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RaISE: A Framework to Characterize Surrogate Models in Scientific Machine Learning

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Context

- **Motivation:** Proliferation of machine learning surrogates in scientific computing
  - Data-driven, constructed with input-output pairs $(\hat{X},\hat{Y})$
  - Physical model structure, often PDE-based
  - Expensive data collection
- Target map f finite- or infinite-dimensional
- Repeated evaluations of surrogate $f_{\hat{X},\hat{Y}}$
- **Goal:** Standardized framework to view surrogates

Characterization Framework

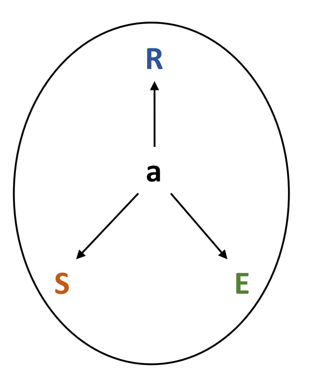

Fig. 1: RaISE framework.

- ***Accuracy (a):*** varies inversely with error

$$\mathcal{E}[f_{\hat{X},\hat{Y}}] = \mathbb{E}_{\hat{X}\sim\mu}\left(\sqrt{\frac{\int_{\mathcal{X}}(f-f_{\hat{X},\hat{Y}})^2\,\mathrm{d}x}{\int_{\mathcal{X}} f^2\,\mathrm{d}x}}\right)$$

- ***Robustness (R):*** constancy of *a* w.r.t. standard deviation σ of additive noise in training outputs

$$R(\sigma) = \gamma\left(\frac{\partial}{\partial\sigma}\log\left(\mathcal{E}[\hat{f}_{\hat{X},\hat{Y}}]\right)\right), \qquad \gamma(x) = \mathrm{e}^{-x}$$

- ***Scalability (S):*** constancy of *a* w.r.t. dimension of input space $d = \dim(\mathcal{X})$

$$S(d) = \gamma\left(\frac{\partial}{\partial d}\log\left(\mathcal{E}[f_{\hat{X}_d,\hat{Y}_d}]\right)\right)$$

- ***Efficiency (E):*** speed of increase in *a* w.r.t. $N = |\hat{X}|$

$$E(N) = 1-\gamma\left(-\frac{\partial}{\partial(\log N)}\log\left(\mathcal{E}[f_{\hat{X},\hat{Y}}]\right)\right)$$

- ***Interpretability (I):*** user-defined convex combination of *R*, *S*, and *E*

$$I(R,S,E) = w_1R + w_2S + w_3E$$
$$w_i \geq 0, \qquad w_1+w_2+w_3 = 1$$

Model Use-Case

$$u_t + \nabla\cdot(\boldsymbol{v}u) + \nabla\cdot(\kappa\nabla u) = g, \qquad \boldsymbol{x}\in[0,1]^2,\ t>0$$

- 2D convection–diffusion with Gaussian source and parameterized velocity field
  - Parameters: KL coefficients, independent and uniformly distributed on $[-1,1]$
  - QoI: State/point-value at final time

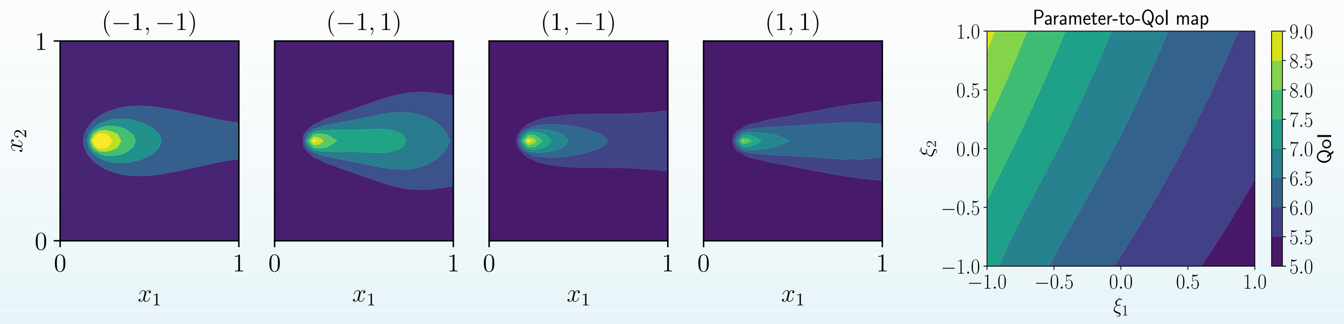

Fig. 2: Final-time concentrations for different parameter choices (left). Scalar response surface (right).

Framework Applied to Surrogates

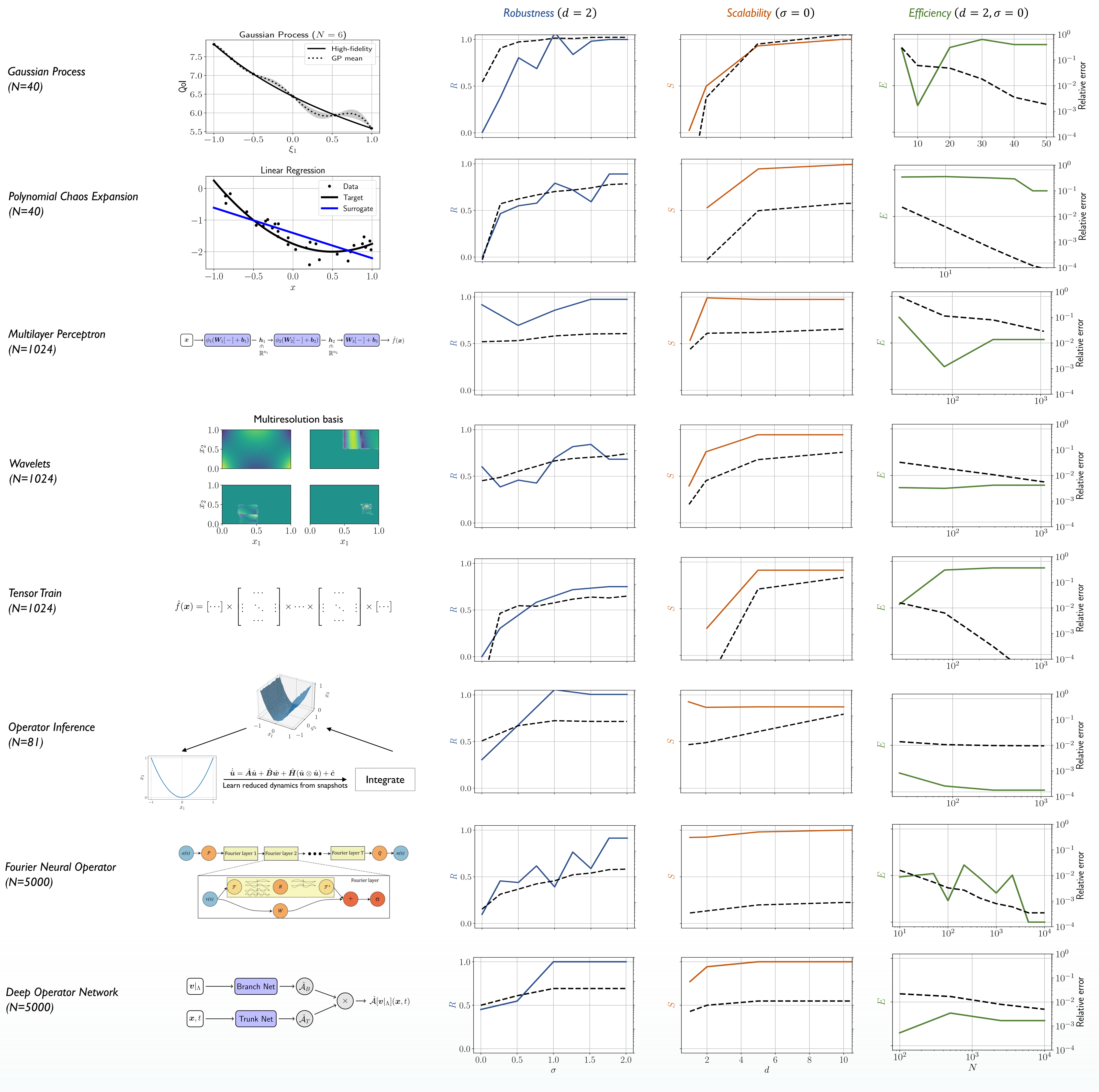

Fig. 3: RaISE applied to function and operator approximation methods. FNO diagram from [Li 2021].

Interpretability Example

- User preferences and application needs will affect interpretability through weights in *I(R, S, E)*
  - User 1: noisy data, large computational budget
    $w_1 = 0.7, \quad w_2 = 0.15, \quad w_3 = 0.15$
  - User 2: noiseless data, small computational budget
    $w_1 = 0.1, \quad w_2 = 0.25, \quad w_3 = 0.65$
  - *R*, *S*, and *E* set to average values over respective domains

Interpretability Ratings

Method	Large noise, large budget	Small noise, small budget
GP	0.63	**0.75**
PCE	0.59	**0.83**
MLP	**0.78**	0.64
Wavelet	0.56	**0.62**
Tensor Train	0.59	**0.76**
OpInf	**0.71**	0.35
FNO	0.48	**0.51**
DeepONet	**0.74**	0.49

Remarks

- Can also use RaISE to demonstrate low-rank structure by fixing size of reduced basis in definition of scalability
- Caveats
  - We do not catch all surrogate features in RaISE (e.g., parallelizability, storage, dependence on regularity)
  - Magnitude **and rate of change** of error are important
  - End-user may want different $\gamma(x)$ across *R*, *S*, and *E*

Summary and Next Steps

- Novel and comprehensive set of metrics to evaluate surrogate models in practice
  - Designed so that ***R***, ***I***, ***S***, and ***E*** range from 0 to 1
- Interpretability depends on robustness, scalability, efficiency, and subjective preferences of decision-maker
- Framework for the community and for Sandia's own surrogate modeling needs
- Manuscript in preparation
  - Large cross-section of methods written accessibly

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References

Z. Li, N. Kovachki, K. Azizzadenesheli, B. Liu, K. Bhattacharya, A. Stuart, A. Anandkumar. "Fourier Neural Operator for Parametric Partial Differential Equations." International Conference on Learning Representations (ICLR), 2021.

Z. M., B. van Bloemen Waanders, A. Gorodetsky, J. D. Jakeman, S. A. McQuarrie, N. H. Nelsen, M. Salloum, N. Winovich. "RaISE: A Framework for Characterizing Surrogate Models in Scientific Computing." In preparation.

Robust Interpretable Scalable Efficient RISE

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