Component specification

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Software components. High level description of the software components such as: *data manager*, which provides a simplified interface to your data and provides application specific features (e.g., querying data subsets); and *visualization manager*, which displays data frames as a plot. Describe at least 3 components specifying: what it does, inputs it requires, and outputs it provides.

PhotokineticAnalysis()

Functions

- PhotokineticAnalysis.check()

  a. Purpose: checks that the inputs for the calculate_theoretical function are correct

- PhotokineticAnalysis.calculate_theoretical()

  a. **Purpose:** Calculates theoretical photouncaging values using the following first order kinetic equation for photouncaging:

  $$\boldsymbol{Y = Y_o + (plateau - Y_o)(1 - \exp(-k * x))}$$

  b. Input:

  i. Array of x values separated by commas.

  ii. Photokinetic constant, k

  c. Output:

  iii. Table of x and corresponding y values (normalized to 1)

  iv. Scatter plot of theoretical data

- PhotokineticAnalysis.calculate_experimental()

  a. Purpose: Calculates the photouncaging constant k using the first order equation from above using raw data inputted from user as an excel file. It uses scipy.optimize.curve_fit to calculate the k value.

  b. Input:

  c. Excel file, formatted such that the first column is labelled with the x value and the corresponding y values labelled

  d. Output:

  v. Table of x and y values

  vi. Kinetic constant

  vii. Data normalized and plotted in a scatter plot

ChemotaxisSimulation

Functions

- ChemotaxisSimulation.cell_movement()

  a. Input:

- n: matrix size or dimensions of the plate area
- m: matrix size or dimensions of the plate area
- CC: location of initial cells in a matrix format where 1 indicates there is a cell
- V: compartment size, which should be set to 1
- rm: motility rate between 0-1, where 1 equates to faster cells
- rp: proliferation rate between 0-1, where 1 equates to max proliferation
- rd: death rate between 0-1, where 1 equates to max death rate
- tf: final dimensionless time of experiment
- C_start: if there is a chemotactic variable applied, when is it applied.
- C_end: if there is a chemotactic variable applied, when does it end.
- rhox: how the chemotactic variable is applied over space (i.e gradient, etc)

b. **Output:**
   i. n * m matrix with final cell positions

- ChemtoaxisSimulation.simulate()
  a. Input:
     ii. Title of movie file to be saved
  b. Output:
     iii. Movie file_name.gif

2. **Interactions to accomplish use cases**. Describe how the above software components interact to accomplish at least one of your use cases.
   a. **Interaction**: All the code uses an the __init__ function initializes the parameters that will then be used in the functions that follow.
   b. Interaction: For calculating theoretical photokinetics, the user can use the check function to see if the input is in the proper format for the calculating_theoretical function.
   c. Interaction: For calculating a kinetic constant from raw data, after uploading the **excel file** and if the user runs the calculate_experimental function it has a function embedded to calculate the experimental data. It does not rely on the other functions.
   d. Interaction: For ChemotaxisSimulation and the modeling cell migration function, cell_movement() produces an n x m matrix of final cell positions following a stochastic simulation for a given input conditions from the users based on their cell type and model and simulate() takes the output matrix of cell_movement to visually plot the movement and generates a movie of the plots over the various time course which are saved as whatever the user file name is inputted as.
3. **Future work**:
   a. Finish creating package
   b. Verify that unittest works when placed in a different folder