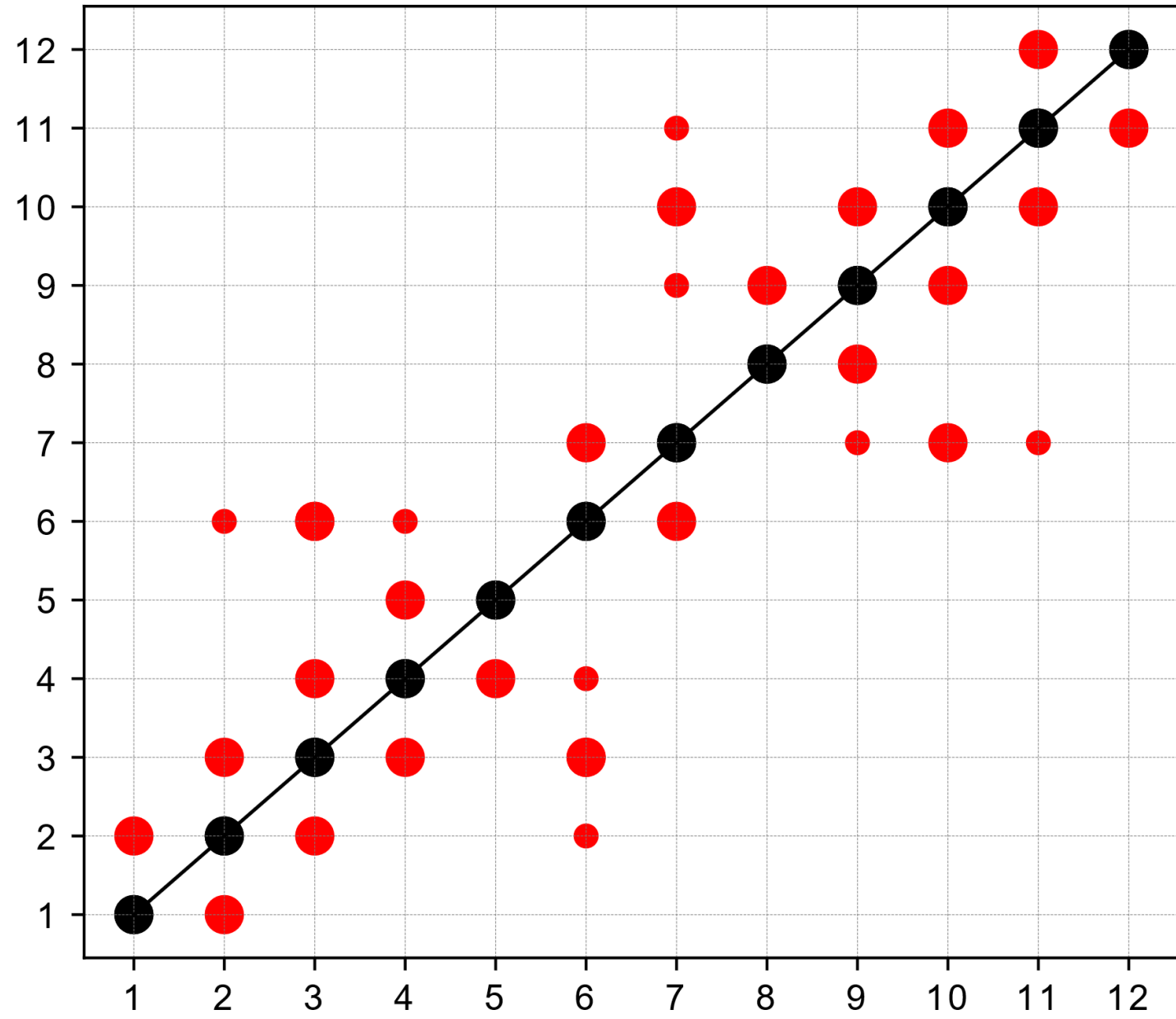
# Písmeno č. 4



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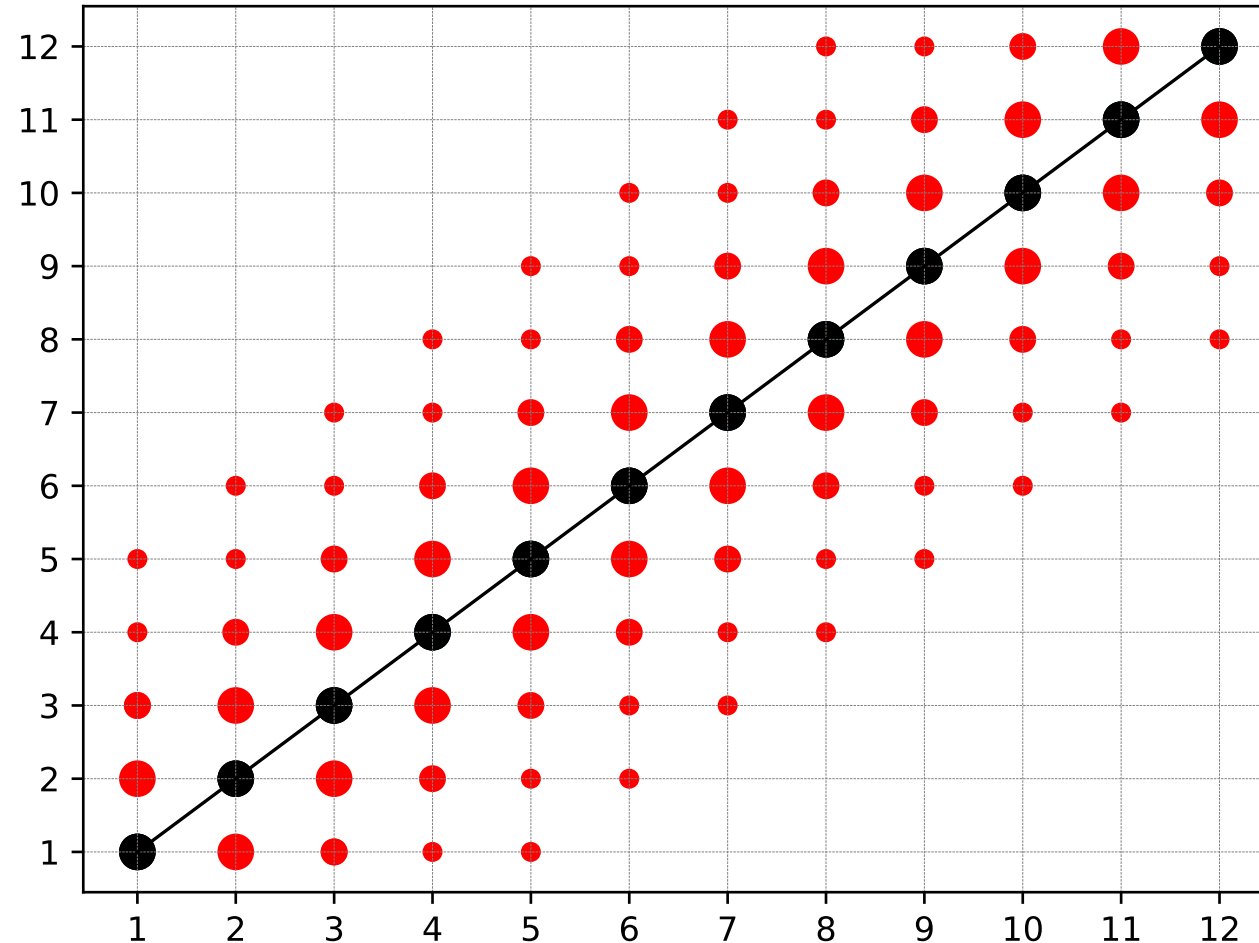


# Písmeno č. 4

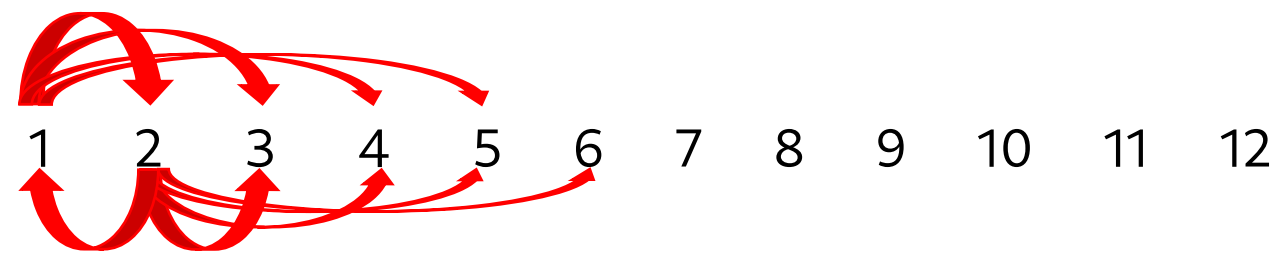
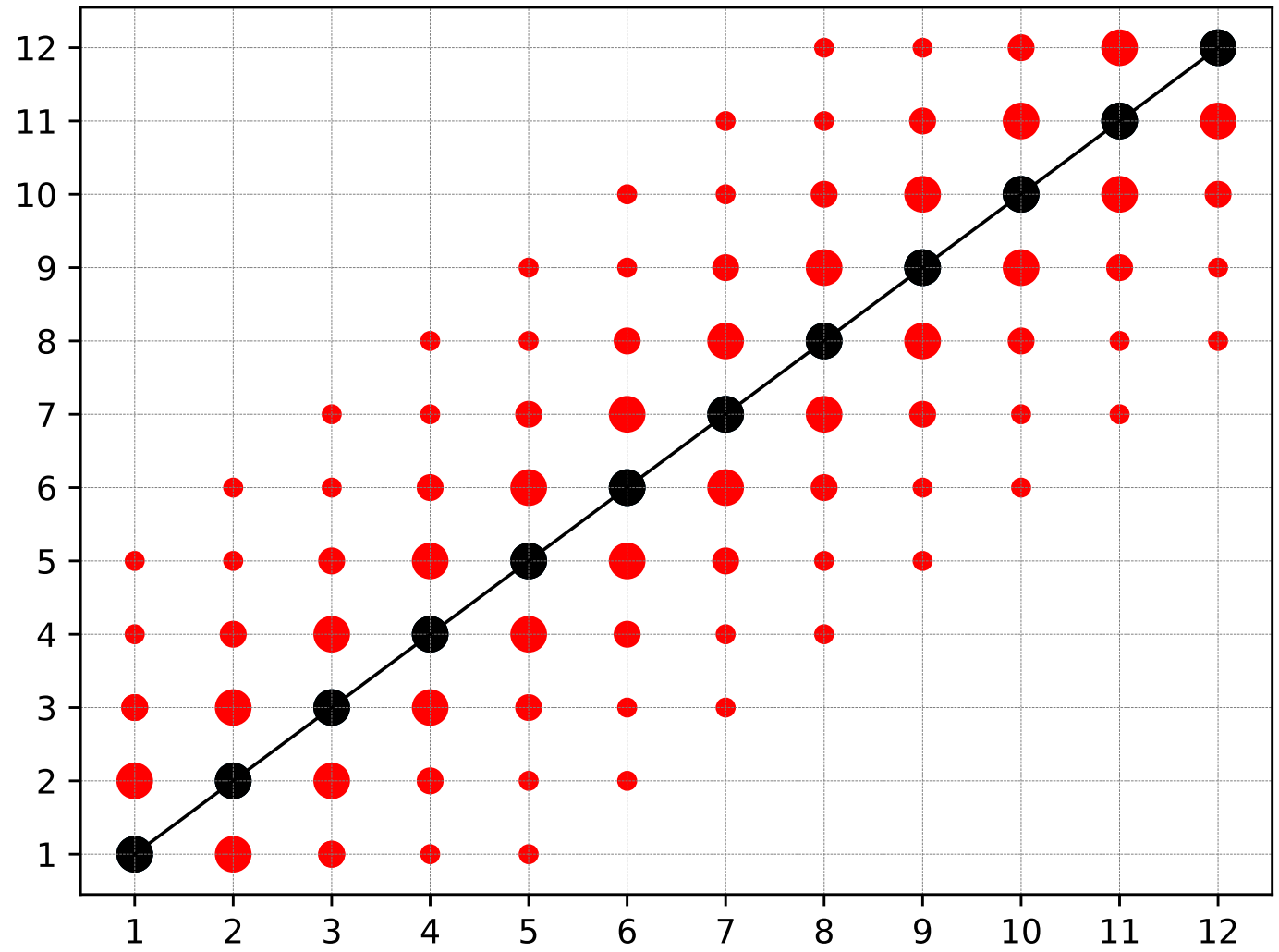


# Zjednoduř. cvičení pro přiřazení NOESY – sekundární struktury

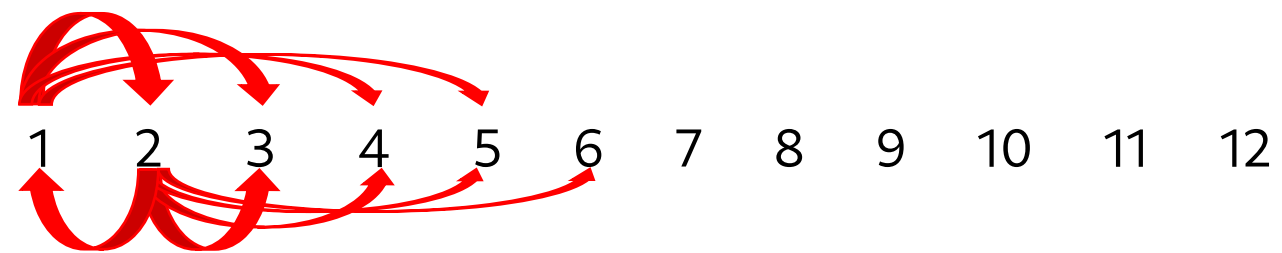
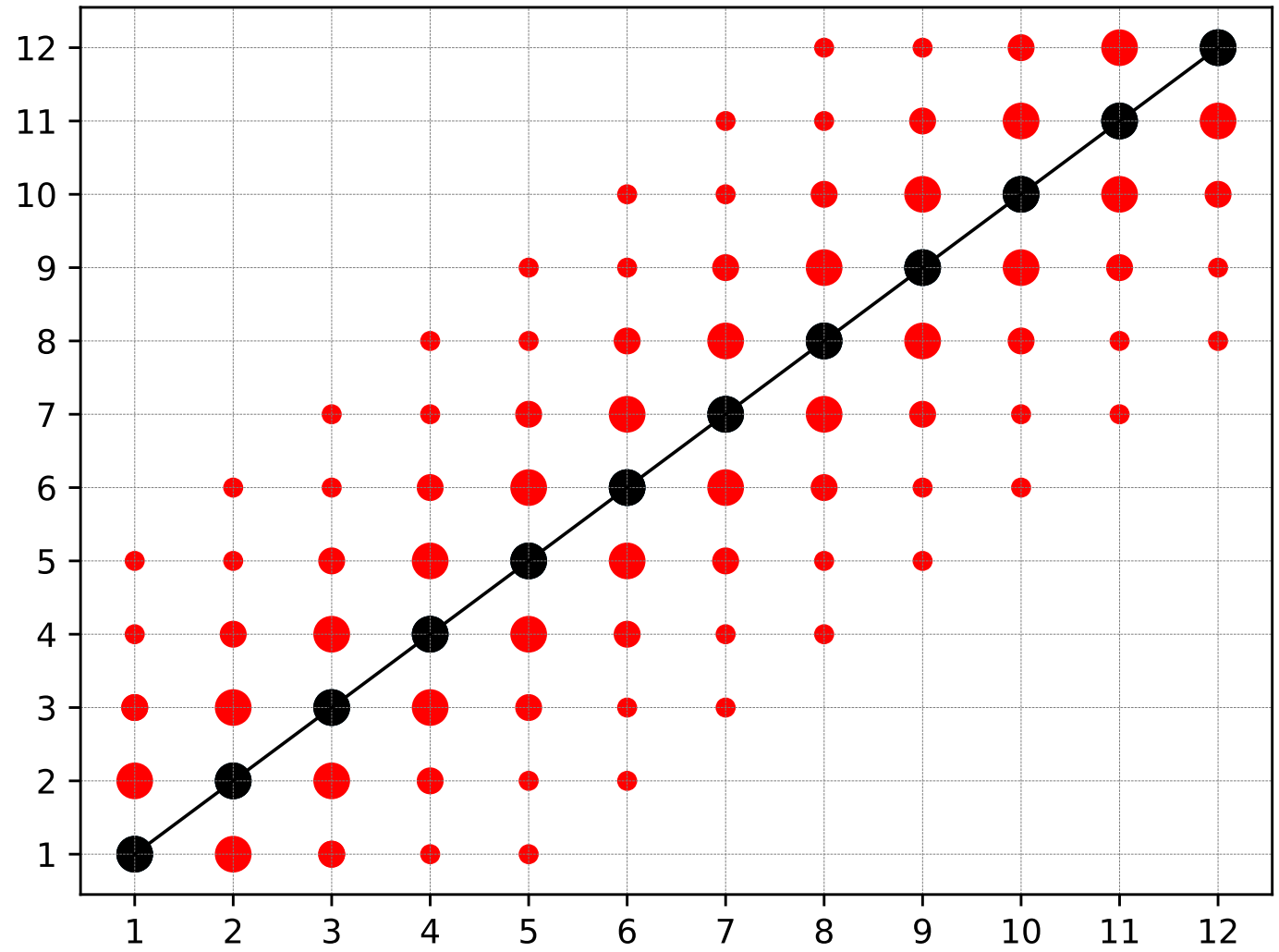
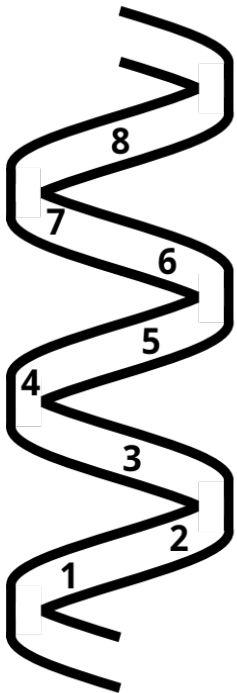
1 signál = jedna aminokyselina  
( $^1\text{H}$  z NH skupiny)



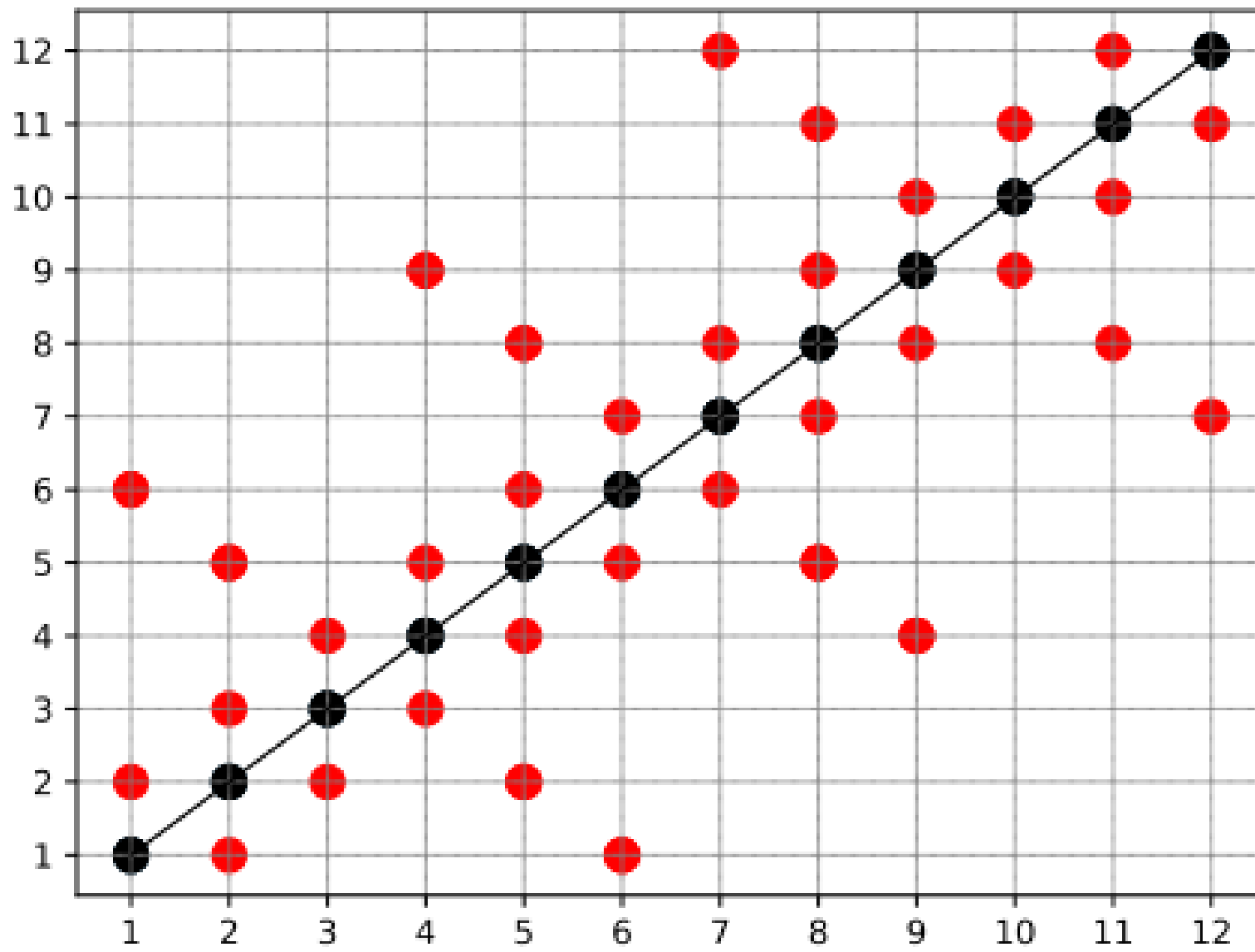
# Sekundární struktura č.1



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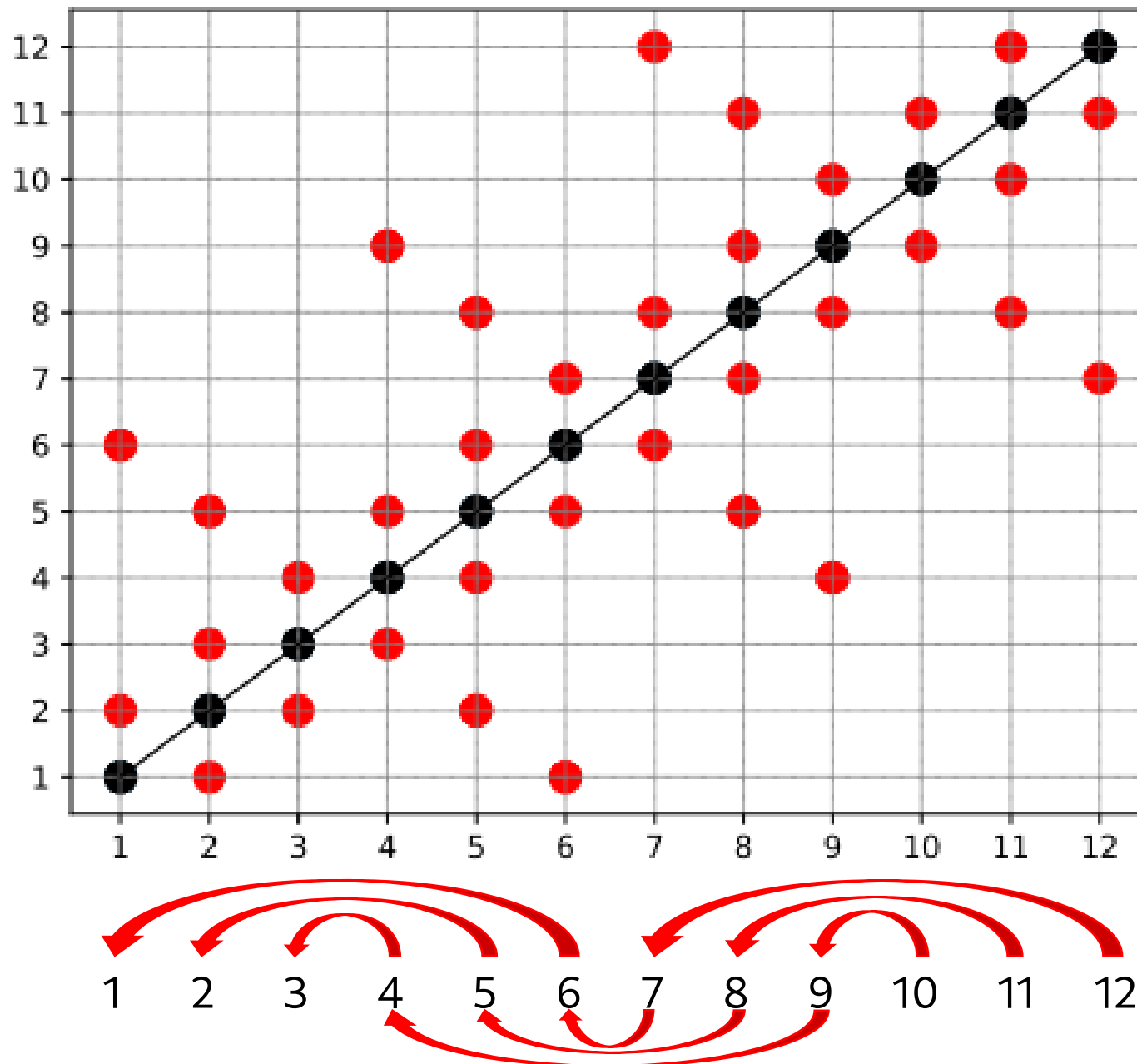


# Sekundární struktura č.2

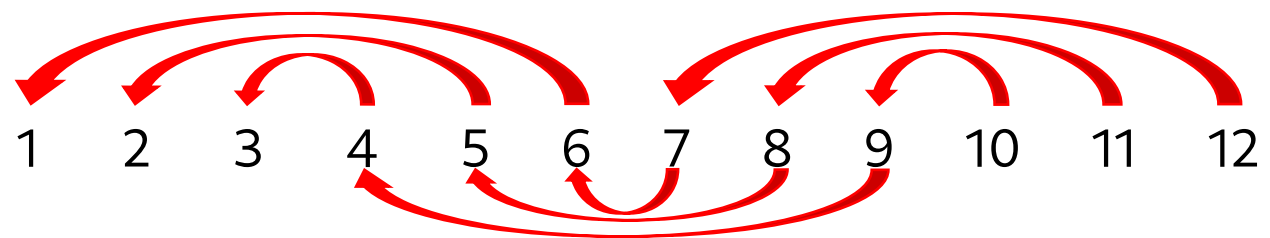
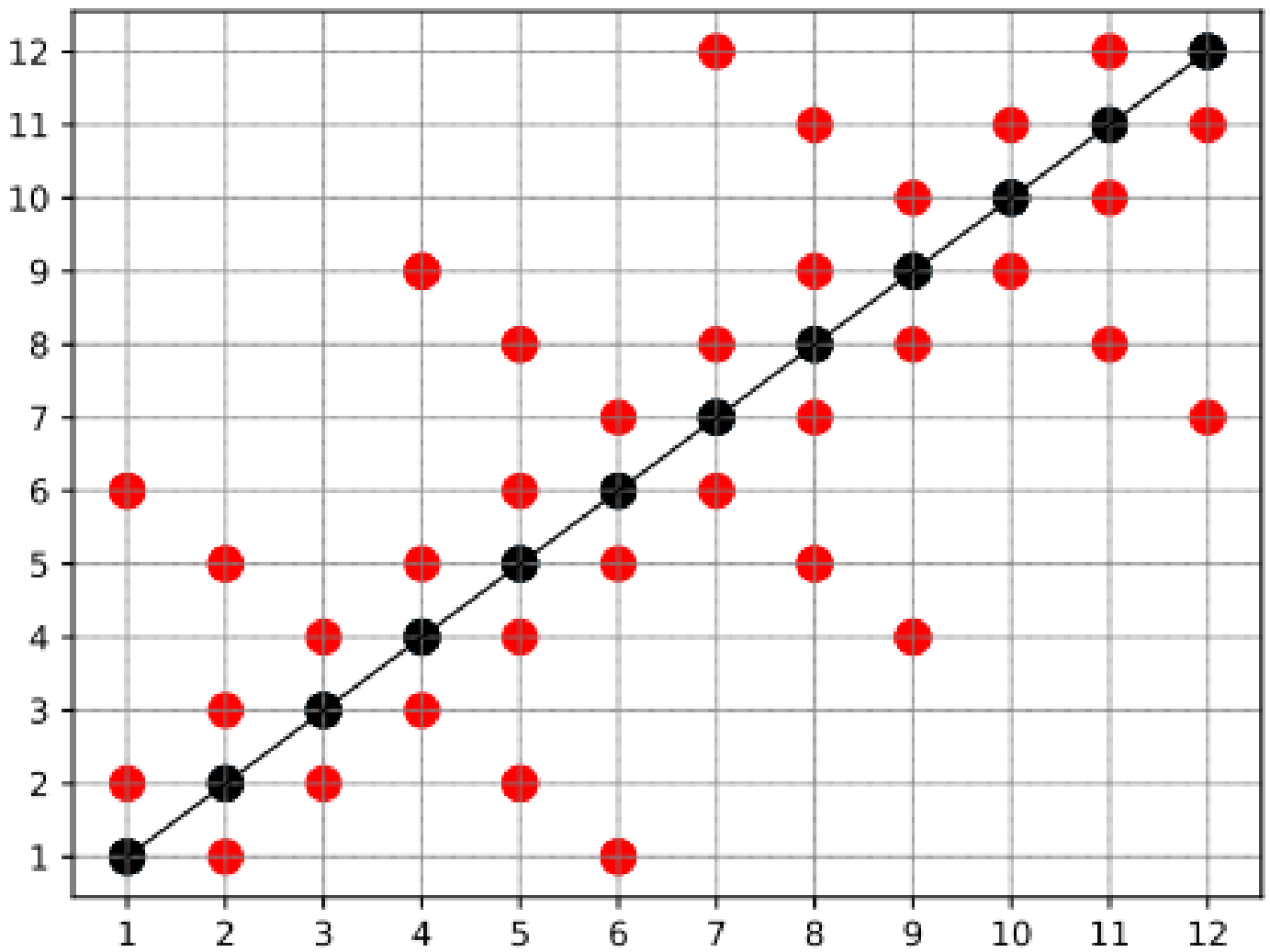
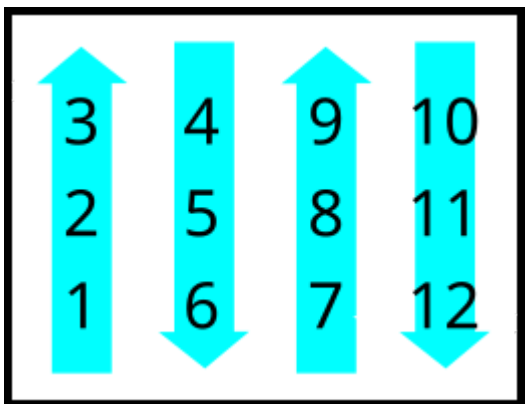




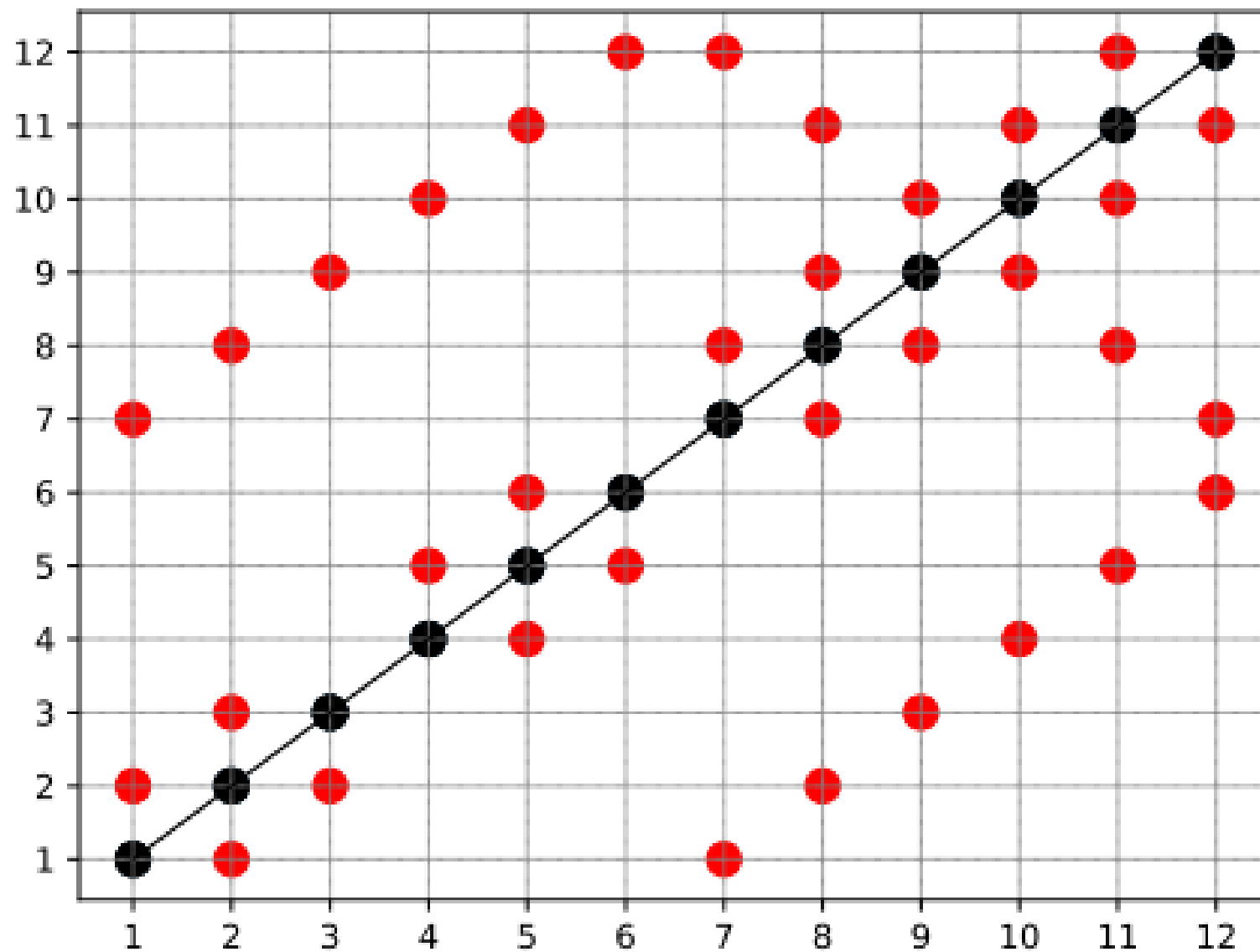
# Sekundární struktura č.2



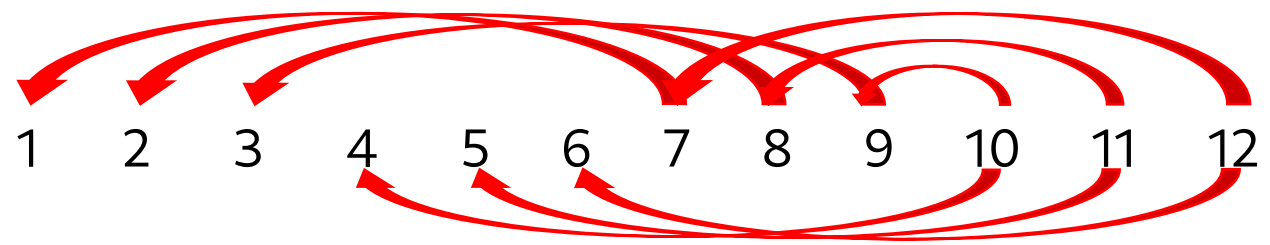
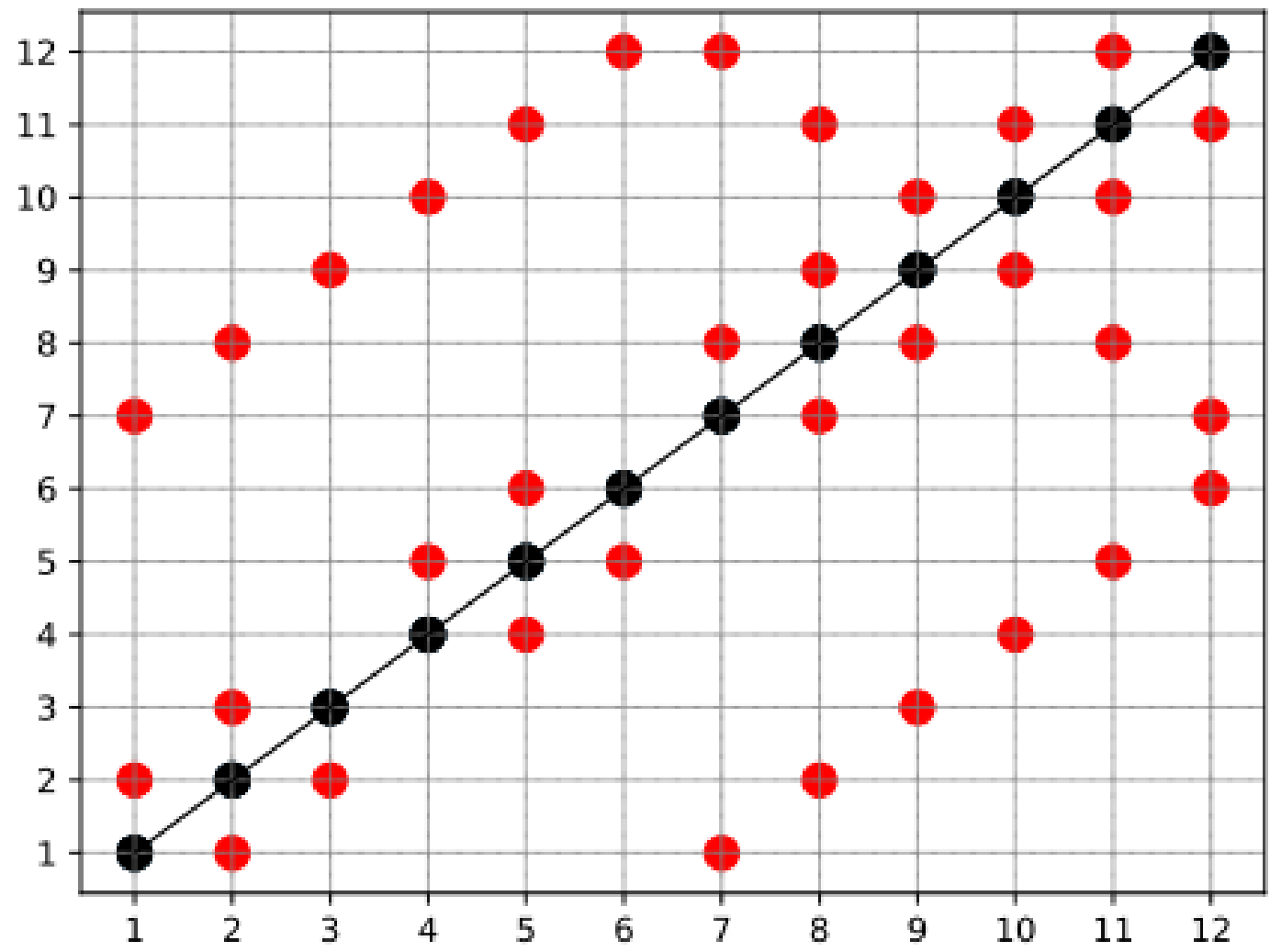
# Sekundární struktura č.2 antiparalelní $\beta$ -sheet



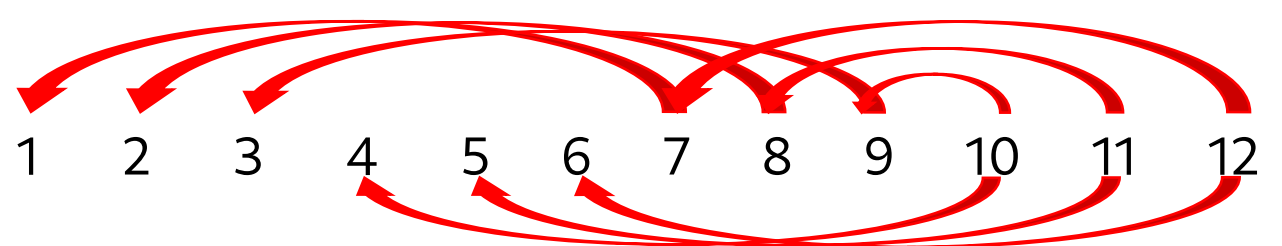
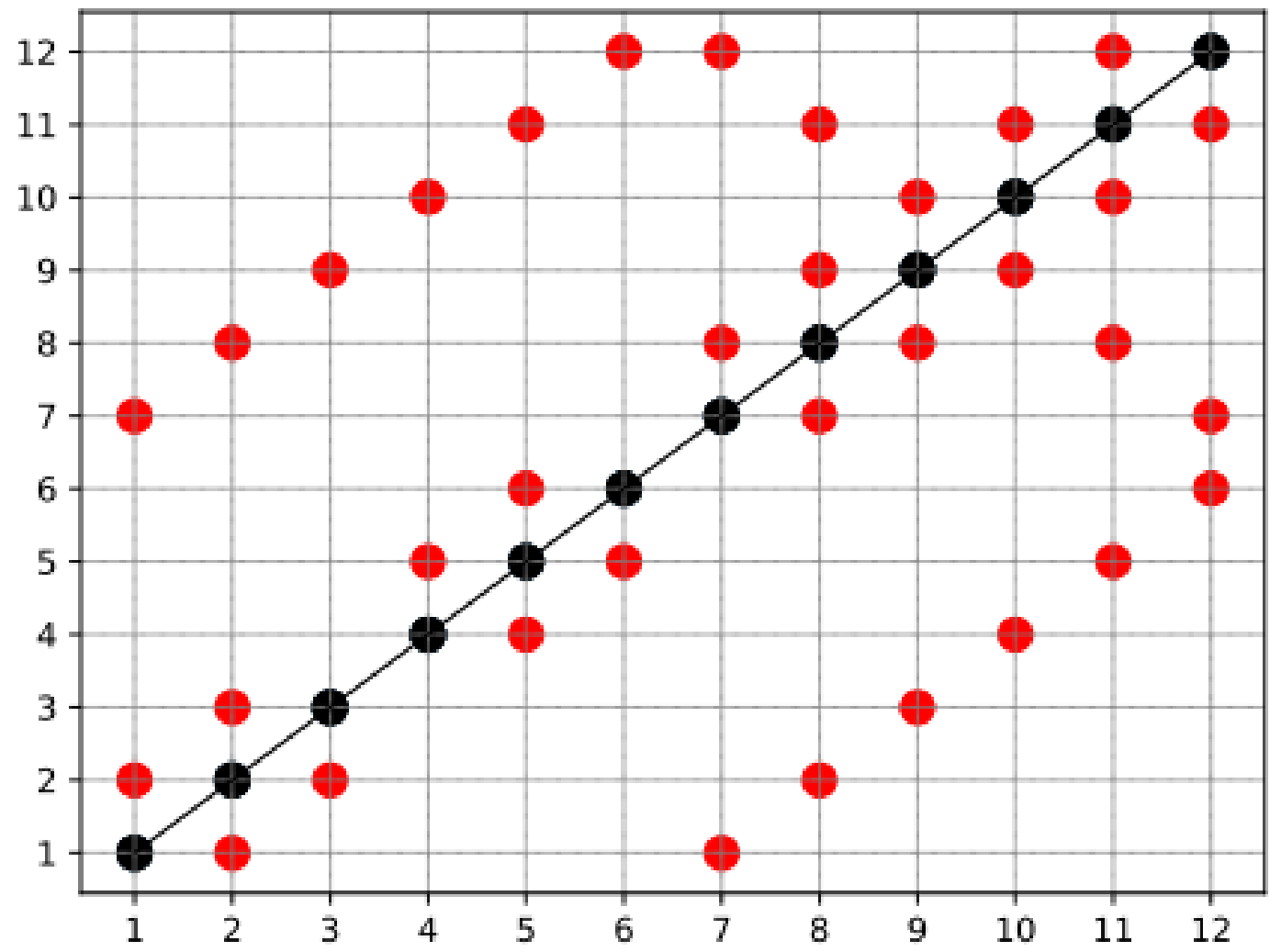
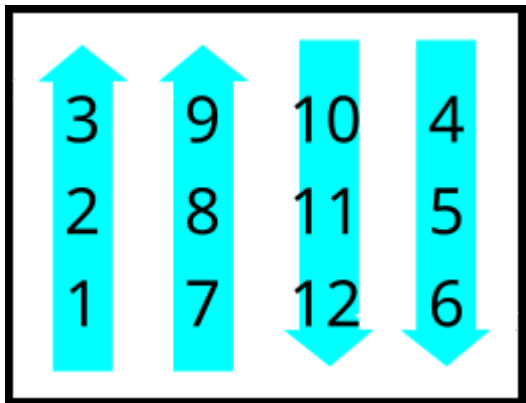
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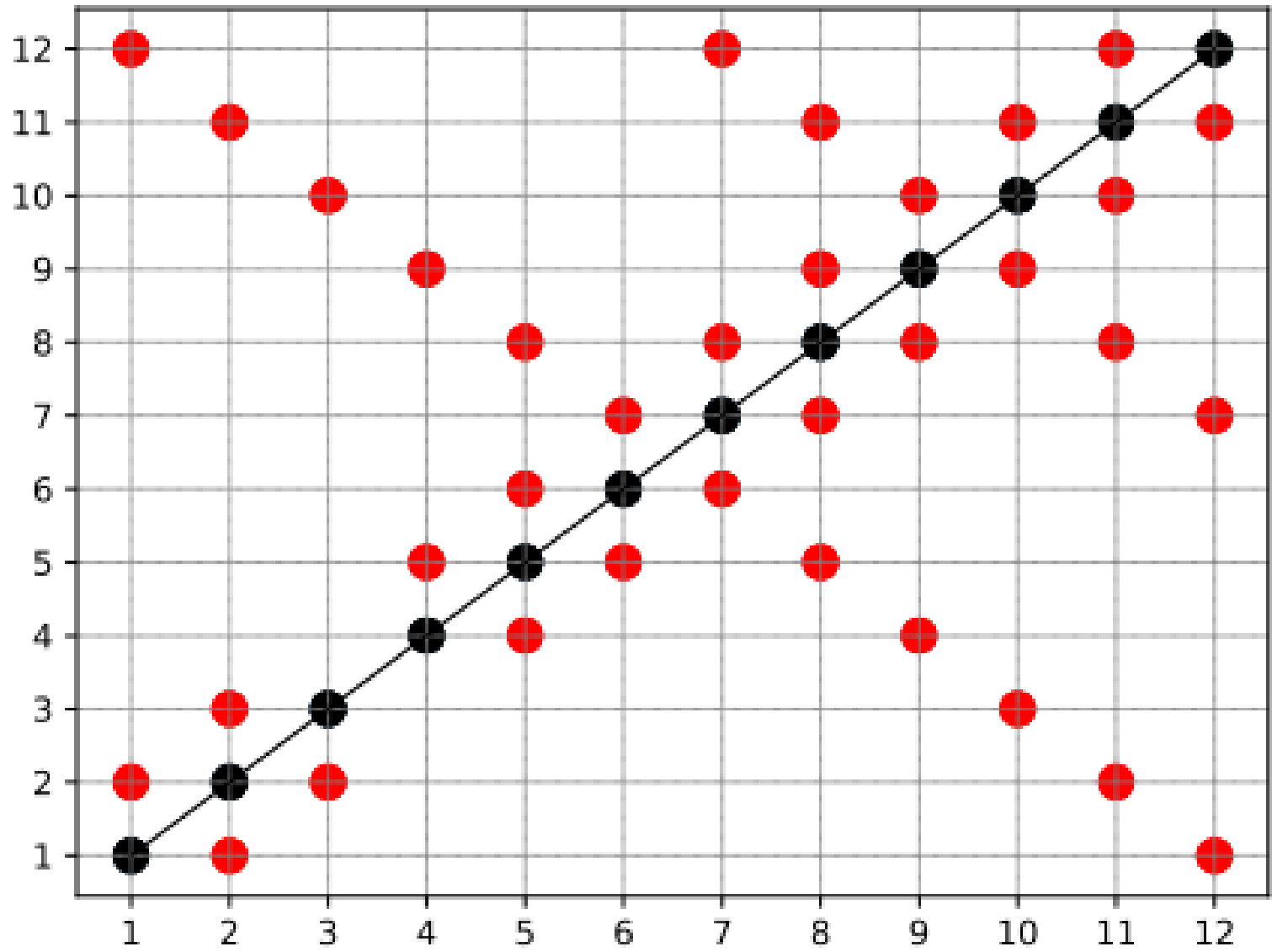
# Sekundární struktura č.3



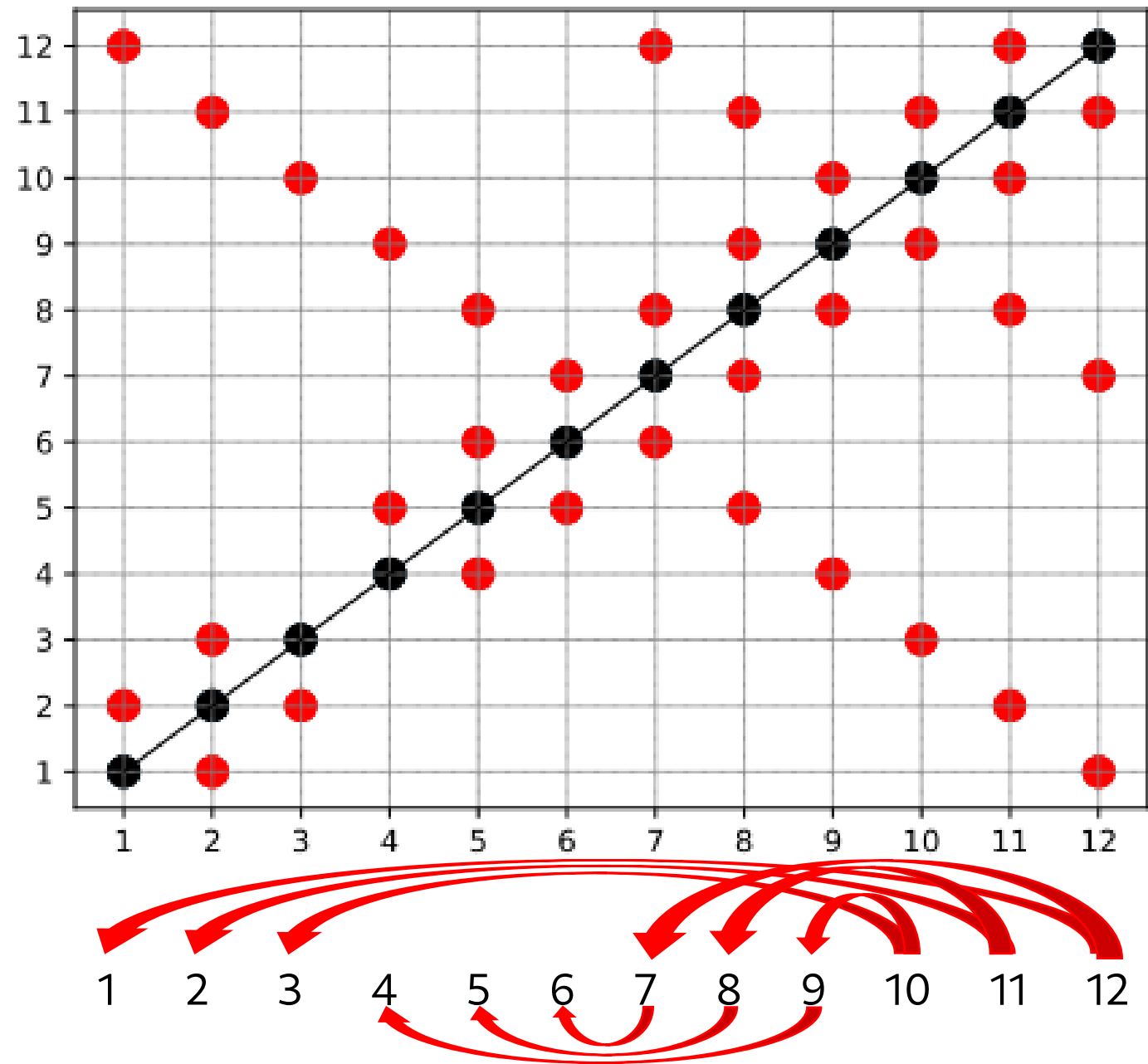
# Sekundární struktura č.3 $\beta$ -sheet



# Sekundární struktura č.4



# Sekundární struktura č.4



# Sekundární struktura č.4 $\beta$ -sheet

