

Probabilistic ODE Solutions in Millions of Dimensions



*Nico Krämer**



Nathanael Bosch*



Jonathan Schmidt*



Philipp Hennig

* Equal contribution

June 27, 2022

EBERHARD KARLS
UNIVERSITÄT
TÜBINGEN



Faculty of Science
Department of Computer Science
Chair for the Methods of Machine Learning



CyberValley

DFG



imprs-is

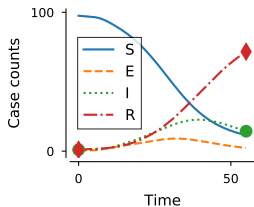
Simulation of ordinary differential equations

Simulation of ordinary differential equations

► ODE: $\dot{y}(t) = f(y(t), t)$, $y(t_0) = y_0 \in \mathbb{R}^d$

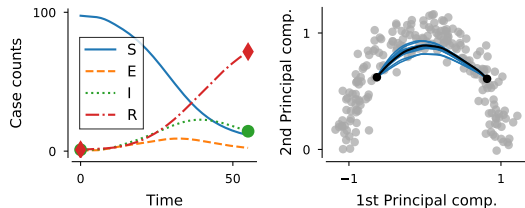
Simulation of ordinary differential equations

- ▶ ODE: $\dot{y}(t) = f(y(t), t)$, $y(t_0) = y_0 \in \mathbb{R}^d$
- ▶ Applications *all over the natural sciences*:
biology, geosciences, fluid dynamics, ...



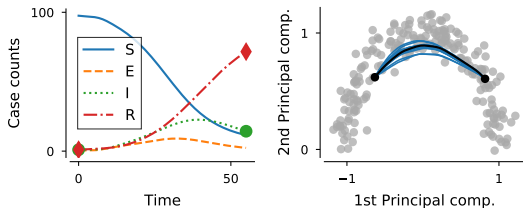
Simulation of ordinary differential equations

- ▶ ODE: $\dot{y}(t) = f(y(t), t)$, $y(t_0) = y_0 \in \mathbb{R}^d$
- ▶ Applications *all over the natural sciences*:
biology, geosciences, fluid dynamics, ...
- ▶ Applications *all over machine learning*:
neural {O, S, P}DEs, PINNs, ...



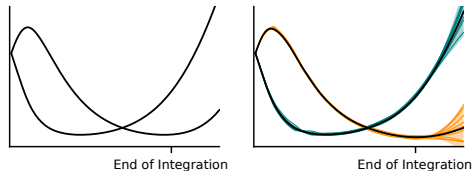
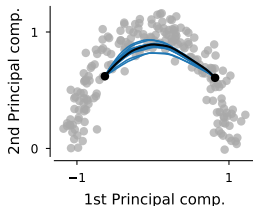
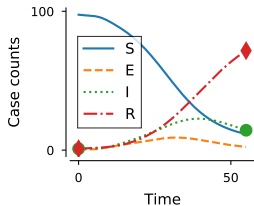
Simulation of ordinary differential equations

- ▶ ODE: $\dot{y}(t) = f(y(t), t)$, $y(t_0) = y_0 \in \mathbb{R}^d$
- ▶ Applications *all over the natural sciences*:
biology, geosciences, fluid dynamics, ...
- ▶ Applications *all over machine learning*:
neural {O, S, P}DEs, PINNs, ...
- ▶ Many dimensions, $d \gg 100$. Think: $d \sim 10^6$



Simulation of ordinary differential equations

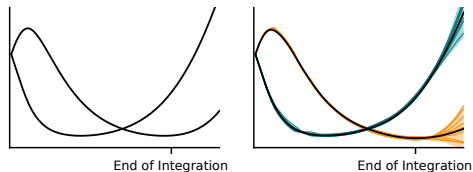
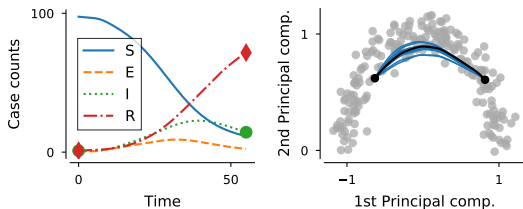
- ▶ ODE: $\dot{y}(t) = f(y(t), t)$, $y(t_0) = y_0 \in \mathbb{R}^d$
- ▶ Applications *all over the natural sciences*: biology, geosciences, fluid dynamics, ...
- ▶ Applications *all over machine learning*: neural {O, S, P}DEs, PINNs, ...
- ▶ Many dimensions, $d \gg 100$. Think: $d \sim 10^6$



- ▶ Any approximation of the posterior distribution $p(y \mid \{\dot{y}(t_n) = f(y(t_n), t_n)\}_{n=0}^N, y(t_0) = y_0)$ approximately solves the ODE

Simulation of ordinary differential equations

- ▶ ODE: $\dot{y}(t) = f(y(t), t)$, $y(t_0) = y_0 \in \mathbb{R}^d$
- ▶ Applications *all over the natural sciences*: biology, geosciences, fluid dynamics, ...
- ▶ Applications *all over machine learning*: neural {O, S, P}DEs, PINNs, ...
- ▶ Many dimensions, $d \gg 100$. Think: $d \sim 10^6$



- ▶ Any approximation of the posterior distribution $p(y \mid \{\dot{y}(t_n) = f(y(t_n), t_n)\}_{n=0}^N, y(t_0) = y_0)$ approximately solves the ODE
- ▶ Complexity $O(d^3)$ per step ⚡⚡

Solution: more structure in the state space

Solution: more structure in the state space

Theorem (Kronecker; simplified)

If the ν th-order prior has Kronecker structure, a single step with the prob. ODE solver costs $O(\nu^3 + d\nu^2)$ in float-ops and $O(d\nu + d^2 + \nu^2)$ in memory.

Solution: more structure in the state space

Theorem (Kronecker; simplified)

If the ν th-order prior has Kronecker structure, a single step with the prob. ODE solver costs $O(\nu^3 + d\nu^2)$ in float-ops and $O(d\nu + d^2 + \nu^2)$ in memory.

Theorem (Independence; simplified)

If the ν th-order prior independent prior dimensions, a single step with the prob. ODE solver costs $O(d\nu^3)$ in float-ops and $O(d\nu^2)$ in memory.

Solution: more structure in the state space

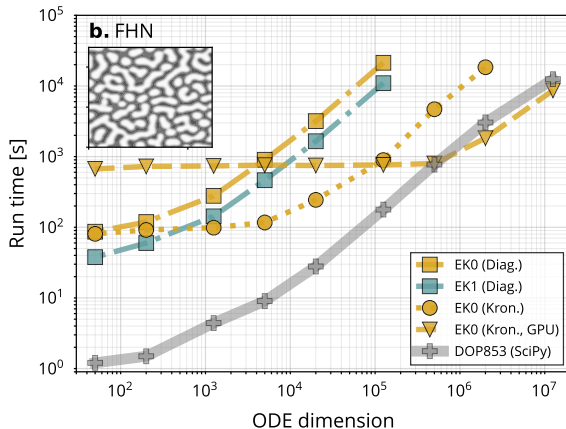
Theorem (Kronecker; simplified)

If the ν th-order prior has Kronecker structure, a single step with the prob. ODE solver costs $O(\nu^3 + d\nu^2)$ in float-ops and $O(d\nu + d^2 + \nu^2)$ in memory.

Theorem (Independence; simplified)

If the ν th-order prior independent prior dimensions, a single step with the prob. ODE solver costs $O(d\nu^3)$ in float-ops and $O(d\nu^2)$ in memory.

a. Run time vs. ODE dimension



Conclusion

Conclusion

- ▶ Structured state spaces accelerate ODE solvers

Conclusion

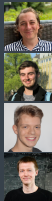
- ▶ Structured state spaces accelerate ODE solvers
- ▶ Simulation of millions of dimensions

Conclusion

- ▶ Structured state spaces accelerate ODE solvers
- ▶ Simulation of millions of dimensions
- ▶ Simulation of PDEs and more

Conclusion

- ▶ Structured state spaces accelerate ODE solvers
- ▶ Simulation of millions of dimensions
- ▶ Simulation of PDEs and more



Nico Krämer (@pnkraemer)

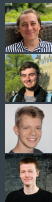
Nathanael Bosch (@NathanaelBosch)

Jonathan Schmidt

Philipp Hennig (@PhilippHennig5)

Conclusion

- ▶ Structured state spaces accelerate ODE solvers
- ▶ Simulation of millions of dimensions
- ▶ Simulation of PDEs and more



Nico Krämer (@pnkraemer)

Nathanael Bosch (@NathanaelBosch)

Jonathan Schmidt

Philipp Hennig (@PhilippHennig5)

Software: <https://github.com/pnkraemer/tornadox>

```
pip install tornadox
```

Paper: <https://arxiv.org/abs/2110.11812>

Come and talk to us. Visit the poster.



Experiment code