

6.7900: Machine Learning

Lecture 16



Lecture start: Tues/Thurs 2:35pm

Who's speaking today? Prof. Tamara Broderick

Course website: gradml.mit.edu

Questions? Ask here or on piazza.com/mit/fall2024/67900/

Materials: Slides, video, etc linked from gradml.mit.edu after the lecture (but there is no livestream)

Last Times

- I. Various supervised learning methods:
linear, polynomial,
trees, forests, neural
networks

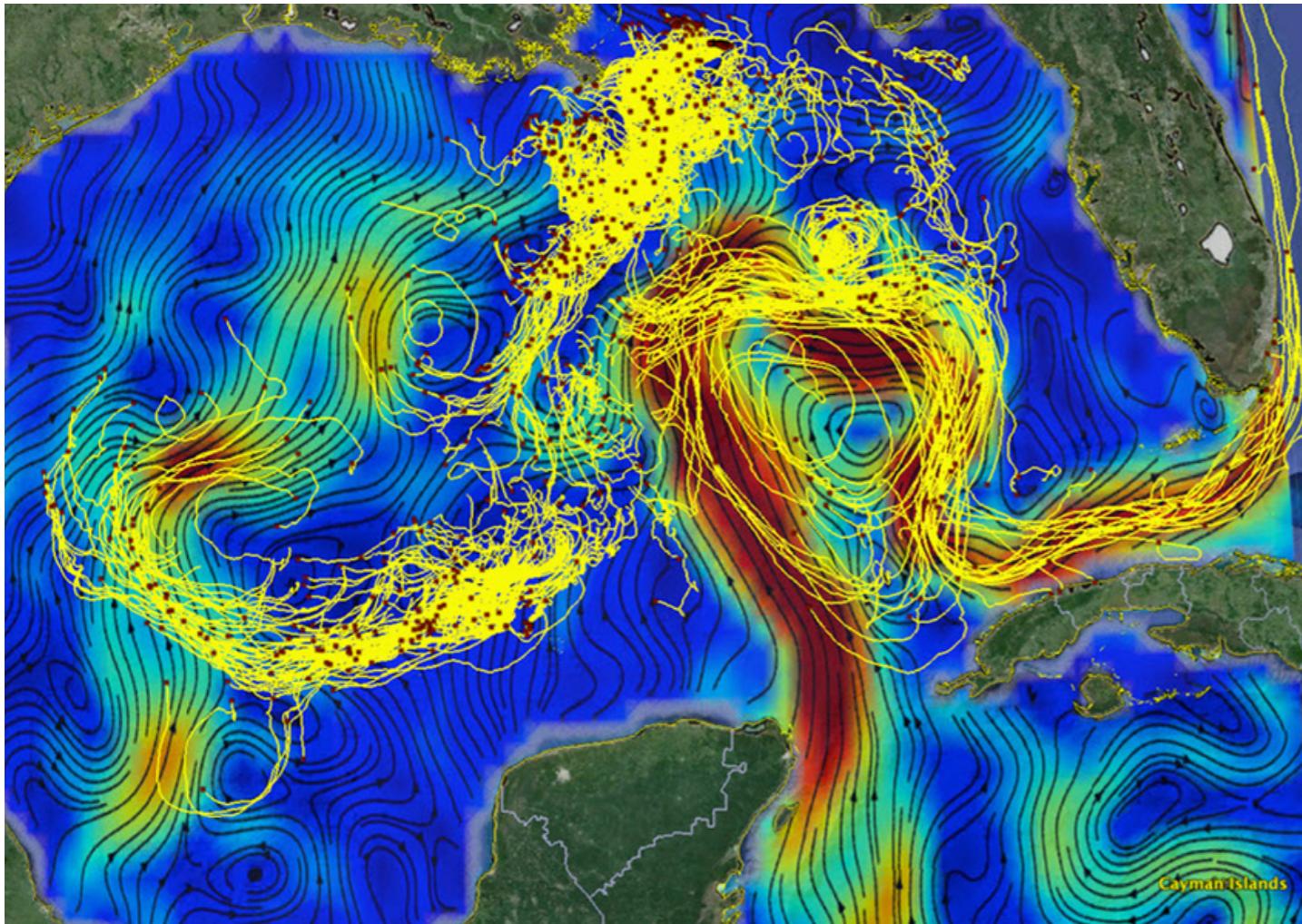
Today

- I. A common motif in spatiotemporal (and similar) data
- II. Gaussian processes:
model and inference

Sub-type of regression

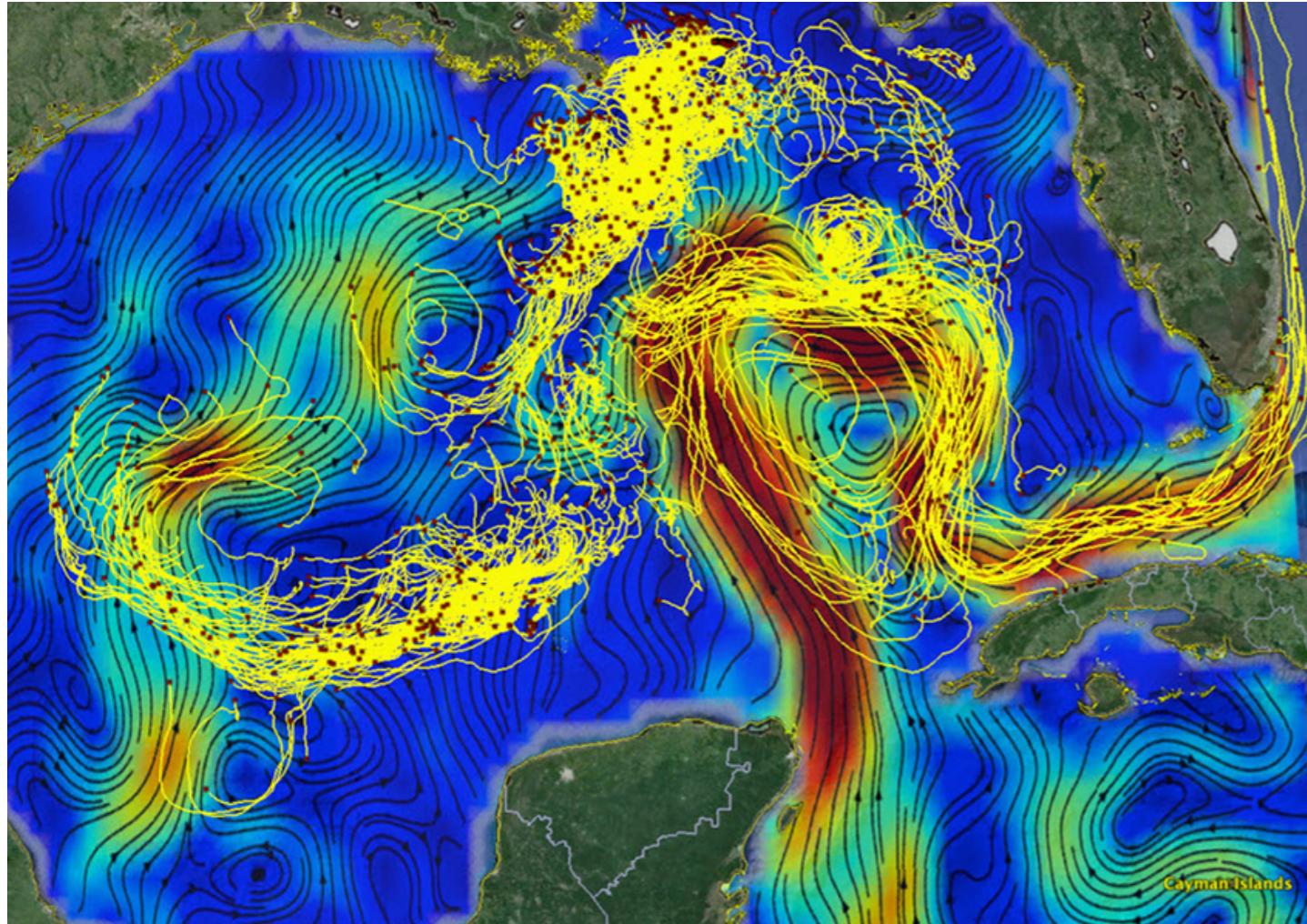
Sub-type of regression

Example:



[Ryan, Özgökmen 2023; Zewe 2023; Gonçalves et al 2019; Lodise et al 2020; Berlinghieri et al 2023]

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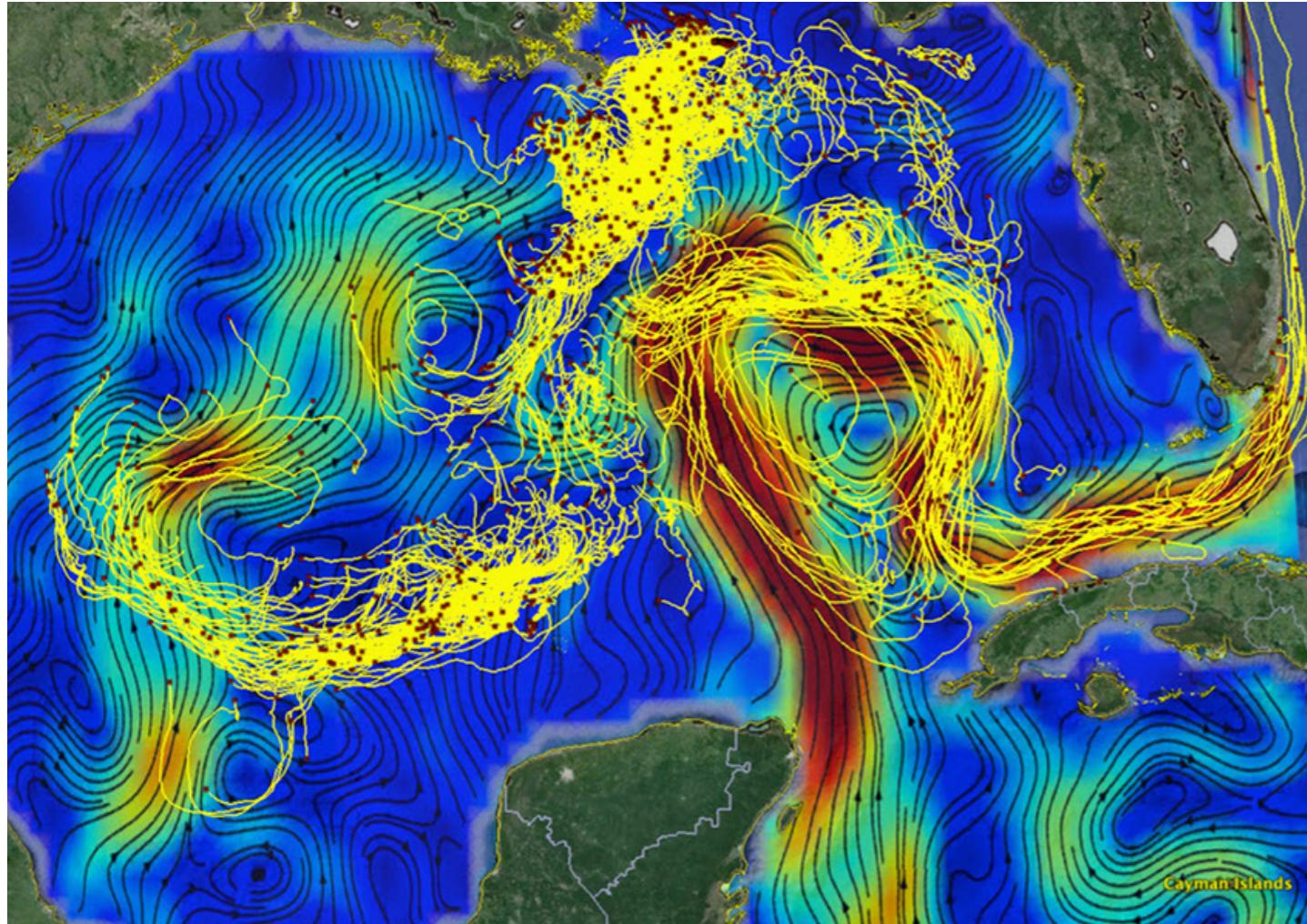


Example:

- The ocean current (velocity vector field) varies by space & time

[Ryan, Özgökmen 2023; Zewe 2023; Gonçalves et al 2019; Lodise et al 2020; Berlinghieri et al 2023]

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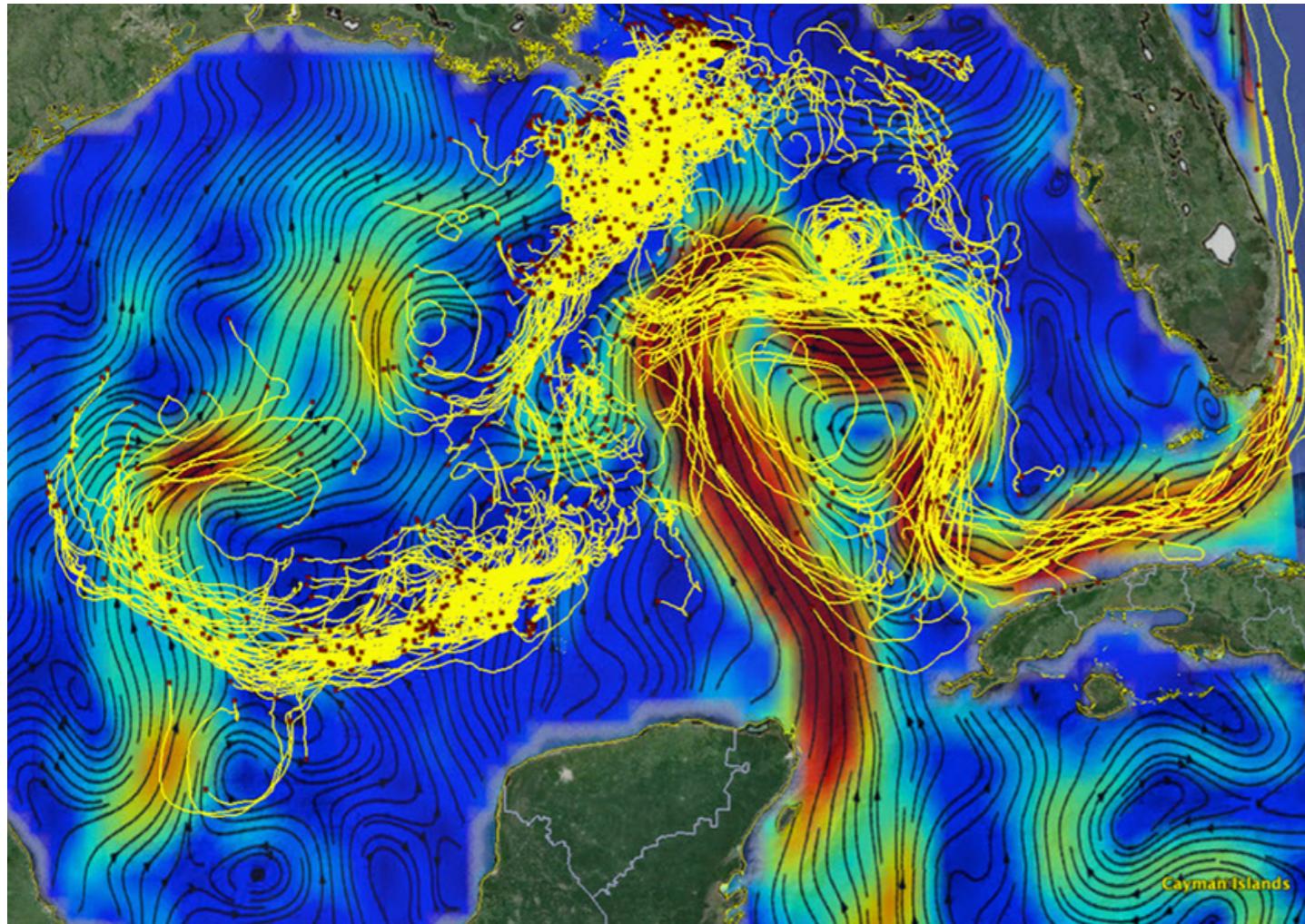


Example:

- The ocean current (velocity vector field) varies by space & time
- Scientists get sparse observations of the current from buoys

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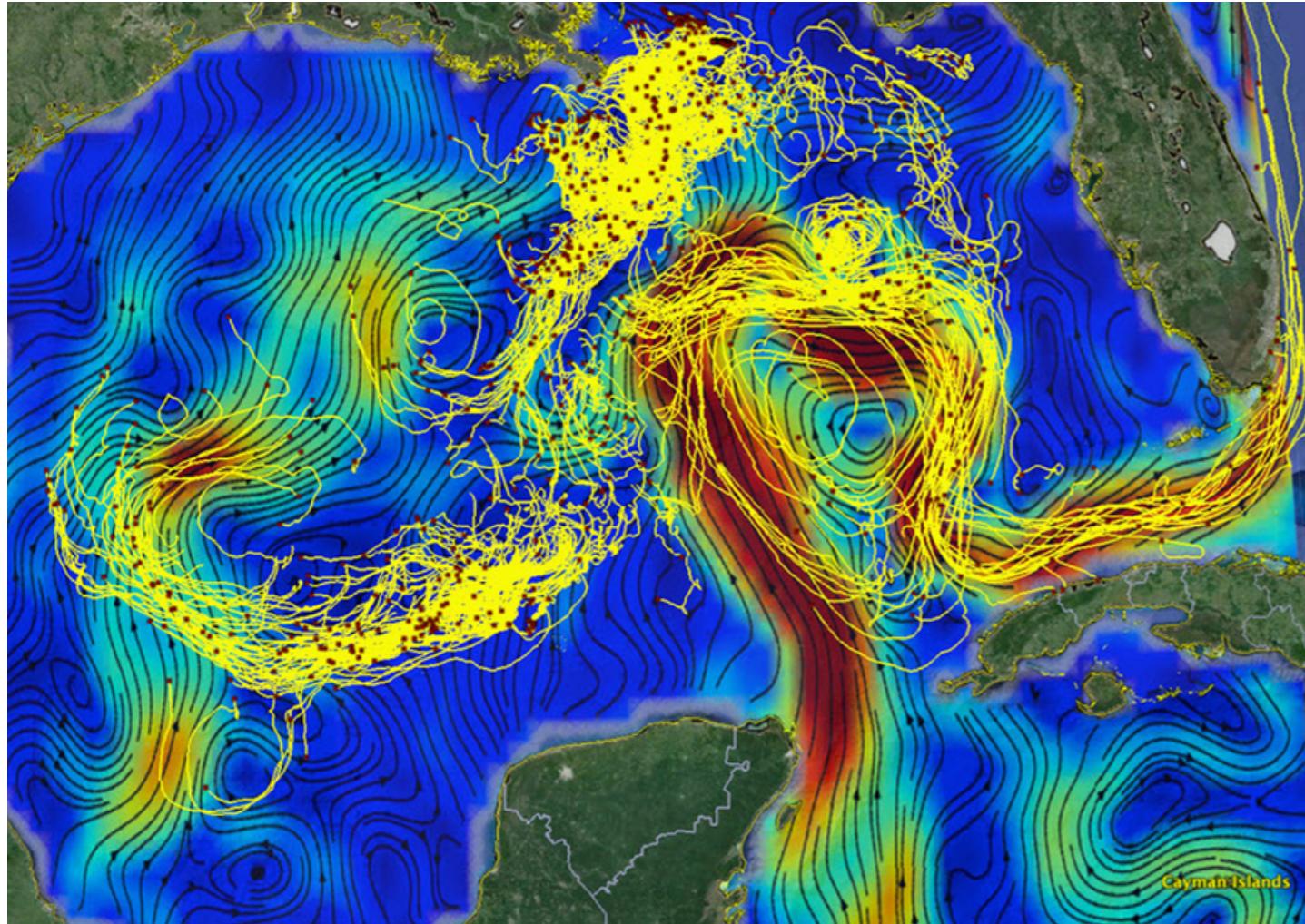


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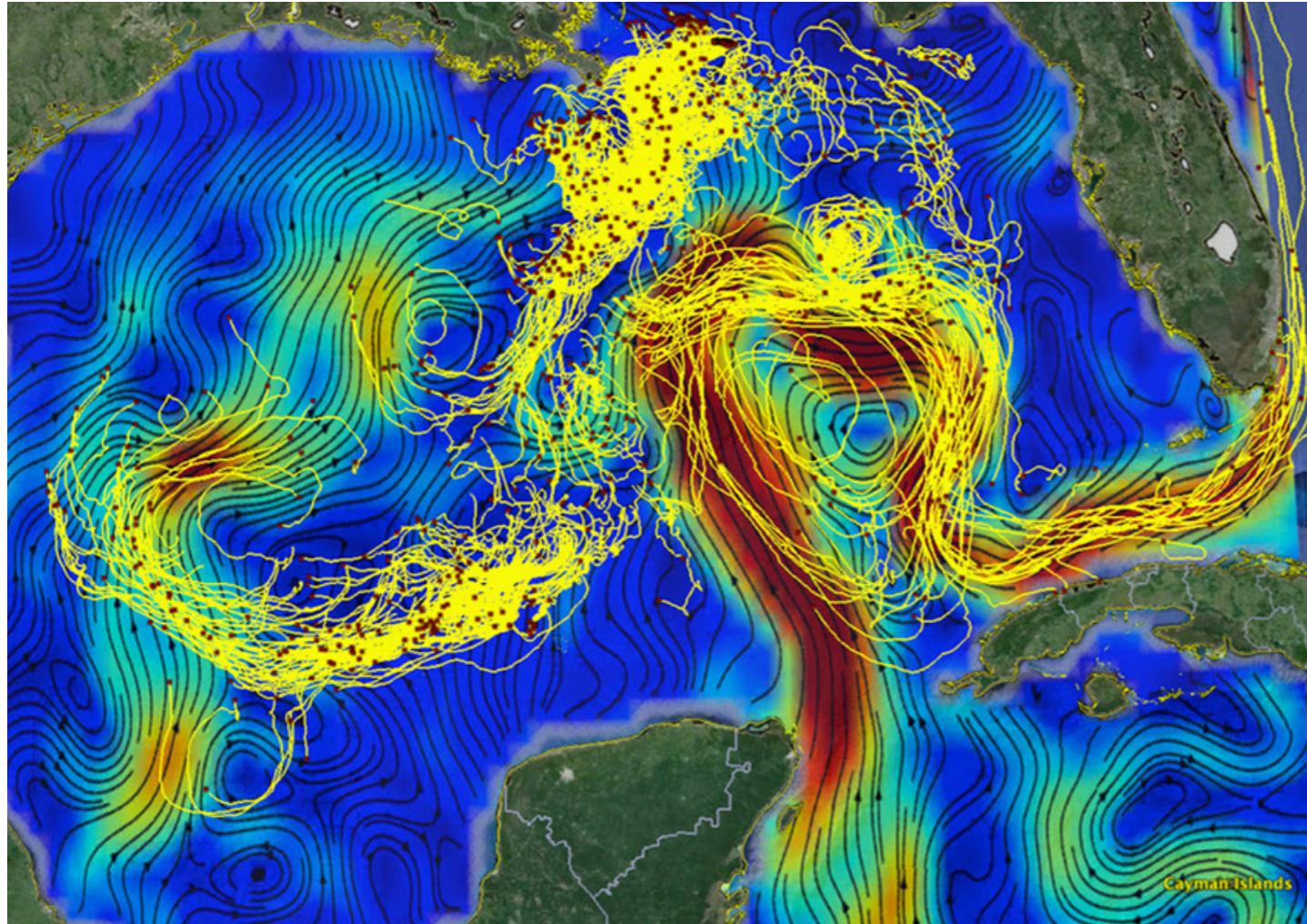
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Challenges: • Data is difficult to collect and sparse

Sub-type of regression



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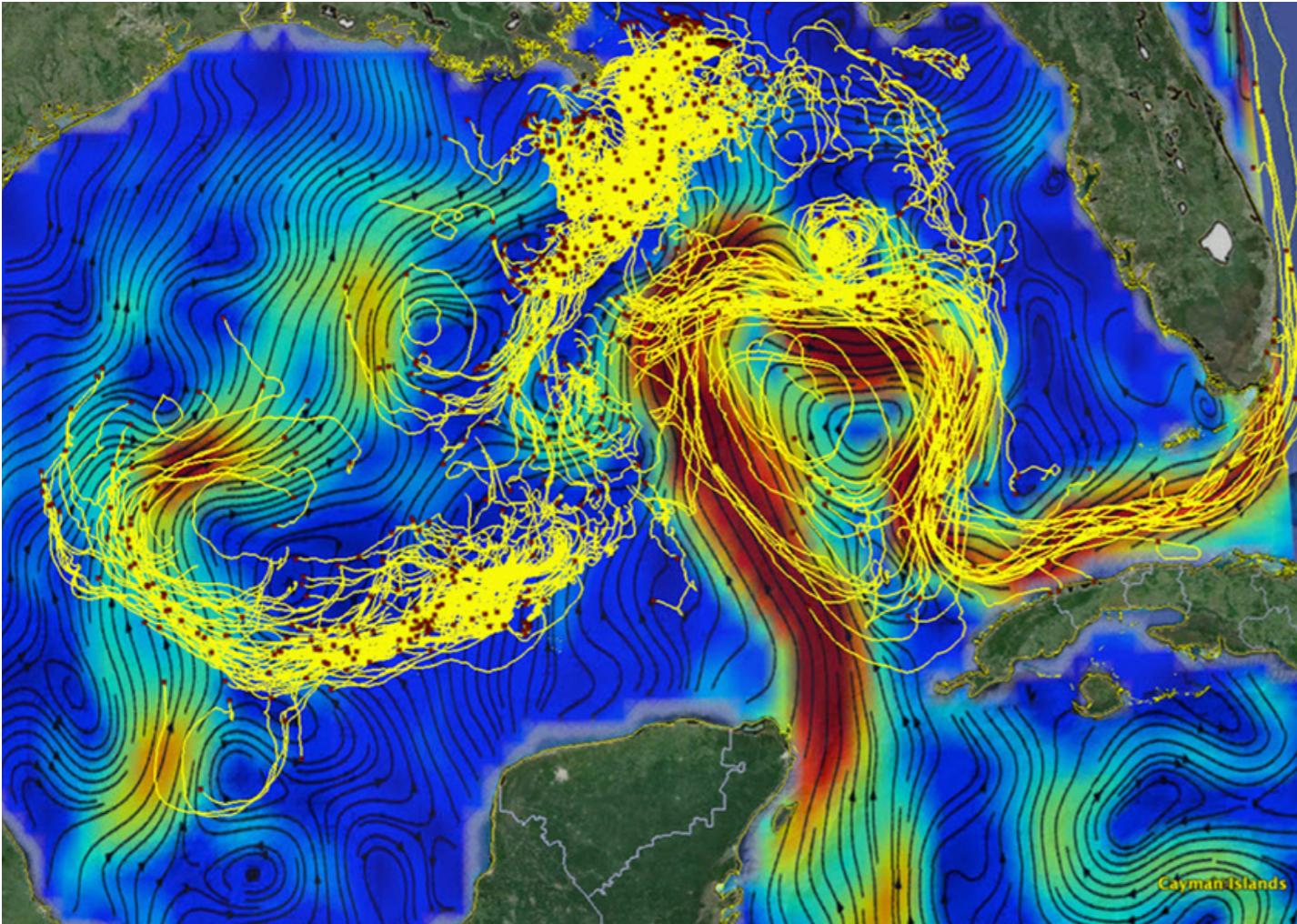
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Challenges:

- Data is difficult to collect and sparse
- Data is not on a grid or discrete structure

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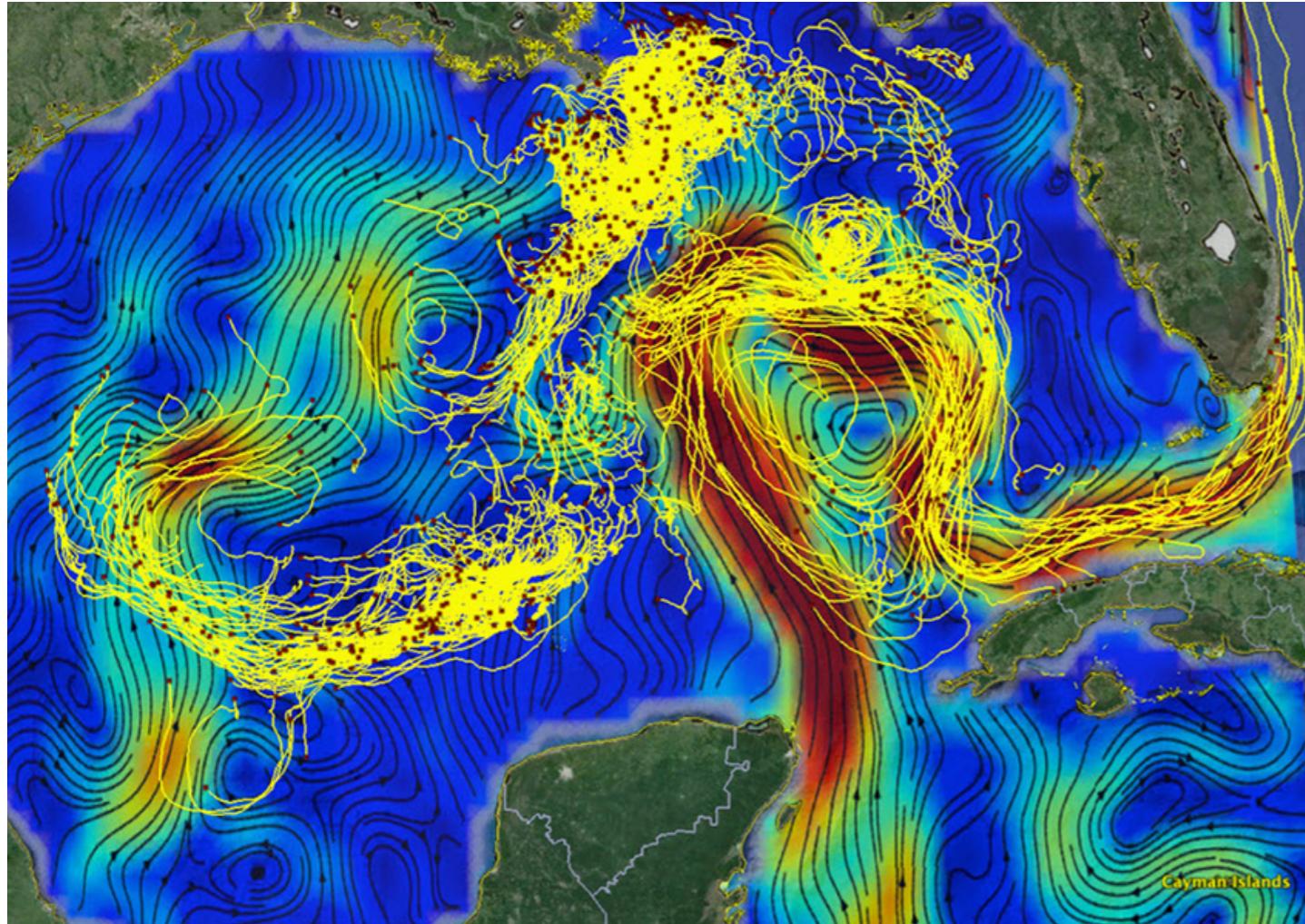
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Challenges:

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- Current is highly nonlinear but smooth in space-time

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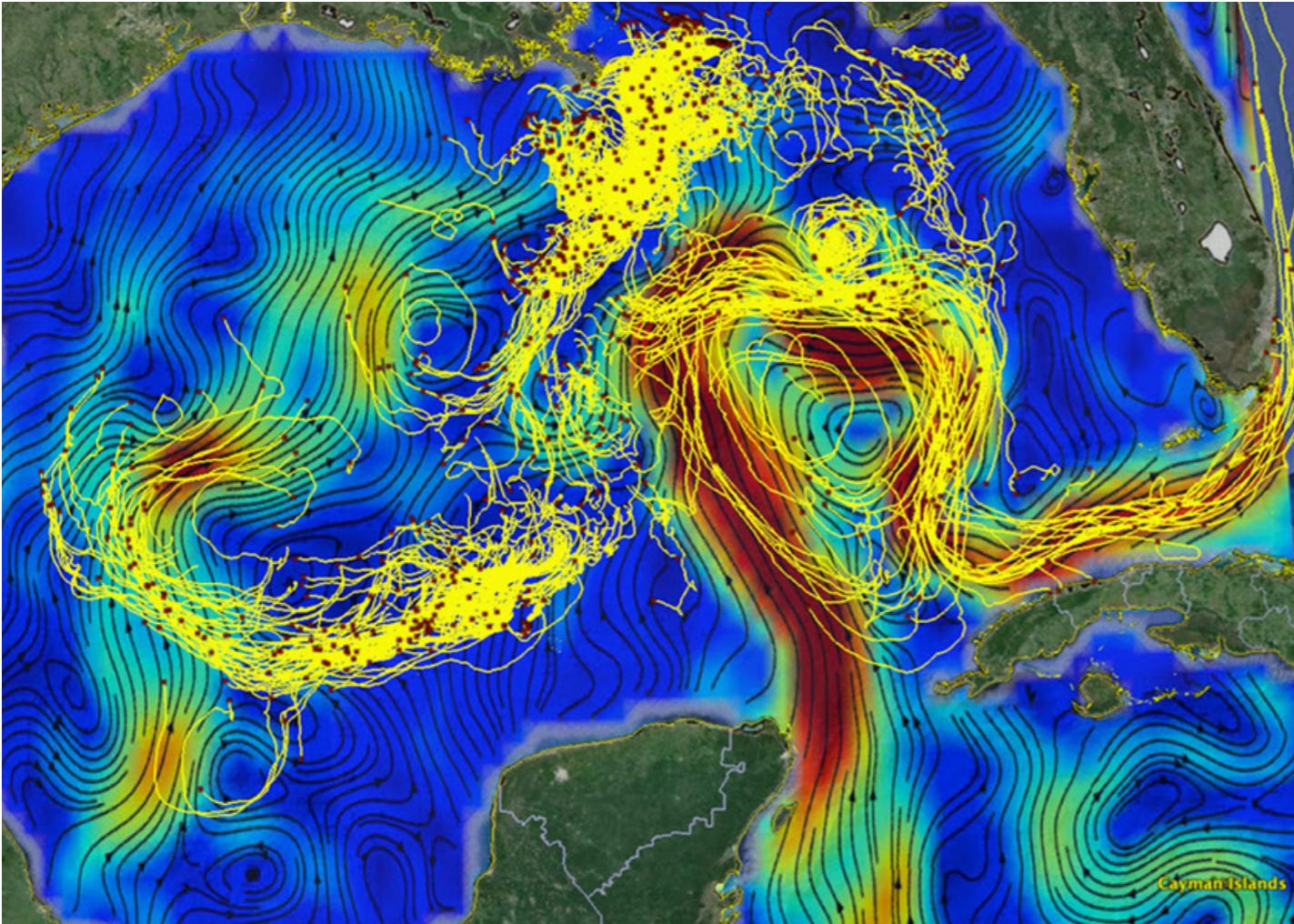
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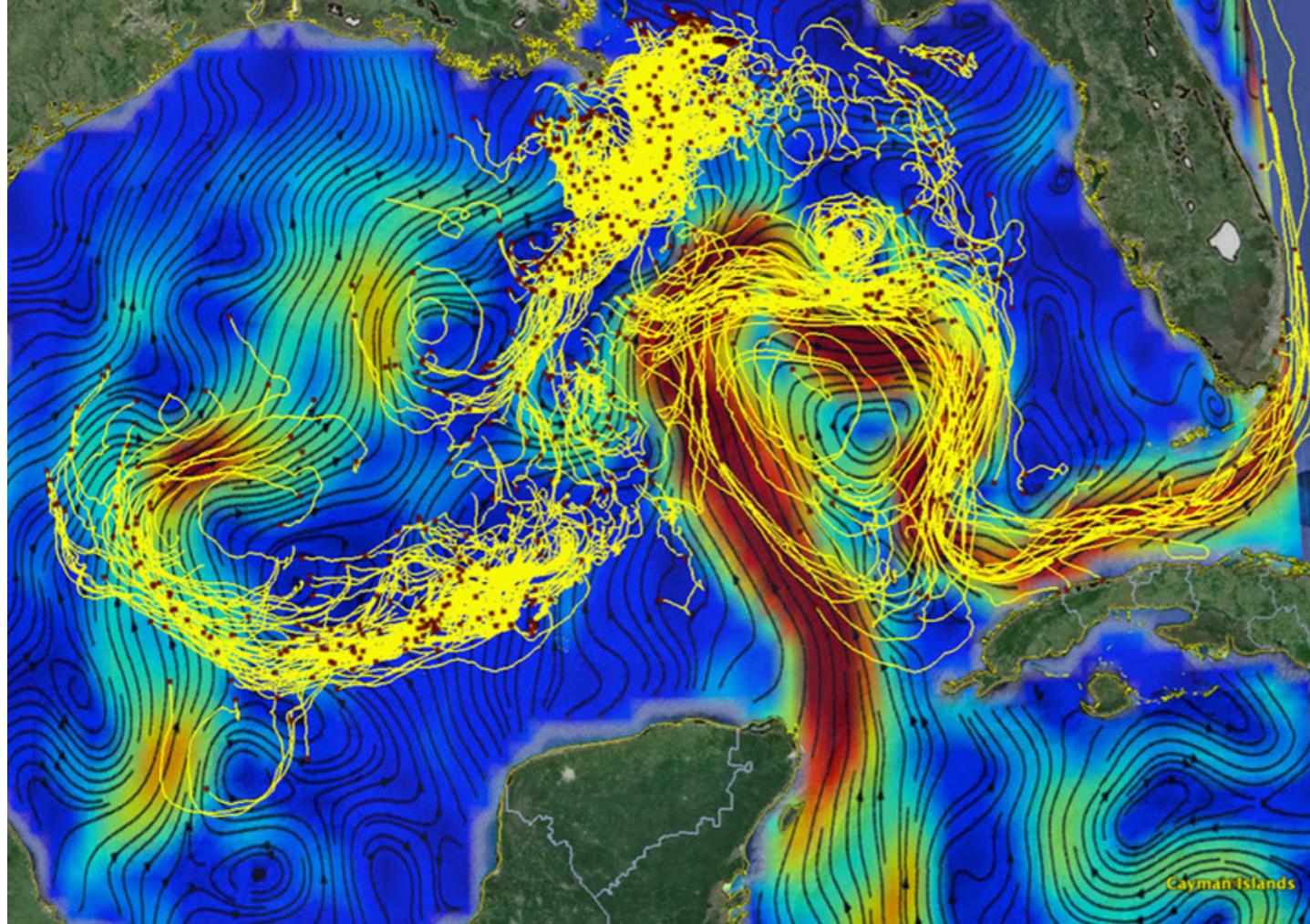
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Many similar problems: e.g. predicting groundwater

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[Belkhiri et al 2020]

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Challenges: • Data is difficult to collect and sparse

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Many similar (low dimensional) problems: e.g. predicting

¹ groundwater quality from well measurements, etc. [Belkhiri et al 2020]

Sub-type of regression

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Example: “Surrogate model”

Sub-type of regression

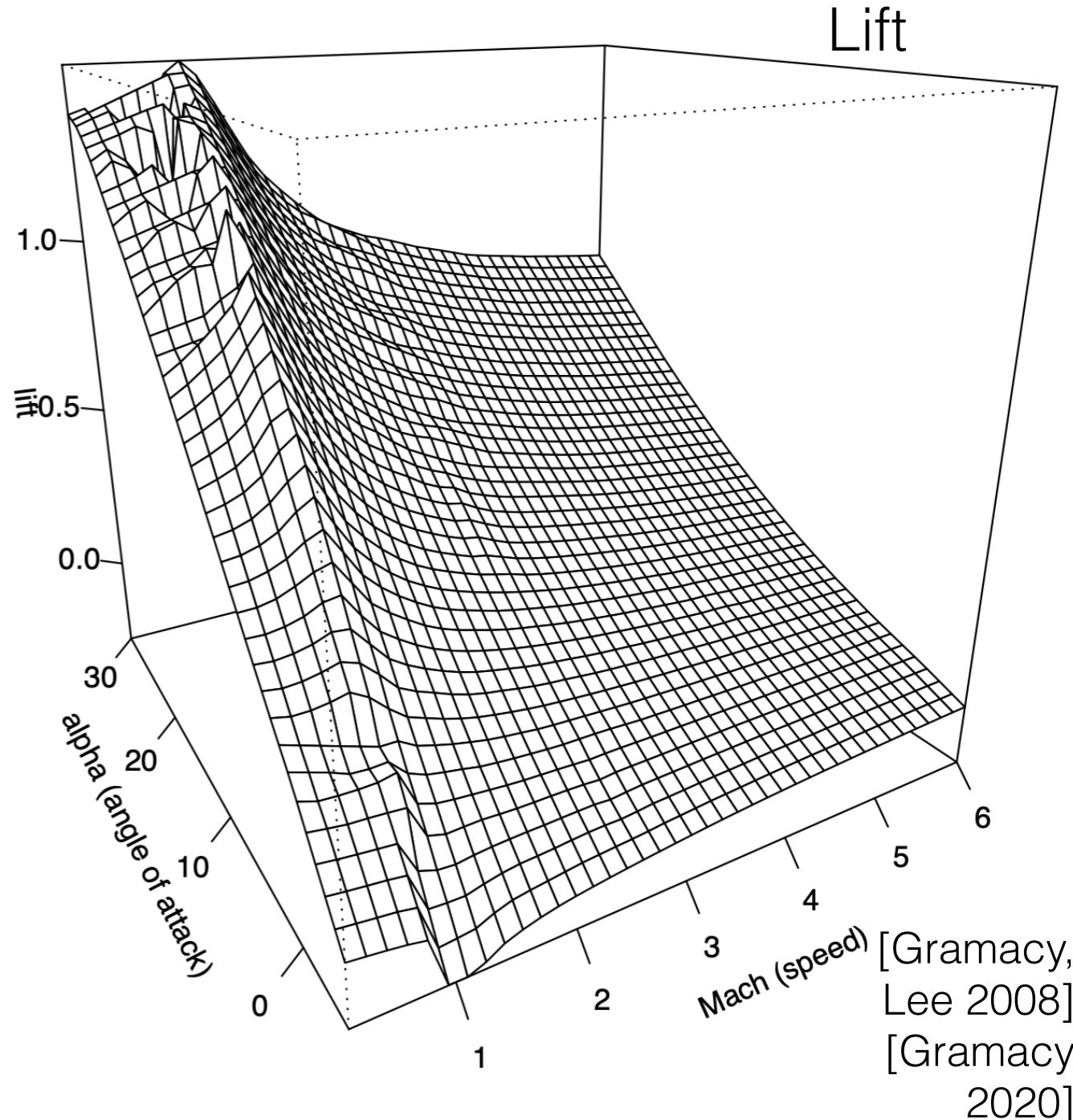
Example: “Surrogate model”

- The lift force of a rocket booster varies as a function of speed at re-entry, angle of attack, and sideslip angle

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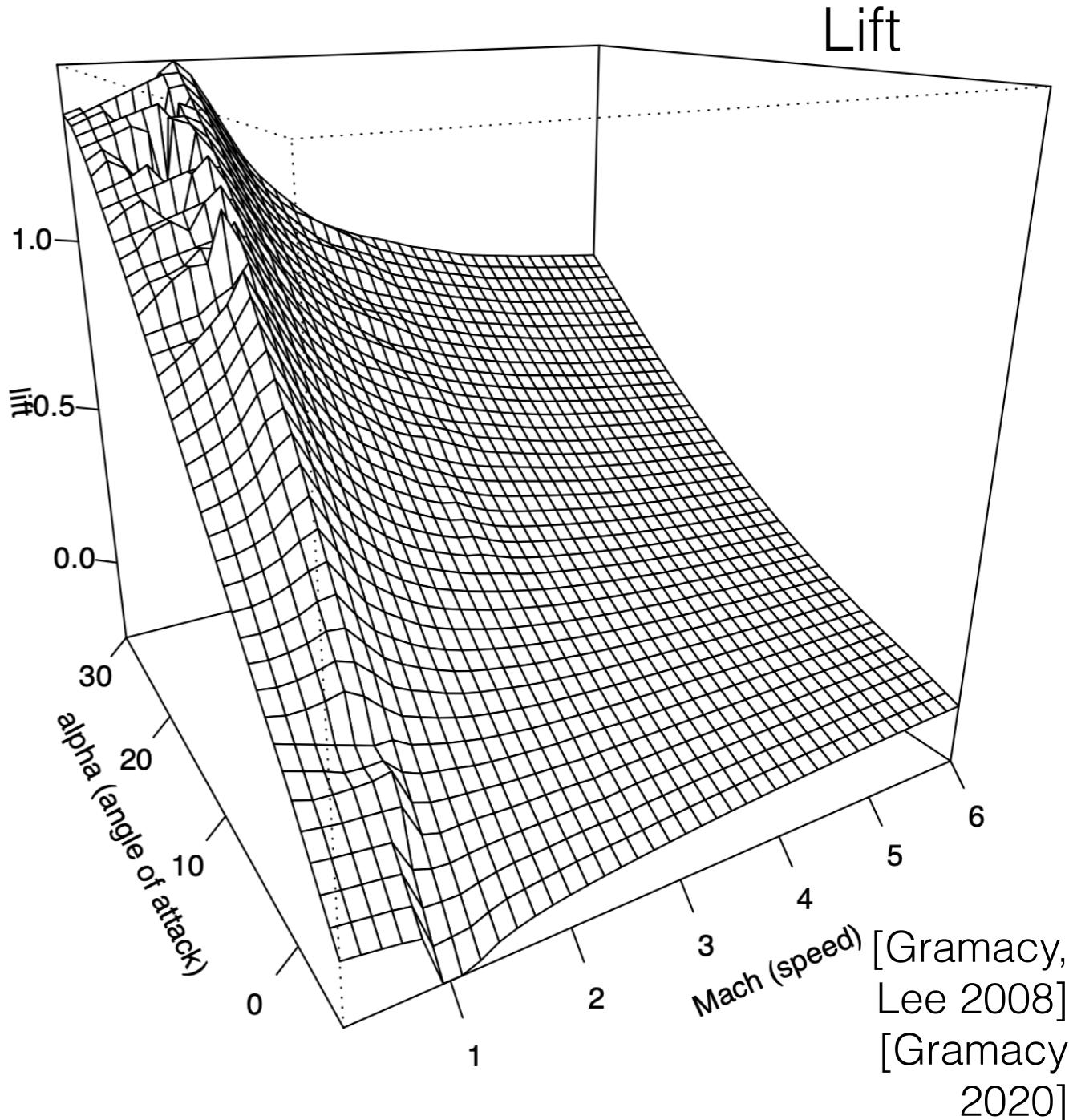
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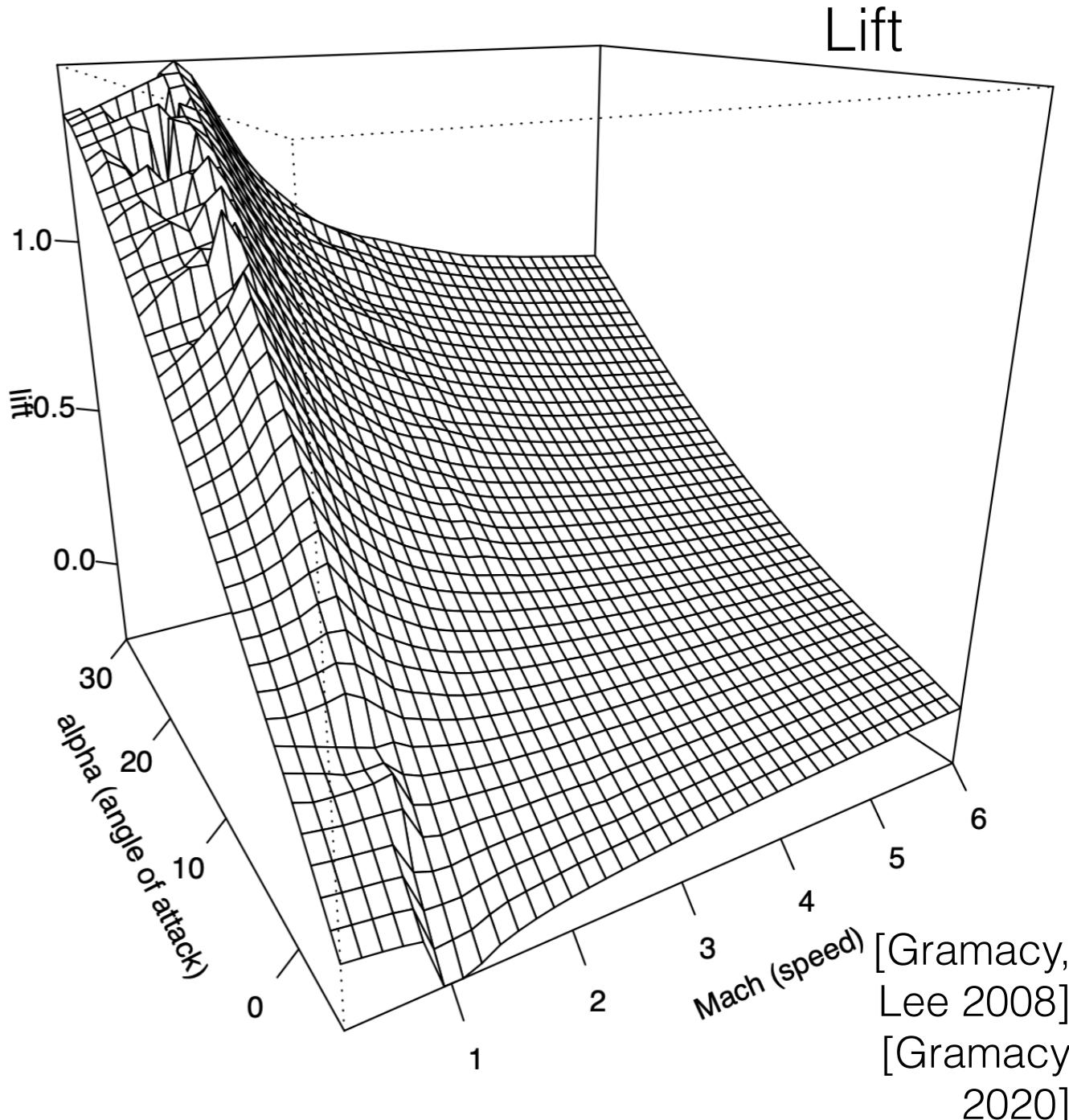
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Example: “Surrogate model”

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- Scientists can run expensive simulations at chosen input settings
- Goal: predict how lift varies as a function of these inputs



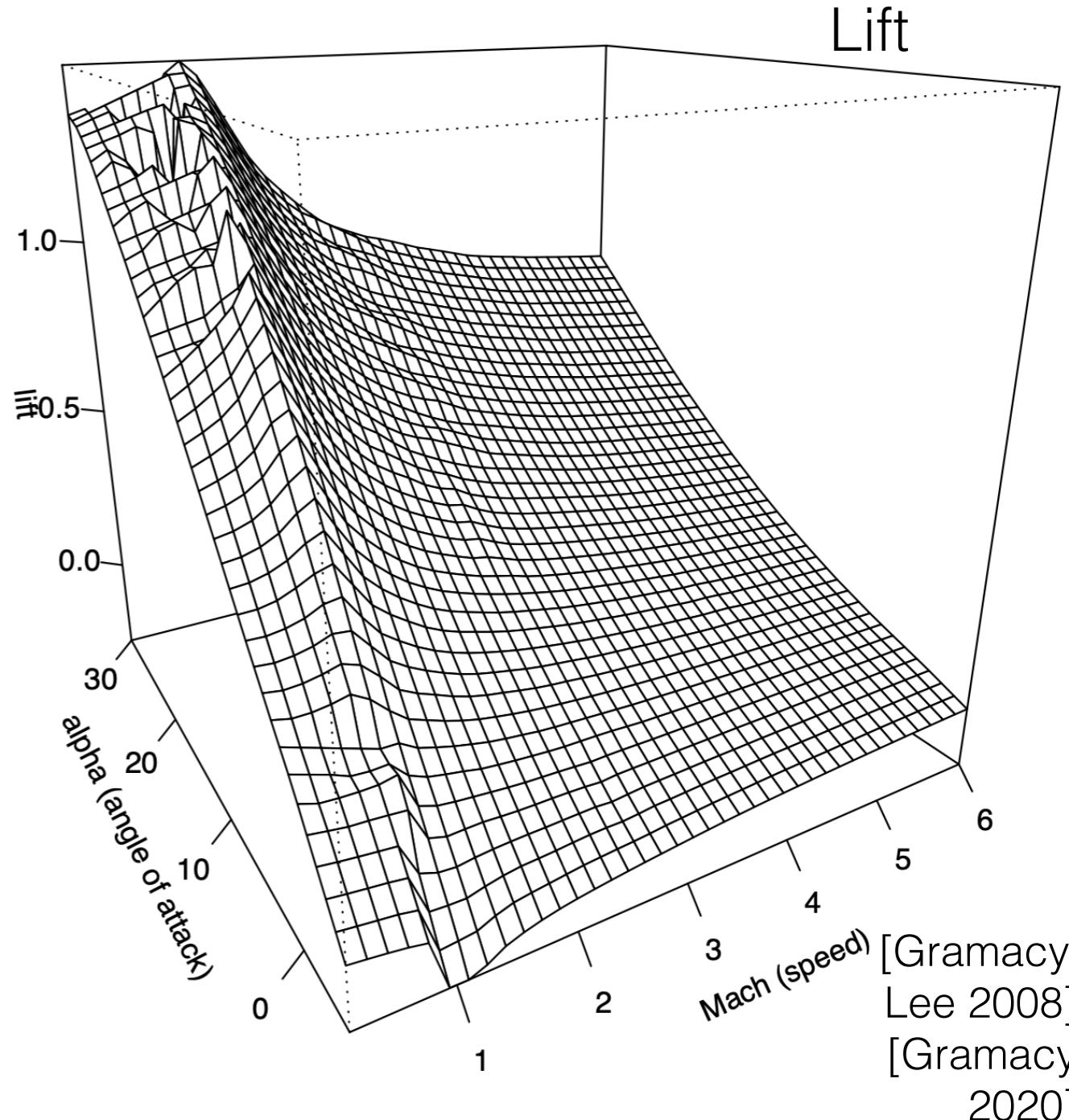
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Challenges:

- Sparse data



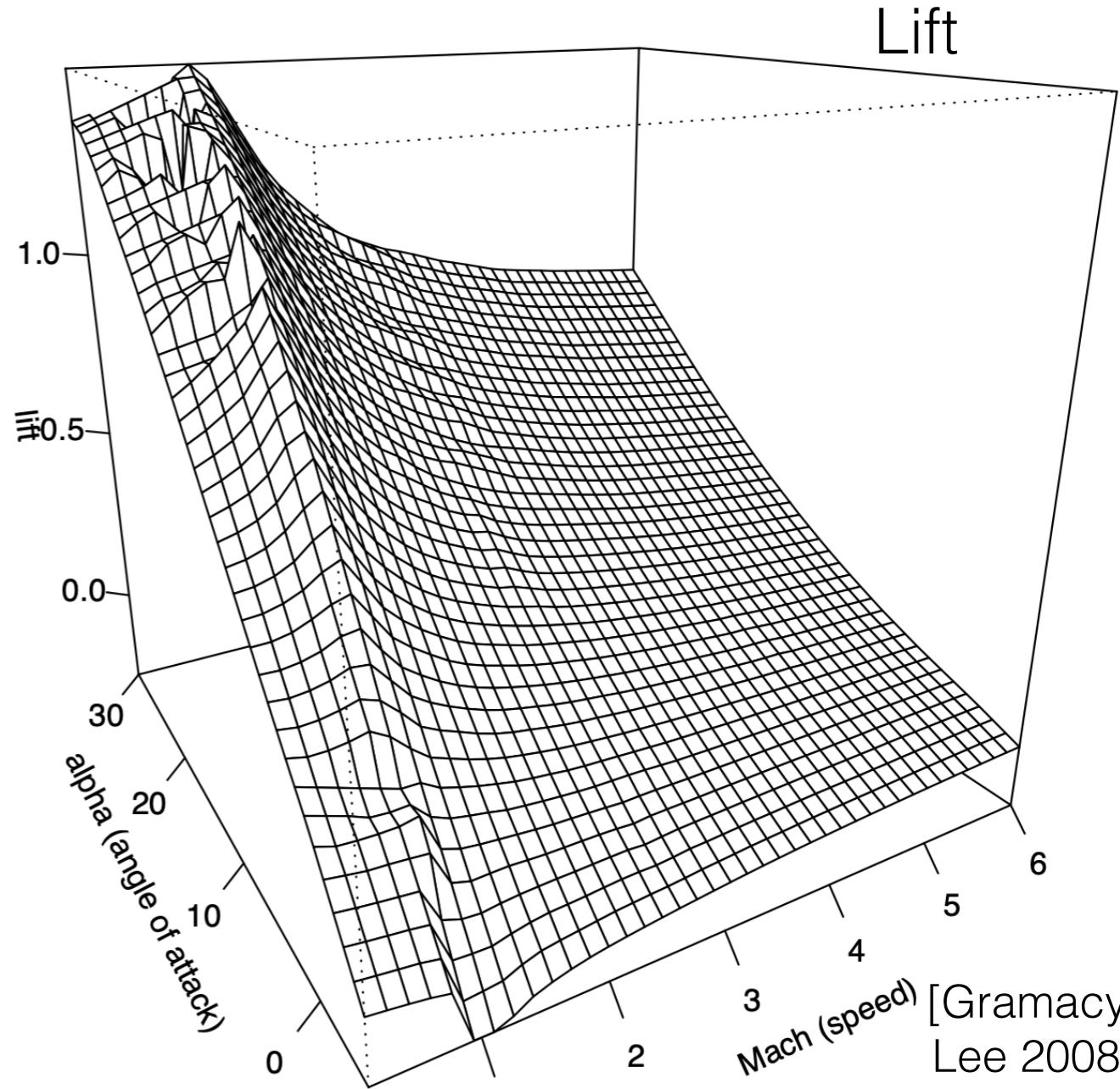
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Challenges:

- Sparse data
- Lift may have a nonlinear relationship to the inputs



Lift

[Gramacy,
Lee 2008]

[Gramacy
2020]

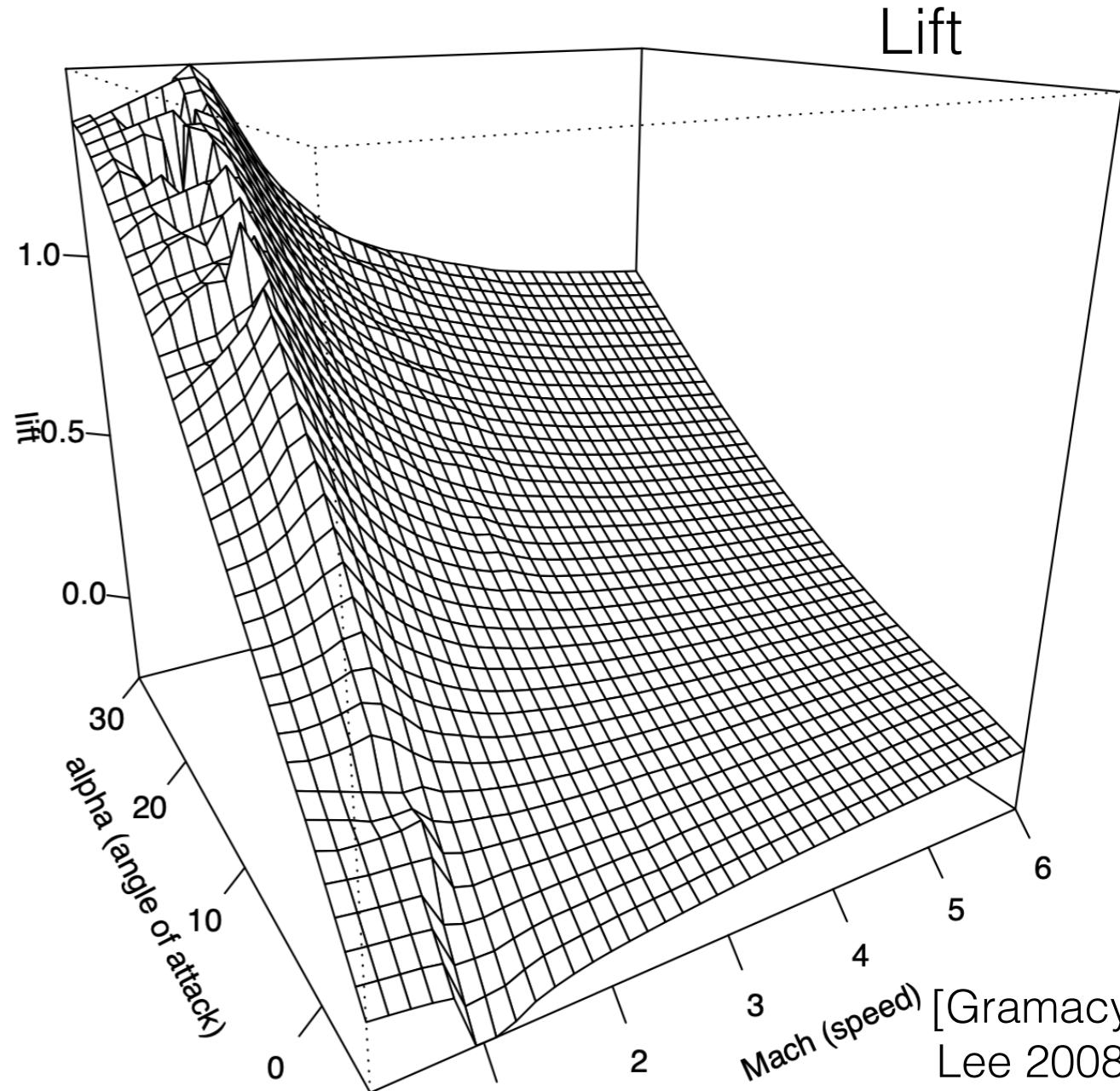
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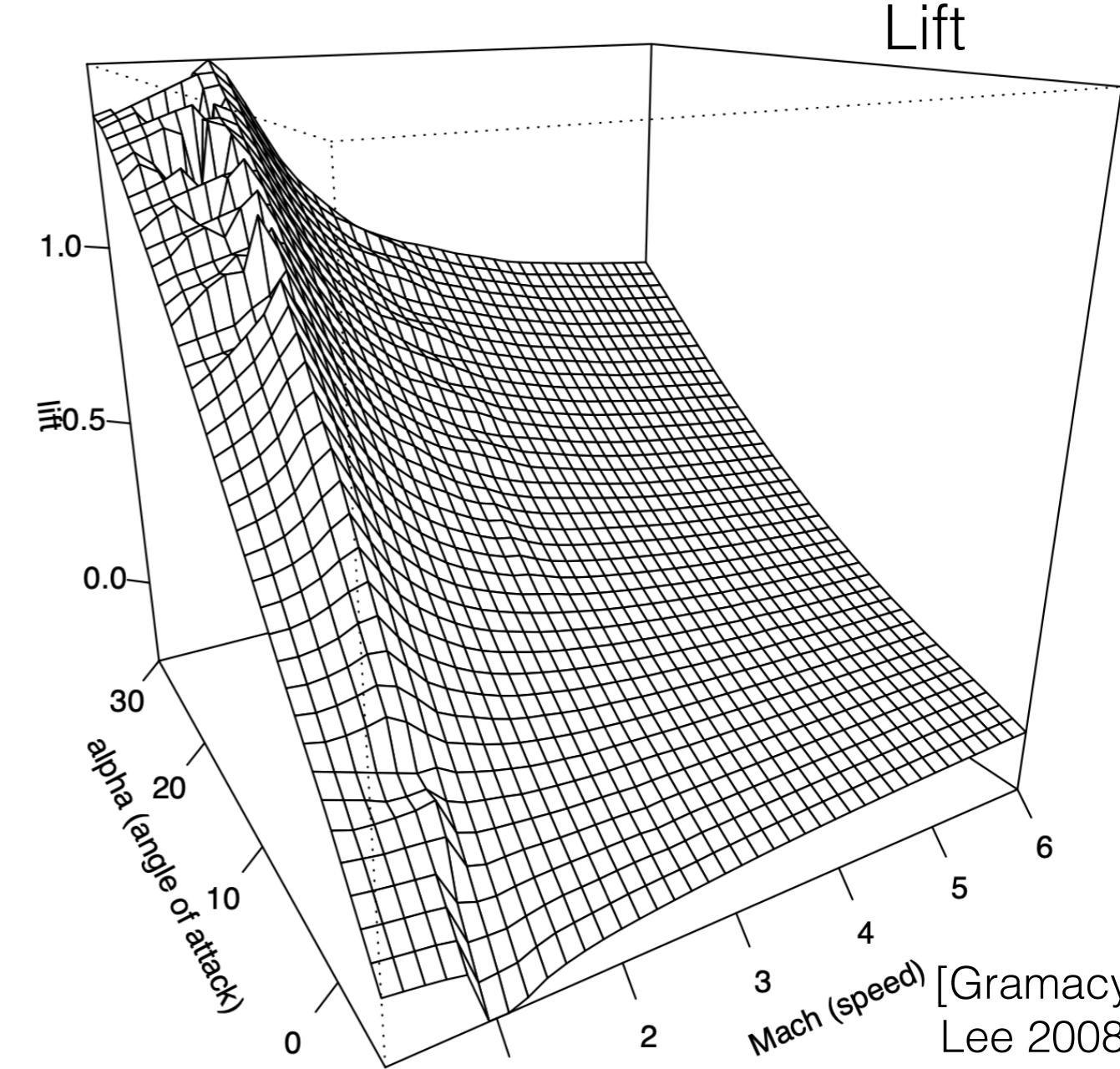
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Challenges:

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Common similar problem: learn (& optimize) performance in ML as a function of scalar hyperparameters



Lift

[Gramacy,
Lee 2008]

[Gramacy
2020]

- 2 • E.g. tune momentum, learning rate, dropout rates, etc.

[Snoek et
al 2012,
2015;

Garnett
2023]

A Bayesian approach

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- $p(\text{unknowns} \mid \text{data})$

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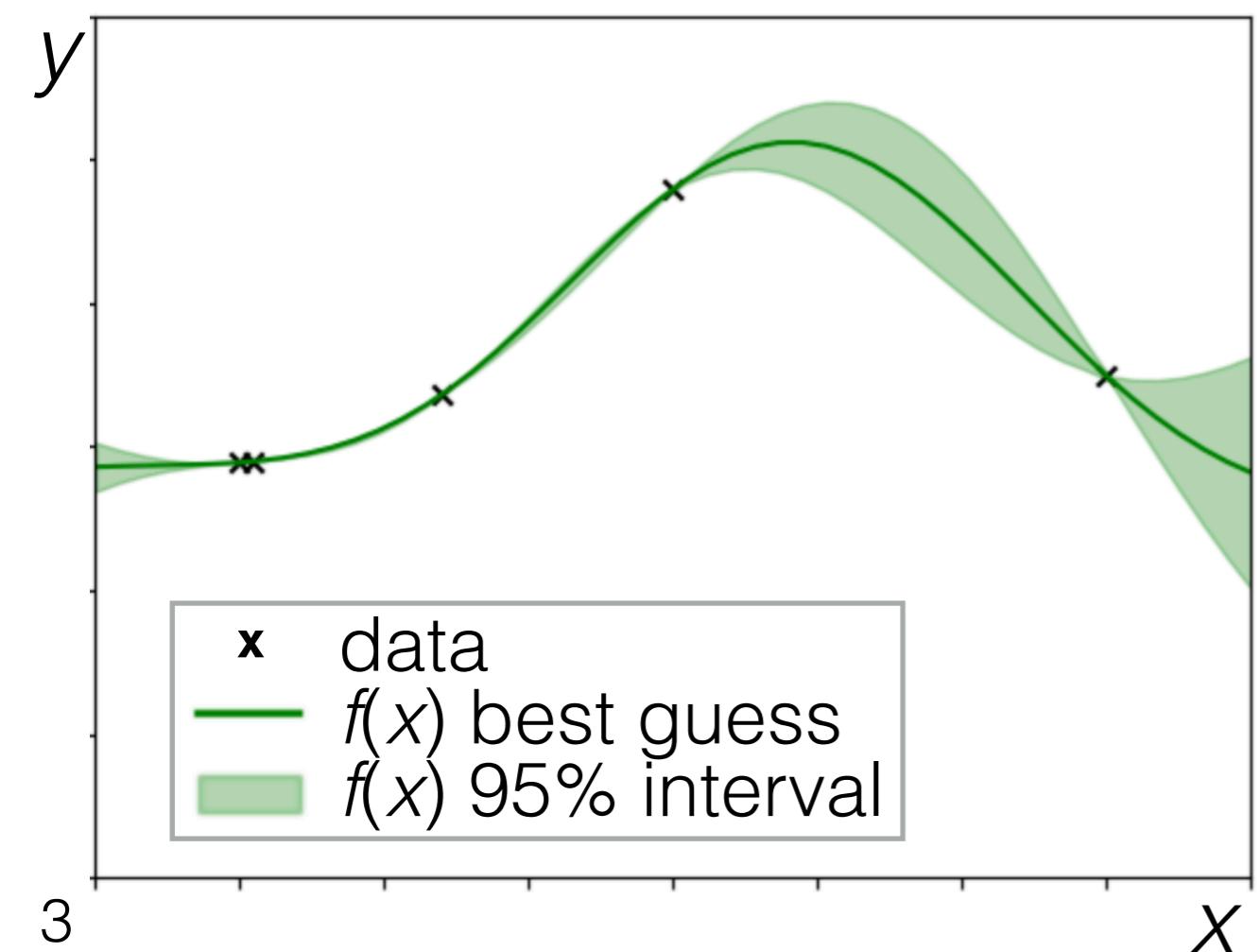
Given the data we've seen, what do we know about the underlying function?



A Bayesian approach

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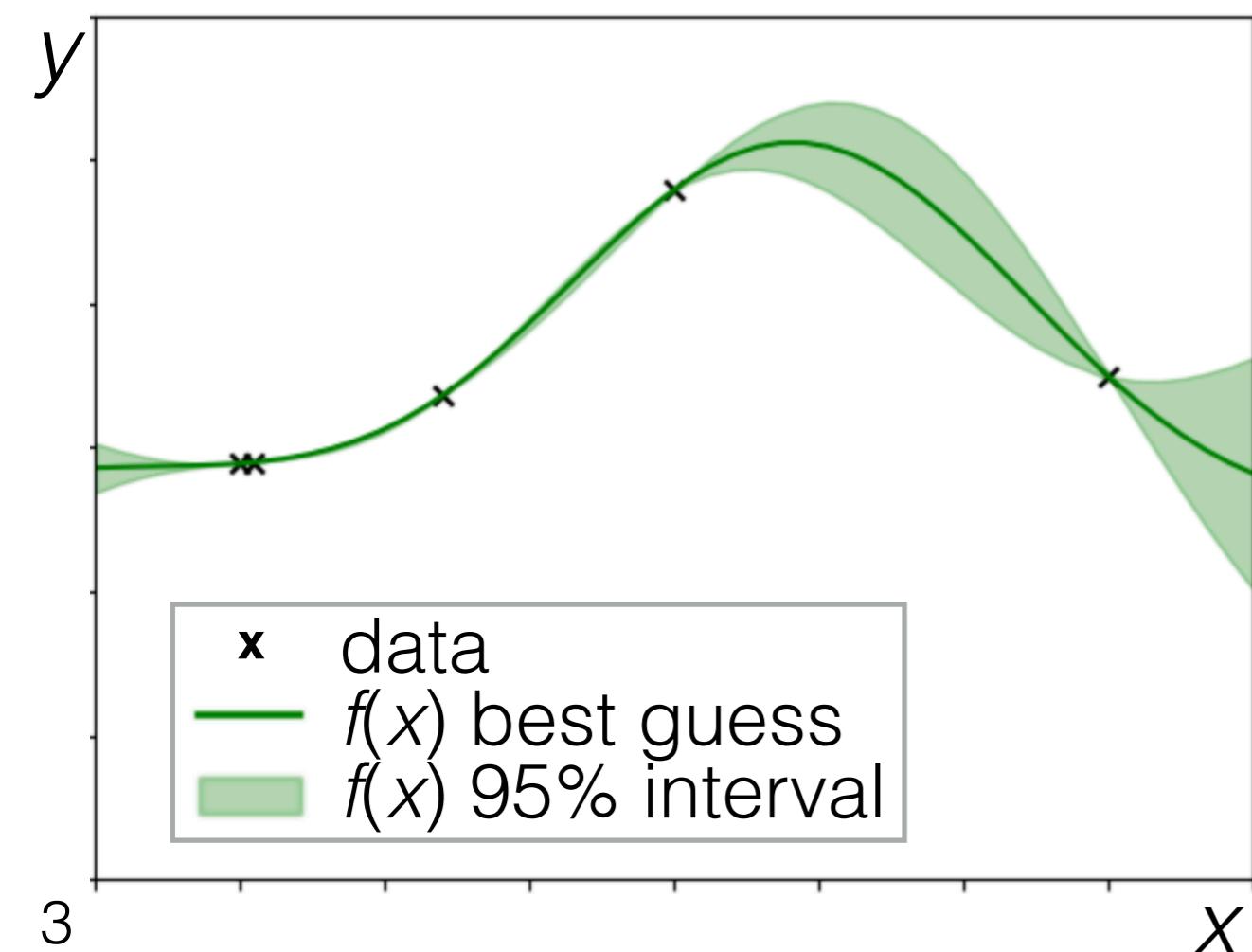
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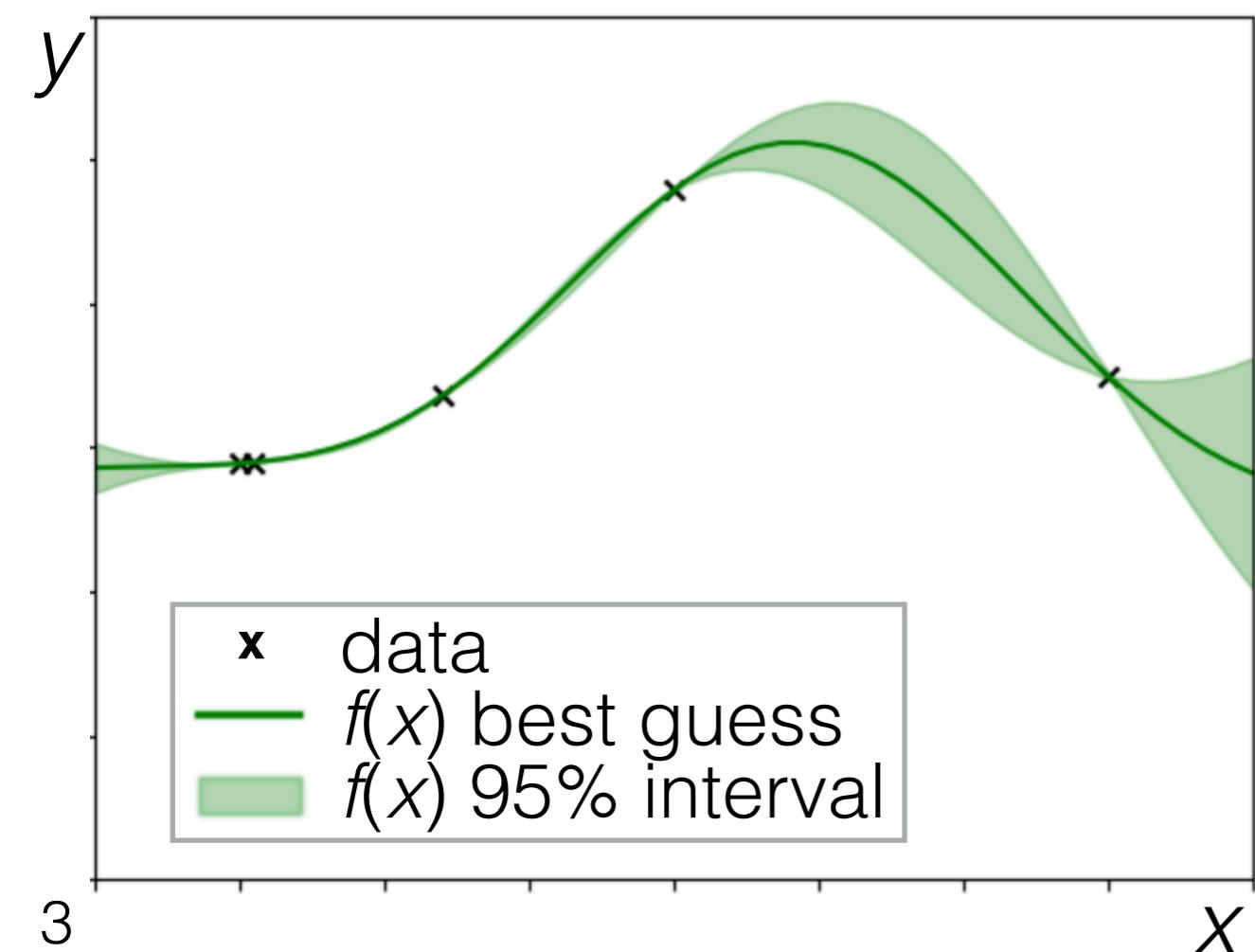


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A model (likelihood & prior) that can generate functions and data of interest

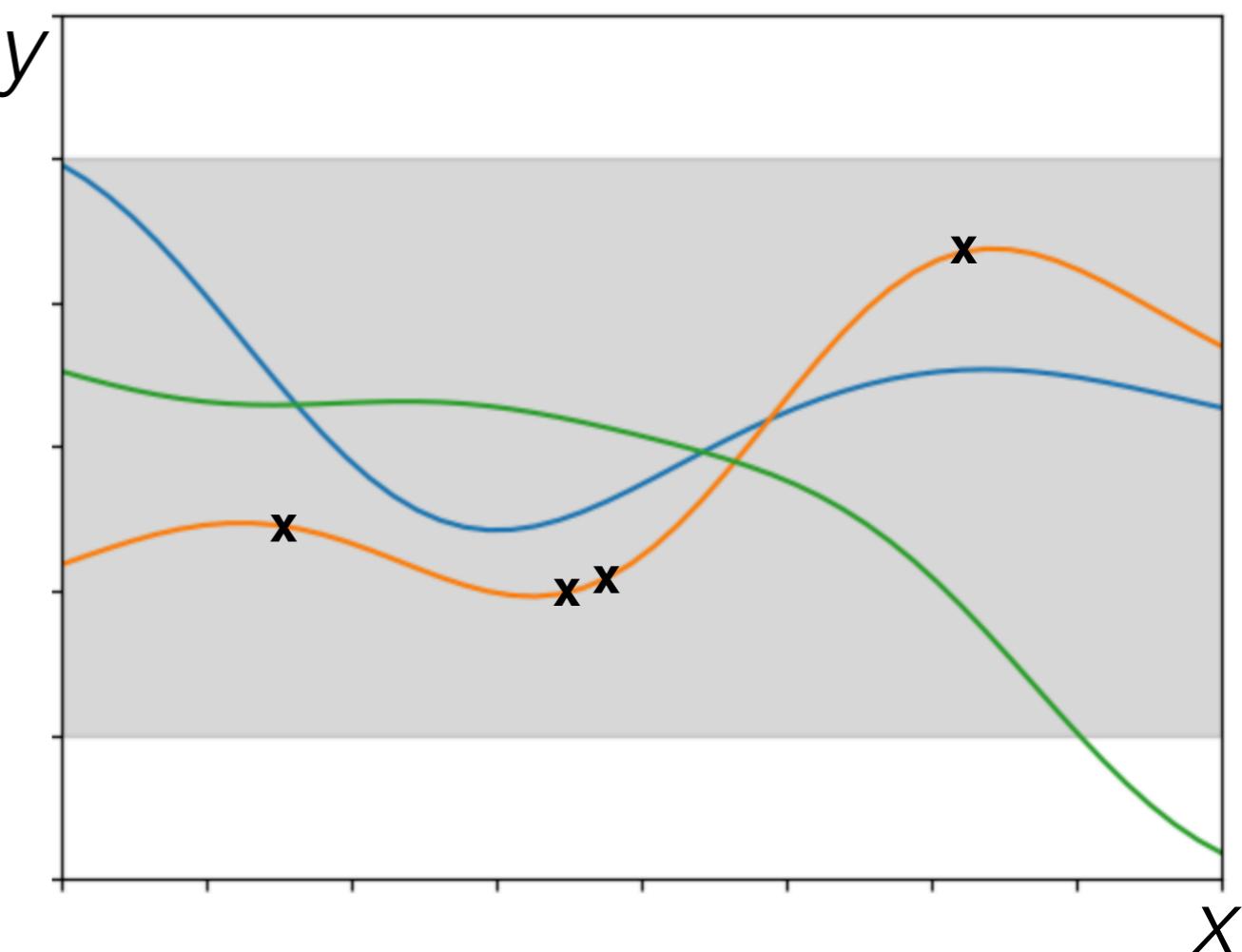
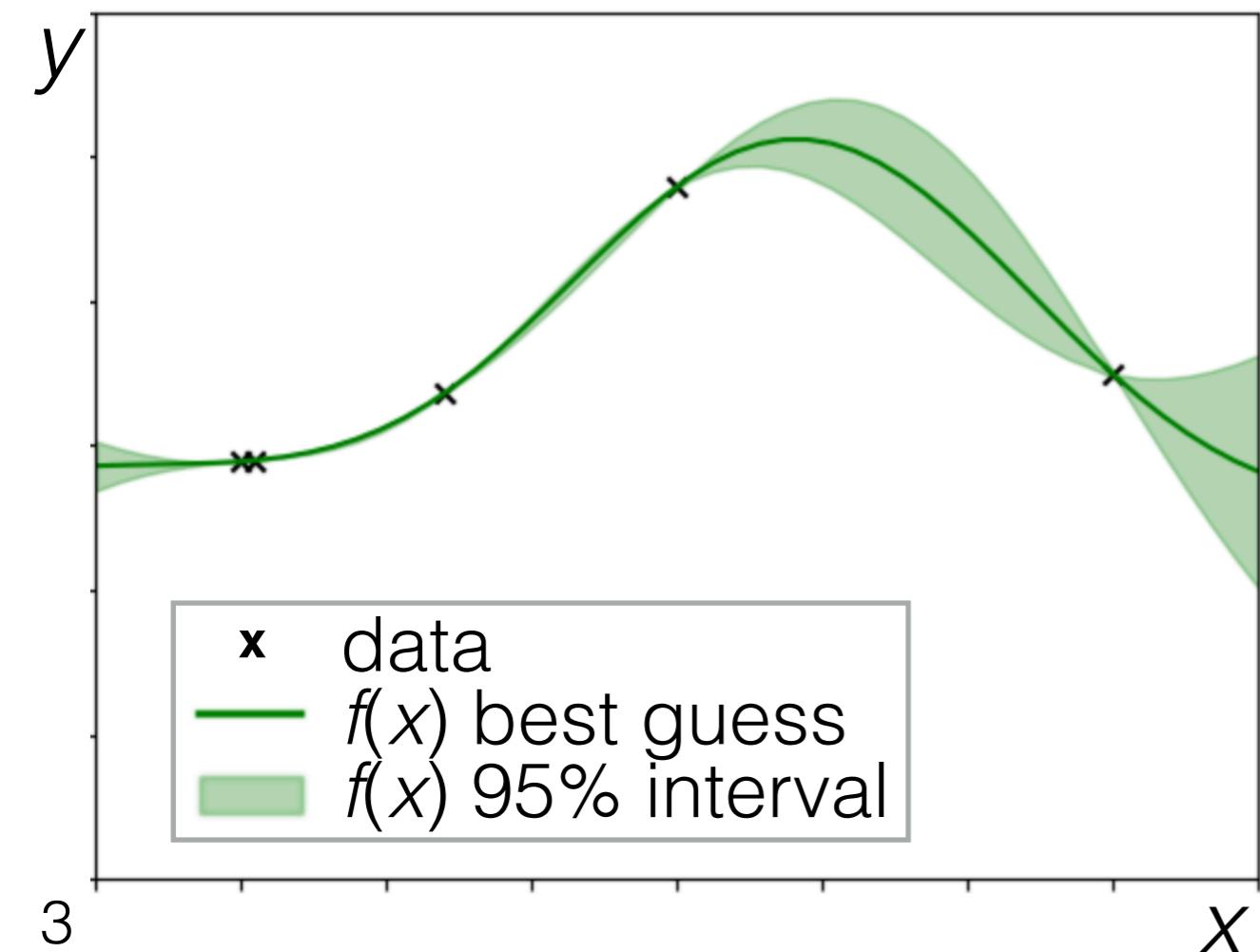


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Multivariate Gaussian using locations

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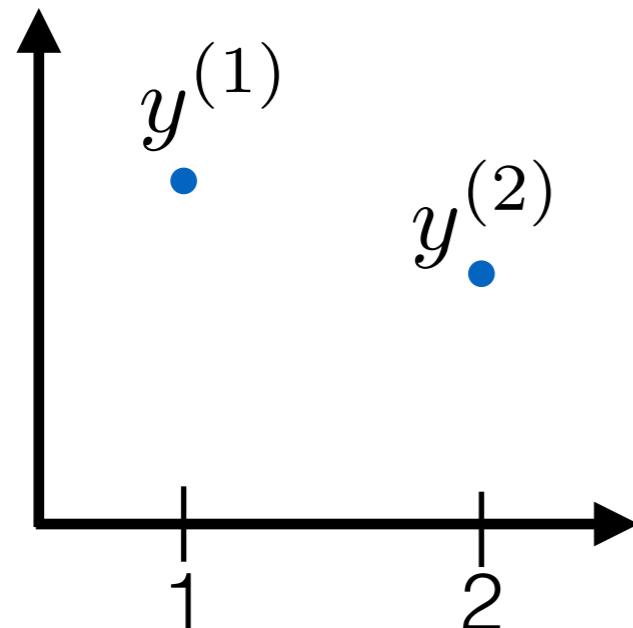
- $M=2$ dimensions: $[y^{(1)}, y^{(2)}]^\top \sim \mathcal{N}(\mu, K)$
 - With $\mu = [0, 0]^\top$ and $K = \sigma^2 \begin{bmatrix} 1 & \rho \\ \rho & 1 \end{bmatrix}$



correlation

Multivariate Gaussian using locations

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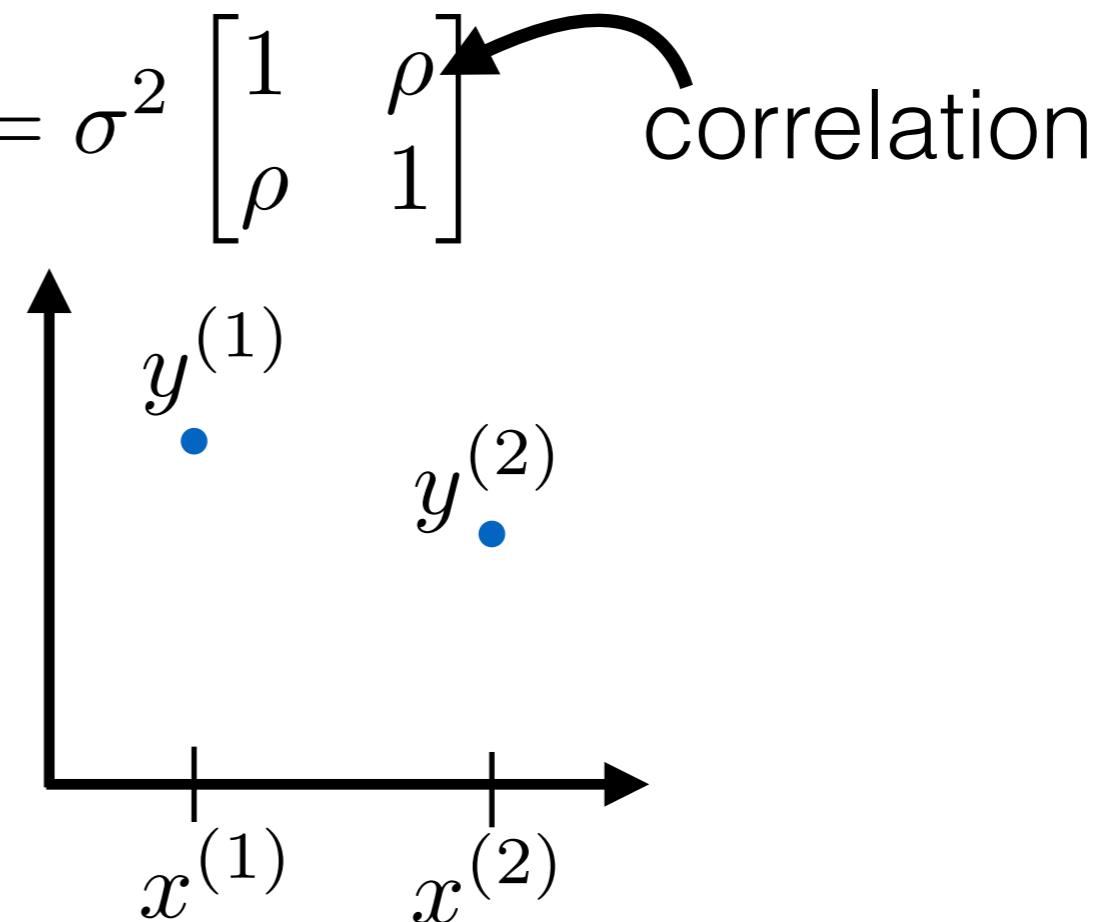
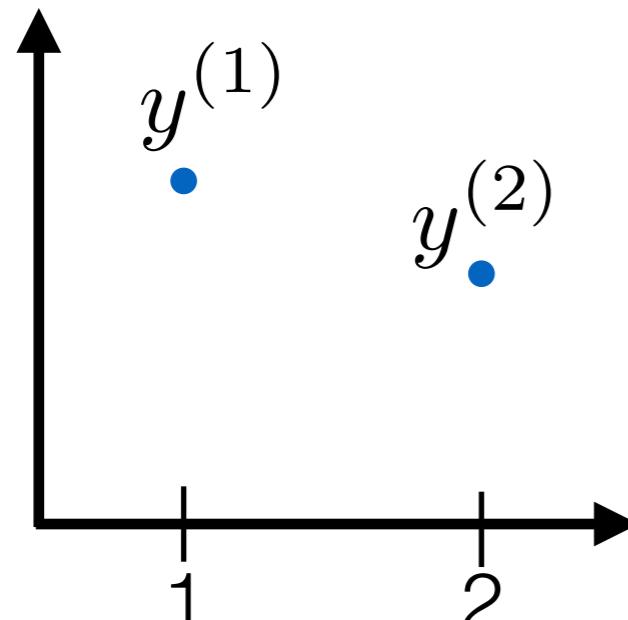


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↑ correlation

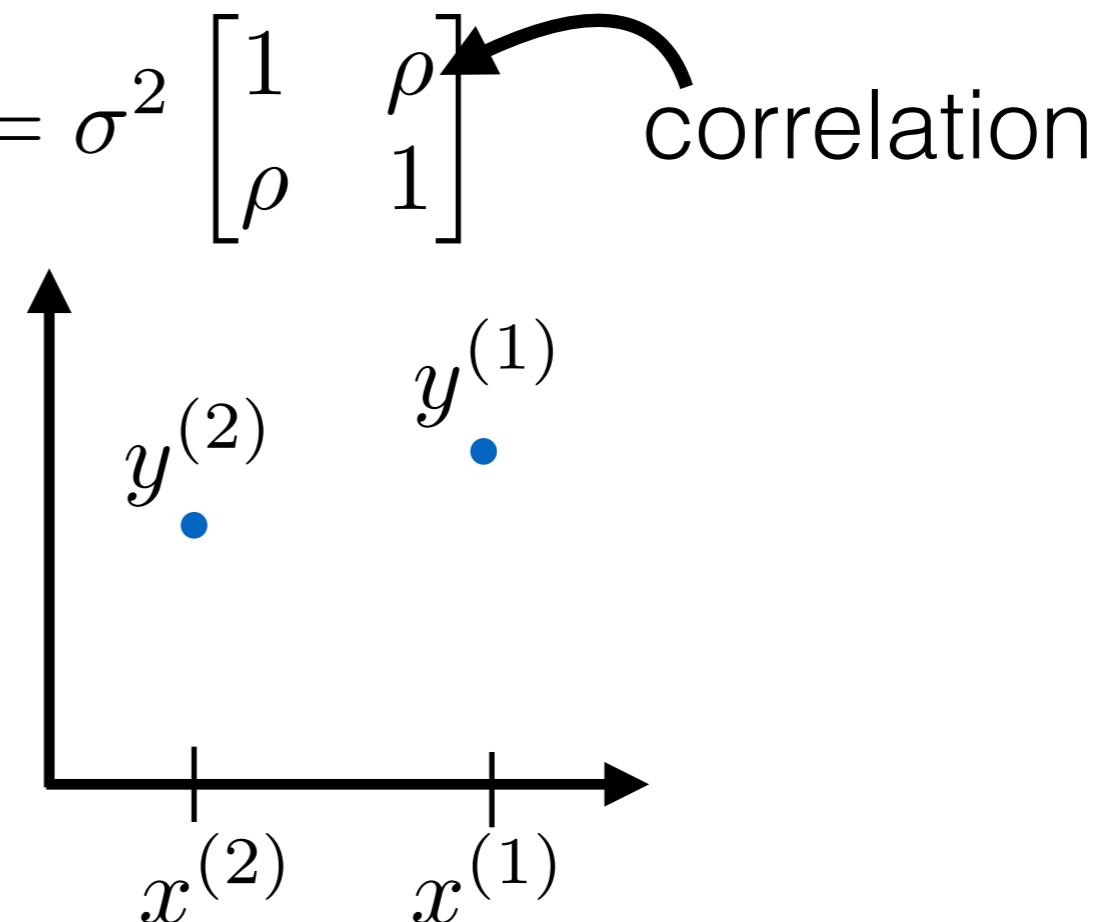
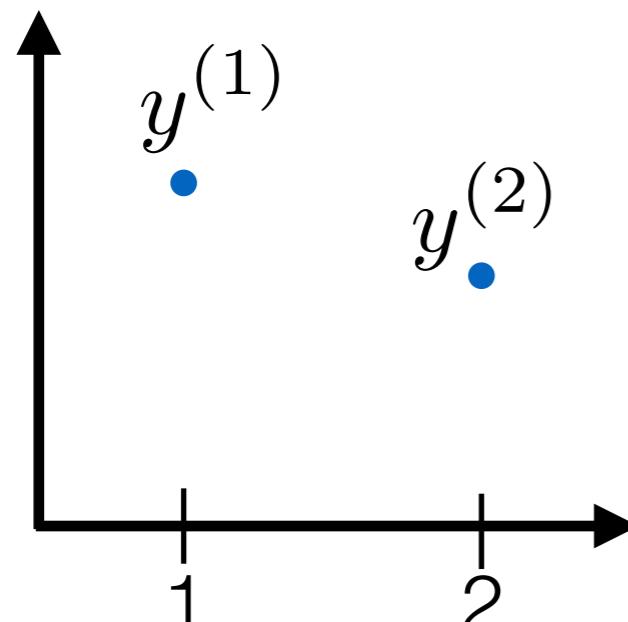
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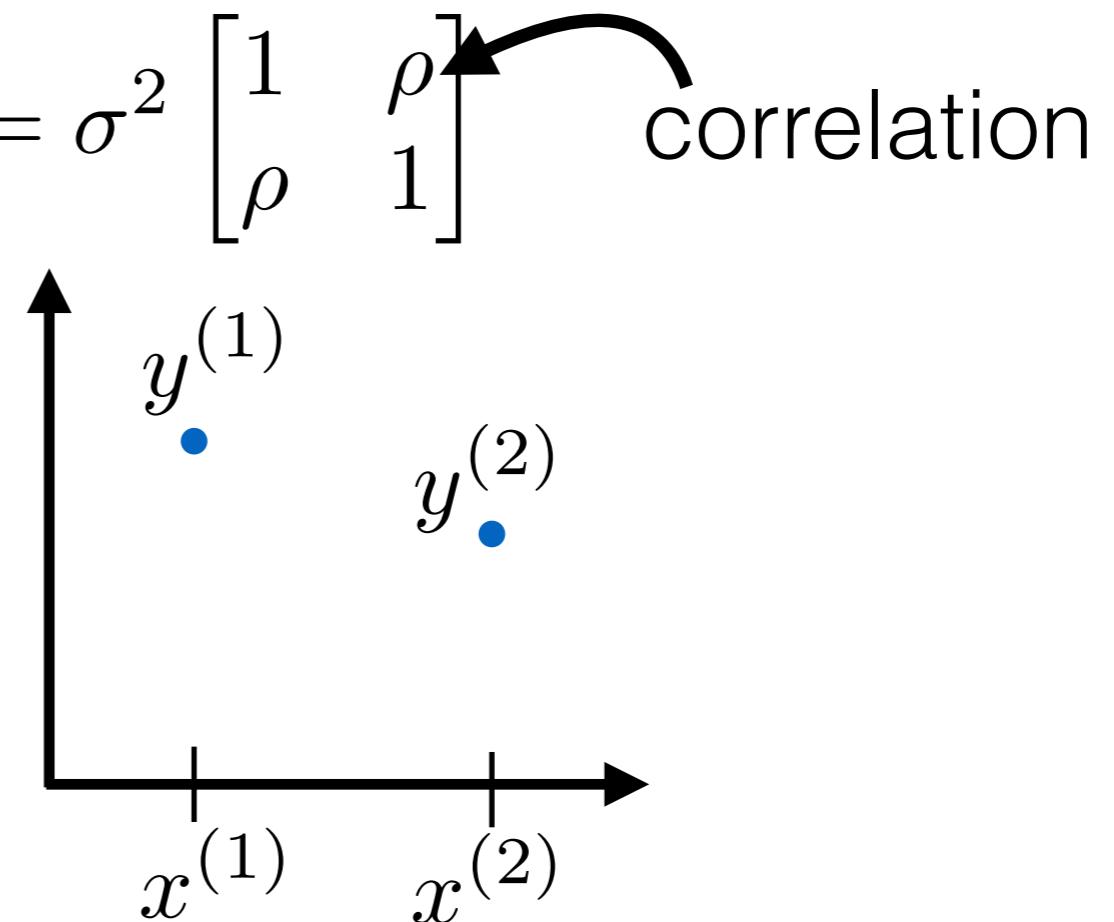
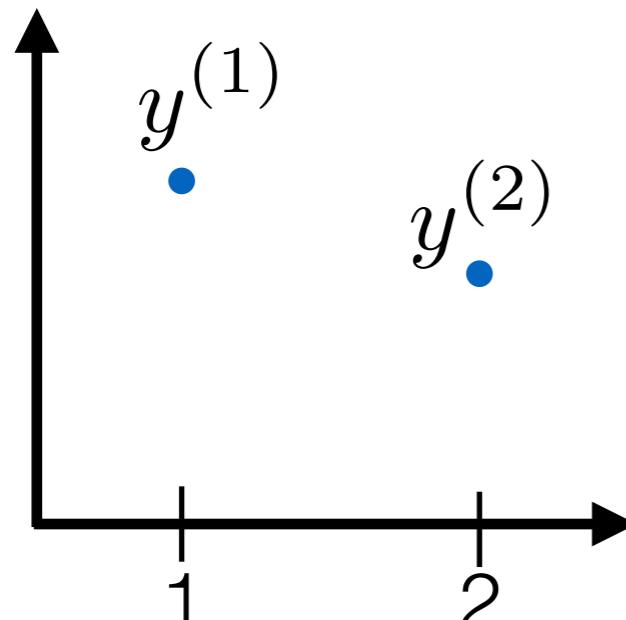
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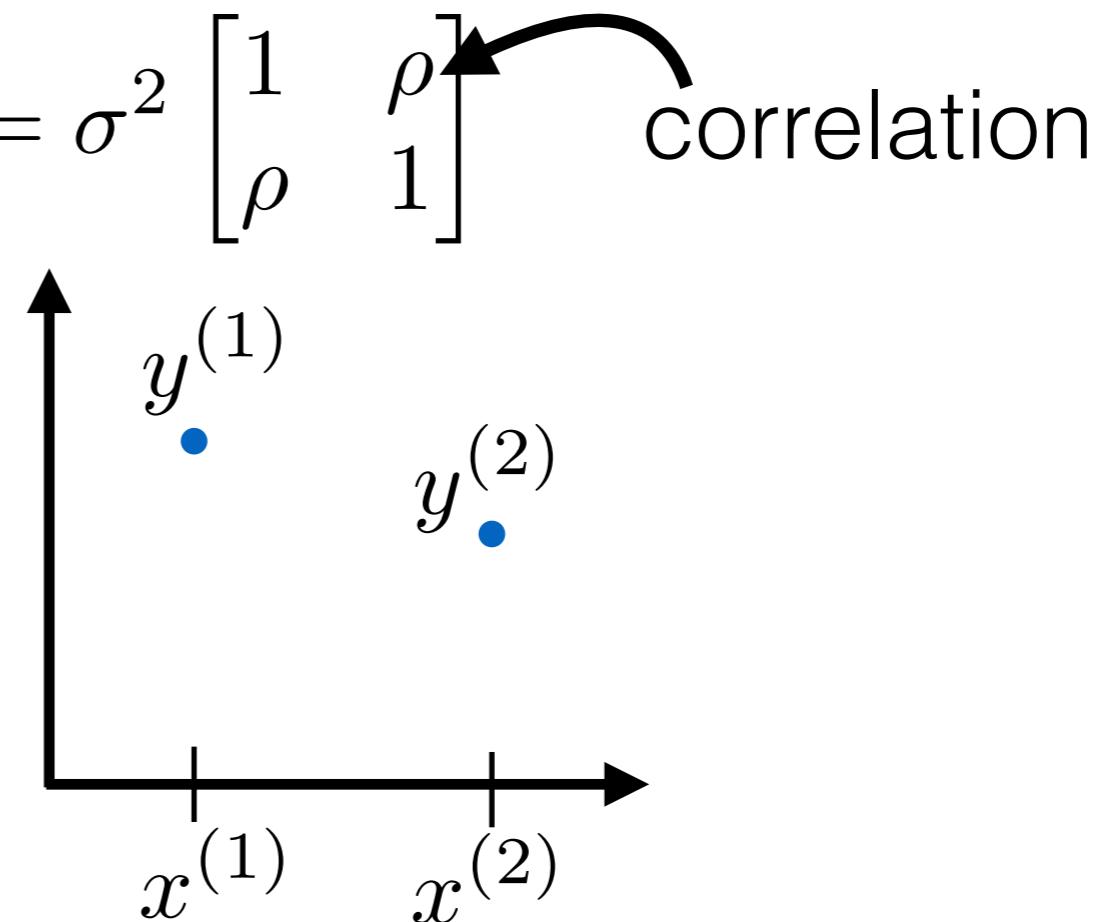
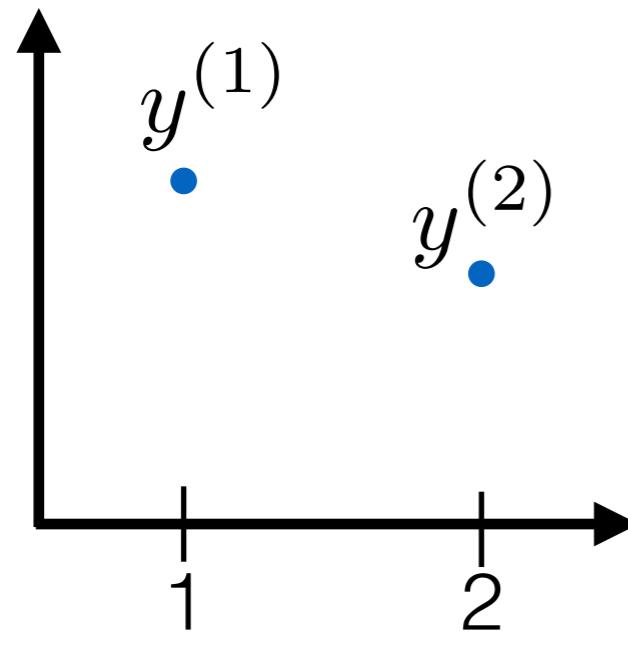
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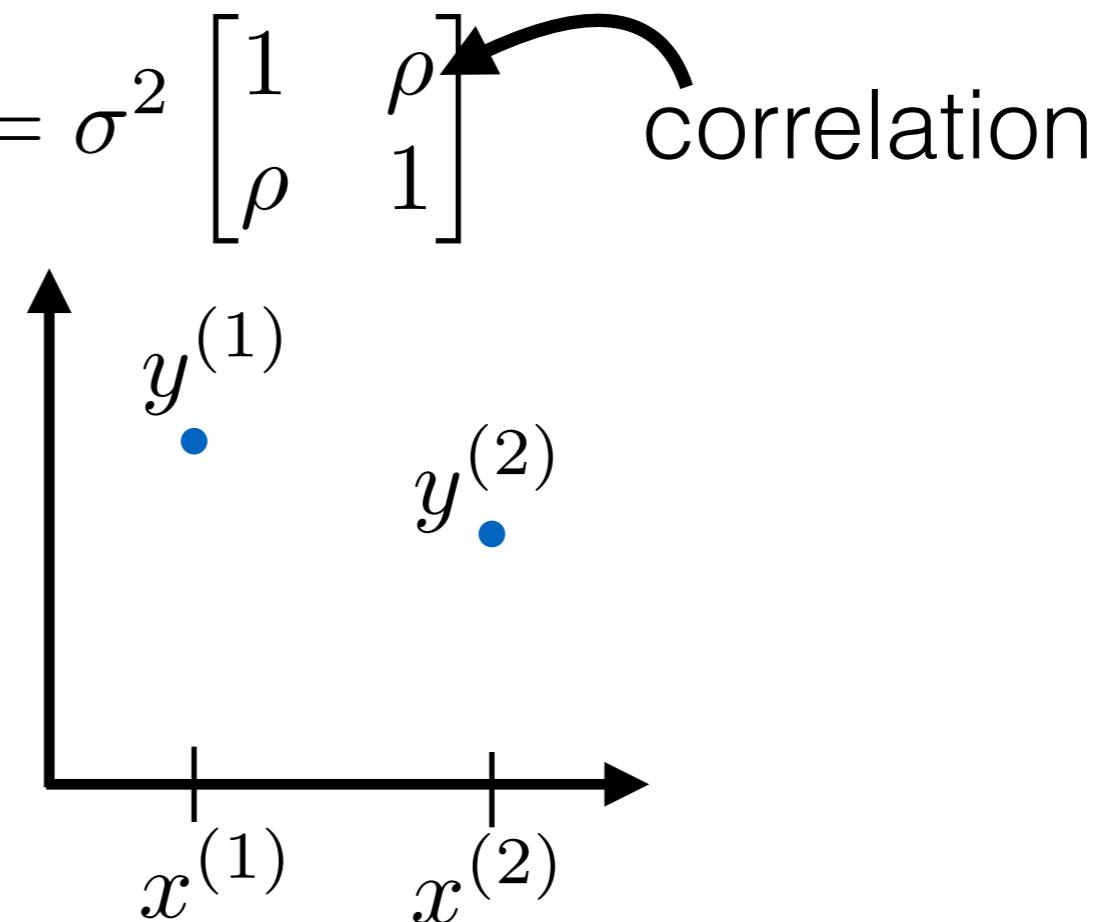
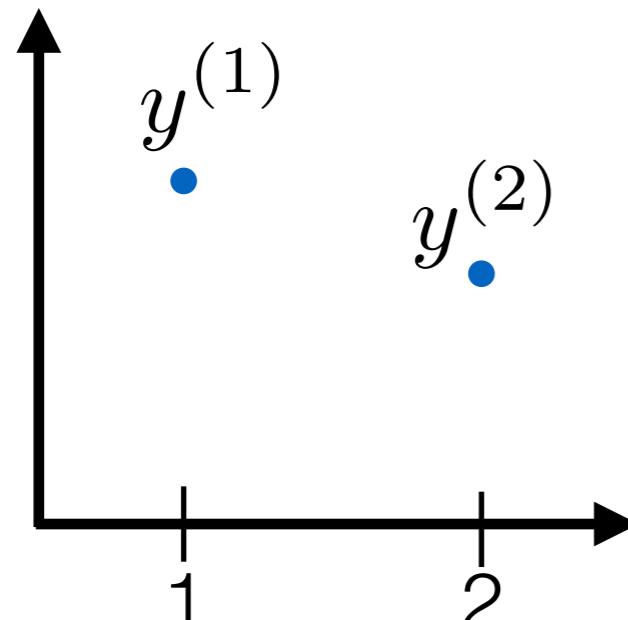
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- What if we let the correlation depend on the x 's?

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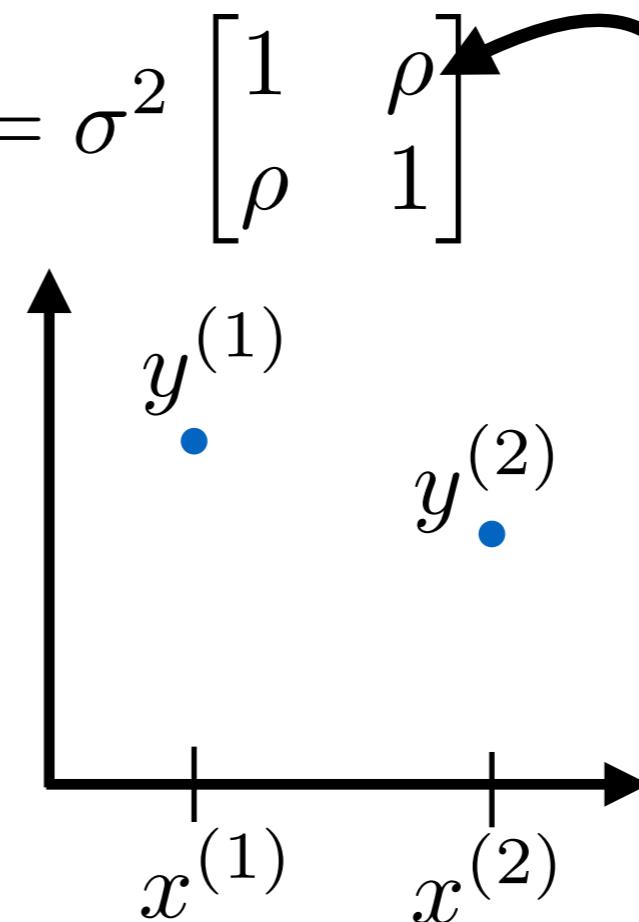
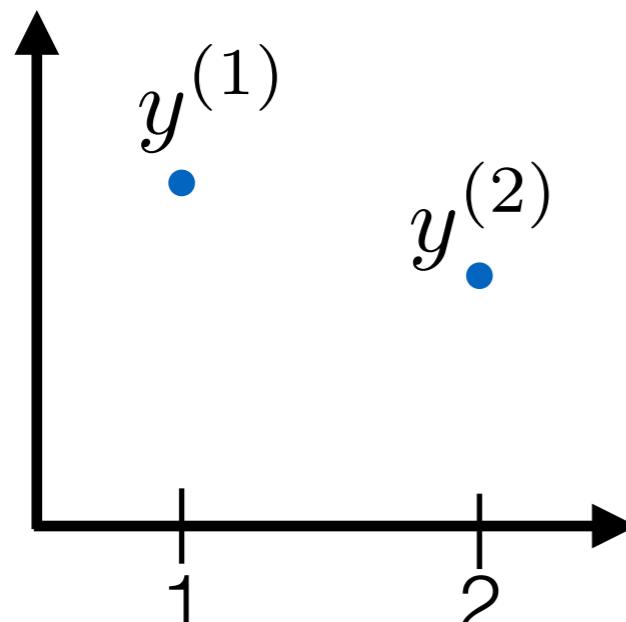
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 - Let $\rho = \rho(|x^{(1)} - x^{(2)}|)$

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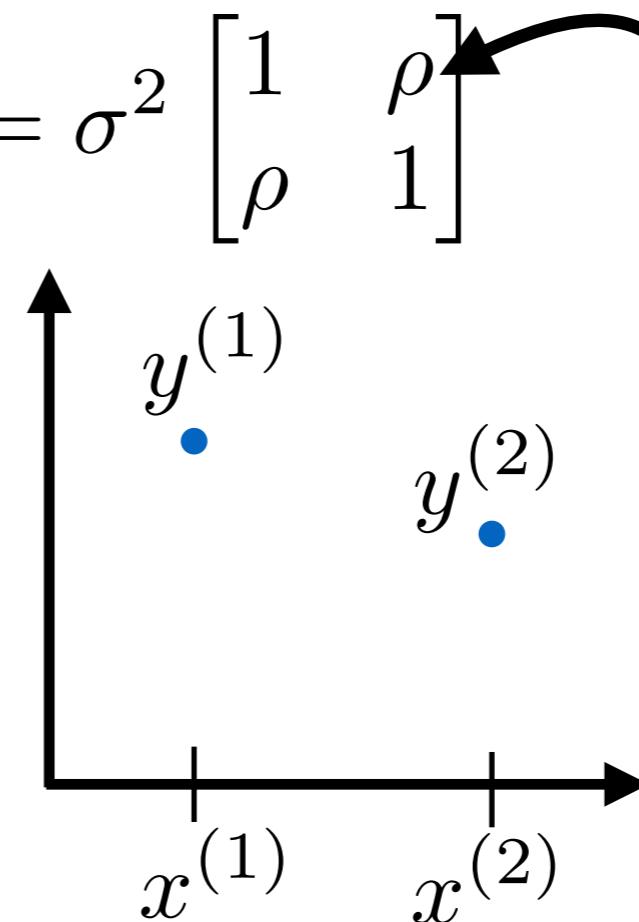
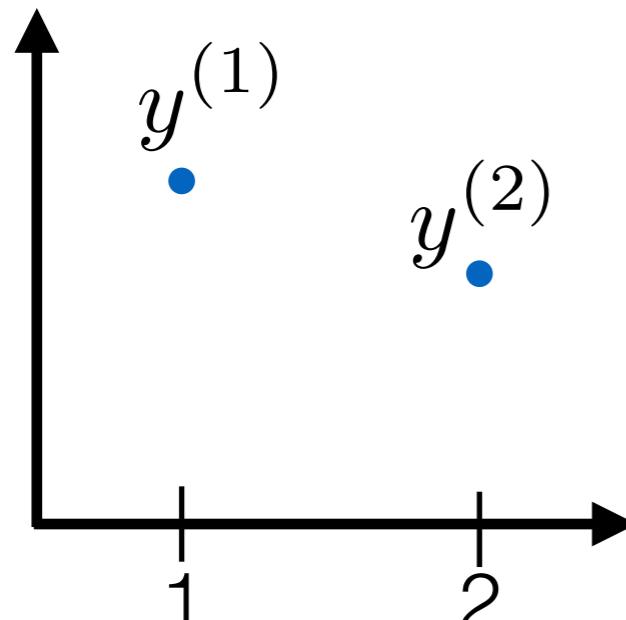
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 - Let $\rho = \rho(|x^{(1)} - x^{(2)}|)$
 - Where the correlation goes to 1 as the x 's get close

Multivariate Gaussian using locations

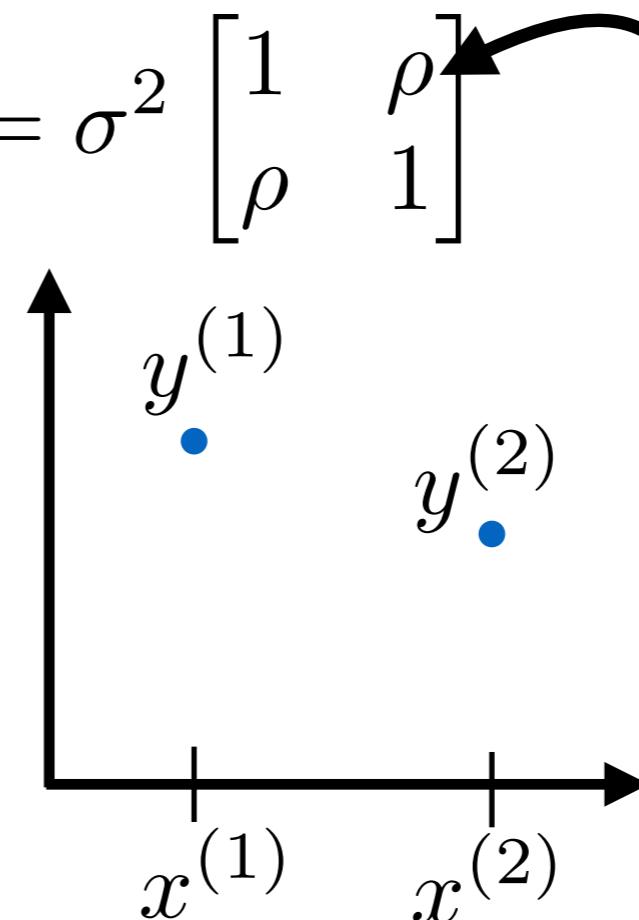
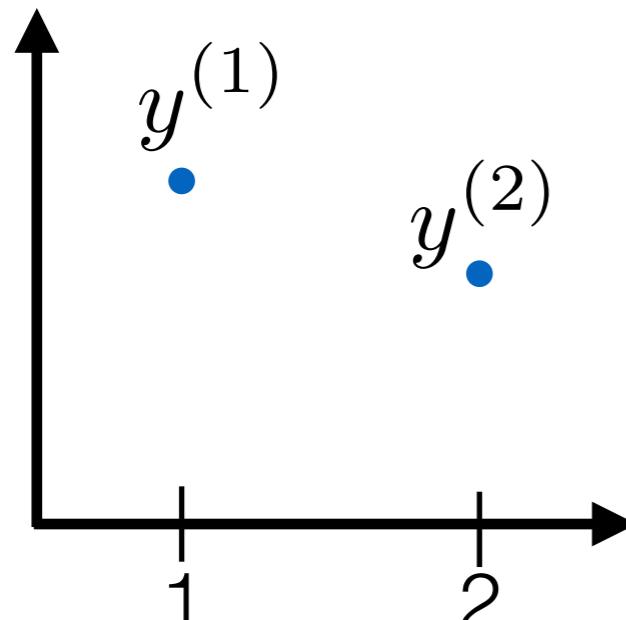
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$$x^{(m)} \in (-\infty, \infty)$$

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- Next: Similar setup but an M -dimensional Gaussian instead of just 2 dimensions
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We just drew random functions from a type of
“Gaussian process”!

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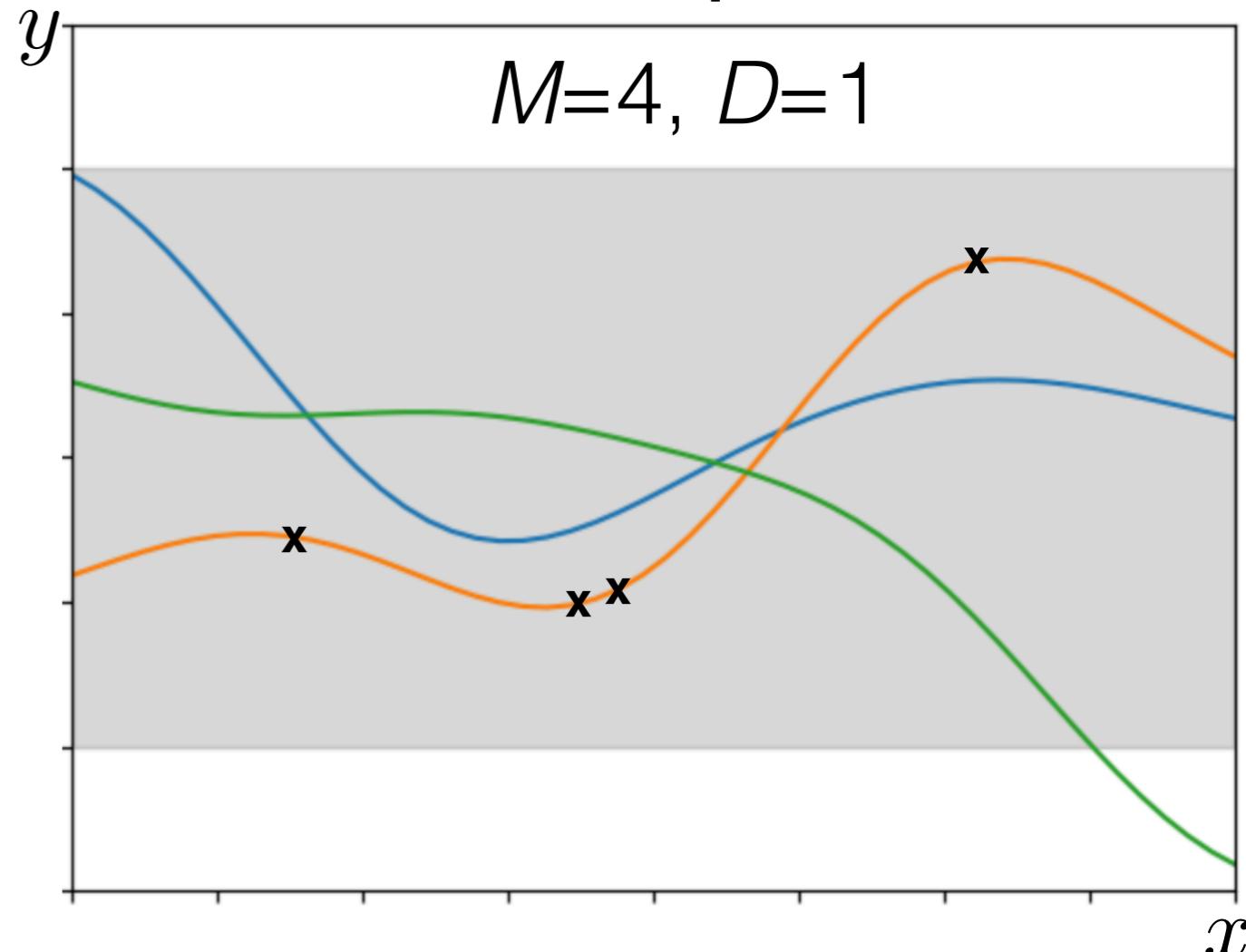
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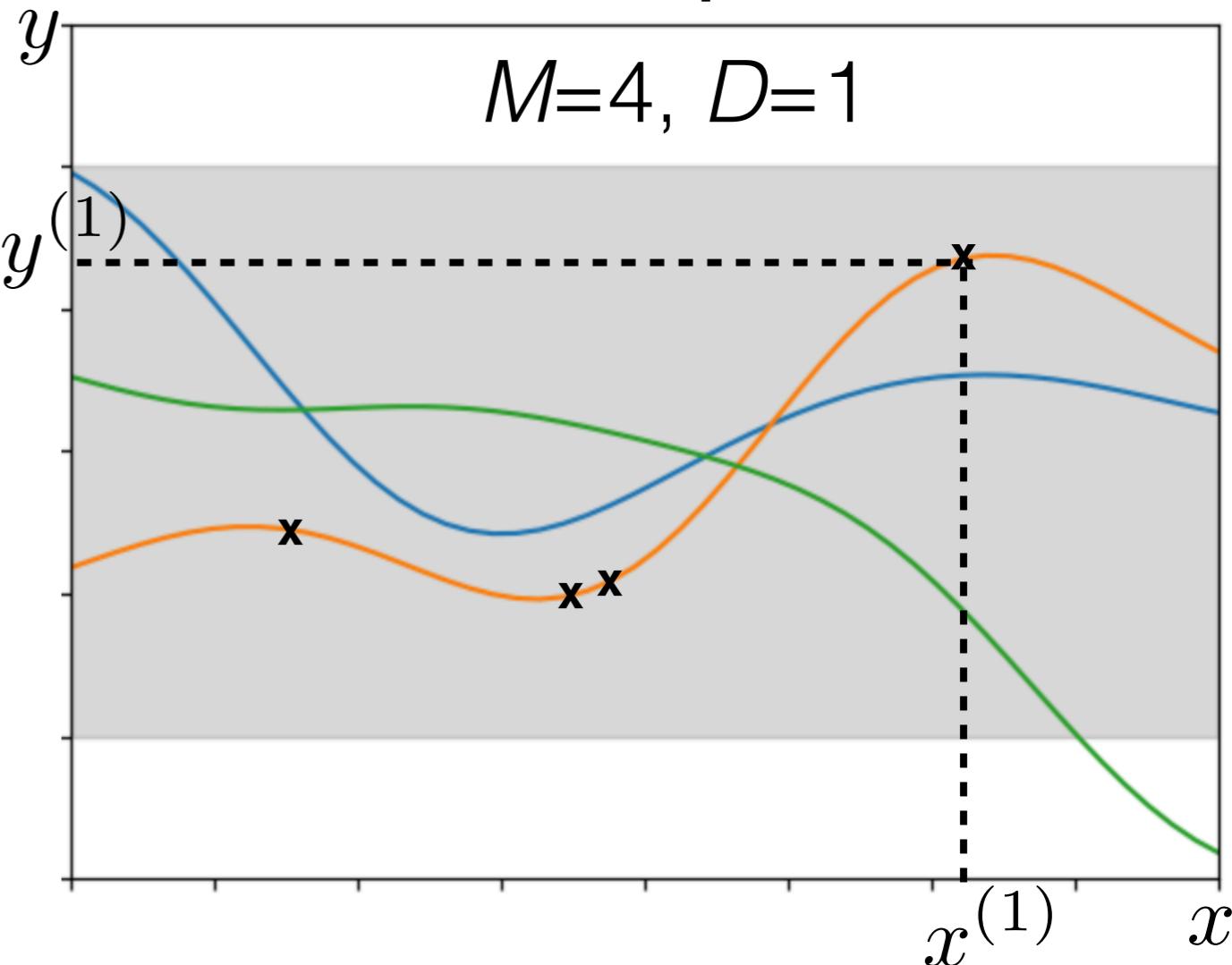
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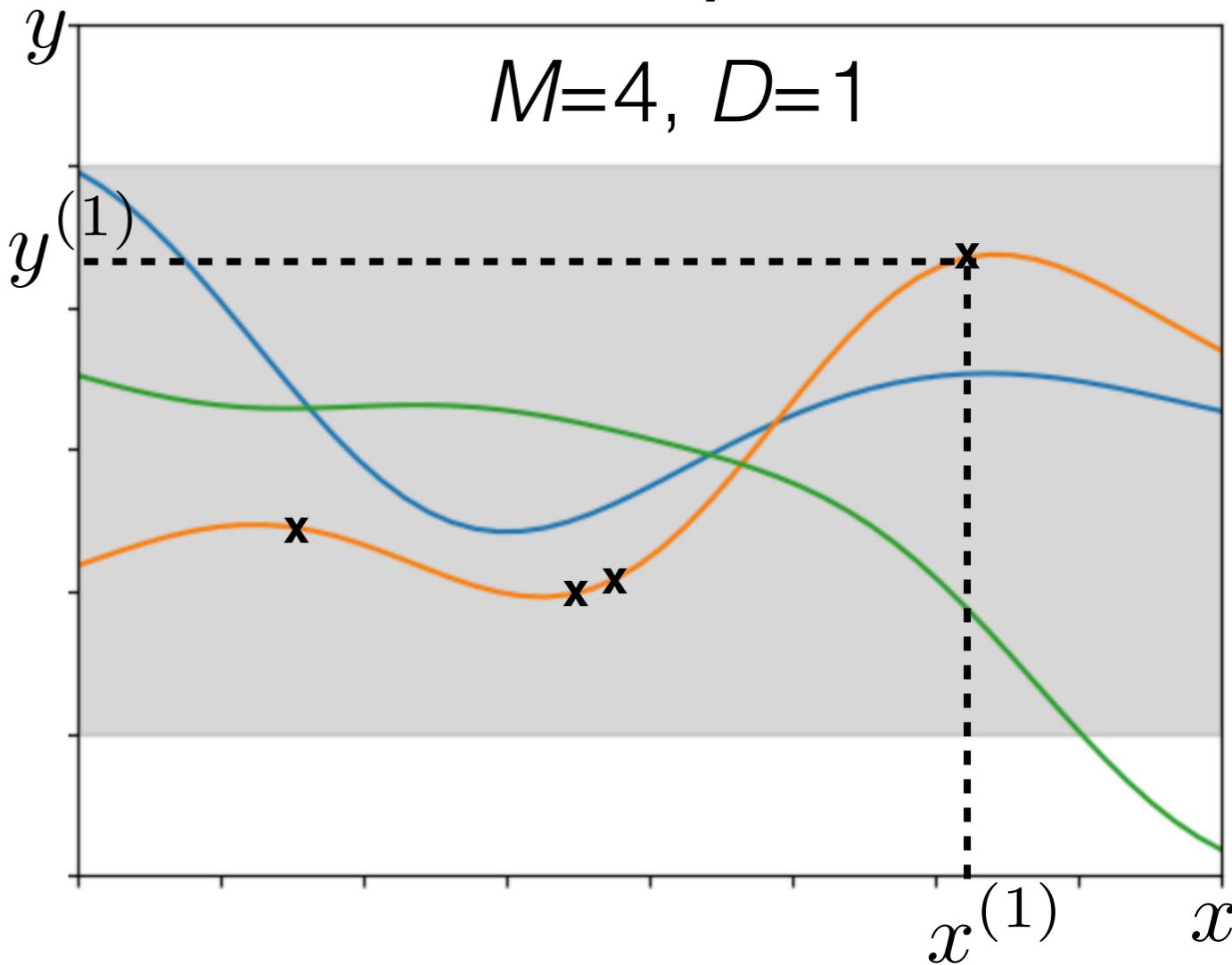
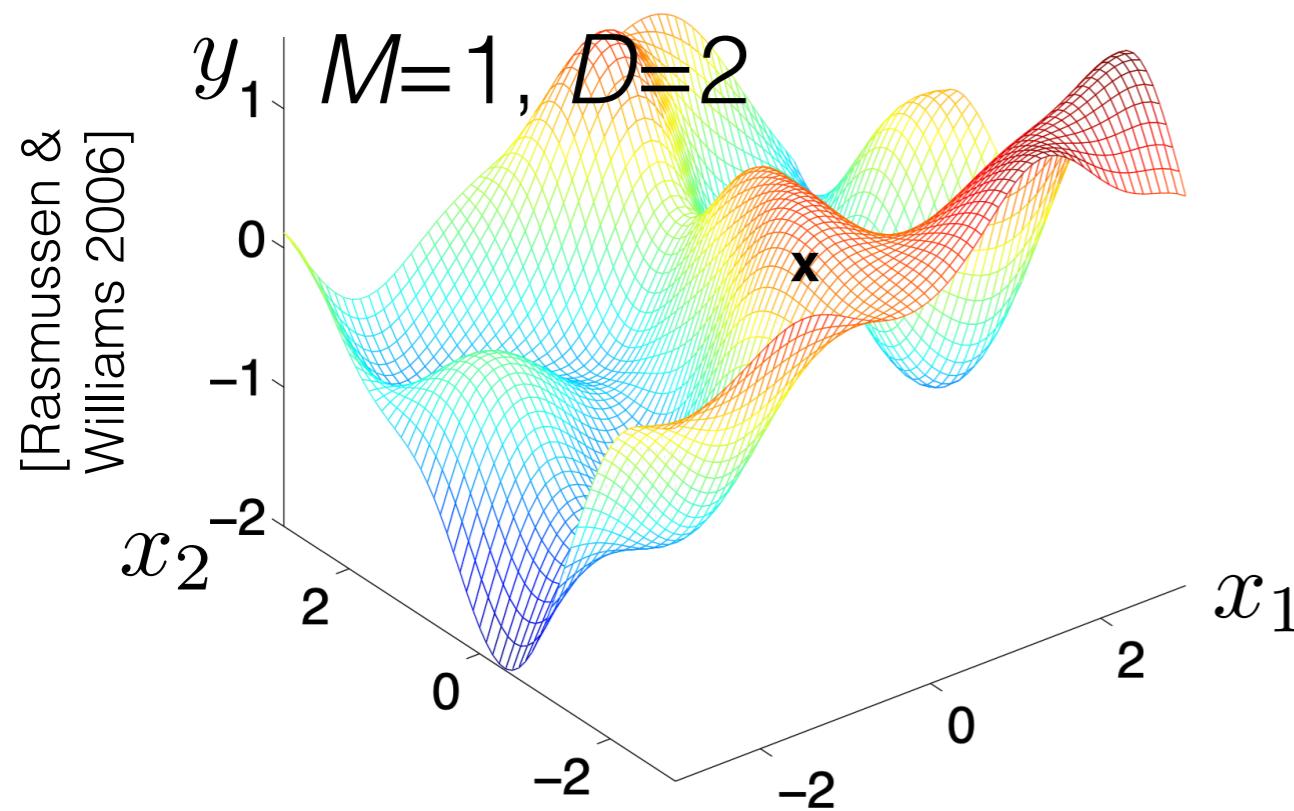
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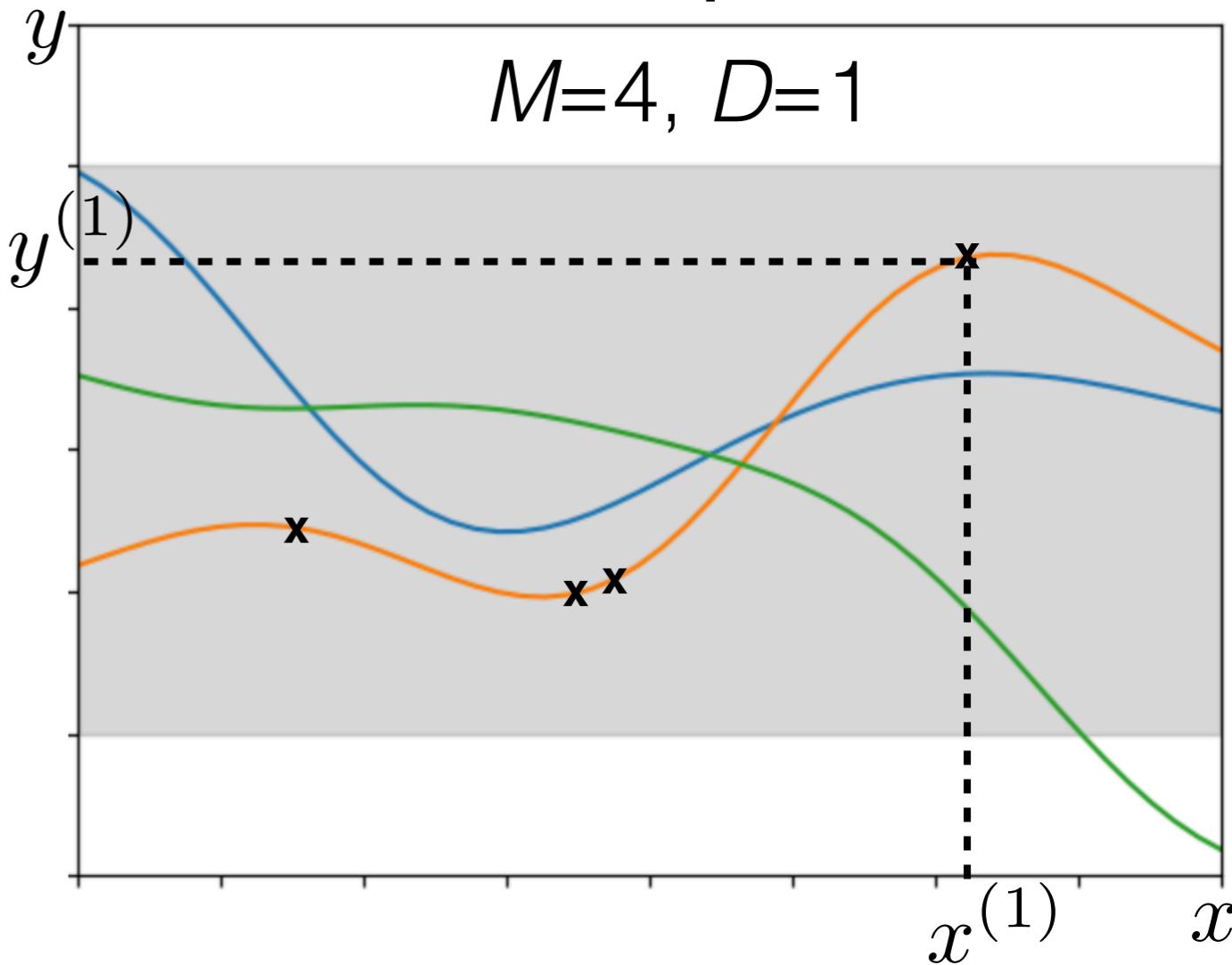
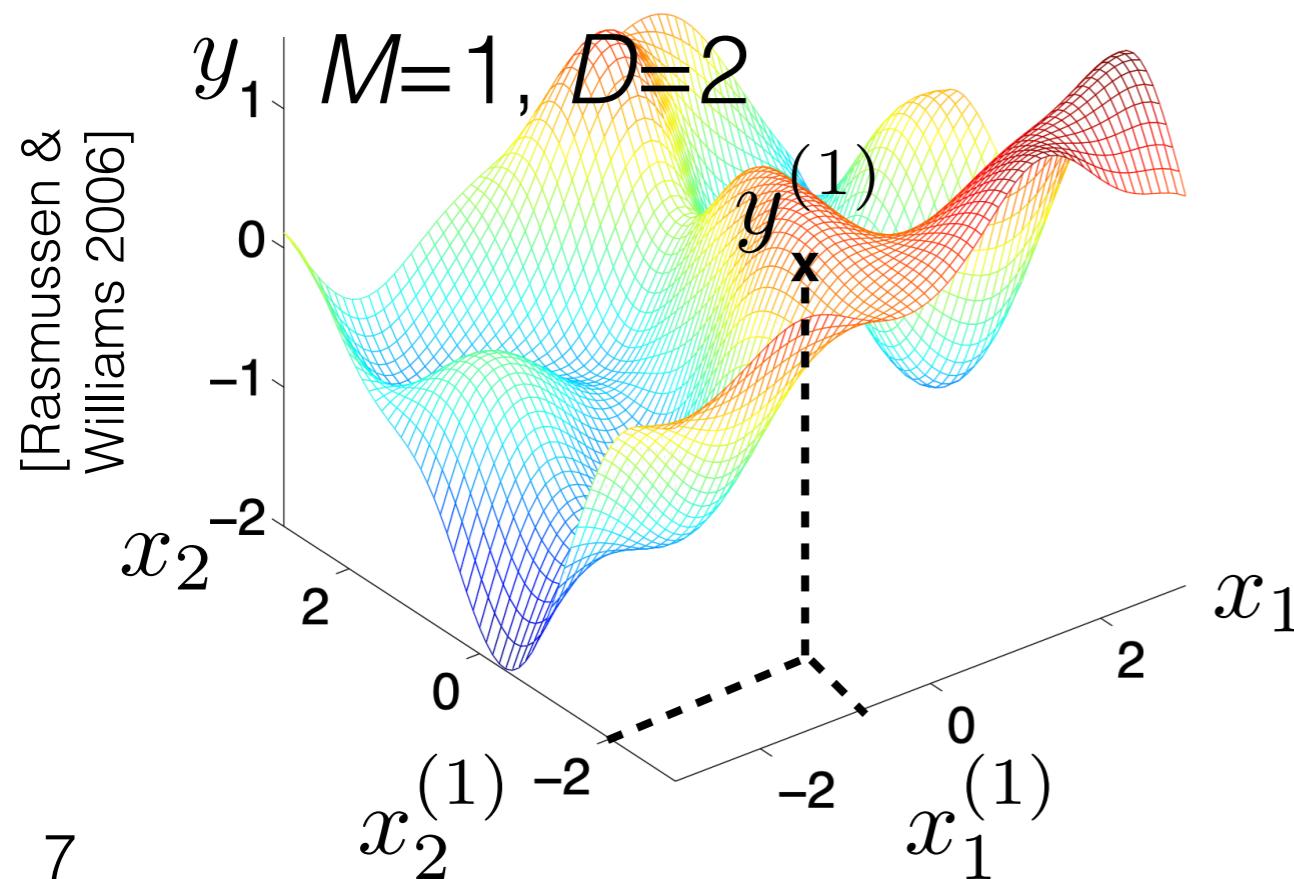
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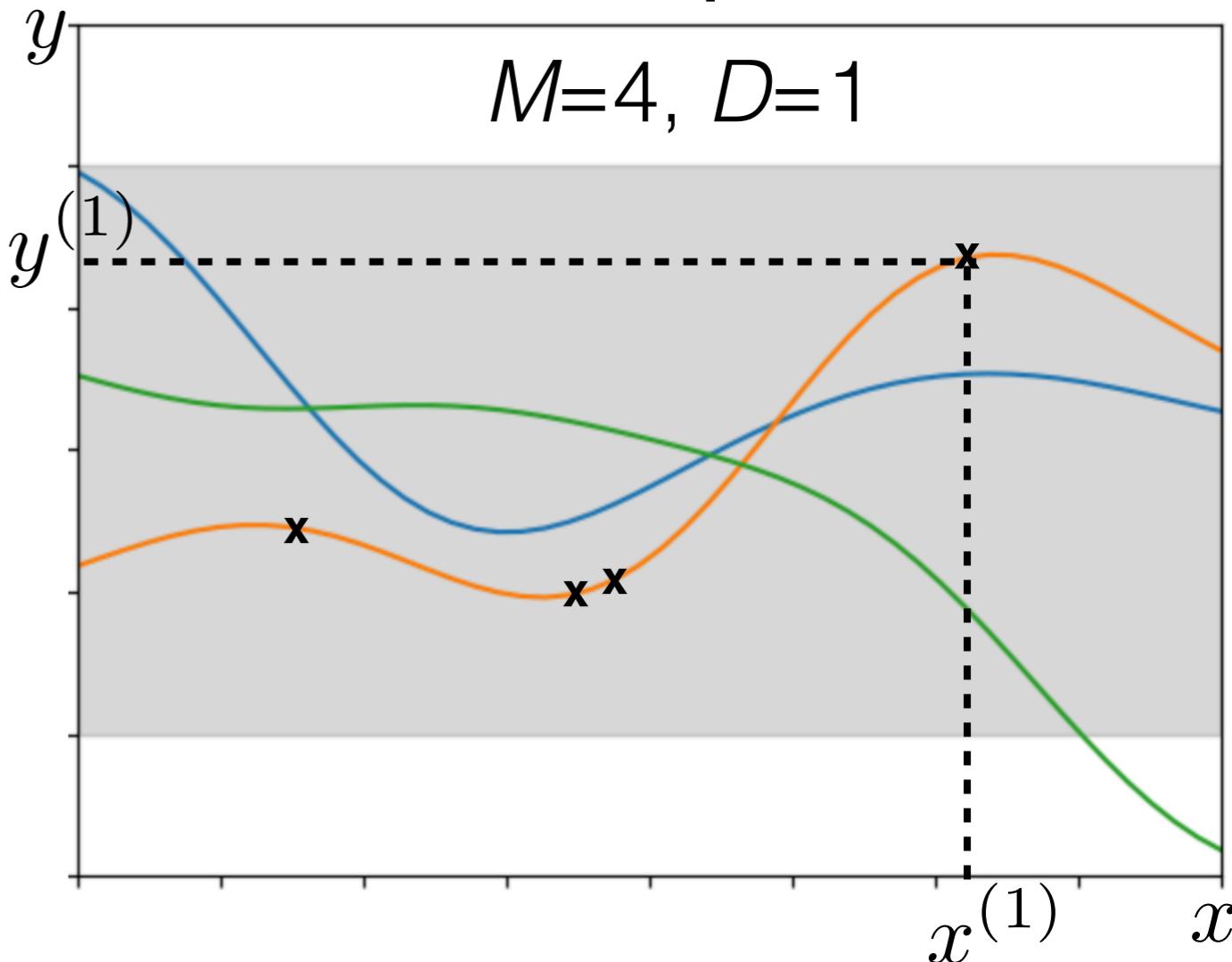
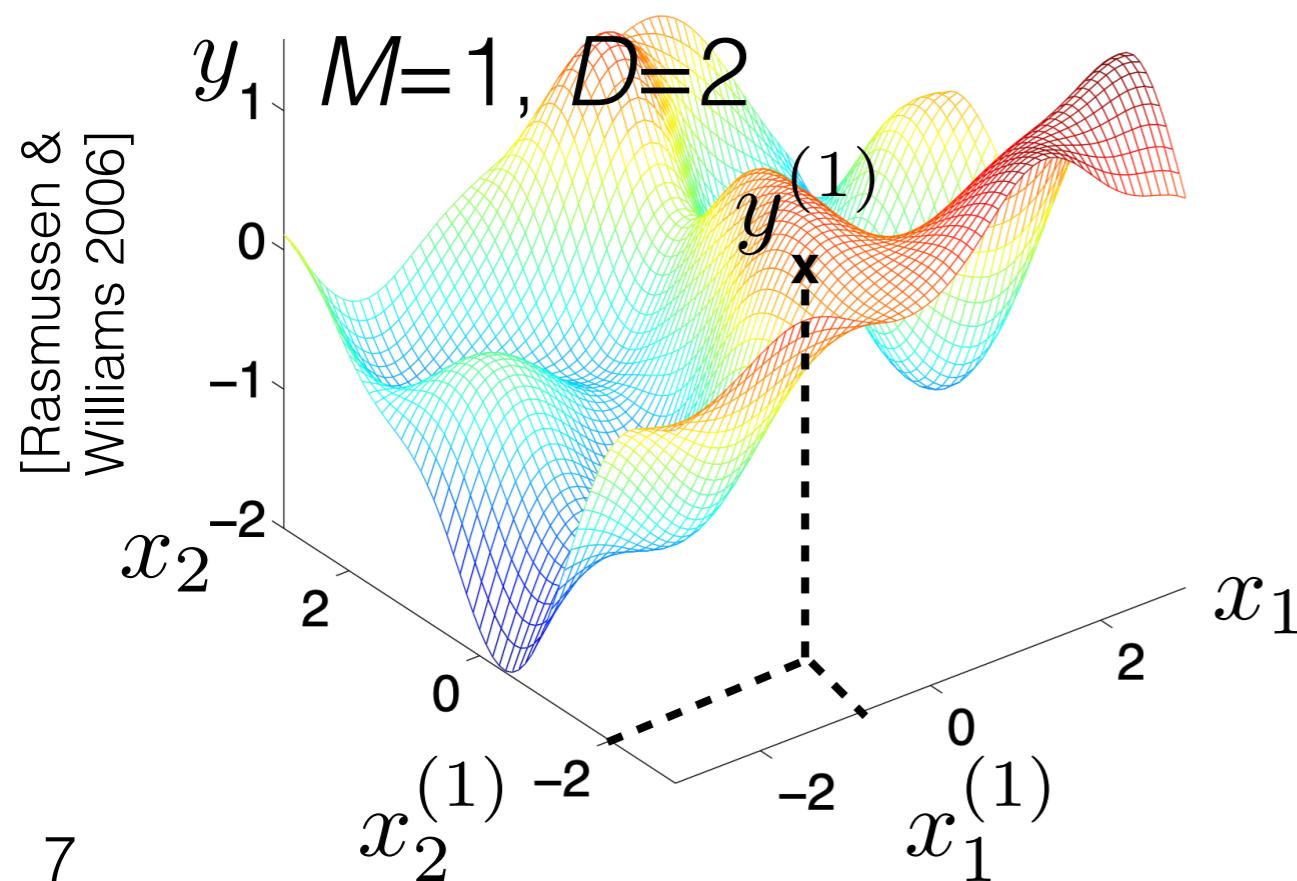
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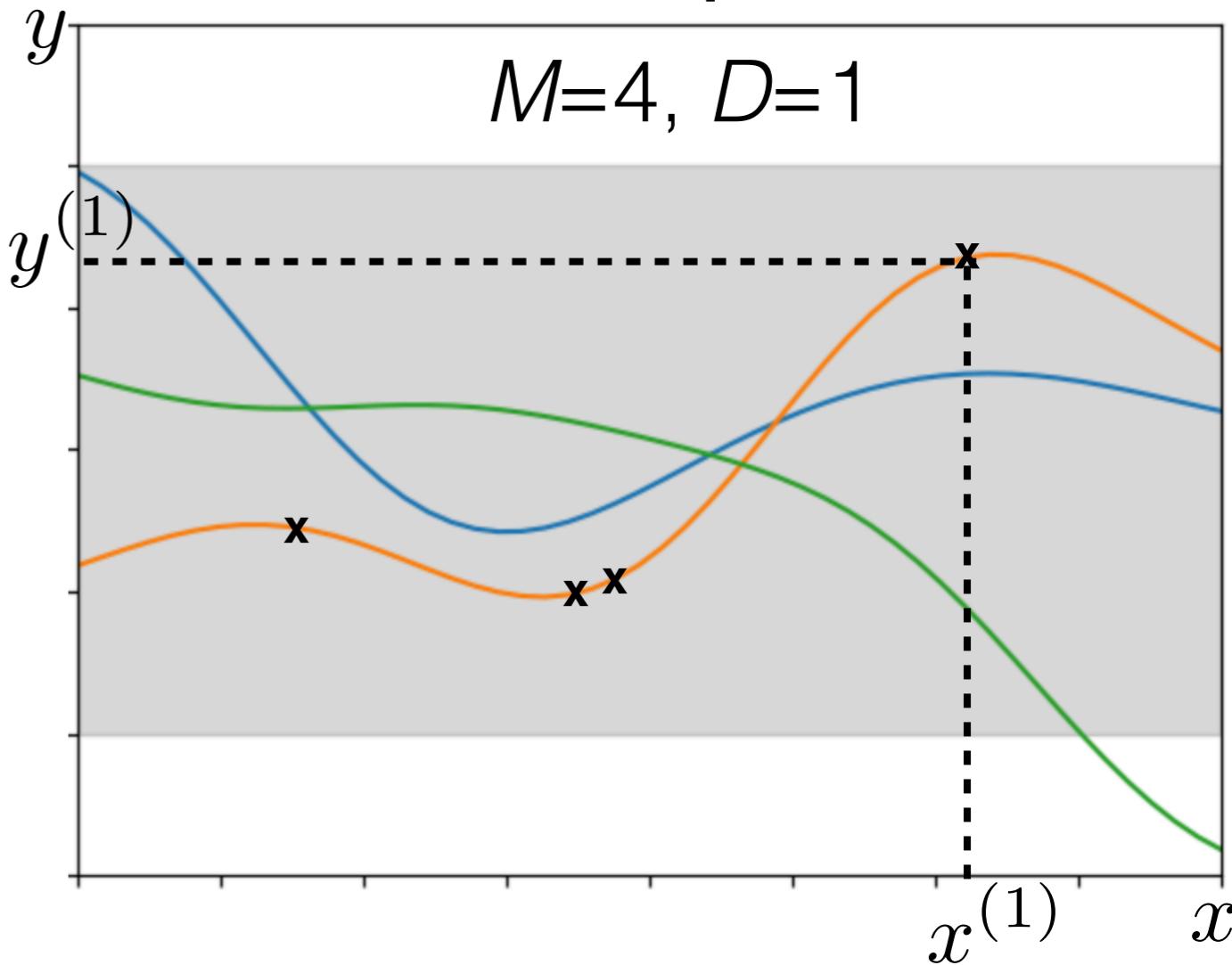
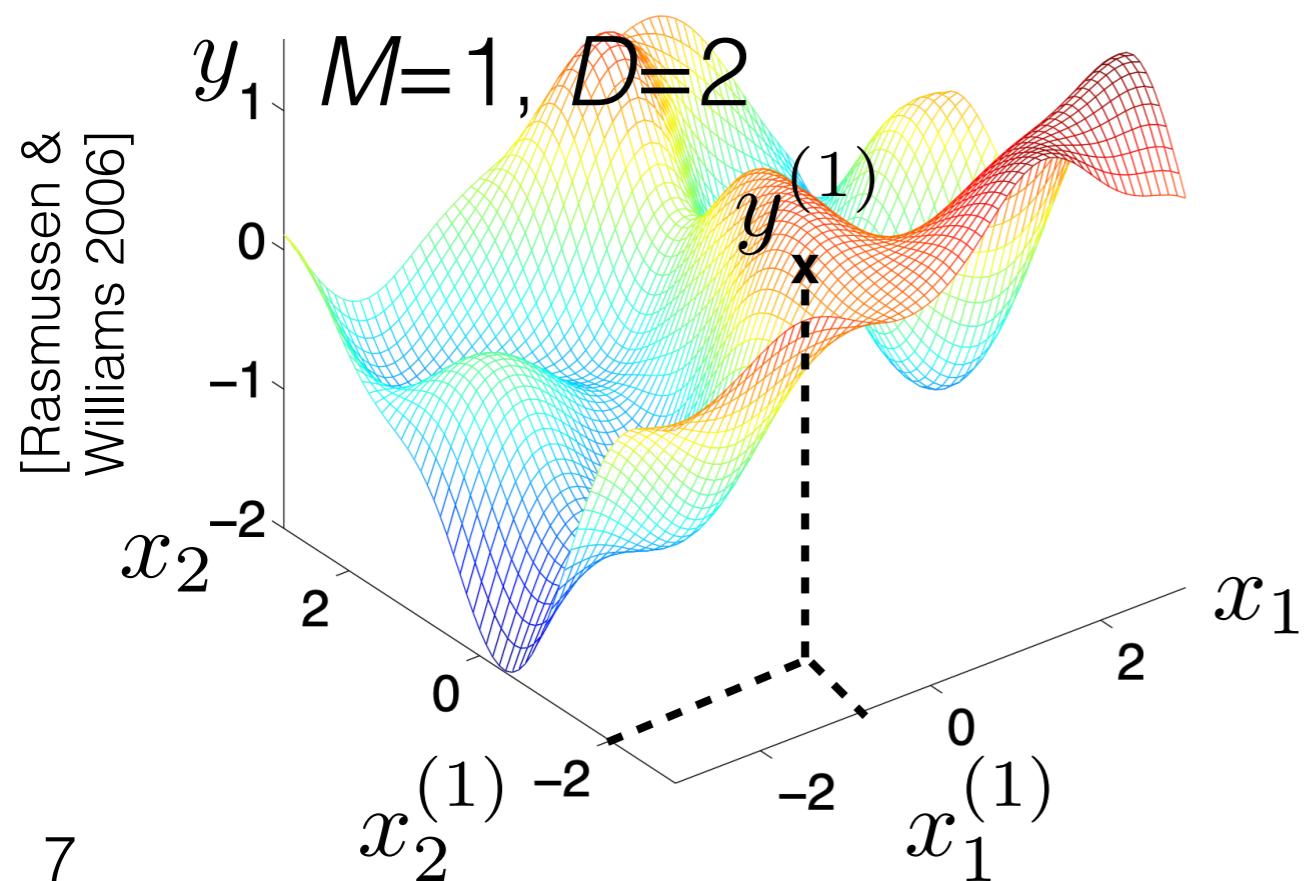
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- Note: all of our real-life examples from the start had number of inputs $D > 1$
- $D = 1$ is much easier to visualize, but might not be representative

Inference about unknowns given data

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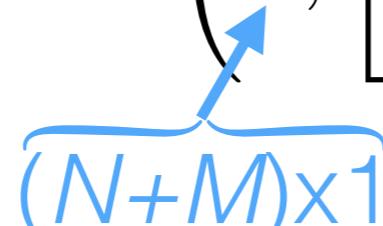
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[demo1,2]

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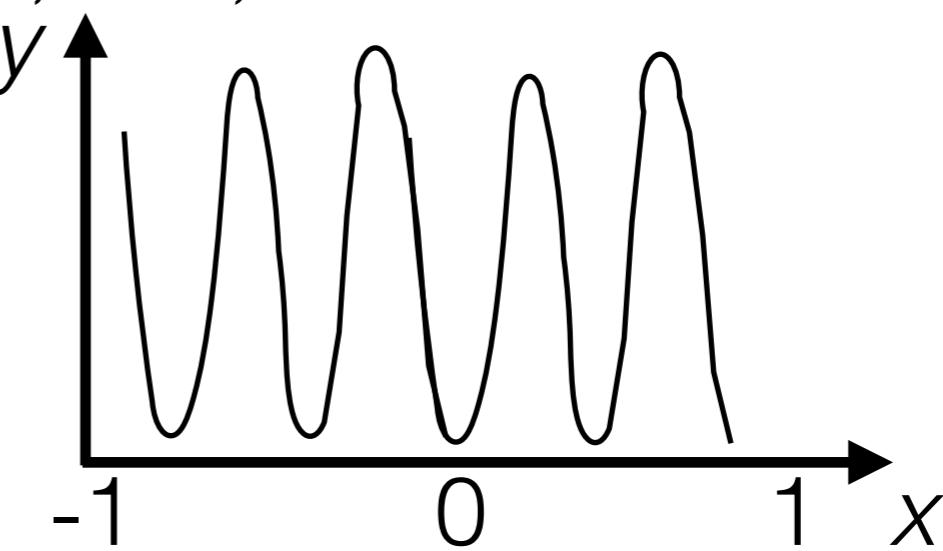
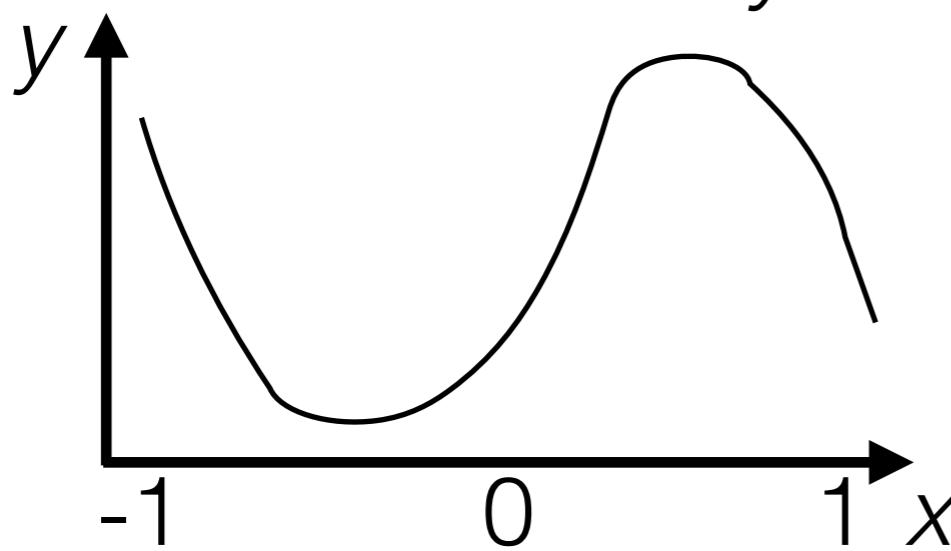
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 - Given those values, now compute and report the mean and uncertainty intervals.

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