Inferring the Dynamics of Underdamped Stochastic Systems

David B. Brückner,[1,†] Pierre Ronceray,[2,†] and Chase P. Broedersz[1,3,*]
[1]Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, Department of Physics, Ludwig-Maximilian-University Munich, Theresienstr. 37, D-80333 Munich, Germany
[2]Center for the Physics of Biological Function, Princeton University, Princeton, New Jersey 08544, USA
[3]Department of Physics and Astronomy, Vrije Universiteit Amsterdam, 1081 HV Amsterdam, The Netherlands

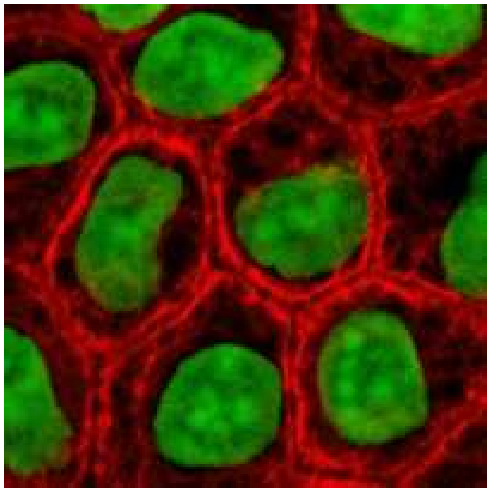
Phys. Rev. Lett. **125**, 058103 – Published 29 July 2020

INFERRING THE DYNAMICS OF UNDERDAMPED STOCHASTIC SYSTEMS

Team 15: Emily Waite, Yu-Huan Wang, Nick Weaver, Michael Wentzel, Yumu Yang, Qiantong Zhong

MOTIVATION

- Goal: Determine equations of motion from data for complex systems
- Methods for deterministic systems and overdamped systems previously developed
- No commonly accepted method for the underdamped case
- New framework: Underdamped Langevin Inference (ULI)



The living cell is an example of a complex system

Image from John Schmidt

LANGEVIN DYNAMICS: THE BASIC EQUATION

- Langevin equation in general:

$$\underbrace{M\ddot{x}}_{F = ma} = \underbrace{-\nabla U(x)}_{\text{Gradient of potential energy, conservative forces in system}} \underbrace{- \gamma\, \dot{x}}_{\text{Damping force}} + \underbrace{\sqrt{2\gamma k_B T}\,\xi(t)}_{\xi(t) \text{ is Gaussian white noise, pre-factor determines strength}}$$

0 for deterministic systems

- γ determines overdamped or underdamped regime
  - Large γ corresponds to overdamped (Brownian) regime → more noise, no average acceleration
  - Small γ corresponds to underdamped regime → less noise, but oscillations & allows overall acceleration

PREVIOUS RESULTS – DETERMINISTIC SYSTEMS

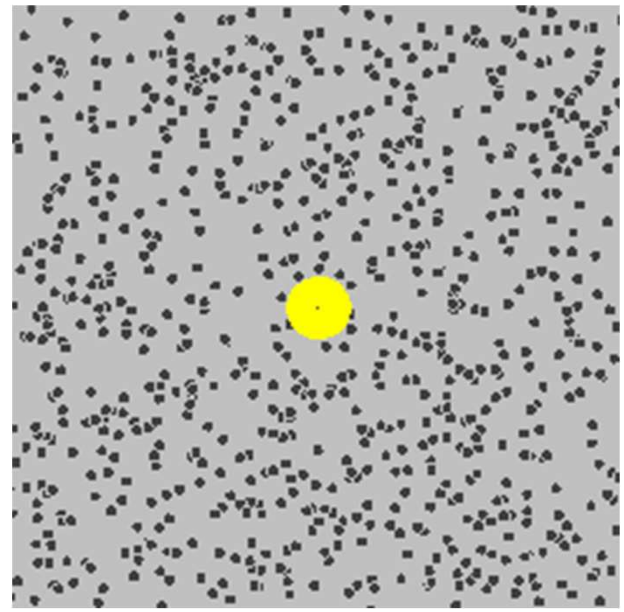
- Systems are complicated but don't contain noise terms
  - Time evolution is fully deterministic, making modelling easier
- Examples: Double pendulum, Lorenz atmospheric model
- Need to capture features without overfitting
- Techniques to achieve found in: Brunton, Proctor, & Kutz (2016) and Daniels & Nemenman (2015)

Lorenz weather model – path through phase space

Gif by Dan Quinn

OVERDAMPED STOCHASTIC SYSTEMS

- Langevin model was developed for the study of molecular systems
  - Example: Brownian motion
  - Can also be applied to other systems
- Level of damping affects level of modelling difficulty
- Methods such as InferenceMap (Beheiry, Dahan, & Masson, 2015) had been developed
- Methods for underdamped systems were much harder to find



Brownian motion of a colloidal particle

Gif by Fransisco Esquembre & Fu Kwun

LARGE AMOUNT OF DATA TO BE ANALYZED

- Examples of underdamped systems:
  - Dust particles in plasma, swarms of insects, and cellular motility
- Recent advances in tracking the members of these systems
  - Enormous amount of new data to be analyzed
- This paper aimed to find a reliable method of analyzing this data and determining the underlying equations of motion

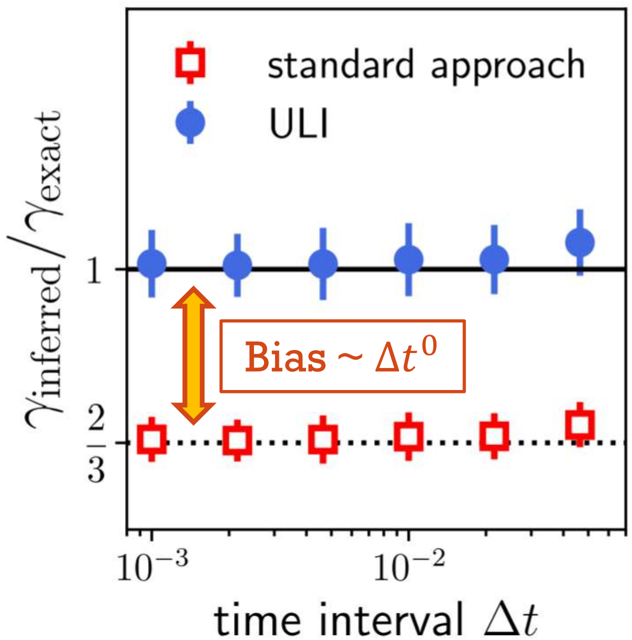
Photo by Damien TUPINIER on Unsplash

CHALLENGES OF GENERALIZING OVERDAMPED LANGEVIN INFERENCE

1. Inconsistent Estimator

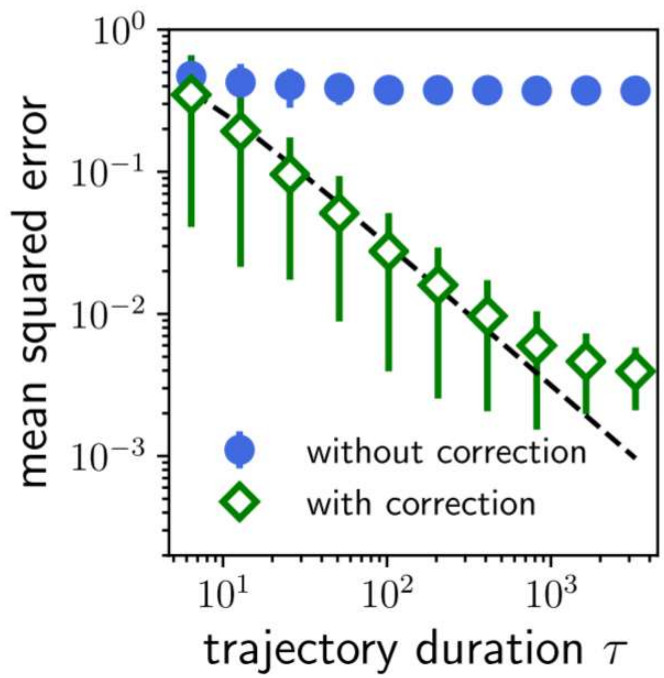
e.g. linear viscous force

$$F(v) = -\gamma v$$



2. Susceptible to Measurement Errors

divergent bias of order Δt^{-3}



A GENERAL METHOD OF SIMULATION

- A general d-dimensional stationary stochastic process $\mathbf{x}(t)$ with components $\{x_\mu(t)\}_{1\leq\mu\leq d}$:

$$\underbrace{\ddot{x}_\mu}_{\text{Acceleration}} = \underbrace{F_\mu(\mathbf{x},\mathbf{v})}_{\text{Force Field}} + \underbrace{\sigma_{\mu\nu}(\mathbf{x},\mathbf{v})}_{\text{Noise Amplitude}}\underbrace{\xi_\nu(t)}_{\text{Gaussian White Noise}}$$

- Project force field and noise amplitude onto an empirical orthonormal basis $\hat{c}_\alpha(\mathbf{x},\mathbf{v})$

RESULTS: ULI ESTIMATORS

$F_\mu(\mathbf{x}, \mathbf{v}) \approx F_{\mu\alpha} \hat{c}_\alpha(\mathbf{x}, \mathbf{v})$

Projection Coefficient For Noise

$$\hat{F}_{\mu\alpha} = \langle \hat{a}_\mu c_\alpha(\mathbf{x}, \hat{\mathbf{v}}) \rangle - \frac{1}{6} \langle (\partial_{v_\nu} c_\alpha(\mathbf{x}, \hat{\mathbf{v}})) \, \widehat{\sigma^2}_{\mu\nu}(\mathbf{x}, \hat{\mathbf{v}}) \rangle$$

Projections of the Accelerations

Correction Term

Force estimator for ~~overdamped~~ underdamped system

MINIMIZE THE MEASUREMENT ERRORS

- Previous estimator for position

$$\mathbf{x}(t) = \mathbf{x}(t)$$

- A more robust estimator

$$\bar{\mathbf{x}} = \frac{1}{3}[\mathbf{x}(t-\Delta t) + \mathbf{x}(t) + \mathbf{x}(t+\Delta t)]$$

- Fails only when the measurement error is comparable to the displacement in a single time step

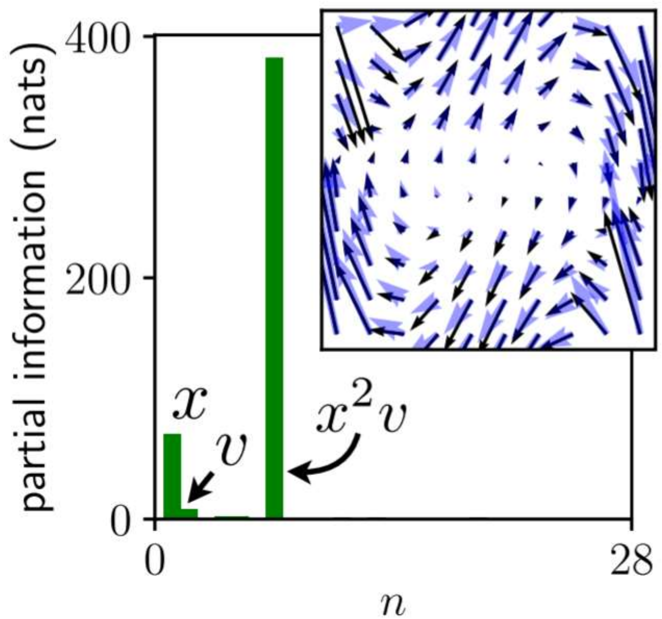
NON-LINEAR DYNAMICS INFERENCE

- Non-Linear System: $\{x, v, x^2, v^2, xv, \ldots\}$
- Which basis functions to choose?
- More is not better
  - 1. Computation load
  - 2. More collective inference errors
- Information (how important it is):

$$\hat{I}_b(n_b) = (\tau/2)\hat{\sigma}_{\mu\nu}^{-2}\hat{F}_{\mu\alpha}\hat{F}_{\nu\alpha} \sim \frac{Force}{noise}$$

e.g. Van der Pol Oscillator

$\{x, v, x^2 v\}$



CRITICAL ANALYSIS

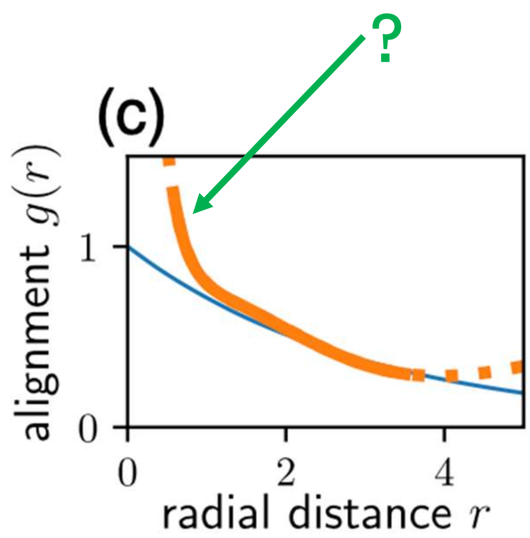
Disconnect between paper & supplementary

- Paper: $\hat{F}_{\mu\alpha} = \langle \hat{a}_\mu c_\alpha(\mathbf{x}, \hat{\mathbf{v}}) \rangle - \frac{1}{6} \langle (\partial_{v_\nu} c_\alpha(\mathbf{x}, \hat{\mathbf{v}}))\, \widehat{\sigma^2}_{\mu\nu}(\mathbf{x}, \hat{\mathbf{v}}) \rangle$
- Supplementary: $\hat{F}_{\mu\alpha} = \langle \hat{a}_\mu c_\alpha(\mathbf{x}, \hat{\mathbf{v}}) \rangle - \frac{1}{2} \langle \widehat{\sigma^2}_{\mu\nu}(\mathbf{x}, \hat{\mathbf{v}}) (\partial_{v_\nu} c_\alpha(\mathbf{x}, \hat{\mathbf{v}})) \rangle$
- Why?
  - In supplemental, $\hat{v} = \frac{x(t+\Delta t) - x(t-\Delta t)}{2\Delta t}$; In paper, $\hat{v} = \frac{x(t) - x(t-\Delta t)}{\Delta t}$
  - Discrepancy is confusing & had to use footnote + lots of searching to figure out why
- Work unnecessarily hard to follow
  - Actual paper gave overview of derivation, but almost had to go to supplemental to actually understand it

CRITICAL ANALYSIS

Limitations of Method

- Could have talked more about range of validity
  - Almost no discussion on the limits in which approximations are valid
- Example:
  - Flock of bird simulation has 6N degrees of freedom
  - "Intuitively, one might expect that ULI should fail dramatically in such a system"
  - "However, by exploiting the particle exchange symmetric and radial symmetry of the interactions, we find that ULI …captures the full force field"
- Limited by choosing a finite basis



BROADER IMPACT: WHAT TO LOOK FOR

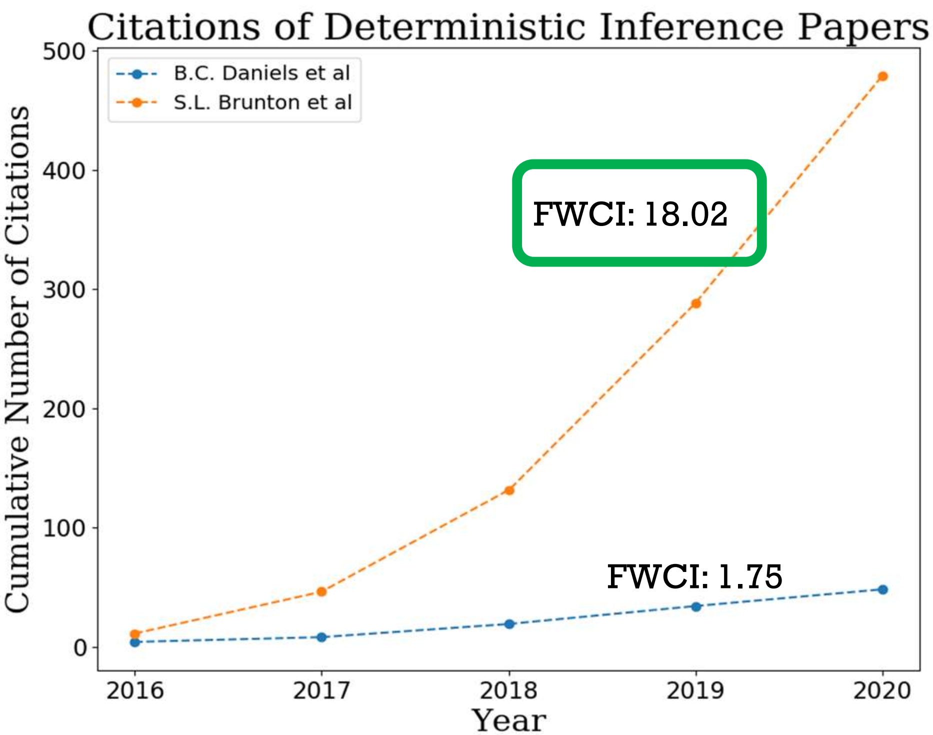
Previous works cited provide frameworks for solving deterministic and overdamped stochastic systems

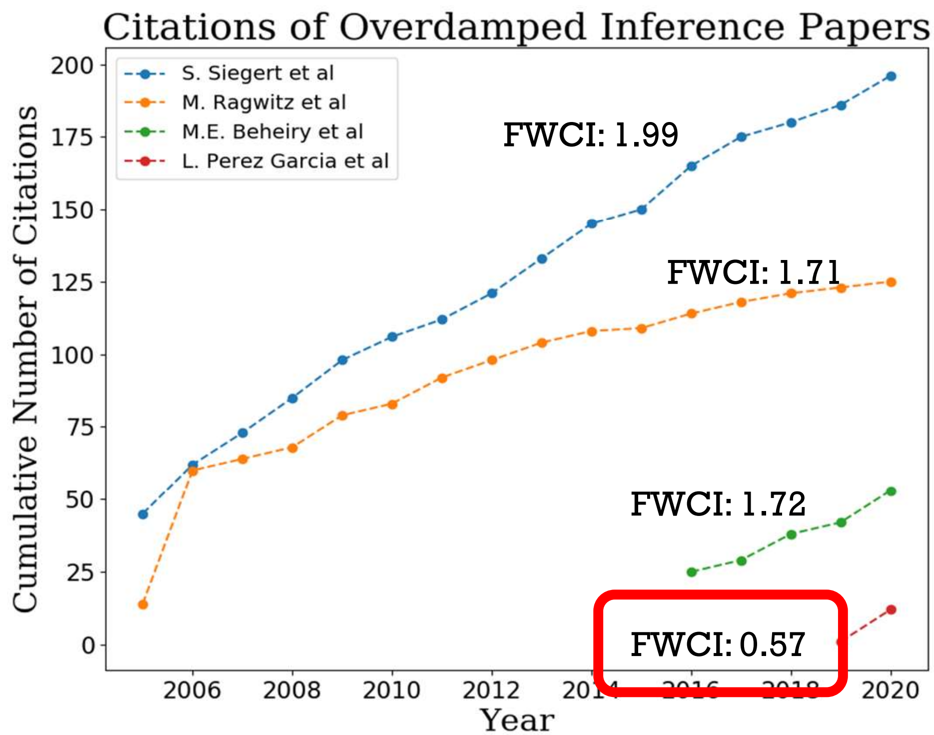
Think of the Underdamped Langevin Inference as the natural next step

Assume that ULI will have similar impacts to papers

Consider BREADTH and INTENSITY of these works

POTENTIAL INTENSITY OF IMPACT

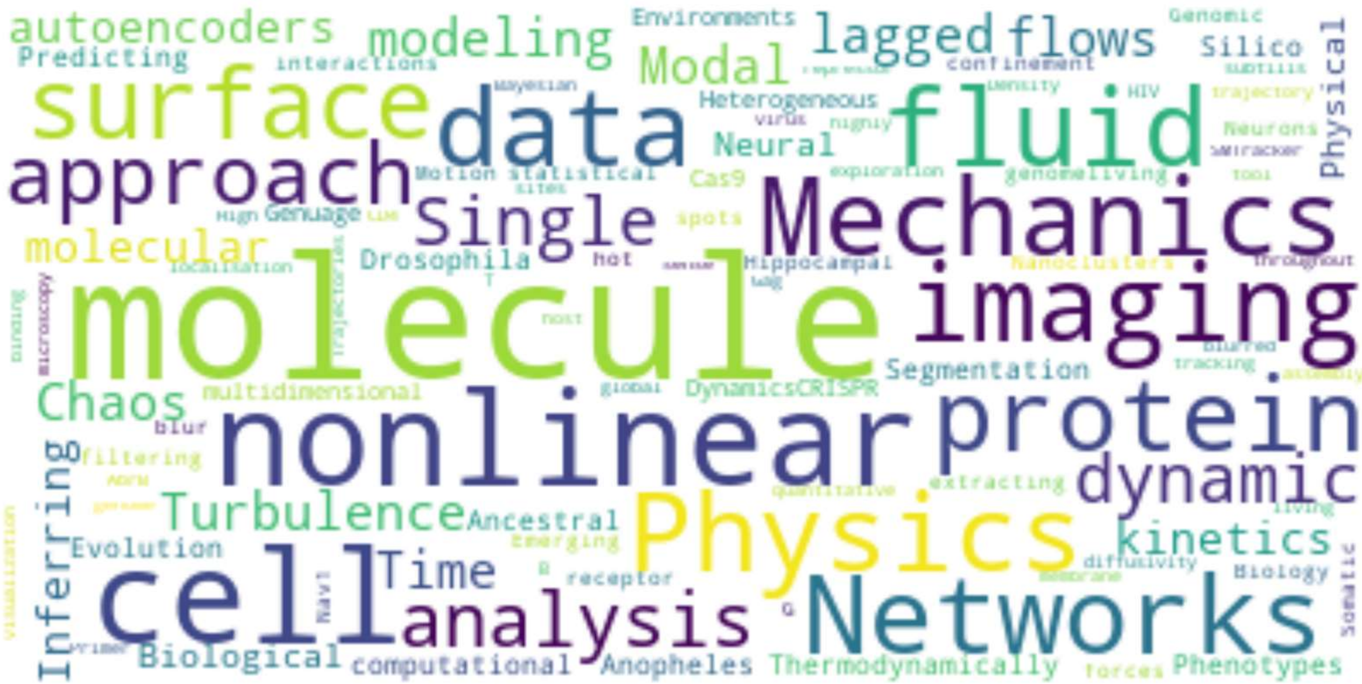




FWCI := Field Weighted Citation Impact

https://www.scopus.com/record/pubmetrics.uri?eid=2-s2.0-85057599516&origin=recordpage

POTENTIAL BREADTH OF IMPACT



Thank you to **Dmitry** for the WordCloud code

WHERE THE FIELD IS GOING

- This paper was published recently so it is unclear what its final impact will end up being
- There is a large amount of data that these techniques could be applied to, so we would expect this paper to be heavily cited over the next few years as these results get applied
- Machine learning is becoming prevalent in all fields
- We will begin to see these inference methods applied with neural networks and machine learning

- NOTE: the code is publicly available on GitHub and so others can immediately begin to apply it to data sets

https://github.com/ronceray/UnderdampedLangevinInference

SUMMARY

Paper:

- Basic history: deterministic & overdamped
- A general framework to write out the equation of motion for underdamped stochastic systems.
- Several cases that ensure the capability of this model.

Our analysis:

- Do somewhat question the limitations of the method, but seems robust for applications that it can be used for
- Has potential to have a large impact on field