www.fresnel.fr

Weakly-supervised inferences of molecular dynamics for fluorescence imaging in physiological environments

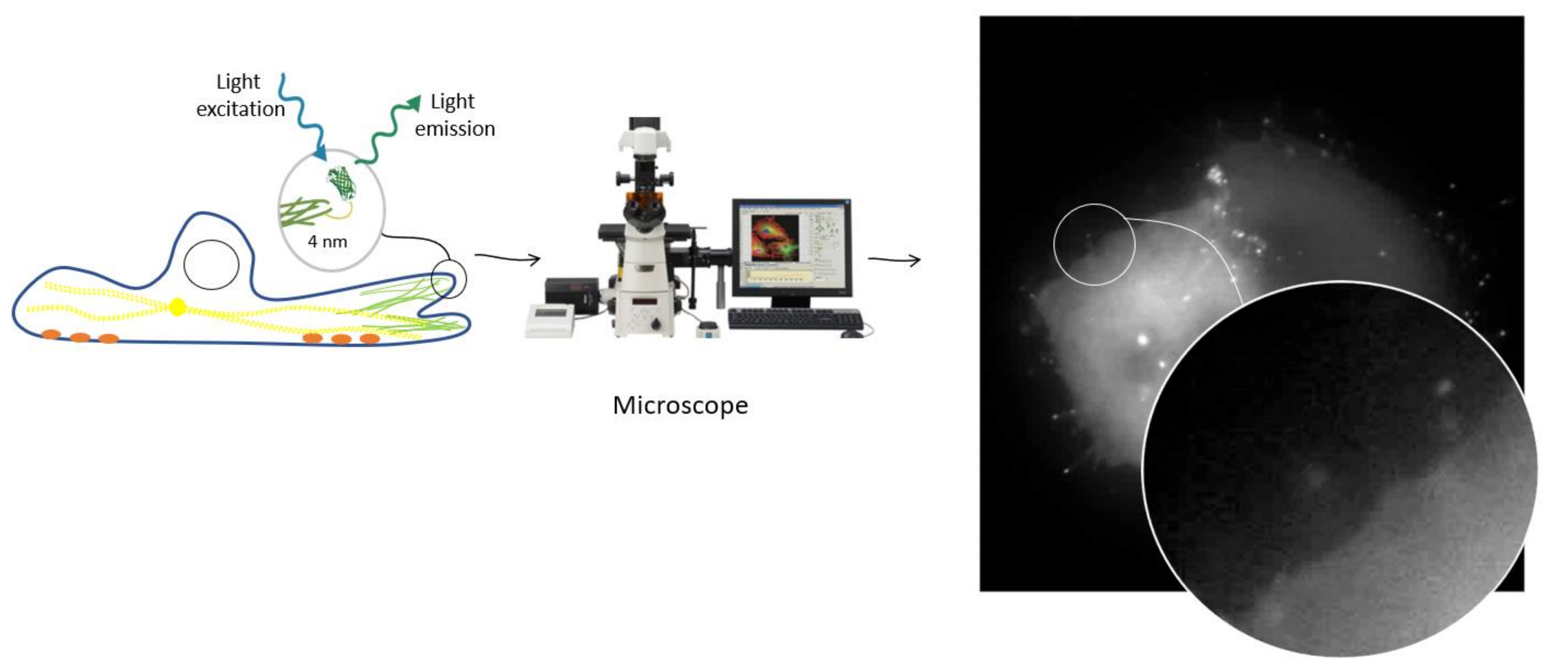
Piyush Mishra, Philippe Roudot

Aix-Marseille University, CNRS, Centrale Méditerranée, Institut de Mathématiques de Marseille, Institut Fresnel, Turing Centre for Living Systems

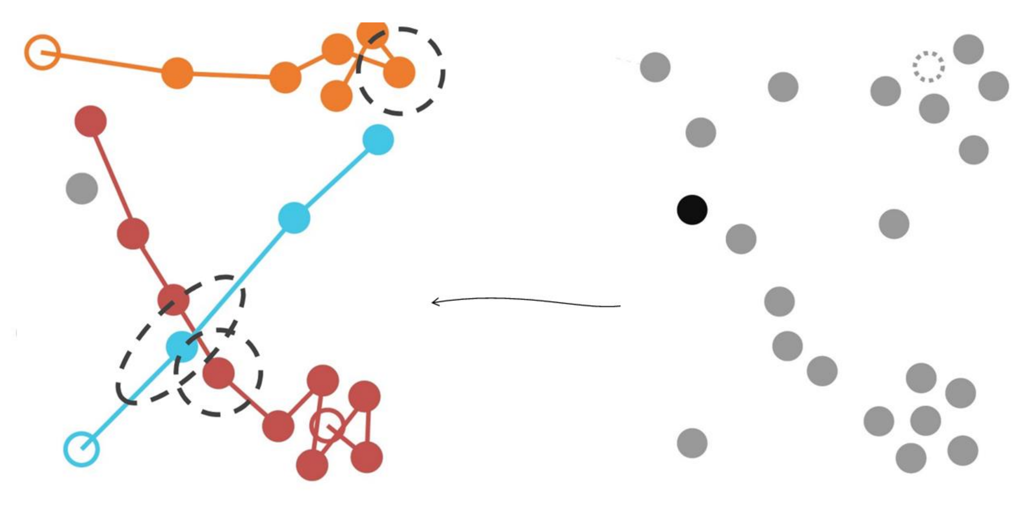
INSTITUT FRESNEL MARSEILLE

A. Context

Measurements from fluorescence microscopy are noisy & cluttered [1]

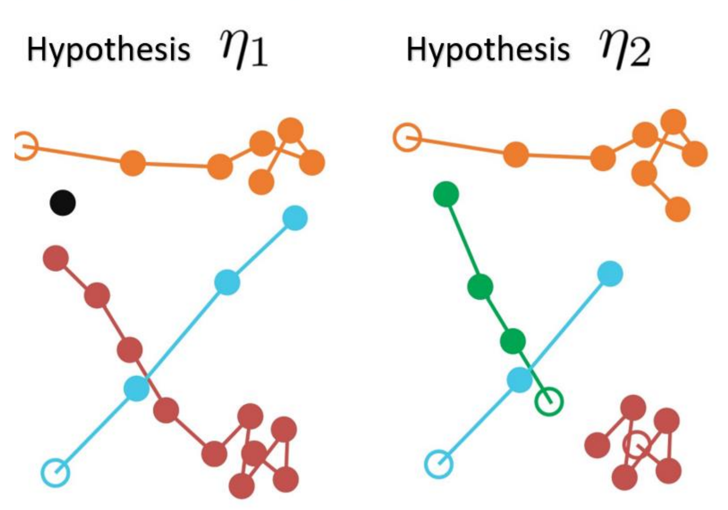


Mapping measurements to trajectories is an inverse data association problem [2]



$\mathbf{X}_t = \{\mathbf{x}_t^i\}_{i \in \Omega_t}$ $\mathbf{Z}_t = \{\mathbf{z}_t^j\}_{i \in D_t}$

Data association is a combinatorially hard problem [3]



$$|\eta_i| \propto n!^t$$

Conventional methods (like MHT) are untractable

$$p(X_t|Z_{1:t}) = p(Z_t|X_t) \int p(X_t|X_{t-1}) p(X_{t-1}|Z_{1:t-1}) dX$$

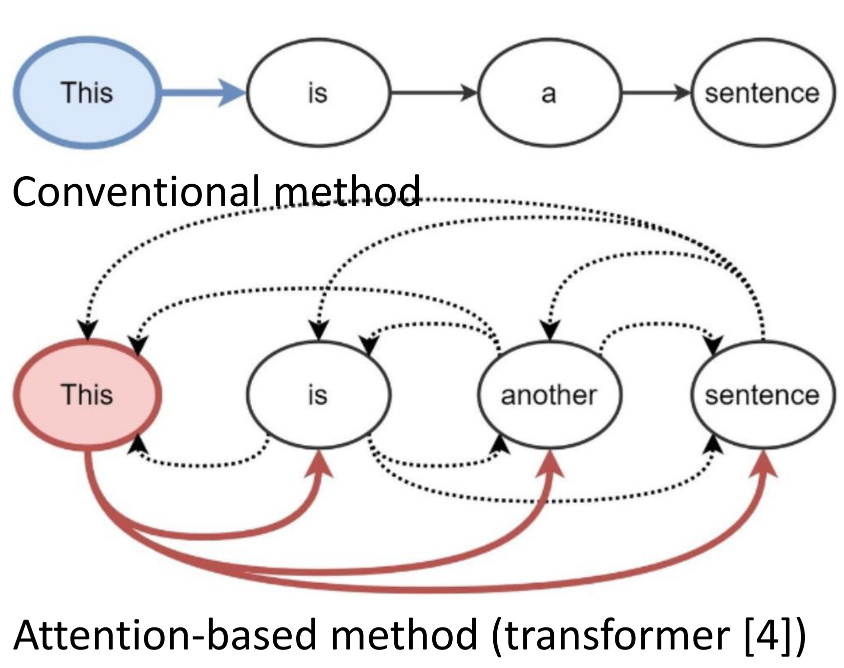
$$\sum_{\eta_i^t \in H_t^i} p(Z_t|X_t, \eta_i^t) p(\eta_i^t|X_t) \int p(X_t|X_{t-1}) p(X_{t-1}|Z_{1:t-1}) dX$$

difficult to account for the super-exponential increase in hypotheses

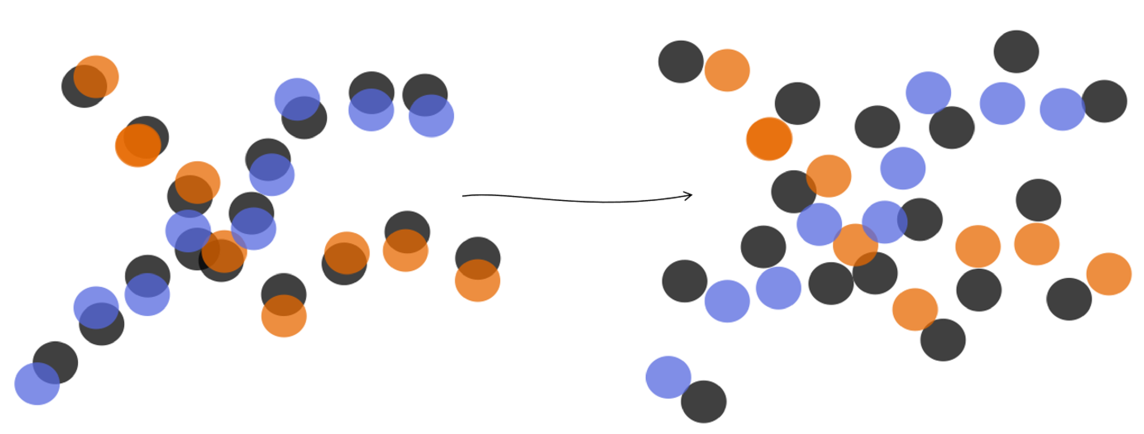
often, we don't have a priori information

Can LLMs be used for long-range sequence-dependencies & combinatorial complexity?

B. Method



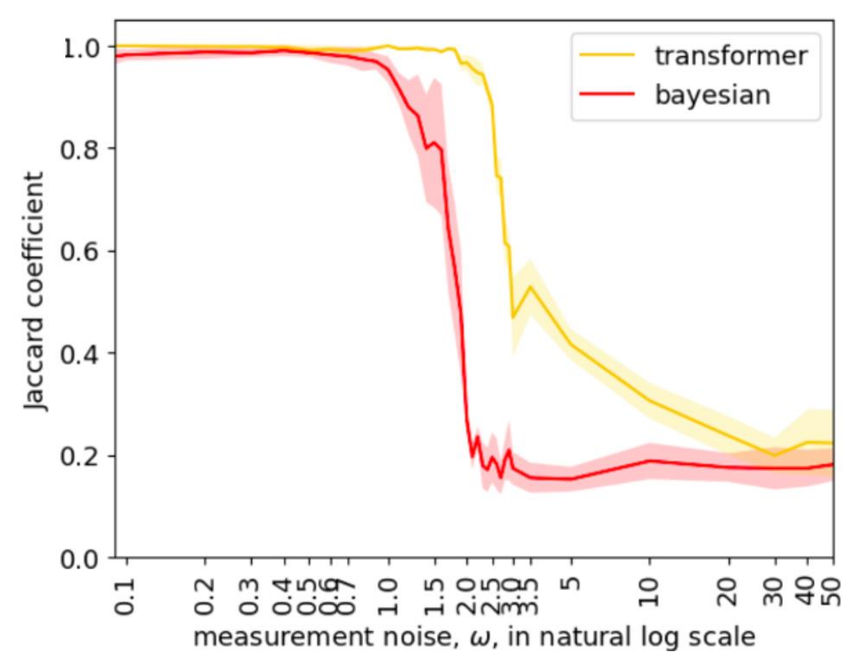
Experimental setup



Simulation of a simple system of 2 particles in 2 dimensions without any false positives & increasing measurement noise following standard Brownian motion

C. Main Results: Transformers are robust for long sequences but MHT remains optimal for short sequences

Robust to increasing noise

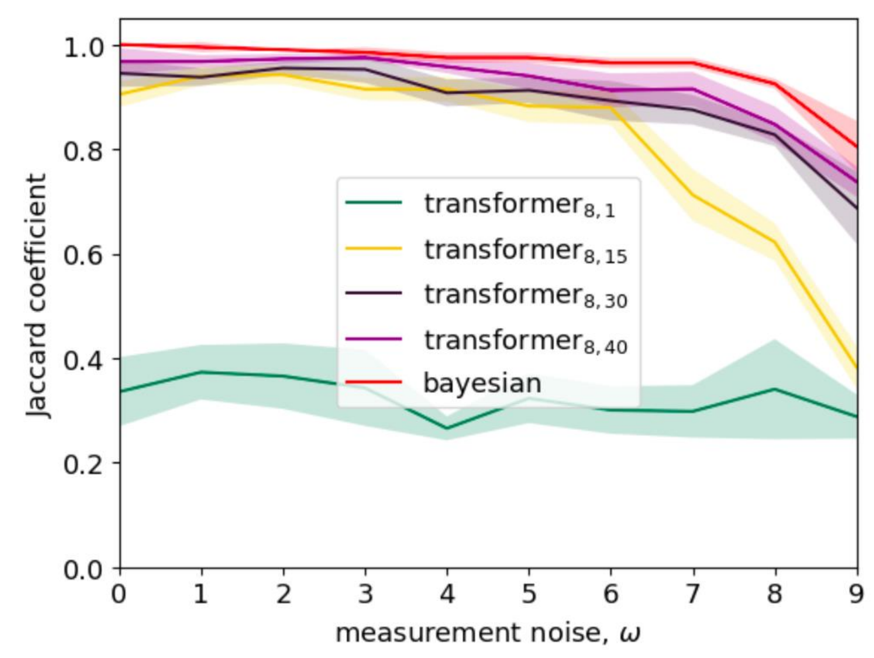


While attention prolongs the noise-cliff, it breaks the same way as MHT does

Hypothesis: MHT would be optimal (and hence, perform best) if it could easily access the entire lookback window.

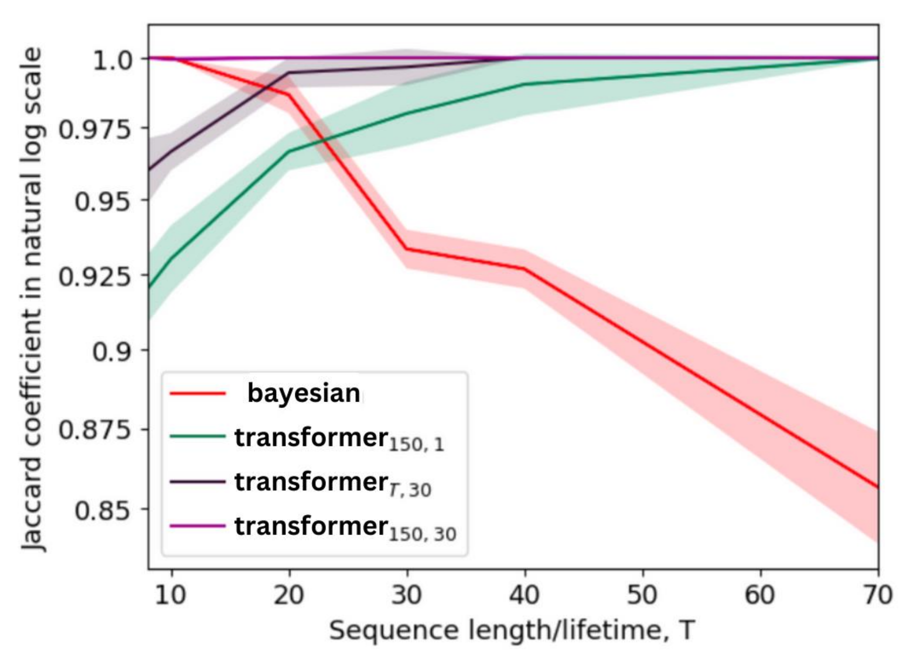
For small sequences, this is still feasible. What happens then?

When MHT is optimal



When MHT is indeed optimal, i.e., for small sequences, attention is unable to match its accuracy

Hint to hybridise?



Emergence of 2 regimes: small sequences where MHT performs better and big sequences where attention performs better

If trained enough times, attention performs better in both regimes!

References:

[1] Vonesch et al, 2006

[2] P. Emami, P. M. Pardalos, 2020

[3] Reid, 1979

[4] Vaswani et al, 2017

Acknowledgements:

The project has received funding from France 2030, the French Government program managed by the French National Research Agency (ANR-16-CONV-0001) and from Excellence Initiative of Aix-Marseille University - A*MIDEX.

cnrs · Aix*Marseille université Socialement engagée · Centrale Méditerranée · CENTURI Turing Centre for Living Systems · Institut Carnot STAR