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PHYS 256B

Term project

2a. ***Goal*****: What is your primary project goal? What you would like to learn?**

I would like to learn how to use epsilon-machine reconstruction methods and/or an information-engine/stochastic sensor framework to model the energetic cost of extracellular electron transfer from an external electron donor (cathode) to a single electroautotrophic bacteria as a function of how predictable the electron donor source (electrode) is. I am interested in how this might impact the gene-expression of such organisms and their strategies for respiration and ultimately their group behavior in a biofilm attached to the cathode. The hypothesis is that an external electron donor that is highly unpredictable is detrimental to the organism and would lead to down-regulation of the genes associated with synthesizing the protein complexes responsible for external electron transfer, which would also reduce conductivity of electroactive biofilms. For this project I will just model a single bacteria. The long term goal would be to extend the model to an entire biofilm to predict its behavior (could be incorporated into my thesis, possibly testable by experiment).

2b. ***System*****: Describe how the dynamical system is nonlinear and time-dependent.**

What's the state space?

The state space is the intercellular pools as defined in equation 1 from Mitra et al., 2015 [6]. The electron transfer channel also has a state (flow rate/fraction of channel capacity of the transfer channel).

What's the dynamic?

The dynamic is the time dependent evolution of this intercellular state space as a function of electron transfer through a bacterial cable, which is driven by an external electron donor (cathode) to which the bacterial cable is attached [3-6]. I would like to develop an equation that predicted the energetic cost/dissipation resulting from changes in the predictability of this external signal (electron transfer rate) similar to work in the field of information thermodynamics [7-8].

Why is the system behavior interesting?

Electroactive microorganisms represent a novel class of organisms whose external electron transfer properties have only been discovered in recent decades. These organisms are the basis of important technological systems such as Microbial Fuel Cells, Microbial electrosynthesis, biological sensors [2]. They are now recognized as being very important in natural systems as well, and electroactive microbes have been found in the deep sub-surface of Earth and the majority of marine settings (marine sediments, hydrothermal vents), where they are capable of accepting or donating electrons directly from or to mineral surfaces [1]. For this reason they may control the fate and transport of metals in natural systems and play an outsized role in global biogeochemical cycles (iron cycle, sulfur cycle, etc.). I also posit they are also ideal model organisms for some of the information thermodynamics concepts, particularly electroautotrophic bacteria that can uptake electrons directly from an electrode (cathode). This is because the thermodynamic driving force (electrode voltage) can be carefully controlled by the experimentalist and cellular heat dissipation could simultaneously be measured. There have been single-cell experiments with such bacteria, so such experimental platforms already exist. This might be a way to experimentally test ideas from the thermodynamics of information which relate to single cells.

2c. ***Dynamical properties***: What dynamical properties are you going to investigate?

The internal cellular state dynamics as a function of electron transport time series data. So the electron transfer channel will have a dynamic which then dictates the dynamic of the internal cellular state. Maybe voltage at the electron donor surface could be incorporated into the model, too.

2d. ***Intrinsic computation properties***: What information processing properties are you going to investigate?

I am interested in communication processes via electron conduction between microbes in the network. Quorum sensing is a microbial communication process based on chemical diffusion of “messenger molecules” that has been studied for decades [3]. It has been posited that electron transfer within microbial biofilms, essentially an electrically connected network of bacteria, may use electron transfer as a communication process as well [1, 3]. However there has been no substantiation of this hypothesis, and apart from the papers I cite here, no work has been done on this topic. Generally speaking I would like to see if epsilon machine reconstruction can help determine if an actual communication process is taking place via electron transfer between microbes, or if the electron transfer is simply an energetic driving force of metabolism. I would also like to recast these phenomena in the framework of stochastic sensors [7, 8], that is, have a method to determine the predictability of a voltage time series or current time series data, as experienced by a single bacteria attached to an external electron donor by a bacterial cable.

2e. ***Methods***: What methods will you use? Why are they appropriate?

To be honest, I am still working on this. It seems to me one would use epsilon machine reconstruction to determine the predictability of the electron channel/signal. I know there are thermodynamic relations (see Still et al., 2012 and Stopnitzky et al. 2019) between heat dissipation and predictability of an external stochastic signal. I need to do further reading/research to determine how I will connect this framework up with the bacterial model I am using.

2f. *Hypothesis: What is your current guess as to what you will find?

See introduction. I think there will be an energetic cost for significant unpredictability of the external electron donor/electron channel that would be detrimental to the bacteria. I can make hypotheses about the phenotypic response to this (down-regulation in genes which code for proteins capable of external electron transfer), but modeling this will be beyond the scope of this particular project given the amount of time I have. This will be done later, building upon the model I develop here.

2g. *Steps*: List the appropriate steps for your investigation; for example, read literature, write simulator, do mathematical analysis, estimate properties from simulation, write up report, and so on.

1. Read literature and better refine specific goals of the project, meet w/ Dr. Crutchfield and any students who are well suited to collaborate on the project. I need to quickly determine which specific tools (epsilon machine, mutual information, info-thermo relations) and equations are best suited to my project. Also need to define the scope so that my goal is reasonable for my time-budget.
2. Define the model and start to work on simulation code, de-bug code, run sanity checks on the code
3. Run simulations, start working on report
4. Complete report, determine next steps, think about how the model can be built upon or refined to either expand to entire biofilm simulations or how one would directly test my model experimentally w/ single cell experiment.

2h. *Time*: Estimate how long each step will take. Can you complete the project within one month?

1. 1 weeks
2. 1.5 week
3. 1 week
4. 0.5 week

It's going to be tight! Ultimately, the feasibility of completing my project within one month will hinge on choosing the appropriate scope. I will consult w/ Dr. Crutchfield about this to do something reasonable. I think if I successfully code up my simulator, can quantitatively characterize the "predictability" of the electron transport channel (i.e. bacterial cable) and simulate the intercellular state dynamics as I vary "predictability" of the channel, and lastly, make some predictions or commentary on the thermodynamic consequences for a single bacteria for increasing channel unpredictability, I will be more than happy. I may have to put aside the latter goal if I am pressed for time.

References:

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7. Still, S., Sivak, D. A., Bell, A. J., & Crooks, G. E. (2012). Thermodynamics of prediction. *Physical review letters*, *109*(12), 120604.

8. Stopnitzky, E., Still, S., Ouldridge, T. E., & Altenberg, L. (2019). Physical limitations of work extraction from temporal correlations. *Physical Review E*, *99*(4), 042115.