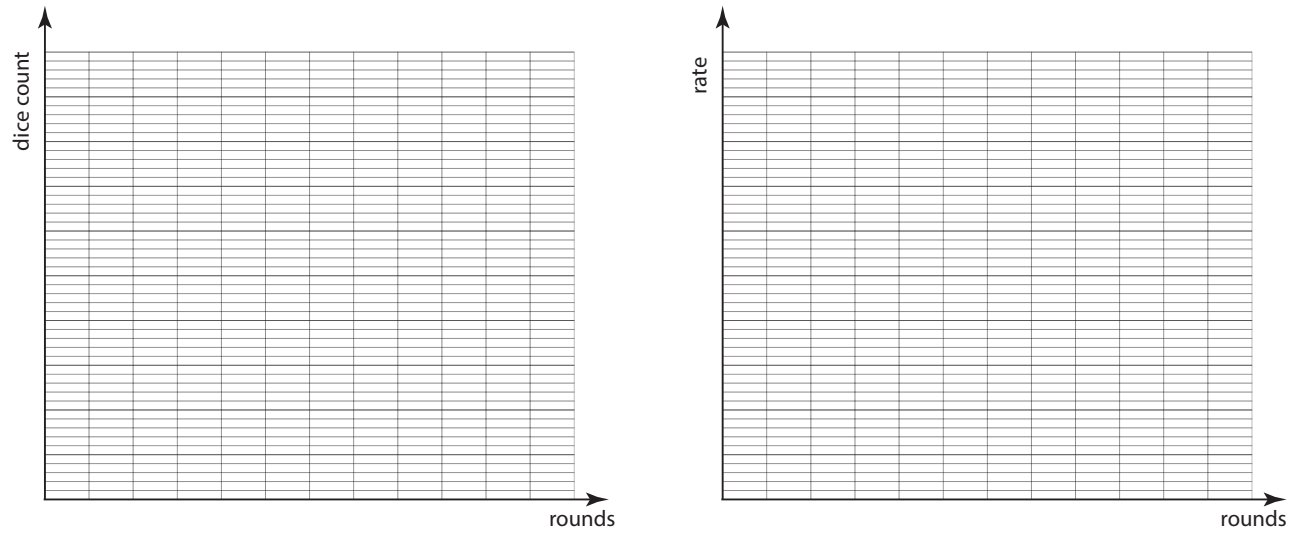
6 - Kinetics simulation - graphical analysis

We continue with the dice simulation found at https://www.jon.hk/app/kineqmsim/ This time extending into a kinetics analysis.

1. **Manual calculation**



(a) Sketch, on the left, the **count** vs **rounds** graph with dieCount = 1000, initialRemain = 1000, dieSide = 100, forward conditions = 20. Allow the simulation to run to round 20.

(b) From count we can get to the rate.

i. How can you calculate the rate for any given round?

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ii. Calculate the instantaneous rate for rounds 2, 6, 10, and 20.

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iii. Sketch, on the right, a **rate** vs **round** graph for the above simulation.

iv. Use your graph to deduce the **initial rate**.

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2. Automating the calculations

What you have done by hand can be automated. The procedure includes:

Clone spreadsheet *File* ⟶ *make a copy*) the spreadsheet from the dicesim link above, and share this link with your group.

Importing data Simulate a dice throw (you can use the same parameters as in Q1). Copy-paste the data into your spreadsheet column A.

Processing Create a new worksheet and transfer columns C–E to it for further processing.

If you need a hint for this section you can unhide (*View* ⟶ *Hidden Sheets*) "dataset 1" and examine it for details.

(a) Add and calculate a new **rate** column. (Use formulae and do not do this by hand!)

(b) For the rate vs rounds graph:

i. Fit a linear curve. What is the equation?

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ii. What evidence supports that a linear function $y = mx + c$ is appropriate for this graph?

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iii. Interpret the function. What does the function suggest? (Hint: examine each of the coefficients in turn.)

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iv. If you doubled the “forwardConditions” parameter in the simulation, how would that affect your coefficients? (Hint: be specific in your prediction. You can test your predictions by generating that exact run.)

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(c) For the dice vs rounds graph, deduce an equation and interpret its significance.

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