Data sampling for surrogate modeling and optimization

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(and others)

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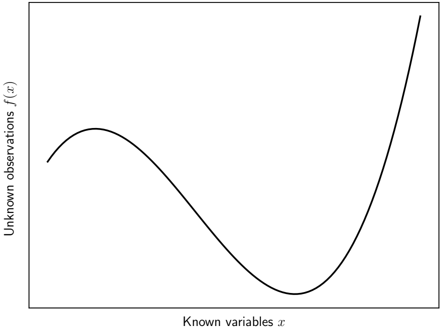
Outlines

Inference problems, the curse of dimensionality, and measure collapse

Modeling for high-dimensional optimization

The fundamental machine learning problem

The fundamental machine learning problem



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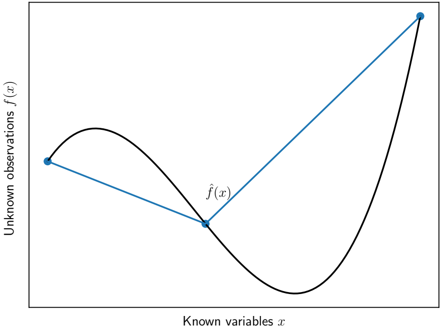
The fundamental machine learning problem



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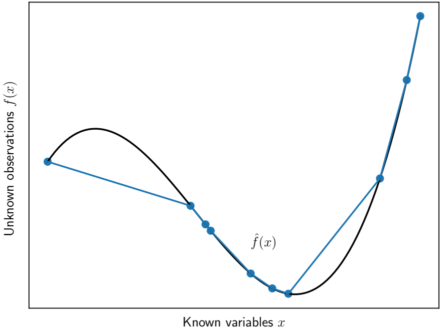

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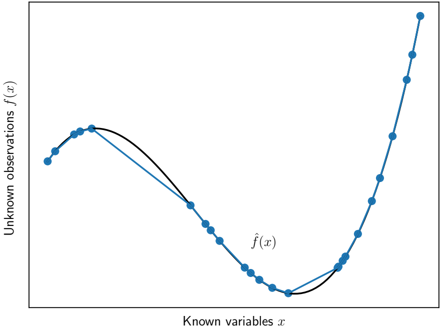

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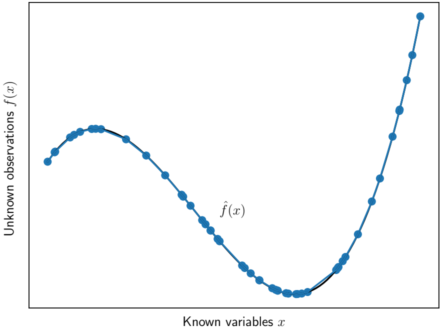

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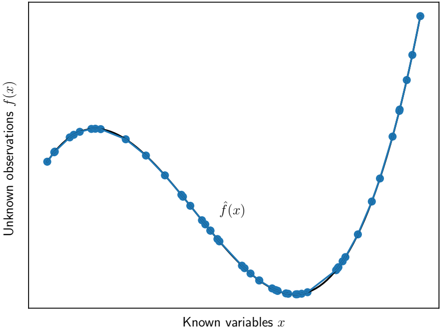
- If we have enough data, it doesn't matter

Some basic numerical analysis results

When $\hat{f}$ is a piecewise linear spline:

For h "small enough" – let q be the querry point

$$|f(q) - \hat{f}(q)| \sim \mathcal{O}(h^2)$$



- h is a "mesh fineness" parameter $\sim$ distance between points in $\mathcal{X}$
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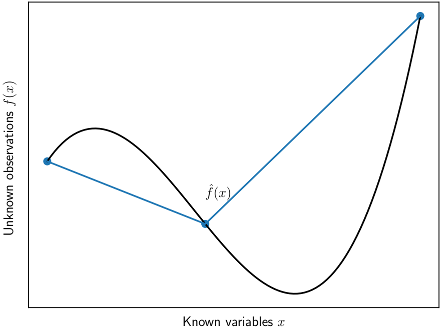

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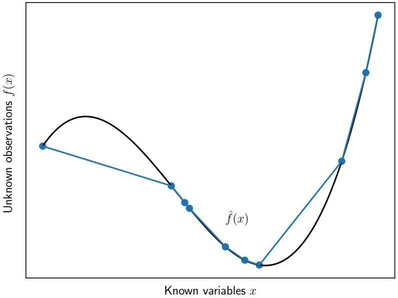
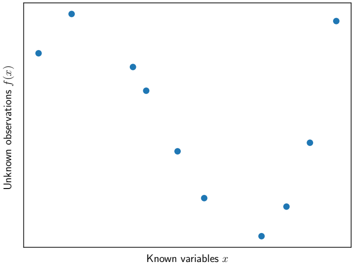
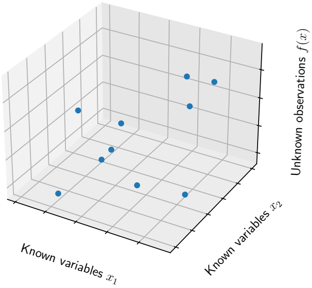


The curse of dimensionality

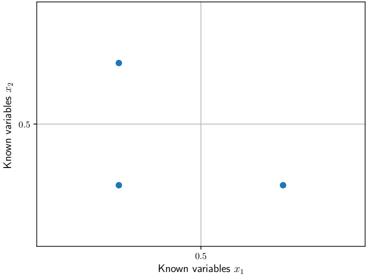


10 training points in 1D



10 training points in 2D

The curse of ~~dimensionality~~ no data



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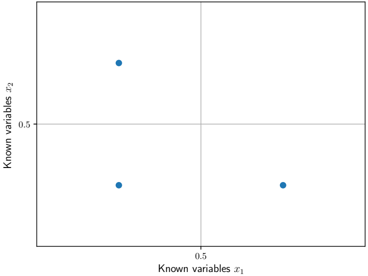
The curse of ~~dimensionality~~ no data



Need data in all quadrants?

- Inference in 2D : $2^2 = 4$
- Inference in 10D : $2^{10} \approx 1000$
- Inference in 100D : $2^{100} \approx 10^{30}$ (orders of magnitude bigger than exascale)
- Many ML problems : inference in 1000+ dimensions

Measure collapse

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If $\mathcal{X}$ are sampled from *any* distribution, $\mu(CH(\mathcal{X})) \to 0$ *exponentially* as d grows

This is called a *concentration of measure*

Gorban and Tyukin, Stochastic separation theorems. *Neural Networks 94*, pp. 255-259 (2017).

Example

Suppose that we uniformly sample $x = (x_1, x_2, \ldots, x_d)$ from $[0,1]^d$

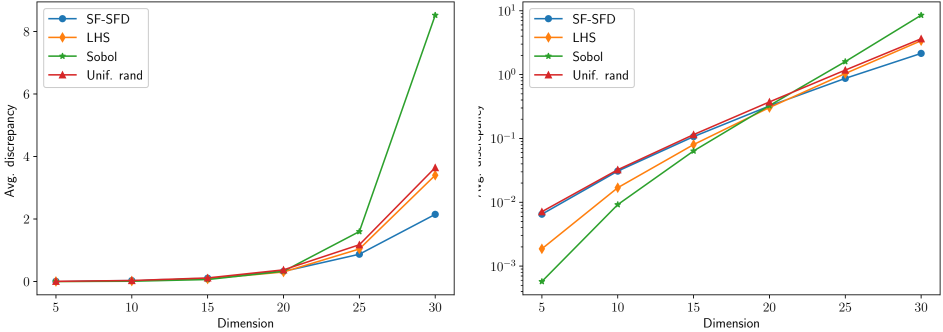
$$\|x - \frac{1}{2}\|_2^2 = \sum_{i=1}^{d} (x_i - \frac{1}{2})^2.$$

$$\mathbb{E}\left[\left(x_i - \frac{1}{2}\right)^2\right] = \int_0^1 \left(u - \frac{1}{2}\right)^2 du = \frac{1}{12}$$

with finite variance ν

By CLT for all $x \in \mathcal{X}$: $\mathbb{E}[\|x - \frac{1}{2}\|_2^2] = \frac{d}{12}$ with variance $\frac{\nu}{d} \to 0$ as $d \to \infty$.

Collapse of some common distributions



Garg, Chang, and Raghavan, Stochastic optimization of Fourier coefficiencts to generate space-filling designs. *To appear in Winter Sim 2023.*

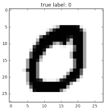
Representation learning solution

“There’s more to machine learning than function approximation”

Representation learning solution

"There's more to machine learning than function approximation"

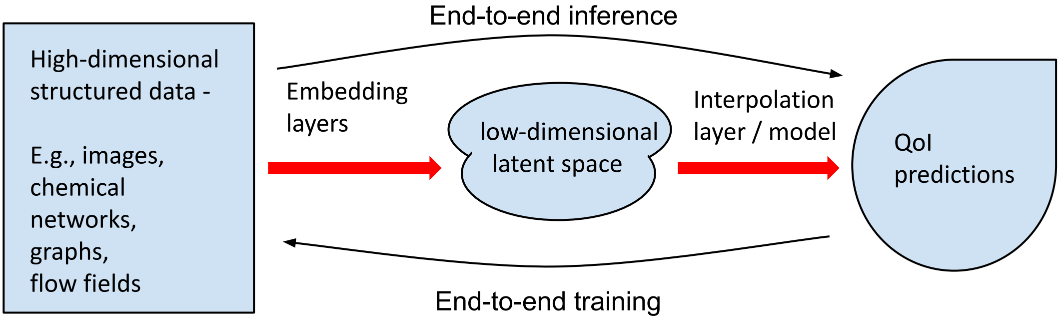
- f is often highly *structured* – MLPs with nothing else are from the 60s



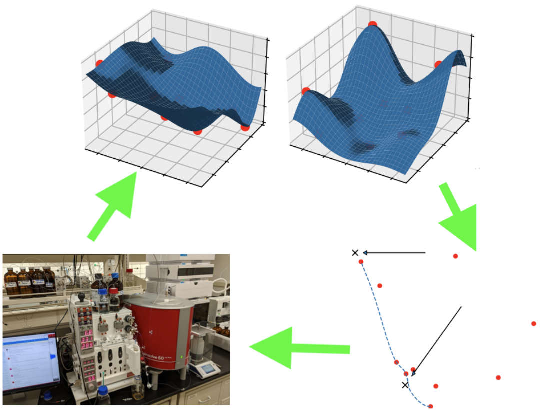
$$\xrightarrow{\quad f \quad} \quad 0$$

28×28 pixels $\neq 784$ dimensions...

Modern deep learning pipeline



Hope in context of optimization



Global modeling is harder than optimization

For optimization, only need model accuracy near the solution...

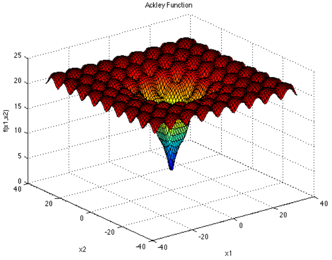
- Global modeling is *significantly harder than optimizing*
- To build a *globally accurate model* over n variables, need $\mathcal{O}(2^n)$ samples
- To build a *locally accurate model* over n variables, need $\mathcal{O}(n)$ samples

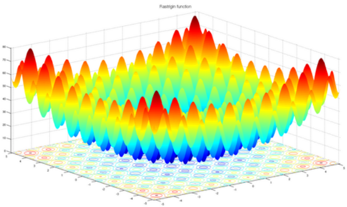
Global optimization

In global optimization literature...

- Balance exploration vs. exploitation
- Drive *global model error* to zero
- Need exponentially many samples to guarantee global convergence

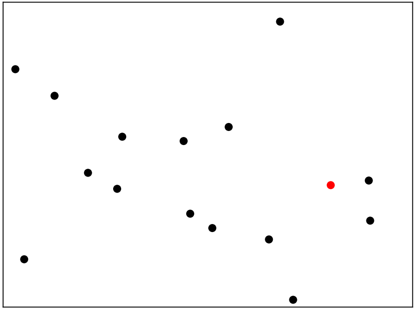
Guarantees convergence for problems with thousands of local minima





Local optimization

- Only exploit – maybe multi-start or large initial search
- Fit a model that is *locally accurate*
  - Sample requirement grows only *linearly with* dimension
- Modification is as simple as putting a *trust-region* around interesting points



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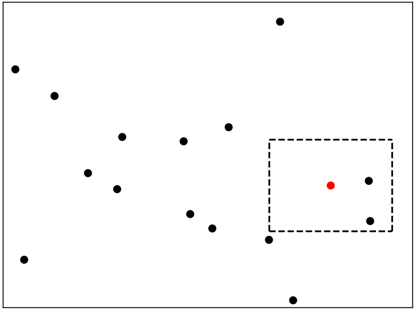

ParMOO

parMOO

Written in Python

Version 0.3.0 is now available on available on `pip`, `conda-forge`, and `GitHub`

`https://github.com/parmoo/parmoo`

`https://parmoo.readthedocs.io`

PyPI

CONDA-FORGE

Chang and Wild. ParMOO: A Python library for parallel multiobjective simulation optimization. *JOSS 8(82):4468 (2023).*