Argonne NATIONAL LABORATORY

Data sampling for surrogate modeling and optimization

Tyler Chang
(and others)

Argonne National Laboratory

ICIAM 2023, Tokyo, Japan
Aug 23, 2023

Outlines

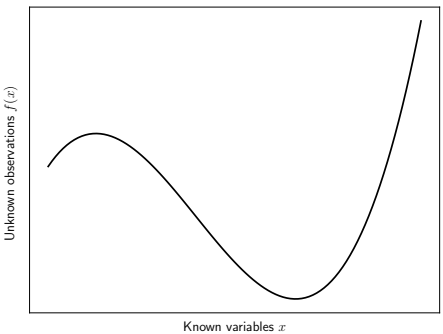
Inference problems, the curse of dimensionality, and measure collapse

Modeling for high-dimensional optimization

Some Applications

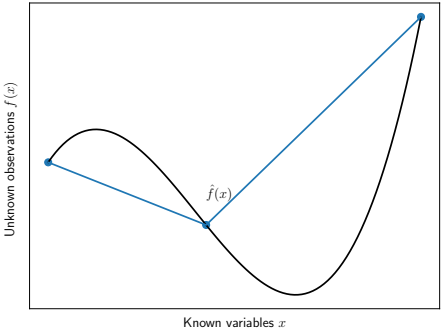
The fundamental machine learning problem

The fundamental machine learning problem



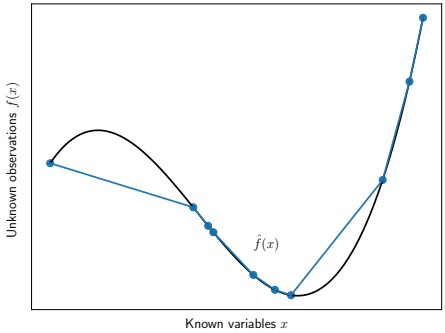
- Want to predict unknown $f(x)$ for observation x

The fundamental machine learning problem



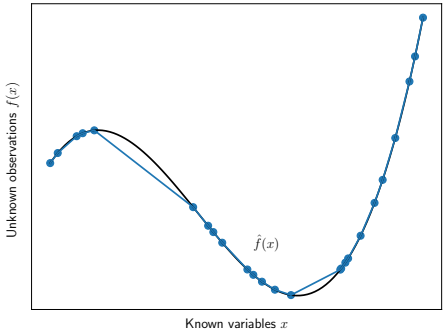
- Want to predict unknown $f(x)$ for observation x
- **ML**: *Learn* approximation $\hat{f} \sim f$ based on *training data* $\mathcal{X}$
- **NA**: fit an interpolant (piecewise-linear) to f on $\mathcal{X}$

The fundamental machine learning problem



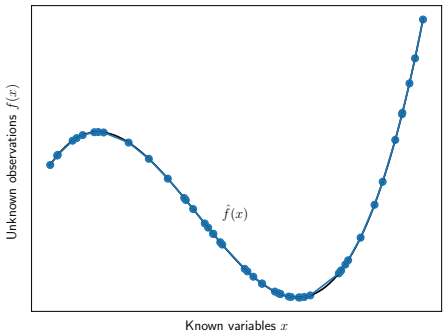
- Want to predict unknown $f(x)$ for observation x
- **ML**: *Learn* approximation $\hat{f} \sim f$ based on *training data* $\mathcal{X}$
- **NA**: fit an interpolant (piecewise-linear) to f on $\mathcal{X}$
- Both cases: more data $\Rightarrow$ better $\hat{f}$

The fundamental machine learning problem



- Want to predict unknown $f(x)$ for observation x
- **ML**: *Learn* approximation $\hat{f} \sim f$ based on *training data* $\mathcal{X}$
- **NA**: fit an interpolant (piecewise-linear) to f on $\mathcal{X}$
- Both cases: more data $\Rightarrow$ better $\hat{f}$
- Real data not perfectly balanced $\Rightarrow$ $\hat{f} \to f$ non-uniformly

The fundamental machine learning problem



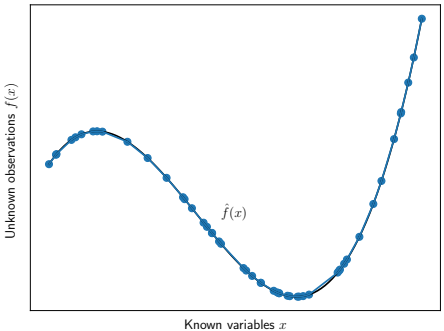
- Want to predict unknown $f(x)$ for observation x
- **ML**: *Learn* approximation $\hat{f} \sim f$ based on *training data* $\mathcal{X}$
- **NA**: fit an interpolant (piecewise-linear) to f on $\mathcal{X}$
- Both cases: more data $\Rightarrow$ better $\hat{f}$
- Real data not perfectly balanced $\Rightarrow$ $\hat{f} \to f$ 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

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



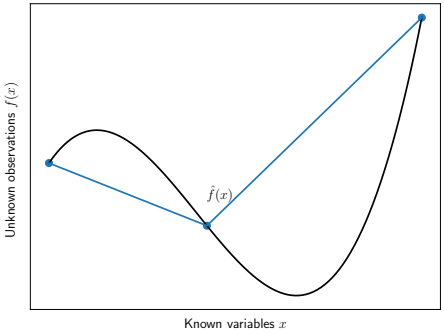
- h is a "mesh fineness" parameter $\sim$ distance between points in $\mathcal{X}$
- For irregular $\mathcal{X}$, h could be the distance from q to the nearest neighbor in $\mathcal{X}$
- Constants proportional to the Lip constant of ∇f

Some basic numerical analysis results

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

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

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



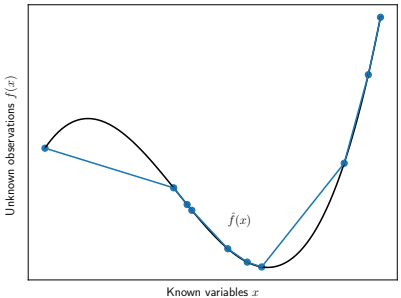
- h is a "mesh fineness" parameter $\sim$ distance between points in $\mathcal{X}$
- For irregular $\mathcal{X}$, h could be the distance from q to the nearest neighbor in $\mathcal{X}$
- Constants proportional to the Lip constant of ∇f

Some basic deep learning

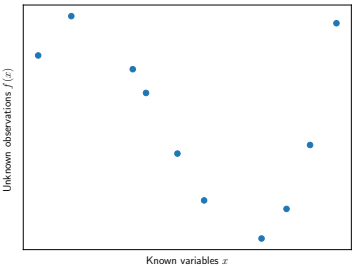
- Train a fully-connected multi-layer perceptron (MLP) using $\mathcal{X}$
- The most popular activation function is ReLU (piecewise linear)
- In modern ML, train as close to zero error as possible (interpolate)

Some basic deep learning

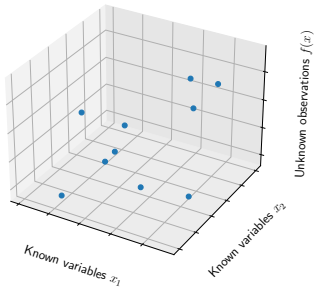
- Train a fully-connected multi-layer perceptron (MLP) using $\mathcal{X}$
- The most popular activation function is ReLU (piecewise linear)
- In modern ML, train as close to zero error as possible (interpolate)



The curse of dimensionality

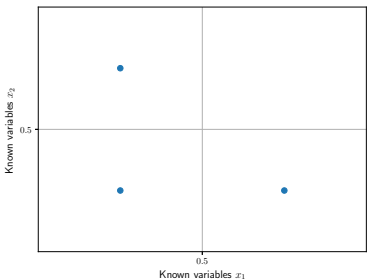


10 training points in 1D



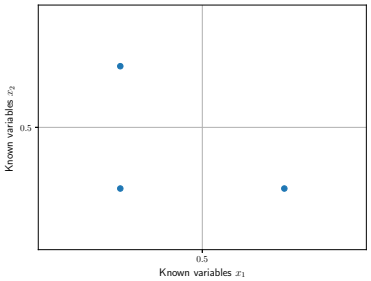
10 training points in 2D

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

Measure collapse

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

Measure collapse

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

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 $CH(\mathcal{X})$

Measure collapse

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

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 $CH(\mathcal{X})$

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 $[0,1]^d$

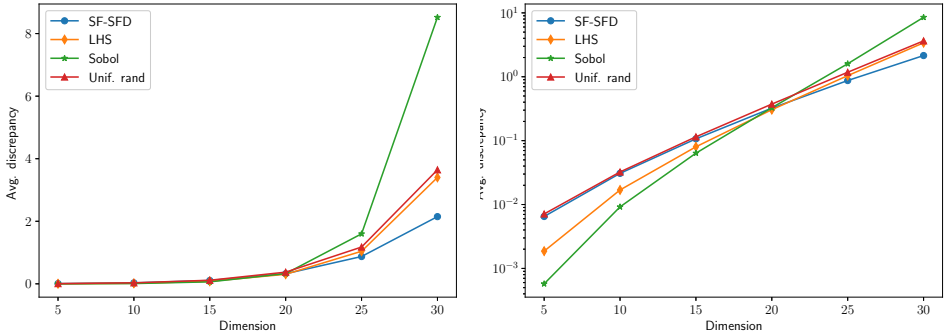
$$\|x - \frac{1}{2}\|_2^2 = \sum_{i=1}^{d} (x_i - \frac{1}{2})^2.$$

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

with finite variance v

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

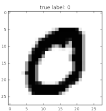
Representation learning solution

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

Representation learning solution

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

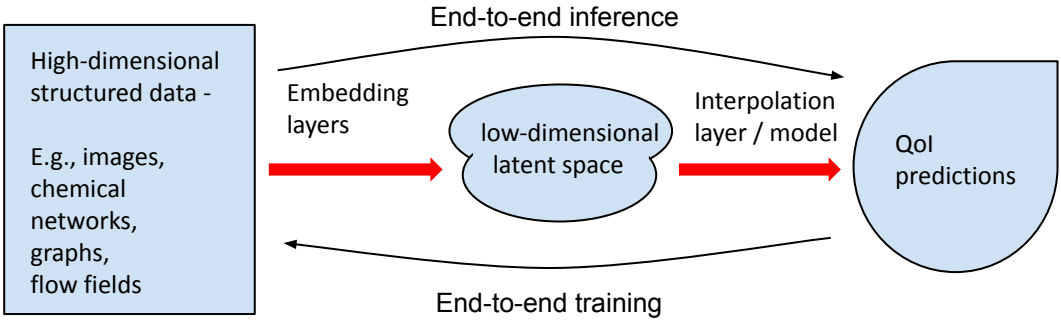
- f is often highly *structured* – MLPs with nothing else are from the 60s



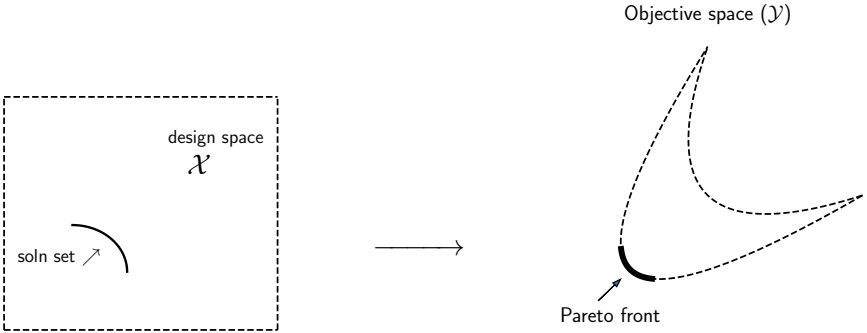
$$\xrightarrow{f} \quad 0$$

28×28 pixels $\neq 784$ dimensions...

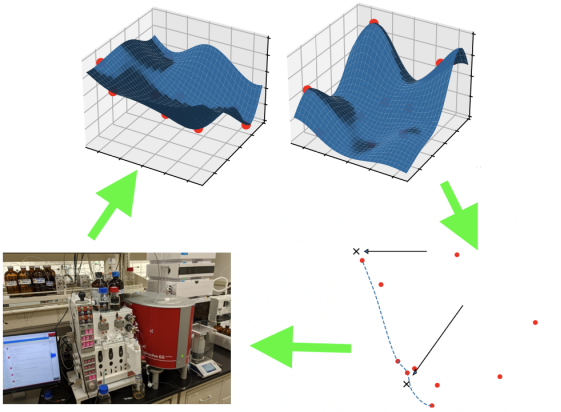
Modern deep learning pipeline



Multiobjective Black-Box Optimization



General Workflow and Data Acquisition

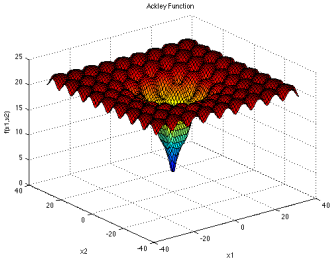


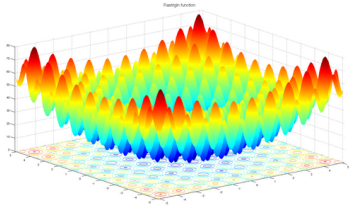
Global optimization

In global optimization literature...

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

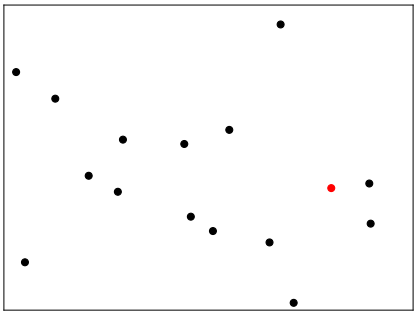
Guarantees convergence for problems with thousands of local minima





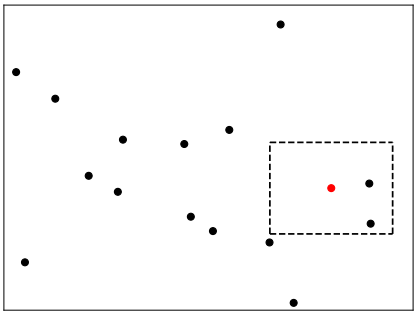
Local optimization

- 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



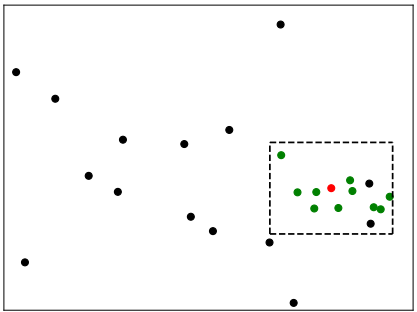
Local optimization

- 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



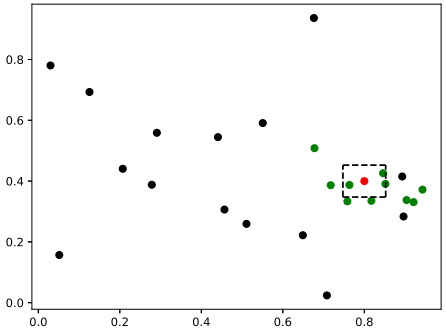
Local optimization

- 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



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



Written in `Python`

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

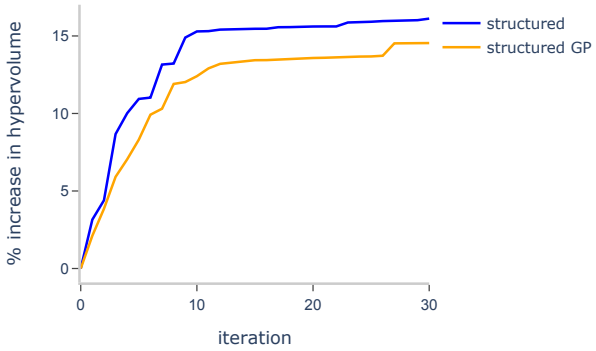
`https://github.com/parmoo/parmoo`

`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

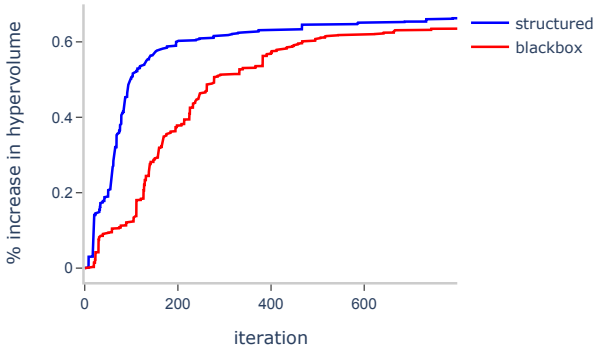
- 6-dimensional latent space embedding of a mixed-variable problem
- 3-objectives electrolyte manufacturing
  - high yield, minimal byproduct, low reaction times
- Running real-world experiments with very limited budget



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)

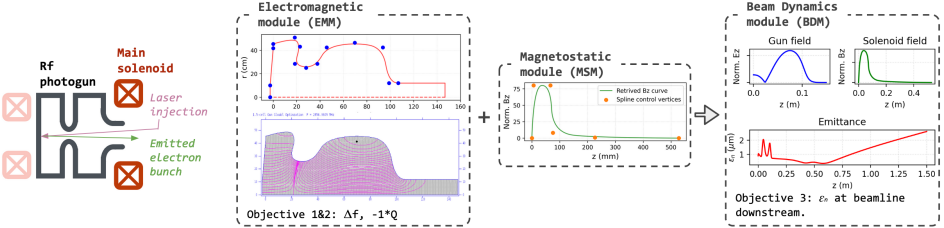
- 13-variable, 3-objective problem
- Higher dimensional, requires trust-region methods



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!
- Optimization rarely truly requires global accuracy

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!
- Optimization rarely truly requires global accuracy
- *But there are other problems that do require global accuracy...*

References

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

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

Chang and Wild. Designing a framework for solving multiobjective simulation optimization problems. Under Review, ArXiv preprint 2304.06881 (2023).

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.

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

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`

This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Advanced Scientific Computing Research, SciDAC program under contract number DE-AC02-06CH11357.