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«Інститут прикладного системного аналізу»

Лабороторна робота № 3
з дисципліни «Моделювання складних систем»

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1 Пошук моделі оптимальної складності

1.1 Задання конфігурацій. Створення вибірок

1.1.1 Тест 1 (вибірка аналогічна вибірці з лабораторної роботи №2)

```
In [761]: config1 = ModelConfig(a=0, b=0.5)
          config1.compile(n=1000)
          config1.generate_noise_and_output()
          config1.show()
```

```
Regressors: m = 5
True parameters: θ = [ 3 -2  1  0  0]
y0 = (3) * x1 + (-2) * x2 + (1) * x3 + (0) * x4 + (0) * x5
Noise generation: σ = 0.3
Sample length: n = 1000
X[:10]:
[[0.04308385 0.27830758 0.26976892 0.39022119 0.49445485]
 [0.35547599 0.48728023 0.29090938 0.17106778 0.44217748]
 [0.23057501 0.05182741 0.35420655 0.33878025 0.43994632]
 [0.09611698 0.12839818 0.18620192 0.42063433 0.26173627]
 [0.091473   0.05942291 0.3604472  0.34968361 0.32910679]
 [0.24643068 0.33150797 0.28024961 0.49592521 0.12985612]
 [0.13910572 0.15118726 0.38102016 0.14029001 0.39970713]
 [0.06306985 0.27847968 0.31756348 0.40461903 0.25243815]
 [0.11870129 0.4192407  0.32457993 0.18718059 0.38507428]
 [0.41681015 0.03932334 0.11500753 0.00913267 0.04140103]]
y[:10]:
[-0.43291385  0.38575983  1.06335113  0.12211829  0.61379791  0.46785321
  1.26450697  0.12539443  0.04208874  1.33072653]
```

1.1.2 Тест 2 (велика вибірка з великою кількістю регресорів)

```
In [762]: config2 = ModelConfig(m=15, s0=10, a=0, b=0.5, theta={'random': [1, 10]})
          config2.compile(n=1000)
          config2.generate_noise_and_output()
          config2.show(5)
```

```
Regressors: m = 15
True parameters: θ = [1.6112567  3.92918486 5.54550484 8.89579123 5.61658096 1.80037743
 1.31102406 4.00562737 7.73951187 8.13889251 0.         0.
 0.         0.         0.        ]
y0 = (1.6112567036457572) * x1 + (3.929184861555827) * x2 + (5.545504835204717) * x3 + (8.895791
Noise generation: σ = 0.3
Sample length: n = 1000
X[:10]:
[[0.17141608 0.08781483 0.01743464 0.29952731 0.16745103 0.24753049
  0.1284215  0.38092612 0.3119313  0.3007671  0.17271201 0.19120914
  0.29735522 0.44397982 0.4809952 ]
```

```
 [0.47869302 0.15824631 0.0570476  0.4013738  0.4536813  0.33610225
  0.07485632 0.24895821 0.18230803 0.14178467 0.32708787 0.2305085
  0.48024906 0.24493323 0.38827829]
 [0.0131716  0.36956987 0.13101176 0.37314593 0.10267952 0.29544454
  0.35293415 0.02098249 0.47523253 0.08506131 0.03398137 0.33780554
  0.48230987 0.47088904 0.03502071]
 [0.17128846 0.2917416  0.43680753 0.42073404 0.24958122 0.08615753
  0.09649508 0.01330002 0.06522511 0.178949   0.2350533  0.25121685
  0.34353518 0.1525882  0.44943699]
 [0.08123586 0.15739996 0.02151389 0.2969259  0.45627141 0.00293347
  0.45785202 0.29677929 0.28126218 0.11094502 0.09498646 0.0181461
  0.07394435 0.19421807 0.45634451]]
y[:10]:
[11.51775111 11.97117785 11.77111645 11.38172423 11.16129411]
```

1.1.3 Тест 3 (власні задачі)

Діабет Для 442 пацієнтів з діабетом, маємо 10 вхідних змінних: - вік - стать - індекс маси тіла - середній артеріальний тиск - шість вимірів сироватки крові,

Вихідна змінна: - кількісний показник прогресії хвороби через рік після вимірювання.

В кожному з цих 10 регресорів елементи відцентровані та поділені на $n\sigma$ (тобто в кожному стовпці сума квадратів елементів становить 1).

```
In [767]: dataframe_path = 'data/diabetes.csv'
          df = pd.read_csv(dataframe_path)
          config3 = ModelConfig(theta='unknown',
                                X=df.loc[:, 'age':'s6'],
                                y=df['target'])
          config3.show(5)
```

```
Regressors: m = 10
True parameters: θ = unknown
Sample length: n = 442
X[:10]:
[[ 0.03807591  0.05068012  0.06169621  0.02187235 -0.0442235  -0.03482076
  -0.04340085 -0.00259226  0.01990842 -0.01764613]
 [-0.00188202 -0.04464164 -0.05147406 -0.02632783 -0.00844872 -0.01916334
   0.07441156 -0.03949338 -0.06832974 -0.09220405]
 [ 0.08529891  0.05068012  0.04445121 -0.00567061 -0.04559945 -0.03419447
  -0.03235593 -0.00259226  0.00286377 -0.02593034]
 [-0.08906294 -0.04464164 -0.01159501 -0.03665645  0.01219057  0.02499059
  -0.03603757  0.03430886  0.02269202 -0.00936191]
 [ 0.00538306 -0.04464164 -0.03638469  0.02187235  0.00393485  0.01559614
   0.00814208 -0.00259226 -0.03199144 -0.04664087]]
y[:10]:
[151.  75. 141. 206. 135.]
```

Оцінка смертності ! TODO: DESCRIBE TASK

Вхідні змінні: - .

Вихідна змінна: - .

```
In [768]: dataframe_path = 'data/death-rate.csv'
          df = pd.read_csv(dataframe_path)
          config3 = ModelConfig(theta='unknown',
                                X=df.loc[:, 'A1':'A15'],
                                y=df['B'])
          config3.X = np.hstack((config3.X, np.ones((config3.n, 1))))
          config3.m += 1
          config3.s += 1
          config3.show(2)
```

```
Regressors: m = 16
True parameters: θ = unknown
Sample length: n = 60
X[:10]:
[[3.600e+01 2.700e+01 7.100e+01 8.100e+00 3.340e+00 1.140e+01 8.150e+01
  3.243e+03 8.800e+00 4.260e+01 1.170e+01 2.100e+01 1.500e+01 5.900e+01
  5.900e+01 1.000e+00]
 [3.500e+01 2.300e+01 7.200e+01 1.110e+01 3.140e+00 1.100e+01 7.880e+01
  4.281e+03 3.600e+00 5.070e+01 1.440e+01 8.000e+00 1.000e+01 3.900e+01
  5.700e+01 1.000e+00]]
y[:10]:
[921.87  997.875]
```

Октан При дослідженні виробничого процесу нафтопереробному заводі вимірюється вміст октану в нафті залежно від кількості 3-х сировинних матеріалів та змінної, що характеризує умови виробництва. Вхідні змінні (5): - одиниця, відповідає вільному члену - кількість матеріалу 1 - кількість матеріалу 2 - кількість матеріалу 3 - кількісний показник умов виробництва

Вихідна змінна: - вміст октану

```
In [769]: dataframe_path = 'data/octane-rating.csv'
          df = pd.read_csv(dataframe_path)
          config3 = ModelConfig(theta='unknown',
                                X=df.loc[:, 'One':'Condition'],
                                y=df['Octane number'])
          config3.show(5)
```

```
Regressors: m = 5
True parameters: θ = unknown
Sample length: n = 82
X[:10]:
[[ 1.      55.33     1.72    54.       1.66219]
 [ 1.      59.13     1.2     53.       1.58399]
 [ 1.      57.39     1.42    55.       1.61731]
```

```
 [ 1.      56.43     1.78    55.       1.66228]
 [ 1.      55.98     1.58    54.       1.63195]]
y[:10]:
[92.19 92.74 91.88 92.8  92.56]
```

House Prices Прогнозування цін на нерухомість.

! TODO: DESCRIBE TASK

Вхідні змінні: - .

Вихідна змінна: - .

```
In [770]: dataframe_path = 'data/house-prices-cleaned.csv'
          df = pd.read_csv(dataframe_path)
          config3 = ModelConfig(theta='unknown',
                                X=df.loc[:, 'MSSubClass':'YrSold'],
                                y=df['SalePrice'])
          config3.show(1)
```

```
Regressors: m = 36
True parameters: θ = unknown
Sample length: n = 1460
X[:10]:
[[4.11087386e+00 4.18965474e+00 9.04204006e+00 7.00000000e+00
  5.00000000e+00 2.00300000e+03 2.00300000e+03 5.28320373e+00
  6.56103067e+00 0.00000000e+00 5.01727984e+00 6.75343792e+00
  6.75343792e+00 6.75110147e+00 0.00000000e+00 7.44483327e+00
  1.00000000e+00 0.00000000e+00 2.00000000e+00 1.00000000e+00
  3.00000000e+00 6.93147181e-01 8.00000000e+00 0.00000000e+00
  2.00300000e+03 2.00000000e+00 5.48000000e+02 0.00000000e+00
  4.12713439e+00 0.00000000e+00 0.00000000e+00 0.00000000e+00
  0.00000000e+00 0.00000000e+00 2.00000000e+00 2.00800000e+03]]
y[:10]:
[12.24769912]
```

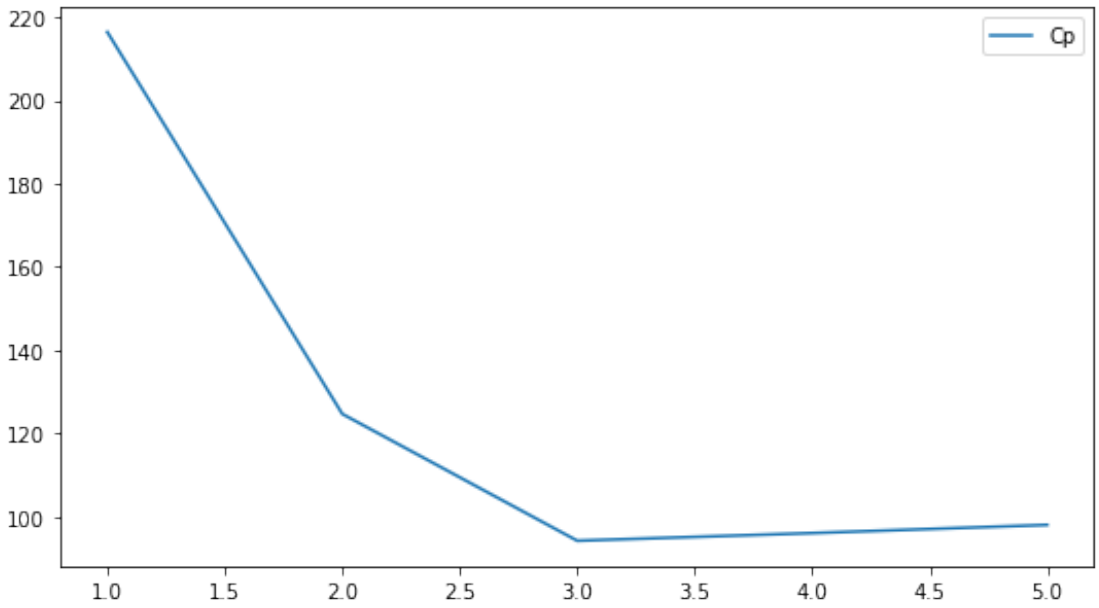
1.2 Пошук моделі. Послідовне включення (метод з лабораторної роботи №2)

1.2.1 Тест 1

```
In [772]: df1 = config1.run_single_RMNK_model_selection(p=None,
                                                        criteria=['Cp'],
                                                        plot=True)
          print()
          df2 = config1.run_single_RMNK_model_selection(p='reverse',
                                                        criteria=['Cp'],
                                                        plot=True)
```

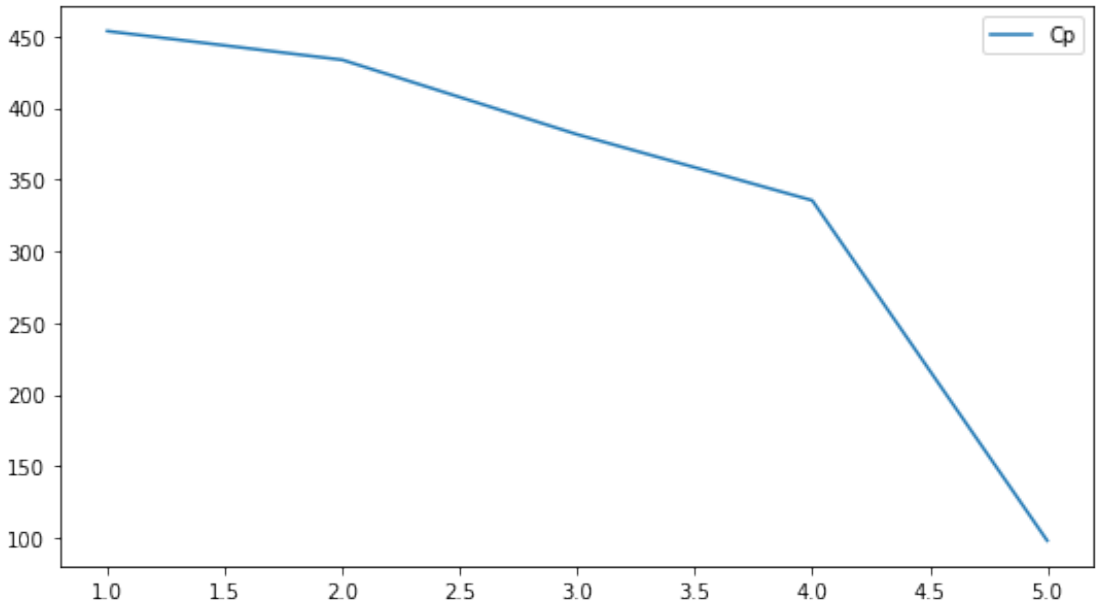
```
=============
DIRECT
```

```
=============
Regressors order: [0 1 2 3 4]
```




```
Optimal:
        s* = 3.0
        regressors = [1, 2, 3]

=============
REVERSE
=============
Regressors order: [4 3 2 1 0]
```

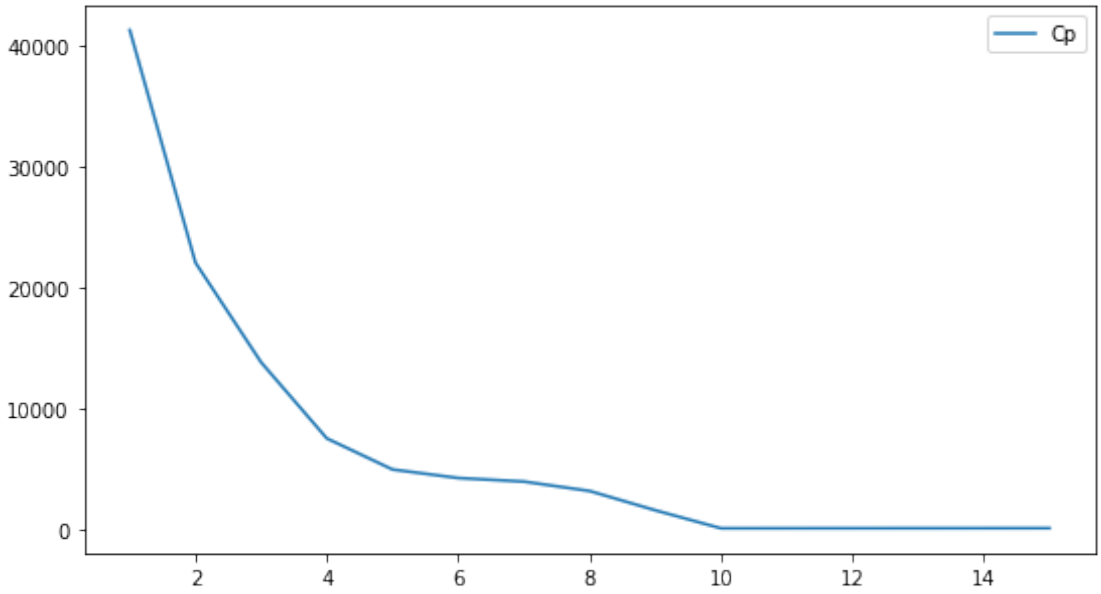



```
Optimal:
        s* = 5.0
        regressors = [1, 2, 3, 4, 5]
```

1.2.2 Тест 2

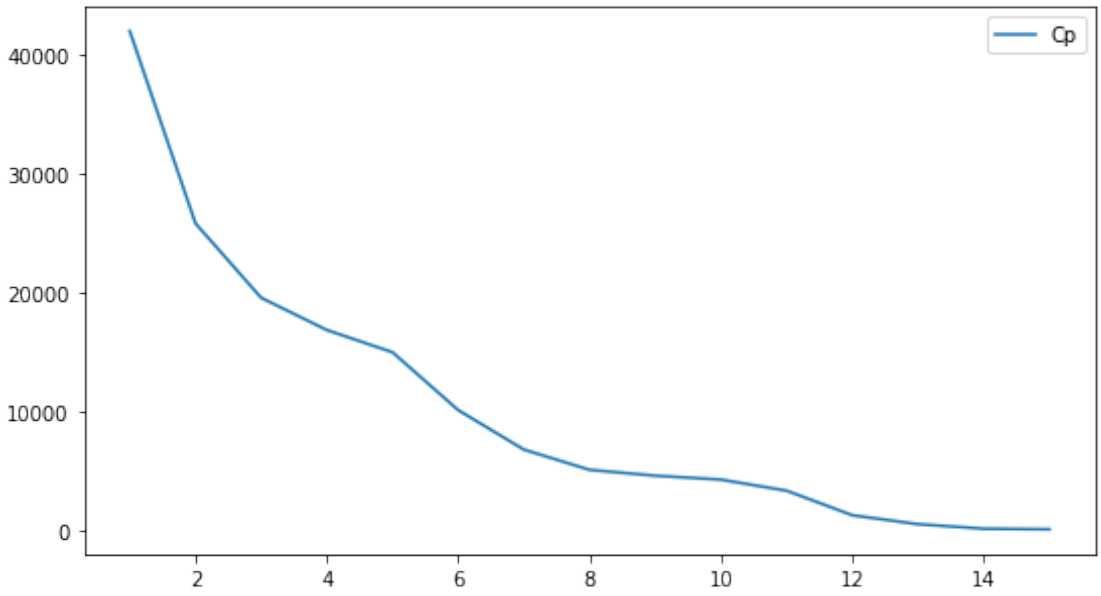
```
In [773]: df1 = config2.run_single_RMNK_model_selection(p=None,
                                                        criteria=['Cp'],
                                                        plot=True)
          print()
          df2 = config2.run_single_RMNK_model_selection(p='reverse',
                                                        criteria=['Cp'],
                                                        plot=True)

=============
DIRECT
=============
Regressors order: [ 0  1  2  3  4  5  6  7  8  9 10 11 12 13 14]
```




```
Optimal:
        s* = 10.0
        regressors = [1, 2, 3, 4, 5, 6, 7, 8, 9, 10]

=============
REVERSE
=============
Regressors order: [14 13 12 11 10  9  8  7  6  5  4  3  2  1  0]
```

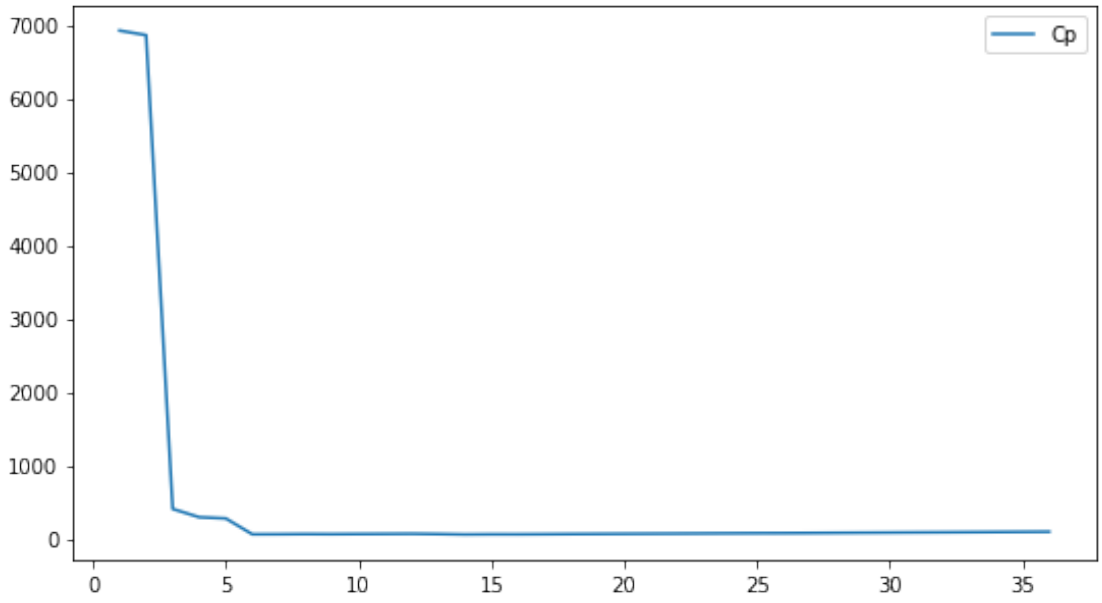


```
Optimal:
        s* = 15.0
        regressors = [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15]
```

1.2.3 Тест 3

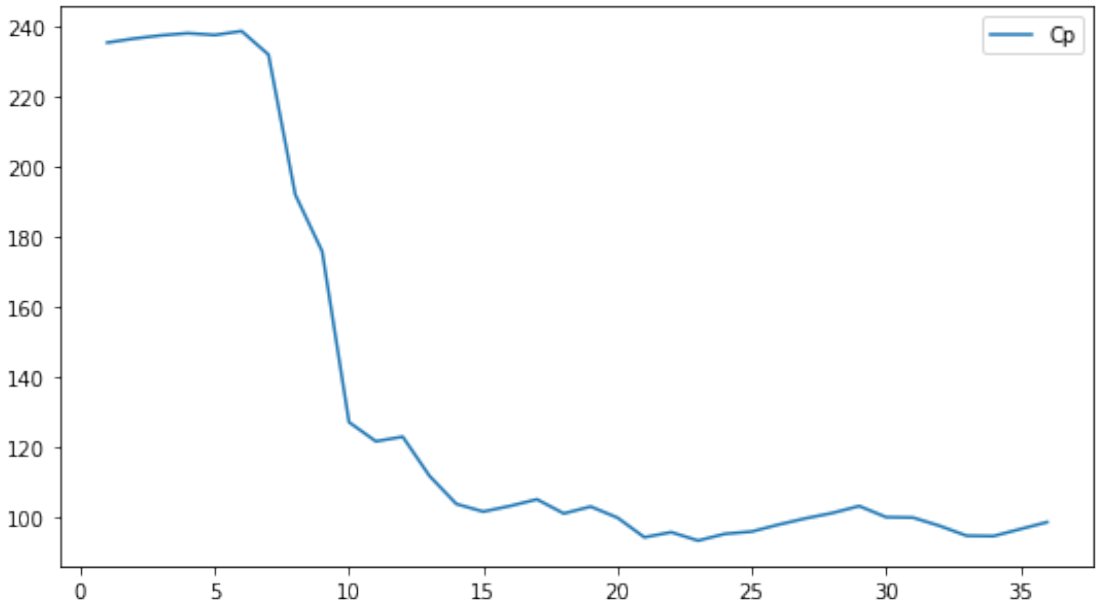
```
In [774]: df1 = config3.run_single_RMNK_model_selection(p=None,
                                                        criteria=['Cp'],
                                                        plot=True)
          print()
          df2 = config3.run_single_RMNK_model_selection(p='reverse',
                                                        criteria=['Cp'],
                                                        plot=True)
```

```
=============
DIRECT
=============
Regressors order: [ 0  1  2  3  4  5  6  7  8  9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
 24 25 26 27 28 29 30 31 32 33 34 35]
```




```
Optimal:
        s* = 14.0
        regressors = [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14]
```

```
=============
REVERSE
=============
Regressors order: [35 34 33 32 31 30 29 28 27 26 25 24 23 22 21 20 19 18 17 16 15 14 13 12
 11 10  9  8  7  6  5  4  3  2  1  0]
```



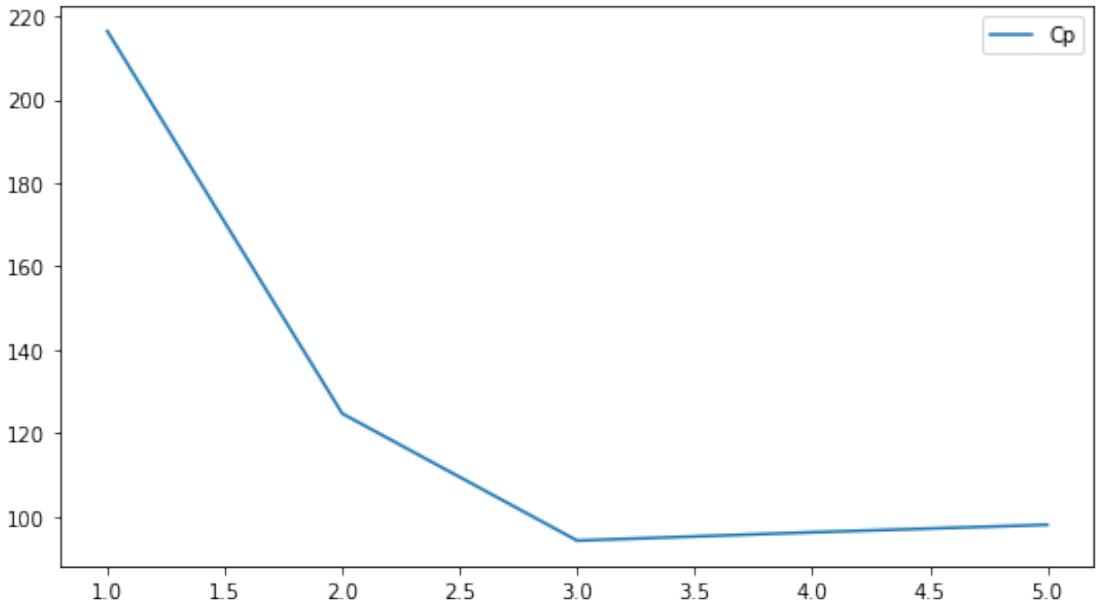

```
Optimal:
        s* = 23.0
        regressors = [14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32
```

1.3 Пошук моделі. Метод кореляційного включення

1.3.1 Тест 1

```
In [775]: df1 = config1.run_single_RMNK_model_selection(p='correlation',
                                                        criteria=['Cp'],
                                                        plot=True)
```

```
=====================
CORRELATION INCLUDING
=====================
Regressors order: [0 1 2 4 3]
```

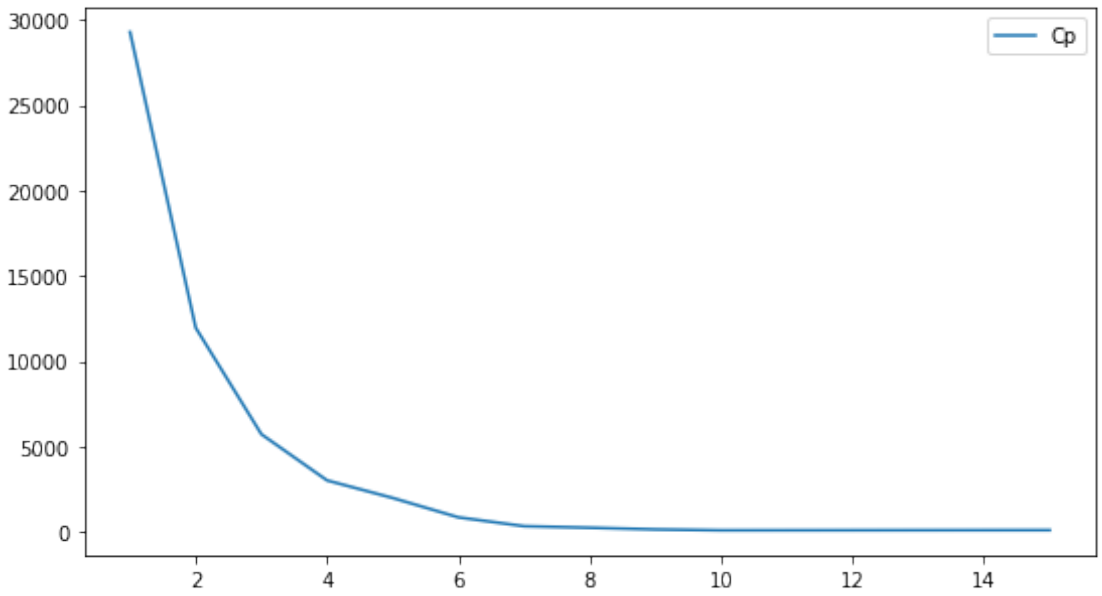



```
Optimal:
        s* = 3.0
        regressors = [1, 2, 3]
```

1.3.2 Тест 2

```
In [776]: df1 = config2.run_single_RMNK_model_selection(p='correlation',
                                                        criteria=['Cp'],
                                                        plot=True)

======================
CORRELATION INCLUDING
======================
Regressors order: [ 3  9  8  2  7  4  1  6  5  0 13 14 12 11 10]
```

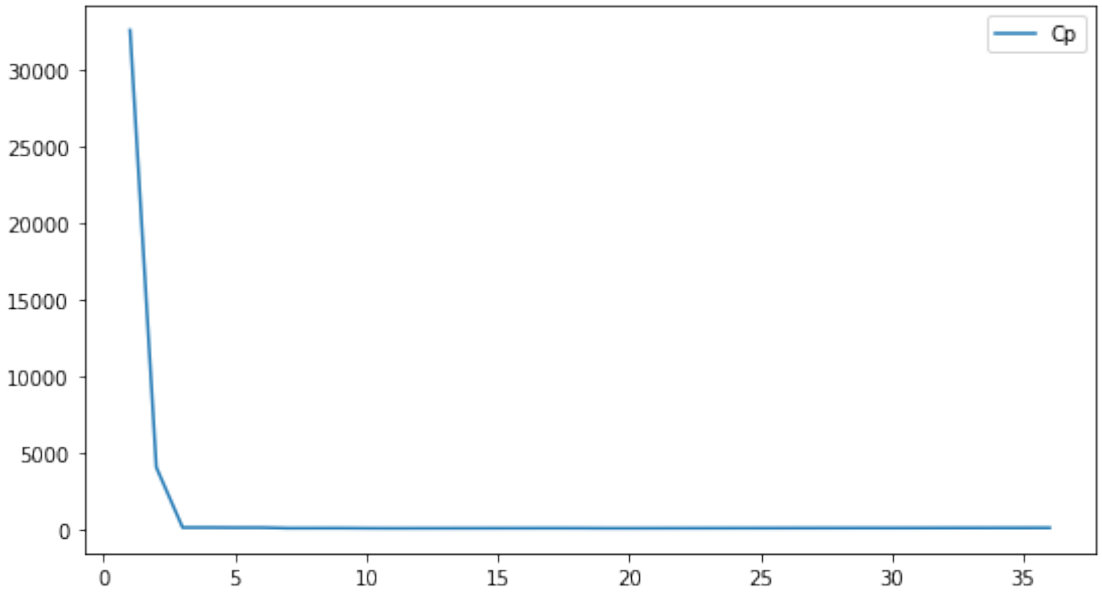



```
Optimal:
        s* = 10.0
        regressors = [1, 2, 3, 4, 5, 6, 7, 8, 9, 10]
```

1.3.3 Тест 3

```
In [777]: df1 = config3.run_single_RMNK_model_selection(p='correlation',
                                                        criteria=['Cp'],
                                                        plot=True)

=====================
CORRELATION INCLUDING
=====================
Regressors order: [26 24  5  1  6  7  3 28 27 22  8 13 25 11 10 29 18 23 15  2 12 20 19 34
 31 16 33  9 35  4 14 30 32  0 21 17]
```




```
Optimal:
        s* = 11.0
        regressors = [2, 4, 6, 7, 8, 9, 23, 25, 27, 28, 29]
```

1.4 Пошук моделі. Метод випадкового включення

1.4.1 Тест 1

```
In [779]: Ks = [10, 20, 50]
          for K in Ks:
              config1.run_single_random_RMNK_model_selection(K=K, criteria=['Cp'],
                                                             main_criterion='Cp')
```

```
================================
RANDOM INCLUDING WITH K = 10
================================

    s*      regressors*         Cp
0  5.0  [1, 2, 3, 4, 5]  98.083822
1  5.0  [1, 2, 3, 4, 5]  98.083822
2  5.0  [1, 2, 3, 4, 5]  98.083822
3  5.0  [1, 2, 3, 4, 5]  98.083822
4  4.0     [1, 2, 3, 5]  96.276951
...
    s*      regressors*         Cp
5  3.0        [1, 2, 3]  94.282328
6  5.0  [1, 2, 3, 4, 5]  98.083822
```

```
7  4.0     [1, 2, 3, 4]  96.115626
8  4.0     [1, 2, 3, 5]  96.276951
9  4.0     [1, 2, 3, 4]  96.115626

Optimal:
        s* = 3.0
        regressors = [1, 2, 3]
================================
RANDOM INCLUDING WITH K = 20
================================

    s*      regressors*         Cp
0  5.0  [1, 2, 3, 4, 5]  98.083822
1  4.0     [1, 2, 3, 4]  96.115626
2  5.0  [1, 2, 3, 4, 5]  98.083822
3  4.0     [1, 2, 3, 4]  96.115626
4  5.0  [1, 2, 3, 4, 5]  98.083822
...
     s*      regressors*         Cp
15  5.0  [1, 2, 3, 4, 5]  98.083822
16  4.0     [1, 2, 3, 5]  96.276951
17  4.0     [1, 2, 3, 5]  96.276951
18  3.0        [1, 2, 3]  94.282328
19  3.0        [1, 2, 3]  94.282328

Optimal:
        s* = 3.0
        regressors = [1, 2, 3]
================================
RANDOM INCLUDING WITH K = 50
================================

    s*      regressors*         Cp
0  3.0        [1, 2, 3]  94.282328
1  4.0     [1, 2, 3, 5]  96.276951
2  4.0     [1, 2, 3, 4]  96.115626
3  3.0        [1, 2, 3]  94.282328
4  5.0  [1, 2, 3, 4, 5]  98.083822
...
     s*      regressors*         Cp
45  5.0  [1, 2, 3, 4, 5]  98.083822
46  4.0     [1, 2, 3, 5]  96.276951
47  5.0  [1, 2, 3, 4, 5]  98.083822
48  5.0  [1, 2, 3, 4, 5]  98.083822
49  4.0     [1, 2, 3, 4]  96.115626

Optimal:
        s* = 3.0
```

```
        regressors = [1, 2, 3]
```

1.4.2 Тест 2

```
In [780]: Ks = [10, 20, 50]
          for K in Ks:
              config2.run_single_random_RMNK_model_selection(K=K, criteria=['Cp'],
                                                             main_criterion='Cp')
```

```
================================
RANDOM INCLUDING WITH K = 10
================================

     s*                                          regressors*          Cp
0  15.0  [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14...  116.237123
1  15.0  [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14...  116.237123
2  15.0  [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14...  116.237123
3  15.0  [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14...  116.237123
4  14.0    [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 14, 15]  114.258229
...
     s*                                          regressors*          Cp
5  15.0  [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14...  116.237123
6  15.0  [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14...  116.237123
7  15.0  [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14...  116.237123
8  15.0  [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14...  116.237123
9  15.0  [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14...  116.237123

Optimal:
        s* = 14.0
        regressors = [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 14, 15]
================================
RANDOM INCLUDING WITH K = 20
================================

     s*                                          regressors*          Cp
0  14.0    [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 15]  114.280158
1  15.0  [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14...  116.237123
2  15.0  [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14...  116.237123
3  14.0    [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 13, 14, 15]  114.453405
4  14.0    [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 12, 13, 14, 15]  114.237896
...
      s*                                          regressors*          Cp
15  14.0    [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 14, 15]  114.258229
16  14.0    [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 13, 14, 15]  114.453405
17  15.0  [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14...  116.237123
18  15.0  [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14...  116.237123
19  15.0  [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14...  116.237123
```

```
Optimal:
        s* = 13.0
        regressors = [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 13, 15]
================================
RANDOM INCLUDING WITH K = 50
================================
```

	s*	regressors*	Cp
0	14.0	[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14]	114.288080
1	14.0	[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14]	114.288080
2	15.0	[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14...	116.237123
3	13.0	[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 12, 14, 15]	112.259362
4	15.0	[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14...	116.237123
...			
	s*	regressors*	Cp
45	15.0	[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14...	116.237123
46	12.0	[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 14]	110.498738
47	15.0	[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14...	116.237123
48	15.0	[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14...	116.237123
49	15.0	[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14...	116.237123

```
Optimal:
        s* = 12.0
        regressors = [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 14]
```

1.4.3 Тест 3

```
In [782]: Ks = [10, 20, 50, 100]
          for K in Ks:
              config3.run_single_random_RMNK_model_selection(K=K, criteria=['Cp'],
                                                             main_criterion='Cp')
```

```
================================
RANDOM INCLUDING WITH K = 10
================================
```

	s*	regressors*	Cp
0	21.0	[1, 2, 4, 5, 7, 8, 9, 11, 13, 15, 16, 20, 23, ...	75.332316
1	19.0	[1, 2, 5, 7, 9, 13, 16, 18, 19, 22, 24, 25, 27...	82.430653
2	22.0	[1, 2, 3, 4, 5, 6, 10, 11, 13, 15, 17, 20, 21,...	78.091102
3	13.0	[3, 4, 5, 6, 8, 9, 12, 15, 16, 18, 23, 26, 28]	56.085399
4	20.0	[1, 4, 5, 9, 10, 12, 13, 16, 17, 19, 23, 24, 2...	75.436484
...			
	s*	regressors*	Cp
5	8.0	[3, 4, 7, 10, 13, 18, 23, 35]	62.258830
6	17.0	[1, 2, 4, 7, 9, 10, 14, 15, 16, 18, 21, 27, 29...	69.731694

```
7  23.0  [2, 3, 7, 8, 9, 10, 11, 14, 16, 17, 18, 19, 20...  87.231527
8  22.0  [1, 2, 4, 5, 6, 8, 12, 14, 16, 18, 20, 21, 22,...  75.364583
9  24.0  [1, 2, 4, 5, 7, 8, 9, 10, 12, 13, 14, 15, 16, ...  80.195423

Optimal:
        s* = 13.0
        regressors = [3, 4, 5, 6, 8, 9, 12, 15, 16, 18, 23, 26, 28]
================================
RANDOM INCLUDING WITH K = 20
================================

     s*                                          regressors*         Cp
0  30.0  [1, 3, 4, 5, 6, 8, 9, 10, 12, 13, 14, 15, 16, ...  87.133982
1  24.0  [1, 2, 3, 4, 5, 6, 7, 9, 10, 13, 14, 16, 17, 1...  76.010921
2  16.0  [1, 2, 5, 6, 10, 12, 14, 16, 17, 18, 19, 22, 2...  71.824050
3  21.0  [1, 2, 3, 4, 7, 8, 11, 15, 16, 17, 18, 19, 20,...  76.634644
4  16.0  [1, 4, 6, 13, 14, 15, 17, 21, 22, 23, 25, 26, ...  71.283410
...
      s*                                          regressors*         Cp
15  26.0  [1, 3, 4, 5, 6, 7, 8, 10, 11, 12, 13, 14, 15, ...  82.392430
16  16.0  [1, 5, 7, 9, 10, 11, 13, 14, 15, 16, 17, 25, 2...  80.362725
17  16.0  [1, 3, 5, 6, 11, 14, 16, 17, 18, 22, 25, 26, 2...  68.556969
18  13.0    [1, 4, 5, 7, 9, 17, 21, 27, 30, 31, 32, 35, 36]  74.879940
19  11.0            [1, 4, 6, 7, 9, 12, 20, 21, 23, 26, 30]  65.816640

Optimal:
        s* = 7.0
        regressors = [3, 4, 5, 6, 16, 26, 28]
================================
RANDOM INCLUDING WITH K = 50
================================

     s*                                          regressors*         Cp
0  17.0  [4, 8, 9, 14, 15, 17, 19, 22, 23, 25, 26, 27, ...  78.082043
1  15.0  [3, 4, 6, 9, 11, 14, 15, 19, 21, 25, 29, 31, 3...  73.891446
2  15.0  [1, 2, 3, 6, 9, 13, 19, 20, 21, 22, 24, 26, 28...  80.762026
3  18.0  [1, 2, 3, 4, 6, 8, 11, 13, 16, 17, 18, 19, 21,...  72.293154
4  12.0      [2, 4, 7, 12, 13, 15, 17, 19, 22, 25, 27, 29]  70.688988
...
      s*                                          regressors*         Cp
45  15.0  [5, 6, 7, 10, 12, 13, 16, 20, 24, 26, 27, 28, ...  67.555766
46  26.0  [1, 3, 5, 6, 7, 8, 9, 12, 14, 16, 18, 19, 20, ...  85.026921
47  27.0  [1, 3, 4, 5, 8, 9, 11, 12, 13, 15, 16, 18, 19,...  86.834162
48  13.0  [1, 4, 7, 11, 13, 14, 19, 22, 23, 24, 25, 33, 36]  67.250935
49  12.0       [3, 4, 6, 7, 12, 14, 16, 21, 25, 27, 28, 30]  58.748351

Optimal:
        s* = 12.0
```

```
        regressors = [3, 4, 6, 7, 12, 14, 16, 21, 25, 27, 28, 30]
================================
RANDOM INCLUDING WITH K = 100
================================

     s*                                          regressors*         Cp
0  19.0  [2, 3, 4, 5, 6, 10, 11, 12, 19, 20, 21, 22, 23...  75.832161
1  18.0  [1, 3, 5, 6, 9, 11, 13, 16, 19, 21, 22, 24, 25...  71.932551
2  12.0       [2, 4, 8, 9, 11, 21, 22, 23, 24, 25, 26, 36]  70.415613
3  15.0  [2, 4, 5, 6, 9, 11, 15, 16, 18, 21, 23, 24, 26...  63.595051
4  21.0  [1, 3, 5, 6, 7, 8, 12, 15, 17, 18, 20, 23, 24,...  90.928419
...
      s*                                           regressors*         Cp
95  14.0  [1, 3, 5, 6, 9, 13, 16, 19, 22, 25, 27, 33, 34...  68.959838
96  25.0  [1, 4, 5, 6, 7, 11, 12, 13, 14, 15, 16, 17, 19...  79.659246
97  19.0  [4, 7, 10, 13, 14, 15, 16, 18, 20, 23, 24, 26,...  75.974088
98  12.0      [1, 3, 4, 10, 11, 17, 19, 22, 23, 24, 31, 36]  70.722923
99   9.0                  [4, 5, 6, 12, 16, 23, 25, 26, 27]  55.254030

Optimal:
        s* = 5.0
        regressors = [4, 7, 12, 13, 16]
```

1.5 Пошук моделі. Метод перебірного включення

1.5.1 Тест 1

```
In [802]: total_df, best_df = config1.run_single_picking_RMNK_model_selection(\
                                                              criteria=['Cp'],
                                                              main_criterion='Cp')

================================
PICKING INCLUDING
================================
Optimal:
        s* = 3.0
        regressors = [1, 2, 3]
```

Таблиця, яка добре демонструє роботу алгоритма (порядок зберігається)

```
In [804]: total_df

Out[804]:       s       regressors          Cp
          0   1.0              [1]  216.391532
          1   1.0              [2]  538.833175
          2   1.0              [3]  380.129151
          3   1.0              [4]  450.597581
```

```
4   1.0              [5]  453.573587
5   2.0           [1, 2]  124.724060
6   2.0           [1, 3]  218.131896
7   2.0           [1, 4]  208.106903
8   2.0           [1, 5]  209.318742
9   3.0        [1, 2, 3]   94.282328
10  3.0        [1, 2, 4]  124.557551
11  3.0        [1, 2, 5]  122.679471
12  4.0     [1, 2, 3, 4]   96.115626
13  4.0     [1, 2, 3, 5]   96.276951
14  5.0  [1, 2, 3, 4, 5]   98.083822
```

1.5.2 Тест 2

```
In [805]: total_df, best_df = config2.run_single_picking_RMNK_model_selection(\
                                                              criteria=['Cp'],
                                                              main_criterion='Cp')

================================
PICKING INCLUDING
================================
Optimal:
        s* = 10.0
        regressors = [1, 2, 3, 4, 5, 6, 7, 8, 9, 10]
```

Таблиця, яка добре демонструє роботу алгоритма (порядок зберігається)

```
In [806]: total_df

Out[806]:         s                                          regressors            Cp
          0     1.0                                                 [1]  41354.994466
          1     1.0                                                 [2]  37630.005797
          2     1.0                                                 [3]  32941.436205
          3     1.0                                                 [4]  29282.190223
          4     1.0                                                 [5]  36730.260511
          5     1.0                                                 [6]  39343.294431
          6     1.0                                                 [7]  39495.098730
          7     1.0                                                 [8]  34653.767187
          8     1.0                                                 [9]  30581.757867
          9     1.0                                                [10]  29854.461825
          10    1.0                                                [11]  44022.317531
          11    1.0                                                [12]  41104.689524
          12    1.0                                                [13]  42800.114205
          13    1.0                                                [14]  40799.957978
          14    1.0                                                [15]  41995.263811
          15    2.0                                             [1, 4]  17284.417147
          16    2.0                                             [2, 4]  16302.798927
          17    2.0                                             [3, 4]  14232.594994
```

```
18    2.0                                                [4, 5]  13945.909409
19    2.0                                                [4, 6]  17043.496668
20    2.0                                                [4, 7]  17846.634431
21    2.0                                                [4, 8]  15899.736951
22    2.0                                                [4, 9]  13061.886973
23    2.0                                               [4, 10]  11966.835111
24    2.0                                               [4, 11]  19331.477751
25    2.0                                               [4, 12]  19181.642813
26    2.0                                               [4, 13]  18745.264177
27    2.0                                               [4, 14]  18211.267525
28    2.0                                               [4, 15]  18527.616071
29    3.0                                            [1, 4, 10]   8700.767740
..    ...                                                   ...           ...
101   9.0                        [1, 2, 3, 4, 5, 6, 8, 9, 10]    145.526558
102  10.0                     [1, 2, 3, 4, 5, 6, 8, 9, 10, 11]    147.459809
103  10.0                     [1, 2, 3, 4, 5, 6, 8, 9, 10, 12]    147.404664
104  10.0                     [1, 2, 3, 4, 5, 6, 8, 9, 10, 13]    147.031402
105  10.0                     [1, 2, 3, 4, 5, 6, 8, 9, 10, 14]    147.386212
106  10.0                     [1, 2, 3, 4, 5, 6, 8, 9, 10, 15]    147.223308
107  11.0                  [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]    108.550762
108  10.0                      [1, 2, 3, 4, 5, 6, 7, 8, 9, 10]    106.550762
109  11.0                  [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 12]    108.347553
110  11.0                  [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 13]    108.544791
111  10.0                      [1, 2, 3, 4, 5, 6, 7, 8, 9, 10]    106.550762
112  11.0                  [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 14]    108.498893
113  11.0                  [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 15]    108.520007
114  11.0                  [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 14]    108.498893
115  12.0              [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 14]    110.498738
116  11.0                  [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 14]    108.498893
117  12.0              [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 12, 14]    110.314425
118  12.0              [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 13, 14]    110.490035
119  12.0              [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 14, 15]    110.460960
120  12.0              [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 14]    110.498738
121  13.0          [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 14]    112.311029
122  12.0              [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 14]    110.498738
123  13.0          [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 13, 14]    112.489985
124  13.0          [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 14, 15]    112.460862
125  13.0          [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 14]    112.311029
126  14.0     [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14]    114.288080
127  13.0          [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 14]    112.311029
128  14.0     [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 14, 15]    114.258229
129  14.0     [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 14, 15]    114.258229
130  15.0  [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14...    116.237123

[131 rows x 3 columns]
```

Таблиця, яка містить глобально кращий результат на кожній ітерації підвищення складності

```
In [797]: best_df
```

Out[797]:

	s*	regressors*	Cp
0	1.0	[4]	29282.190223
1	2.0	[4, 10]	11966.835111
2	3.0	[4, 9, 10]	5730.487062
3	4.0	[3, 4, 9, 10]	3026.765316
4	5.0	[3, 4, 5, 9, 10]	1535.515926
5	6.0	[2, 3, 4, 5, 9, 10]	829.992514
6	7.0	[2, 3, 4, 5, 8, 9, 10]	346.640527
7	8.0	[2, 3, 4, 5, 6, 8, 9, 10]	218.295380
8	9.0	[1, 2, 3, 4, 5, 6, 8, 9, 10]	145.526558
9	10.0	[1, 2, 3, 4, 5, 6, 7, 8, 9, 10]	106.550762
10	10.0	[1, 2, 3, 4, 5, 6, 7, 8, 9, 10]	106.550762
11	10.0	[1, 2, 3, 4, 5, 6, 7, 8, 9, 10]	106.550762
12	10.0	[1, 2, 3, 4, 5, 6, 7, 8, 9, 10]	106.550762
13	10.0	[1, 2, 3, 4, 5, 6, 7, 8, 9, 10]	106.550762
14	10.0	[1, 2, 3, 4, 5, 6, 7, 8, 9, 10]	106.550762

1.5.3 Тест 3

```
In [798]: total_df, best_df = config3.run_single_picking_RMNK_model_selection(\
                                                        criteria=['Cp'],
                                                        main_criterion='Cp')

================================
PICKING INCLUDING
================================
Optimal:
        s* = 7.0
        regressors = [3, 4, 5, 6, 9, 16, 26]
```

Таблиця, яка добре демонструє роботу алгоритма (порядок зберігається)

```
In [799]: total_df
```

Out[799]:

	s	regressors	Cp
0	1.0	[1]	6922.622699
1	1.0	[2]	171607.168945
2	1.0	[3]	595.423285
3	1.0	[4]	8072.403830
4	1.0	[5]	8415.507144
5	1.0	[6]	158.358196
6	1.0	[7]	175.164569
7	1.0	[8]	208501.298773
8	1.0	[9]	69222.239836
9	1.0	[10]	187787.682459
10	1.0	[11]	19886.729830

11	1.0		[12]	5277.995979
12	1.0		[13]	280.697357
13	1.0		[14]	119107.026909
14	1.0		[15]	207716.568406
15	1.0		[16]	208.827496
16	1.0		[17]	124823.714740
17	1.0		[18]	199572.038985
18	1.0		[19]	20872.240938
19	1.0		[20]	131690.187233
20	1.0		[21]	15268.403104
21	1.0		[22]	3751.889765
22	1.0		[23]	10822.918605
23	1.0		[24]	107593.708684
24	1.0		[25]	4139.687219
25	1.0		[26]	28801.198215
26	1.0		[27]	32587.576839
27	1.0		[28]	109136.079786
28	1.0		[29]	95121.691000
29	1.0		[30]	182670.791806
..	...		...	...
772	31.0	[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14...		89.120961
773	32.0	[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14...		90.880558
774	33.0	[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14...		92.767377
775	32.0	[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14...		90.880558
776	33.0	[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14...		92.800002
777	32.0	[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14...		90.880558
778	33.0	[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14...		92.878469
779	31.0	[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14...		89.120961
780	32.0	[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14...		90.880558
781	33.0	[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14...		92.855271
782	32.0	[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14...		90.880558
783	33.0	[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14...		92.767377
784	34.0	[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14...		94.695102
785	31.0	[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14...		89.120961
786	32.0	[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14...		90.880558
787	33.0	[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14...		92.767377
788	34.0	[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14...		94.766422
789	34.0	[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14...		94.739615
790	32.0	[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14...		90.880558
791	33.0	[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14...		92.767377
792	34.0	[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14...		94.695102
793	35.0	[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14...		96.693792
794	33.0	[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14...		92.767377
795	34.0	[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14...		94.695102
796	35.0	[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14...		96.668793
797	32.0	[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14...		90.880558
798	33.0	[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14...		92.767377
799	34.0	[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14...		94.695102

```
800  35.0  [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14...      96.693792
801  36.0  [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14...      98.667221

[802 rows x 3 columns]
```

Таблиця, яка містить глобально кращий результат на кожній ітерації підвищення складності

```
In [800]: best_df
```

Out[800]:

	s*	regressors*	Cp
0	1.0	[6]	158.358196
1	2.0	[6, 16]	78.361004
2	3.0	[4, 6, 16]	54.822413
3	4.0	[3, 4, 6, 16]	49.481128
4	5.0	[3, 4, 5, 6, 16]	47.128611
5	6.0	[3, 4, 5, 6, 9, 16]	45.398392
6	7.0	[3, 4, 5, 6, 9, 16, 26]	44.912894
7	7.0	[3, 4, 5, 6, 9, 16, 26]	44.912894
8	7.0	[3, 4, 5, 6, 9, 16, 26]	44.912894
9	7.0	[3, 4, 5, 6, 9, 16, 26]	44.912894
10	7.0	[3, 4, 5, 6, 9, 16, 26]	44.912894
11	7.0	[3, 4, 5, 6, 9, 16, 26]	44.912894
12	7.0	[3, 4, 5, 6, 9, 16, 26]	44.912894
13	7.0	[3, 4, 5, 6, 9, 16, 26]	44.912894
14	7.0	[3, 4, 5, 6, 9, 16, 26]	44.912894
15	7.0	[3, 4, 5, 6, 9, 16, 26]	44.912894
16	7.0	[3, 4, 5, 6, 9, 16, 26]	44.912894
17	7.0	[3, 4, 5, 6, 9, 16, 26]	44.912894
18	7.0	[3, 4, 5, 6, 9, 16, 26]	44.912894
19	7.0	[3, 4, 5, 6, 9, 16, 26]	44.912894
20	7.0	[3, 4, 5, 6, 9, 16, 26]	44.912894
21	7.0	[3, 4, 5, 6, 9, 16, 26]	44.912894
22	7.0	[3, 4, 5, 6, 9, 16, 26]	44.912894
23	7.0	[3, 4, 5, 6, 9, 16, 26]	44.912894
24	7.0	[3, 4, 5, 6, 9, 16, 26]	44.912894
25	7.0	[3, 4, 5, 6, 9, 16, 26]	44.912894
26	7.0	[3, 4, 5, 6, 9, 16, 26]	44.912894
27	7.0	[3, 4, 5, 6, 9, 16, 26]	44.912894
28	7.0	[3, 4, 5, 6, 9, 16, 26]	44.912894
29	7.0	[3, 4, 5, 6, 9, 16, 26]	44.912894
30	7.0	[3, 4, 5, 6, 9, 16, 26]	44.912894
31	7.0	[3, 4, 5, 6, 9, 16, 26]	44.912894
32	7.0	[3, 4, 5, 6, 9, 16, 26]	44.912894
33	7.0	[3, 4, 5, 6, 9, 16, 26]	44.912894
34	7.0	[3, 4, 5, 6, 9, 16, 26]	44.912894
35	7.0	[3, 4, 5, 6, 9, 16, 26]	44.912894

2 Висновки

! TODO: Write down conclusions

3 Код програми

3.1 Імпорт необхідних бібліотек, налаштування

```
In [623]: import numpy as np
          import pandas as pd
          from scipy.integrate import odeint
          from itertools import permutations
          import matplotlib.pyplot as plt
          %matplotlib inline

          from pylab import rcParams
          rcParams['figure.figsize'] = 9, 5
```

3.2 Реалізація МНКО

```
In [624]: def RMNK(X, y, s=None, sigma_estimation=None, verbose=False,
                   deep_verbose=False, create_dataframe=False):
              assert X.ndim == 2 and X.shape[1] > 0
              m = X.shape[1]
              if m > 1:
                  if create_dataframe:
                      w, H_inv, RSS, df = RMNK(X[:,:-1], y, s, sigma_estimation,
                                               verbose, deep_verbose, create_dataframe)
                      if s and m > s:
                          return w, H_inv, RSS, df
                  else:
                      w, H_inv, RSS = RMNK(X[:,:-1], y, s, sigma_estimation,
                                           verbose, deep_verbose, create_dataframe)
                      if s and m > s:
                          return w, H_inv, RSS
                  # w is of shape = [m-1, 1]; H_inv is of shape = [m-1, m-1]
                  h = (X[:,:-1].T @ X[:,-1]).reshape(-1,1) # shape = [m-1, 1]
                  eta = X[:,-1].T @ X[:,-1] # shape = [1, 1]
                  alpha = H_inv @ h # shape = [m-1, 1]
                  beta = eta - h.T @ alpha # shape = [1, 1]
                  beta_inv = 1 / beta # shape = [1, 1]
                  gamma = X[:,-1].T @ y # shape = [1, 1]
                  nu = beta_inv * (gamma - h.T @ w) # shape = [1, 1]
                  w = np.vstack((w - nu * alpha, nu))  # shape = [m, 1]
                  H_next_inv = np.vstack((np.hstack((H_inv + beta_inv * alpha @ alpha.T,
                                                     (- beta_inv * alpha).reshape(-1, 1))),
                                          np.hstack((-beta_inv * alpha.T, beta_inv))))
                  RSS_next = (RSS - nu.flatten() ** 2 * beta.flatten())[0]
```

```
else: # 1
    H_inv = np.array([[0]])
    eta = beta = X[:,-1].T @ X[:,-1]
    beta_inv = 1 / beta
    alpha = h = np.array([0])
    gamma = X[:,-1].T @ y
    nu = np.array([beta_inv * gamma])
    w = np.array([nu])
    H_next_inv = np.array(beta_inv).reshape(1, 1)
    RSS_next = (y.T @ y - y.T @ X[:,-1].reshape(-1, 1) @ w)[0]
    if create_dataframe:
        if sigma_estimation is None:
            df = pd.DataFrame(columns=['s', 'RSS', 'Cp', 'FPE'])
        else:
            df = pd.DataFrame(columns=['s', 'RSS', 'Cp_simple',
                                       'Cp', 'FPE'])

if verbose:
    print('================================================')
    print('\tStep {}'.format(m))
    print('================================================')
    if deep_verbose:
        print('h_{}:\t\t{}'.format(m, h.reshape(-1,1)[:,0]))
        print('eta_{}:\t\t{}'.format(m, eta))
        print('alpha_{}:\t{}'.format(m, alpha.reshape(-1,1)[:,0]))
        print('beta_{}:\t\t{}'.format(m, beta))
        print('gamma_{}:\t{}'.format(m, gamma))
        print('nu_{}:\t\t{}'.format(m, nu))
        print('================================================')
    print('> θ_{}: {}'.format(m, w[:, 0]))
    print('> H_{}_inv:\n{}'.format(m, H_next_inv))
    print('> RSS_{}: {}'.format(m, RSS_next))
if create_dataframe:
    n = y.shape[0]
    FPE = (n + m) / (n - m) * RSS_next
    Cp_simple = RSS_next + 2 * m
    if sigma_estimation is None:
        df = df.append({'s': m, 'RSS': RSS_next,
                        'Cp': Cp_simple, 'FPE': FPE},
                       ignore_index=True)
    else:
        Cp = RSS_next + 2 * sigma_estimation * m
        df = df.append({'s': m, 'RSS': RSS_next,
                        'Cp_simple': Cp_simple,
                        'Cp': Cp, 'FPE': FPE},
                       ignore_index=True)
    return w, H_next_inv, RSS_next, df
```

```
        return w, H_next_inv, RSS_next
```

3.3 Реалізація класу моделювання і усіх необхідних методів

```
In [745]: class ModelConfig():
        m = 5
        n = 10
        n_grid = [10, 30, 100]
        theta = np.array([3, -2, 1, 0, 0])
        a = 0
        b = 2
        sigma = 0.3
        s0 = 3
        s = m

        def __init__(self, m=None, s0=None, theta=None, a=None, b=None,
                     X=None, y=None):
            if m:
                self.m = m
                self.s = m
            if s0:
                self.s0 = s0
            if theta:
                if isinstance(theta, dict) and theta['random']:
                    self.theta = np.zeros(self.m)
                    self.theta[:self.s0] = np.random.uniform(*theta['random'],
                                                             size=self.s0)
                elif theta == 'unknown':
                    assert X is not None, 'Please provide data (X)'
                    assert y is not None, 'Please provide target values as well (y)'
                    self.theta = theta
                else:
                    self.theta = theta
            if a:
                self.a = a
            if b:
                self.b = b
            if X is not None:
                assert y is not None, 'Please provide target values as well (y)'
                self.X = np.array(X)
                self.y = np.array(y)
                (self.n, self.m) = X.shape
                self.s = self.m
            else:
                self.compile()

        def generate_noise_and_output(self):
            self.ksi = np.random.normal(0, self.sigma, size=self.n)
```

```
        self.y = self.X @ self.theta + self.ksi

    def compile(self, n=None, sigma=None):
        if n:
            self.n = n
        if sigma:
            self.sigma = sigma
        self.X = np.random.uniform(self.a, self.b, size=(self.n, self.m))
        self.generate_noise_and_output()

    def show(self, n_limit=10):
        print('Regressors: m = {}'.format(self.m))
        print('True parameters: θ = {}'.format(self.theta))
        if not isinstance(self.theta, str):
            equation_str = ''
            for i, theta_i in enumerate(self.theta):
                equation_str += ' + ({}) * x{}'.format(theta_i, i+1)
            equation_str = 'y0 = '+ equation_str[3:]
            print(equation_str)
            print('Noise generation: σ = {}'.format(self.sigma))
        print('Sample length: n = {}'.format(self.n))
        print('X[:10]:\n{}'.format(self.X[:n_limit]))
        print('y[:10]:\n{}'.format(self.y[:n_limit]))

    def show_estimations(self):
        print('RSS(m) = {:5.5}'.format(self.RSS))
        print('σ* = {:5.5}'.format(self.sigma_hat ** .2))

    def estimate_sigma(self):
        _, _, self.RSS = RMNK(self.X, self.y, s=self.s,
                              verbose=False, create_dataframe=False)
        self.sigma_hat = self.RSS ** 2 / (self.X.shape[0] - self.X.shape[1])

    def run_grid_RMNK_model_selection(self):
        self.estimate_sigma()
        for i, n in enumerate(self.n_grid):
            for j, sigma in enumerate(self.sigma_grid):
                self.compile(n, sigma)
                print('-------------------------------------------------------------'
                print('\t\t\tSAMPLE #{}'.format(i * len(self.n_grid) + j + 1))
                print('-------------------------------------------------------------'
                print('\t\tCONFUGURATIONS & DATA')
                self.show()
                print('\n\t\tRLSM ITERATIONS')
                theta_pred, _, _, df = RMNK(self.X, self.y, s=self.s,
                                            verbose=True, create_dataframe=True)
                print('\n\t\t\tRESULTS')
                print('\nPARAMETERS')
```

```
            print('True values:\tθ: {}'.format(self.theta))
            print('Estimates:\tθ*: {}'.format(theta_pred[:,0]))
            plt.plot(df['s'], df['RSS'], label='RSS')
            plt.plot(df['s'], df['Cp'], label='Cp')
            plt.plot(df['s'], df['FPE'], label='FPE')
            plt.legend()
            plt.show()
            print(df)
            print('s* by Cp:  {}'.format(np.array(df['Cp']).argmin()+1))
            print('s* by FPE: {}'.format(np.array(df['FPE']).argmin()+1))
            print()

    def run_single_RMNK_model_selection(self, p=None, plot=False,
                                        criteria=['Cp', 'FPE', 'RSS']):
        """Single RMNK

        p : str in ['direct', 'reverse', 'correlation'] or list
            if list: permutation indices
            if str: how to create permutation
        """
        if p == 'reverse':
            print('=============\nREVERSE\n=============')
            p = np.flip(np.arange(self.m), axis=0)
        elif p == 'correlation':
            print('====================\nCORRELATION INCLUDING\n====================
            correlations = np.abs(np.cov(self.X.T, self.y.T)[-1,:-1])
            p = np.argsort(-correlations)
        elif isinstance(p, list):
            print('=============\nCUSTOM\n=============')
        else:
            print('=============\nDIRECT\n=============')
            p = np.arange(self.m)
        print('Regressors order: {}'.format(p))
        theta_pred, _, _, df = RMNK(self.X[:,p], self.y, s=self.s,
                                    verbose=False, create_dataframe=True)

        df['regressors'] = [str(sorted(p[:int(s)]+1)) for s in df.s]
        for criterion in criteria:
            df[criterion] = np.round(df[criterion], 6)
        if plot:
            for criterion in criteria:
                plt.plot(df['s'], df[criterion], label=criterion)
                plt.legend()
                plt.show()
        df = df.sort_values(by=criteria).reset_index()\
                    [['s', 'regressors'] + criteria]
        self.s_opt, self.regressors_opt = df.loc[0, ['s','regressors']]
        print('Optimal:')
```

```
        print('\ts* = {}\n\tregressors = {}'.format(self.s_opt,
                                                    self.regressors_opt))
        return df

    def run_single_full_RMNK_model_selection(self,
                                             criteria=['Cp', 'FPE', 'RSS']):
        print('=============\nBRUT FORCE\n=============')
        total_df = pd.DataFrame()
        for p in permutations(range(self.m)):
            p = np.array(p)
            theta_pred, _, _, df = RMNK(self.X[:,p], self.y, s=self.s,
                                        verbose=False, create_dataframe=True)
            df['regressors'] = [str(sorted(p[:int(s)]+1)) for s in df.s]
            total_df = pd.concat([total_df, df], axis=0)
        for criterion in criteria:
            total_df[criterion] = np.round(total_df[criterion], 6)
        total_df = total_df.drop_duplicates()
        total_df = total_df.sort_values(by=criteria).reset_index()\
                   [['s', 'regressors'] + criteria]
        return total_df

    def run_single_random_RMNK_model_selection(self, K=20,
                                               criteria=['Cp', 'FPE', 'RSS'],
                                               main_criterion='Cp'):
        print('================================\nRANDOM INCLUDING WITH K = {}\n=======
        permutations = [np.random.permutation(self.m) for k in range(K)]
        total_df = pd.DataFrame()
        best_df = pd.DataFrame()
        self.main_criterion_value = np.Inf
        for p in permutations:
            p = np.array(p)
            theta_pred, _, _, df = RMNK(self.X[:,p], self.y, s=self.s,
                                        verbose=False, create_dataframe=True)
            df['regressors'] = [str(sorted(p[:int(s)]+1)) for s in df.s]
            df = df.sort_values(by=criteria).reset_index()
            main_criterion_value = df.loc[0, main_criterion]
            if main_criterion_value < self.main_criterion_value:
                self.main_criterion_value = main_criterion_value
                self.theta_pred = theta_pred
                self.s_opt, self.regressors_opt = df.loc[0,
                                                         ['s', 'regressors']]
            total_df = pd.concat([total_df, df], axis=0)
            best_df = pd.concat([best_df, df.loc[0:0]], axis=0)
        for criterion in criteria:
            total_df[criterion] = np.round(total_df[criterion], 6)
            best_df[criterion] = np.round(best_df[criterion], 6)
        total_df = total_df.drop_duplicates()
        total_df = total_df.sort_values(by=criteria).reset_index()\
```

```
                [['s', 'regressors'] + criteria]
        best_df = best_df.rename(columns={'s': 's*',
                                 'regressors': 'regressors*'}).reset_index()\
                  [['s*', 'regressors*'] + criteria]
        print()
        print(best_df[:5])
        print('...')
        print(best_df[-5:])
        print()
        print('Optimal:')
        print('\ts* = {}\n\tregressors = {}'.format(self.s_opt,
                                                   self.regressors_opt))
        return total_df, best_df

    def run_single_picking_RMNK_model_selection(self,
                                                criteria=['Cp', 'FPE', 'RSS'],
                                                main_criterion='Cp'):
        print('================================\nPICKING INCLUDING\n==================
        total_df = pd.DataFrame()
        best_df = pd.DataFrame()
        self.main_criterion_value = np.Inf
        remained_indices = list(range(self.m))
        regressors_indices = []
        while len(remained_indices) > 0:
            local_main_criterion_value = np.Inf
            for i in remained_indices:
                p = np.array(regressors_indices + [i])
                theta_pred, _, _, df = RMNK(self.X[:,p], self.y, s=len(p),
                                            verbose=False, create_dataframe=True)
                df['regressors'] = [str(sorted(p[:int(s)]+1)) for s in df.s]
                df = df.sort_values(by=criteria).reset_index()
                main_criterion_value = df.loc[0, main_criterion]
                if main_criterion_value < local_main_criterion_value:
                    local_main_criterion_value = main_criterion_value
                    local_df = df[:1]
                    local_i = i
                if main_criterion_value < self.main_criterion_value:
                    self.main_criterion_value = main_criterion_value
                    self.theta_pred = theta_pred
                    self.s_opt, self.regressors_opt = df.loc[0, ['s', 'regressors']]
                total_df = pd.concat([total_df, df], axis=0)
            regressors_indices += [local_i]
            remained_indices.remove(local_i)
            best_df = pd.concat([best_df, local_df], axis=0)
        for criterion in criteria:
            total_df[criterion] = np.round(total_df[criterion], 6)
            best_df[criterion] = np.round(best_df[criterion], 6)
        total_df = total_df.drop_duplicates().reset_index()\
```

```
                    [['s', 'regressors'] + criteria]
#         total_df = total_df.sort_values(by=criteria).reset_index()\
#                     [['s', 'regressors'] + criteria]
        best_df = best_df.rename(columns={'s': 's*',
                                 'regressors': 'regressors*'}).reset_index()\
                  [['s*', 'regressors*'] + criteria]
        print('Optimal:')
        print('\ts* = {}\n\tregressors = {}'.format(self.s_opt,
                                                   self.regressors_opt))
        return total_df, best_df
```