

Bridging Biology and Artificial Intelligence: Opportunities, Tools, Challenges, and Ethical Considerations

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Artificial intelligence (AI) is now widely used in biological research. It helps researchers analyse large datasets, identify patterns, and make predictions that are difficult to obtain by manual analysis alone. In genomics, AI can relate DNA sequence to gene regulation and variant effects. In structural biology, deep-learning systems such as AlphaFold have greatly improved protein-structure prediction. AI is also being used in drug discovery, medical data analysis, ecology, and biodiversity monitoring. These advances are important, but they do not remove the need for biological reasoning or experimental validation. Model performance depends strongly on the quality and diversity of training data, while many high-performing models remain difficult to interpret. The use of genomic and clinical data also raises concerns about privacy, fairness, accountability, and unequal access to computational resources. This review examines major applications of AI in biology, summarizes the main computational approaches, and compares their strengths and limitations. It also considers ethical issues and identifies areas where human judgement remains essential. AI is most useful when it supports, rather than replaces, biological expertise, careful experimental design, and transparent scientific decision-making.

Keywords: artificial intelligence, machine learning, deep learning, genomics, protein structure, drug discovery, ecology, bioethics

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1. Introduction

Biology has become a data-intensive science. High-throughput sequencing, cryo-electron microscopy, single-cell profiling, imaging, and remote sensing can generate more information than traditional manual approaches can efficiently process. Machine learning has therefore become increasingly useful because it can detect complex patterns in large and high-dimensional datasets (Ching et al., 2018).

The rapid growth of AI in biology is not simply a change in computing power. It is also changing the way biological questions are framed. Earlier computational approaches often depended on features selected in advance by researchers. Modern deep-learning models can learn useful representations directly from raw sequence, image, or molecular data. This has created new opportunities, but it has also made model behaviour harder to interpret in biological terms.

Enthusiasm about AI should therefore be balanced with caution. A highly accurate prediction is not automatically a biological explanation. Models can also fail when they are applied to populations, species, laboratories, or environmental conditions that differ from the data used for training. In biomedical settings, such errors can have direct consequences for patients and clinical decisions.

This review has three aims. First, it examines major applications of AI in genomics, protein science, drug discovery, biomedicine, and ecology. Second, it describes the main computational approaches used in these fields. Third, it considers the limitations and ethical questions that become important when AI systems influence research, health care, conservation, or other biological decisions. The review focuses on a central question: where does AI genuinely extend biological research, and where is human interpretation still indispensable?

2. Opportunities: AI Applications Across Biology

2.1 Genomics and Gene Regulation

Genomics was one of the earliest areas of biology to benefit from deep learning. Convolutional and recurrent neural networks have been used to learn sequence patterns associated with chromatin accessibility, transcription-factor binding, splicing, and genetic variation (Eraslan et al., 2019).

These models are useful because they can analyse sequence directly rather than depending entirely on manually selected features.

The main advantage is scale. A model can screen very large numbers of variants or sequence regions and identify candidates for further study. This is especially valuable in non-coding regions, where experimental annotation is incomplete. However, prediction alone does not establish biological function. A model may identify a sequence pattern that is statistically informative without revealing the molecular mechanism that makes the pattern important. Experimental validation therefore remains essential, particularly when predictions are used to infer causality.

2.2 Protein Structure and Function

Protein-structure prediction is one of the clearest examples of the impact of AI on biology. AlphaFold achieved very high accuracy in CASP14 and showed that deep learning could predict the three-dimensional structure of many proteins with a level of accuracy that had previously been difficult to reach computationally (Jumper et al., 2021). This has made structural information available for many proteins that lack experimentally determined structures.

The benefit is immediate for hypothesis generation. Predicted structures can guide mutagenesis, domain analysis, docking, and the interpretation of disease-associated variants. They can also help researchers decide which proteins or regions deserve detailed experimental study. Yet predicted structure should not be treated as a complete description of protein function. Proteins are dynamic, may adopt several conformations, and often depend on ligands, membranes, post-translational modifications, or interaction partners. AI-based structural prediction therefore complements structural experiments; it does not make them unnecessary.

2.3 Drug Discovery and Development

Drug discovery involves repeated decisions about targets, candidate molecules, toxicity, pharmacological properties, and clinical response. Machine-learning approaches are now used at many of these stages, including target prioritization, virtual screening, molecular-property prediction, biomarker discovery, and analysis of pathology images (Vamathevan et al., 2019).

AI is particularly useful for reducing a very large search space. It can rank compounds or experiments so that laboratory resources are directed toward more promising candidates. This can improve efficiency, but it does not eliminate the biological causes of drug failure. A model trained on incomplete chemical or biological data may perform well on a benchmark and still fail on novel compounds or patient populations. For this reason, the value of AI in drug discovery depends on prospective testing, careful validation, and integration with experimental pharmacology.

2.4 Ecology and Environmental Biology

AI has also expanded the scale of ecological monitoring. Deep-learning methods can classify camera-trap images, identify organisms from sound recordings, analyse satellite or drone imagery, and estimate species distributions from large observational datasets (Christin et al., 2019). These tasks are important because ecological datasets often contain thousands or millions of observations that cannot be reviewed manually within a useful time frame.

Automated classification can support faster biodiversity assessment and conservation planning. At the same time, ecological data have their own sources of bias. Sampling is often uneven across regions, seasons, habitats, and species. Rare species may be poorly represented in training data, while common species may dominate model performance. The ecological meaning of a prediction must therefore be considered together with sampling design and field knowledge.

2.5 Broader Biomedical Applications

In biomedicine, AI is being studied for patient classification, disease subtyping, prognosis, image interpretation, and treatment prediction. Deep learning has shown promise in many of these areas, but the size of reported improvements varies substantially across studies and applications (Ching et al., 2018).

This variation is important. Biomedical models are often evaluated on retrospective datasets collected under particular clinical conditions. Performance may decline when the same model is used in a different hospital, population, or workflow. The clinically relevant question is therefore not only whether a model is accurate, but whether it remains reliable when used outside the environment in which it was developed.

Table 1: Comparative view of major AI applications in biology

Area	Main contribution of AI	Major strength	Important limitation
Genomics	Sequence-to-function prediction and variant prioritization	Handles very large sequence datasets	Prediction may not reveal causal mechanism
Protein science	Structure prediction and functional hypothesis generation	Rapid access to structural hypotheses	Dynamics and biological context may be missing
Drug discovery	Compound ranking, property prediction, biomarker analysis	Reduces experimental search space	Performance depends on chemical and biological coverage of training data
Biomedicine	Classification, prognosis, imaging and treatment prediction	Can integrate complex clinical and molecular data	External validation and fairness remain major concerns
Ecology	Species identification, remote sensing and distribution modelling	Allows analysis at large spatial and temporal scales	Sampling bias and rare-species underrepresentation can distort results

3. Tools and Methods

The AI toolkit used in biology includes both classical machine-learning methods and deep-learning architectures. Random forests, support vector machines, and gradient-boosted trees remain useful when datasets are structured, moderate in size, or when some degree of interpretability is important. Deep learning is more commonly used for raw, high-dimensional data such as sequences, images, and complex signals (Eraslan et al., 2019).

Convolutional neural networks are effective for image-like patterns and have also been adapted to biological sequences. Recurrent networks were designed for sequential data, although transformer-based models are now widely used when long-range relationships in sequences are important. Graph neural networks are well suited to molecules and interaction networks because atoms, residues, proteins, or other entities can be represented as nodes connected by edges. Generative models can create new molecular or sequence candidates and are therefore being explored in drug discovery and synthetic biology.

The choice of algorithm should follow the biological question rather than current popularity. A complex model is not automatically better. Smaller and more interpretable models may be preferable when the dataset is limited or when the research objective is to understand which variables are driving a prediction. Conversely, deep models may be appropriate when the available data are large enough and the predictive task involves highly complex patterns.

Data infrastructure is as important as model architecture. Public genomic, structural, chemical, imaging, and ecological repositories have made many AI applications possible. However, the usefulness of these resources depends on accurate annotation, consistent metadata, suitable benchmarks, and access to sufficient computing infrastructure (Ching et al., 2018). Poorly curated data can produce sophisticated models with unreliable biological conclusions.

4. Challenges and Limitations

Several limitations occur across almost every biological application of AI. The first is data quality. Biological datasets are often smaller, noisier, more heterogeneous, and more context-dependent than datasets used in some other areas of AI (Ching et al., 2018). Differences in laboratory protocols, instruments, populations, species, or sampling conditions can create patterns that a model learns even when those patterns are not biologically meaningful.

A second limitation is generalizability. Strong performance on an internal test set does not guarantee reliable performance in another laboratory, hospital, ecosystem, or population. External validation is therefore necessary when the intended use extends beyond the original dataset.

A third problem is interpretability. Some deep-learning systems can make accurate predictions without providing a clear explanation that maps onto known biological mechanisms. This becomes especially important when a prediction is used to guide an experiment, assign clinical risk, or support a policy decision. In such settings, researchers need to distinguish between a model that is useful for prediction and a model that improves scientific understanding.

Finally, AI can create a false sense of certainty. A numerical probability or confidence score may appear precise even when the underlying data are incomplete. Biological uncertainty should therefore be reported explicitly, and model outputs should be interpreted alongside experimental evidence and domain expertise.

5. Ethical Considerations

As AI moves from exploratory research into clinical and applied decision-making, ethical questions become more important. Four issues are especially relevant: bias and fairness, privacy and data governance, transparency and accountability, and the broader social and dual-use implications of biological AI.

5.1 Bias and Fairness

Algorithmic bias can arise when training data do not represent the population in which a model is used. It can also arise from the choice of labels or proxy variables. Obermeyer et al. (2019) showed this clearly in a health-care algorithm that used previous health-care spending as a proxy for health need. Because spending reflected unequal access to care, the system underestimated the needs of Black patients compared with White patients who were similarly ill.

The lesson is broader than a single algorithm. A dataset can appear large and still be systematically unrepresentative. Fairness therefore requires examination of who is included in the training data, which variables are used as proxies, and whether errors are distributed equally across relevant groups.

5.2 Privacy and Data Governance

Genomic and health data require particular care because they can reveal sensitive information about individuals and, in some cases, their biological relatives. Responsible use of such data requires informed consent, secure stewardship, and clear rules about who may use the data and for what purpose (Char et al., 2018).

These questions become harder when datasets are shared across institutions or used to train commercial models. Data can move farther than the original participant expected, while responsibility for later uses may become unclear. Governance therefore needs to address the full life cycle of data, not only the point at which it is first collected.

5.3 Transparency and Accountability

When an AI model influences a biological or clinical decision, responsibility cannot be assigned to the model itself. Researchers, software developers, institutions, and professionals who act on model outputs all have roles in validation and oversight. Char et al. (2018) emphasize the need for clear frameworks that define these responsibilities in health care.

Transparency is also necessary for scientific reproducibility. Researchers should report the source of training data, important preprocessing steps, validation strategy, performance limits, and known sources of bias. Without this information, an apparently strong result may be difficult to reproduce or evaluate independently.

5.4 Dual-Use and Broader Societal Impact

Generative biological models can support legitimate work in molecule design and protein engineering, but some of the same capabilities could be misused. This creates a dual-use problem in which open scientific progress must be balanced against reasonable safeguards. The appropriate response is not to treat all biological AI as dangerous, but to evaluate risk according to capability, access, and intended use.

Equity is another concern. Training large models can require expensive computing systems, proprietary datasets, and specialized expertise. If these resources remain concentrated in a small number of institutions or companies, the scientific benefits of AI may also become concentrated. Wider access to well-curated public data, transparent tools, and shared computational infrastructure can help reduce this imbalance.

6. Critical Synthesis: What AI Adds and What It Does Not Replace

The studies considered in this review point to a consistent pattern. AI is strongest when the main problem is scale, ranking, classification, or detection of complex statistical patterns. It can examine more sequences, images, molecules, or ecological observations than a researcher could inspect manually. It can also identify candidates that deserve experimental attention.

Its weakness appears when prediction is confused with explanation. In genomics, a sequence feature predicted to be regulatory still needs biological validation. In structural biology, a predicted fold does not fully describe protein dynamics or cellular context. In drug discovery, a promising computational score does not establish efficacy or safety. In ecology, automated species recognition does not correct for poor sampling design. Across these fields, AI changes where researchers begin an investigation, but it does not remove the need for experiments, field observations, and mechanistic reasoning.

This distinction is important for evaluating future claims. The most convincing biological AI studies are likely to be those in which computational predictions and experimental evidence strengthen each other. AI should therefore be judged not only by benchmark accuracy, but also by whether it produces reproducible, biologically meaningful, and testable knowledge.

7. Future Directions

Future progress will depend on both technical improvement and better scientific practice. More interpretable models may help researchers connect predictions with biological mechanisms. Biologically informed architectures may also reduce the tendency of models to learn irrelevant correlations when useful prior knowledge is available.

More diverse and representative datasets are needed, especially in biomedical research. Multimodal models that combine sequence, structure, imaging, and clinical information may provide a more complete view of biological systems, but they will also require careful validation because errors from several data sources can be combined in the same model.

Another priority is reproducibility. Shared benchmarks, transparent reporting, open evaluation datasets, and independent validation can make it easier to distinguish genuine progress from performance that depends on a particular dataset. Ethical and regulatory frameworks will also need to develop alongside technical capabilities, especially where privacy, clinical responsibility, or dual-use concerns are involved.

For biologists, an equally important future direction is training. Researchers do not all need to become AI specialists, but they should understand enough about model development, validation, bias, and uncertainty to evaluate AI-based claims critically. Productive collaboration between biologists and computational scientists will depend on this shared scientific language.

8. Conclusion

Artificial intelligence has expanded what can be analysed in modern biology. It can help interpret genomes, predict protein structures, prioritize drug candidates, classify biomedical data, and process ecological observations at unprecedented scale. These are substantial gains, but they should not be described as a replacement for biological expertise.

The central challenge is to connect prediction with understanding. Reliable biological AI requires high-quality data, appropriate validation, transparent reporting, and careful attention to bias, privacy, and accountability. The strongest research will combine computational power with experimental evidence and domain knowledge. Used in this way, AI can become a valuable partner in biological discovery while remaining subject to the same standards of reproducibility, critical evaluation, and ethical responsibility that apply to other scientific methods.

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