

Geometric Considerations when Surrogate Modeling for Multiobjective Optimization

Tyler Chang^a, Manisha Garg^{a,b}, and Stefan Wild^a

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^bDept. of Mathematics, Univ. Illinois Urbana Champaign

SIAM MDS 2022

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The Geometry of a Bad Dataset

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Outlines

Problem Setting and Some Background

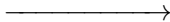
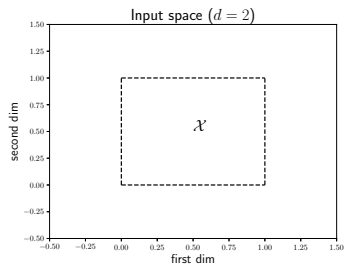
My Story with Interpolation Methods

The Geometry of Bad Data

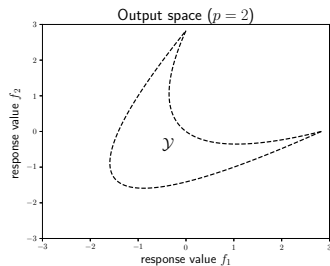
A Proposed Solution

Problem Setting and Some Background

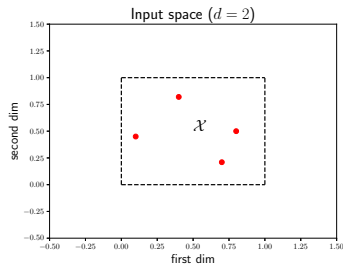
Multivariate Interpolation



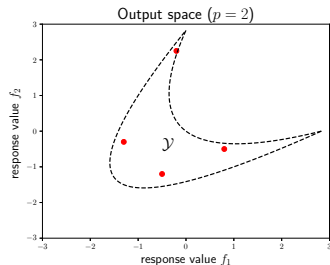
$$F : \mathcal{X} \rightarrow \mathcal{Y}$$



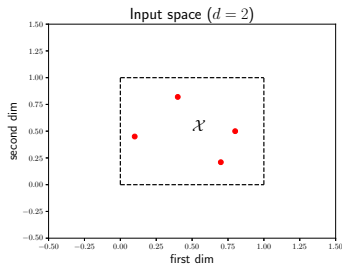
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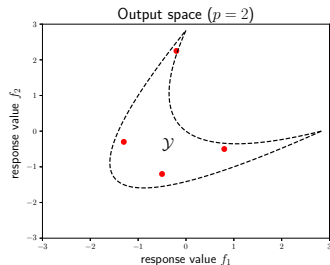
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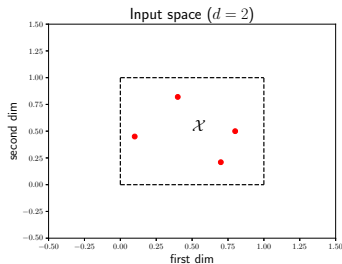


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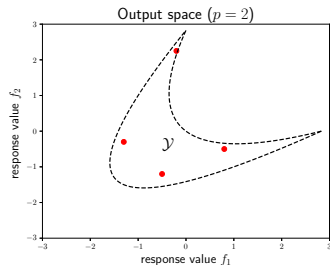


Given a set of n points \mathcal{P} in \mathcal{X} , find $\hat{F} \approx F$ such that $\hat{F}(\mathbf{x}) = F(\mathbf{x})$ for all $\mathbf{x} \in \mathcal{P}$

Multivariate Interpolation



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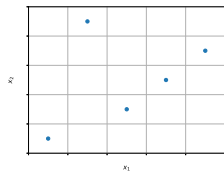


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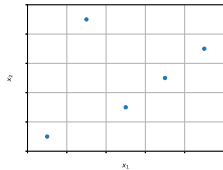
Suppose $\mathcal{X} \subset \mathbb{R}^d$ and $\mathcal{Y} \subset \mathbb{R}^p$, and F is continuous

My Motivation: Multiobjective RSM

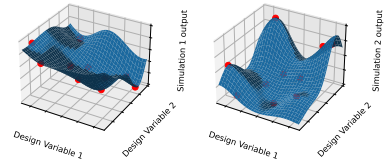
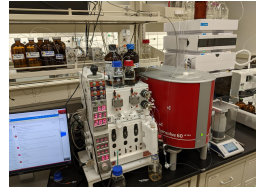
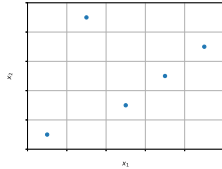
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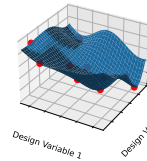
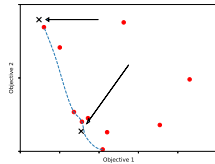
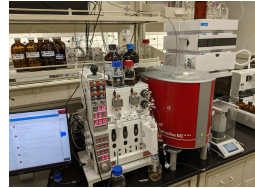
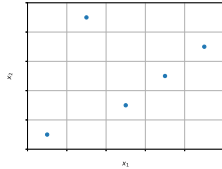
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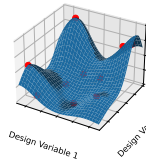
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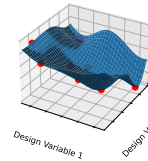
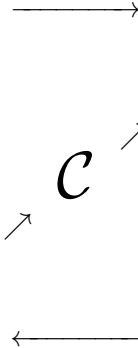
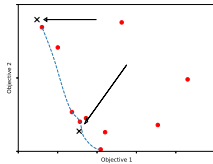
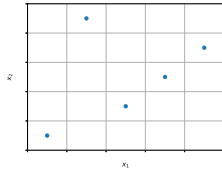


Simulation 1 output

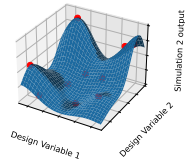


Simulation 2 output

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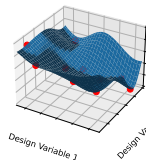
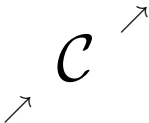
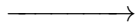
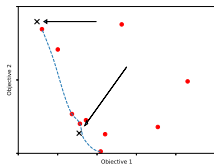
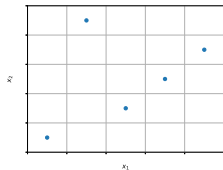


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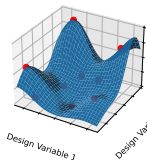


Simulation 2 output

My Motivation: Multiobjective RSM



Simulation 1 output



Simulation 2 output

<https://github.com/parmoo/parmoo>

Interpolation Techniques

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- ▶ “Classical” interpolation techniques
 - ▶ Polynomial interpolation
 - ▶ B-spline interpolation
 - ▶ RBF interpolants
 - ▶ generalized Shepard’s methods
 - ▶ **Piecewise linear interpolation**

My Story with Interpolation Methods

Piecewise Linear Interpolation

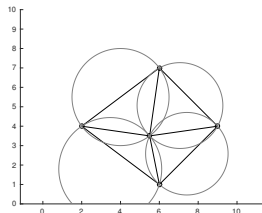
- ▶ Let $\mathcal{T}(\mathcal{P})$ be a d -dimensional triangulation of \mathcal{P} .
- ▶ Given an interpolation point $q \in \mathcal{CH}(\mathcal{P})$, let \mathcal{S} be a simplex in $\mathcal{T}(\mathcal{P})$ with vertices s_1, \dots, s_{d+1} such that $q \in \mathcal{S}$.
- ▶ Then there exist unique *convex weights* w_1, \dots, w_{d+1} such that $q = \sum_{i=1}^{d+1} w_i s_i$.

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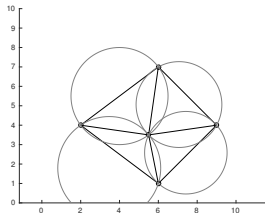
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Chang et al. 2020. Algorithm 1012: DELAUNAYSPARSE. ACM TOMS 46(4), Article No. 38.



Error Rates for Piecewise Linear Interpolants

For an individual component function F_i :

- ▶ Let ∇F_i be λ -Lipschitz in the 2-norm
- ▶ For $\mathcal{S} \in \mathcal{T}$ containing q ,
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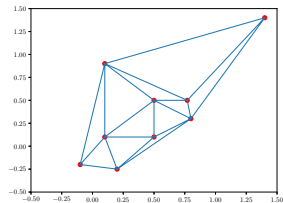
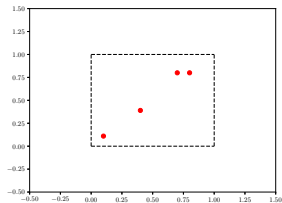
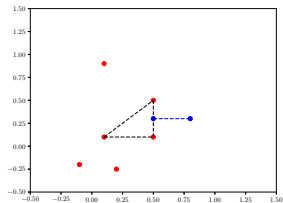
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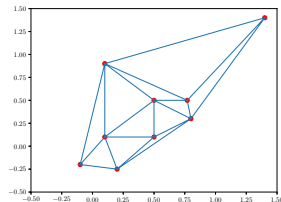
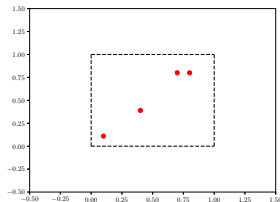
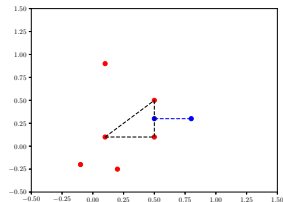
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*Lux, Watson, **Chang**, et al. 2021. Interpolation of sparse high-dimensional data. Numerical Algorithms 88(1), 281–313.*

Issues Solving Real-World Problems

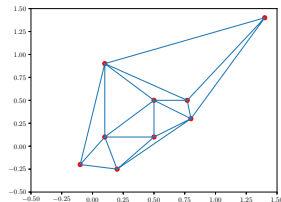
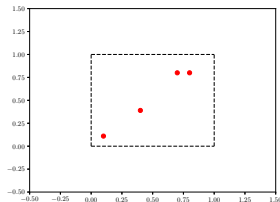
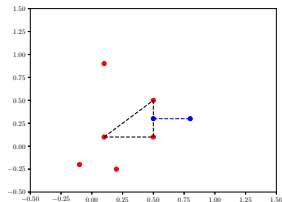


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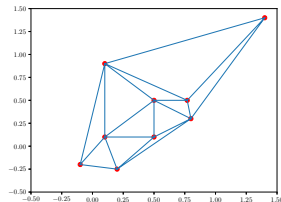
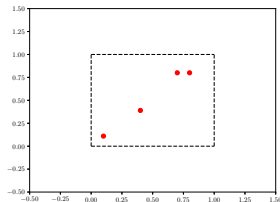
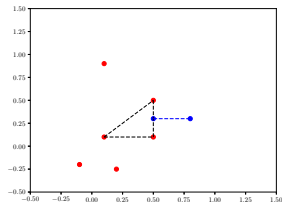
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- ▶ Too many extrapolation points (information lost in projection)
- ▶ “Flat” data set – cannot (accurately) triangulate
- ▶ Several massive simplices (high error-rate, poor conditioning)

What does the theory say?

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Gorban et al. 2017. Stochastic separation theorems. Neural Networks 94, 255-259.

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Let \mathcal{P} be randomly sampled by a distribution μ , then

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My take:

Yes, it does... and it's bad.

The Geometry of Bad Data

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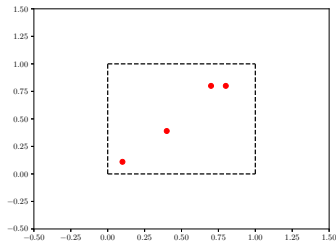
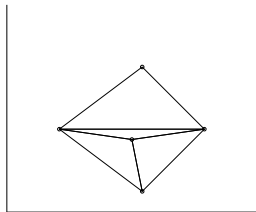
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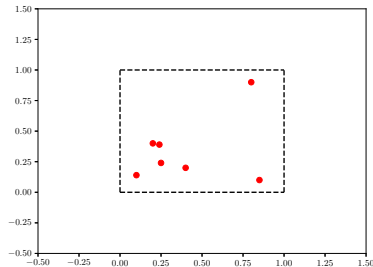
- ▶ Simplices are long and narrow
- ▶ κ_S term blows up
- ▶ \hat{F}_T is hard to compute and low accuracy
- ▶ Ex: data lies close to a lower-dimensional manifold



What Could Go Wrong: Data imbalance

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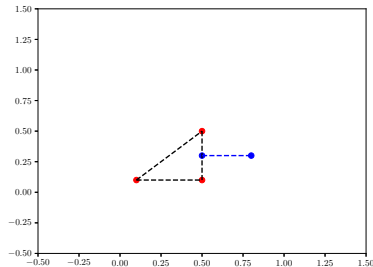
- ▶ Data accumulates in subregions of \mathcal{X}
- ▶ ξ stays large in less-dense regions of \mathcal{X}
- ▶ Can also result in poor conditioning, but they are not the same
- ▶ Called *high discrepancy*



What Could Go Wrong: Extrapolation

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- ▶ $\hat{F}_{\mathcal{T}}$ is only defined in the $\mathcal{CH}(\mathcal{P})$
- ▶ Will have to project q into $\mathcal{CH}(\mathcal{P})$ and interpolate projection
- ▶ Low accuracy when residual is large
- ▶ When $\mathcal{CH}(\mathcal{P})$ is a small subset of \mathcal{X} , overall accuracy can be poor



Same Issues for RBFs/GPs

$$\hat{F}_{RBF} = \omega^\top \begin{bmatrix} e^{-\|x_1 - x\|^2 / \sigma} \\ e^{-\|x_2 - x\|^2 / \sigma} \\ \vdots \\ e^{-\|x_n - x\|^2 / \sigma} \end{bmatrix}$$

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where $A\omega = y$ and

$$A = \begin{bmatrix} 1 & e^{-\|x_1 - x_2\|^2/\sigma} & \dots & e^{-\|x_1 - x_n\|^2/\sigma} \\ e^{-\|x_2 - x_1\|^2/\sigma} & 1 & \dots & e^{-\|x_2 - x_n\|^2/\sigma} \\ \vdots & \vdots & & \vdots \\ e^{-\|x_n - x_1\|^2/\sigma} & e^{-\|x_n - x_2\|^2/\sigma} & \dots & 1 \end{bmatrix} \quad y = \begin{bmatrix} F(x_1) \\ F(x_2) \\ \vdots \\ F(x_n) \end{bmatrix}$$

RBF/GP Conditioning and Accuracy

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- ▶ As we seek higher accuracy, data points get closer together
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- ▶ Decrease the shape parameter σ to keep A nonsingular

RBF/GP Conditioning and Accuracy

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- ▶ “Uncertainty principle” – for real-world datasets, cannot have accuracy and solvability

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- ▶ When \hat{F} interpolates, conditions for fully linearity reduce to geometric conditions
 - ▶ $d + 1$ model points in ball are affinely independent
- ▶ Only accurate within ball
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 - ▶ no convergence in low-density regions

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Real-world datasets have zero-volume in high-dimensions, which leads to all of the properties

A Proposed Solution

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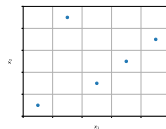
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- ▶ Latin hypercubes
 - ▶ Stratifies sample – good for linear models
 - ▶ No theory for nonlinear models
 - ▶ Heuristically good in practice and cheap to calculate

Stochastic Fourier SFD

- Desired sample size
- Performance criteria

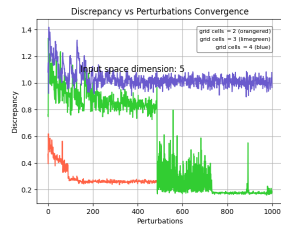
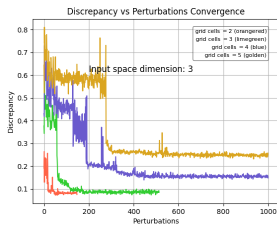
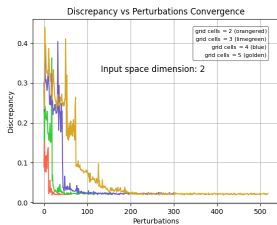


COBYLA



$$\alpha_1 e^{2\pi i x} + \alpha_2 e^{2\pi i (2x)} + \dots$$

Preliminary Results



E-mail: `tchang@anl.gov`

Code: `github.com/thchang/sf-sfd`

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