# PhytoProm:

## mineração e processamento de DNA para análise de enriquecimento de elementos cis regulatórios

# Sobre mim

## Filipe Medeiros

- Ciência da computação - UNICAP
- Iniciação científica - Lab. Gen. Biotecnologia Veg. UFPE
- Engenheiro de inteligência artificial - Cloudia

## Tópicos

- Tecnologias utilizadas
- Atividades desempenhadas
  - Mineração
  - Processamento
  - Análise exploratória
  - Visualização dos dados

# Tecnologias utilizadas









# Ciclo de vida da ciência dos dados

# Mineração dos dados

## Jaspar

| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| A | [13 | 13 | 03 | 01 | 54 | 01 | 01 | 01 | 00 | 03 | 02 | 05] |
| C | [13 | 39 | 05 | 53 | 00 | 01 | 50 | 01 | 00 | 37 | 00 | 17] |
| G | [17 | 02 | 37 | 00 | 00 | 52 | 03 | 00 | 53 | 08 | 37 | 12] |
| T | [11 | 00 | 09 | 00 | 00 | 00 | 00 | 52 | 01 | 06 | 15 | 20] |

Matriz de peso e posição

Tamanho: 489 matrizes

## PhytoMine API

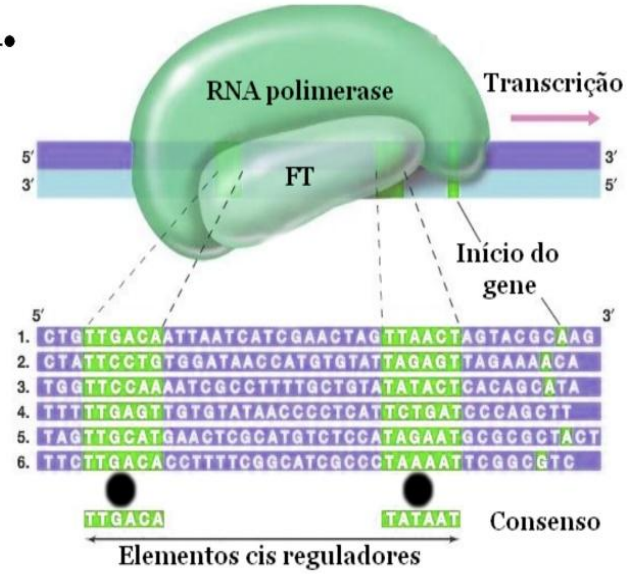
>Vigun04g127700 5000 upstream
TTTAATCCTTCATCTTTCGAAATACGTG
AATTTAATCATTTTAATCAAATTTTGTTA
AATTTGTTTGATATTTTGTACGTATTTC
ACGATTATATTTGAATTGTTTATAGTGT
TTAACACATTTTTGCTTTAATATTAAGTT
AAATACTATTATAA…

FASTA em JSON

Tamanho: 29.722 promotores

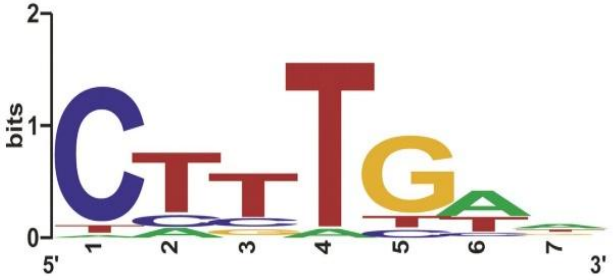
# Dados obtidos

**A.**




**B.**

| | 1 | 2 | 3 | 4 | 5 | 6 | 7 |
|---|---|---|---|---|---|---|---|
| A | 1 | 4 | 1 | 2 | 0 | 17 | 13 |
| C | 28 | 5 | 5 | 0 | 3 | 3 | 2 |
| G | 0 | 0 | 4 | 0 | 25 | 1 | 7 |
| T | 2 | 22 | 21 | 29 | 4 | 10 | 9 |
| | 31 | 31 | 31 | 31 | 31 | 31 | 31 |



# Limpeza dos dados

In [12]:

```
df['Matrix'] = df['Matrix'].apply(lambda x: probability(x))
df['Matrix'] = df['Matrix'].apply(lambda x: x.transpose())
df
```

Out[12]:

| | ID | Name | A | C | G | T | Matrix |
|---|---|---|---|---|---|---|---|
| 0 | >MA0020.1 | Dof2 | [21, 21, 21, 0, 3, 7] | [0, 0, 0, 0, 14, 6] | [0, 0, 0, 21, 2, 3] | [0, 0, 0, 0, 2, 5] | [[1.0, 1.0, 1.0, 0.0, 0.14285714285714285, 0.3... |
| 1 | >MA0021.1 | Dof3 | [21, 21, 21, 0, 0, 6] | [0, 0, 0, 0, 10, 6] | [0, 0, 0, 21, 3, 9] | [0, 0, 0, 0, 8, 0] | [[1.0, 1.0, 1.0, 0.0, 0.0, 0.2857142857142857]... |
| 2 | >MA0034.1 | Gam1 | [4, 10, 3, 23, 25, 1, 3, 6, 10, 5] | [6, 5, 13, 1, 0, 24, 14, 0, 11, 19] | [11, 7, 0, 1, 0, 0, 6, 19, 0, 1] | [4, 3, 9, 0, 0, 0, 2, 0, 4, 0] | [[0.16, 0.4, 0.12, 0.92, 1.0, 0.04, 0.12, 0.24... |
| 3 | >MA0044.1 | HMG-1 | [0, 0, 0, 0, 0, 6, 3, 0, 0] | [5, 0, 4, 2, 1, 1, 5, 1, 8] | [8, 3, 0, 10, 0, 3, 0, 2, 1] | [0, 10, 9, 1, 12, 3, 5, 10, 4] | [[0.0, 0.0, 0.0, 0.0, 0.0, 0.46153846153846156... |
| 4 | >MA0045.1 | HMG-I/Y | [3, 7, 9, 3, 11, 11, 11, 3, 4, 3, 8, 8, 9, 9, ... | [5, 0, 1, 6, 0, 0, 0, 3, 1, 4, 5, 1, 0, 5, 0, 7] | [4, 3, 1, 4, 3, 2, 2, 2, 8, 6, 1, 4, 2, 0, 3, 0] | [2, 4, 3, 1, 0, 1, 1, 6, 1, 1, 0, 1, 3, 0, 0, 5] | [[0.21428571428571427, 0.5, 0.6428571428571429... |
| 5 | >MA0053.1 | MNB1A | [15, 15, 15, 0, 3] | [0, 0, 0, 0, 9] | [0, 0, 0, 15, 0] | [0, 0, 0, 0, 3] | [[1.0, 1.0, 1.0, 0.0, 0.2], [0.0, 0.0, 0.0, 0.... |
| 6 | >MA0054.1 | myb.Ph3 | [19, 64, 63, 4, 10, 10, 13, 3, 28] | [3, 1, 0, 62, 27, 2, 8, 17, 1] | [2, 2, 2, 3, 16, 53, 0, 1, 0] | [46, 3, 5, 1, 17, 5, 49, 49, 41] | [[0.2714285714285714, 0.9142857142857143, 0.9,... |

# Extrair elementos cis regulatórios

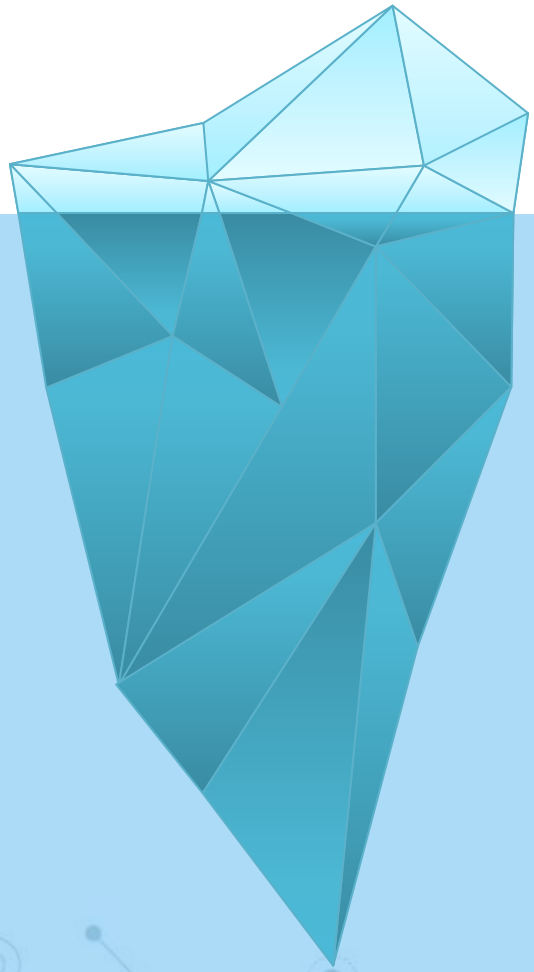
In [14]:
```
1 lista = combinatoria(df['A'][0], df['C'][0], df['G'][0], df['T'][0])
2 print (lista)
```

```
['AAAGAA', 'AAAGCA', 'AAAGGA', 'AAAGTA', 'AAAGAC', 'AAAGCC', 'AAAGGC', 'AAAGTC', 'AAAGAG', 'AAAGCG', 'AAAGGG', 'AAA
GTG', 'AAAGAT', 'AAAGCT', 'AAAGGT', 'AAAGTT']
```

$$4^{30} = 1{,}15.10^{18}$$

Impraticável

# Problemas



## Grande número de elementos cis regulatórios

A busca de um grande número de sub-strings torna o processamento do modelo inviável mesmo para um único promotor.

## Dupla fita do DNA

Um DNA possui duas fitas gênicas: uma positiva e outra negativa. A análise se concentra apenas na fita positiva para poupar processamento. Isso implica que deve ser feita a busca pelo elemento cis regulatório em forma de complemento reverso para emular a busca na fita negativa.

## Solução

| Gray code | Base | IUPAC | Gray code | Base | IUPAC |
|---|---|---|---|---|---|
| 0000 | - | # | 1100 | A\|C | M |
| 0001 | T | T | 1101 | A\|C\|T | H |
| 0011 | G\|T | K | 1111 | A\|C\|G\|T | N |
| 0010 | G | G | 1110 | A\|C\|G | V |
| 0110 | C\|G | S | 1010 | A\|G | R |
| 0111 | C\|G\|T | B | 1011 | A\|G\|T | D |
| 0101 | C\|T | Y | 1001 | A\|T | W |
| 0100 | C | C | 1000 | A | A |

Modelo de consenso da IUPAC (International Union of Pure and Applied Chemistry)

| | 1 | 2 | 3 | 4 | 5 | 6 | 7 |
|---|---|---|---|---|---|---|---|
| A | 1 | 4 | 1 | 2 | 0 | 17 | 13 |
| C | 28 | 5 | 5 | 0 | 3 | 3 | 2 |
| G | 0 | 0 | 4 | 0 | 25 | 1 | 7 |
| T | 2 | 22 | 21 | 29 | 4 | 10 | 9 |

1 2 3 4 5 6 7

[H, H, N, W, B, N, N]

# Aplicando ao novo modelo

In [24]:

```
#Cria uma coluna no data frame para o complemento reverso (a coluna só recebe o motivo reverso)
df['ReverseComplement'] = df['Motifs'].apply(lambda x: x[::-1])
#Calcula o complemento do motivo (para resultar no complemento reverso)
df.ReverseComplement.apply(lambda x: reverseComplement(x))
df
```

Out[24]:

| | ID | Name | A | C | G | T | Matrix | Motifs | ReverseComplement |
|---|---|---|---|---|---|---|---|---|---|
| 0 | >MA0020.1 | Dof2 | [21, 21, 21, 0, 3, 7] | [0, 0, 0, 0, 14, 6] | [0, 0, 0, 21, 2, 3] | [0, 0, 0, 0, 2, 5] | [[1.0, 1.0, 1.0, 0.0, 0.14285714285714285, 0.3... | [A, A, A, G, C, A] | [T, G, C, T, T, T] |
| 1 | >MA0021.1 | Dof3 | [21, 21, 21, 0, 0, 6] | [0, 0, 0, 0, 10, 6] | [0, 0, 0, 21, 3, 9] | [0, 0, 0, 0, 8, 0] | [[1.0, 1.0, 1.0, 0.0, 0.0, 0.2857142857142857]... | [A, A, A, G, Y, G] | [C, R, C, T, T, T] |
| 2 | >MA0034.1 | Gam1 | [4, 10, 3, 23, 25, 1, 3, 6, 10, 5] | [6, 5, 13, 1, 0, 24, 14, 0, 11, 19] | [11, 7, 0, 1, 0, 0, 6, 19, 0, 1] | [4, 3, 9, 0, 0, 0, 2, 0, 4, 0] | [[0.16, 0.4, 0.12, 0.92, 1.0, 0.04, 0.12, 0.24... | [G, A, Y, A, A, C, C, G, M, C] | [G, K, C, G, G, T, T, R, T, C] |
| 3 | >MA0044.1 | HMG-1 | [0, 0, 0, 0, 0, 6, 3, 0, 0] | [5, 0, 4, 2, 1, 1, 5, 1, 8] | [8, 3, 0, 10, 0, 3, 0, 2, 1] | [0, 10, 9, 1, 12, 3, 5, 10, 4] | [[0.0, 0.0, 0.0, 0.0, 0.0, 0.46153846153846156... | [S, T, Y, G, T, A, Y, T, Y] | [R, A, R, T, A, C, R, A, S] |
| 4 | >MA0045.1 | HMG-I/Y | [3, 7, 9, 3, 11, 11, 11, 3, 4, 3, 8, 8, 9, 9, ... | [5, 0, 1, 6, 0, 0, 0, 3, 1, 4, 5, 1, 0, 5, 0, 7] | [4, 3, 1, 4, 3, 2, 2, 2, 8, 6, 1, 4, 2, 0, 3, 0] | [2, 4, 3, 1, 0, 1, 1, 6, 1, 1, 0, 1, 3, 0, 0, 5] | [[0.21428571428571427, 0.5, 0.6428571428571429... | [C, A, A, C, A, A, A, T, G, G, M, A, A, M, A, Y] | [R, T, K, T, T, K, C, C, A, T, T, T, G, T, T, G] |
| 5 | >MA0053.1 | MNB1A | [15, 15, 15, 0, 3] | [0, 0, 0, 0, 9] | [0, 0, 0, 15, 0] | [0, 0, 0, 0, 3] | [[1.0, 1.0, 1.0, 0.0, 0.2], [0.0, 0.0, 0.0, 0.... | [A, A, A, G, C] | [G, C, T, T, T] |

# Pré-processamento

```
In [30]:
1 searchLog = ecrMiner(genome, df)
2 searchLog
```

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| **757970** | >MA0021.1 | Dof3 | [A, A, A, G, Y, G] | [C, R, C, T, T, T] | VigunL002200 | [435, 1972] | [413] | 940.000000 | 3 |
| **757971** | >MA0053.1 | MNB1A | [A, A, A, G, C] | [G, C, T, T, T] | VigunL002200 | [1972] | [153, 1785] | 1303.333333 | 3 |
| **757972** | >MA0064.1 | PBF | [A, A, A, G, Y] | [R, C, T, T, T] | VigunL002200 | [160, 435, 713, 859, 1289, 1393, 1597, 1972] | [153, 349, 414, 780, 1308, 1624, 1785, 1870] | 1043.812500 | 16 |
| **757973** | >MA0121.1 | ARR10 | [A, G, A, T, Y, Y, K, C] | [G, K, R, R, A, T, C, T] | VigunL002200 | [1328, 1499] | [] | 1413.500000 | 2 |
| **757974** | >MA0562.1 | PIF5 | [T, C, A, C, R, T, G, S] | [S, C, A, Y, G, T, G, A] | VigunL002200 | [1334] | [] | 1334.000000 | 1 |
| **757975** | >MA0932.1 | AHL12 | [A, A, W, W, W, W, T, T] | [A, A, W, W, W, W, T, T] | VigunL002200 | [83, 126, 127, 178, 179, 180, 204, 246, 650, 6... | [83, 126, 127, 178, 179, 180, 204, 246, 650, 6... | 624.684211 | 38 |
| **757976** | >MA0933.1 | AHL20 | [A, A, T, T, A, A, W, T] | [A, W, T, T, A, A, T, T] | VigunL002200 | [1514, 1518] | [613, 1510, 1514] | 1333.800000 | 5 |
| **757977** | >MA0934.1 | AHL25 | [A, W, T, T, A, A, W, T] | [A, W, T, T, A, A, W, T] | VigunL002200 | [338, 613, 1510, 1514, 1518] | [338, 613, 1510, 1514, 1518] | 1098.600000 | 10 |

# Processamento

```
In [7]: 1 df
```

Out[7]:

| | ID | Name | Matrix | Motifs | ReverseComplement | Genome | Cluster |
|---|---|---|---|---|---|---|---|
| **0** | >MA0020.1 | Dof2 | [[1. 1. 1. 0. ... | ['A', 'A', 'A', 'G', 'C', 'A'] | ['T', 'G', 'C', 'T', 'T', 'T'] | 5 | 1 |
| **1** | >MA0021.1 | Dof3 | [[1. 1. 1. 0. ... | ['A', 'A', 'A', 'G', 'Y', 'G'] | ['C', 'R', 'C', 'T', 'T', 'T'] | 1 | 1 |
| **2** | >MA0034.1 | Gam1 | [[0.16 0.4 0.12 0.92 1. 0.04 0.12 0.24 0.4 ... | ['G', 'A', 'Y', 'A', 'A', 'C', 'C', 'G', 'M', ... | ['G', 'K', 'C', 'G', 'G', 'T', 'T', 'R', 'T', ... | 91 | 1 |
| **3** | >MA0044.1 | HMG-1 | [[0. 0. 0. 0. ... | ['S', 'T', 'Y', 'G', 'T', 'A', 'Y', 'T', 'Y'] | ['R', 'A', 'R', 'T', 'A', 'C', 'R', 'A', 'S'] | 21726 | 31 |
| **4** | >MA0045.1 | HMG-I/Y | [[0.21428571 0.5 0.64285714 0.21428571 ... | ['C', 'A', 'A', 'C', 'A', 'A', 'A', 'T', 'G', ... | ['R', 'T', 'K', 'T', 'T', 'K', 'C', 'C', 'A', ... | 25575 | 36 |
| **5** | >MA0053.1 | MNB1A | [[1. 1. 1. 0. 0.2]\n [0. 0. 0. 0. 0.6]... | ['A', 'A', 'A', 'G', 'C'] | ['G', 'C', 'T', 'T', 'T'] | 79 | 1 |
| **6** | >MA0054.1 | myb.Ph3 | [[0.27142857 0.91428571 0.9 0.05714286 ... | ['T', 'A', 'A', 'C', 'C', 'G', 'T', 'T', 'W'] | ['W', 'A', 'A', 'C', 'G', 'G', 'T', 'T', 'A'] | 7181 | 12 |
| **7** | >MA0064.1 | PBF | [[1. 1. 1. 0. 0.0625]\n [0. ... | ['A', 'A', 'A', 'G', 'Y'] | ['R', 'C', 'T', 'T', 'T'] | 2 | 1 |
| **8** | >MA0082.1 | squamosa | [[0.36666667 0. 0.8 0.53333333 ... | ['M', 'C', 'A', 'W', 'A', 'W', 'A', 'T', 'R', ... | ['A', 'T', 'T', 'W', 'C', 'Y', 'A', 'T', 'W', ... | 27431 | 35 |
| **9** | >MA0096.1 | bZIP910 | [[0.42857143 0. 0. 1. ... | ['M', 'T', 'G', 'A', 'C', 'G', 'T'] | ['A', 'C', 'G', 'T', 'C', 'A', 'K'] | 957 | 5 |
| **10** | >MA0097.1 | bZIP911 | [[0.03030303 0.51515152 0. 0. ... | ['G', 'R', 'T', 'G', 'A', 'C', 'G', 'T', 'G', ... | ['G', 'K', 'K', 'C', 'A', 'C', 'G', 'T', 'C', ... | 29717 | 39 |
| **11** | >MA0120.1 | id1 | [[0.04166667 0.125 0.04166667 0. ... | ['T', 'T', 'K', 'Y', 'C', 'C', 'Y', 'T', 'W', ... | ['C', 'G', 'A', 'W', 'A', 'R', 'G', 'G', 'R', ... | 178 | 2 |

# Análise exploratória

In [13]:
```
df['p-value'] = 0
df['p-value'] = df.apply(lambda x: stats.fisher_exact([[x['vigna_genome'], x['Cluster']], [vigna_genome, cluster]
```

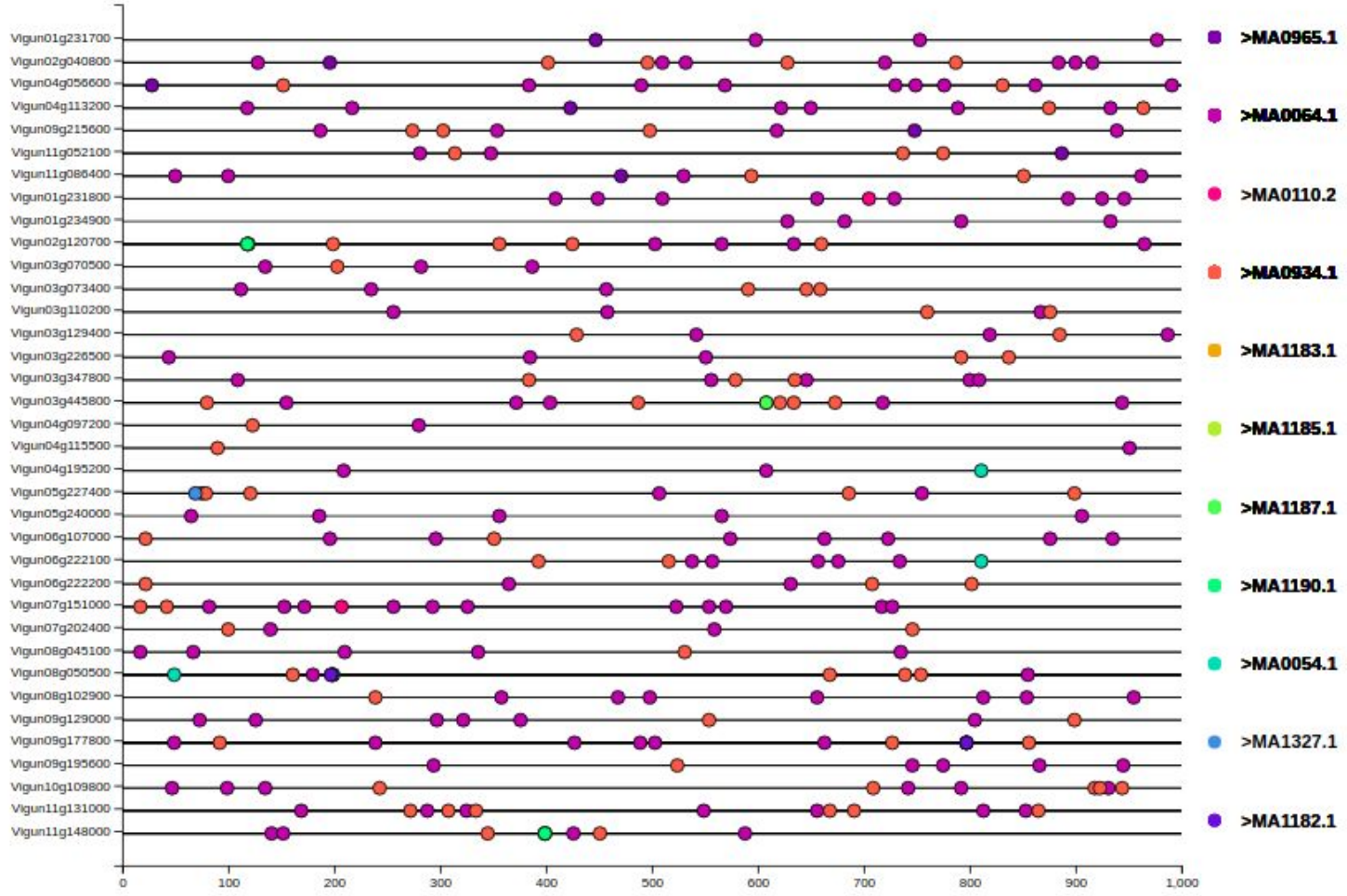
In [14]:
```
df
```

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 9 | >MA0054.1 | myb.Ph3 | Myb | [[0.2714285714285714, 0.9142857142857143, 0.9,... | ['T', 'A', 'A', 'C', 'C', 'G', 'T', 'T', 'W'] | ['W', 'A', 'A', 'C', 'G', 'G', 'T', 'T', 'A'] | 534 | 3 | 0.037485 |
| 10 | >MA0064.1 | PBF | Dof | [[1.0, 1.0, 1.0, 0.0, 0.0625], [0.0, 0.0, 0.0,... | ['A', 'A', 'A', 'G', 'Y'] | ['R', 'C', 'T', 'T', 'T'] | 203249 | 251 | 0.166510 |
| 11 | >MA0082.1 | squamosa | SBP | [[0.36666666666666664, 0.0, 0.8, 0.53333333333... | ['M', 'C', 'A', 'W', 'A', 'W', 'A', 'T', 'R', ... | ['A', 'T', 'T', 'W', 'C', 'Y', 'A', 'T', 'W', ... | 105 | 0 | 1.000000 |
| 12 | >MA0096.1 | bZIP910 | bZIP | [[0.42857142857142855, 0.0, 0.0, 1.0, 0.0, 0.0... | ['M', 'T', 'G', 'A', 'C', 'G', 'T'] | ['A', 'C', 'G', 'T', 'C', 'A', 'K'] | 2410 | 1 | 0.393155 |
| 13 | >MA0097.1 | bZIP911 | bZIP | [[0.030303030303030304, 0.5151515151515151, 0.... | ['G', 'R', 'T', 'G', 'A', 'C', 'G', 'T', 'G', ... | ['G', 'K', 'K', 'C', 'A', 'C', 'G', 'T', 'C', ... | 9 | 0 | 1.000000 |
| 14 | >MA0110.2 | ATHB-5 | Homeobox | [[0.0, 0.11764705882352941, 0.0555555555555555... | ['B', 'G', 'Y', 'C', 'C', 'A', 'A', 'T', 'T', ... | ['C', 'A', 'A', 'T', 'A', 'A', 'T', 'T', 'G', ... | 7 | 1 | 0.010786 |
| 15 | >MA0120.1 | id1 | C2H2 | [[0.041666666666666664, 0.125, 0.0416666666666... | ['T', 'T', 'K', 'Y', 'C', 'C', 'Y', 'T', 'W', ... | ['C', 'G', 'A', 'W', 'A', 'R', 'G', 'G', 'R', ... | 53 | 0 | 1.000000 |
| 16 | >MA0121.1 | ARR10 | ARR-B | [[0.9333333333333333, 0.0, 0.9333333333333333,... | ['A', 'G', 'A', 'T', 'Y', 'Y', 'K', 'C'] | ['G', 'K', 'R', 'R', 'A', 'T', 'C', 'T'] | 4534 | 7 | 0.682771 |
| 17 | >MA0123.1 | abi4 | B4 | [[0.0, 0.24489795918367346, 0.0, | ['C', 'G', 'S', 'Y', 'G', 'C', | ['G', 'G', 'G', 'G', 'G', 'C', 'R', | 10 | 0 | 1.000000 |

# Análise de enriquecimento

| Family | ID | Motifs | Scientific Library(PubMed) | Reverse Complement | Vigna Genome | Cluster | p-value |
|---|---|---|---|---|---|---|---|
| Myb | >MA0054.1 | ['T', 'A', 'A', 'C', 'C', 'G', 'T', 'T', 'W'] | myb.Ph3 | ['W', 'A', 'A', 'C', 'G', 'G', 'T', 'T', 'A'] | 534 | 3 | 0,03865570777721362 |
| Dof | >MA0064.1 | ['A', 'A', 'A', 'G', 'Y'] | PBF | ['R', 'C', 'T', 'T', 'T'] | 203249 | 244 | 0,04692722453436693 |
| Homeobox | >MA0110.2 | ['B', 'G', 'Y', 'C', 'C', 'A', 'A', 'T', 'T', 'A', 'T', 'T', 'G'] | ATHB-5 | ['C', 'A', 'A', 'T', 'A', 'A', 'T', 'T', 'G', 'G', 'R', 'C', 'V'] | 7 | 2 | 6,732757488997154e-05 |
| HMGA factors | >MA0934.1 | ['A', 'W', 'T', 'T', 'A', 'A', 'W', 'T'] | AHL25 | ['A', 'W', 'T', 'T', 'A', 'A', 'W', 'T'] | 99148 | 162 | 0,034801162706162944 |
| bHLH | >MA0965.1 | ['N', 'K', 'C', 'A', 'C', 'G', 'T', 'G', 'M', 'N'] | BIM2 | ['N', 'K', 'C', 'A', 'C', 'G', 'T', 'G', 'K', 'N'] | 1843 | 7 | 0,015248479858376891 |
| Myb-related | >MA1182.1 | ['A', 'G', 'A', 'T', 'A', 'T', 'T', 'T', 'T', 'T', 'T', 'T'] | At3g09600 | ['A', 'A', 'A', 'A', 'A', 'A', 'A', 'T', 'A', 'T', 'C', 'T'] | 252 | 2 | 0,04817833118087982 |
| Myb-related | >MA1183.1 | ['A', 'G', 'A', 'T', 'A', 'T', 'T', 'T', 'T', 'T', 'T'] | At5g52660 | ['A', 'A', 'A', 'A', 'A', 'A', 'T', 'A', 'T', 'C', 'T'] | 558 | 4 | 0,007966603499479863 |
| Myb-related | >MA1185.1 | ['A', 'G', 'A', 'T', 'A', 'T', 'T', 'T', 'T', 'T'] | LHY1 | ['A', 'A', 'A', 'A', 'A', 'T', 'A', 'T', 'C', 'T'] | 1275 | 5 | 0,03324558491325824 |
| Myb-related | >MA1187.1 | ['A', 'G', 'A', 'T', 'A', 'T', 'T', 'T', 'T', 'T'] | LCL1 | ['A', 'A', 'A', 'A', 'A', 'T', 'A', 'T', 'C', 'T'] | 1275 | 5 | 0,03324558491325824 |
| Myb-related | >MA1190.1 | ['A', 'G', 'A', 'T', 'A', 'T', 'T', 'T', 'T', 'T', 'T'] | At4g01280 | ['A', 'A', 'A', 'A', 'A', 'A', 'T', 'A', 'T', 'C', 'T'] | 558 | 4 | 0,007966603499479863 |
| Homeobox | >MA1327.1 | ['W', 'W', 'W', 'N', 'W', 'T', 'A', 'A', 'T', 'T', 'A', 'A', 'T', 'T', 'A', 'A', 'T', 'W', 'A', 'W', 'T', 'W'] | ATHB23 | ['W', 'A', 'W', 'T', 'W', 'A', 'T', 'T', 'A', 'A', 'T', 'T', 'A', 'A', 'T', 'T', 'A', 'W', 'N', 'W', 'W', 'W'] | 226 | 2 | 0,03971075700540519 |

# Visualização dos dados



**As famílias de elementos cis regulatórios Dof, Homeobox, Myb-related e bHLH na espécie da planta *Vigna unguiculata* (Feijão macassar) são fortes candidatos a regulação da via metabólica de fenilpropanóides, responsável pela produção de óleos essenciais, produto largamente utilizado na indústria no controle de fungos, e portanto, de grande interesse biotecnológico.**

# Muito obrigado!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