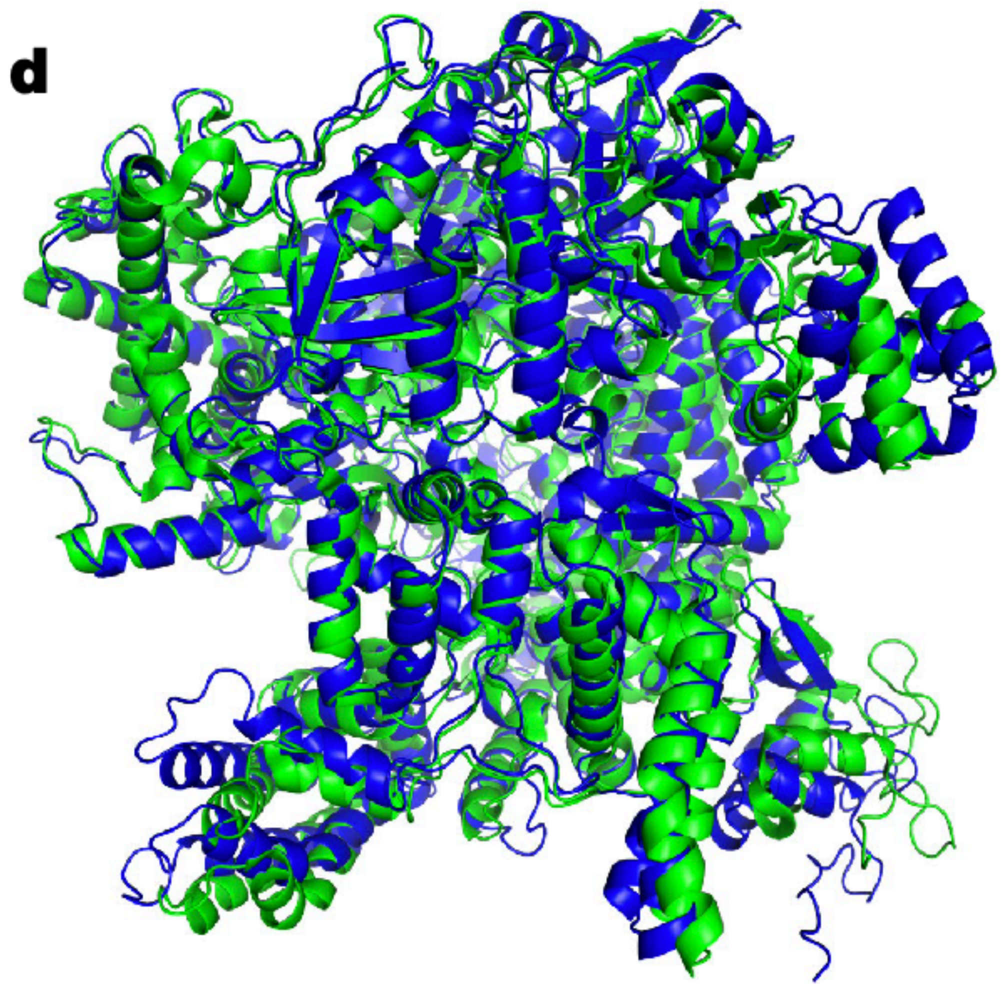
Mathematical Uncertainty Mitigation in Machine Learning (for Science)

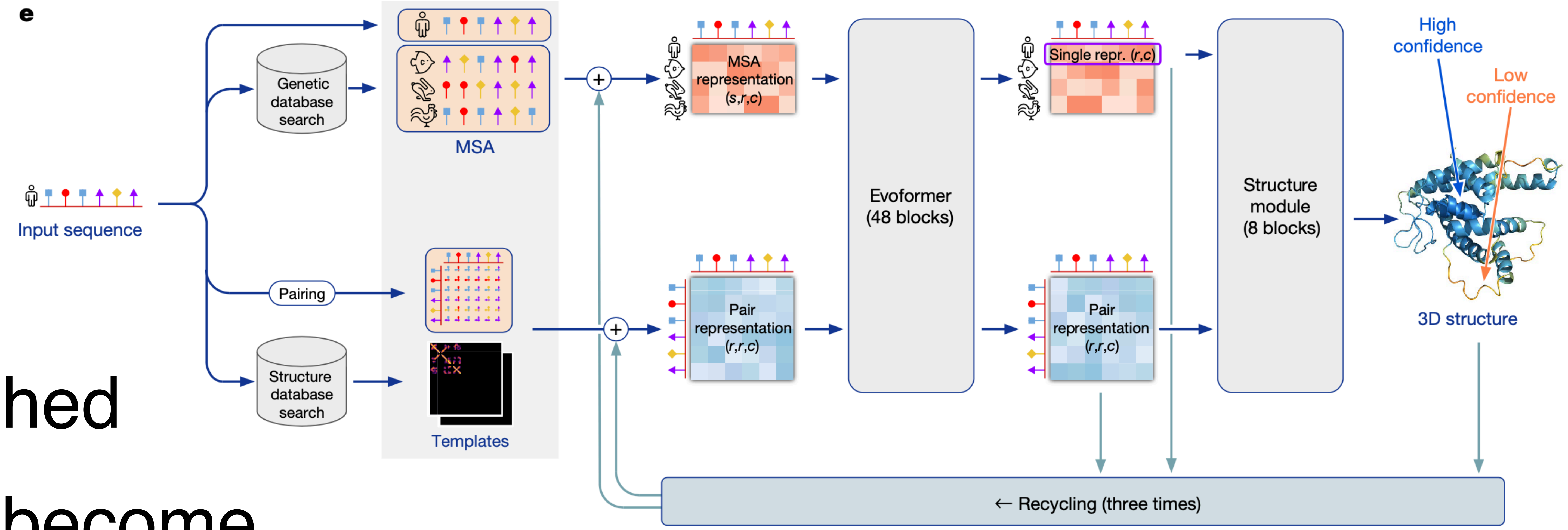
AIM NWO Grant Pitch

Patrick Forré

Motivation



- The success of **huge AI models** like AlphaFold or ChatGPT, is mainly due to:
    - flexible, scalable models,
    - big engineering effort,
    - **huge data sets**.
- For such big data sets the attached **uncertainties** arguably tend to become **minimal**.



- Jumper, J et al. Highly accurate protein structure prediction with AlphaFold. Nature (2021).

Problems for typical / scientific data sets

- In contrast, typical or **scientific data sets** are rather **small** ($n \lesssim p$ case),
- leading to **increased** data and model **uncertainties** and/or **complexities**,
- **requiring** sophisticated **uncertainty/complexity mitigation** strategies,
- **necessitating** proper **mathematical analysis with guarantees**!

  - We identify **3 major areas** (not necessarily disjoint) for the AIM community to engage in.

Pillar A - Uncertainty / complexity quantification

- Besides the usual model output, also **quantify** data and model **uncertainty/ complexity** reliably.
- Possible research directions (examples):
    - statistical/causal hypothesis testing (e.g. e-variables)
    - conformal predictions
    - Gaussian processes
    - statistical and singular learning theory
    - stochastic optimization

Pillar B - Uncertainty / complexity reduction via domain knowledge

- Use **domain** or **expert knowledge** to **reduce** the model **complexity** and/or data **uncertainty**.
- Domain/expert knowledge can be conveyed through:
    - models,
    - implicit biases (graph or geometric structures, symmetries, etc.),
    - simulators,
    - differential equations (ordinary/partial/stochastic).
- Possible research directions (examples):
    - geometric and topological machine learning
    - physics-informed machine learning, operator learning
    - simulation-based inference and optimization
    - causal, dynamical and generative modelling

Pillar C - Robustification against uncertainty / complexity

- Identify sources of uncertainty and **make** the machine learning model output **more robust against uncertainty**.
- Several approaches and research directions (examples):
    - dimensionality reduction (e.g. PCA, ICA),
    - representation learning (deep, structured, causal),
    - denoising techniques,
    - other data-driven robustifcation techniques (e.g. order statistics, etc.)

Applications in science and society?

- Optional, but **desirable** are **application areas in science and society**:
    - medical imaging
    - weather modelling
    - drug discovery
    - molecule and material sciences
    - liquid chromatography
    - astro-physics
    - gene expression data
    - animal movement prediction and tracking
    - AI fairness and safety
    - social networks

The key points

- clear narrative:
  - huge AI models ($n \gg p$) vs. scientific ML models ($n \lesssim p$)
  - (unreliable) engineering vs. mathematical guarantees
  - optional: useful applications in science and society
  - feasibility proven with our joint previous publication record
- broad umbrella project:
  - easily allows AIM community to participate
  - can be narrowed down (if necessary)

Interested? - What to think about

- To which pillar are you mostly connected to? A, B, C or some combination?
- Think about one PhD student engaging in:
  - one **proper mathematical project** (Def./Lem./Thm.-style)
    - for publication in (more) mathematical machine learning journal,
  - one project with knowledge transfer from mathematics to machine learning, **applying mathematical concepts to machine learning** (benchmark data sets)
    - for publication in machine learning conference,
  - one project **applying developed methods in science or society** (real data sets)
    - for publication in some science journal.

Example - 3D medical imaging

- application area: 3D medical imaging
  - domain knowledge: contains $\mathrm{SO}(3)$-symmetries
    - geometric deep learning (pillar B)
- study $\mathrm{SO}(3)$-representations, propose $\mathrm{SO}(3)$-equivariant convolutional neural network and study corresponding universal approximation theorem.
- implement the above neural network, apply it to 3D image/video benchmark data sets and record performance.
- apply the above method to real 3D medical images for specific prediction or segmentation tasks.

Thank you for your attention!

Questions?