The curse of dimensionality

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Argonne National Laboratory

CAA&CM Argonne Student Visit
Sep 28, 2023

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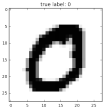

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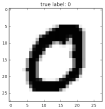

$\xrightarrow{f}$ 0

"The dog jumped over the ..." $\xrightarrow{f}$ "fence"

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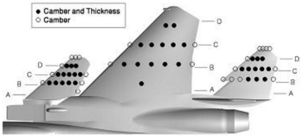

Nonparametric aircraft geometry (photo from NASA Langley).

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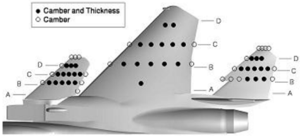

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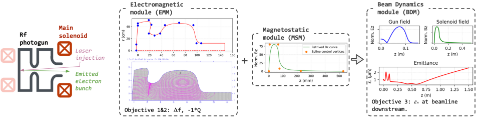

Particle accelerator designs (photo from simulation run on HPCs at Argonne).

The fundamental machine learning problem

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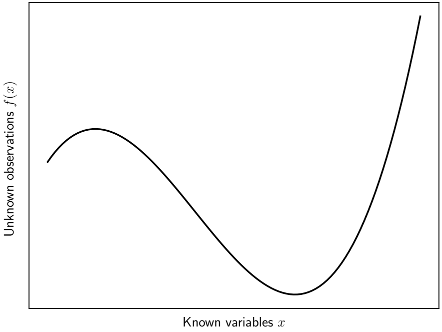
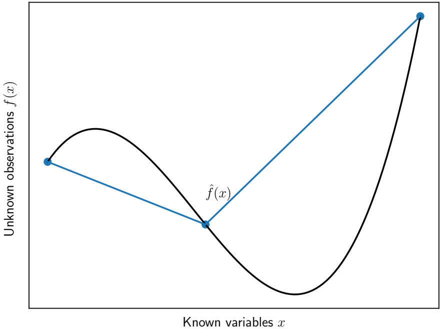


- Want to predict unknown $f(x)$ for observation x

The fundamental machine learning problem



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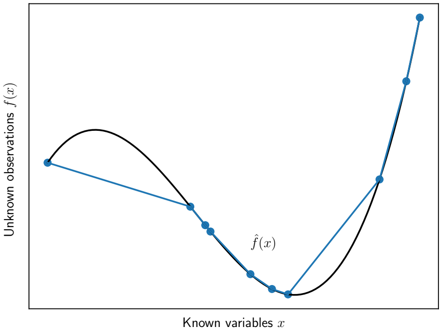

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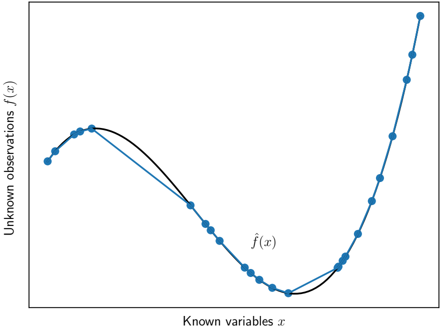

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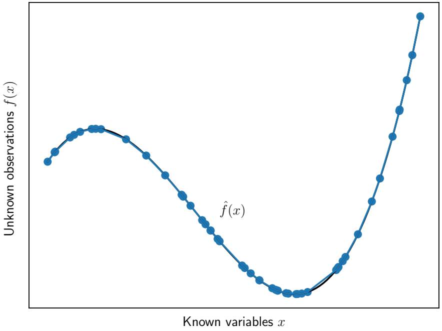

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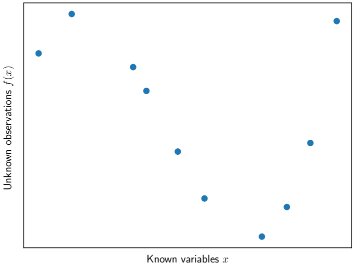
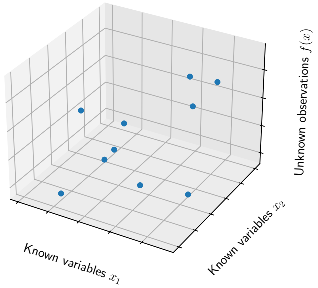
- If we have enough data, it doesn't matter

The curse of dimensionality

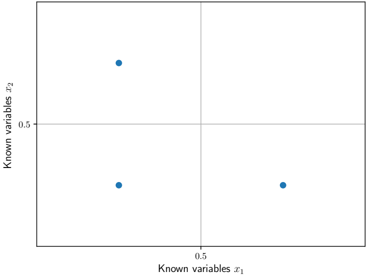


10 training points in 1D



10 training points in 2D

The curse of ~~dimensionality~~ no data



Need data in all quadrants?

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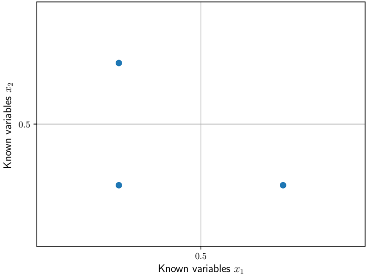
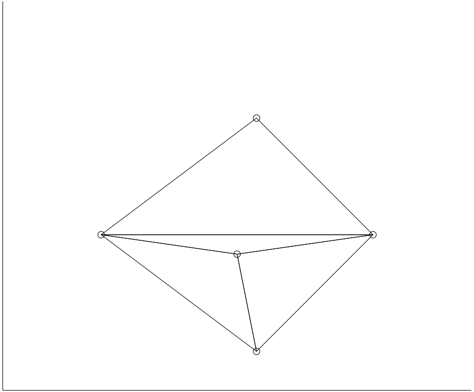


Need data in all quadrants?

- 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

The curse of ~~dimensionality~~ too much data

Classical methods to "connect the dots" in high-dimensions (from applied math literature) rely on meshing:



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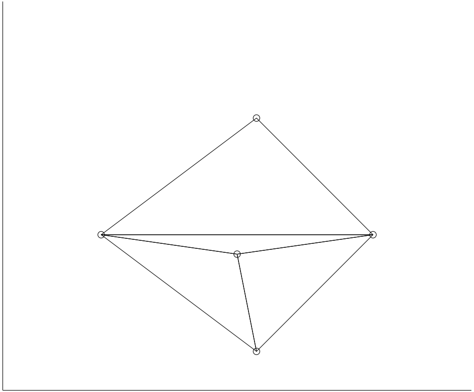

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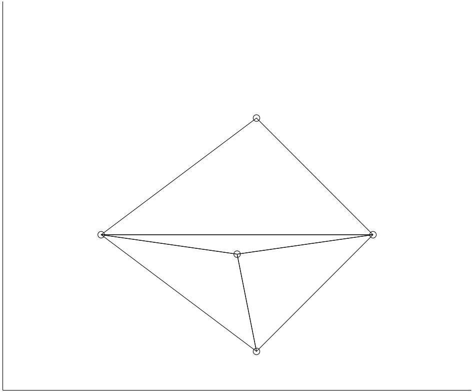

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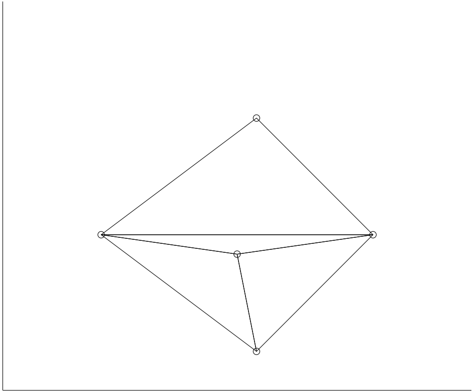

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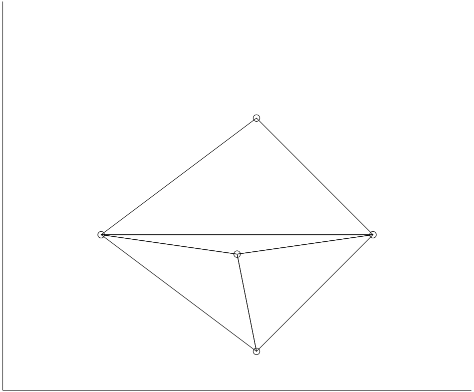

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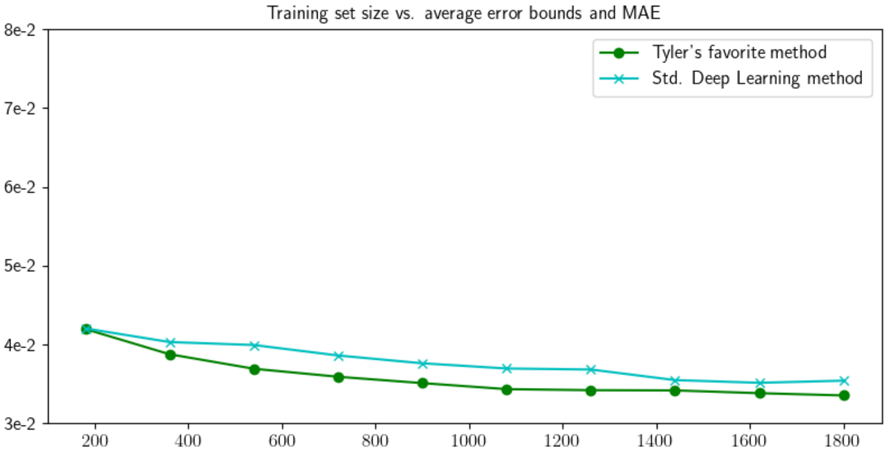
- **Impossible for large data sets**

Results for some methods



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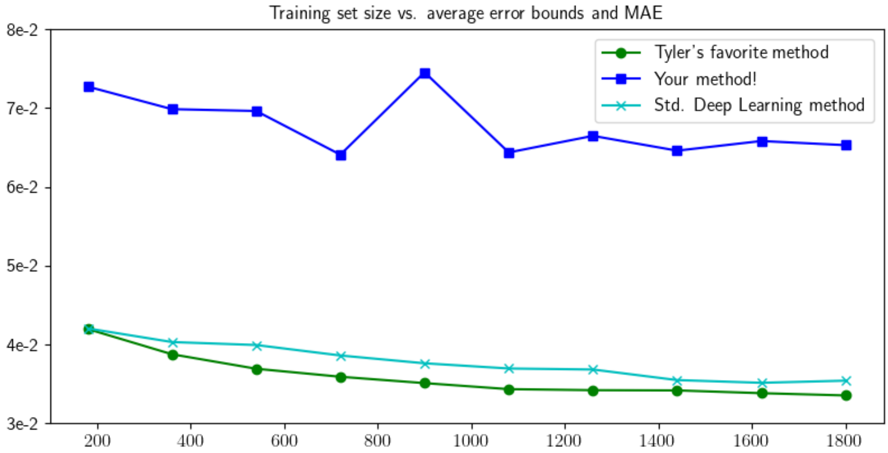

Questions

Everything is a function

The fundamental ML problem (multidimensional inference)

The curse of dimensionality

- Not enough data to make accurate predictions
- Too much data for many "classical" methods

Data from some existing methods

Some courses to take

Math:

- Advanced linear algebra
- Numerical analysis
- Functional analysis

CS:

- Data structures & algorithms
- Parallel computing
- Data analysis and/or Machine learning