## Investigating Metabolic Phenomena Using Information Theory

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## 1 Updates

A key development that has come about because of this collaboration is the idea that information theory can be used to quantify the performance of a model. This is a result of treating a model as an entity that compresses the data that it describes. Models that better compress the data generated by a process are more useful for the purposes of optimization and control. From this, a framework for the analysis and selection of systems biological model has come about. Prior to this work, biological modelers have relied upon either qualitative arguments or error-based metrics to distinguish one model from another. The drawback of these approaches is that they are subjective or do not simultaneously gauge a model's fit and complexity. The framework that we have developed seeks to provide a novel, quantitative way to evaluate the performance of systems biological models. It not only measures each model's ability to fit the data but also each model's ability to provide succinct description of the data. Models with high degrees of complexity are penalized despite their accurate representations of the data.

This idea is useful for systems biological modelers who can employ a number of mathematical approximations to describe a single system. We have illustrated the power of this idea in a recently submitted journal publication detailed below and will be sharing it during a conference presentation this coming November at the Annual AIChE conference in a topical session related to biological modeling. If there is any funding left for the grant, it will be used for travel to this conference. The total expenses for travel should be in the range of  $\sim$ \$1,500.

## 2 Presentations

- DeVilbiss, Frank, Maxim Raginsky, and Doraiswami Ramkrishna. "An Information Theoretic Approach to the Model Selection Problem in Systems Biology." Paper #TBD, AIChE Annual Meeting, Salt Lake City, Utah, November 8-13, 2015.
- DeVilbiss, Frank, Mano R. Maurya, Shakti Gupta, Aravinda Mandli, Shankar Subramaniam and Doraiswami Ramkrishna. "Prediction of Gene Expression Using Goal-Directed Metabolic Models." Paper #TBD, AIChE Annual Meeting, Salt Lake City, Utah, November 8-13, 2015.

## 3 Publications

Acknowledged are both Prof. Raginsky and Pablo. The Center is also acknowledged.

• DeVilbiss, Frank, and Doraiswami Ramkrishna. "Addressing the Need for a Model Selection Framework in Systems Biology Using Information Theory." Proc. of the IEEE (submitted)