Potsdam Institute for
Climate Impact Research

Leibniz
Association

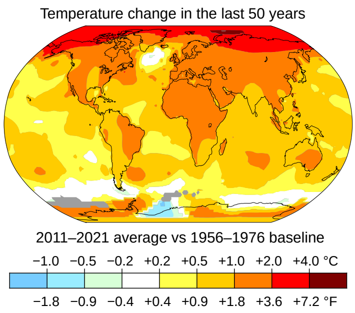
Nonparametric Estimation of Ordinary Differential Equations

Christof Schötz

PIK Future Lab: AI in the Anthropocene

March 9, 2023
German Probability and Statistics Days, Essen

- **Weather** and **climate** models



Source: Wikimedia

- **Weather** and **climate** models
- Classical physics-driven models: numerically solve Navier–Stokes partial **differential equations**

Navier–Stokes

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} - \nu \nabla^2 \mathbf{u} = -\frac{1}{\rho} \nabla p + \mathbf{g}$$

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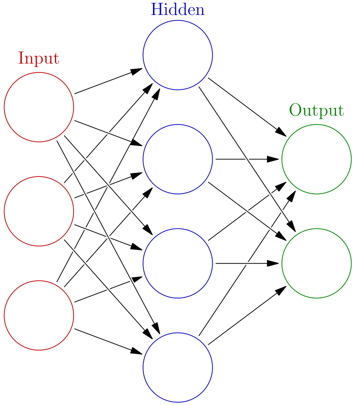
- New data-driven models: train **neural network** on weather observations



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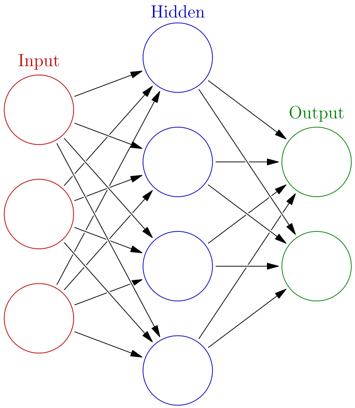
  Neural network as **nonparametric** estimator



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- **Theory** (convergence rates) of
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$$\left\|\hat{f}(x) - f(x)\right\| = \mathbf{O}_p\left(n^{-\frac{2\beta}{2\beta+d}}\right)$$

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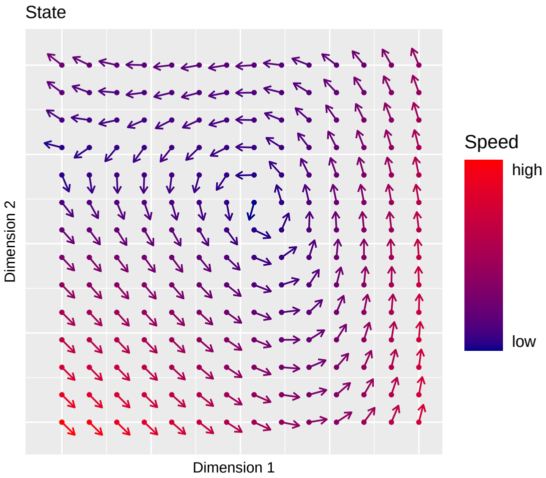
  Neural network as **nonparametric** estimator
- **Theory** (convergence rates) of
  nonparametric differential equation estimation?
- Start simple:
  Autonomous first-order deterministic
  ordinary differential equation (ODE)
  with measurement noise

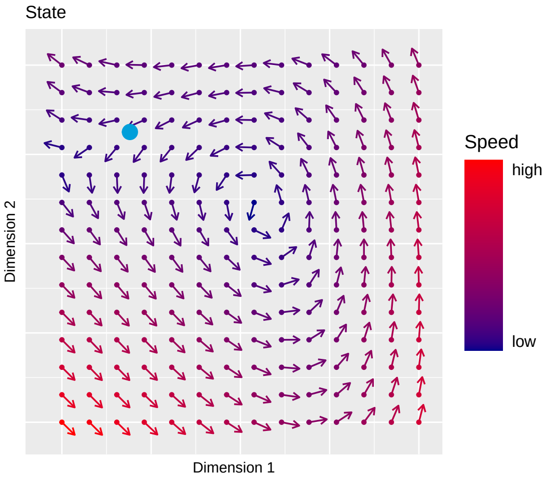
$$\dot{u} = f(u)$$

$$Y_i = u(t_i) + \epsilon_i$$

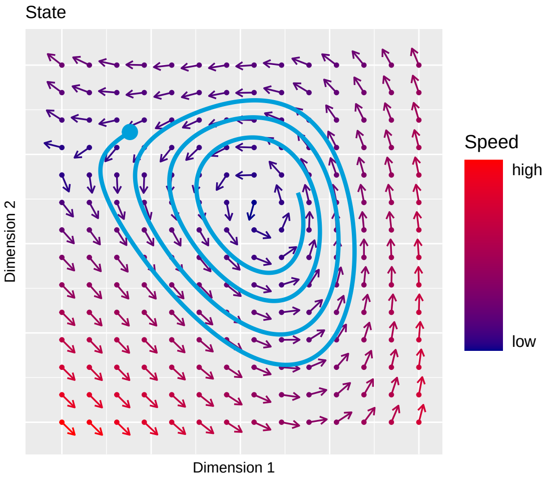
$f : \mathbb{R}^d \to \mathbb{R}^d$



$f : \mathbb{R}^d \to \mathbb{R}^d$ $u_0 \in \mathbb{R}^d$



$f \colon \mathbb{R}^d \to \mathbb{R}^d$ $\qquad$ $u_0 \in \mathbb{R}^d$ $\qquad$ $T > 0$ $\qquad$ $u \colon [0, T] \to \mathbb{R}^d,\ \dot{u}(t) = f(u(t)),\ u(0) = u_0$



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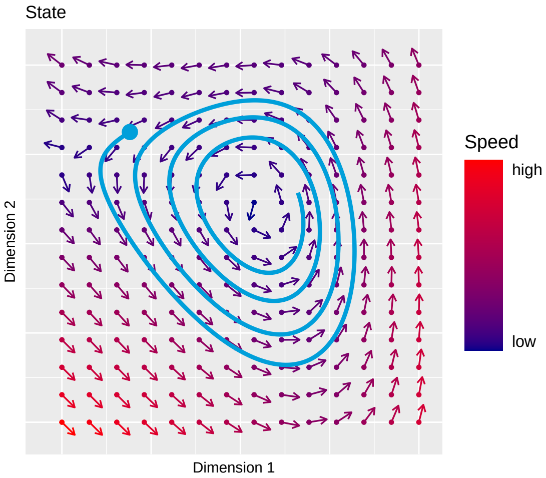

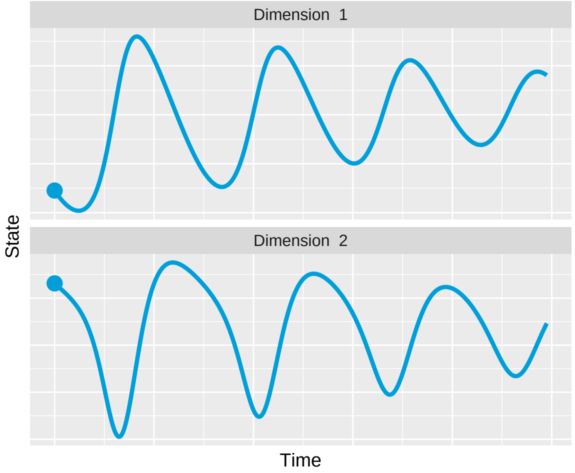

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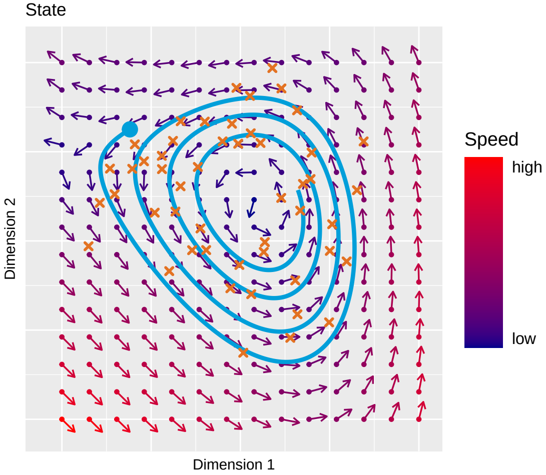
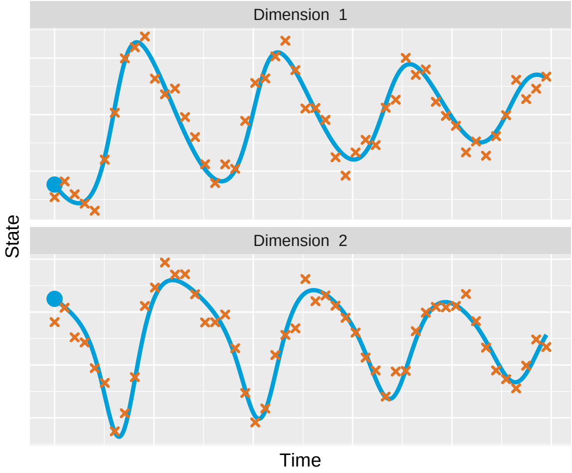
For $i = 1, \dots, n:$ $\quad t_i = T/n$ $\quad Y_i = u(t_i) + \epsilon_i$ $\quad \epsilon_i \overset{iid}{\sim} \mathcal{N}(0, \sigma^2 I_d)$





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- **Nonparametric approaches** without rate of convergence:
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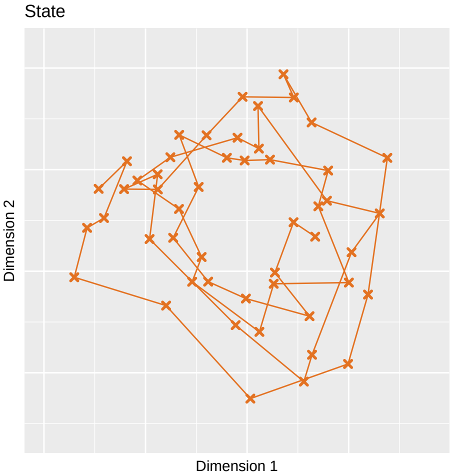
- **Goal:** Upper bound assuming $f\colon \mathbb{R}^d \to \mathbb{R}^d$ is β-times continuously differentiable:

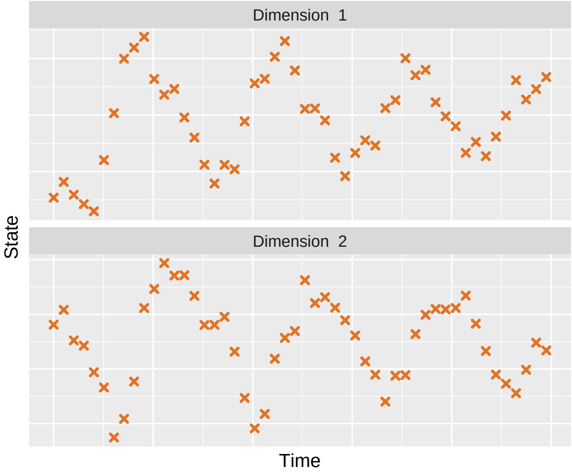
$$\left\| \hat{f}(x) - f(x) \right\| = \mathbf{O}_p\left(n^{-\alpha}\right)$$

$$\alpha = ?$$

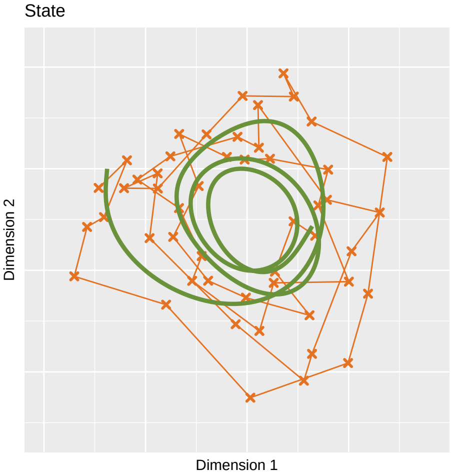
Ansatz 1:
Snake Model and Trajectory Estimation

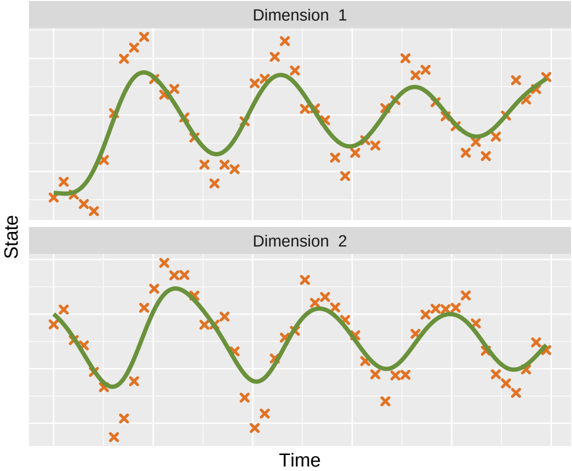
Observations $(Y_i, t_i)_{i=1,\dots,n}$



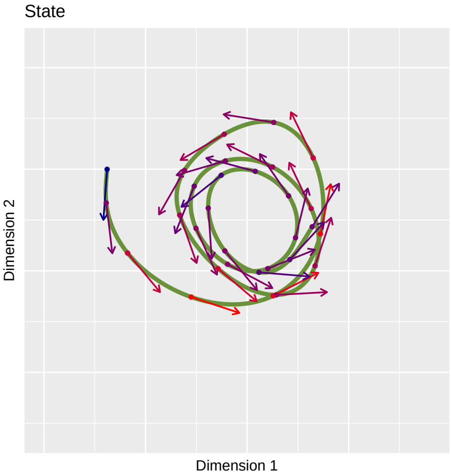


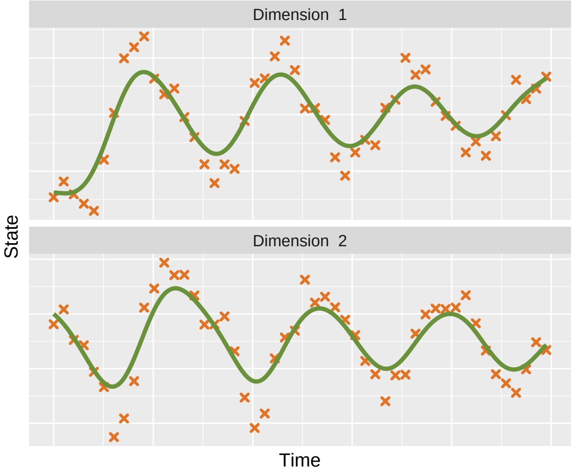
Nonparametric time–state regression, e.g., local linear $\Longrightarrow \hat{u}$



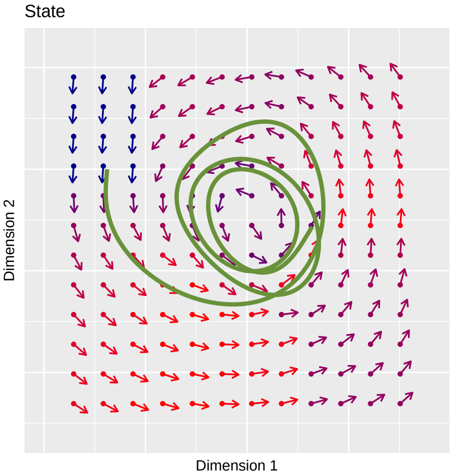


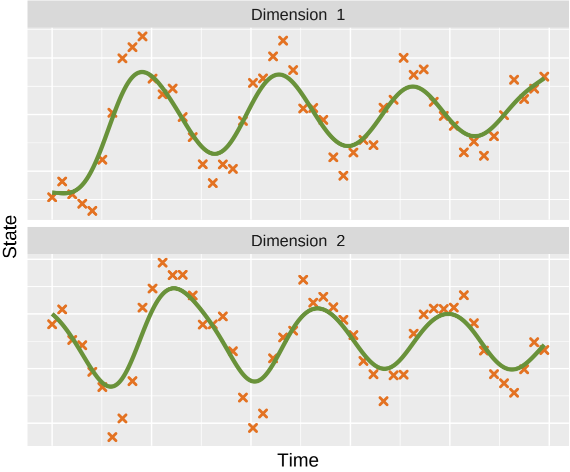
Nonparametric time–state regression, e.g., local linear with **derivative** $\Longrightarrow (\hat{u}, \hat{\dot{u}})$





$(\hat{u}, \hat{\dot{u}}) \Longrightarrow$ nearest neighbor **interpolation** $\Longrightarrow \hat{f}$





Theorem

Let

- $\hat{f}$: *trajectory estimation*
- $\delta \geq 0$

Assume f *is* $(\beta = 1)$*–smooth.*
Then

$$\sup_{x \in \mathrm{B}_\delta(u([0,T]))} \left\| \hat{f}(x) - f(x) \right\| = \mathbf{O}_p\left(\delta + T^{\frac{1}{5}} \left(\frac{n}{\log n} \right)^{-\frac{1}{5}} \right)$$

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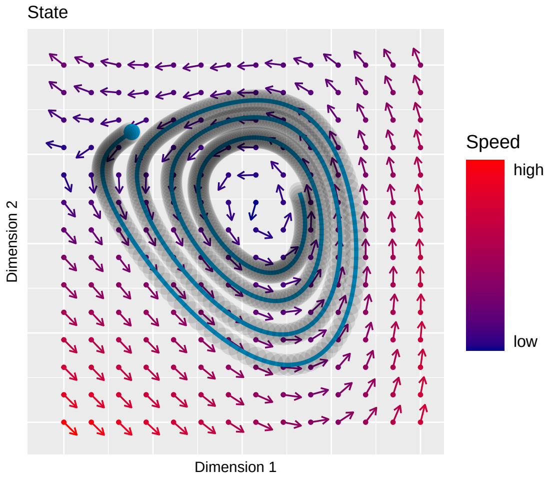

Corollary (Optimal Trade-Off)

Let $\delta := \sup_{x\in[0,1]^d} \inf_{t\in[0,T]} \|u(t) - x\|$.
Assume

- f *is* $(\beta = 1)$*-smooth*
- $T = \mathbf{O}\left(\left(\frac{n}{\log n}\right)^{\frac{d-1}{4+d}}\right)$
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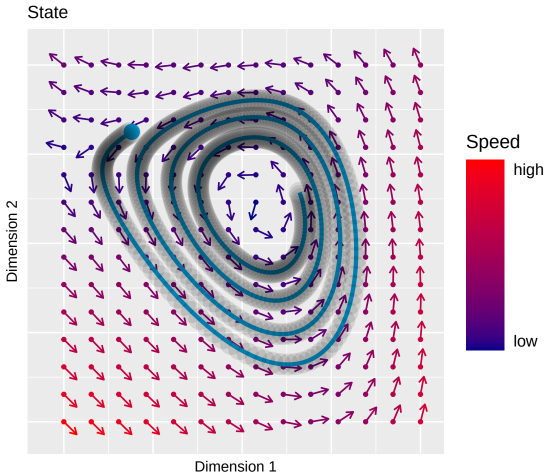

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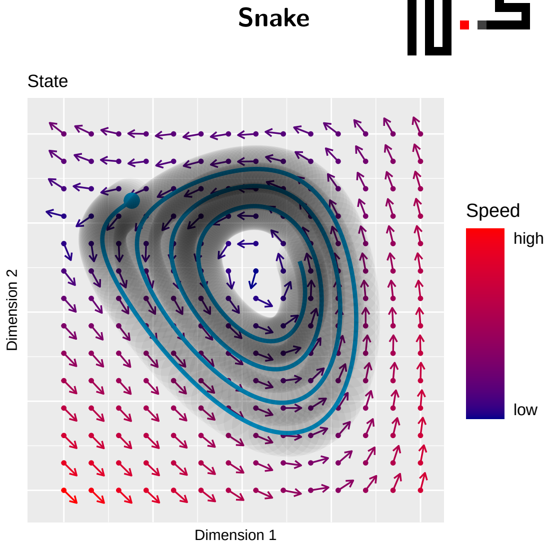

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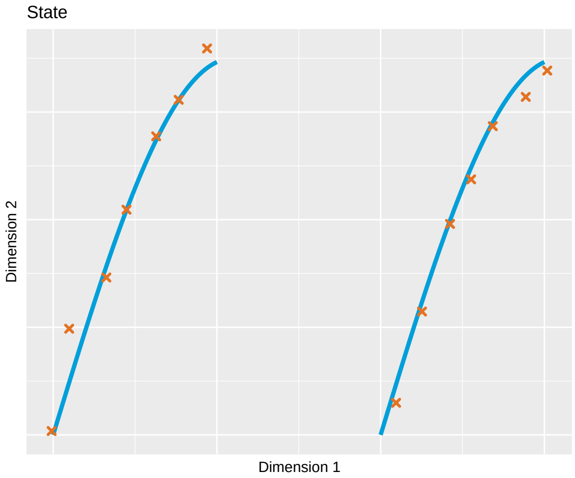

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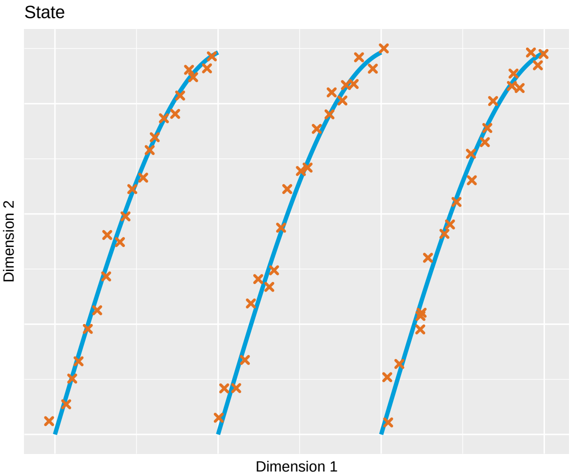

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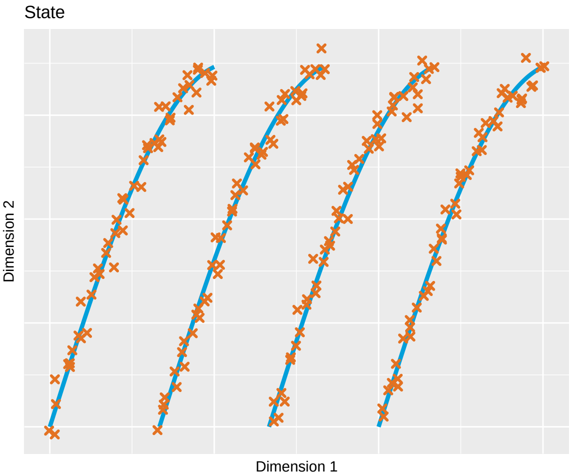

Generalization to arbitrary $\beta \in \mathbb{N}$

Theorem

Let $\hat{f}$ be trajectory estimation with rate-optimal nonparametric estimator + polynomial interpolation. Assume

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- Same rate as estimating derivative ($r = 1$) of ($b = \beta + 1$)-smooth regression function $g \colon \mathbb{R}^d \to \mathbb{R}$

$$\left\| \hat{g}^{(r)}(x) - g^{(r)}(x) \right\| = \mathbf{O}_p\left(n^{-\frac{b-r}{2b+d}}\right)$$

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- Awkward assumption for best rate
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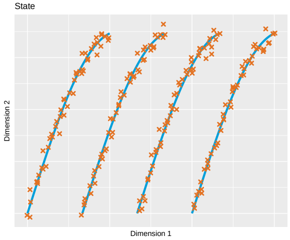
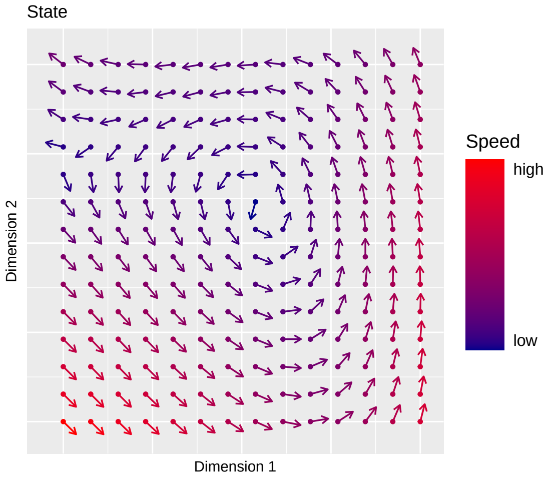
- State smoothness is ignored



Ansatz 2:
Stubble Model and Increment Estimation

Stubble Model:

- Let $U(f, x, t)$ solve $\dot{u} = f(u), u(0) = x$
- Grid $x_i \in [0,1]^d$, $i = 1, \ldots, n$
- Step size $s > 0$
- Observation $Y_i = U(f, x_i, s) + \epsilon_i$



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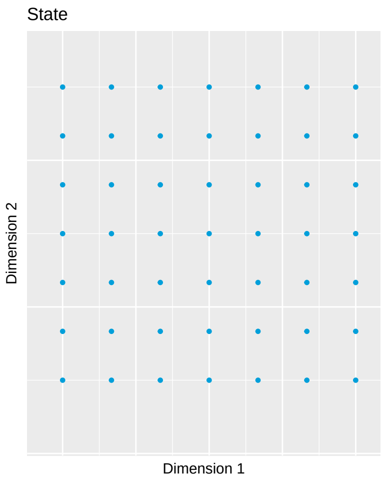

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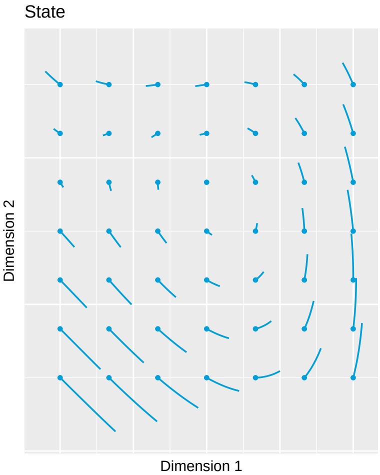

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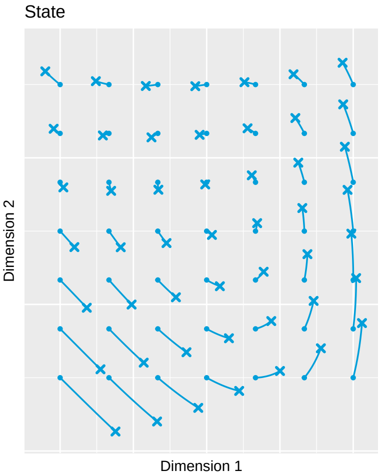

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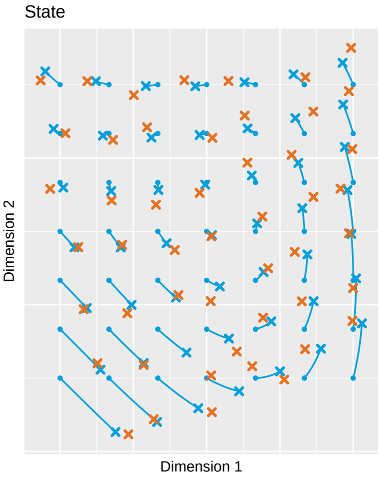

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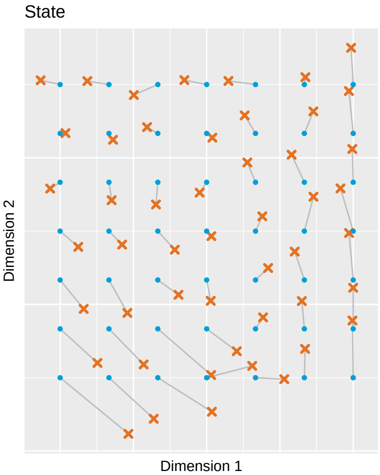
Increment Estimation:

- Estimate Increment $x \mapsto U(f, x, s) - x$
- Nadaraya–Watson estimator $\hat{\imath} \colon \mathbb{R}^d \to \mathbb{R}^d$ on data $(Y_i - x_i,\ x_i)_{i=1,\ldots,n}$

Stubble



Stubble Model:

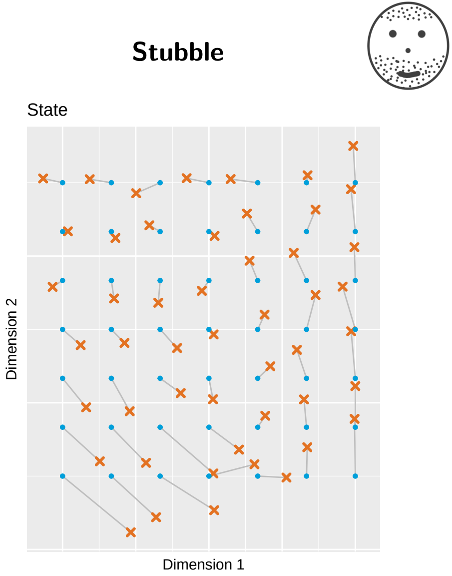
- Let $U(f, x, t)$ solve $\dot{u} = f(u), u(0) = x$
- Grid $x_i \in [0, 1]^d$, $i = 1, \dots, n$
- Step size $s > 0$
- Observation $Y_i = U(f, x_i, s) + \epsilon_i$

Increment Estimation:

- Estimate Increment $x \mapsto U(f, x, s) - x$
- Nadaraya–Watson estimator $\hat{\iota}\colon \mathbb{R}^d \to \mathbb{R}^d$ on data $(Y_i - x_i,\ x_i)_{i=1,\dots,n}$

Scaled Increment Estimator of f:

$$\hat{f}(x) := \frac{1}{s}\hat{\iota}(x)$$



Theorem

Assume f *is* $(\beta = 1)$*-smooth.*
Then, for $x_0 \in [0,1]^d$,

$$\left\| \hat{f}(x_0) - f(x_0) \right\| = \mathbf{O}_p\left(s + s^{-\frac{2}{2+d}} n^{-\frac{1}{2+d}} \right) .$$

Corollary

Assume

- f *is* $(\beta = 1)$*-smooth*
- $s = \mathbf{O}\left(n^{-\frac{1}{4+d}} \right)$

Then, for $x_0 \in [0,1]^d$,

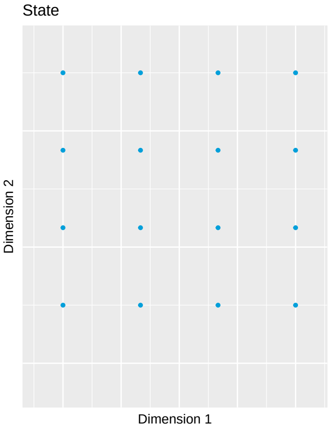
$$\left\| \hat{f}(x_0) - f(x_0) \right\| = \mathbf{O}_p\left(n^{-\frac{1}{4+d}} \right) .$$

Generalization to arbitrary $\beta \in \mathbb{N}$

- Observe β points at for each x_i,

$$Y_{i,j} = U(f, x_i, js) + \epsilon_{i,j}$$

$i = 1, .., n, j = 1, .., \beta$



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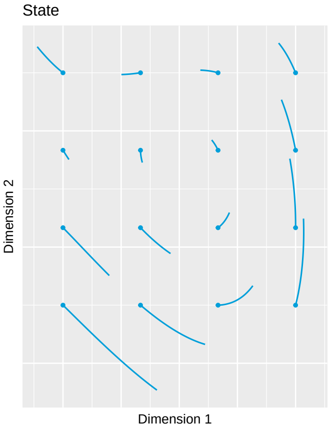

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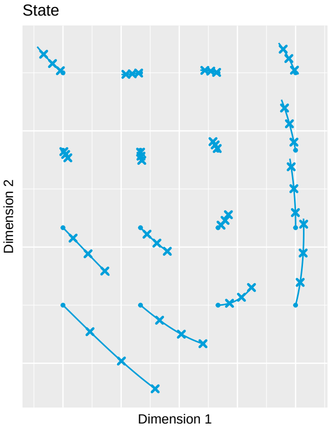

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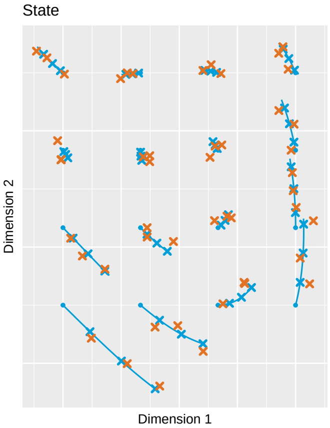

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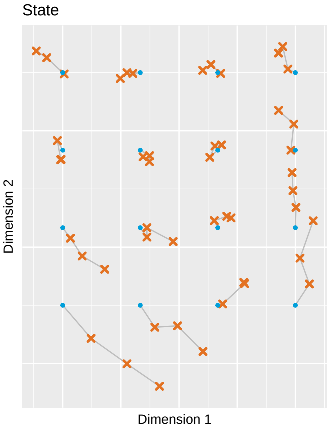

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- For each $j = 1, .., \beta$:
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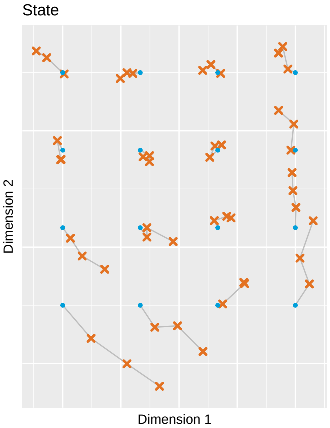

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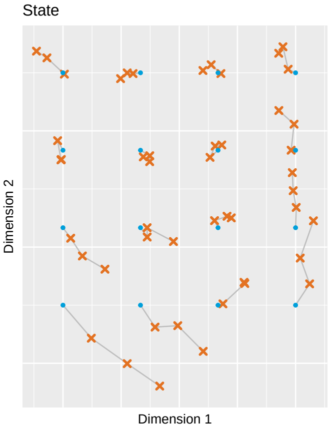

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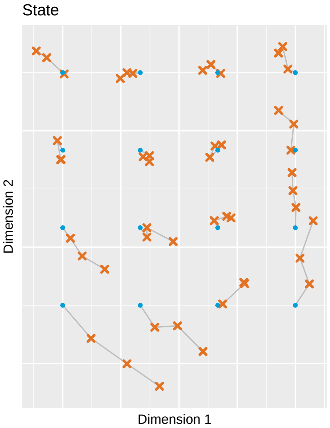

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Theorem

Assume

- f *is* β*-smooth*
- $s = \mathbf{O}\left(n^{-\frac{1}{2(\beta+1)+d}}\right)$

Then, for $x_0 \in [0, 1]^d$,

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Conclusion

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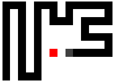
Snake 

- few long trajectories
- cover area of interest by trajectory
- estimate trajectory (time $\rightarrow$ state)
- interpolate in state space (state $\rightarrow$ state)

Stubble 

- many short trajectories
- cover area of interest by initial conditions
- estimate increments (state $\rightarrow$ state)
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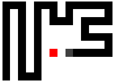
$$\left\| \hat{f}(x) - f(x) \right\| = \mathbf{O}_p\left(n^{-\frac{\beta}{2(\beta+1)+d}} \right)$$

Conclusion

Snake



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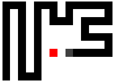
Conjecture: This is the Minimax-Rate for β-Hölder smooth f.

Snake 

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Thanks!

Slides: https://github.com/chroetz/GPSD23slides/

Chen, R. T. Q., Y. Rubanova, J. Bettencourt, and D. Duvenaud (2018). "Neural Ordinary Differential Equations". In: *Proceedings of the 32nd International Conference on Neural Information Processing Systems*. NIPS'18. Montréal, Canada: Curran Associates Inc., pp. 6572–6583.

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