Data sampling for surrogate modeling and optimization

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(and others)

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Outlines

The fundamental machine learning problem

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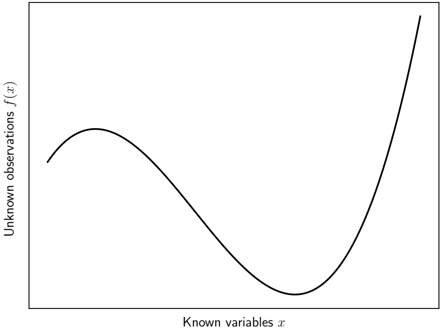
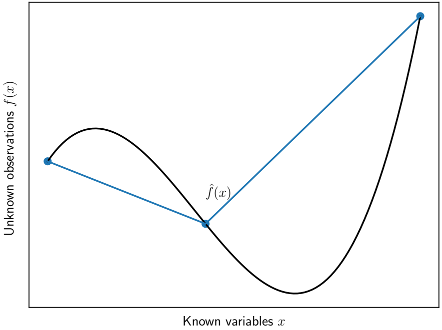


- Want to predict unknown $f(x)$ for observation x

The fundamental machine learning problem



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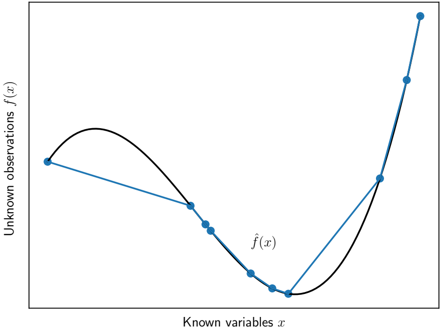

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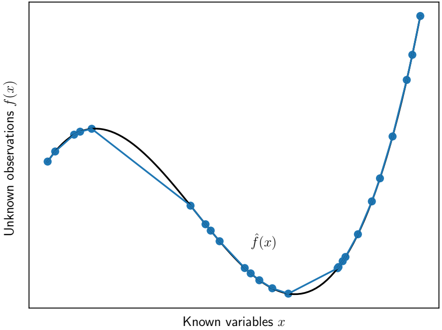

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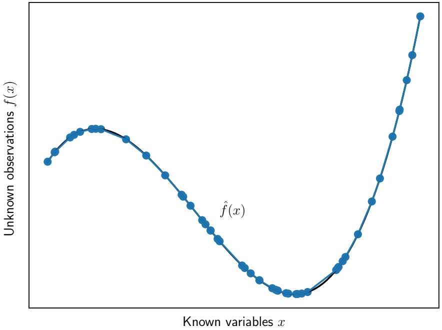

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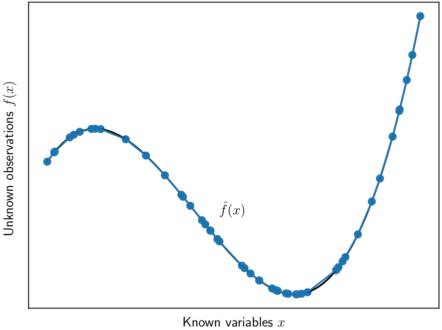
- Real data not perfectly balanced $\Rightarrow$ $\hat{f} \to f$ non-uniformly
- If we have enough data, it doesn't matter

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 $\mathcal{X}$
- For irregular $\mathcal{X}$, h could be the distance from q to the nearest neighbor in $\mathcal{X}$
- Constants proportional to the Lip constant of ∇f

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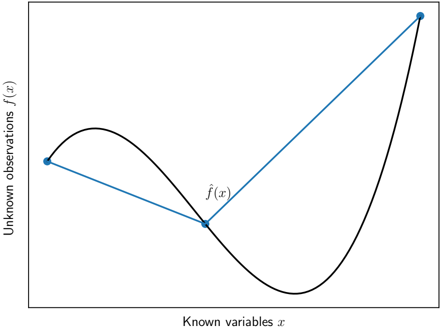

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Some basic deep learning

- Train a fully-connected multi-layer perceptron (MLP) using $\mathcal{X}$
- The most popular activation function is ReLU (piecewise linear)
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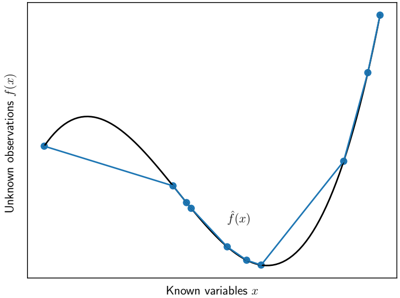
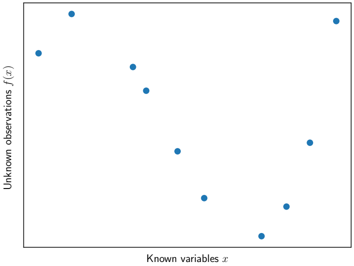
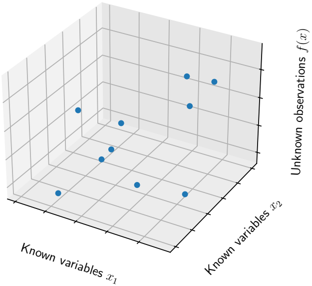


The curse of dimensionality

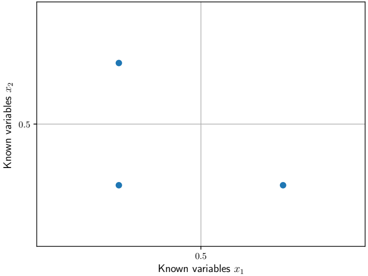


10 training points in 1D



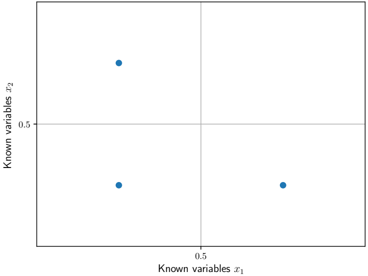
10 training points in 2D

The curse of ~~dimensionality~~ no data



Need data in all quadrants?

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

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Can we still make good predictions where we **do** have data?

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No, because we have no data anywhere

We measure where we *might* have enough data to make a prediction using the "convex hull" of the training data $CH(\mathcal{X})$

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We measure where we *might* have enough data to make a prediction using the "convex hull" of the training data $CH(\mathcal{X})$

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 $[0,1]^d$

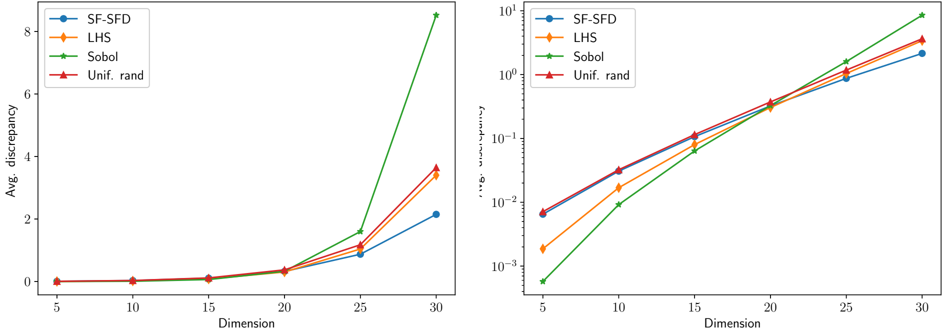
$$\|x - \frac{1}{2}\|_2^2 = \sum_{i=1}^{d} (x_i - \frac{1}{2})^2.$$

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

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”

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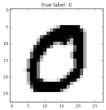
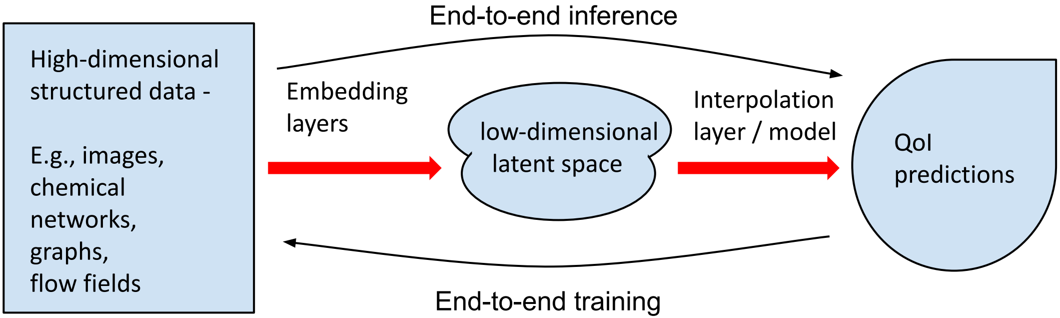
- f is often highly *structured* – MLPs with nothing else are from the 60s



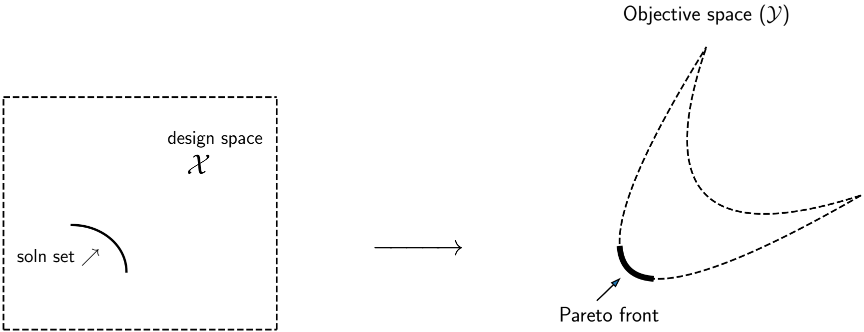
$$\xrightarrow{f} \quad 0$$

28×28 pixels $\neq 784$ dimensions...

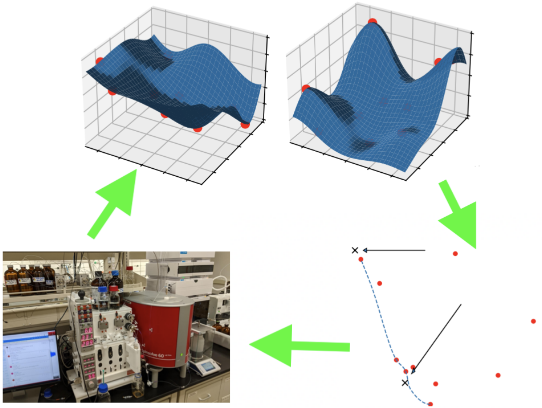
Modern deep learning pipeline



Multiobjective Black-Box Optimization



General Workflow and Data Acquisition

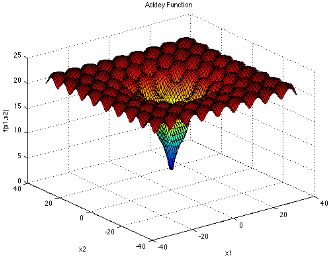


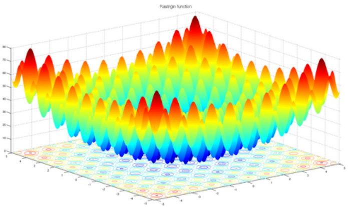
Global optimization

In global optimization literature...

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

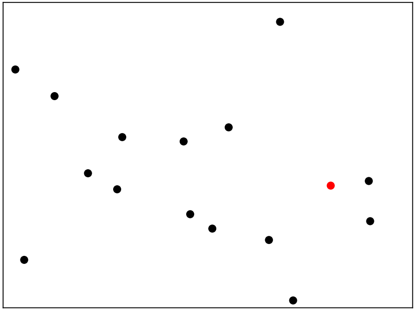
Guarantees convergence for problems with thousands of local minima





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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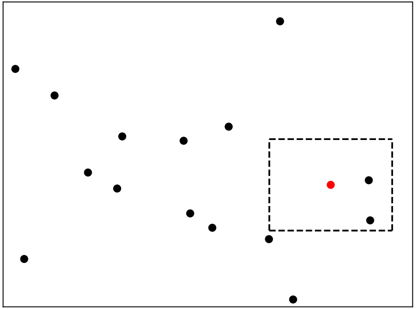

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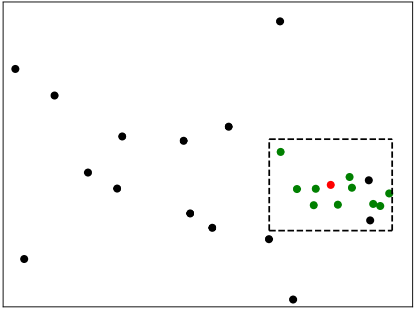

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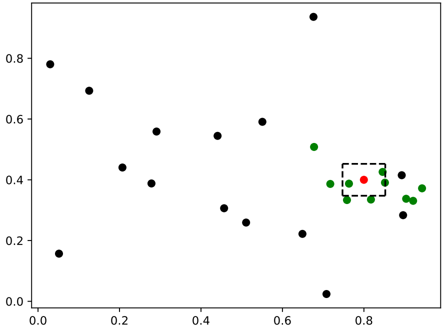


ParMOO

parMOO

Written in `Python`

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

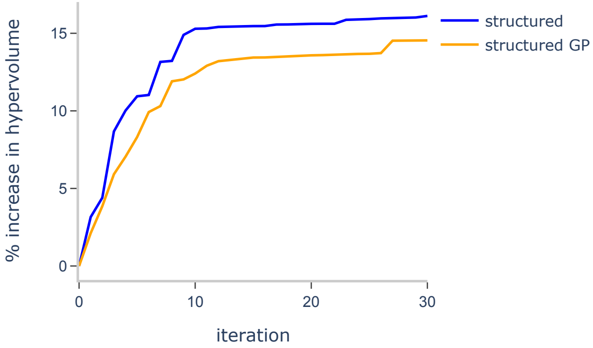
`https://github.com/parmoo/parmoo`

`https://parmoo.readthedocs.io`

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

Chemical Design on a Limited Budget

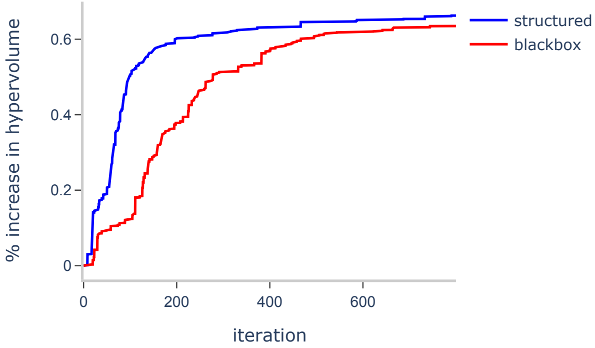
- 6-dimensional latent space embedding of a mixed-variable problem
- 3-objectives electrolyte manufacturing
  - high yield, minimal byproduct, low reaction times
- Running real-world experiments with very limited budget



Chang et al. A framework for fully autonomous design of materials via multiobjective optimization and active learning: challenges and next steps *In ICLR 2023, Workshop on ML4Materials.*

Fayans Model Calibration (Inverse Problem)

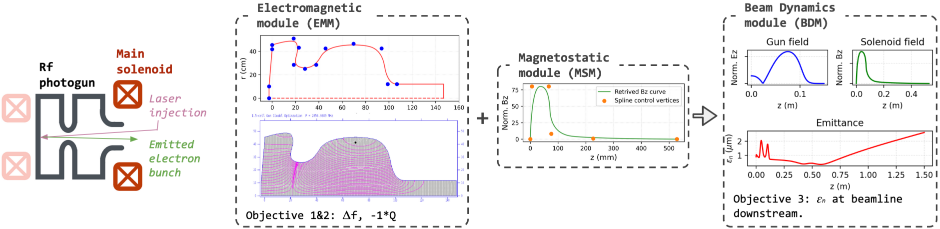
- 13-variable, 3-objective problem
- Higher dimensional, requires trust-region methods



Chang and Wild. Designing a framework for solving multiobjective simulation optimization problems. *Under review, preprint https://arxiv.org/abs/2304.06881.*

Particle Accelerator Beam Design

- 22-variable, 2-objective problem
- 3 physics constraints, nearly impossible to satisfy
- Matched well-known reference gun geometry with just **1300** true simulation evaluations



Chen, Chang, et al. An Integrated Multi-Physics Optimization Framework for Particle Accelerator Design. *Under review.*

Some Conclusions

- Doing anything global (modeling, optimization, etc.) in high-dimensions is very hard (maybe impossible)
- Easier to identify low-dimensional structures and model these *locally*
  - In my experience, giving up global accuracy is the only thing that scales to big problems
- Some problems (optimization) don't necessarilly require global accuracy
  - Don't demand it if you don't need it!
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- Some problems (optimization) don't necessarilly require global accuracy
  - Don't demand it if you don't need it!
- Optimization rarely truly requires global accuracy
- *But there are other problems that do require global accuracy...*

References

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Resources

GitHub: `github.com/parmoo/parmoo`

Pip: `pip install parmoo`
Conda: `conda install --channel=conda-forge parmoo`

Test problems: `github.com/parmoo/parmoo-solver-farm`

`tchang@anl.gov`

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