

Optimal Control and Decision Making Under Uncertainty for Digital twins





Krithika Manohar Mechanical Engineering

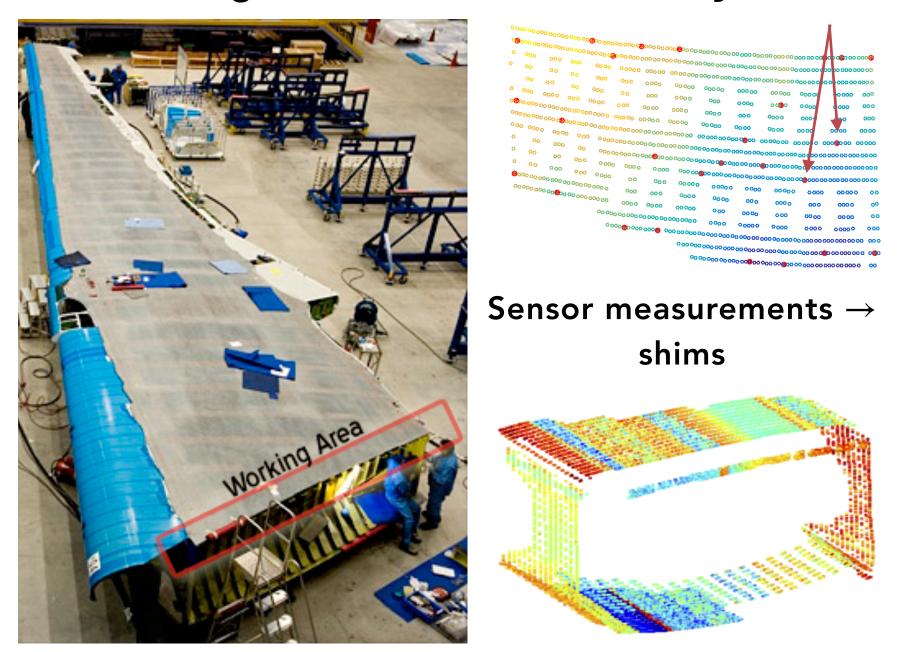


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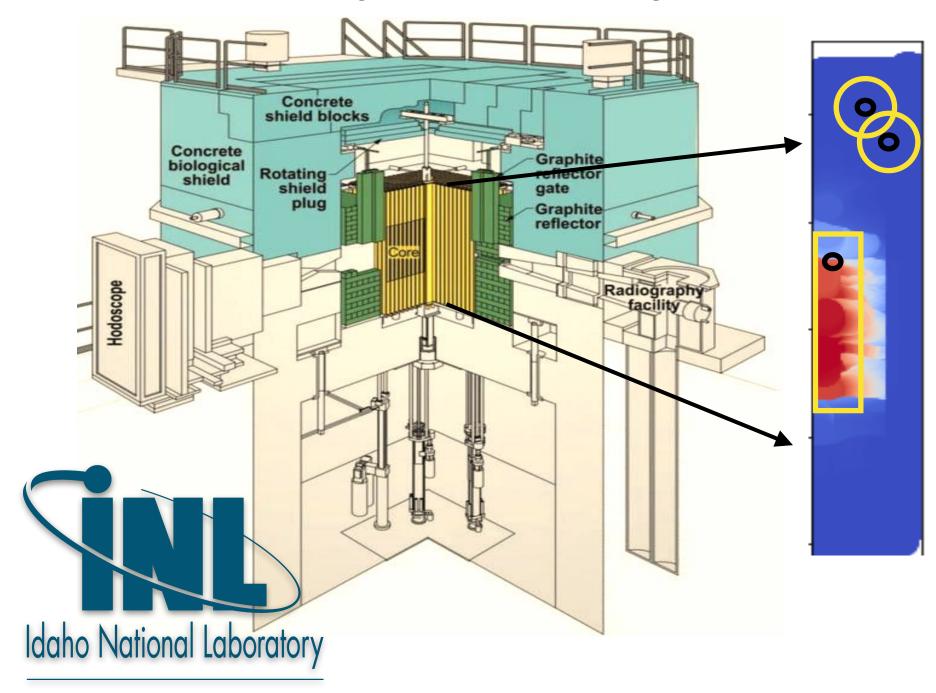
Data-Driven Sensing

- Data-driven sensor placement optimization
 - Choice of measurements crucial for real-time estimation and control
 - Physical resources with placement constraints and deployment cost
 - Uncertainty quantification, interpretability

Large-scale aircraft assembly

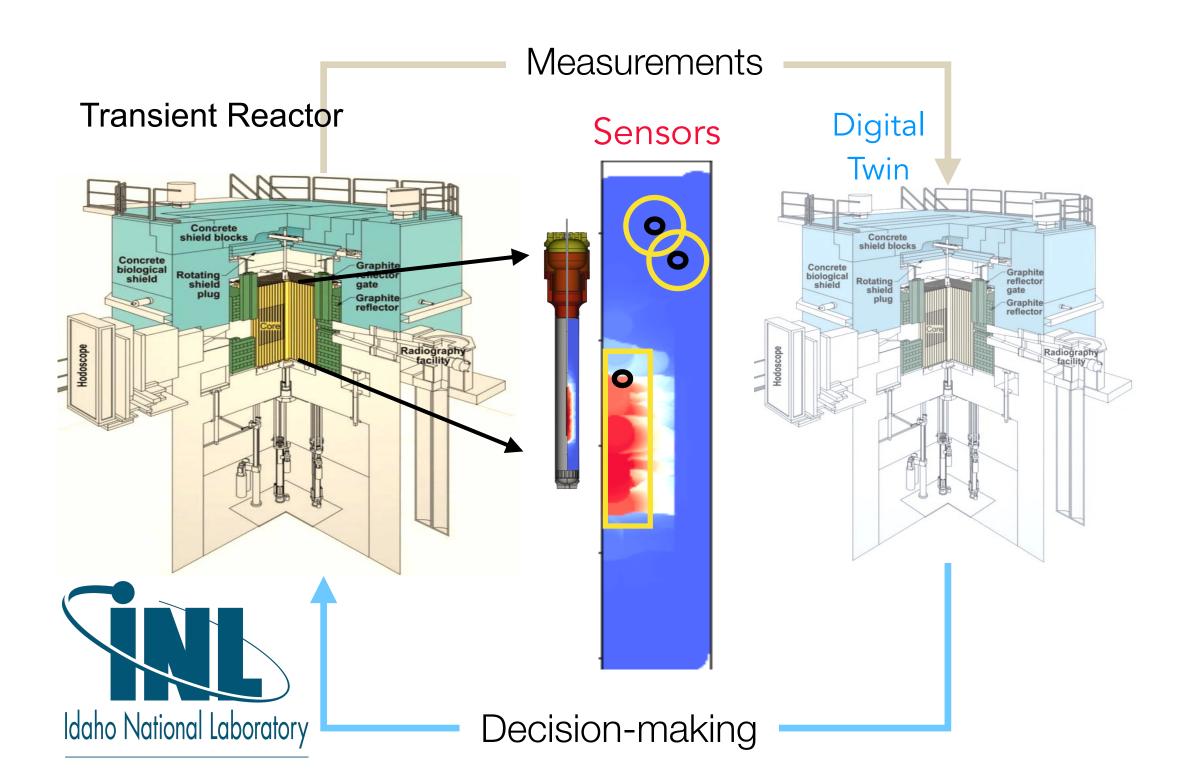


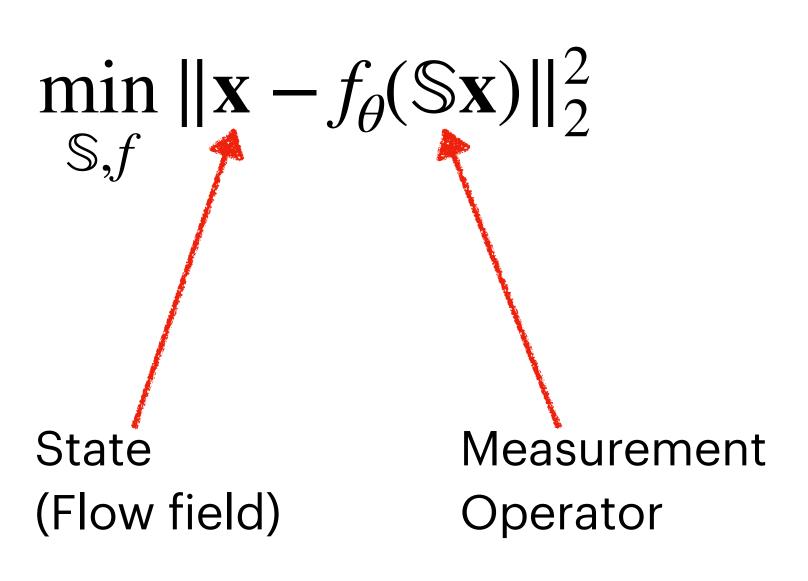
Sparse Sensing in Nuclear Energy Systems



Core challenges

- Detect, characterize sensor failure/perturbation
- Model discrepancy between virtual & physical spaces
- Uncertainty quantification- expected performance
- Interpretability- non convex, non differentiable optimization landscape



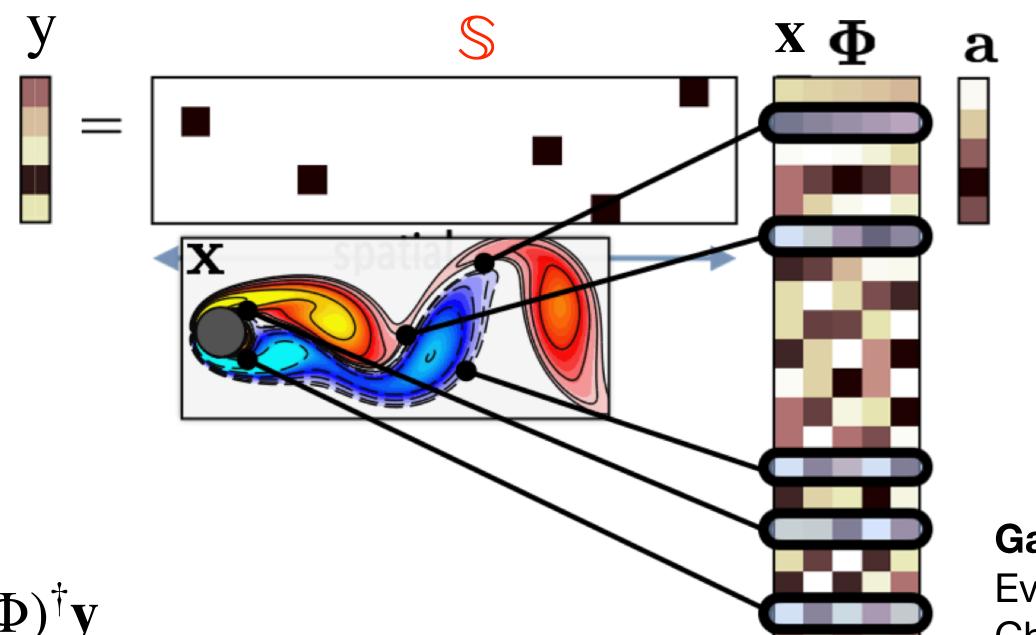


Sparse sensor allocation in nuclear reactors

Problem setting

Sensor measurements $\mathbf{y} = \mathbf{S}\mathbf{x} + \boldsymbol{\xi}$

Represent state in a low-dimensional basis $\mathbf{x} pprox \Phi \mathbf{a}$



Reconstruction $\hat{\mathbf{x}} = \Phi(\mathbb{S}\Phi)^{\dagger}\mathbf{y}$

$$Var(\mathbf{a} - \hat{\mathbf{a}}) \propto det[(\mathbb{S}\Phi_r)^T \mathbb{S}\Phi_r]^{-1}$$

 $\mathbf{x} \in \mathbb{R}^n$ $\Phi \in \mathbb{R}^{n \times r}$ $\mathbb{S} \in \{0,1\}^{p \times r}$

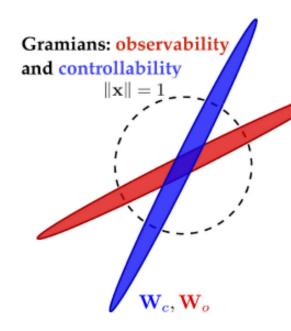
Gappy Reconstruction/Interpolation

Everson & Sirovich 1995 (gappy POD) Chaturantabut & Sorensen 2010 (DEIM) Manohar, Brunton, Kutz, Brunton 2018 Manohar, Kutz & Brunton, IEEE TAC 2021 Drmac & Gugercin 2016 (QDEIM)

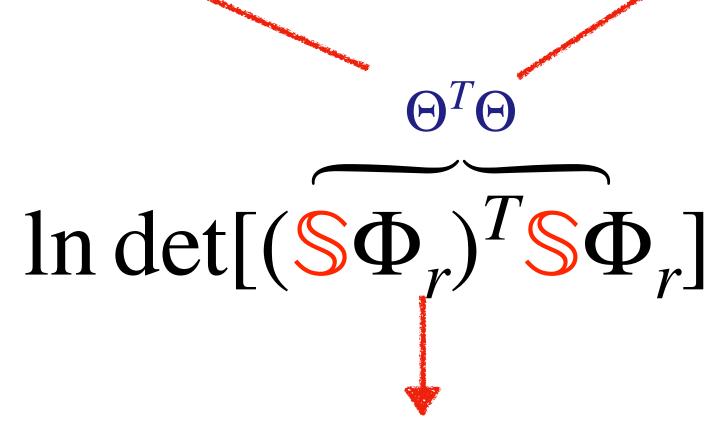
Objective function at a glance

$tr(\mathbf{\Theta}^T\mathbf{\Theta})$

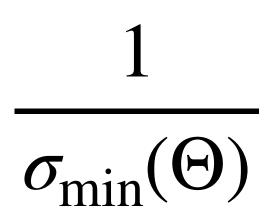
- ullet Observability, H_2 norm optimal
 - Chen & Rowley 2016
 - Manohar et al 2021



Measure	Formula	Geometry		
Generalized variance	$\det(\mathbf{\Sigma}) = \Pi_i \lambda_i$	area, (hyper)volume		
Average variance	$\operatorname{tr}(\mathbf{\Sigma}) = \sum_{i} \lambda_{i}$	linear sum		
Maximal variance	$\lambda_{ m max}$	maximum dispersion		



- When submodular, greedy near-D-optimal
- Probabilistic view (max volume ellipsoid)
 - Joshi & Boyd 2016
 - Kakasenko, Alexanderian et al, arXiv 2025



- Empirical Interpolation $p \ge r$
- Drmac & Gugercin 2016
- Perherstofer et al 2020

Bayesian Inference Setting

Prior over modal coefficients

$$p(\mathbf{a}) = \exp\left(-\frac{1}{2}\mathbf{a}^T S^{-2}\mathbf{a}\right)$$

Likelihood

$$\ln p(\mathbf{y} \mid \mathbf{a}) = -\frac{1}{2\eta^2} (\mathbf{y} - \mathbf{\Theta}\mathbf{a})^T (\mathbf{y} - \mathbf{\Theta}\mathbf{a}) - \frac{1}{2}\mathbf{a}^T S^{-2}\mathbf{a}$$

MAP estimate

$$\mathbf{a} = \left(S^{-2} + \frac{\Theta^T \Theta}{\eta}\right)^{-1} \frac{\Theta^T \mathbf{y}}{\eta}$$





Andrei Klishin Nathan Kutz

D-optimal design

MAP estimate

$$\mathbf{a} = \left(S^{-2} + \frac{\mathbf{\Theta}^T \mathbf{\Theta}}{\eta}\right)^{-1} \frac{\mathbf{\Theta}^T \mathbf{y}}{\eta}$$

Hamiltonian of a given sensor set γ

$$\mathbf{a} = \left(\underbrace{S^{-2} + \frac{\Theta^T \Theta}{\eta}}^{\mathbf{O}^T \mathbf{O}} \right)^{-1} \frac{\Theta^T \mathbf{y}}{\eta}$$

$$\mathcal{H}(\gamma) \equiv -\ln \det A = E_b - \operatorname{tr} \ln \left(\mathbf{I} + \frac{\Theta S^2 \Theta^T}{\eta^2} \right)$$

Decompose into sums over 1pt, 2pt, s pt interactions:

$$\mathcal{H}(\gamma) = E_b - \operatorname{tr} \ln \left(\mathbf{I} + \frac{1}{\eta^2} (\mathbf{D} + \mathbf{R}) \right)$$

$$= E_b - \operatorname{tr} \ln (\mathbf{I} + \eta^{-1} \mathbf{D})$$

$$+ \sum_{s=1}^{\infty} \frac{(-1)^s}{s!} \operatorname{tr} \left(\left[\eta^{-2} \mathbf{R} (\mathbf{I} + \eta^{-2} \mathbf{D})^{-1} \right]^s \right)$$

Klishin, Kutz & KM (2023) arXiv:2307.11838

Two-point Energy Approximation

$$\mathcal{H}_{2pt}(\gamma) \equiv -\operatorname{tr} \ln(\mathbf{I} + \eta^{-2}\mathbf{D})$$
$$+ \frac{1}{2}\operatorname{tr}\left(\left[\eta^{-2}\mathbf{R}(\mathbf{I} + \eta^{-2}\mathbf{D})^{-1}\right]^{2}\right)$$

Express as dot products of sensing vectors (columns of measurement-basis product)

$$G \equiv \Theta S$$
 $\mathcal{H}_{2pt}(\gamma) \equiv \sum_i h_i + \sum_{i,j} J_{ij}$ Sensor 2-pt energy (crosstalk)

Sensor 1-pt energy

$$h_i = -\ln(1 + \mathbf{g}_i \cdot \mathbf{g}_i/\eta^2) \le 0$$

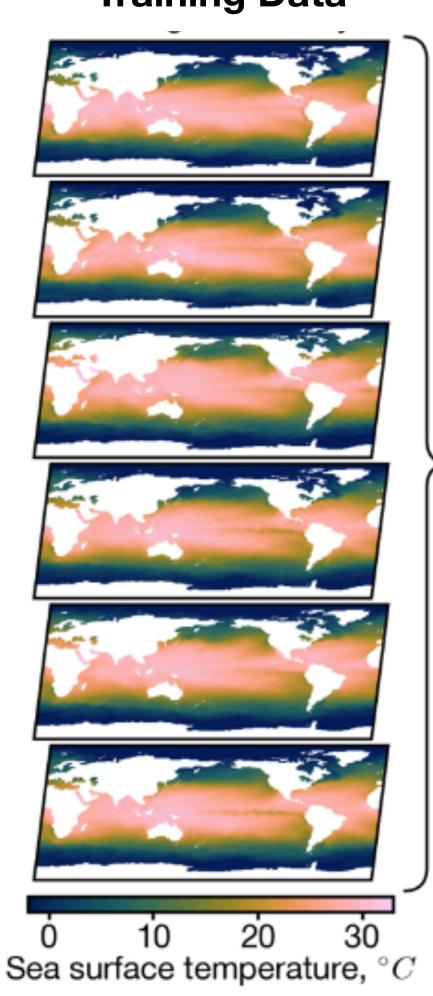
Attracted to high-variance locations

$$I_{ij} = \frac{(\mathbf{g}_i \cdot \mathbf{g}_j/\eta^2)^2}{\left(1 + \mathbf{g}_i \cdot \mathbf{g}_i/\eta^2\right)\left(1 + \mathbf{g}_j \cdot \mathbf{g}_j/\eta^2\right)} \ge 0$$

Repelled from correlated sensors

Two-point greedy sensor placement



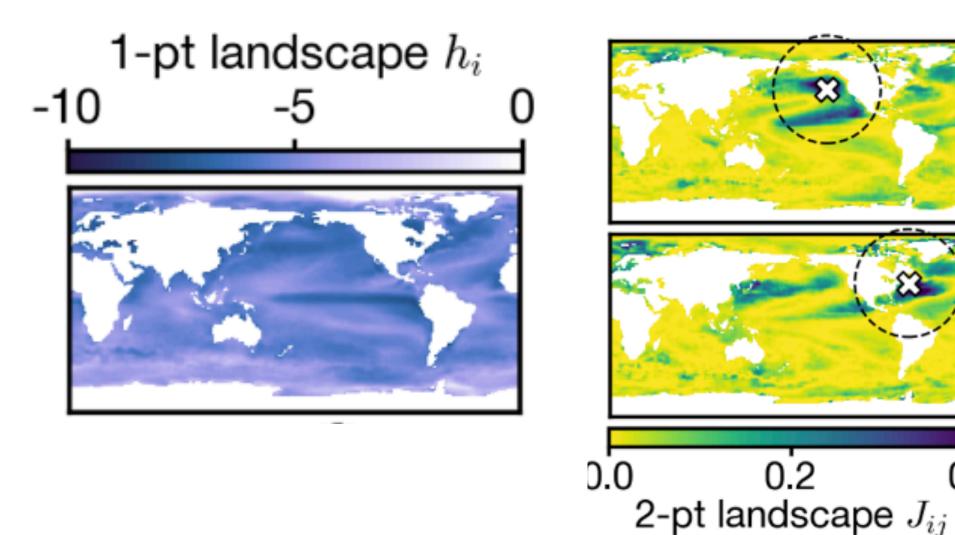


Greedy strategy for selection of the next sensor aims to minimize sensor 1- and 2- body interactions (crosstalk) O(nrp)

$$q = \arg\min_{q \notin \gamma} (h_q + 2 \sum_{i \in \gamma} J_{iq}); \ \gamma \leftarrow q$$

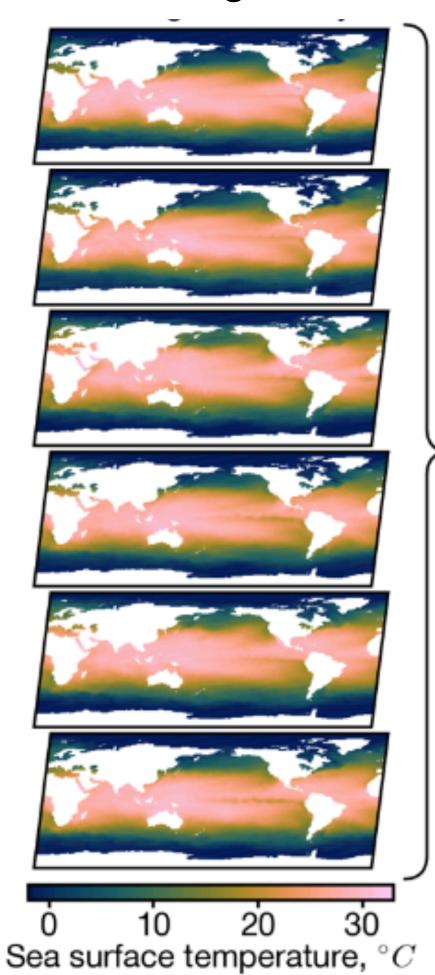
Two-point interactions provide a sensor optimization landscape

→ Alternatives to the minimizer for emerging design constraints



Two-point Energy Approximation

Training Data

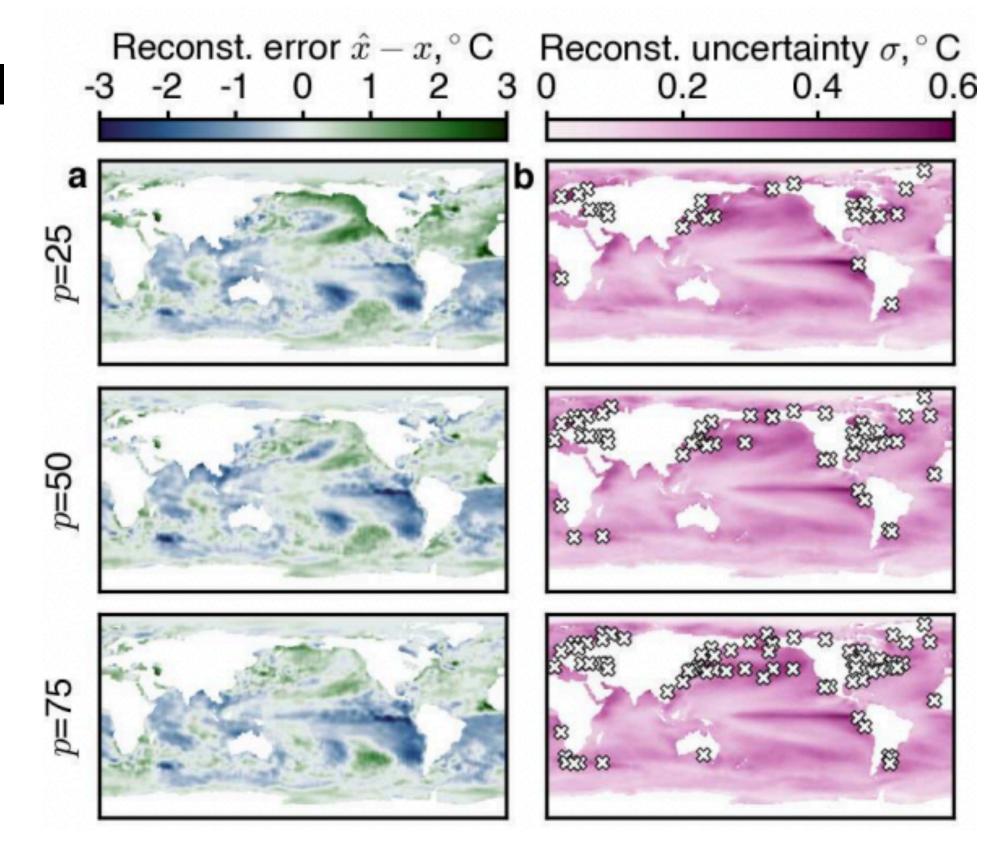


State reconstruction fluctuation propagated from sensor reading

Compute only diagonal part of the covariance matrix $\langle \Delta \mathbf{x} \Delta \mathbf{x}^T \rangle$

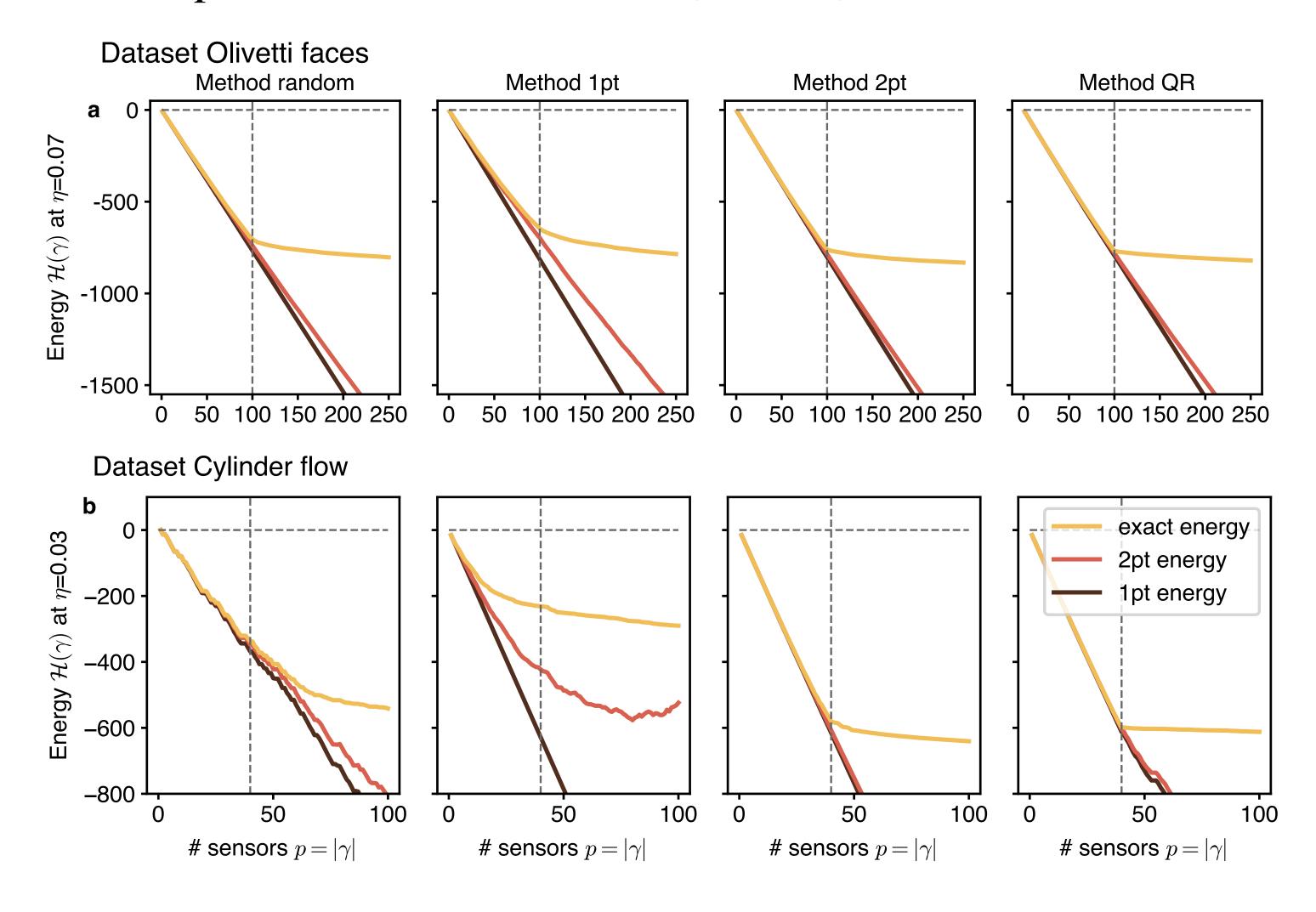
$$B = \Phi_r A^{-1} \frac{\Theta^T}{\eta^2}$$

$$\sigma_i = \eta \sqrt{\sum_j B_{ij}^2}$$

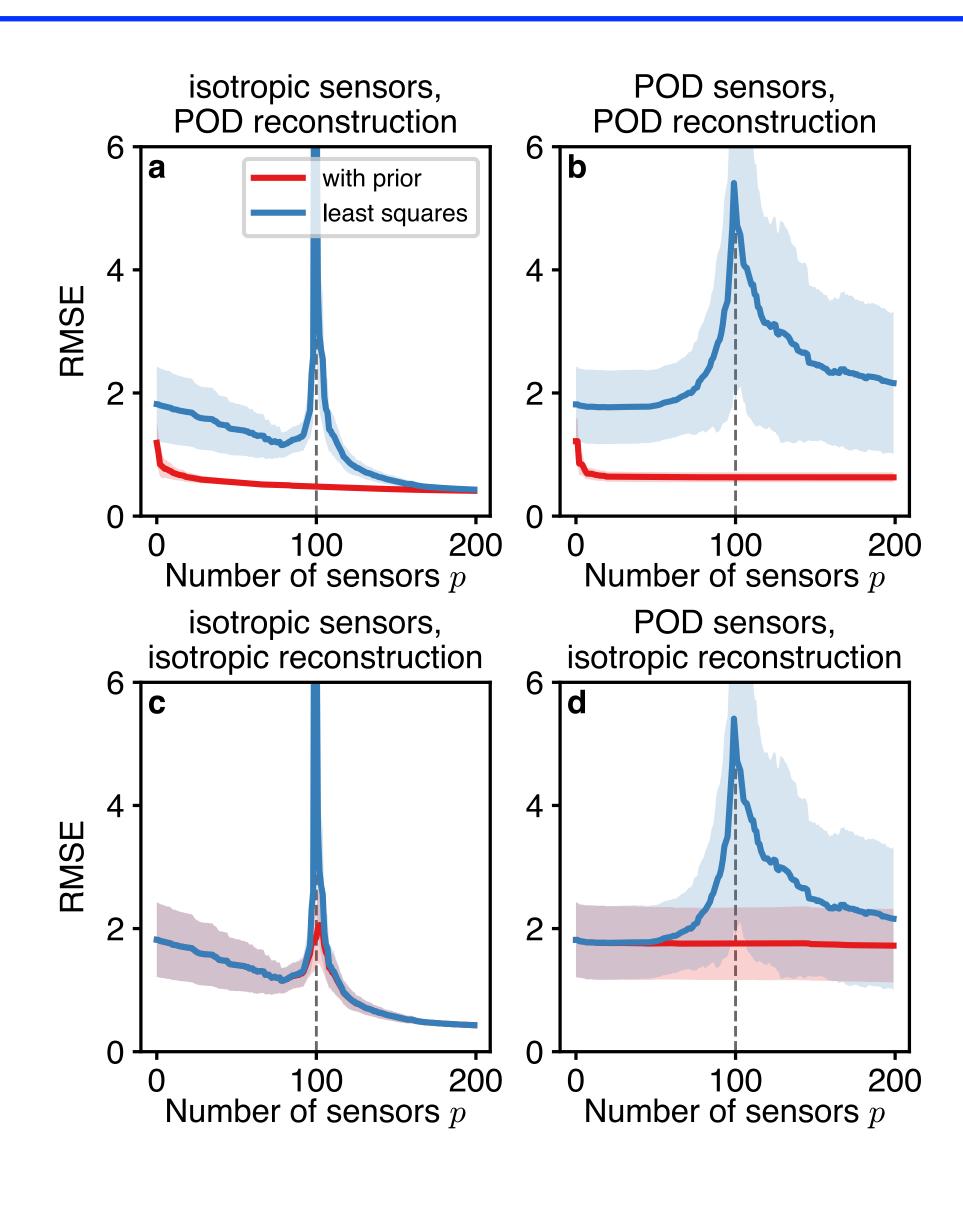


Validity of approximation

For small p (no. sensors) 2pt energy is a good approximation



Effect of Data-Driven Prior

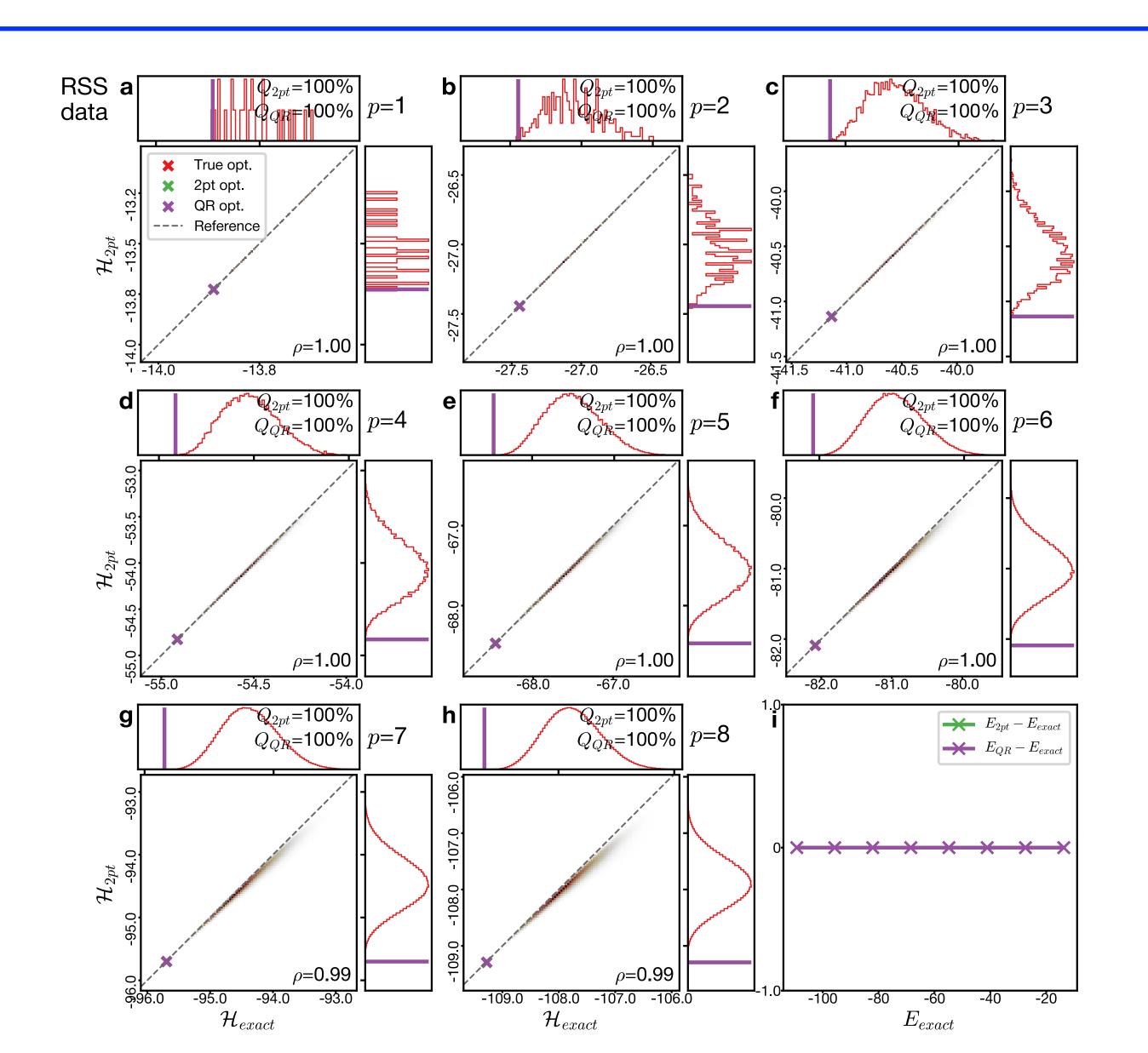


- Data-driven prior $S = \Sigma^2 / \sqrt{n-1}$
- Isotropic prior $S = \sigma_{prior} I$
- Mitigates CPQR instability when p = r
- Outlook: Error covariance decomposition

Outlook: Analytic expression for RMSE curve

$$\mathbf{K} = \underbrace{\mathbf{\Psi}_{c} \mathbf{B}_{0} \mathbf{B}_{0}^{T} \mathbf{\Psi}_{c}^{T}}_{\text{subleading modes}} + \underbrace{\mathbf{\Psi}_{r} \mathbf{B}_{1} \mathbf{B}_{1}^{T} \mathbf{\Psi}_{r}^{T}}_{\text{leading modes}} + \underbrace{\mathbf{\Psi}_{r} \mathbf{B}_{2} \mathbf{B}_{2}^{T} \mathbf{\Psi}_{r}^{T}}_{\text{contamination}} + \underbrace{\mathbf{\Psi}_{r} \mathbf{B}_{3} \mathbf{B}_{3}^{T} \mathbf{\Psi}_{r}^{T}}_{\text{noise}}$$

Comparison to exhaustive search

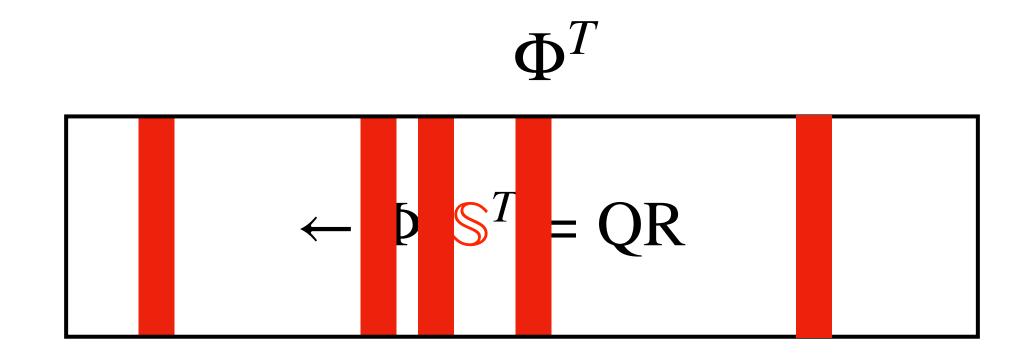


Column-Pivoted QR

Minimize error covariance of estimation $\mathbb{S}_{\star} = \arg\max \sigma((\mathbb{S}\Phi_r)^T \mathbb{S}\Phi_r)$

$$\mathbb{S}_{\star} = \arg\max_{\mathbb{S}} \sigma((\mathbb{S}\Phi_r)^T \mathbb{S}\Phi_r)$$

$$Var(\mathbf{a} - \hat{\mathbf{a}}) \propto det[(\$\Phi_r)^T \$\Phi_r]^{-1}$$

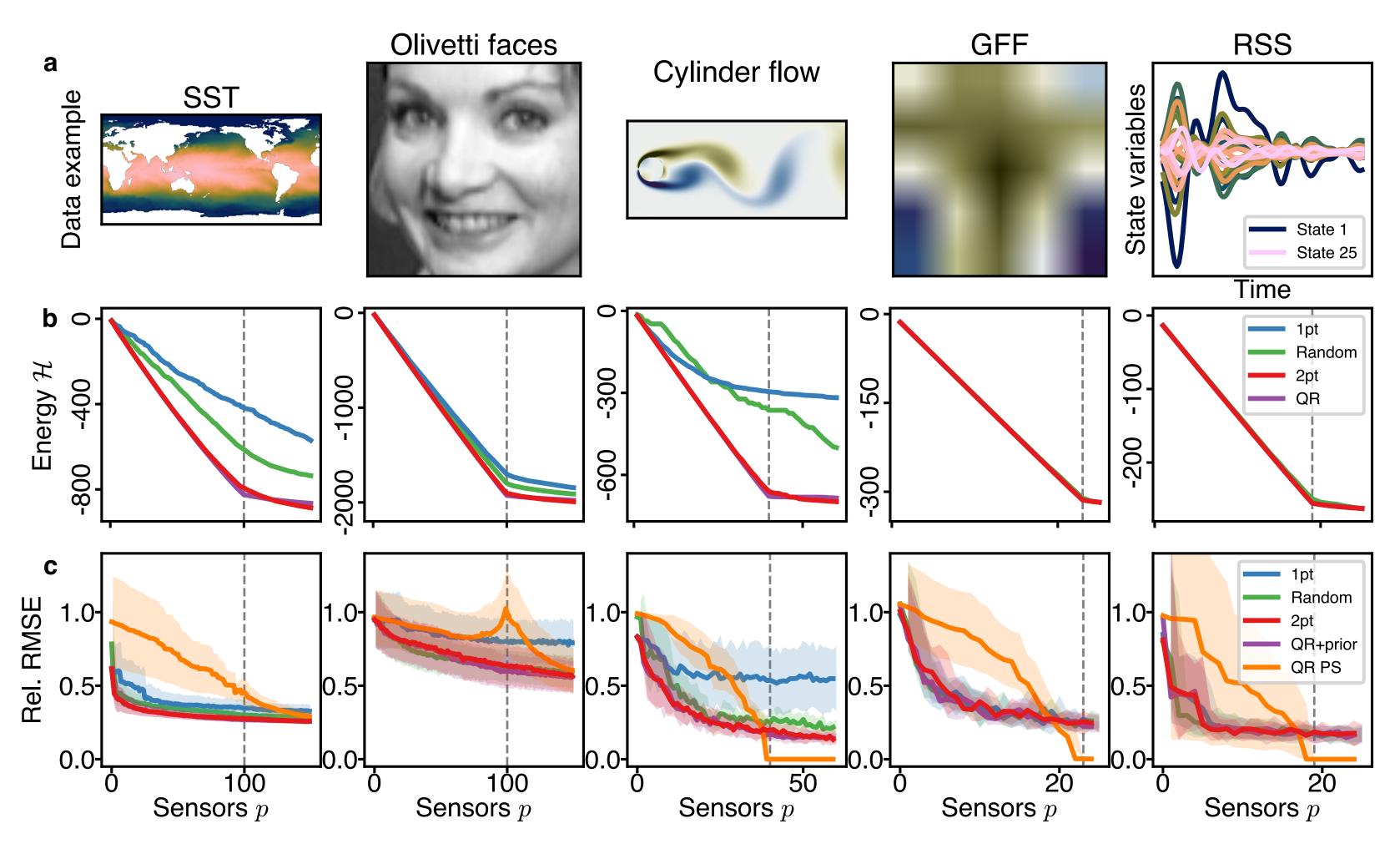


$$\det \Theta^T \Theta = \prod_i R_{ii}^2$$

Efficient interpolation points $O(nr^2)$

Drmac and Gugercin 2016 KM, Brunton, Kutz & Brunton, IEEE CSM 2018 KM, Kutz & Brunton, IEEE TAC 2021 Peherstofer et al, 2020 (ODEIM p > r)

Reconstruction results

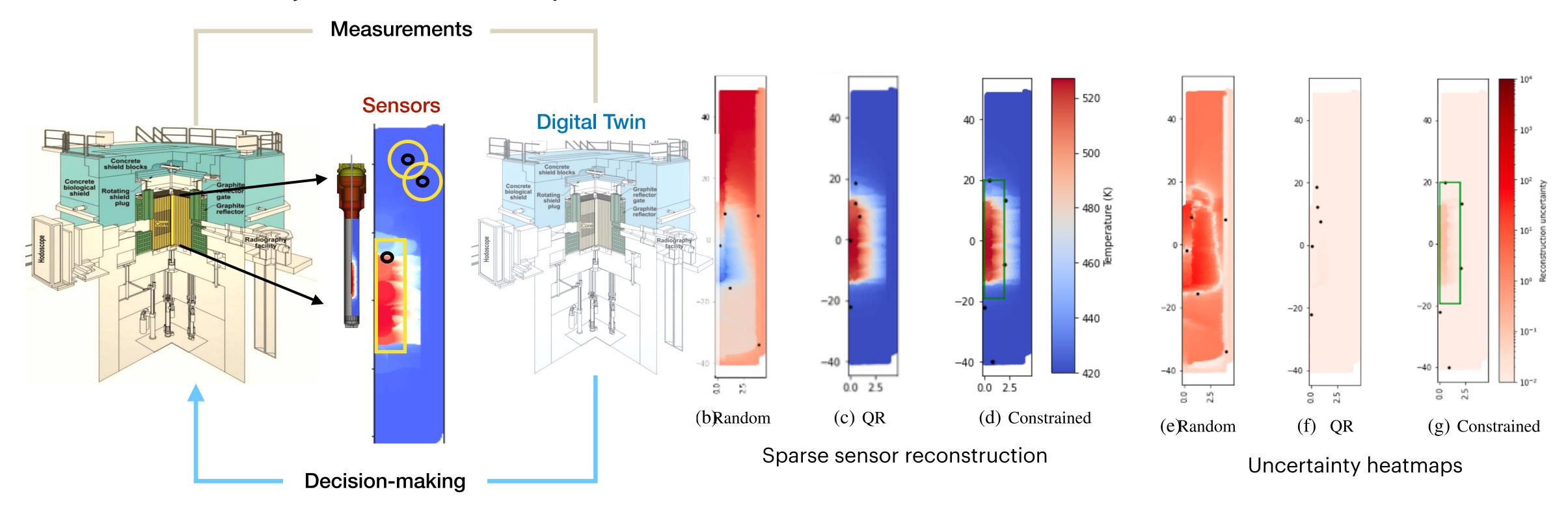


CPQR and 1pt consistently underperform 2pt greedy and data-driven prior

Constrained Sensing for Nuclear DTs



Reconstruct temperature field from optimized, spatially constrained measurements Heater adjacent sensors optimize reconstruction





Karnik, Abdo, Perez, Yoo, Cogliati, Skifton, Calderoni, Brunton & KM, arXiv:2306.13637 *IEEE Sensors Journal* (2024)

Outlook: sensor information criteria

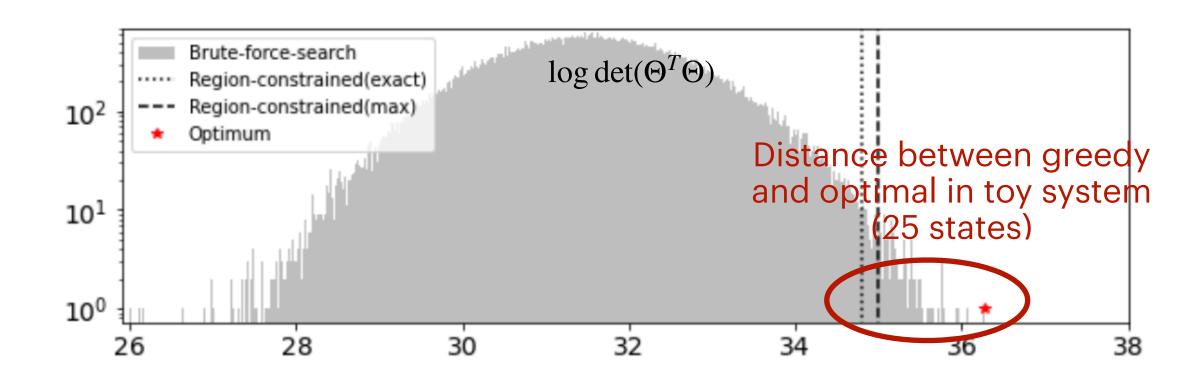
• A set function submodular if $f(\gamma \cup \{s\}) - f(\gamma)$ is monotone decreasing $\forall s \in V$ (Diminishing returns) $\ln \det \mathbb{S}W_c \mathbb{S}^T$

Summers et al, 2016

• Ex. Observability/controllability metrics, mutual information, neural estimation Belghazi, Bengio, et al., ICML (2018)

$$\arg\min_{\gamma}I(X_{\gamma};X_{S\setminus\gamma})$$

Krause et al, JMLR, 2008 Gaussian Processes



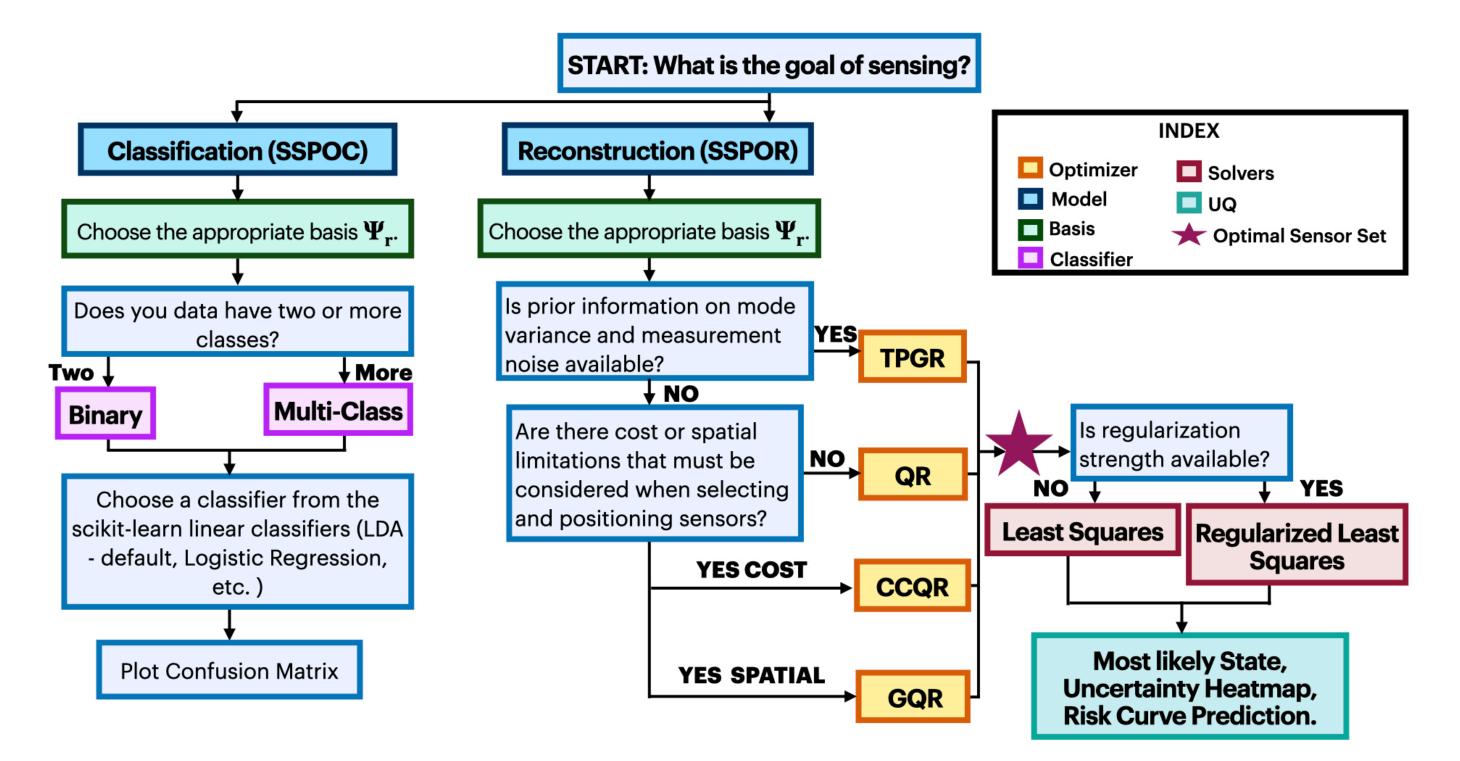
PySensors 2.0

Open-source code and benchmark datasets



Code 2: Implementation of the Two Point Greedy Optimizer

```
basis = ps.basis.SVD(n_basis_modes=r)
  optimizer = ps.optimizers.TPGR(n_sensors, noise, prior)
  model = ps.SSPOR(basis=basis, optimizer=optimizer)
  model.fit(data)
  sensors=model.get_selected_sensors()
  one_pt_landscape = model.one_pt_energy_landscape(prior, noise)
  two_pt_landscape = model.two_pt_energy_landscape(prior, noise, sensors)
```



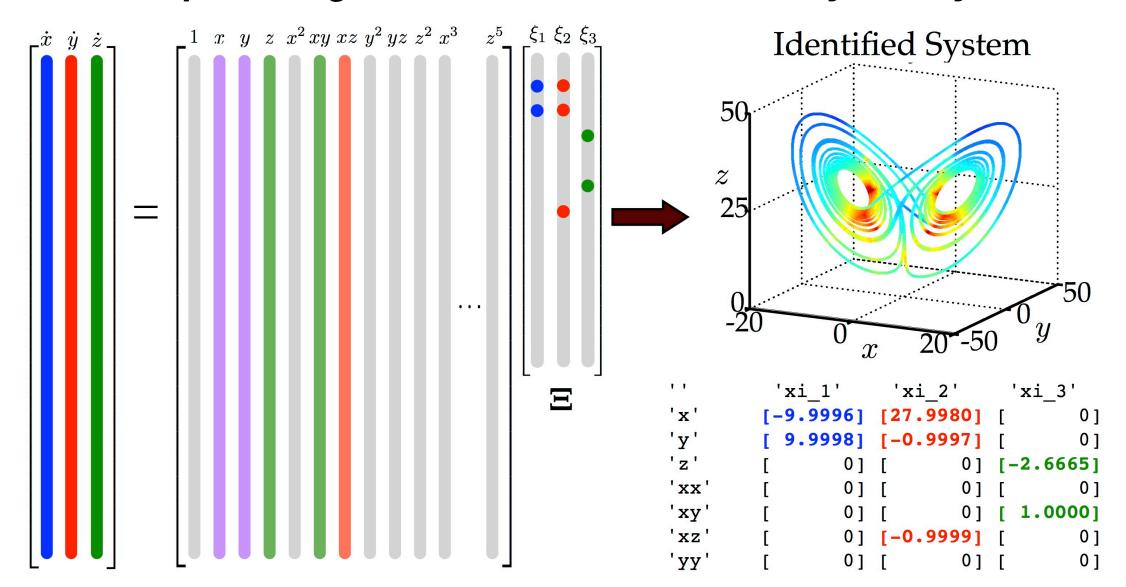


Karnik, Bhangale, Abdo, Klishin, Cogliati, Brunton, Kutz, Brunton & Manohar, arXiv 2509.08017 (2025)

Nonlinear System Identification

- Goal: learn ODEs, laws of motion from trajectory data
- Nonconvex optimization = many solutions
- When is recovery possible: trajectory length n, Δt , noise η
- Hyperparameters: sparsity λ , resolution ρ

Sparse regression in constrained library: SINDy



Brunton, Proctor, Kutz, PNAS (2016)

SINDy sparse regression loss function

$$\Xi_l = \arg\min_{\Xi} \frac{1}{2\rho^2} \sum_t (\dot{x}_l - \Theta^T(x) \cdot \Xi_l)^2 + \lambda ||\Xi_l||_p$$
 Sparsifying for $p \le 1$

Statistical mechanics for SINDy







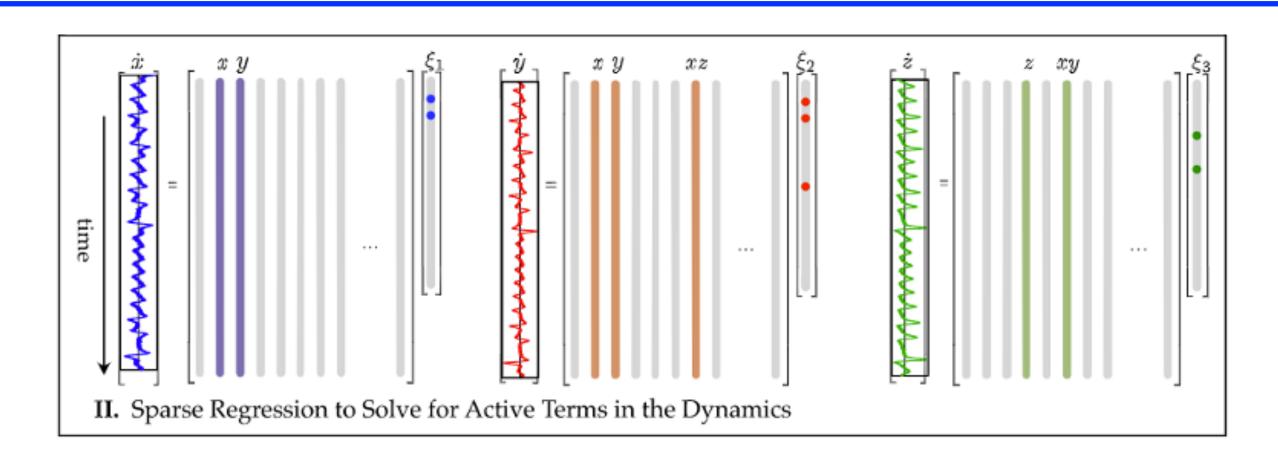
Andrei Klishin Joseph Bakarji Nathan Kutz

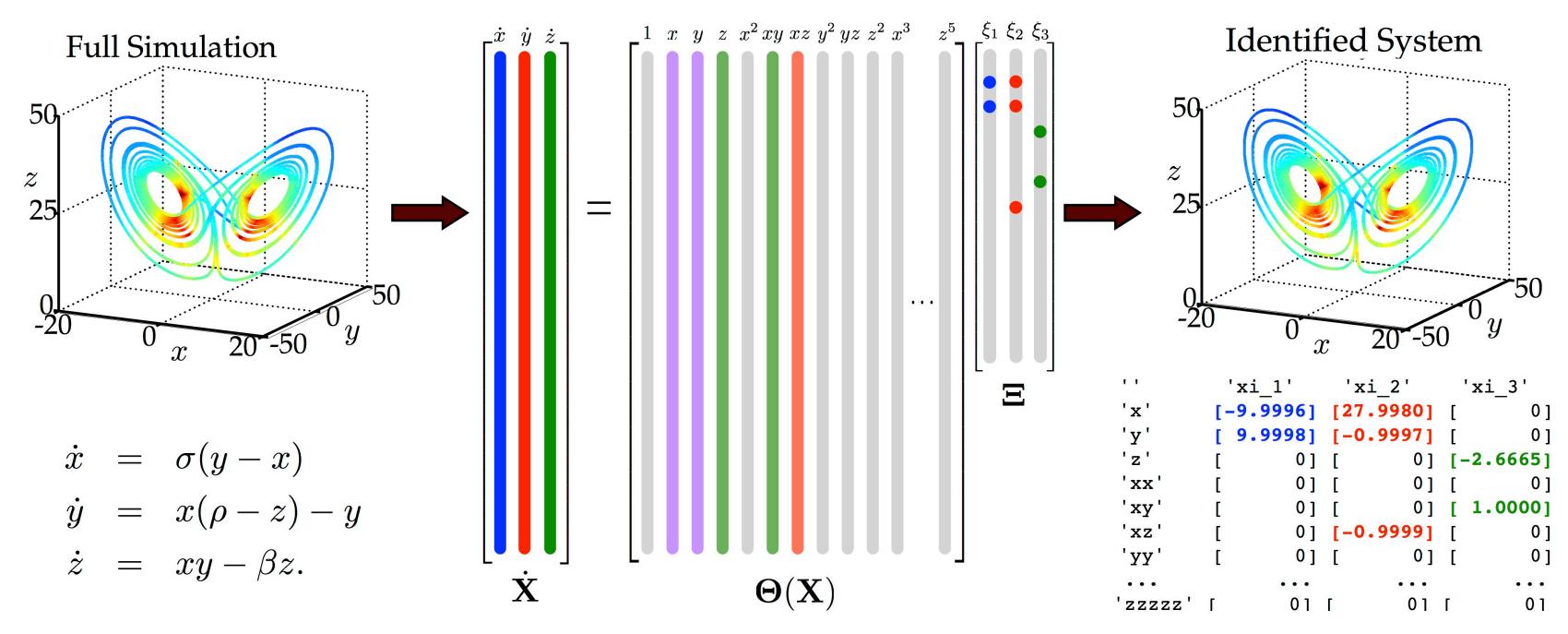
Sparse Identification of Nonlinear Dynamics

Identify ODE from trajectory data

$$\dot{x}_l = f_l(\overrightarrow{x}) \approx \sum_{i=1}^{N} \Theta_i(\overrightarrow{x}) \Xi_{il}$$

where $\Theta_i(\overrightarrow{x})$ is an overcomplete nonlinear library and Ξ_{il} is sparse

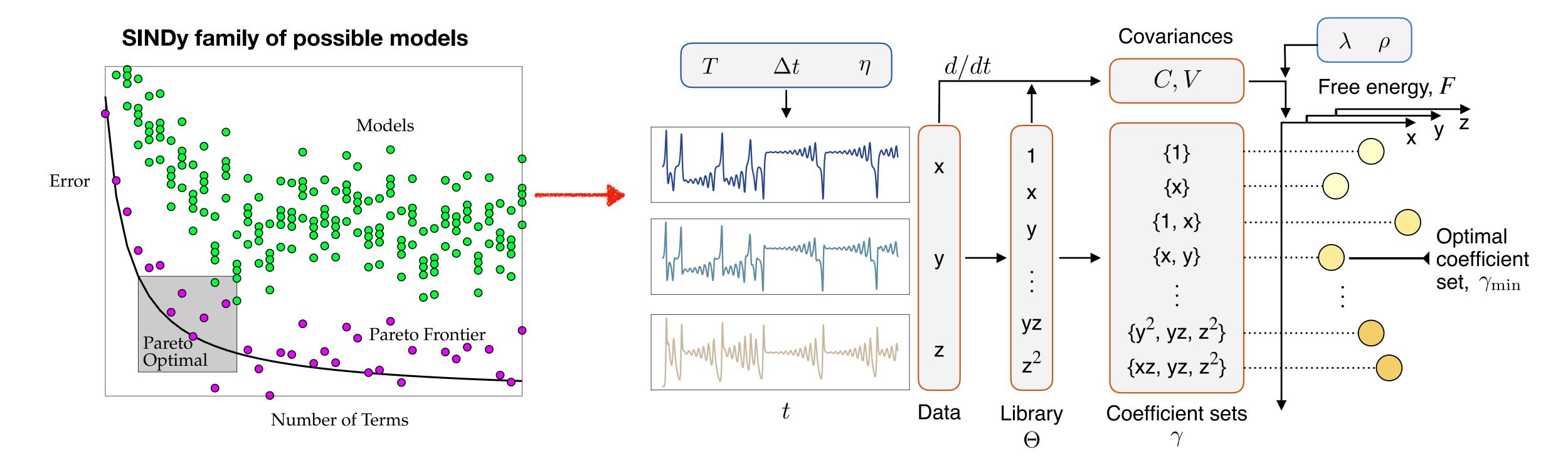




Brunton, Proctor, Kutz, PNAS (2016)

Nonlinear System Identification - ZSINDy

- Closed form posterior for l_0 SINDy: $p(\Xi \mid x) = \frac{1}{Z} \left(-\frac{1}{2\rho^2} \sum_t (\dot{x} \Theta^T \Xi)^2 \Lambda ||\Xi||_0 \right)$ Free energy criterion ranks models
- ullet Predicts model transition behavior with changing Λ
- Identifies Lotka-Volterra from Mahaffy population dataset



Nonlinear System Identification - ZSINDy

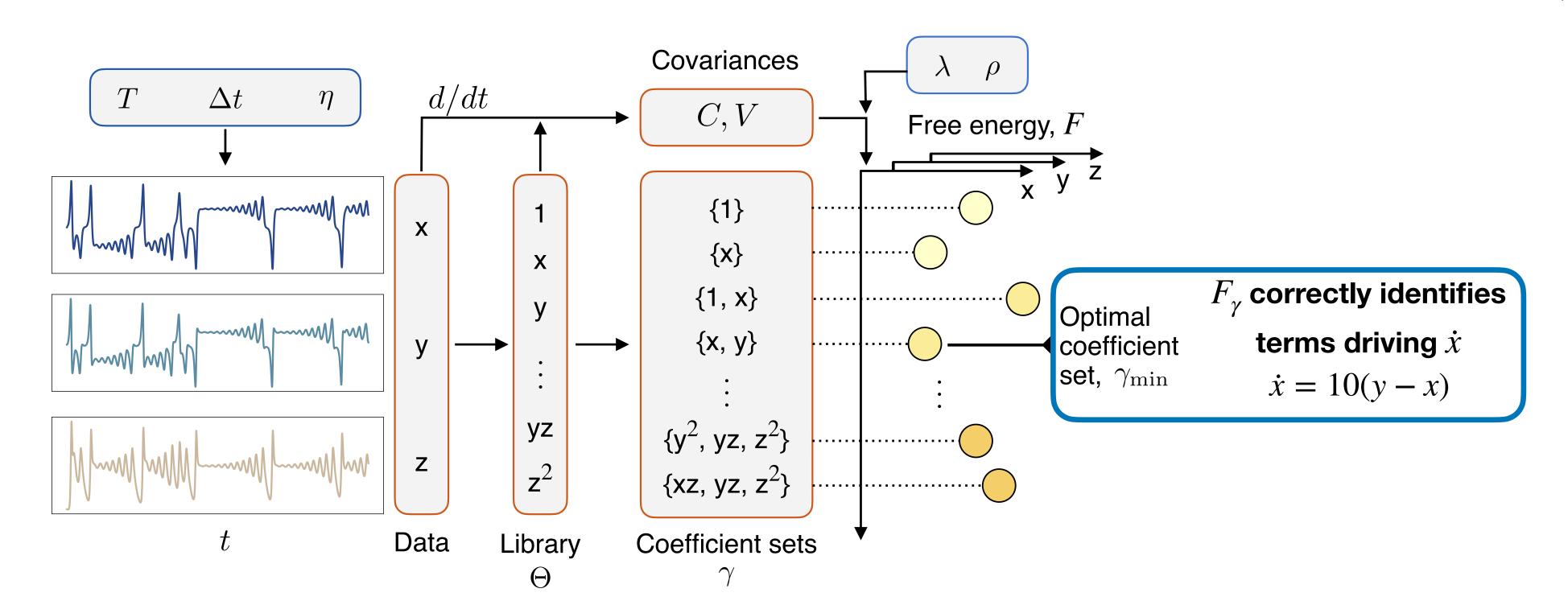
Recast SINDy as Bayesian inference problem, characterize optimization landscape of different coefficient sets γ using statistical mechanics

Statistical "free energy" characterizes optimal set
$$\gamma_{\min}$$

$$F_{\gamma} = \frac{1}{2\rho^2} \sum_{t} \dot{x}^2 - \underbrace{\frac{|\gamma|}{2} \ln(2\pi\rho^2) + \frac{1}{2} \ln \det C_{\gamma}}_{natural\ sparsity} - \underbrace{\frac{1}{2\rho^2} V_{l,\gamma}^T C_{\gamma}^{-1} V_{l,\gamma}}_{O(n)\ LS\ fit} + \underbrace{\frac{|\gamma| n \cdot \lambda}{explicit}}_{explicit}$$

$$p(\Xi \mid x) = \frac{\sum_{\gamma} p(\Xi \mid \gamma, x) Z_{\gamma}}{\sum_{\gamma} Z_{\gamma}}$$

Factorized posterior over γ weighted by $Z_{\gamma}=e^{-F_{\gamma}}$



Nonlinear System Identification - ZSINDy

Factorized posterior over coefficient sets γ weighted by $Z_{\gamma}=e^{-F_{\gamma}}$

$$p(\Xi \mid x) = \frac{\sum_{\gamma} p(\Xi \mid \gamma, x) Z_{\gamma}}{\sum_{\gamma} Z_{\gamma}}$$

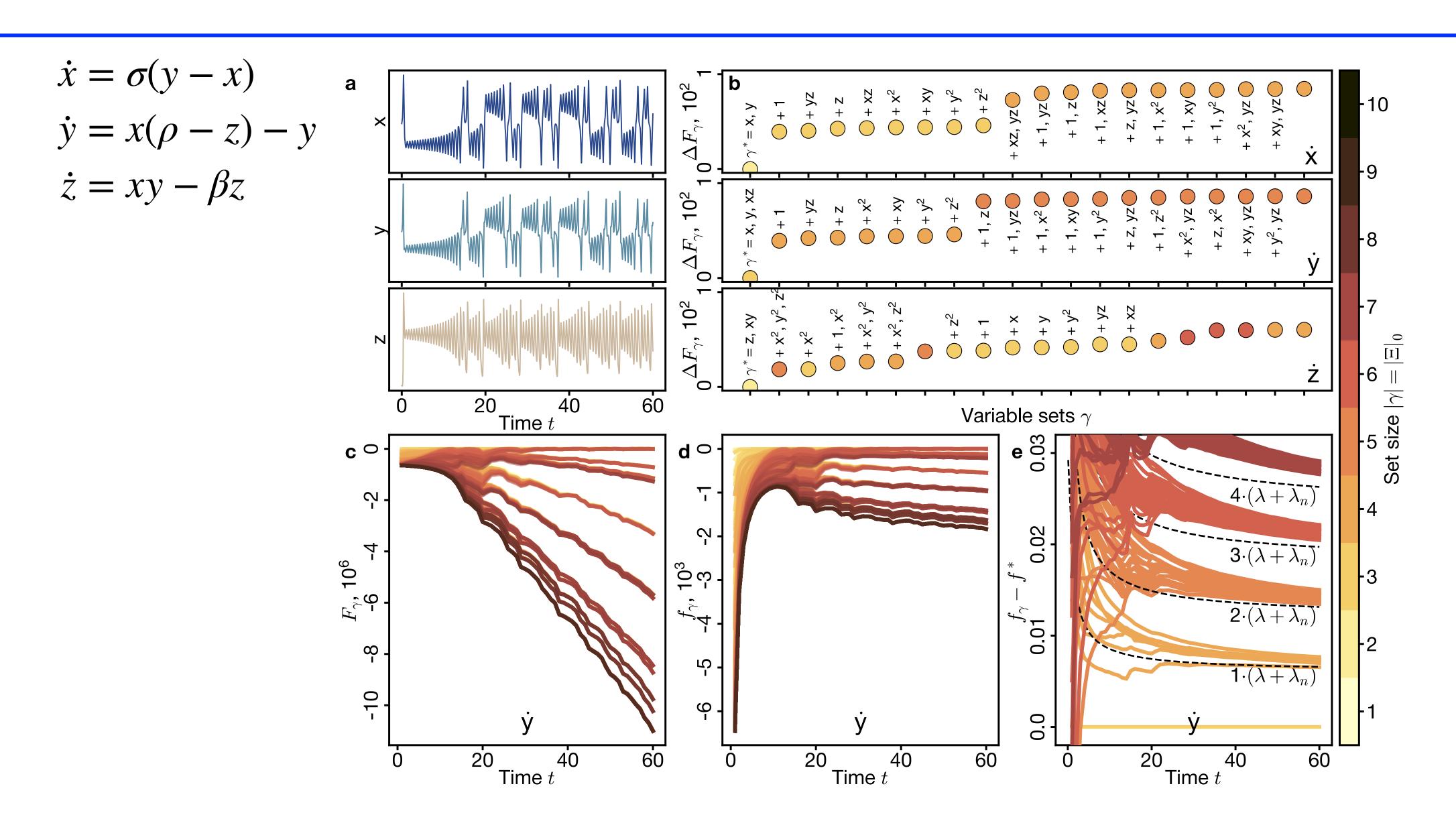
Bernoulli-Gaussian prior

$$p(\Xi) = \prod_{i} \frac{1}{1 + e^{-\Lambda}} (\delta(\Xi_i) + w(\Xi_i)e^{-\Lambda})$$

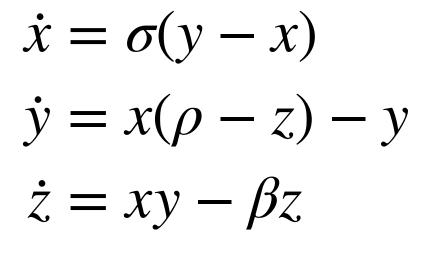
 $F_{\gamma} = -\ln Z_{\gamma}$: Minimizer set identifies l_0 optimal solution

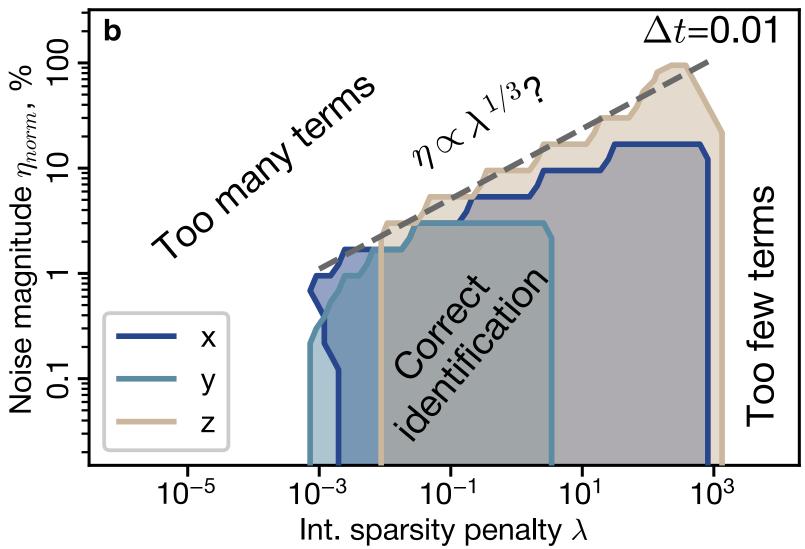
$$F_{\gamma} \propto -\frac{|\gamma|}{2} \ln(2\pi\rho^{2}) + \frac{1}{2} \ln \det C_{\gamma} - \underbrace{\frac{1}{2\rho^{2}} V_{l,\gamma}^{T} C_{\gamma}^{-1} V_{l,\gamma}}_{O(n) LS \ fit} + \underbrace{|\gamma| n \cdot \lambda}_{explicit}$$

Identification of optimal coefficient set

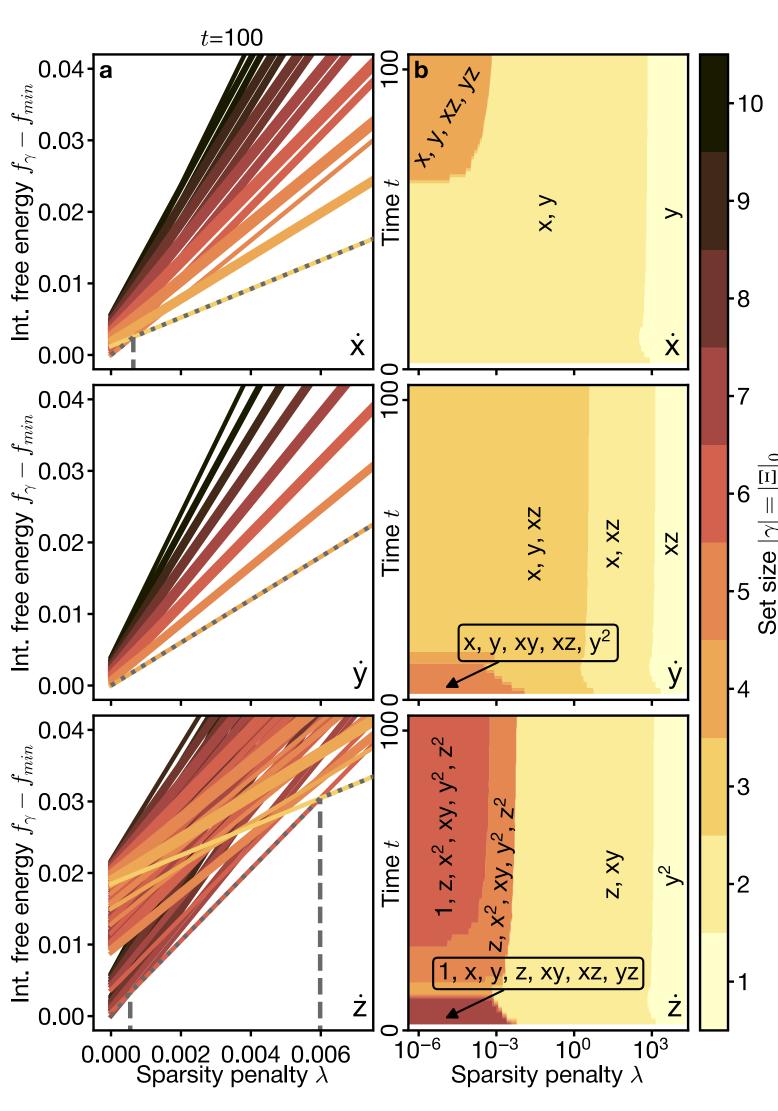


When is inference possible

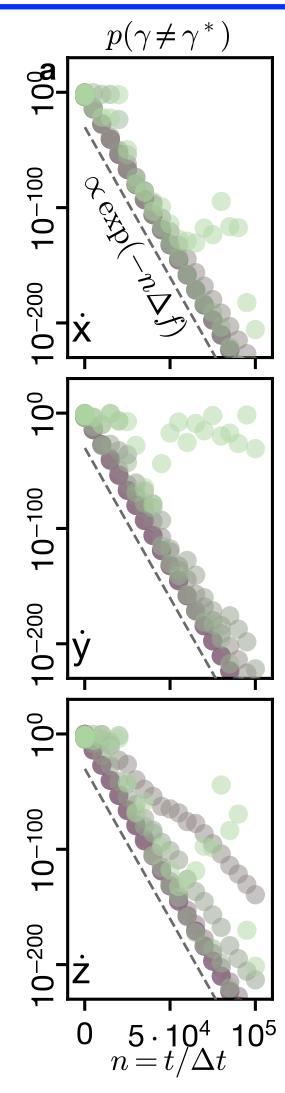




Critical noise levels for inference



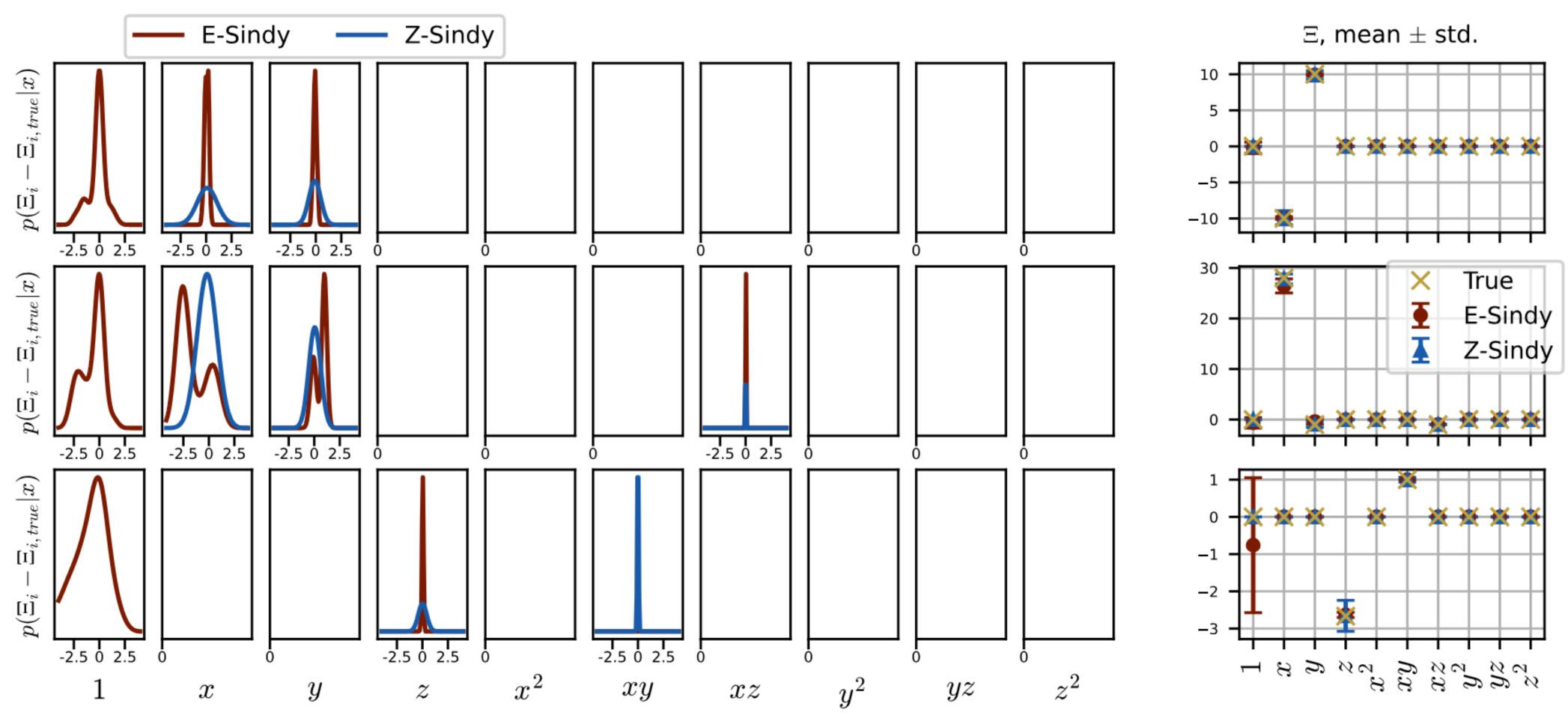
Sharp transitions of coefficient sets with increasing sparsity penalty



Probability of selecting suboptimal set decays exponentially w/ trajectory length $p(\gamma^*) \approx 1 - e^{-n\Delta f}$

Comparison with Ensemble SINDy

- E-SINDy fits distributions to bootstrapped ensemble models
- Z-SINDy consistently identifies sparser solutions



Klishin, Bakarji, Kutz & Manohar, Phys. Rev. Research 2025



Long-Term Forecasting

- Williams, J. P., Kutz, J. N., & Manohar, K. (2024). Reservoir computing for system identification and predictive control with limited data. arXiv preprint arXiv:2411.05016.
- Klishin, A. A., Bakarji, J., Kutz, J. N., & Manohar, K. (2025). Statistical mechanics of dynamical system identification. *Physical Review Research*, 7(3), 033181.
- Peng, M., Kaptanoglu, A. A., Hansen, C. J., Stevens-Haas, J., Manohar, K., & Brunton, S. L. (2025). Extending the trapping theorem to provide local stability guarantees for quadratically nonlinear models. *Physics of Fluids*, 37(10).
- Salazar, Manohar, & Banerjee. Online Kernel Dynamic Mode Decomposition for Real-Time Time Series Forecasting with Adaptive Windowing (In preparation)

Predictive shimming in large-scale assembly

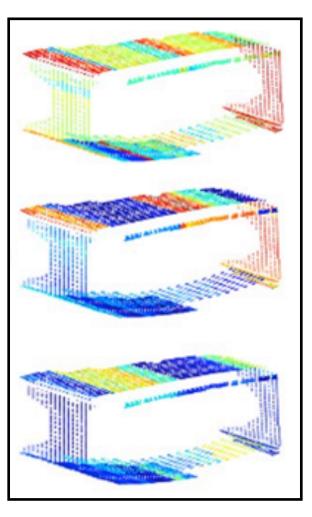
787 Wing-to-Body Join

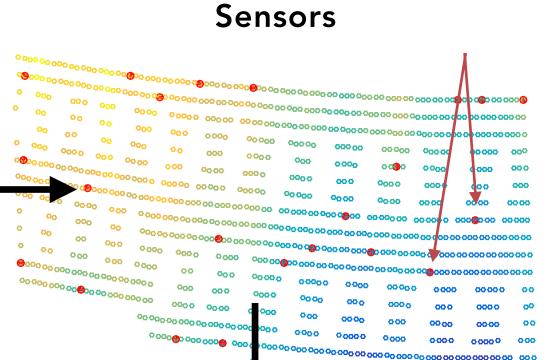


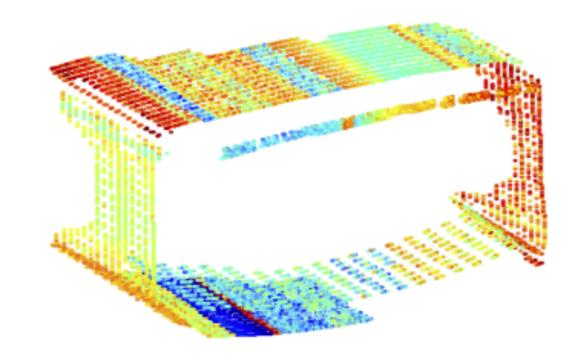
Training data: 10,000 gap measurements (truth data) for 50 aircraft

Data from individual aircraft

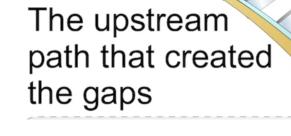
Dominant patterns Modes







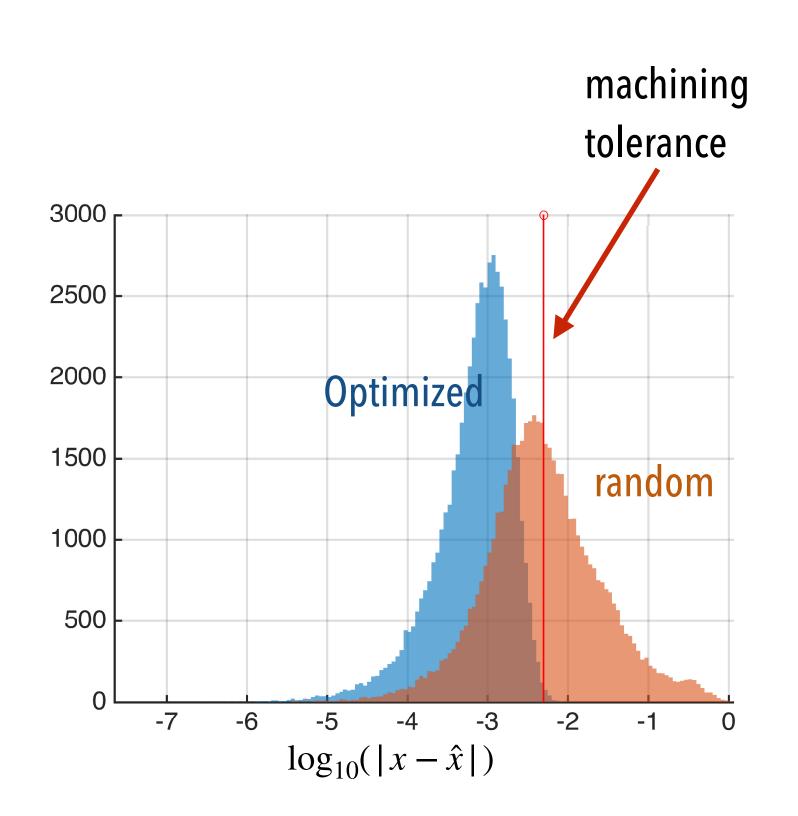
Predicted shims





Predictive shimming in large-scale assembly

99% unknown gaps within 0.005" with 30X less measurement



Shim No.	1	2	3	4	5	6	7
Percent Accurate Optimal sensors (avg)	97.90 26	98.05 26	$99.82 \\ 25$	$99.94 \\ 26$	$99.99 \\ 25$	99.03 26	99.97 25
Total points	1003	1116	453	692	709	768	664

