Data sampling for surrogate modeling and optimization

Tyler Chang

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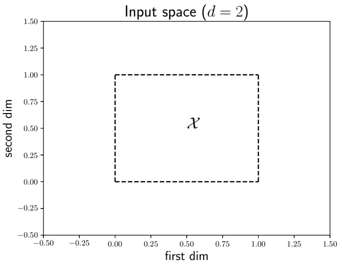
Outlines

Problem Setting and Some Background

Multivariate Interpolation



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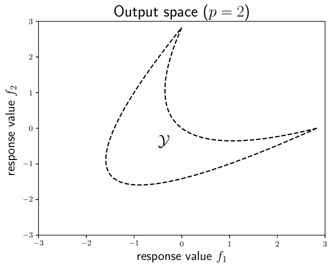
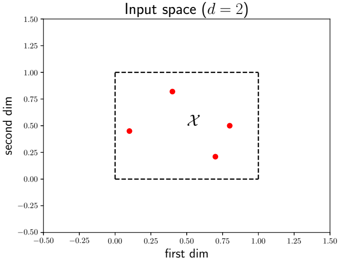


Multivariate Interpolation



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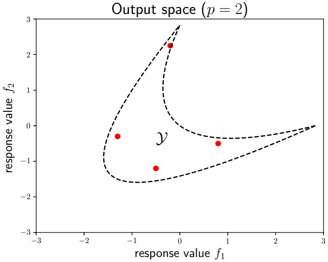

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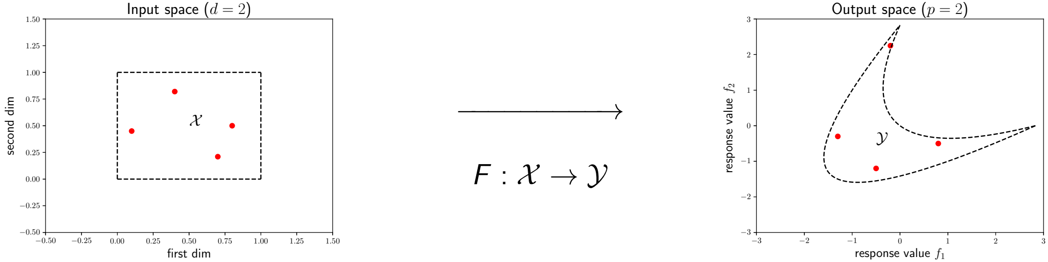

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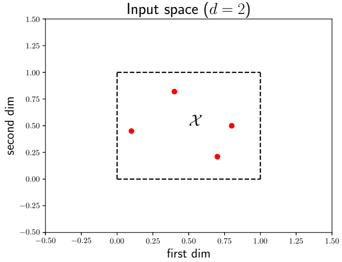

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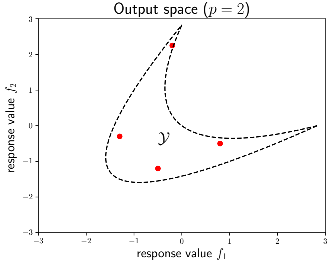

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Suppose $\mathcal{X} \subset \mathbb{R}^d$ and $\mathcal{Y} \subset \mathbb{R}^p$, and F is continuous

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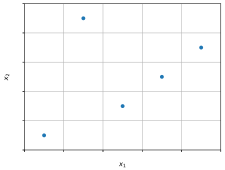

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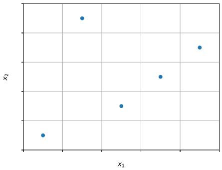

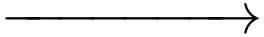

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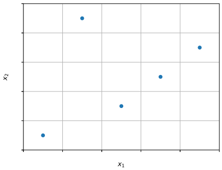

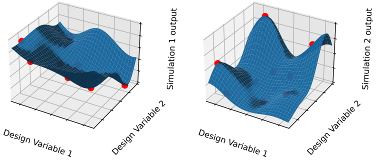

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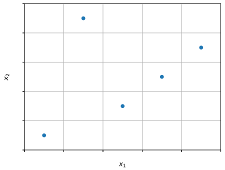

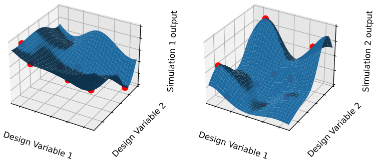

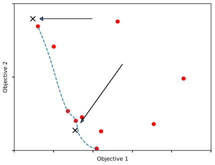

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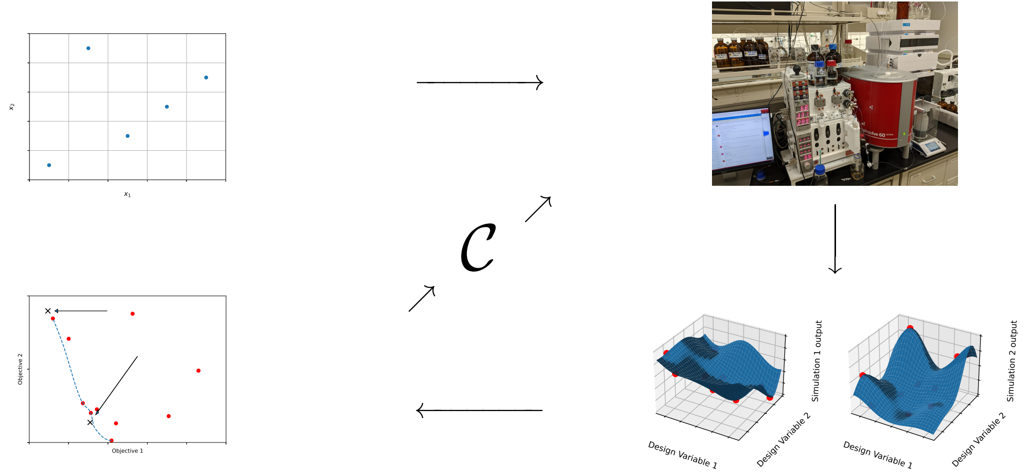

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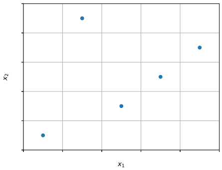

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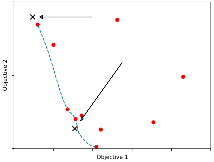

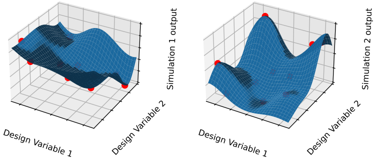

https://github.com/parmoo/parmoo

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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 $s_1, \ldots, s_{d+1}$ such that $q \in \mathcal{S}$.
- Then there exist unique *convex weights* $w_1, \ldots, w_{d+1}$ such that $q = \sum_{i=1}^{d+1} w_i s_i$.

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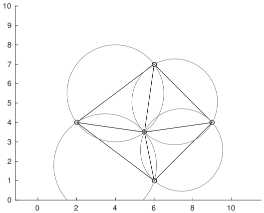

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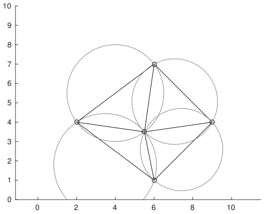

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Chang *et al. 2020. Algorithm 1012: DELAUNAYSPARSE. ACM TOMS 46(4), Article No. 38.*

Error Rates for Piecewise Linear Interpolants

For an individual component function F_i:

- Let ∇F_i be λ-Lipschitz in the 2-norm
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Lux, Watson, ***Chang****, et al. 2021. Interpolation of sparse high-dimensional data. Numerical Algorithms 88(1), 281–313.*

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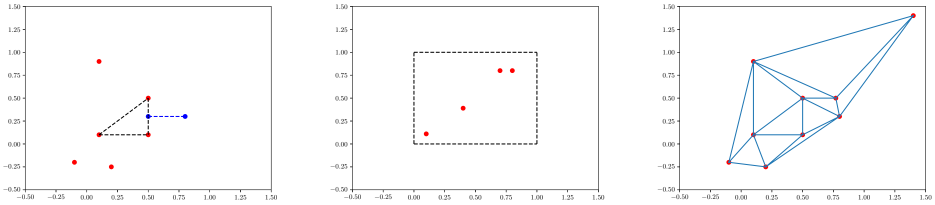

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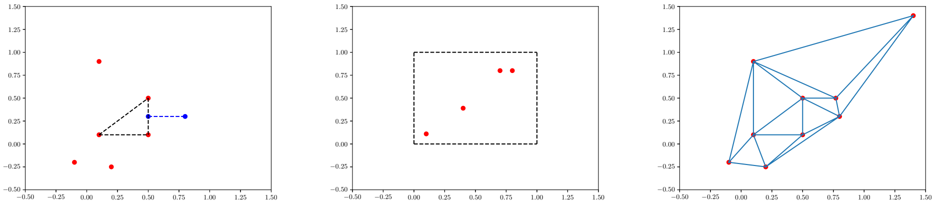

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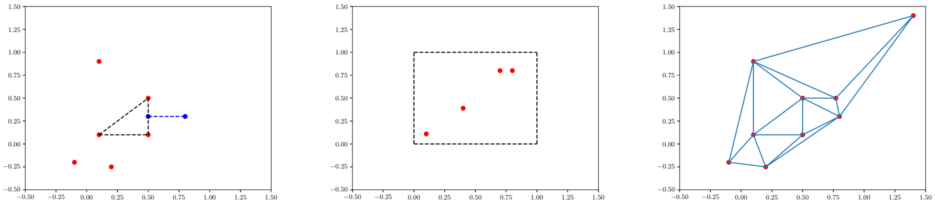

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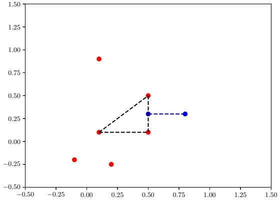

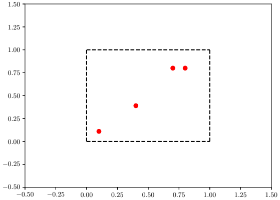

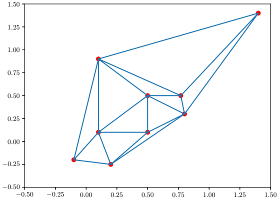

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- Several massive simplices (high error-rate, poor conditioning)

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My take:
Yes, it does... and it's bad.

The Geometry of Bad Data

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What Could Go Wrong: Poor data conditioning

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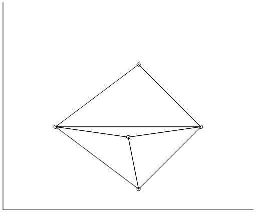
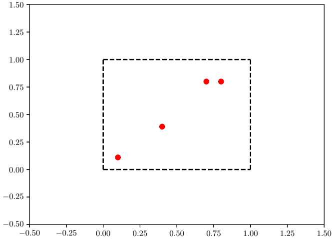
- Simplices are long and narrow
- $\kappa_{\mathcal{S}}$ term blows up
- $\hat{F}_{\mathcal{T}}$ is hard to compute and low accuracy
- Ex: data lies close to a lower-dimensional manifold





What Could Go Wrong: Data imbalance

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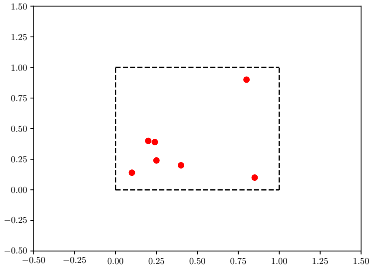
- Data accumulates in subregions of $\mathcal{X}$
- ξ stays large in less-dense regions of $\mathcal{X}$
- Can also result in poor conditioning, but they are not the same
- Called *high discepancy*



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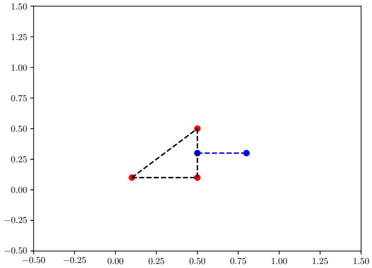
- $\hat{F}_{\mathcal{T}}$ is only defined in the $\mathcal{CH}(\mathcal{P})$
- Will have to project q into $\mathcal{CH}(\mathcal{P})$ and interpolate projection
- Low accuracy when residual is large
- When $\mathcal{CH}(\mathcal{P})$ is a small subset of $\mathcal{X}$, overall accuracy can be poor



Same Issues for RBFs/GPs

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where $A\omega = y$ and

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- "Uncertainty principle" – for real-world datasets, cannot have accuracy and solvability

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for all $\|x - x_0\| < \delta$.

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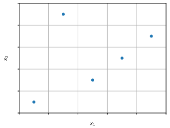
- Latin hypercubes
  - Stratifies sample – good for linear models
  - No theory for nonlinear models
  - Heuristically good in practice and cheap to calculate

Stochastic Fourier SFD

- Desired sample size
- Performance criertia

$\longrightarrow$



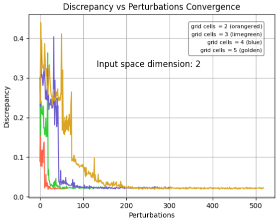
$\downarrow$

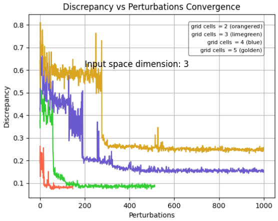
$$\alpha_1 e^{2\pi i x} + \alpha_2 e^{2\pi i (2x)} + \dots$$

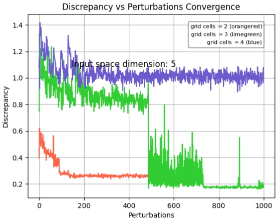
$\longleftarrow$

`COBYLA`

Preliminary Results







Resources

E-mail: tchang@anl.gov

Code: github.com/thchang/sf-sfd

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