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Project 2: Enzyme Kinetics, Reproduce all of Figure 2 from "Quasiequilibrium approximation of fast reaction kinetics in stochastic biochemical Systems"

The objective for this project was to implement a Monte Carlo simulation of a common enzyme catalyzed reaction using the Gillespie algorithm. This system is characterized by the following equations:

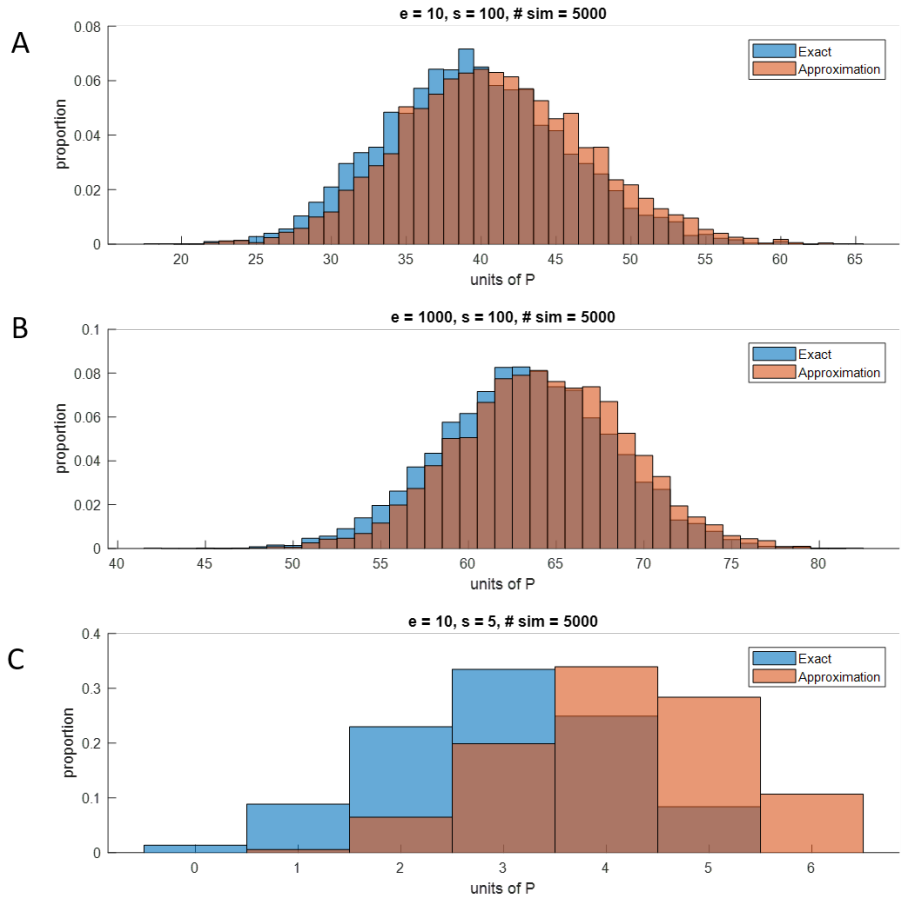
Reaction 1: $E + S \xrightarrow{c_2} E \cdot S$

Reaction 2: $E \cdot S \xrightarrow{c_3} E + S$

Reaction 3: $E \cdot S \xrightarrow{c_1} E + P$

Where reactions 1 and 2 represent the fast reactions in the system, due to rapid coupling of enzyme and substrate, while reaction 3 represents the slow reaction in the system.

To model the system, Monte Carlo simulation of 5k runs is obtained through application of the Gillespie algorithm on the chemical master equation. An exact and approximate solution is obtained for the system, with the exact solution modeling the propensity functions of all three reactions, while the latter models only the slow reaction (3), assuming that fluctuations in the fast reactions are negligible with regards to product production.



End proportion of product (PMF of DA process) at end of times (A) t =40s, (B) t=10s, and (C) t=10s.

Exact PMF (blue), Approximate PMF (orange).

Quantity of enzyme (e) and substrate (s) available at time of simulation is indicated in title.

5000 simulations were run per plot.

Simulations for (e,s,t) = (10,5,10) frequently timed out early, owing to full expenditure of substrate. These results were terminated early, with the final result (e,s,p) = (10,0,5) accepted as the final outcome. Approximate solution shifts distribution towards the right favoring more product, with the shift more pronounced at low initial counts of enzyme and substrate. For exact PMF, median for simulations represented in figures A, B, and C were 39, 63, and 3 molecules of P respectively, while for the approximate PMF, median was 41, 64, and 4. Standard deviation for exact PMF for figures A, B, C respectively were 6.10, 4.88, and 1.14, while approximate PMF standard deviations were 6.23, 4.80, and 1.10. Dispersion in each distribution for exact and approximate PMFs is relatively similar, with PMFs following a relatively Gaussian distribution. These result strengthen the validity of the approximation for this system, as the exact and approximate results exhibit similar characteristics.