Global Optimization over Compact Domains

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Joint work with Mohab Safey El Din and Emmanuel Trélat
Ongoing work with Alexander Demin

Partially supported by Grant FA8665-20-1-7029 of the EOARD-AFOSR

October 24, 2025

MAX PLANCK INSTITUTE
OF MOLECULAR CELL BIOLOGY
AND GENETICS

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$$\text{Find all } x^\star \in \mathcal{C} \text{ s.t. } f(x^\star) \leq f(x) \text{ for all } x \text{ near } x^\star$$

Motivational Example: The Hölder Table Function

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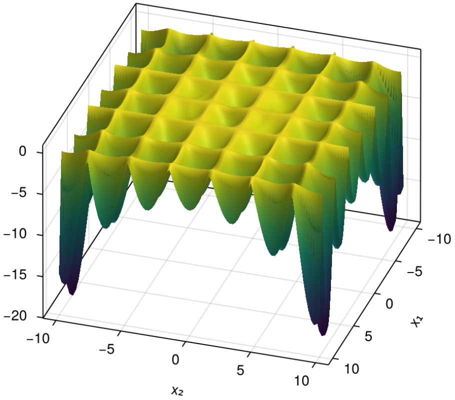

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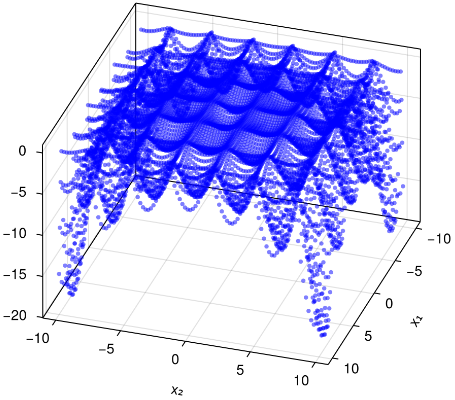

Critical Points Capture of The Hölder Table Function

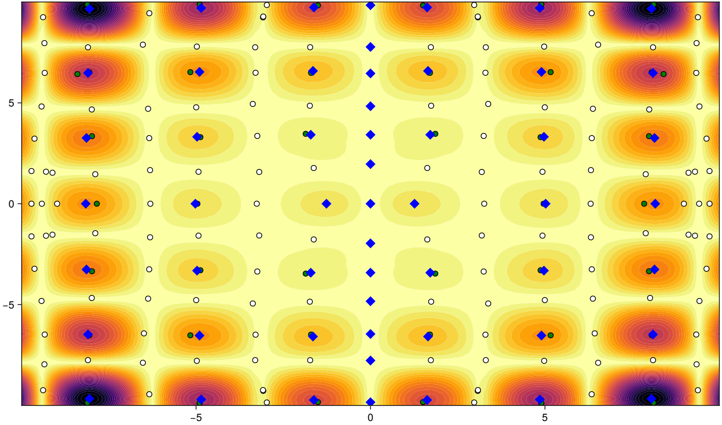

Figure: Level sets and critical points of $w_{18,\mathcal{S}}$

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- For $\lambda > 0$, $\rho > 0$ define

$$\mathscr{C}_{\lambda}^{m,\rho}(\mathcal{C}) = \{f \in \mathscr{M}^m(\mathcal{C}) \mid \min \operatorname{spec}(f) \geq \lambda, \max_{x \in \mathcal{C}} \|d^j f(x)\| \leq \rho, j \leq m\}$$

where $\mathscr{M}^m(\mathcal{C})$ = m-times diff. Morse functions on $\mathcal{C}$

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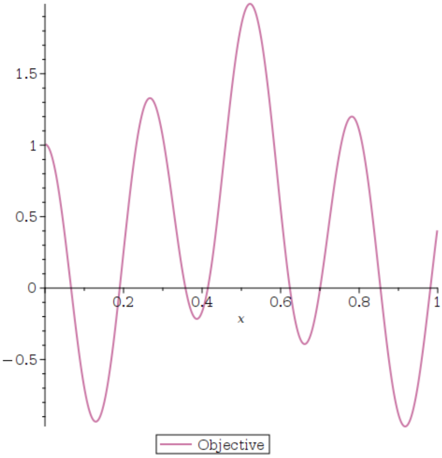
   - Initiate local optimization methods at the computed points

L^∞ vs L^2 Polynomial Approximant



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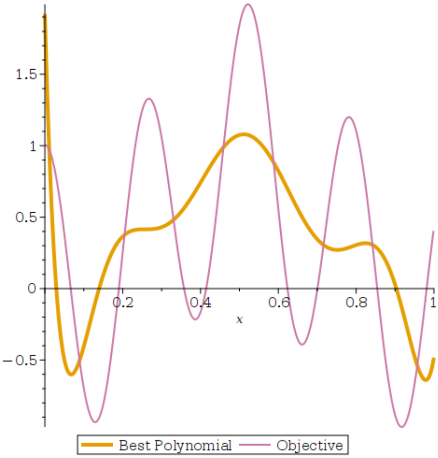

$$\| f \|_{\mathcal{L}^\infty} = \max_{x \in \mathcal{C}} |f(x)|. \quad (1)$$

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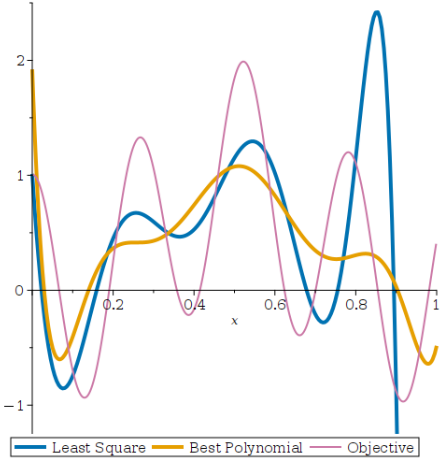

$$\| f \|_{\mathcal{L}^2} = \left(\int_{\mathcal{C}} f(x)^2 \mathrm{d}\mu \right)^{\frac{1}{2}} . \tag{2}$$

Chebyshev Polynomials

[1] Keaton J. Burns et al. "Dedalus: A flexible framework for numerical simulations with spectral methods". *Phys. Rev. Res.* 2 (2 Apr. 2020), p. 023068. DOI: 10.1103/PhysRevResearch.2.023068. URL: https://link.aps.org/doi/10.1103/PhysRevResearch.2.023068.

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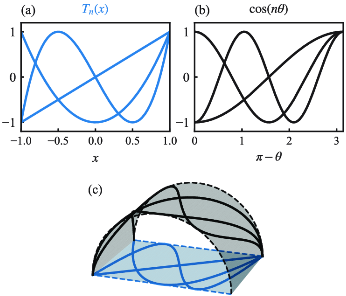

Figure: Dedalus[1]

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$$\int_{\mathcal{C}} T_m(x) T_n(x) \mathrm{d}\mu = \gamma_n \delta_{mn}$$

where $\gamma_n > 0$

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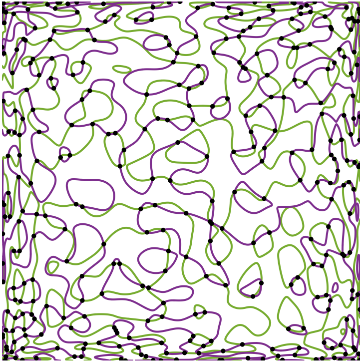

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Let $f \in \mathscr{C}_{\lambda}^{m,\rho}(\mathcal{C})$ with $m \geq \max(3, \beta n + 1)$, where $\beta = \frac{\ln(3)}{2\ln(2)}$.
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Constants dependency:

- A_1: dimension n, smoothness m, regularity ρ, parameter δ
- A_2: dimension n, parameter δ

Probabilistic Least Squares Polynomials

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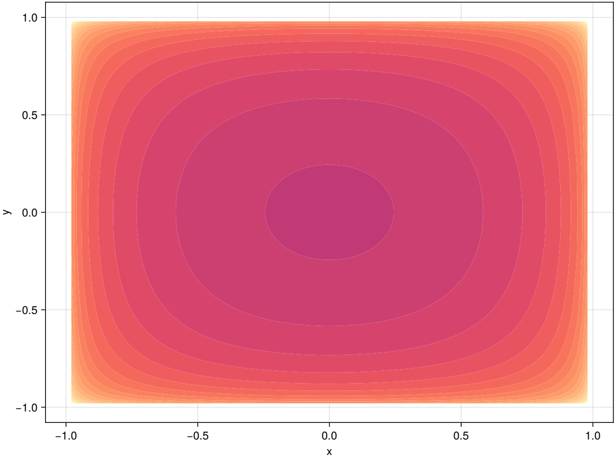

Figure: probability density of μ.

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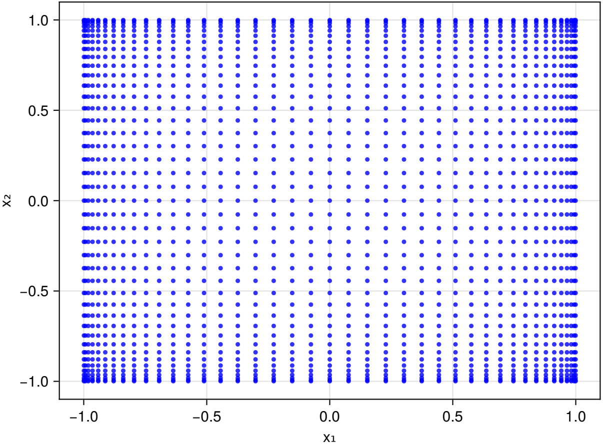

Figure: Discretization of μ.

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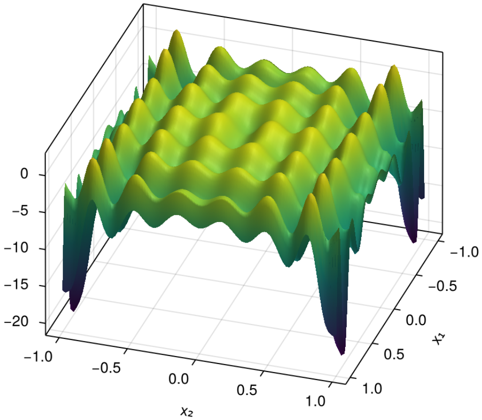

Figure: w_{18}

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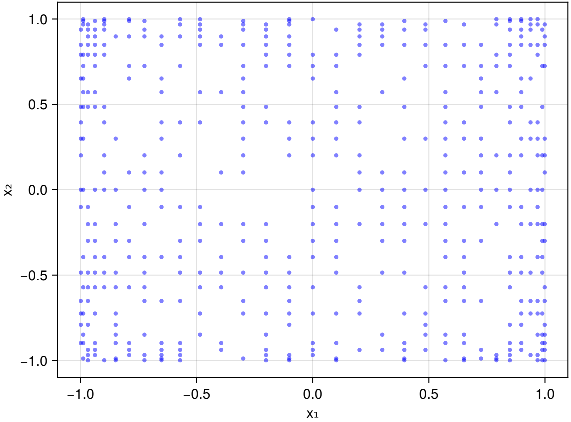

Figure: reduced sample set $\mathcal{S}$.

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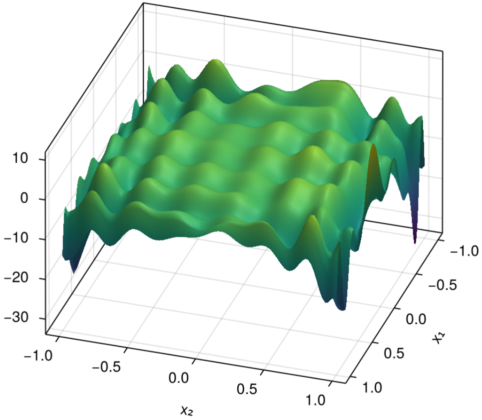

Figure: $w_{18,\mathcal{S}}$.

Probabilistic Bounds

[2] Giovanni Migliorati, Fabio Nobile, and Raúl Tempone. "Convergence estimates in probability and in expectation for discrete least-squares with noisy evaluations at random points". *Journal of Multivariate Analysis* 142 (2015), pp. 167–182. ISSN: 0047-259X. DOI: https://doi.org/10.1016/j.jmva.2015.08.009. URL: https://www.sciencedirect.com/science/article/pii/S0047259X15001931.

Probabilistic Bounds

Theorem:[2] if the number of samples k satisfies

$$\frac{\binom{n+d}{n}^{\frac{\ln(3)}{2\ln(2)}}}{\delta + (1-\delta)\ln(1-\delta)} \leq \frac{k}{\ln(k) + \ln(6\alpha^{-1})}, \tag{3}$$

then with probability at least $1-\alpha$, we have

$$\| w_{d,\mathcal{S}} - f \|^2_{\mathcal{L}^2} \leq \left(1 + \frac{C(\delta)}{\alpha \ln(6k\alpha^{-1})}\right) e_d(f)^2, \tag{4}$$

where

$$C(\delta) = \frac{4\left(\delta + (1-\delta)\ln(1-\delta)\right)}{(1-\delta)^2}, \tag{5}$$

[2] Giovanni Migliorati, Fabio Nobile, and Raúl Tempone. "Convergence estimates in probability and in expectation for discrete least-squares with noisy evaluations at random points". *Journal of Multivariate Analysis* 142 (2015), pp. 167–182. ISSN: 0047-259X. DOI: https://doi.org/10.1016/j.jmva.2015.08.009. URL: https://www.sciencedirect.com/science/article/pii/S0047259X15001931.

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Convergence in L^2

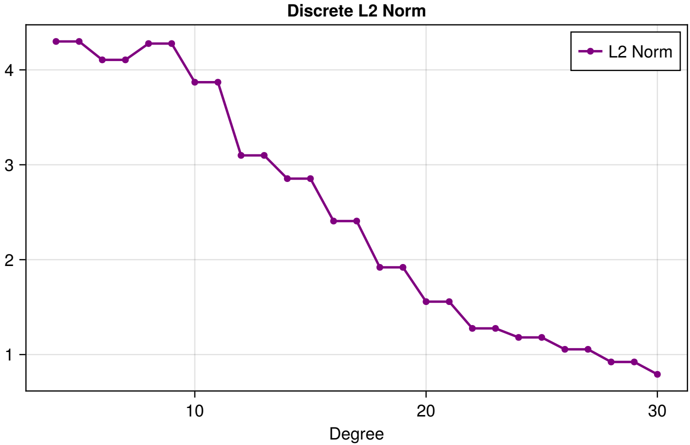

Figure: Error in $\mathcal{L}^2$-norm of the approximant

Convergence of Local Minimizers

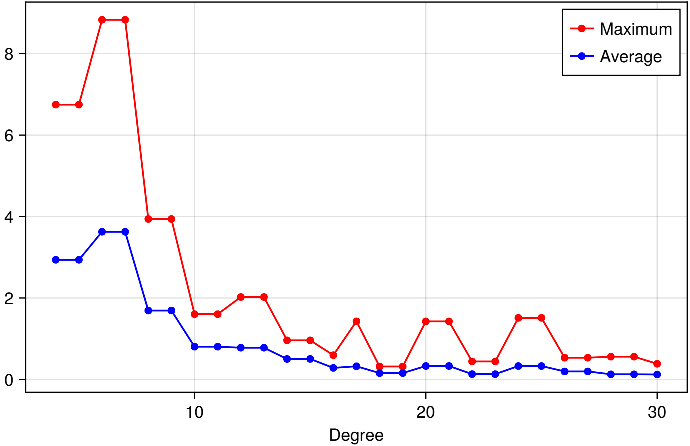

Figure: Distance from local minimizers to nearest critical point.

Tolerance to Noise

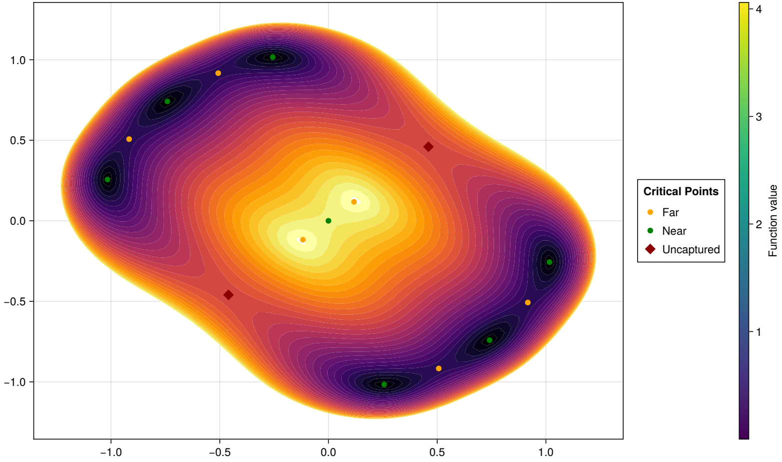

Figure: Deuflhard function

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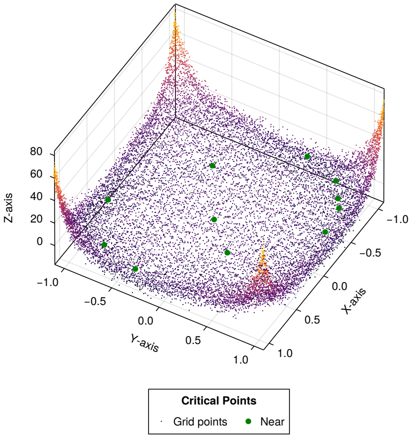

Figure: Noisy Deuflhard function

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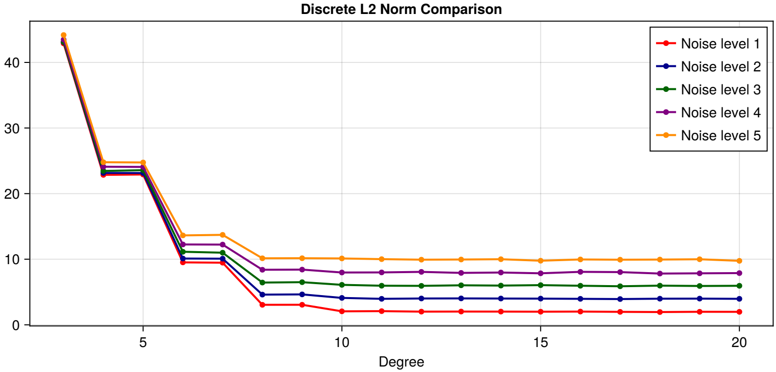

Figure: Noisy Deuflhard L2-norm approximation

Tolerance to Noise

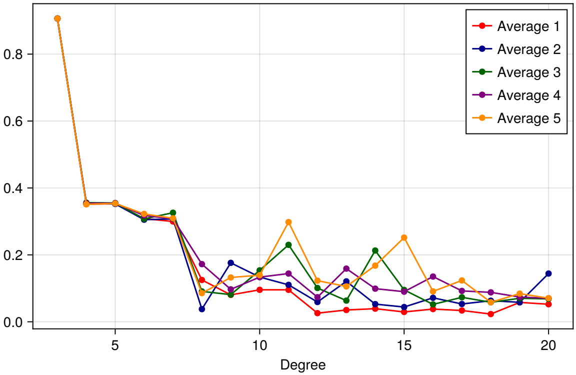

Figure: Noisy Deuflhard convergence of critical points

3D Function Example

$$f(x, y, z) = e^{\sin(50x_1)} + \sin(60e^{x_2})\sin(60x_3) + \sin(70\sin(x_1))\cos(10x_3) + \sin(\sin(80x_2)) - \sin(10(x_1 + x_3)) + \frac{x_1^2 + x_2^2 + x_3^2}{4} \quad (6)$$

ODE System: Parameter Estimation Problem

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Given data: $D = ((t_1, \boldsymbol{y}_1), \ldots, (t_n, \boldsymbol{y}_n))$, where $\boldsymbol{y}_i$ is measured at time t_i

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$$f(\boldsymbol{\mu}) = \sum_{i=1}^{N} \left(\boldsymbol{y}(t_i; \boldsymbol{\mu}) - \boldsymbol{y}_{\text{target}}(t_i) \right)^2$$

where $\boldsymbol{y}(t_i; \boldsymbol{\mu})$ is the computed response at time t_i for parameters $\boldsymbol{\mu}$, and $\boldsymbol{y}_{\text{target}}(t_i)$ is the target response.

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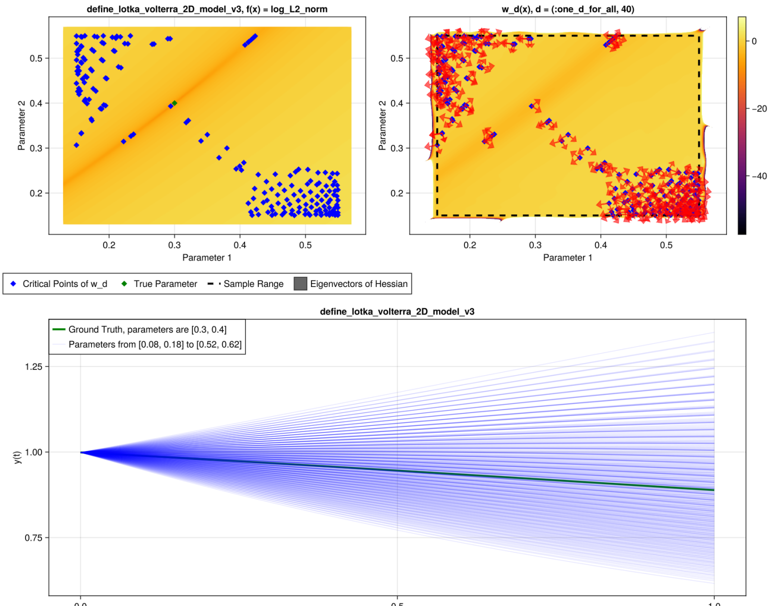
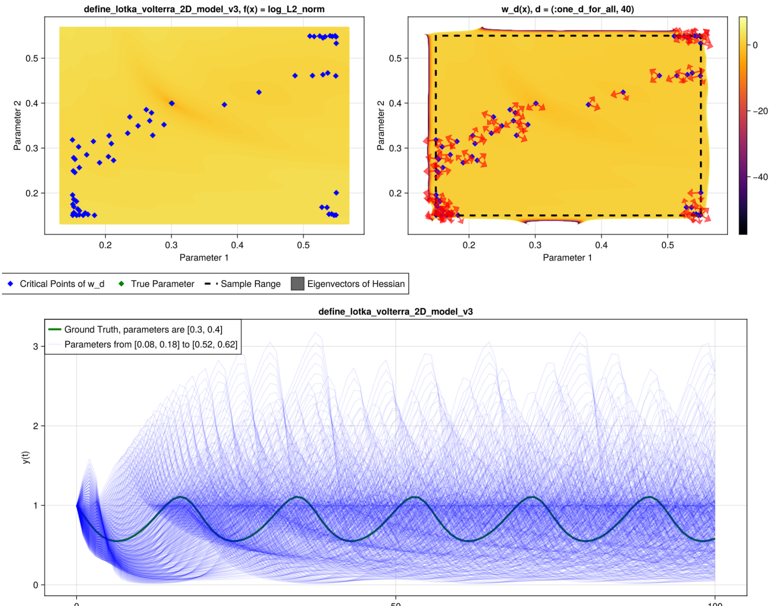
The recovered critical points serve as initial guesses for local optimization methods.

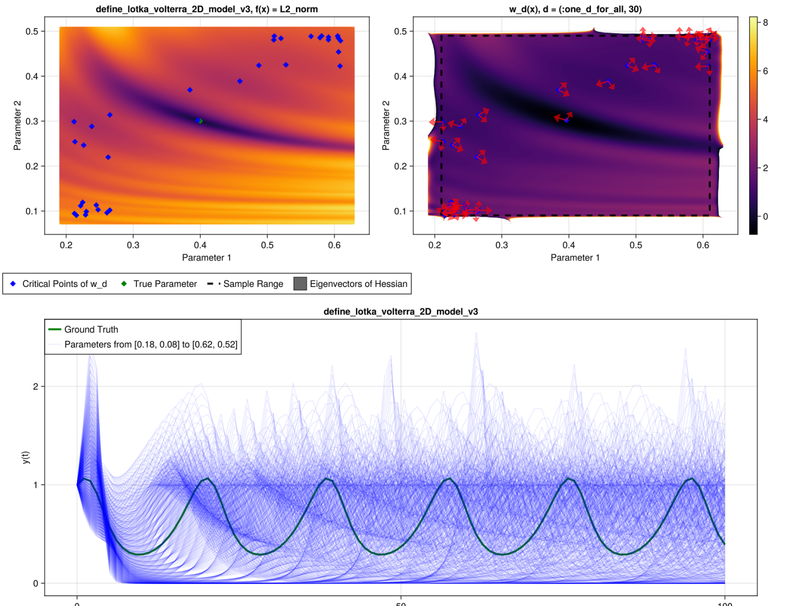
Parameter Estimation Lotka-Volterra: (t=1)



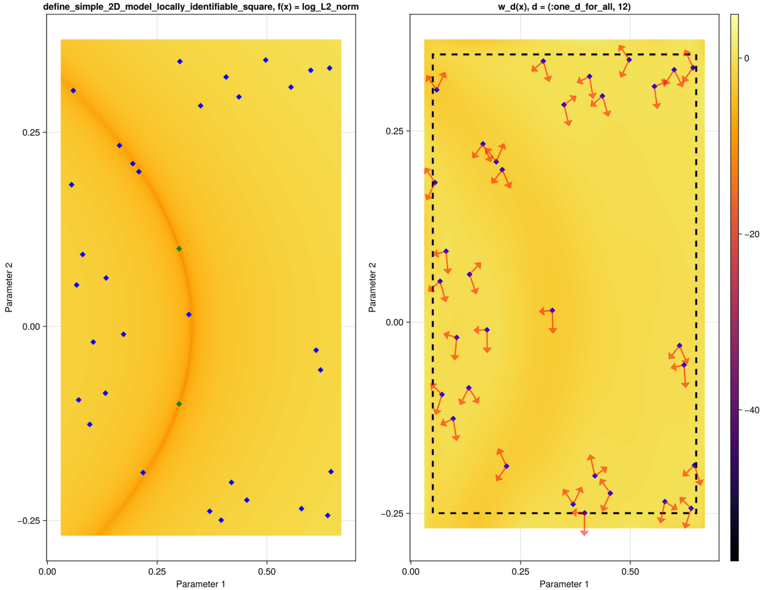
Parameter Estimation Lotka-Volterra (t=100)



Parameter Estimation Lotka-Volterra (t=100)



Locally Identifiable Model



Thank You! I

- Matthieu Dolbeault, David Krieg, and Mario Ullrich. "A sharp upper bound for sampling numbers in $\mathcal{L}^2$". *Applied and Computational Harmonic Analysis* 63 (2023), pp. 113–134. ISSN: 1063-5203. DOI: https://doi.org/10.1016/j.acha.2022.12.001. URL: https://www.sciencedirect.com/science/article/pii/S1063520322000999
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- Mohab Safey El Din, Georgy Scholten, and Emmanuel Trélat. "Probabilistic algorithm for computing all local minimizers of Morse functions on a compact domain". working paper or preprint. 2025. URL: https://hal.sorbonne-universite.fr/hal-05160251