Data for Tutorial 4

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1 Problem 1:

You and your friend have an assignment from your boss to analyze how fast a secret chemical A can react into another secret chemical B.

$$A \to B$$

You and your buddy have run an experiment for the reaction in a batch reactor and got this data points below. We assume your friend likes Python as much as you do and as a good friend he has imported everything into Python arrays.

```
time_array = array([   0.,  125.,  250.,  375.,  500.,  625.,  750.,  875., 1000.,
       1125., 1250., 1375., 1500., 1625., 1750., 1875., 2000., 2125.,
       2250., 2375., 2500., 2625., 2750., 2875.])

C_A_array = array([10.28148623,  8.92676003,  7.47370739,  7.20498621,  6.01448975,
        4.85174028,  4.68868558,  4.01410753,  3.94055544,  3.04186757,
        2.40544184,  2.62290428,  2.18704979,  1.31502537,  1.03730156,
        2.28837979,  0.45062549,  1.43886825,  1.26808295,  1.24125421,
        0.28353151,  0.90117414,  0.74132173,  0.73710597])
```

You know that `time_array` corresponds to time and `C_A_array` to $C_A(t)$.
You also know that it is the first order reaction, i.e:
$-r_A = kC_A$
Now $\dfrac{dC_A}{dt} = -kC_A$ and the solution is $C_A(t) = C_{A0} \cdot e^{-kt}$
Your boss says that you and your friend need to give him a reaction constant k otherwise your whole company won't be able to deliver a new product and will experience significant difficulties (especially after the recent tax reform). You suspect $C_{A0} = 10moles$, but it would be nice to check that as well.
What should we do?

1.1 Problem 2:

Fitting another function:
$dC_A/dt = -k$
The exact solution here would be
$C_A = C_{A0} - kt$
Our Experimental data is:

```python
import numpy as np
time_array = np.array([ 0.        ,  0.30612245,  0.6122449 ,  0.91836735,  1.2244898 ,
        1.53061224,  1.83673469,  2.14285714,  2.44897959,  2.75510204,
        3.06122449,  3.36734694,  3.67346939,  3.97959184,  4.28571429,
        4.59183673,  4.89795918,  5.20408163,  5.51020408,  5.81632653,
        6.12244898,  6.42857143,  6.73469388,  7.04081633,  7.34693878,
        7.65306122,  7.95918367,  8.26530612,  8.57142857,  8.87755102,
        9.18367347,  9.48979592,  9.79591837, 10.10204082, 10.40816327,
       10.71428571, 11.02040816, 11.32653061, 11.63265306, 11.93877551,
       12.24489796, 12.55102041, 12.85714286, 13.16326531, 13.46938776,
       13.7755102 , 14.08163265, 14.3877551 , 14.69387755, 15.        ])

C_A_array = np.array([10.07639696,  9.91832079,  9.88786894,  9.86452614,  9.94122765,
        9.84390408,  9.67133   ,  9.83831594,  9.85882335,  9.80157275,
        9.84539316,  9.55091516,  9.61587477,  9.66549779,  9.49617392,
        9.55431562,  9.35852625,  9.49039332,  9.38783532,  9.44147304,
        9.40256963,  9.29987479,  9.14910022,  9.40193543,  9.15306236,
        9.35110886,  9.21753824,  9.04908686,  9.23874406,  9.02922114,
        9.01426505,  9.07687961,  9.03789781,  8.74373902,  8.93811106,
        8.89792648,  8.92497756,  8.9052101 ,  8.69154187,  8.83577787,
        8.6515694 ,  8.8865218 ,  8.43442155,  8.63970657,  8.5779596 ,
        8.6386648 ,  8.64805349,  8.37248495,  8.60161561,  8.64226331])
```

We need to find C_A0 and k ?

2 Problem 3:

Your boss asked you to try another reaction and get parameters from there.

$$2A- > B$$

Your boss told you that it is probably a second order reaction $-r_A = k[C_A]^2$.

Your friend has helped you out with the design equation and the exact solution for the current system:

$dC_A/dt = -kC_A = -kC_A^2$

The exact solution here would be

$1/C_A = kt + 1/C_{A0}$

Your friend suggested that it would be better to plot $1/C_A$ instead of C_A. You think it is a great idea. Conveniently, your data is presented in the neccesseary format:

Time:

```python
time_array = array([ 0.        ,  0.41666667,  0.83333333,  1.25      ,  1.66666667,
        2.08333333,  2.5       ,  2.91666667,  3.33333333,  3.75      ,
        4.16666667,  4.58333333,  5.        ,  5.41666667,  5.83333333,
        6.25      ,  6.66666667,  7.08333333,  7.5       ,  7.91666667,
        8.33333333,  8.75      ,  9.16666667,  9.58333333, 10.        ])
```

and $1/C_A(time)$:

```
CA_inv_array = array([0.09955774, 0.10041539, 0.10164106, 0.10040534, 0.10151214,
       0.1027833 , 0.10252228, 0.10259392, 0.10369246, 0.10371607,
       0.10400771, 0.10517007, 0.10549644, 0.10558765, 0.10639114,
       0.10600782, 0.10506377, 0.10734534, 0.10655902, 0.10820498,
       0.1077726 , 0.10985819, 0.10912644, 0.11053292, 0.10939707])
```

Your task is to find parameters k and C_A0 from the experimental data.