Computational Science via Machine Learning (aka *Reverse Engineering*)

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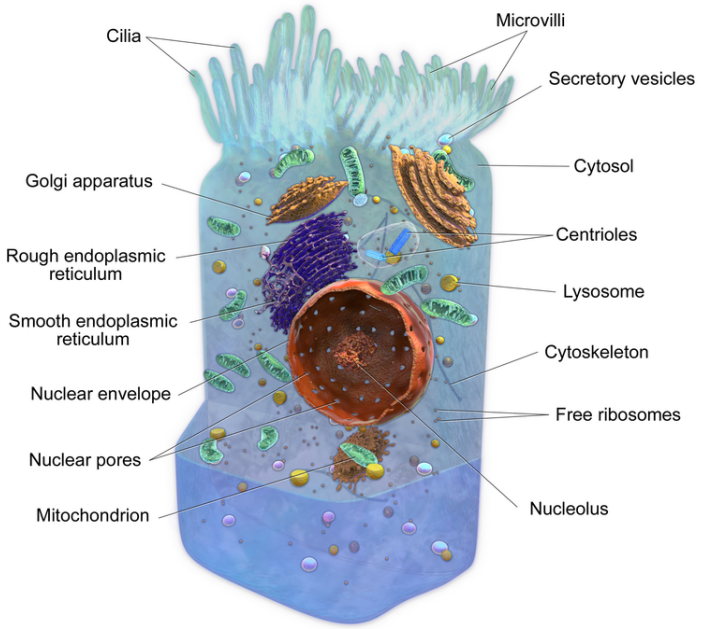
I have striven not to laugh at human actions, not to weep at them, nor to hate them, but to understand them.

Baruch Spinoza

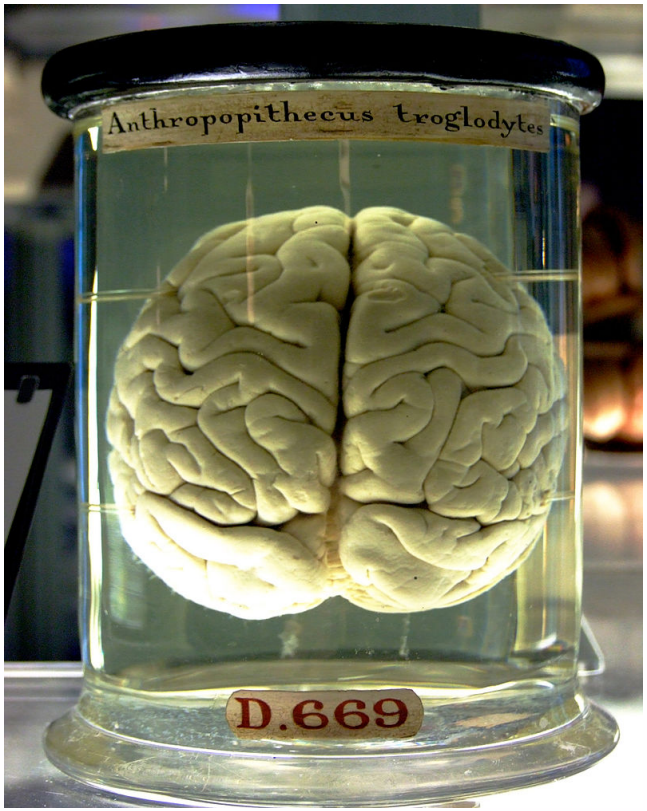
Terminology and Jargon

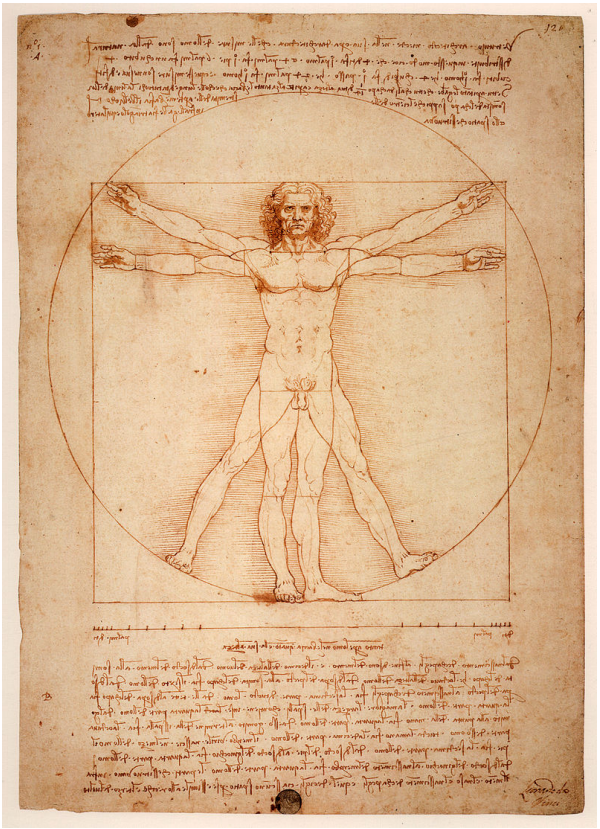
- Scientific computing / Computational science: Trying to understand natural systems (physical, chemical, biological, cognitive, social) by means of mathematical modelling and computational simulation
- Data science / Data mining: Algorithms and techniques for discovering patterns and relationships in data sets
- Machine Learning: Using such patterns/relationships to learn useful input-output mappings that can provide predictive models
- *Reverse Engineering:* In a way combines all of the above; using machine learning for data-driven model and parameter selection for scientific computing

Natural systems



Anatomy of a Cell



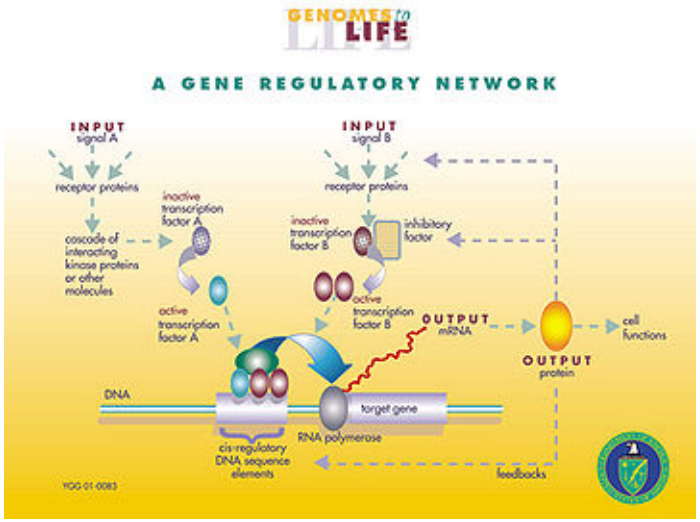


The scientific understanding of life and mind in terms of information, computation, and feedback control.

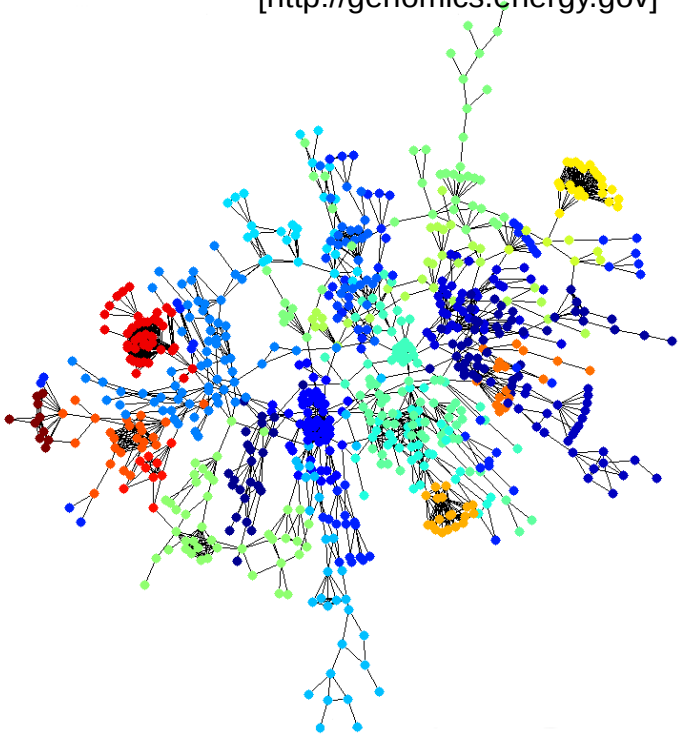
Steven Pinker

[Systems Biology, Cognitive Science]

Reverse engineering the circuitry of biology



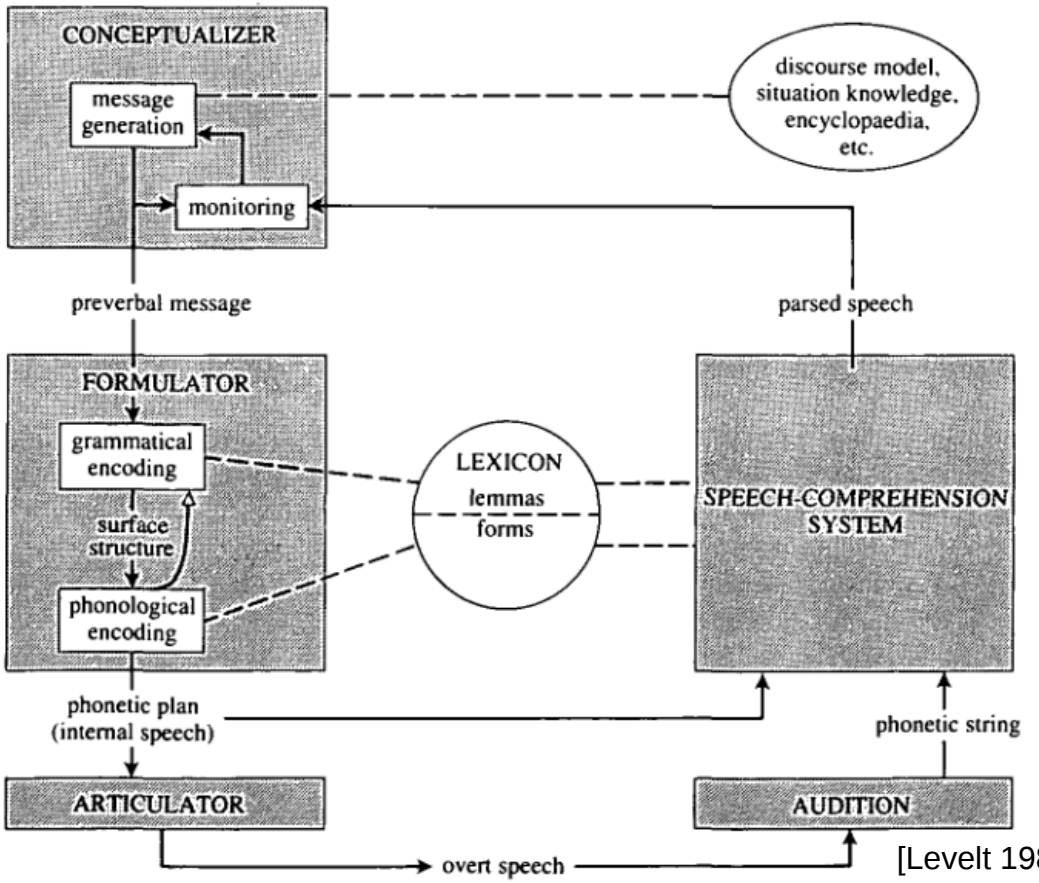
[http://genomics.energy.gov]



- Biological cells are essentially bags of interacting genes/proteins, which combine to carry out the various processes of life
- Given experimental data about how the concentration levels of proteins respond to various kinds of stimuli, can we try to recover the relationships of regulation and control between different genes/proteins?
- This can be thought of as learning the structure of a dynamical system, given some input/output characteristics
- We are looking at a range of approaches for mathematically modelling and learning these regulatory networks, such as Petri Nets, ODEs, and Markov Nets

How do we produce and comprehend language?

Sentence	Dependency Length
[उत्तर प्रदेश में] [गंगा और यमुना] [उफान पर] हैं ।	[10]
[उत्तर प्रदेश में] [उफान पर] [गंगा और यमुना] हैं ।	[11]
[गंगा और यमुना] [उत्तर प्रदेश में] [उफान पर] हैं ।	[10]
[गंगा और यमुना] [उफान पर] [उत्तर प्रदेश में] हैं ।	[11]
[उफान पर] [उत्तर प्रदेश में] [गंगा और यमुना] हैं ।	[12]
[उफान पर] [गंगा और यमुना] [उत्तर प्रदेश में] हैं ।	[12]



[Levelt 1989]

- What factors drive production choice amongst competing variants?
- How does this vary across languages? (Currently looking at Hindi-Urdu and English)
- Can we model the integration of different factors, like dependency and expectation effects, in a cognitively motivated model?
- Can machine learning be useful in determining such a model, and can it also tell us about human language learning?
- How does production relate to comprehension?
- Do we produce sentences that are more easily comprehended? Can reading time and eye-tracking data tell us about production as well?

Connections, Applications

- Biological systems (gene/protein networks) are essentially being modelled in terms of information flows and processing; machine learning being used to help uncover underlying structure – may be relevant to a variety of systems involving either physical or informational flows
- On the systems biology side: Modelling and engineering synthetic fuel-producing microorganisms
- On the cognitive science side: Modelling and influencing human energy usage decisions
- Common challenges: How do we combine domain knowledge and expertise with data-driven modelling? How do we deal with noise and uncertainty? Can we do *domain-aware* machine learning, rather than just domain-general?

Scientists create renewable fossil fuel alternative using bacteria

by Gail Wilson
02 September 2014

Researchers have engineered the harmless gut bacteria E.coli to generate renewable propane.

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Household energy use: Applying behavioural economics to understand consumer decision-making and behaviour

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ABSTRACT

Household energy conservation has emerged as a major challenge and opportunity for researchers, practitioners and policymakers. Consumers also seem to be gaining greater awareness of the value and need for sustainable energy practices, particularly amid growing public concerns over greenhouse gas emissions and climate change. Yet even with adequate knowledge of how to save energy and a professed desire to do so, many consumers still fail to take noticeable steps towards energy efficiency and conservation. There is often a sizeable discrepancy between peoples' self-reported knowledge, values, attitudes and intentions, and their observable behaviour—examples include the well-known 'knowledge-action gap' and 'value-action gap'. But neither is household energy consumption driven primarily by financial incentives and the rational pursuit of material interests. In fact, people sometimes respond in unexpected and undesirable ways to rewards and sanctions intended to shift consumers' cost–benefit

The same stream of life that runs through my veins night and day runs through the world and dances in rhythmic measures. It is the same life that shoots in joy through the dust of the earth in numberless blades of grass and breaks into tumultuous waves of leaves and flowers.

Rabindranath Tagore