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Plant Breeding Biomolecular Classification in Quantum Bayesianism (QBism) Physics-Informed Neural Network Architecture

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Brief Communication

Plant Breeding Biomolecular Classification in Quantum Bayesianism (QBism) Physics-Informed Neural Network Architecture

Barbara S. Keary, Karriem A.J. Perry

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Plant science, in particular plant breeding, with its emphasis on gene manipulation and therefore large data sets, can benefit from greater penetration of ML and DL tools for solutions to problems from Multi-classification (*M*-class) and optimization to anomaly detection to time-series analysis and forecasting (Sammut, 2017; Yoosefzadeh-Najafabadi, 2021). Machine Learning (ML) is a primary component of Artificial Intelligence (AI) (Sammut, 2017) and it contributes to plant science using specifically designed Artificial Neural Networks (ANN) to inference biomolecular classification. Deep learning (DL) contributes to plant science by simulating biochemical behaviors and assisting with the spatial analysis of plant evolution. A majority of the improvements made in machine learning (ML) and deep learning (DL) are not fully explored by disciplines outside of computer science, the physical sciences, engineering, and mathematics (Davies et al., 2021). Plant science will advance more rapidly if it makes better use of related advances in the partner sciences of ML and DL to solve the growing complexity of challenges in food security.

Classical DL, defined as inference calculated on a classical information system, has positively affected biotechnological processes in a variety of plant species (Yoosefzadeh-Najafabadi et al. 2021). However, Qbism, defined as quantum Bayesianism, has not been fully exploited by simulations for the plant sciences (Bharadwaj, 2018; Rovelli, 2022). Moreover, the rapid pace at which computational advances evolve is a product of the ML model's loss function, for example the unformed loss function of Sum of Squared Errors (SSE) resulting in computation and environmental energy waste and algorithm non-convergence (Berrar, 2018). Notwithstanding, the technology associated with physico-biological/chemical technologies has progressed concurrently with classical ML evolutions. (Sajjan et al., 2021).

Leveraging the full capacity of AI techniques and connecting somewhat disparate forms of mathematics to accelerate scientific discovery in discipline-dependent domains requires a comprehensive and incisive understanding of AI constraints and capabilities as derived from problem statements and hypotheses development, through to model selection and tuning--much like the effectiveness robotics researchers experience when using Physical Artificial Intelligence (PAI); (Davies et al., 2021). No two ML models behave the same and this exclusivity is amplified when considering the application of Relational Quantum Machine Learning (RQML) methods, a derivation of Scientific ML alternatively (SciML), directed at biomolecular processes (Rovelli, 2022; Yoosefzadeh-Najafabadi et al. 2021). More specifically, our research will evolve

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into a derivation of a physics-informed Multiclassification (M -class) intelligent agent designated as *Relational Quantum-Informed Neural Network* or RQINN (Rovelli, 2022).

Classical neural networks may encounter datatypes causing computational intractability or conditions comparable to those seen in $\#NP$ -type problems from relatively common anomalies as noisy, time series, streaming datasets and predictions of biomolecular processes containing robust molecules composed of (> 15) non-hydrogen atoms (Berrar, 2018; Yoosefzadeh-Najafabadi et al. 2021). Considering plant breeding as the end-goal, the initial challenge may include deciding the most utilitarian physical approach to employ, for instance chemical versus biological and establishing the applicable partial differential equation (PDE); (Berrar, 2018; Yoosefzadeh-Najafabadi et al. 2021).

The trajectory taken for this research communication describes predictive analysis for a given biological process in advanced molecular plant breeding commonly referred to as gene editing have yet to begin exploration into scientific machine learning, the benefits of which are in initial stages for physics-informed and plant science (Yoosefzadeh-Najafabadi et al. 2021). These potential RQINN exploits will positively impact the trajectory of a number of crucial areas in molecular plant science; as described by Bharadwaj (2018); these areas include, but are not limited to, genome editing in plant breeding; plant-based edible vaccines, RNA Interference (RNAi) biotechnology, sustainable agriculture supporting food security, and many other areas. These advances provide enhanced granularity by describing some of the emerging technologies, or new plant breeding technology, associated with the plant sciences (Berrar, 2018; Bharadwaj, 2018).

A vital method in evaluating and understanding physical traits associated with a given species is the use of the *breeder's equation* (Kelly, 2011). As with a majority of PDEs, solving for an unknown function, for instance f in $f(x)$, is dependent on myriad factors not initially identifiable (Farlow 2012). Therein lies the importance in knowledge of the structure of those data and how relations among metadata, example include nodes and the composition of entities, objects, elements (Koller, 2007). Moreover, due to the complexity of biological systems, these domains often provide favorable test-beds for often intractable M -class from a classical optic (Sammur et al., 2017). Considering the QBism perspective, we are allowed to update our understanding of the breeder's equation as more data are made available (Rovelli, 2022). This update of data does not interfere with the initial data quality and potentially enhances the classifier at convergence or the understanding of the observer (Koller, 2007).

It is questionable that conducting biological computation is obstinate to the point of rendering the operation inconsequential (Berrar, 2018). This postulation is non-linear and should be considered subjective without the presence of a comprehensive problem statement and successive hypotheses development, a necessary exercise in preparation for discretization of experimental data (Farlow, 2012). Moreover, this inherent complexity accompanying biological data effects both binary and M -class problems (Sammur et al., 2017). Finally, let us briefly consider a utilitarian aspect of the breeder's equation, where Z represents the central limit of an unidentified trait of a species population. From a PDE point of observation, this is equivalent to some unknown function $f(x)$; (Farlow 2012). Moreover, $\Delta Z = h^2 S$ denotes the breeder's equation *rate of change* over time and should indicate to plant scientists or ML engineers that time series analysis and forecasting may produce a useful modeling alternative or exists as an

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independent model (Kelly, 2011). Consider that S signifies a *selection differential* and if this numeric value is a non-negative integer, then the equations indicate preference toward higher generation species trait values (Kelly, 2011). The significance of h^2 is the inference is not beholden to the knowledge of gene-specific effects on off-spring trait heritability (Kelly, 2011).

The intent of this short communication is to promote further interests in the utility ML modelling can offer to plant sciences. As ML modelling performance improves and other aspects of computation are available, for example *quantum vs. classical* computing, the probability of computational intractability will decrease as will the likelihood of adverse computational environmental effects. If these factors reach equilibrium the potential for more effective plant breeding experiments using ML modelling will significantly benefit both fields of research.

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