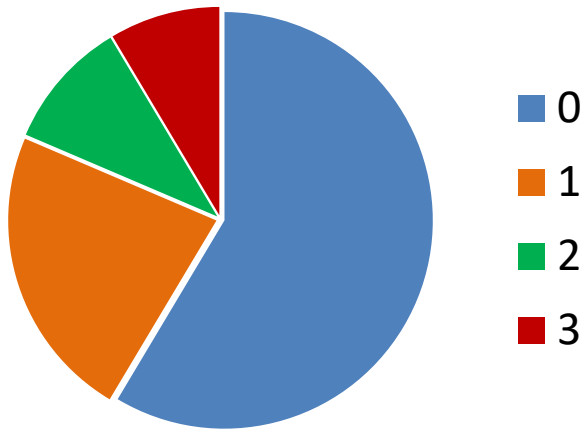


Квантовые вычисления: применения

Артем Корюкин

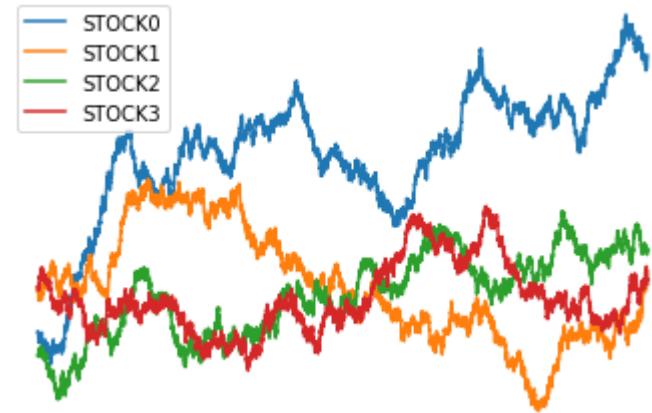
Оптимизация портфолио с помощью квантовых компьютеров

Портфель активов



```
# Set parameters for assets and risk factor
num_assets = 4      # set number of assets to 4
q = 0.5             # set risk factor to 0.5
budget = 2          # set budget as defined in the problem
```

optimal value: [1. 0. 1. 0.]



```
q2 = 0.5           #Set risk factor to 0.5
budget2 = 3         #Set budget to 3
bounds = [[0,2] for x_i in range(num_assets)]
```

optimal value: [2. 0. 1. 0.]

Высокодоходный портфель активов
(акций) с минимальными рисками

Расчет запрещенной зоны молекул OLED

OLED (органический
светодиод)

```
from qiskit_nature.drivers import Molecule
from qiskit_nature.drivers.second_quantization import ElectronicStructureDriverType, ElectronicStructureMoleculeDriver

# PSPCz molecule
geometry = [['C', [-0.2316640, 1.1348450, 0.6956120]],
            ['C', [-0.8886300, 0.3253780, -0.2344140]],
            ['C', [-0.1842470, -0.1935670, -1.3239330]],
            ['C', [1.1662930, 0.8801450, -1.4737160]],
            ['C', [1.8089230, 0.8832220, -0.5383540]],
            ['C', [1.1155860, 1.4218050, 0.5392780]],
            ['S', [3.5450920, 1.2449890, -0.7349240]],
            ['O', [3.8606900, 1.0881590, -2.1541690]],
            ['C', [4.3889120, -0.0620730, 0.1436780]],
            ['O', [3.8088290, 2.4916780, -0.0174650]],
            ['C', [4.6830900, 0.1064460, 1.4918230]],
            ['C', [5.3364470, -0.9144080, 2.1705280]],
            ['C', [5.6895490, -2.0818670, 1.5007820]],
            ['C', [5.4000540, -2.2323130, 0.1481350]],
            ['C', [4.7467230, -1.2180160, -0.5404770]],
            ['N', [-2.2589180, 0.0399120, -0.0793330]],
            ['C', [-2.8394600, -1.2343990, -0.1494160]],
            ['C', [-4.2635450, -1.0769890, 0.0660760]],
            ['C', [-4.5212550, 0.2638010, 0.2662190]],
            ['C', [-3.2669630, 0.9823890, 0.1722720]],
            ['C', [-2.2678900, -2.4598950, -0.3287380]],
            ['C', [-3.1299420, -3.6058560, -0.3236210]],
            ['C', [-4.5179520, -3.4797390, -0.1395160]],
            ['C', [-5.1056310, -2.2512990, 0.0536940]],
            ['C', [-5.7352450, 1.0074800, 0.5140960]],
            ['C', [-5.6563790, 2.3761270, 0.6274610]],
            ['C', [-4.4287740, 3.0501460, 0.5083650]],
            ['C', [-3.2040560, 2.3409470, 0.2746950]],
            ['H', [-0.7813570, 1.5286610, 1.5426490]],
            ['H', [-0.7079140, -0.7911480, -2.0611600]],
            ['H', [1.7161320, -0.2933710, -2.3302930]]]
```

=== GROUND STATE ENERGY ===

```
* Electronic ground state energy (Hartree): -4043.632437386191
  - computed part: -0.766114826099
  - ActiveSpaceTransformer extracted energy part: -4042.866322560092
```

=== EXCITED STATE ENERGIES ===

```
1:
* Electronic excited state energy (Hartree): -4043.426320955958
* Electronic excited state energy (Hartree): -4043.426320955959
> Total excited state energy (Hartree): -4043.426320955959
2:
* Electronic excited state energy (Hartree): -4043.394874376457
* Electronic excited state energy (Hartree): -4043.394874376457
> Total excited state energy (Hartree): -4043.394874376457
3:
* Electronic excited state energy (Hartree): -4043.085273016712
* Electronic excited state energy (Hartree): -4043.085273016712
> Total excited state energy (Hartree): -4043.085273016712
```

```
bandgap = qeom_results.computed_energies[1] - qeom_results.computed_energies[0]
bandgap # in Hartree
```

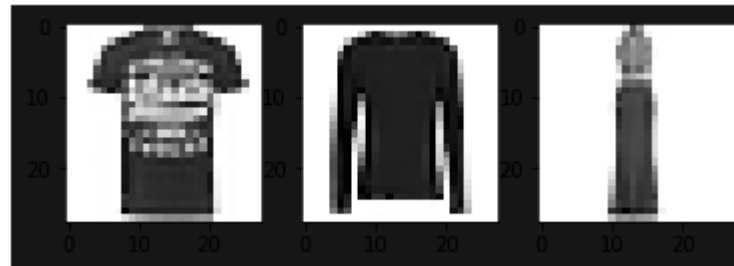
0.20611643023268267

Дисплеи,
внутренняя квантовая
эффективность (IQE) от
25% к 100%

Qiskit Nature

Классификация изображений

```
LABELS = [0, 2, 3]
num_labels = len(LABELS)
for i in range(num_labels):
    ax = fig.add_subplot(1, num_labels, i+1)
    img = sample_train[labels_train==LABELS[i]][0].reshape((28, 28))
    ax.imshow(img, cmap="Greys")
```



Prediction: [0 0 3 3 3 3 0 2 0 0 3 0 2 2 3 2 3 0 3 0]

Упаковка рюкзака



```
val = [5,6,7,8,9]  
wt = [4,5,6,7,8]  
W = 18
```

```
result:  
  optimal function value: 21.0  
  optimal value: [0. 1. 1. 1. 0.]  
  status: SUCCESS  
  
  index of the chosen items: [1, 2, 3]
```

Оптимизация замен аккумуляторов

Количество циклов;
деградация
(количество циклов).

0	1
5; 1.	8; 3.
3; 1.	4; 2.
3; 2.	5; 3.
6; 1.	12; 2
9; 1.	10; 4
7; 1.	11; 3
1; 2.	2; 3.

Оптимальное расписание
замены батарей.

$$\max_{z \in \{0,1\}^n} \sum_{t=1}^n (1 - z_t) \lambda_1^t + z_t \lambda_2^t$$

$$s. t. \sum_{t=1}^n [(1 - z_t) c_1^t + z_t c_2^t] \leq C_{max}$$

```
L1 = [5,3,3,6,9,7,1]
L2 = [8,4,5,12,10,11,2]
C1 = [1,1,2,1,1,1,2]
C2 = [3,2,3,2,4,3,3]
C_max = 16
```

```
result: [1. 1. 1. 1. 0. 1. 0.]
total revenue: 50
```

Спасибо за внимание!