

Fighting the Curse of Dimensionality in Uncertainty Quantification

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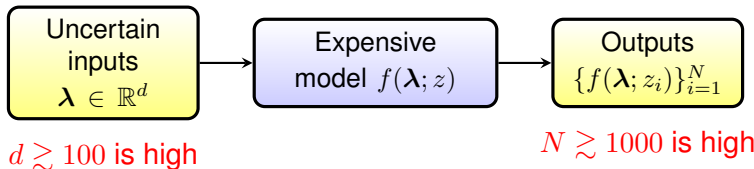
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Where High Dimensionality Hurts Us

Mostly: surrogates *for* UQ (forward UQ) $\Rightarrow$ at the end: UQ *for* surrogates



λ : uncertain parameters; z : 'certain' conditions — space, time, QoI id, ...

High-d inputs

- many uncertain parameters, BCs, field-valued inputs
- *e.g.* transport/rate coefficients

Hurts: too many runs

High-d outputs

- fields, profiles, spectra, time series
- *e.g.* temperature across the globe, strain stress curves

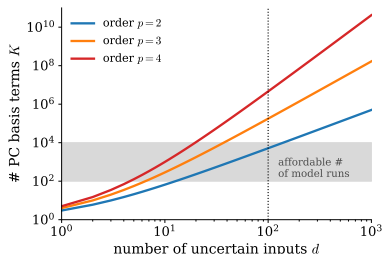
Hurts: too many surrogates

High-d Inputs: Surrogates Hit the Wall

- UQ stands on surrogates:
propagation, sensitivity, calibration
need 10^4 – 10^6 model evaluations
- e.g. Polynomial chaos (PC)
surrogate

$$f(\lambda) \approx \sum_{k=0}^{K-1} c_k \Psi_k(\xi)$$

- Number of terms $K = \frac{(d+p)!}{d! p!}$
 $d = 100, p = 3 \Rightarrow K = 176,851$
- Regression needs $N \gtrsim K$ runs;
expensive models give $N \sim 10^2$ – 10^3



- Tensor-product quadrature: m^d points
- Other surrogates, e.g., GPs, NNs, also struggle similarly.

Need to find, and exploit, low-dimensional structure

Good News: Effective Dimension is Often Low

- In practice:
only a few inputs, a few interactions, or a few directions matter
- Turn the curse into a *blessing of dimensionality* [\[Donoho, 2000\]](#)

Screen	global sensitivity (Sobol, Morris)	which inputs?
Sparsify	compressive sensing, basis pursuit	which basis terms?
Rotate	active subspaces, ridge functions	which combinations?

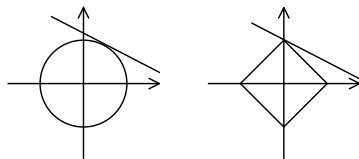
- Reframing the input yields a smaller problem for *any* surrogate: PC, GP, NN
- PC surrogates give Sobol indices for free from their coefficients [\[Sudret, 2008; Crestaux, 2009\]](#). For others, Monte-Carlo sampling can estimate them.

Sparse Learning: (Bayesian) Compressive Sensing

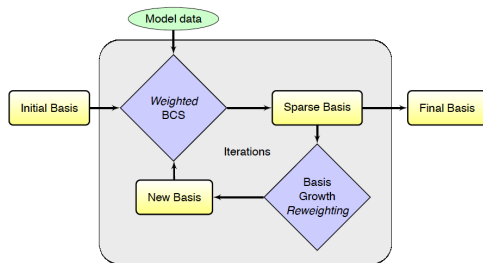
- Underdetermined regression, $N < K$: $\mathbf{y} \approx \mathbf{P}\mathbf{c}$, $P_{ik} = \Psi_k(\xi_i)$
- Sparsity via ℓ_1 regularization (CS, LASSO, basis pursuit)

$$\underset{\mathbf{c}}{\operatorname{argmin}} \|\mathbf{y} - \mathbf{P}\mathbf{c}\|_2^2 + \alpha \|\mathbf{c}\|_1$$

- Bayesian CS: sparsity priors $\Rightarrow$ prunes irrelevant terms; coefficients *with uncertainties* (UQ for surrogates) [Ji, 2008; Babacan, 2010]
- Iterative basis growth: raise the order only for surviving terms [Sargsyan, 2014; Jakeman, 2015]

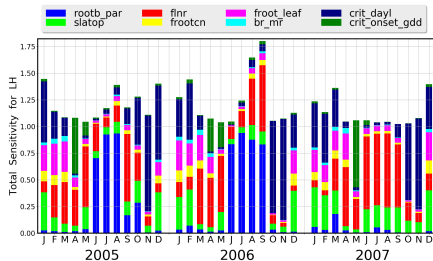


ℓ_2 vs ℓ_1 : the ℓ_1 ball finds sparse solutions

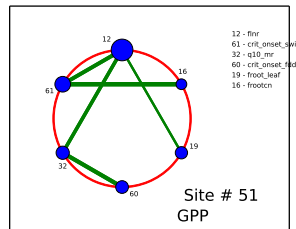


Sparse PC in Action: E3SM Land Model

- ~ 70 uncertain parameters; a single-site run takes ~ 10 hrs
- BCS finds ~ 200 relevant basis terms in a 50-dimensional space
- Sensitivities come for free from the PC coefficients: rank inputs, find key couplings



Total sensitivity of latent heat flux, per month



Main (nodes) & joint (edges) effects, GPP

[Sargsyan *et al.*, IJUQ 2014; Ricciuto *et al.*, JAMES 2018]

Active Subspaces: Rotate, then Reduce

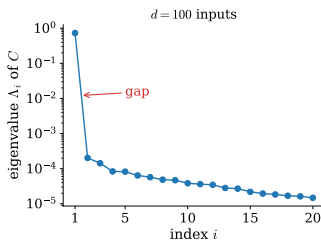
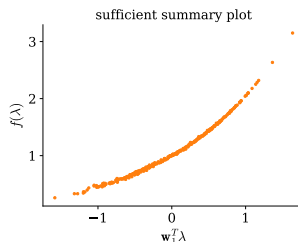
- Seek a few important linear combinations of the inputs

$$f(\boldsymbol{\lambda}) \approx g(\mathbf{W}_1^T \boldsymbol{\lambda}), \quad \mathbf{W}_1 \in \mathbb{R}^{d \times r}, \quad r \ll d$$

- Eigen-decompose the gradient covariance; an eigenvalue gap reveals r

$$\mathbf{C} = \mathbb{E} [\nabla f \nabla f^T] = \mathbf{W} \boldsymbol{\Lambda} \mathbf{W}^T$$

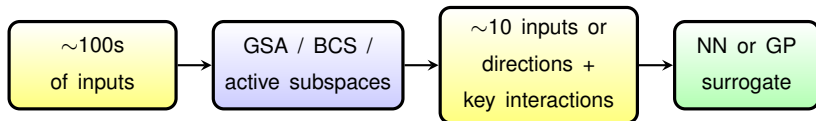
- Needs gradients: adjoints, finite differences, or a global (e.g. quadratic) fit



P. Constantine, E. Dow, Q. Wang, “Active subspace methods in theory and practice: applications to kriging surfaces”, *SIAM J. Sci. Comput.*, 36(4), 2014
 P. Constantine, *Active Subspaces*, SIAM, 2015

What About Neural Networks?

- NN surrogates cope with many inputs better than PC, but
 - they are data hungry; expensive models give 10^2 – 10^3 runs
 - black box: no sensitivities or interpretability for free
 - UQ for NNs is harder (next subtalk)
- Recommendation: **screen first, then learn**



- Sobol indices from a sparse PC fit on the *same* runs add interaction information

High-d Outputs: Too Many Surrogates

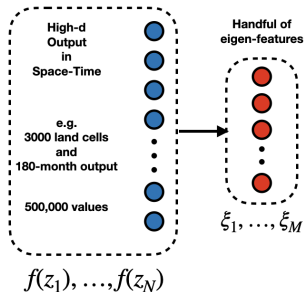
- Output is a field $f(\lambda; z)$ over conditions $z = \text{space, time, mode number, } \dots$
 $\Rightarrow N$ values per run
 - E3SM land model: $4000 \text{ cells} \times 180 \text{ months} = 720,000$
 - Materials: A density field on a 100×100 mesh = 10,000
 - Chemistry: Concentration of 5 species at 100 pressure levels = 500
- Naive approach: N separate surrogates
 - cost grows with N
 - ignores correlations across z ; predictions can be noisy/inconsistent
 - calibration: pointwise likelihood over N correlated data misspecified
- But neighboring outputs are strongly correlated $\Rightarrow$ low-rank structure

Reduce first, then build surrogates in the latent space

Karhunen-Loève Expansion: the UQ sibling of SVD

$$f(\boldsymbol{\lambda}; z) \approx \bar{f}(z) + \sum_{m=1}^M \xi_m(\boldsymbol{\lambda}) \sqrt{\mu_m} \phi_m(z)$$

- (μ_m, ϕ_m) : eigenpairs of the output covariance $C(z, z')$, estimated from an ensemble of runs
- $\xi_m(\boldsymbol{\lambda})$: latent features; uncorrelated, zero mean, unit variance
- Discrete form: SVD of the centered ensemble matrix $F = U \Sigma V^T$ (a.k.a. PCA, POD, EOF)
- Truncate at $M \ll N$, keeping, e.g., 99% of variance: $\sum_{m=1}^M \mu_m / \sum_m \mu_m > 0.99$
- Same tool for field-valued *inputs*, e.g. uncertain transport-coefficient profiles
- Nonlinear alternatives: autoencoders, diffusion maps



[Ghanem & Spanos, 1991; Higdon *et al.*, 2008; Kontolati *et al.*, 2022; Mueller *et al.*, 2025]

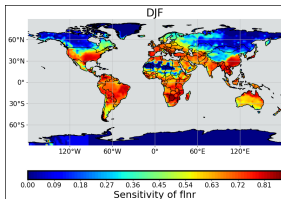
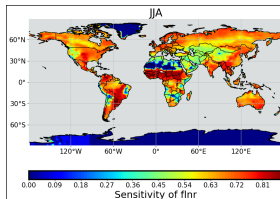
KL+PC Surrogate: Sensitivities at every z

- PC for each latent feature, $\xi_m(\lambda) \approx \sum_{k=0}^{K-1} c_{mk} \Psi_k(\lambda)$; plug into KL and **swap the sums**

$$\begin{aligned} f(\lambda; z) &\approx \bar{f}(z) + \sum_{m=1}^M \sum_{k=0}^{K-1} c_{mk} \Psi_k(\lambda) \sqrt{\mu_m} \phi_m(z) \\ &= \sum_{k=0}^{K-1} c_k(z) \Psi_k(\lambda), \quad c_k(z) = \bar{f}(z) \delta_{k0} + \sum_{m=1}^M c_{mk} \sqrt{\mu_m} \phi_m(z) \end{aligned}$$

- $\Rightarrow$ a PC expansion at every z : closed-form mean, variance, Sobol indices ($\mathbb{K}_i$: basis terms involving λ_i only)

$$\mathbb{V}[f(z)] = \sum_{k \geq 1} c_k^2(z) \|\Psi_k\|^2, \quad S_i(z) = \sum_{k \in \mathbb{K}_i} c_k^2(z) \|\Psi_k\|^2 / \mathbb{V}[f(z)]$$



Main-effect sensitivity of ELM GPP to fLNR, per grid cell

(shown: KLNN + sampling; KLPC gives such maps analytically)

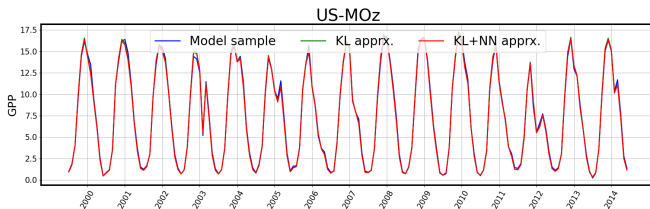
[Mueller *et al.*, JUQ 2025;
Sargsyan *et al.*, in review]

Surrogate in the Latent Space: KL+NN

- One multi-output surrogate $\lambda \mapsto (\xi_1, \dots, \xi_M)$, then decode back to the field

$$f(\lambda; z) \approx \bar{f}(z) + \sum_{m=1}^M \xi_m^{NN}(\lambda) \sqrt{\mu_m} \phi_m(z)$$

- NN instead of PC: flexible, all M outputs at once; GSA only by sampling
- Errors: KL truncation + surrogate $\Rightarrow$ **UQ for surrogates**

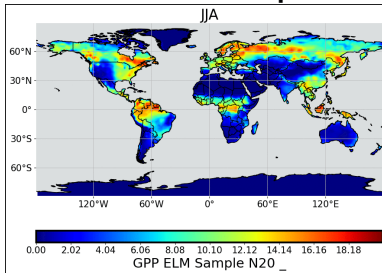


E3SM land, 96 sites $\times$ 180 months: one NN, 8 latent outputs
instead of 17,280 separate surrogates

Example: E3SM Land Model

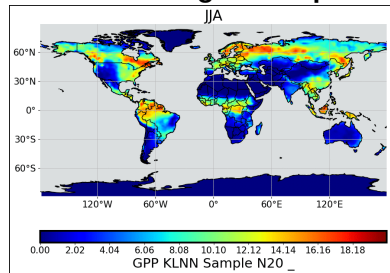
- 10 uncertain parameters, 275 training runs
- Output: gross primary productivity (GPP), 4000 cells $\times$ 4 seasons = 16,000 values
- KL: 16,000 $\rightarrow$ 11 latent dimensions; NN surrogate on the latent features

ELM model sample



several hours per run

KLNN surrogate sample



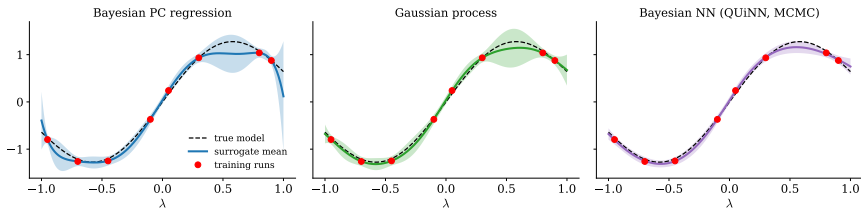
$\sim$ 1 second per run

[Sargsyan *et al.*, in review]

Flipping the Question: UQ *for* Surrogates

So far: surrogates *for* UQ (forward UQ) $\Rightarrow$ Now: UQ *for* surrogates

- Few expensive runs $\Rightarrow$ surrogate error can rival parametric uncertainty
- Bayesian regression gives the surrogate its own uncertainty
 - Bayesian PC: posterior on the coefficients c [Sargsyan, 2017]
 - Bayesian CS: sparse *and* uncertain coefficients
 - Gaussian process: posterior variance
 - UQ for NN surrogates (*e.g.* the QUiNN library)
(*e.g.* see next subtalk)



Why UQ for Surrogates Matters

- **Calibration (inverse UQ):** surrogate error enters the likelihood

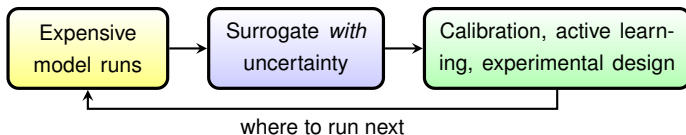
$$y_i = f_s(\boldsymbol{\lambda}; z_i) + \epsilon_i^{\text{surr}} + \epsilon_i^{\text{data}}$$

$$\Rightarrow L(\boldsymbol{\lambda}) \propto \prod_i \mathcal{N}(y_i; \mu_s(\boldsymbol{\lambda}; z_i), \sigma_{\text{data}}^2(z_i) + \sigma_{\text{surr}}^2(\boldsymbol{\lambda}; z_i))$$

- ignore σ_{surr} $\Rightarrow$ overconfident, biased posteriors
- in latent space: add surrogate variance per KL mode

- **Outer-loop activities** need trustworthy surrogate errors

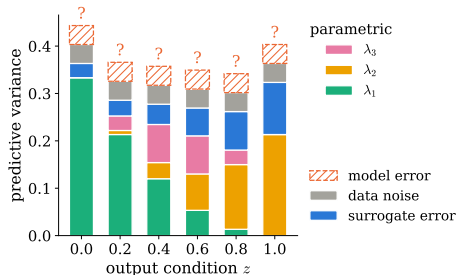
- active learning: run the model where the surrogate is least certain
- experimental design: which experiment best constrains $\boldsymbol{\lambda}$?
- model comparison and selection



Uncertainty Attribution

- Split the predictive variance at each condition z (law of total variance)

$$\text{Var}[y(z)] = \underbrace{\sum_i V_i(z)}_{\text{parametric (Sobol)}} + \underbrace{\sigma_{\text{surr}}^2(z)}_{\text{surrogate error}} + \underbrace{\sigma_{\text{data}}^2(z)}_{\text{data noise}} + \underbrace{\sigma_{\delta}^2(z)}_{\text{model error}}$$



Where to invest:

parametric $\Rightarrow$ calibrate

surrogate $\Rightarrow$ more runs

noise $\Rightarrow$ better data

model $\Rightarrow$ improve model

**Calibration (inverse UQ) and
model error: stories for another day**

[Kennedy & O'Hagan, 2001; Sargsyan, Huan & Najm, 2019]

Software: PyTUQ

- Python Toolkit for Uncertainty Quantification
- <https://github.com/sandialabs/pytuq>
- The Python offspring of UQTK (C++/Python)
- A FASTMath (SciDAC) library; BSD-3 license

PyTUQ



surrogates	PC, NN; multi-output KL-based workflows
lreg	Bayesian regression, sparse regression, BCS
linred	Karhunen-Loève, SVD
gsa	global sensitivity analysis (Sobol indices)
minf	Bayesian inference: MCMC, likelihoods, model error
rv, ftools, optim	random variables, integration, optimization

- **QUINN**: UQ library for PyTorch NNs via probabilistic wrappers (MCMC, variational, Laplace, SWAG, deep ensembles)
<https://github.com/sandialabs/quinn>

Summary

- Surrogates *for* UQ, inputs ($d \gtrsim 100$): exploit low effective dimension
 - screen (sensitivity), sparsify (BCS), rotate (active subspaces)
 - pre-screening makes NN/GP surrogates easier to train and interpret
- Surrogates *for* UQ, outputs ($N \gtrsim 1000$): exploit correlations
 - KL/SVD down to a handful of latent features; KL+PC gives sensitivities at every z
 - build surrogates *and* calibrate in the latent space
- UQ *for* surrogates:
 - needed for predictions, calibration likelihoods, active learning, experimental design
 - *e.g.* see Julie's talk next: quantify NN uncertainty
- Inverse UQ / Model Calibration (not covered here)
 - Uncertainty attribution: decompose predictive variance into parametric, surrogate, data, and model contributions
 - Model error: often critically overlooked
- Software
 - PyTUQ: Python toolkit for UQ <https://github.com/sandialabs/pytuq>
 - QUIINN: UQ for PyTorch NNs <https://github.com/sandialabs/quinn>

Literature: High-d Inputs

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Literature (cont.)

Thank you!

High-d outputs

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UQ for surrogates

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Software

PyTUQ: github.com/sandialabs/pytuq

QUiNN: github.com/sandialabs/quinn

UQTk: www.sandia.gov/uqtoolkit

Calibration in the Latent Space

- Project observations $g(z)$ onto the same KL basis

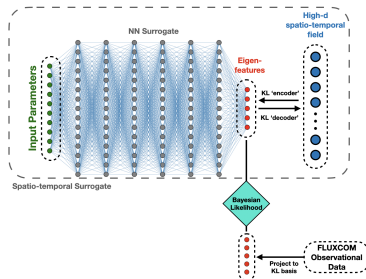
$$\eta_m = \langle g - \bar{f}, \phi_m \rangle / \sqrt{\mu_m}$$

- Pointwise likelihood (naive): N correlated residuals treated as independent

$$L(\lambda) \propto \exp \left(- \sum_{i=1}^N \frac{(g(z_i) - f(\lambda; z_i))^2}{2\sigma_i^2} \right)$$

- Latent likelihood: $M \ll N$ uncorrelated features

$$L(\lambda) \propto \exp \left(- \sum_{m=1}^M \frac{(\eta_m - \xi_m^{NN}(\lambda))^2}{2\sigma^2} \right)$$



Cheap surrogate
+ low-d likelihood
⇒ feasible MCMC

σ^2 should include
surrogate error
⇒ UQ for surrogates