Unlocking Growth Potential at the Intersection of AI, Robotics, and Synthetic Biology

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ABSTRACT

Growth Potential at the Crossroads of Artificial Intelligence, Robotics, and Synthetic Biology. Biomedical and bioengineering advancements are impeded by our incapacity to foretell how biological systems will act. We are unable to extrapolate behaviour on a large scale from studies conducted on a small scale, nor can we foretell how changes to genotype will impact phenotype. Recent advances in machine learning have made it possible to get the necessary predictive power without a deep mechanical knowledge. Having said that, training them requires massive amounts of data. In order to create a wide variety of biological systems with good reproducibility, the quantity and quality of data needed can only be met by combining synthetic biology with automation. Advancements in predictive biology and better machine learning algorithms can be achieved through consistent funding of research into the areas of synthetic biology, machine learning, and automation.

Keywords: Machine Learning; Automation; Synthetic Biology

Introduction

A shift from a descriptive to a design science has occurred within biology during the last 20 years, leading to significant changes in the field. Synthetic biology and genetic engineering were both initiated by the revelation of DNA as a storehouse of genetic information and recombinant DNA as a powerful tool for editing it. Beyond the traditional focus on description and cataloguing in biology (e.g., Linnaean taxonomic classification or phylogenetic tree development), synthetic biologists now seek to engineer biological systems to meet specific requirements (e.g., producing a specific quantity of a medicinal drug or specifically invading a particular type of cancer cell) [1–5].

From creating renewable biofuels to fight climate change to enhancing human health, this shift towards industrialised synthetic biology is anticipated to impact the vast majority of human endeavours. Synthetic spider silk and leather, vegan burgers that taste like meat, sustainable skin-rejuvenating cosmetics, renewable biodiesel that powers Rio de Janeiro's public bus system, and many more examples are currently available for purchase.

In this effort, new tools enable us to bioengineer cells faster than ever: CRISPR-enabled genetic editing has revolutionized our ability to edit DNA in vivo, DNA synthesis productivity improves as fast as Moore’s law, transcriptomics data volume has a doubling rate of 7 months, and high-throughput workflows for proteomics and metabolomics are emerging. Furthermore, the miniaturization and automation of these techniques through microfluidic chips promise a future where data analysis rather than data production will be the bottleneck in biological research.

Obstacles to an Exponential Increase in Synthetic Biology Productivity

However, despite new tools and exponentially increasing data volumes, synthetic biology cannot yet fulfill its true potential due to our inability to predict the behavior of biological systems. Arguably, the most pressing problems are our inability to predict the phenotype of biological systems when their DNA is altered, and the difficulty of using small scale experiments to predict the behavior at large scales [6-18]. In general, while we can make the DNA changes we intend on target cells, the end result on their behavior is usually unpredictable.4 This limitation has led to a traditional bioengineering approach that involves randomizing exper- imental efforts hoping for an improved result, or using arduously gathered biological intuition. This approach is hardly scalable, and has resulted in long development times: for example, it took 150 person-years of effort for heterologous expression of the 16-enzyme artemisinin pathway, and 575 person-years of effort for DuPont's 1,3-propanediol. Furthermore, we lack the ability to extrapolate large-scale behavior from small-scale experiments. In bioengineering, a key bottleneck is designing fermentation systems that reliably scale up lab results (1−100 mL) to commercial volumes (100−106 L). Failure to do so and meet production timelines resulted in the past in the inability to address high-volume production, economic losses, and significantly decreased investment in the field. Amyris, for example, had to announce major changes to its financing, strategy, and production targets after falling significantly short of their target of producing nine million liters of farnesene. In biomedical applications, we cannot use information on cell culture experiments to reliably extrapolate the implications on human health. This short-coming forces researchers to rely on proxy systems (animal models) such as mice, rats, pigs, monkeys, or rabbits. These animal models imperfectly represent human biology in biomedicine: the average rate of successful translation from animal models to clinical cancer trials is less than 8%. These failures significantly contribute to the billion dollar figures routinely cited for new drug development. While these two problems (predicting phenotype from DNA and scaled behavior) are perhaps more evident in the field of synthetic biology, they are shared with (and inherited from) the rest of biology. For example, it would be transformative to predict (1) plant phenotype from its genome, (2) soil microbial community impact on its environment and globally on Earth's climate from the study of pure cultures, or (3) mammalian metabolism from single cell studies. Any advance in these two problems will positively impact other subfields of biology. Further hurdles facing synthetic biology (e.g., product extraction and downstream purification, supplement precursor cost, toxicity, long-term stability, reproducibility, cross-talk) are important, but less generally impactful if solved [19-39].

Machine Learning's Predictive Capabilities

Machine learning can provide predictive power without the need for detailed mechanistic understanding, by learning the underlying regularities in experimental data. Training data is used to statistically link a set of inputs to a set of outputs through models that are expressive enough to represent almost any relationship, without being encumbered by biased assumptions. In this vein, machine learning has been used to predict pathway dynamics, optimize pathways through trans- lational control, diagnose skin cancer, detect tumors in breast tissues, and predict DNA and RNA protein-binding sequences.8−10 Furthermore, machine learning can be used to design synthetic biology systems: it can be used to learn the relationship between phenotype and the genetic parts used in genetic circuits, thus allowing more stable circuits. But machine learning algorithms are data-hungry: they require abundant data to be trained and be effective. The current revolution in machine learning was enabled not by new techniques, but rather by (1) rising processing power and (2) the availability of massive training libraries. Image identification in the field of artificial vision would have most likely not attained superhuman performance if it had to be trained on photographs recorded on photographic film and physically shipped from photographers to artificial intelligence researchers. The availability of large image libraries enabled by automated digital image acquisition through charge-coupled device (CCD) cameras, and its dispersal through the Internet, have been key to its development [40-65].

Machine Learning Needs Automation to be Truly Effective

We cannot produce the quantity and quality of data needed for effective machine learning without using automation. The situation we face in biology is akin to using mailed paper pictures: most assays are low-throughput and manual, and most phenotypic data is produced and analyzed within the same lab. Although this is beginning to change, the rate is not fast enough to support machine learning approaches (except for the field of genomics). To make matters worse, historical data not always meet the requirements for machine learning to be effective (e.g., lack of standardized data collection), so it is important that new data are collected with these needs in mind. Competitions such as the Critical Assessment of methods of protein Structure Prediction (CASP) provide a good example of how to promote community effort for this purpose.

Large-scale high-quality data is necessary but not sufficient: proper experimental design is fundamental to leverage machine learning. Opportunities in this area run in both directions: high-quality data generation for training machine learning algorithms necessitates experimental designs that carefully consider the different effects influencing the response; and machine learning can be used to choose the next set of experiments in order to improve experimental data quality and reduce the estimation errors. In this area, “robot scientists” (chemical experiment planners) have proven successful in synthetic chemistry, and are expected to play an important role in synthetic biology [66-89].

Hence, we need to invest in capabilities that couple machine learning algorithms with high-throughput, fast-turnaround, automated phenotyping approaches, to solve biological problems whose solution is of wide applicability, Possible approaches involve robotic liquid handler platforms, microfluidics, or cloud laboratories. Future challenges include acquiring data in real time, developing comprehensive noninvasive assays, taking the human out of the loop, and developing workflows and data standards that ensure reproducibility.

Academic research would greatly benefit from this approach, which is already being used in industry. The availability of large amounts of high-quality data would enable computational biologists to produce robust theories without the need of running their own experimental facilities, and the theory produced by these data sets would allow experimentalists to better design experiments and tackle questions of general relevance. Furthermore, this division of labor would enable higher productivity and allow for addressing more ambitious biological questions. Indeed several academic biofoundries have recently appeared, which can provide the ideal environment for the integration of synthetic biology, machine learning, and automation, if properly directed and resourced.

Conclusion

A significant opportunity lies in the integration of synthetic biology, machine learning, and automation, enabling disruptive changes in both biology and computer science. This integration can not only produce transformational synthetic biology applications for the production of biomaterials, biofuels and biomedical applications, but also enable a better mechanistic understanding. Unlike for other domains where machine learning is leveraged productively , for many of the current synthetic biology applications we have a significant (but not complete) knowledge of the underlying processes. Coupling the predictive ability of machine learning models with the possibilities afforded by new synthetic biology tools to easily modify the system components will allow us to probe and expand our mechanistic understanding. We expect this improved understanding to help us generate new types of machine learning algorithms: after all, machine learning staples such as genetic algorithms and artificial neural networks were inspired by biological analogies. This integration will require a tight multidisciplinary collaboration among biologists, mathe- maticians, engineers, chemists, physicists, and computer scientists in order to be successful.

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