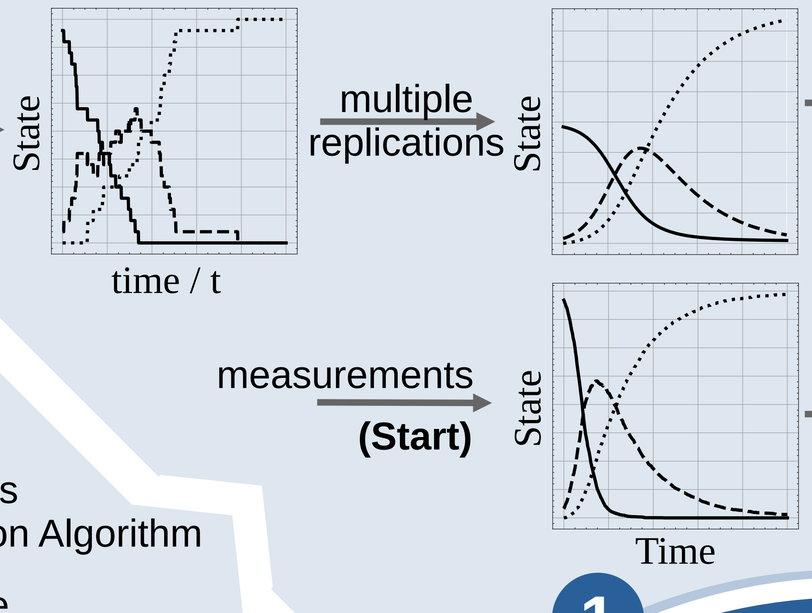
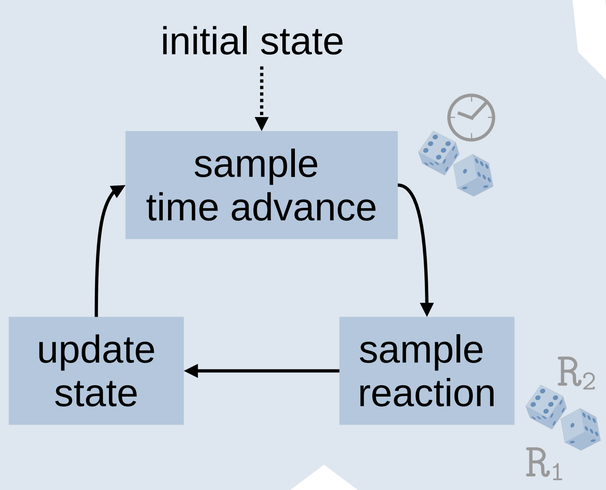
Universität Rostock
Traditio et Innovatio

VAC visual & analytic computing

Learning Reaction Networks by Gradient Descent



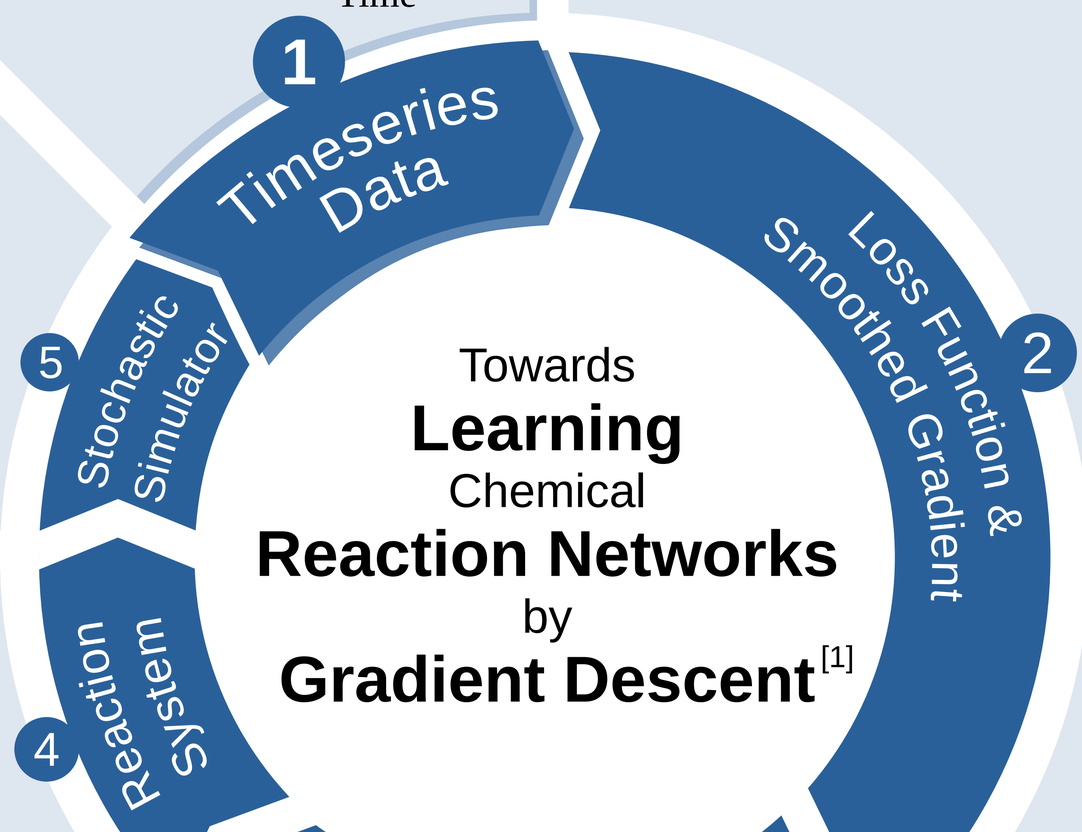
Gillespie's Stochastic Simulation Algorithm

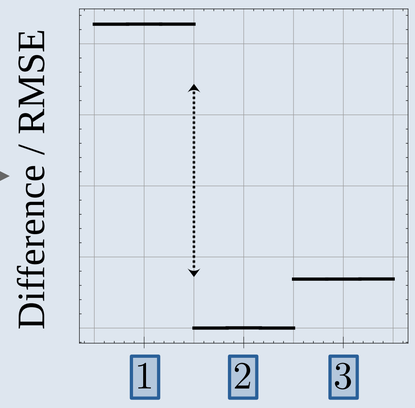


rate (continuous) coefficient (discrete)

$$\begin{aligned} \mathrm{R}_1 &: 1S + 1I \xrightarrow{0.02} 2I \\ \mathrm{R}_2 &: 1I \xrightarrow{5.00} 1R \end{aligned}$$

reaction system model (ground truth)



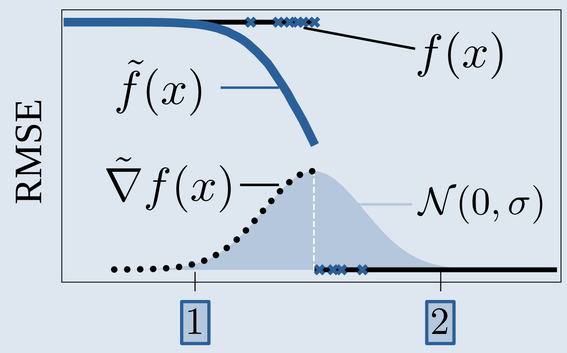


$$\begin{aligned} S + I &\xrightarrow{0.02} ?\, I \\ I &\xrightarrow{5.00} R \end{aligned}$$

➔ Loss surface wrt. discrete coefficients has jumps ↕

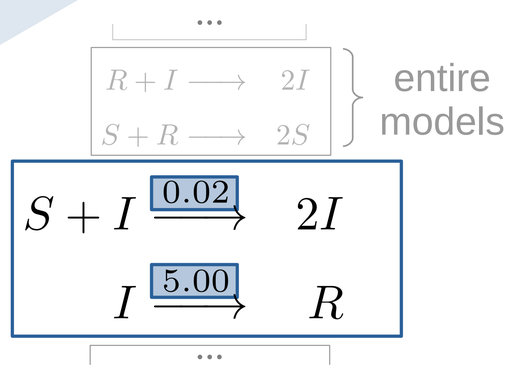
➔ Gradient undefined

Solution:
Smoothing Gradient Estimator [2]

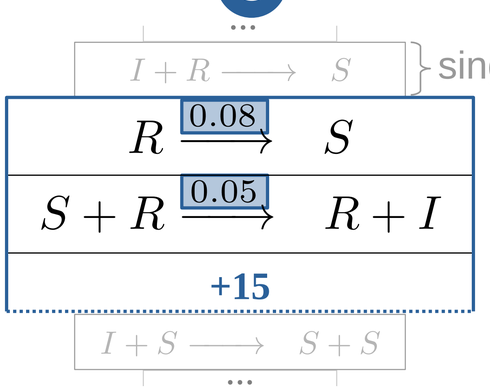


$$\tilde{\nabla} f(\mathbf{x}) = \frac{1}{N} \sum_{i=1}^{N} \frac{f(\mathbf{x} + \sigma \mathbf{u}) - f(\mathbf{x})}{\sigma} \mathbf{u}$$

" = " Gradient of f convolved with a normal distribution via Monte Carlo sampling; $\mathbf{u} \sim \mathcal{N}(0, I)$



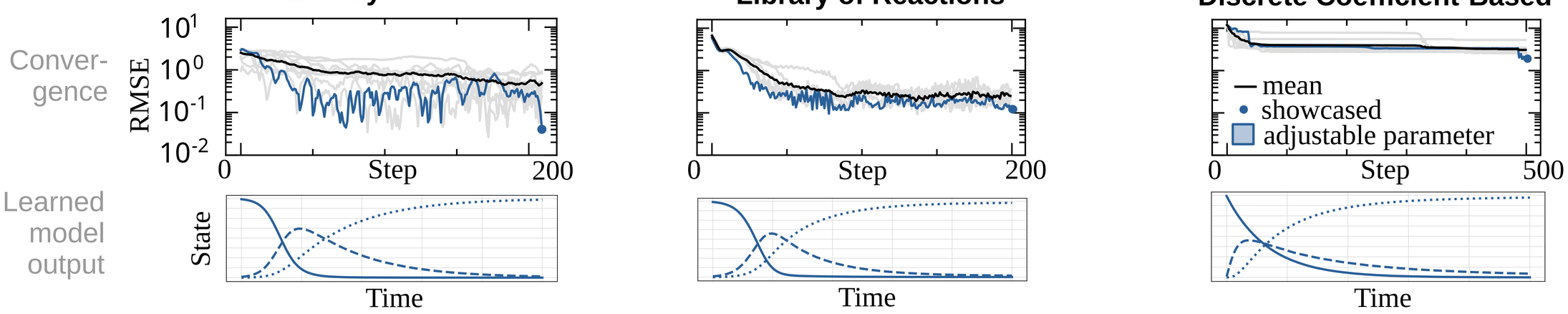
Library of Models



Library of Reactions

$$\begin{aligned} 1S + 0I + 0R &\xrightarrow{7.20} 0S + 2I + 0R \\ 0S + 2I + 0R &\xrightarrow{0.01} 0S + 0I + 1R \end{aligned}$$

Discrete Coefficient-Based



Conclusions

➔ Smoothed Gradient Descent as-is can already **recover models close to the ground truth**
➔ Main **challenge:** neighboring solutions in **coefficient space** may not produce similar output
➔ **Reparametrization** of discrete-continuous search space would **improve convergence**

Get the paper!

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[1] Poster based on: J. N. Kreikemeyer, P. Andelfinger, and A. M. Uhrmacher. 2024. Towards Learning Stochastic Population Models by Gradient Descent. In Proceedings of the 38th ACM SIGSIM Conference on Principles of Advanced Discrete Simulation (SIGSIM-PADS '24). ACM, New York, NY, USA, 88–92.
[2] Gradient Estimator based on: Y. Nesterov, V. Spokoiny. 2017. Random Gradient-Free Minimization of Convex Functions. Found Comput Math17, 527–566.

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