# Data sampling for surrogate modeling and optimization

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# Outlines

Inference problems and high-dimensional modeling

Modeling for high-dimensional optimization

# The fundamental machine learning problem

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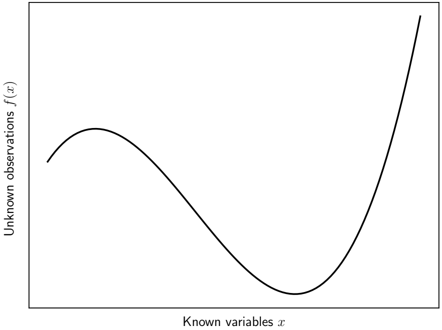


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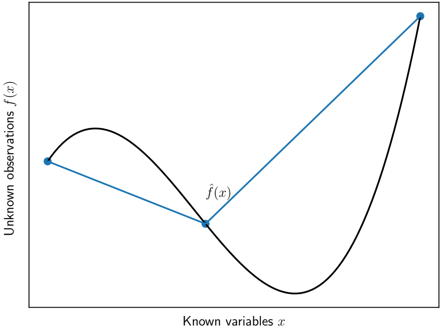


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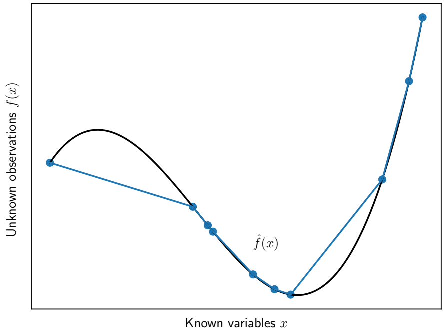


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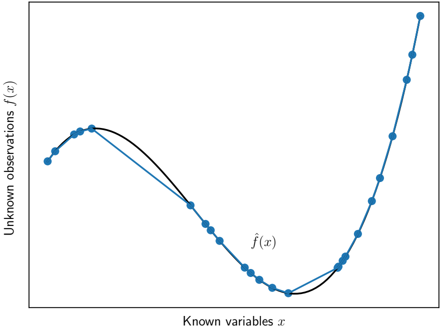


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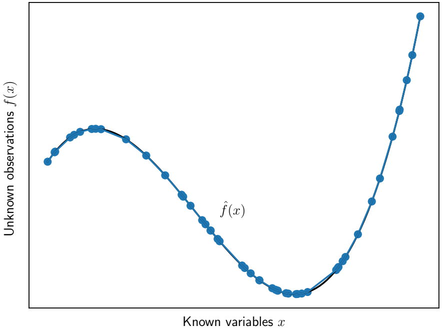


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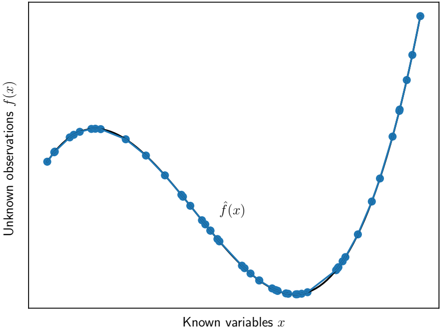
- If we have enough data, it doesn't matter

# 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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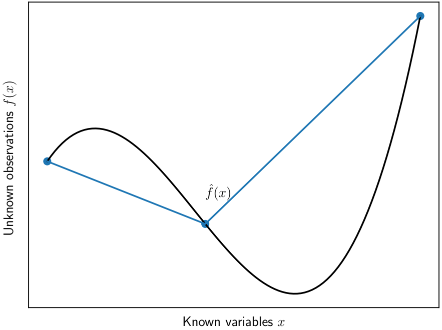


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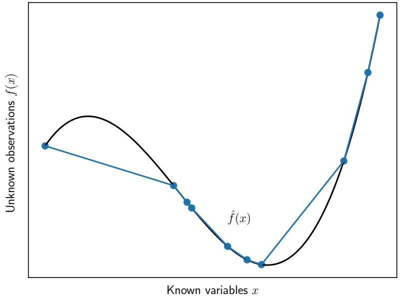

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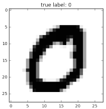
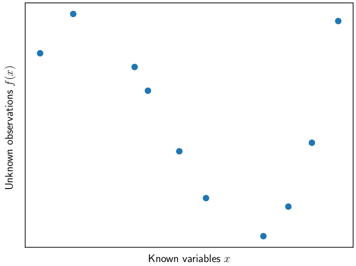
- $f$ is often highly *structured* – MLPs with nothing else are from the 60s



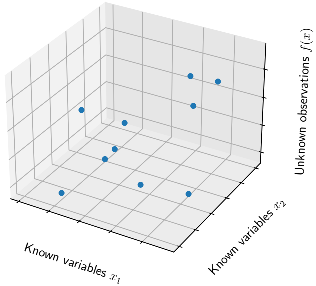

$$\xrightarrow{f} \quad 0$$

$28 \times 28$ pixels $\neq 784$ dimensions...

# The curse of dimensionality

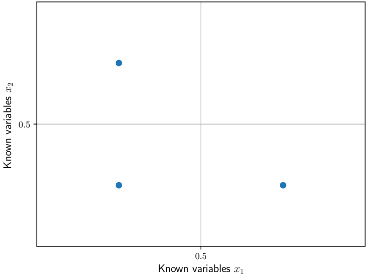



10 training points in 1D




10 training points in 2D

# The curse of ~~dimensionality~~ no data

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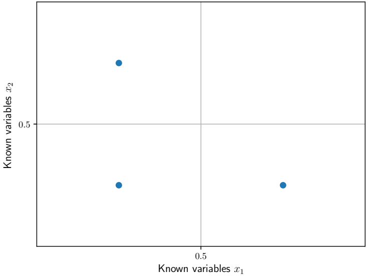


Need data in all quadrants?

- 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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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 $x = (x_1, x_2, \dots, x_d)$ from $[0,1]^d$

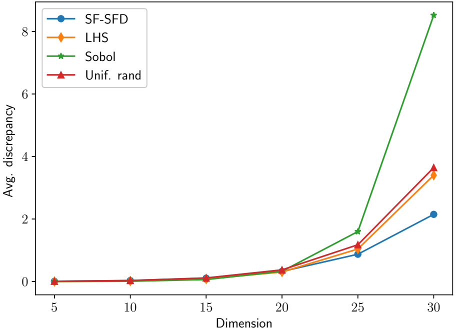
$$\|x - \frac{1}{2}\|_2^2 = \sum_{i=1}^{d} (x_i - \frac{1}{2})^2.$$

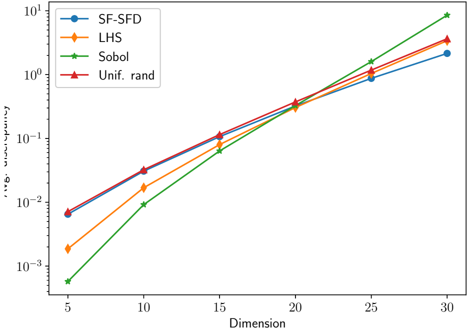
$$\mathbb{E}\left[\left(x_i - \frac{1}{2}\right)^2\right] = \int_0^1 \left(u - \frac{1}{2}\right)^2 du = \frac{1}{12}$$

with finite variance $\nu$

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 $d \to \infty$.

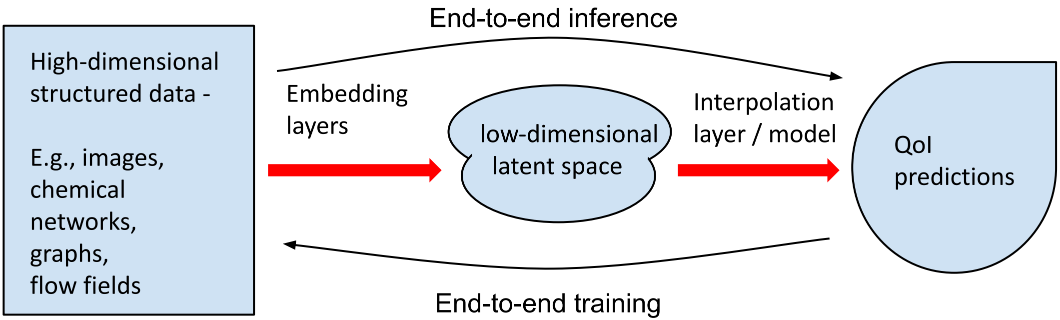
# Collapse of some common distributions



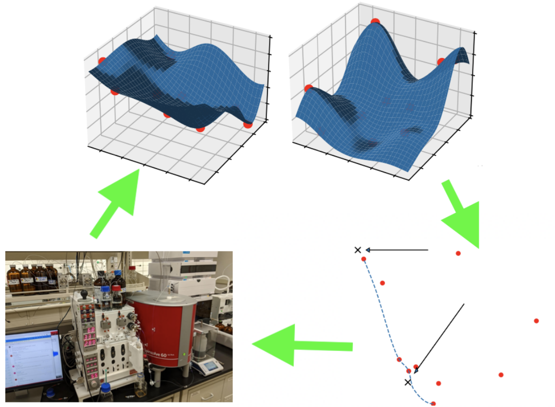




Garg, Chang, and Raghavan, Stochastic optimization of Fourier coefficiencts to generate space-filling designs. *To appear in Winter Sim 2023*.

# 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