Problem 1. Fractional in Time Advection Dispersion - Moments

Consider the fractional in time advection dispersion equation

$$\frac{\partial^\gamma C}{\partial t^\gamma} + u\frac{\partial C}{\partial x} = D\frac{\partial^2 C}{\partial x^2} \qquad 0 < \gamma < 1 \tag{1}$$

Prove what was written in class about how the spatial moments will scale in time for a pulse initial condition, that is

$$m_0 = 1 \qquad m_1 \sim t^\alpha \qquad m_2 \sim t^{2\alpha} \tag{2}$$

where $m_n(t) = \int_{-\infty}^{\infty} x^n C(x,t)dx$. As an aside for you more mathematical types, can you show by induction that to leading order $m_n \sim t^{n\alpha}$ for any integer n.

Problem 2. Fractional in Time Dispersion - Reactions

Consider the same reaction problem we have considered many times in this class $A+B \rightarrow C$ and consider the reaction to be instantaneous, that is $C_A C_B = 0$. A, B and C can move by fractional in time diffusion, that is

$$\frac{\partial^\gamma C_i}{\partial t^\gamma} = D\frac{\partial^2 C_i}{\partial x^2} \pm r \qquad 0 < \gamma < 1 \qquad i = A, B, C \tag{3}$$

The initial conditions are

$$C_A(t=0) = H(-x) \qquad C_B(t=0) = H(x) \qquad C_C(t=0) = 0 \tag{4}$$

For the standard diffusion case $\gamma = 1$ we showed that the mass of C will grow like the square root of time, that is

$$M_C = \int_{-\infty}^{\infty} C_C dx = \sqrt{\frac{4Dt}{\pi}} \sim t^{\frac{1}{2}} \tag{5}$$

Can you tell me how the mass M_C will scale with time when $0 < \gamma < 1$? Indeed, if you can, try to give me the whole answer (not just the scaling - but the scaling itself is valuable).

What happens if we add advection now i.e. equation (3) becomes something like (1)). Can you still solve the problem in the same way? Why or why not? Can you still tell me something about the scaling in that case? Do not make any big calculations here - just explain your reasoning.

Problem 3. Bernoulli CTRW - A simple correlated CTRW

The Spatial Markov Model is a complex implementation of a correlated random walk, but in many settings what is called a Bernoulli model can actually capture a range of complex behaviors. Consider the following Langevin equation

$$x_{n+1} = x_n + \Delta x \qquad\qquad t_{n+1} = t_n + \tau_n \tag{6}$$

which is the same as the standard CTRW equation, but instead of drawing τ from $\psi(\tau)$ we draw it from $\psi(\tau_{n+1}|\tau_n)$, that is the next step is conditioned on the previous one, just like the SMM. But

$$\tau_{n+1} = \tau_n \tag{7}$$

with probability P OR

$$\tau_{n+1} = \tau \tag{8}$$

with probability $1 - P$. That is the time step is the same as the last with probability P or it is completely random with probability $1 - P$.

Implement the random walks with the distributions described in class slides (exponential, power law). The codes, as implemented in class, are available online in Codes for Chapter 15 folder. Implement the same CTRWs with P=0, 0.2, 0.4, 0.6, 0.8 and 1 and compare the resulting distributions. Note P=0 is the uncorrelated case. Discuss and explain similarities and differences.

SEE BELOW FOR OPTIONAL in 2020 - TO GET PRACTICE WITH CTRW TOOLBOX - DO AFTER SEMESTER ENDS IF YOU LIKE

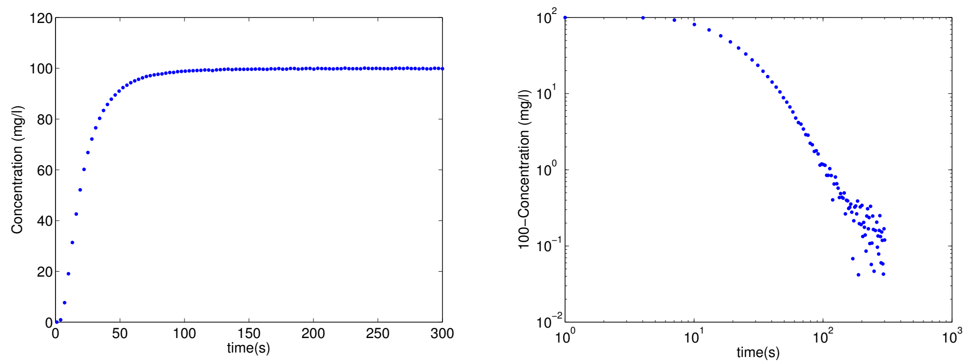

Figure 1: Breakthrough Curves for Problem 3.

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Problem 4. CTRW Tool box

The data shown in figure 1 is from a column experiment. The column is 50 cm long and a breakthrough curve is measured for a step input of concentration where the influent concentration steps from 0 to 100 mg/L. There is evidence of power law tailing in the BTC. The instrument you are using has a resolution of about 0.1 mg'L and you can see that the there is noise in the tail when plotted on the log-log axes in such a way that highlights tailing effects (second panel in figure 1).
Use the CTRW toolbox to obtain best fits to the data for both and Advection-Dispersion Model (ADE) as well as a CTRW with a truncated power law (TPL). Report the 2 parameters for the ADE and the 5 parameters for the TPL. Discuss matches and mismatches and in particular address whether you think there is any added benefit to the five parameter CTRW model over the 2 parameter ADE and explain carefully why you feel this way.

The data can be obtained from the class website under the link for Data for Homework 8. This file contains a single parameter a. The first column in a is time and the second one is concentration.

Problem 5. CTRW - Real Data

The data in figure 2 was obtained from a tracer test in a stream. It is noisy, but what is impressive about this data is that it spans so many orders of magnitude of concentration, something that is typically difficult to do with any conventional methods.

Try to estimate to the best of your ability the parameters that you might use for a CTRW model or any other model of your choosing should you so desire. You can try to use the CTRW optimization toolbox, but it is very hard to do and your best bet is probably to estimate some of the parameters ahead of time using any information you might have and then tweak the others to see if you can match what is observed by simply plotting the solution

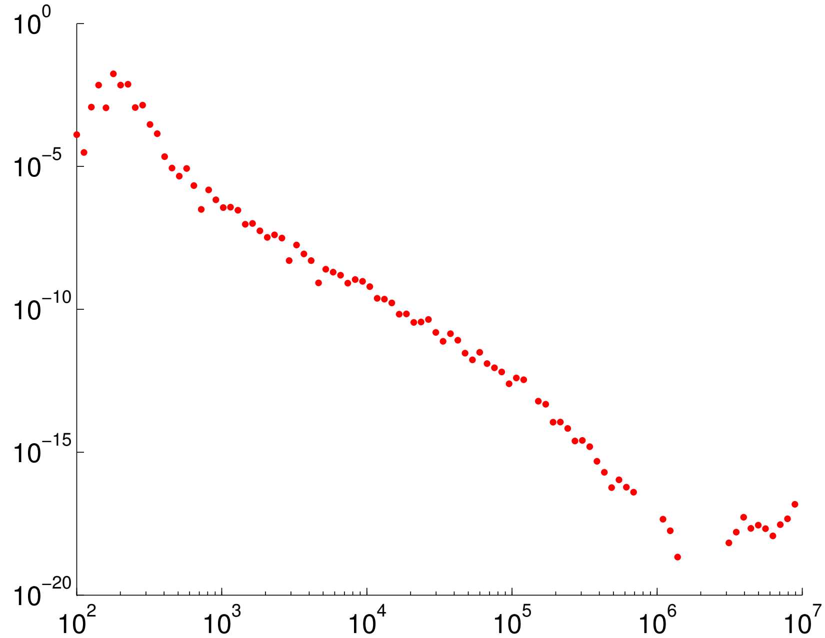

Figure 2: Breakthrough Curves for Problem 4.

with the CTRW toolbox routines. Don't be shy about distrusting certain parts of the curve if you so desire, but discuss it if you do so. This will be potentially painful as you will see just by playing around with parameters how sensitive and unstable CTRW solutions can be. But it is a useful endeavor if you pay close attention to how solutions change with changes in parameters. The data can be obtained from the class website under the link for Data for Homework 8. This file contains a single variable a. The first column in a is time and the second one is concentration. The mass has already been appropriately normalized.

In your final results report the v and D you obtain (don't worry about correcting for length of the river - if you're curious the BTC was measured 110 m downstream of the injection point).