

Artificial Intelligence in Bioinformatics

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Content

Introduction

Vaccine Development

Gene Editing

Protein Folding

Presentations are communication tools that can be used as

Conclusion

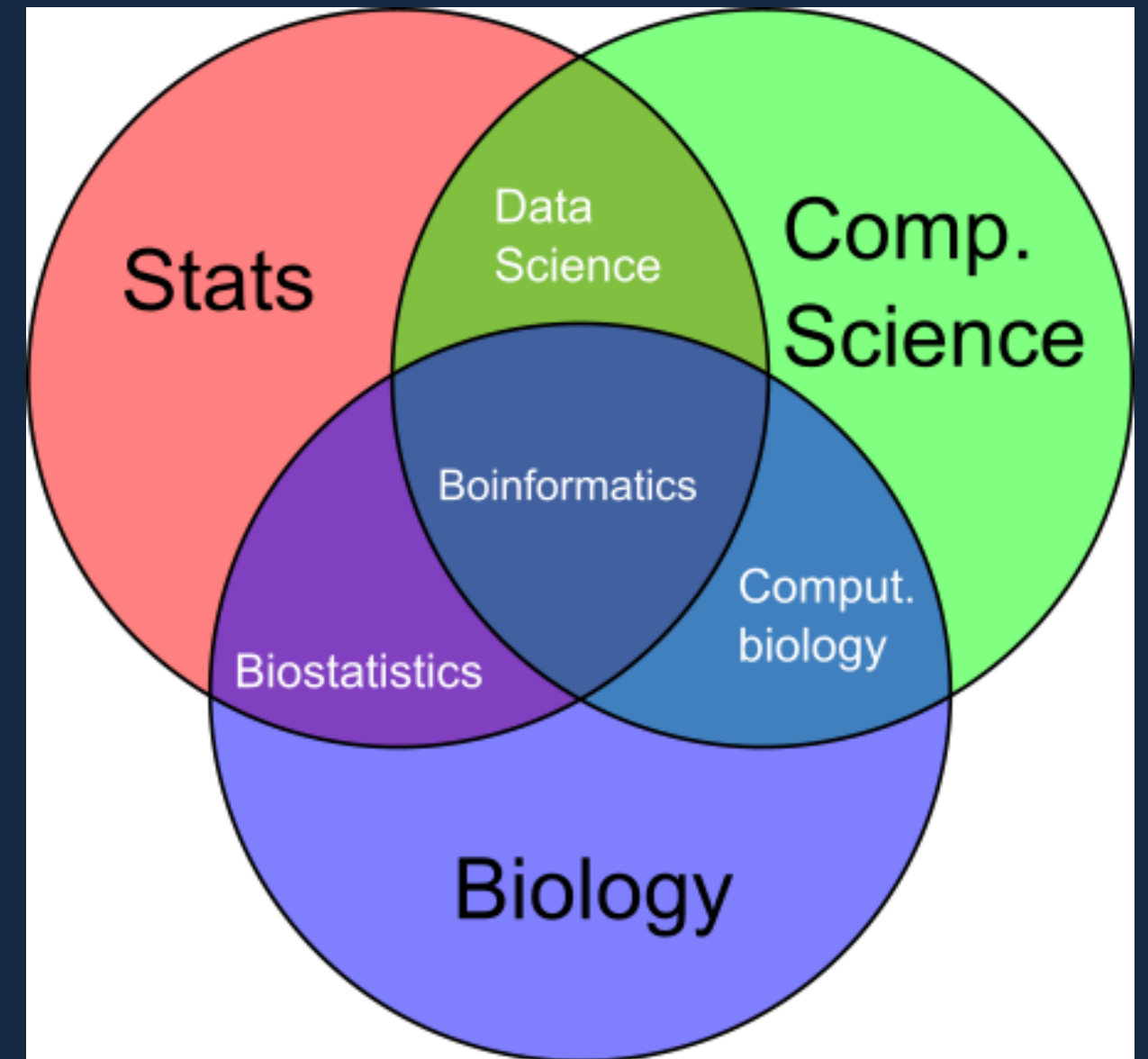
Introduction

What is Bioinformatics?

- Acquisition, Storage and Analysis of biological data using computer science and statistics

Why is it important/Uses?

- Vaccine development
- Gene analysis and editing
- Protein structure analysis and prediction



Vaccine Development

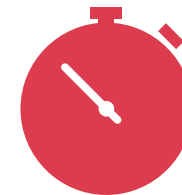
Role of AI in Vaccine Development



Challenges



Solution



Application



Impact

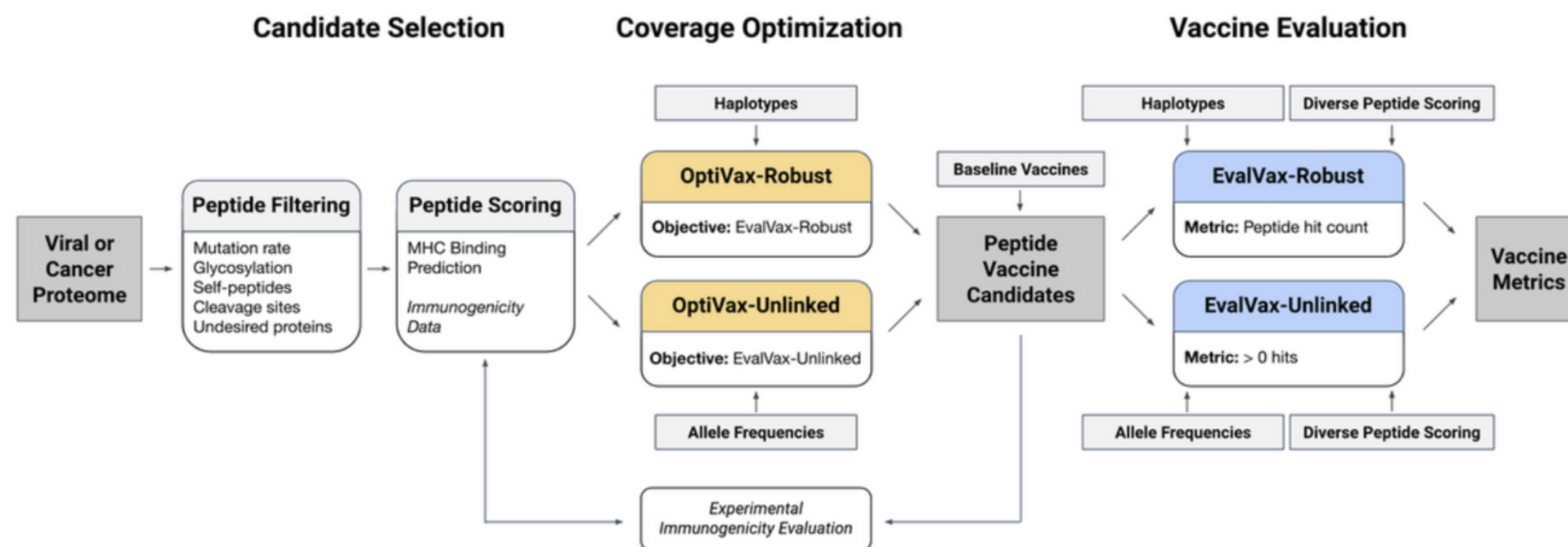
The background of the slide features a stylized illustration of a person with brown hair, wearing a white lab coat, looking at a laptop. The laptop screen displays several data visualizations, including a donut chart, a bar chart with an upward-pointing arrow, and another bar chart. The overall color palette is light blue and white, with some brown and dark blue accents. The title is presented in a dark blue rounded rectangle on the left side of the slide.

Challenges of Vaccine Development

- Data sets are often so messy and challenging that scientists historically haven't even attempted these sorts of analyses.
- AI cannot replace or speed up the most crucial, time-consuming aspect of vaccine development – human and animal trials.

Solution to challenges of Vaccine Development

MIT has developed an OptiVAX algorithm which searches for optimal binding pairs of peptides and human cell surface receptor proteins. It is composed of a novel assembly of eleven existing machine learning search programs. Its objective function is the information about optimal population coverage fed to it by the second algorithm, EvalVax, which analyzes frequency of genetic variants across the population.



Applications of Vaccine Development

- Deep learning and AI has allowed for better computation times and solutions to complex problems.
- Along with vaccine development, AI has also helped in vaccine rollout and distribution.
- An important application of AI is the planning and hypothesis testing that's flexible enough to adjust quickly to new information so that decisions can be made based on the best available evidence.
- AI can also provide insights on patients that are likely to react to the vaccination, given their medical history and demographics information.

IMPACT OF VACCINE DEVELOPMENT

2 to 3 million

Deaths prevented per annum with correct production of Vaccines

- AI is a powerful catalyst, as these tools are helping researchers understand the virus and its structure, and predict which of its components will provoke an immune response—a key step in vaccine design.
- AI has also helped scientists track the virus's genetic mutations over time, information that will determine any vaccine's value in the years to come.

Gene Editing

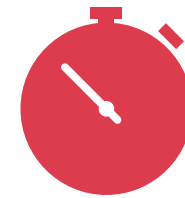
Role of AI in Gene Editing



Challenges



Solution



Application

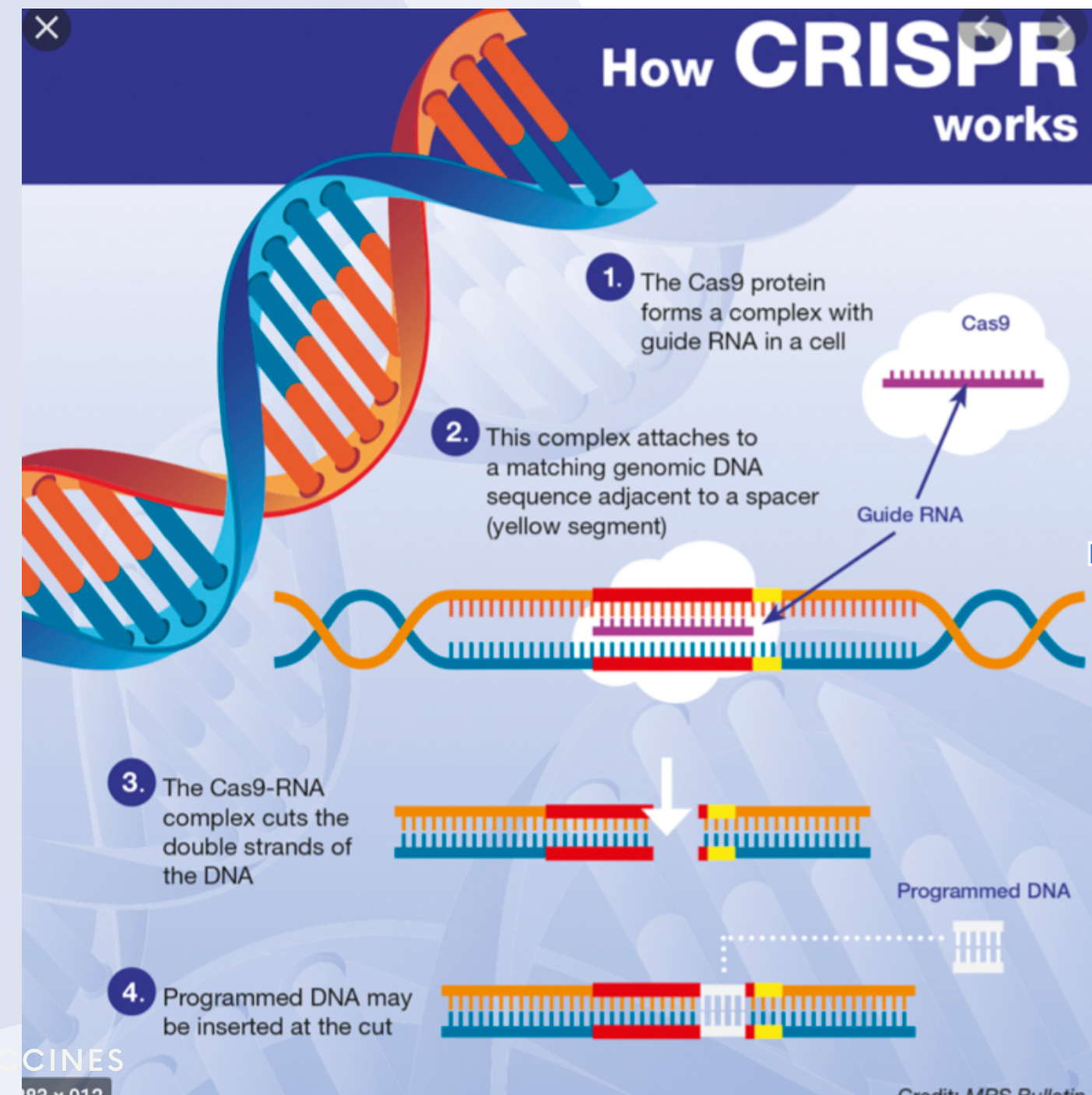


Impact

Challenges of Gene Editing

The issue in calculating accuracy and how to safely use Artificial intelligence while following ethics.

How to improve editing efficiency in Crispr which is the main gene editing mode.



Solution to Incorporate Ai in Gene Editing

A multi-step process to go by ethics and improve efficiency and editing accuracy

Engineering sgRNA

Engineering sgRNA with multiple accuracy to make sure the RNA is edited accurately

Choose mRNA

Use compatibility algorithms to fine the most compatible RNA and compare various suitors to improve efficiency.

Check Edits

Using MITs inDelphi algorithm check possible edits and check if the edits by using the innacuracy check in inDelphi

Modulate Cas9

Using inDelphi modulate the main gene for insertion and make sure to keep the inaccuracy in check with scale.

Regulatory Approval

Check through regulatory approval through experts to avoid long term error.



Applications of Gene Editing

- By using machine learning algorithms to compare the different gene expression levels in malignant and normal tissue samples of a patient diagnosed with cancer, predictions can be made about which genes have been mutated in that patient's DNA.
- The algorithms would train and make these predictions based on how often a gene is expressed in a malignant sample and compare this to the same gene in a normal sample, adding new information with each new set of data that it is fed.
- Machine learning algorithms are useful in identifying where the alteration must be made and how to ensure that the DNA strand is repaired properly afterwards, reducing potential for mistakes throughout the process.

Impact of incorporating AI in Gene Editing

**Improved
accuracy and
efficiency.**

**Increased
trust in
Crispr**

**Large-
scale trial**

Protein Folding

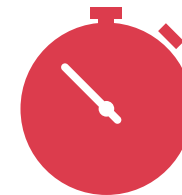
Role of AI in Protein Folding



Challenges



Solution



Application



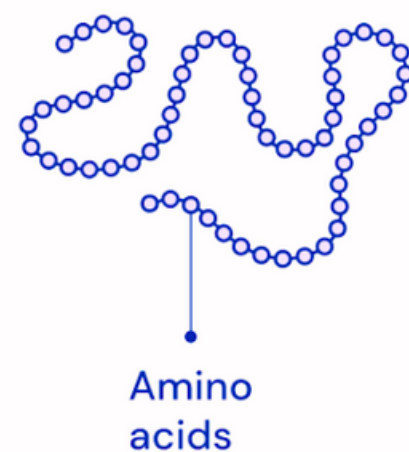
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Challenges in Protein folding and predicting its structure

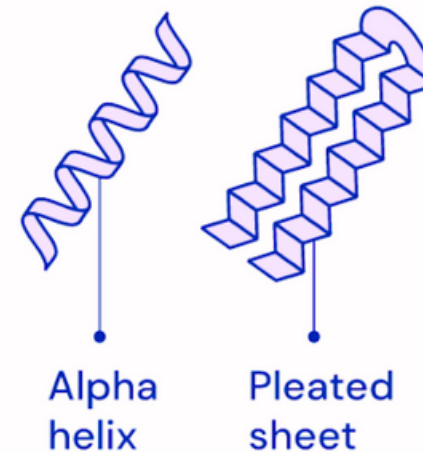
Challenges

- Proteins support practical functions that are essential to life
- Function of protein dependent on its 3 dimensional shape
- Predicting shape of protein is near impossible
- Has been a grand central problem for past 50 years

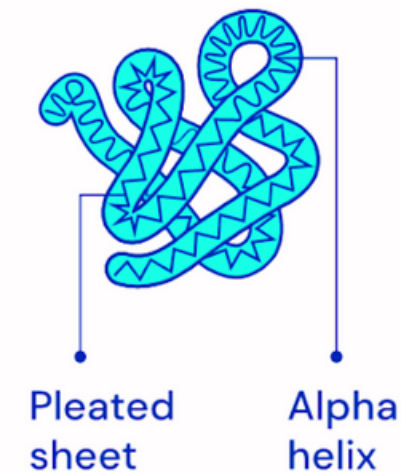
Every protein is made up of a sequence of amino acids bonded together



These amino acids interact locally to form shapes like helices and sheets



These shapes fold up on larger scales to form the full three-dimensional protein structure



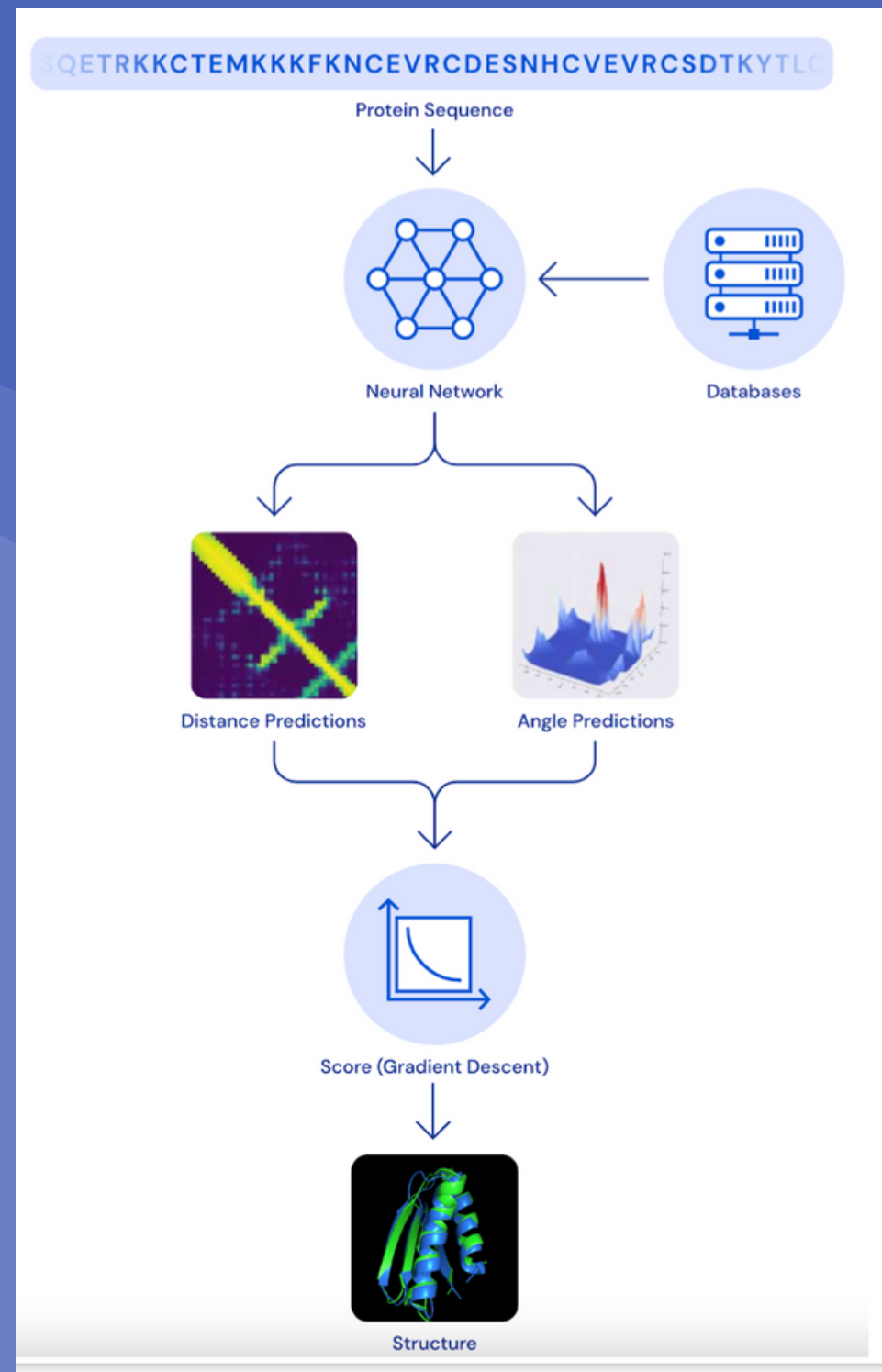
Proteins can interact with other proteins, performing functions such as signalling and transcribing DNA



Solution to challenges of Protein Folding

- Current methods to determine protein structure information involves manual inspection of individual molecules
- AI could help consolidate gene information to predict the structure of a given protein
- CASP was established as a global competition to accelerate research and measure progress on the protein structure predictions

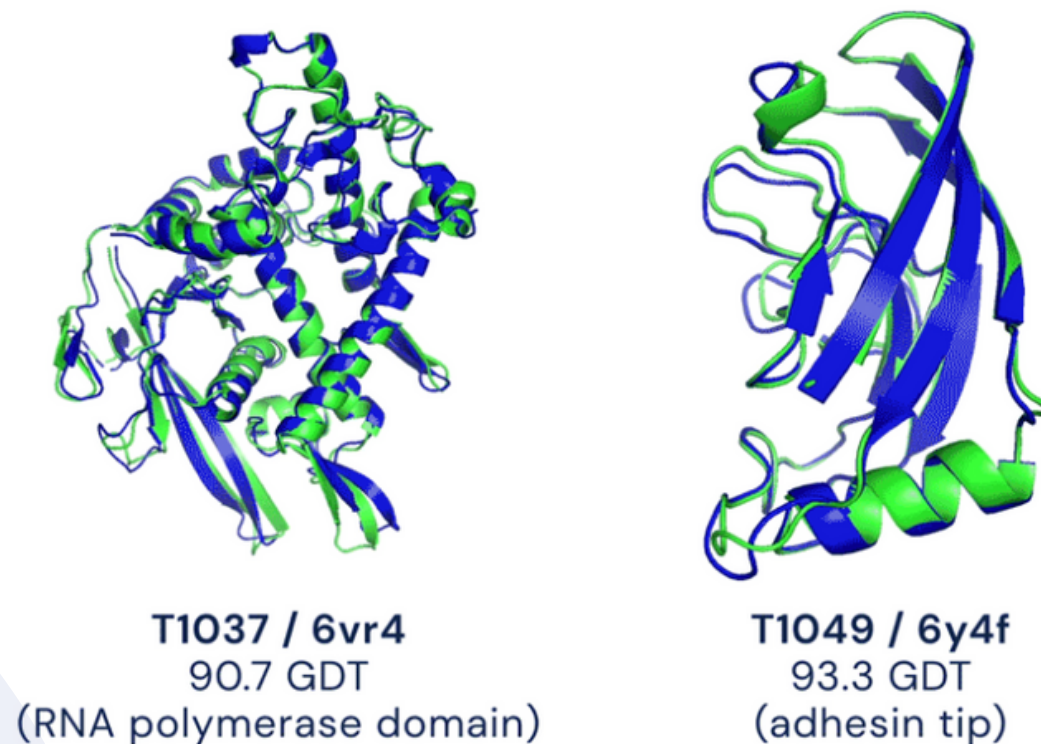
Applications of Protein Folding



- Alpha Fold from Deepmind has proposed a novel AI-based solution to predict the structure of protein
- Their solution relies on deep neural networks that are trained to predict properties of the protein from its genetic sequence
- The properties the networks predict are: distances between pairs of amino acids and angles between chemical bonds that connect those amino acids

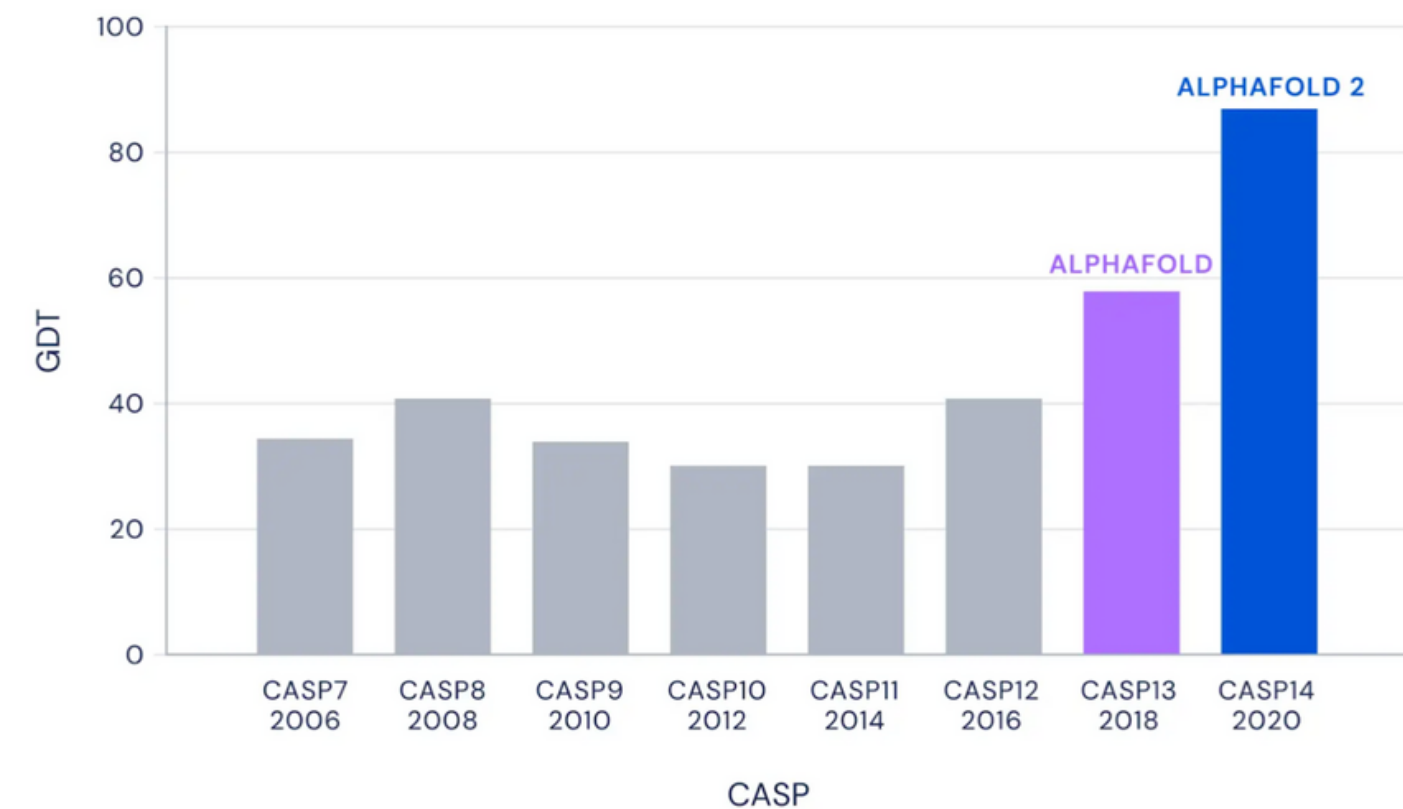
IMPACT OF INCORPORATING AI IN PROTEIN FOLDING

- Overall majority structures had higher levels of prediction accuracies than threshold level of 90 GDT
- In some cases, Alpha Fold performed better than experimental results



● Experimental result
● Computational prediction

Median Free-Modelling Accuracy



Conclusion

Bioinformatics

Vaccine Development

Human/Animal Trials (aka Data); OptiVAX Algorithm; better computation/solution; tracking mutations, catalyst

Gene Editing

Crispr; Improving the process; Improved Accuracy and Efficiency

Protein Folding

Deriving 3D shape of protein; Predicting structure using AI; Alpha Fold; Higher prediction Accuracy

Thank You!