

Gaussian Processes for Regression: Models, Algorithms, and Applications

Tamara Broderick
Associate Professor
MIT

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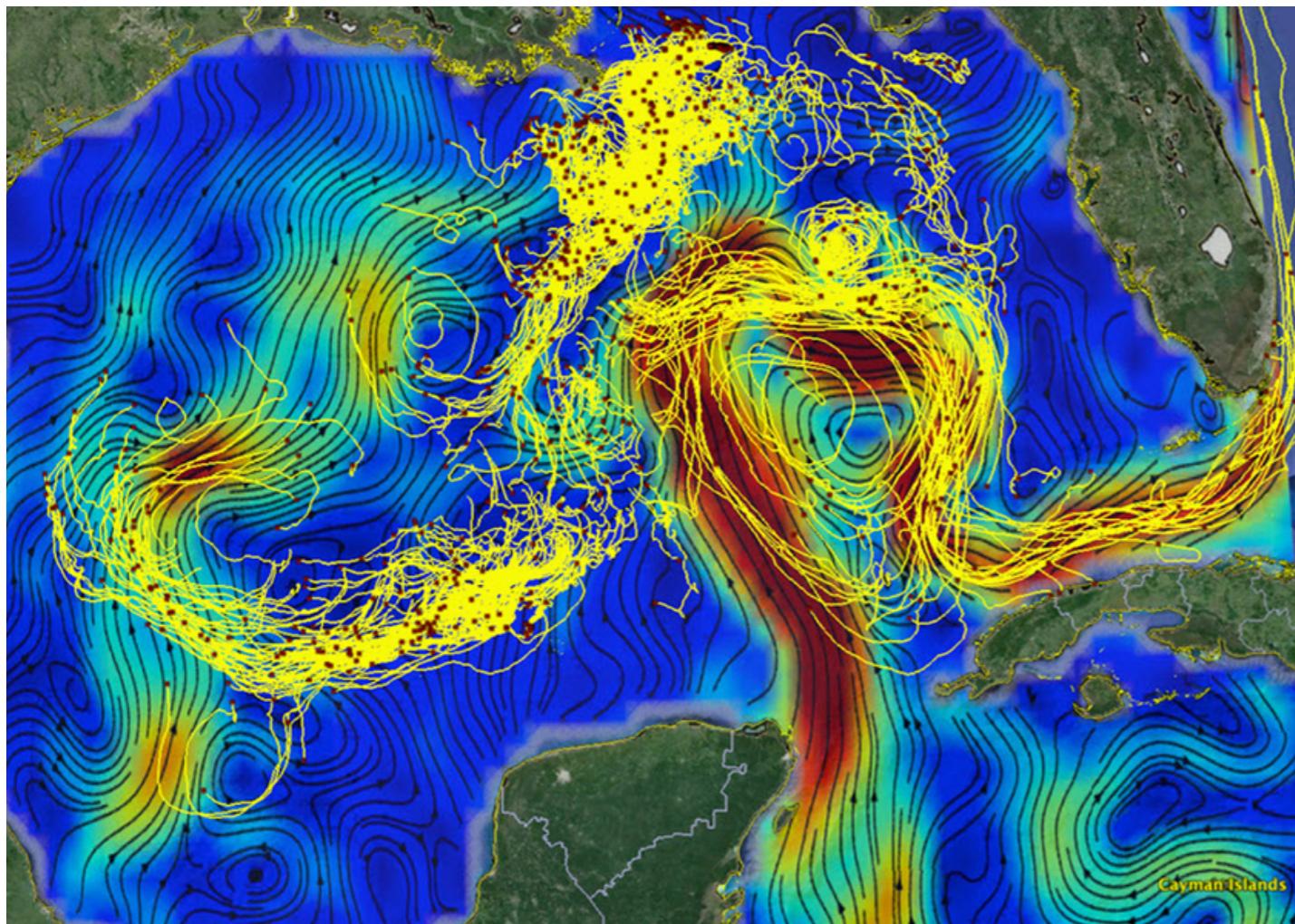
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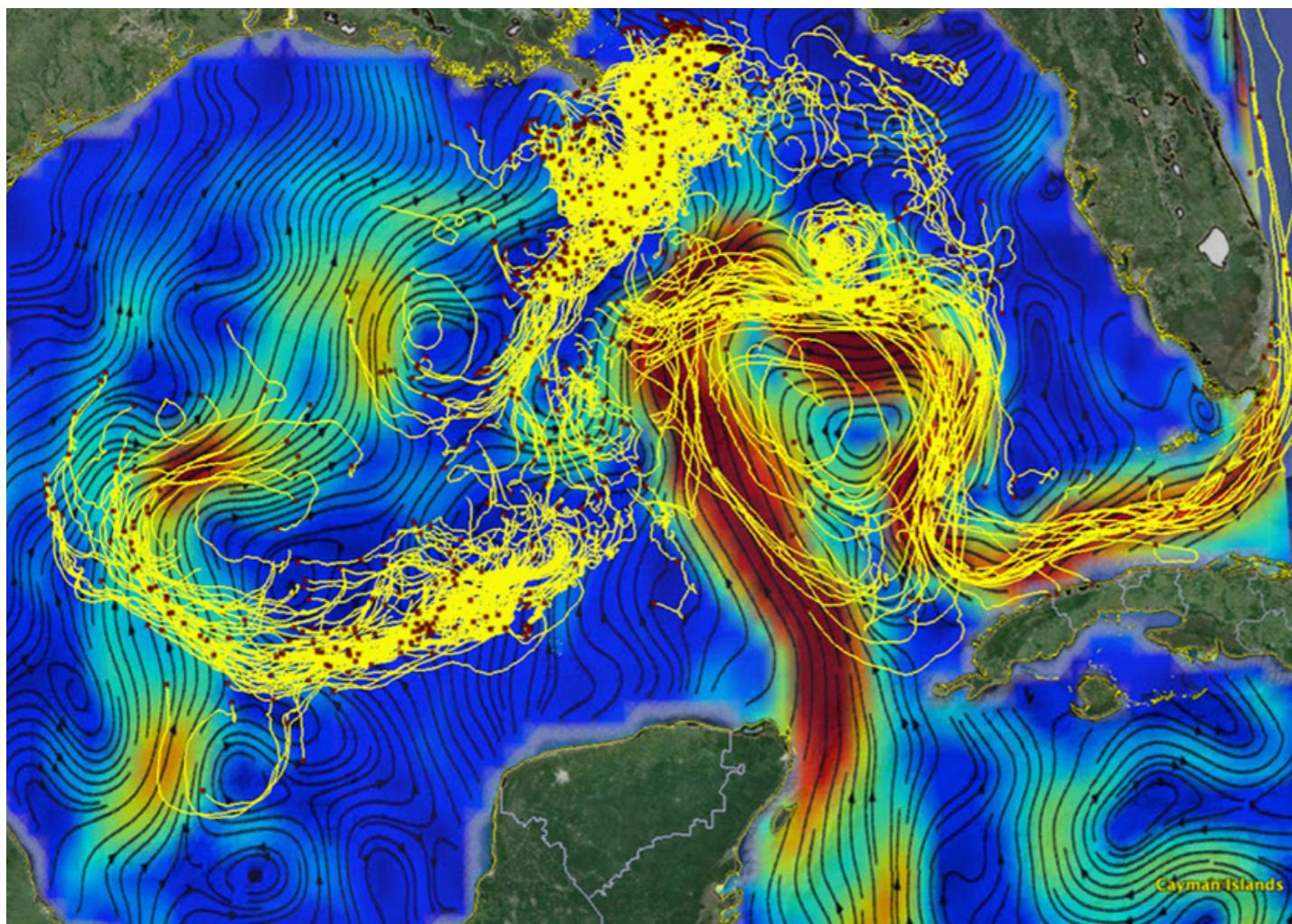


Example:

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

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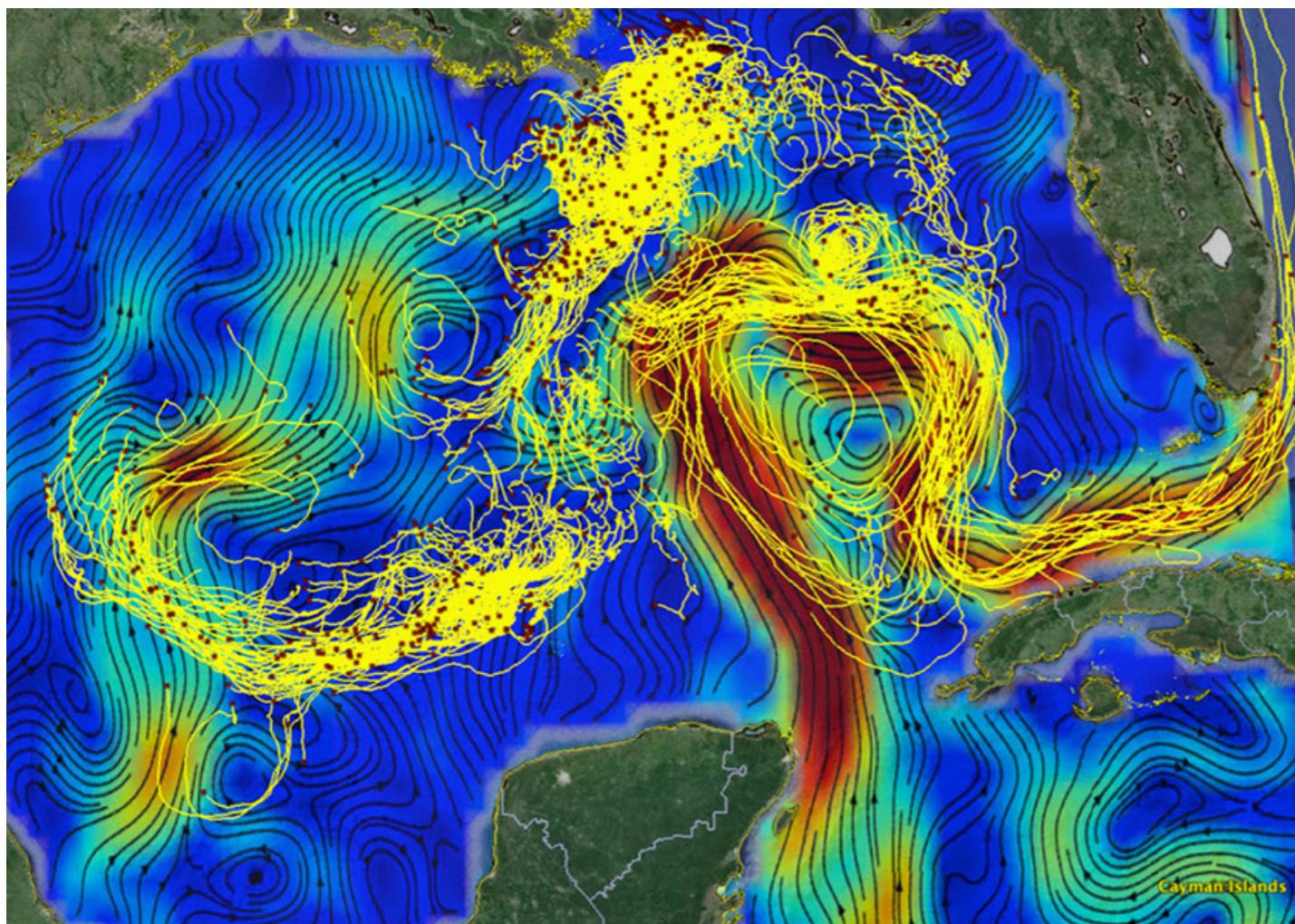
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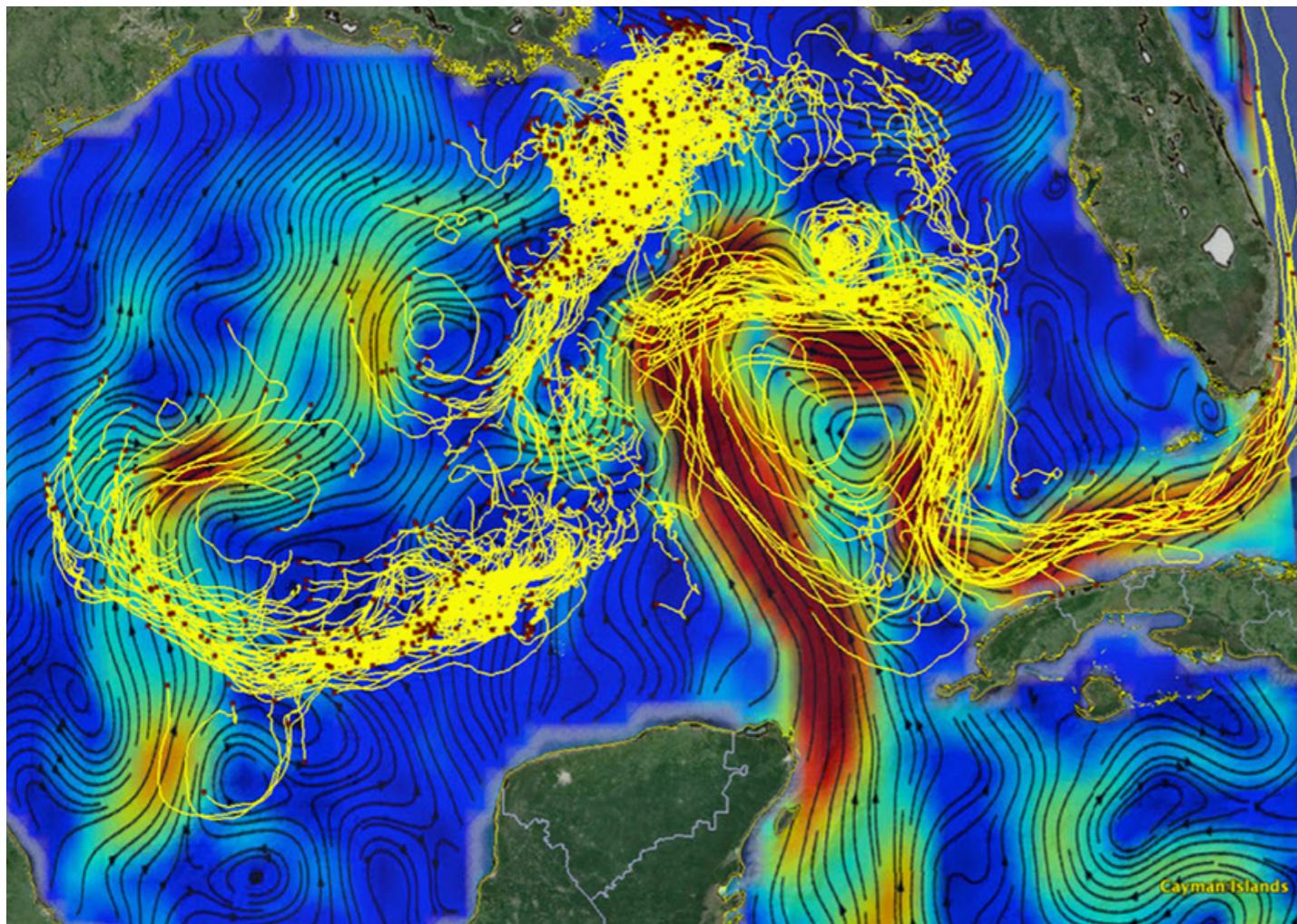
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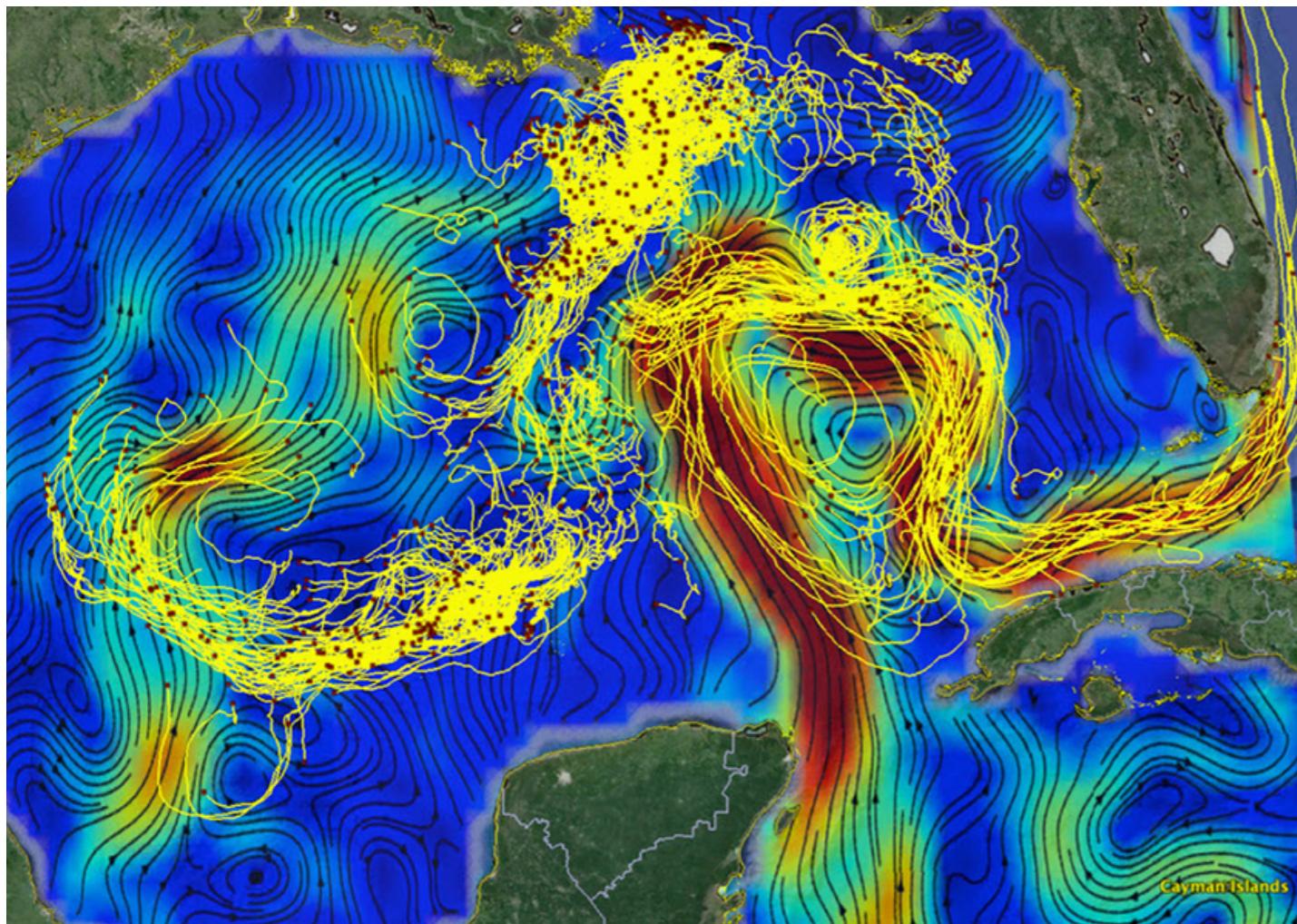
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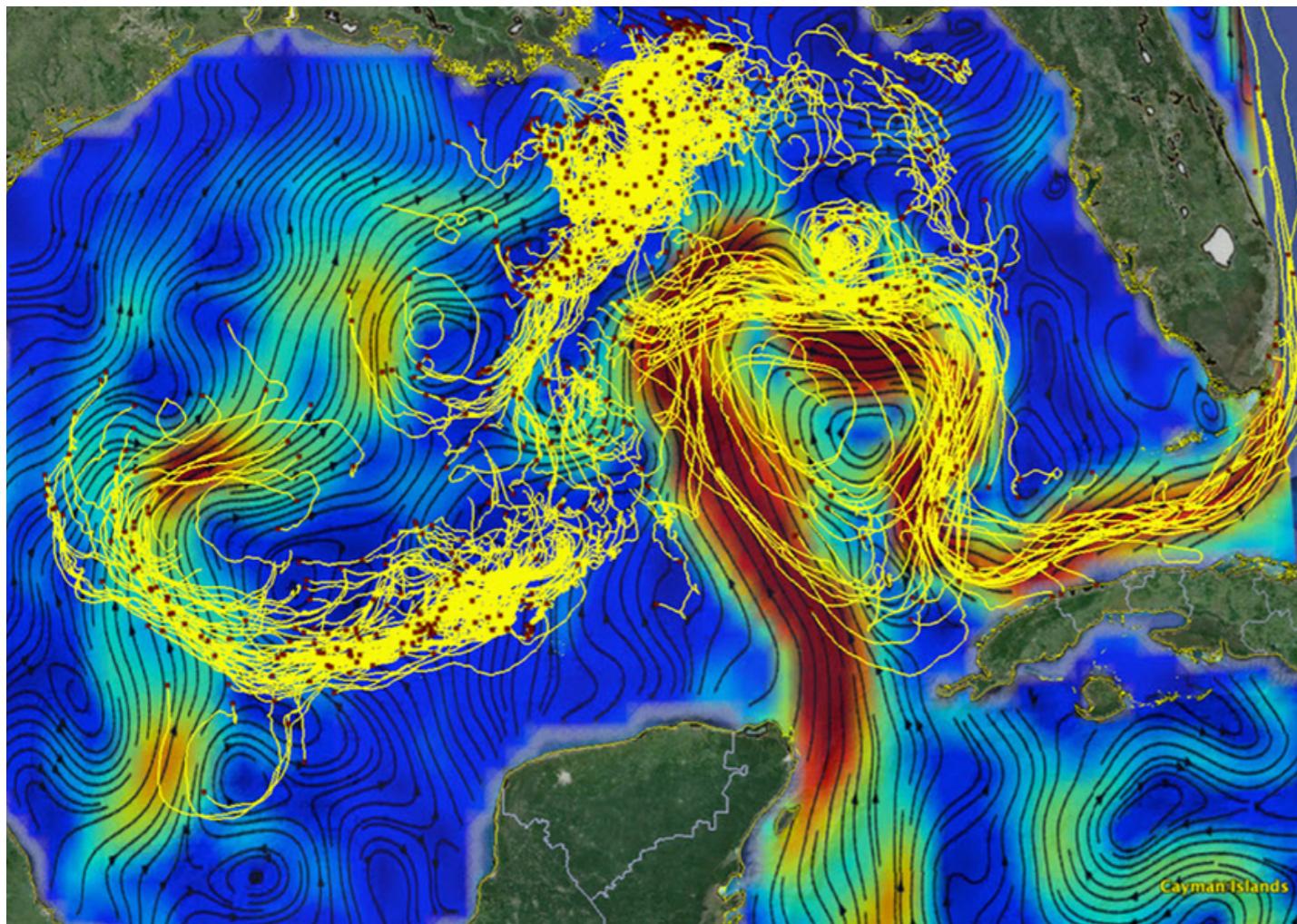
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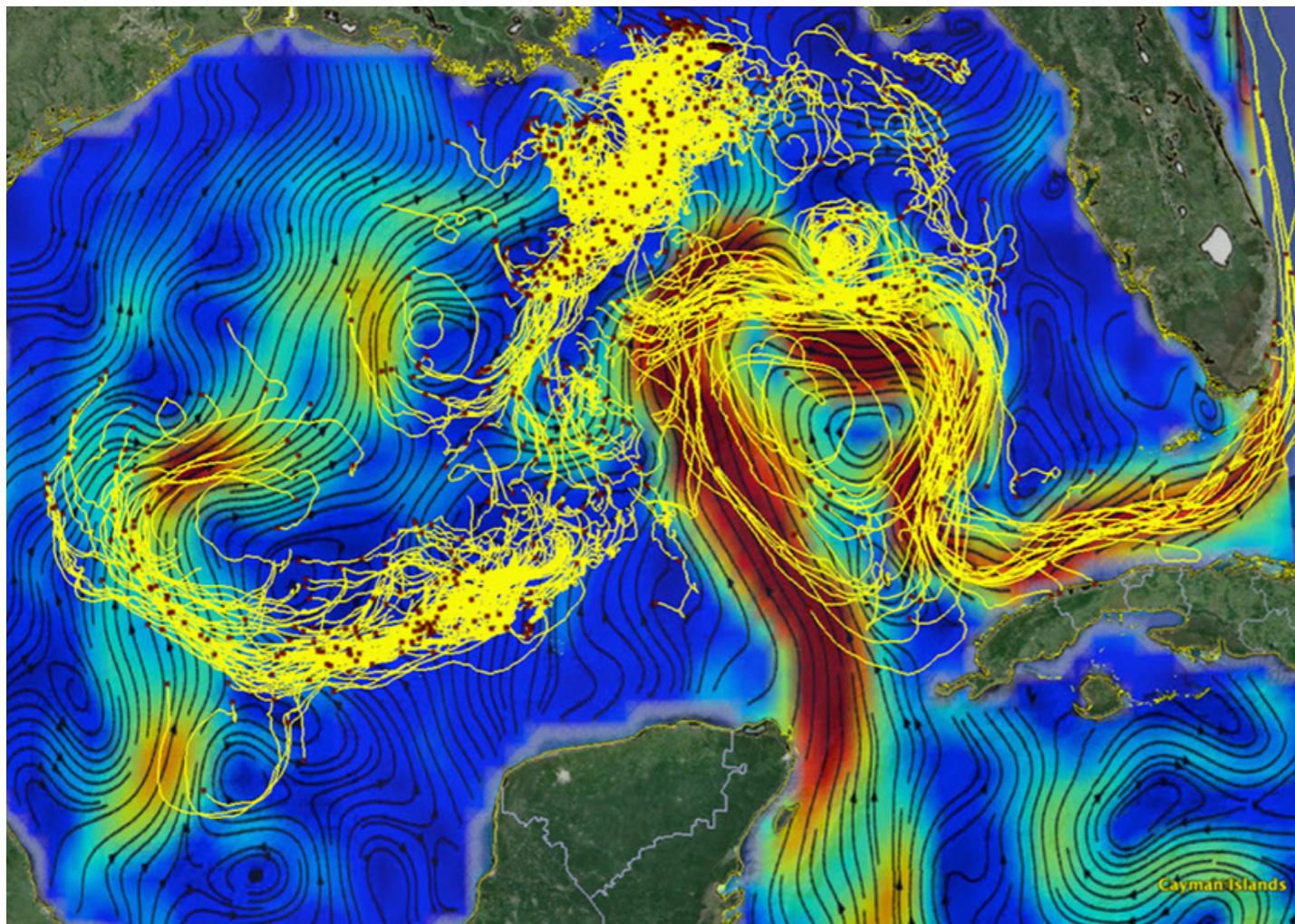
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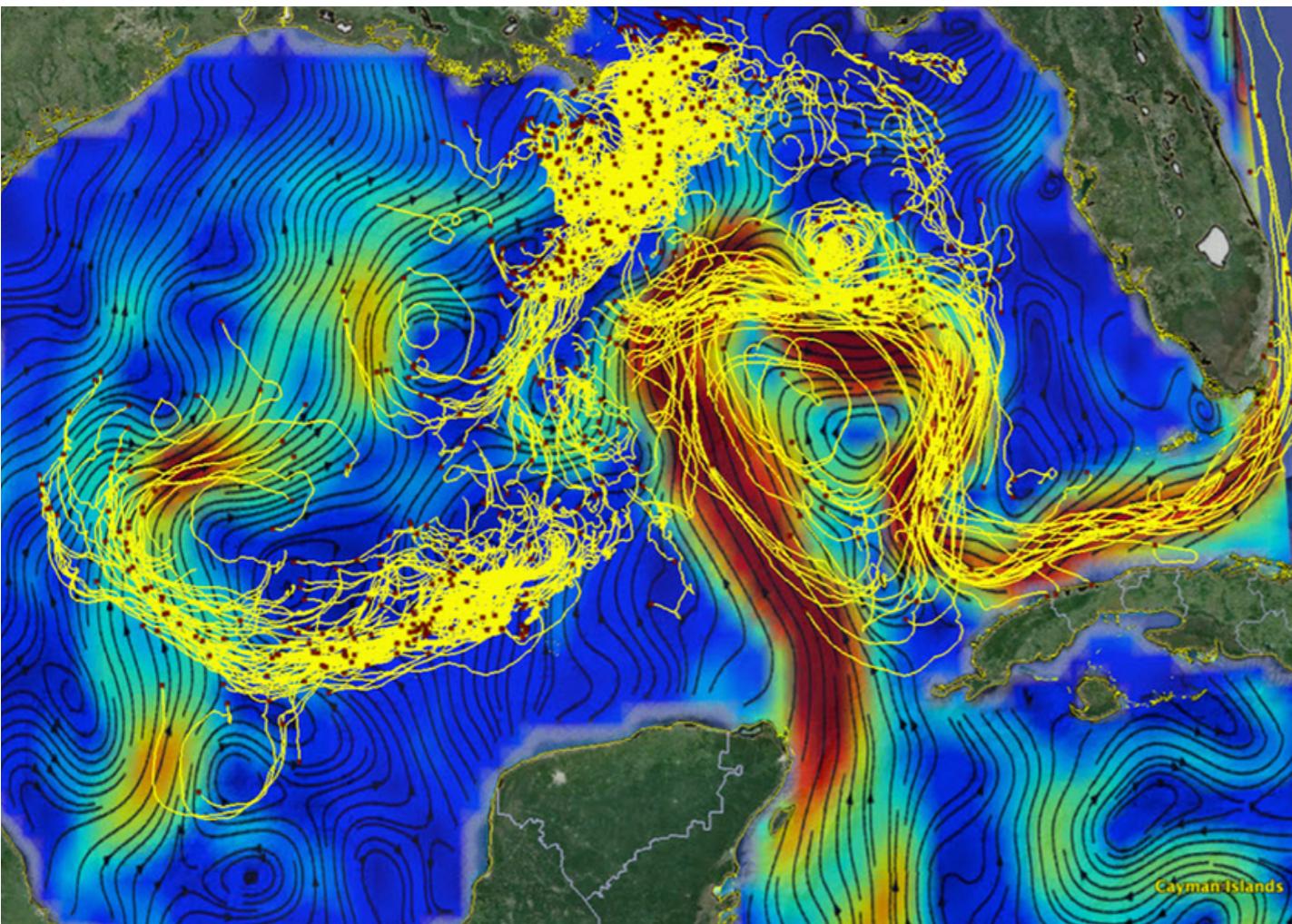
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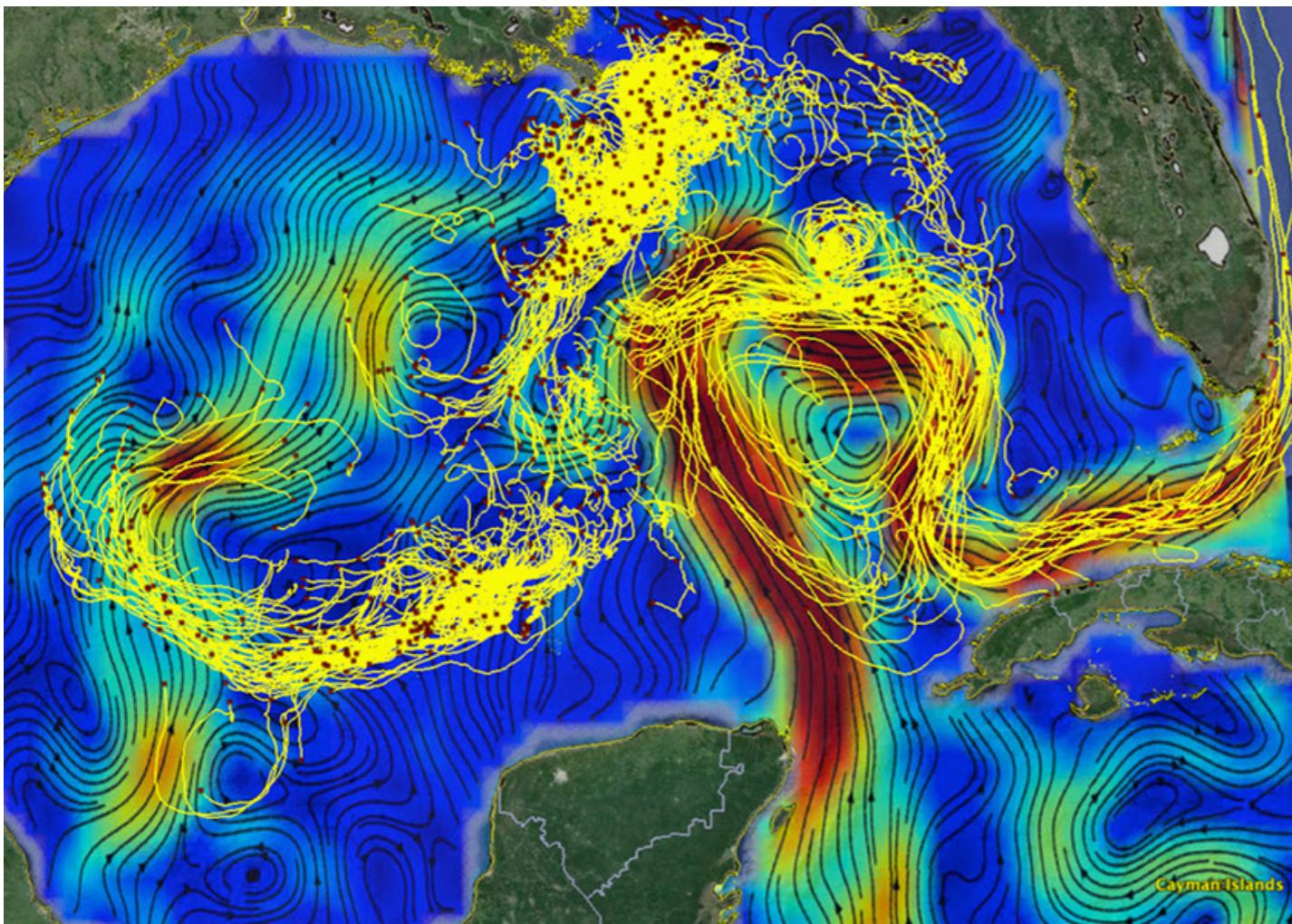
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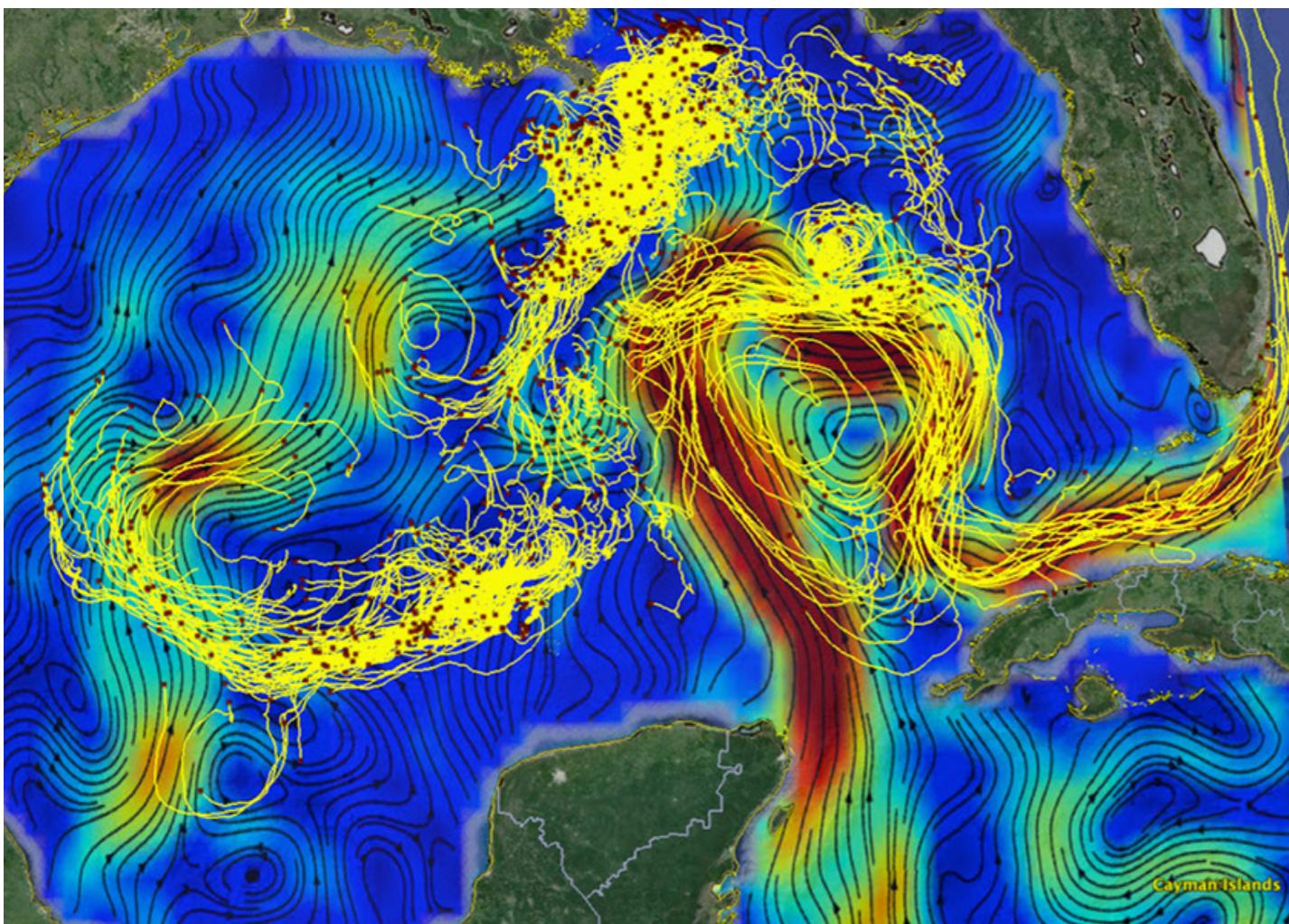
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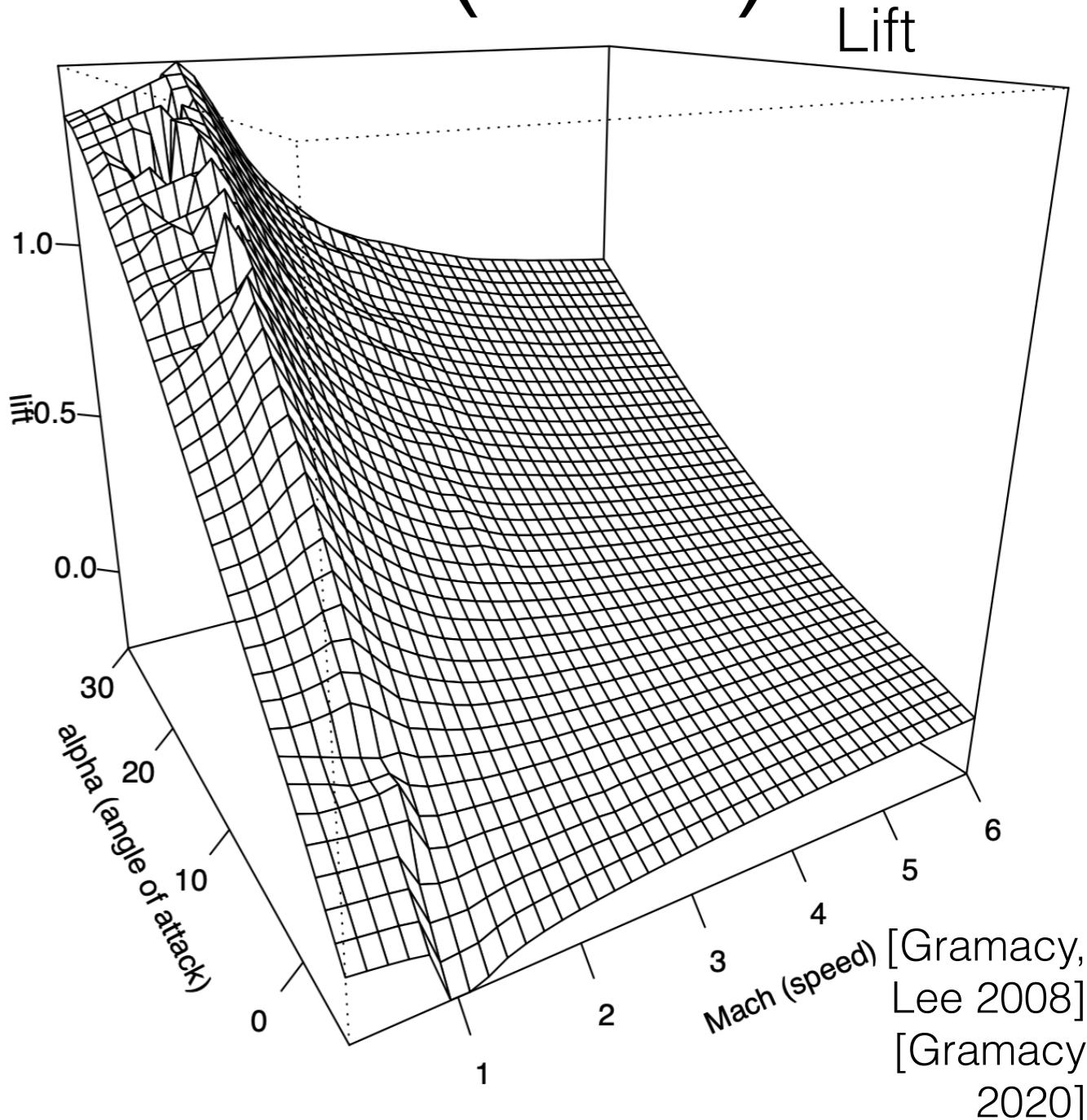
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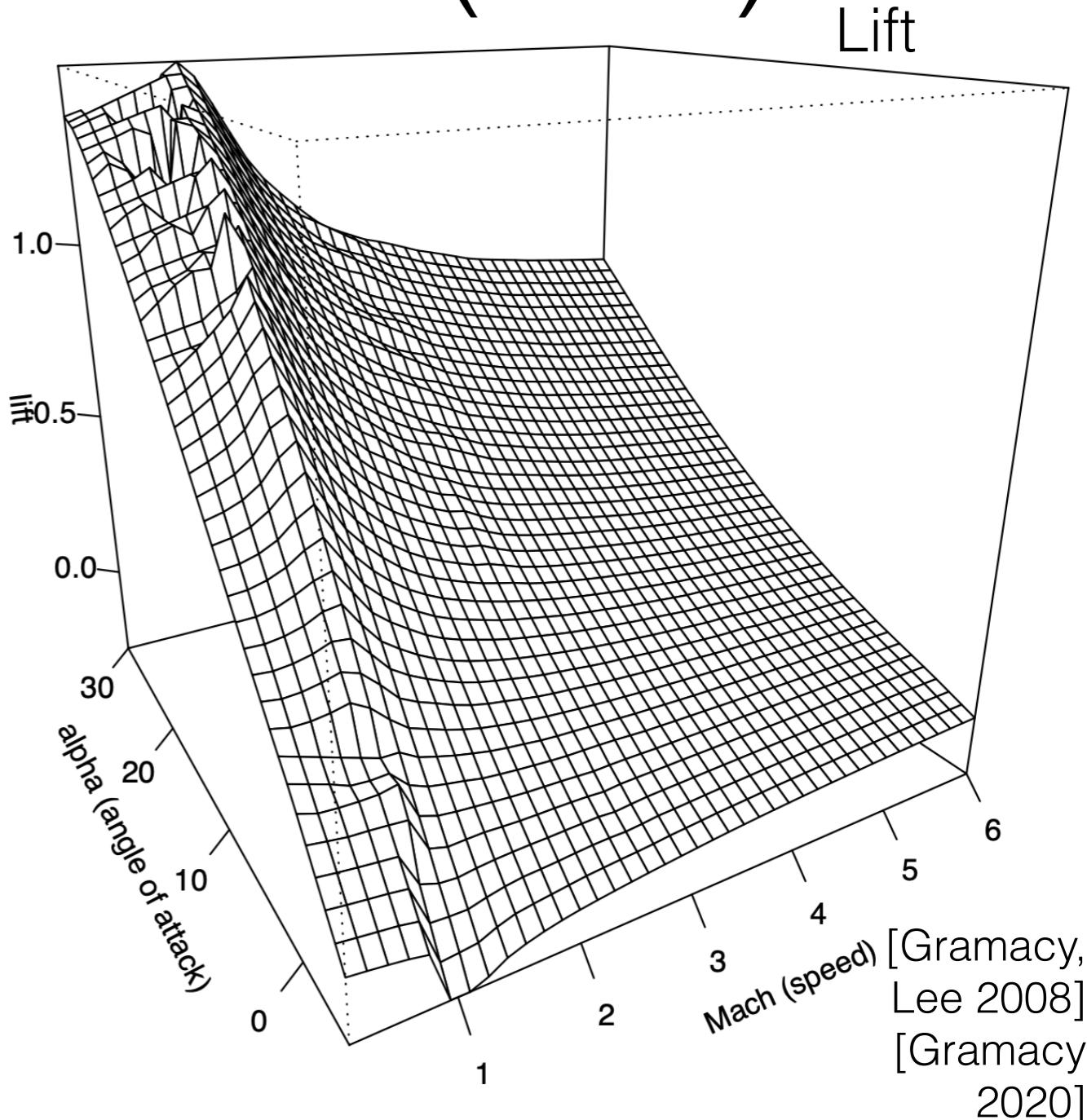
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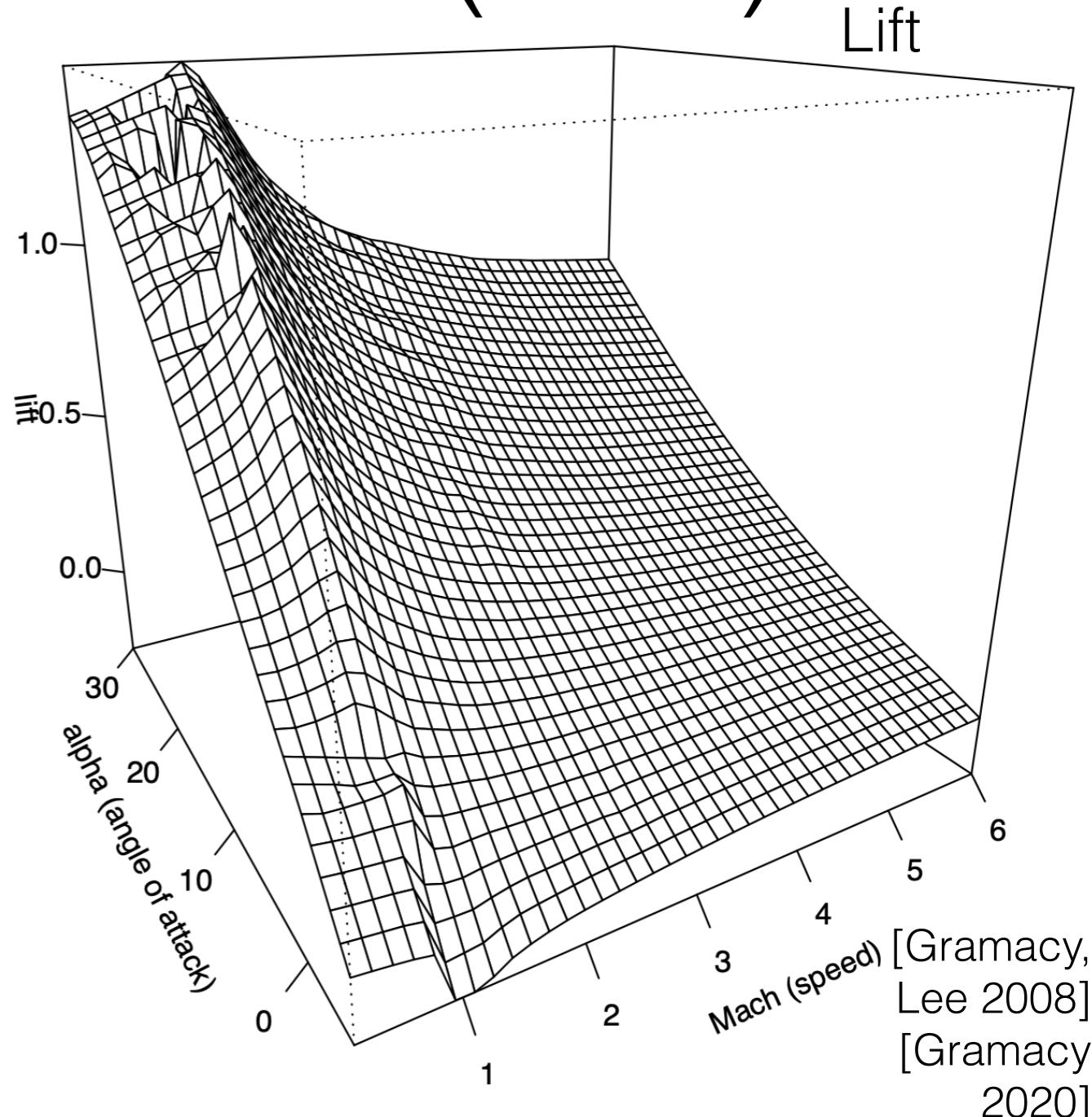
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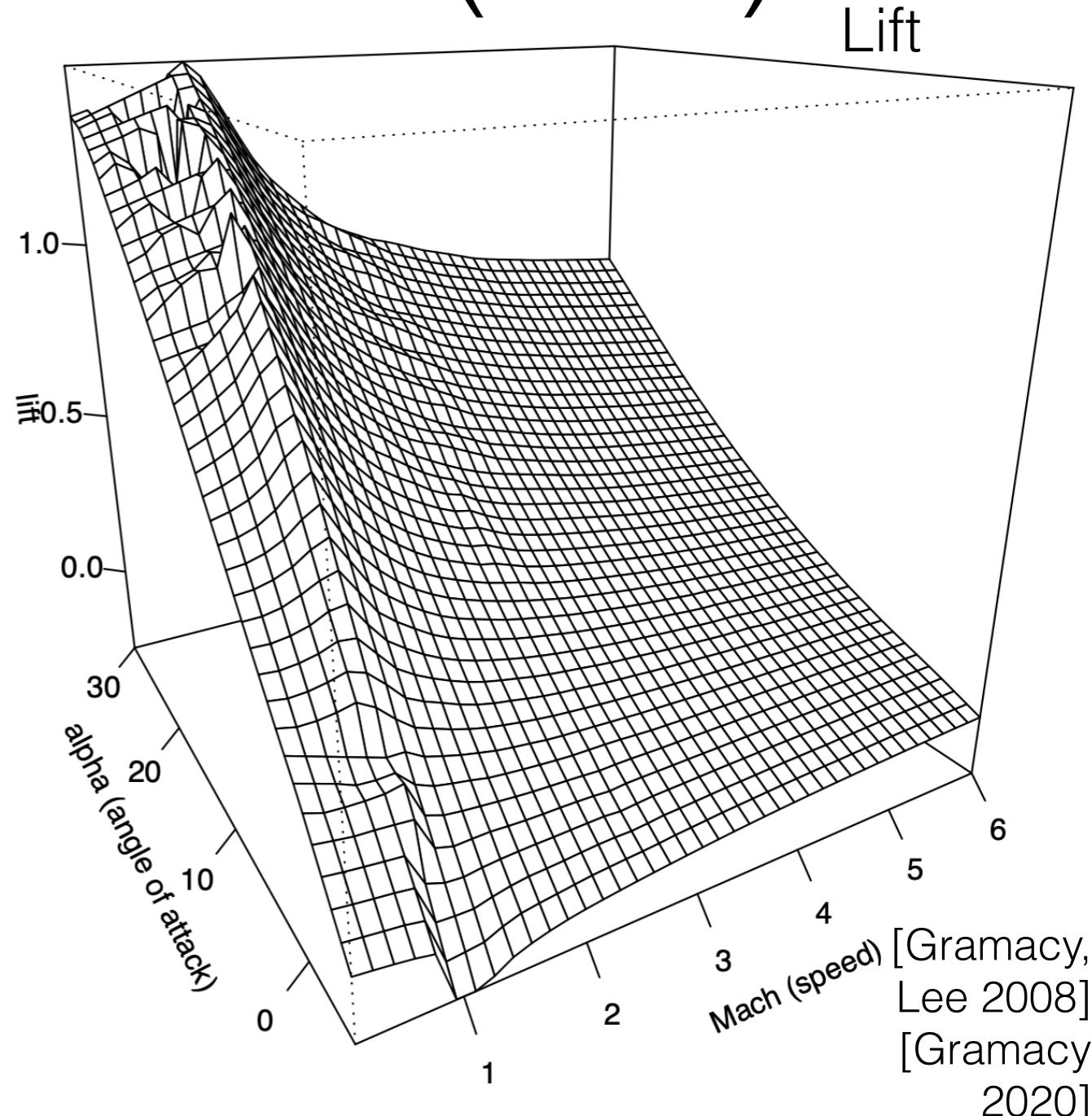
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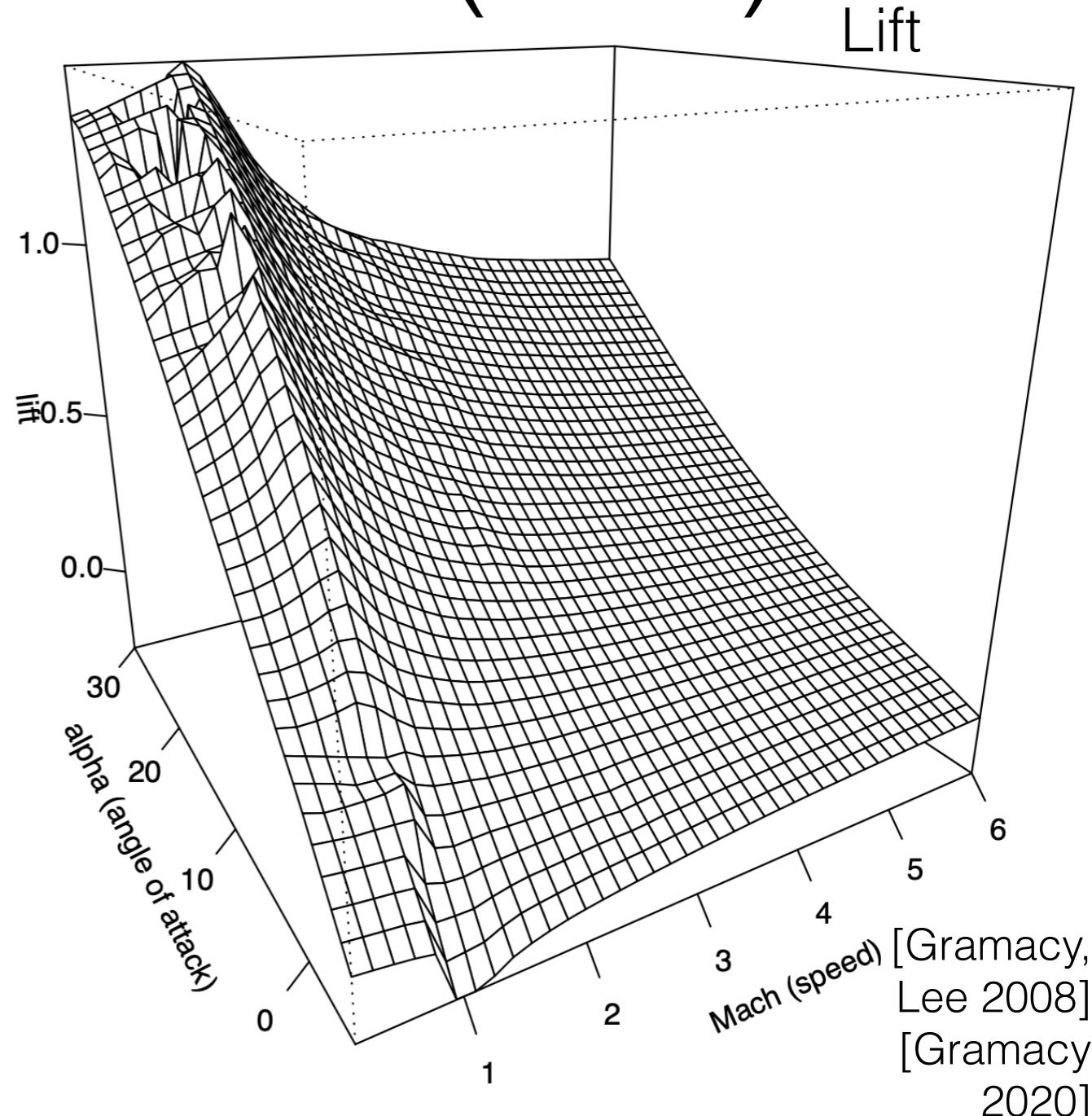


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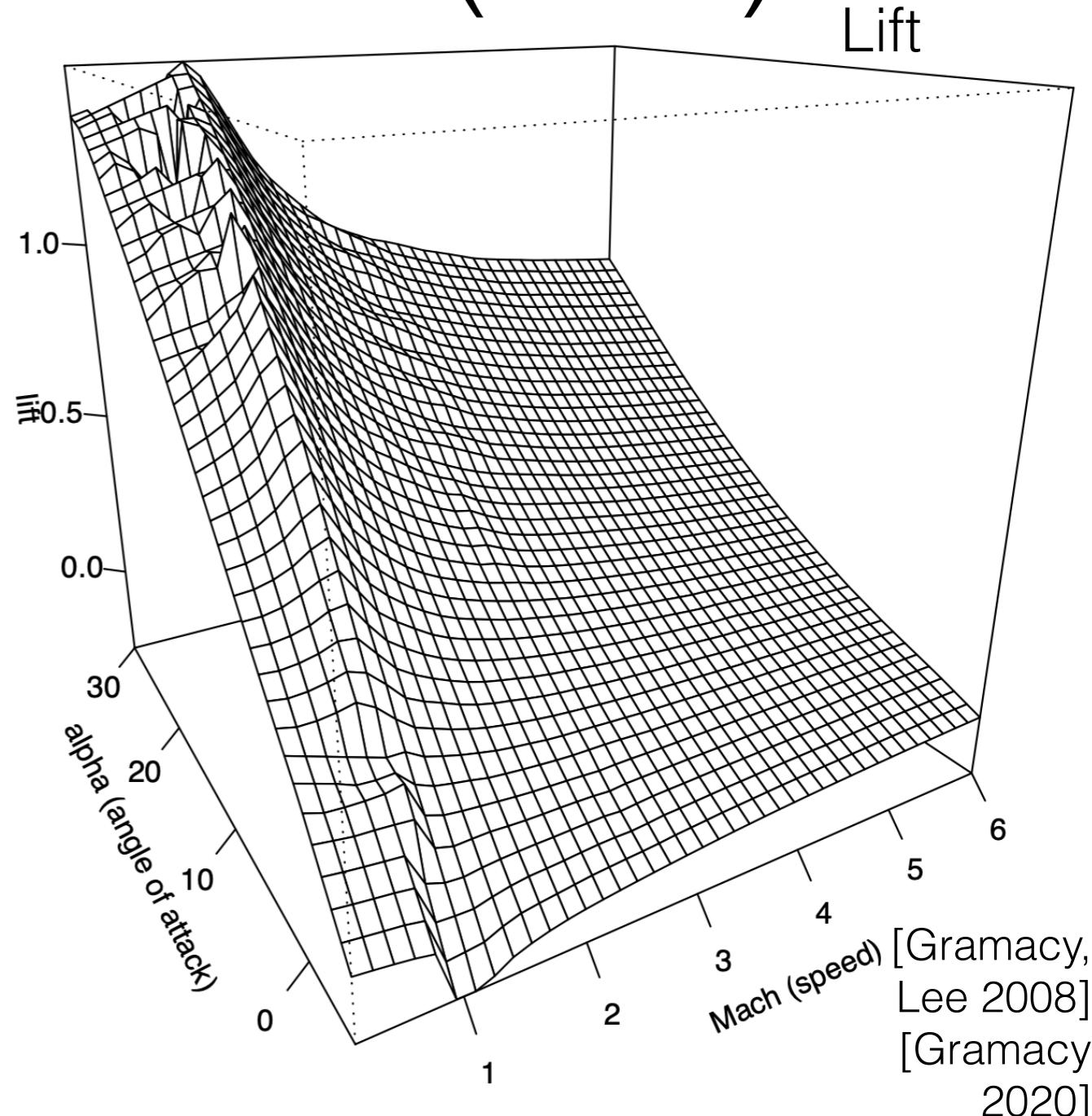
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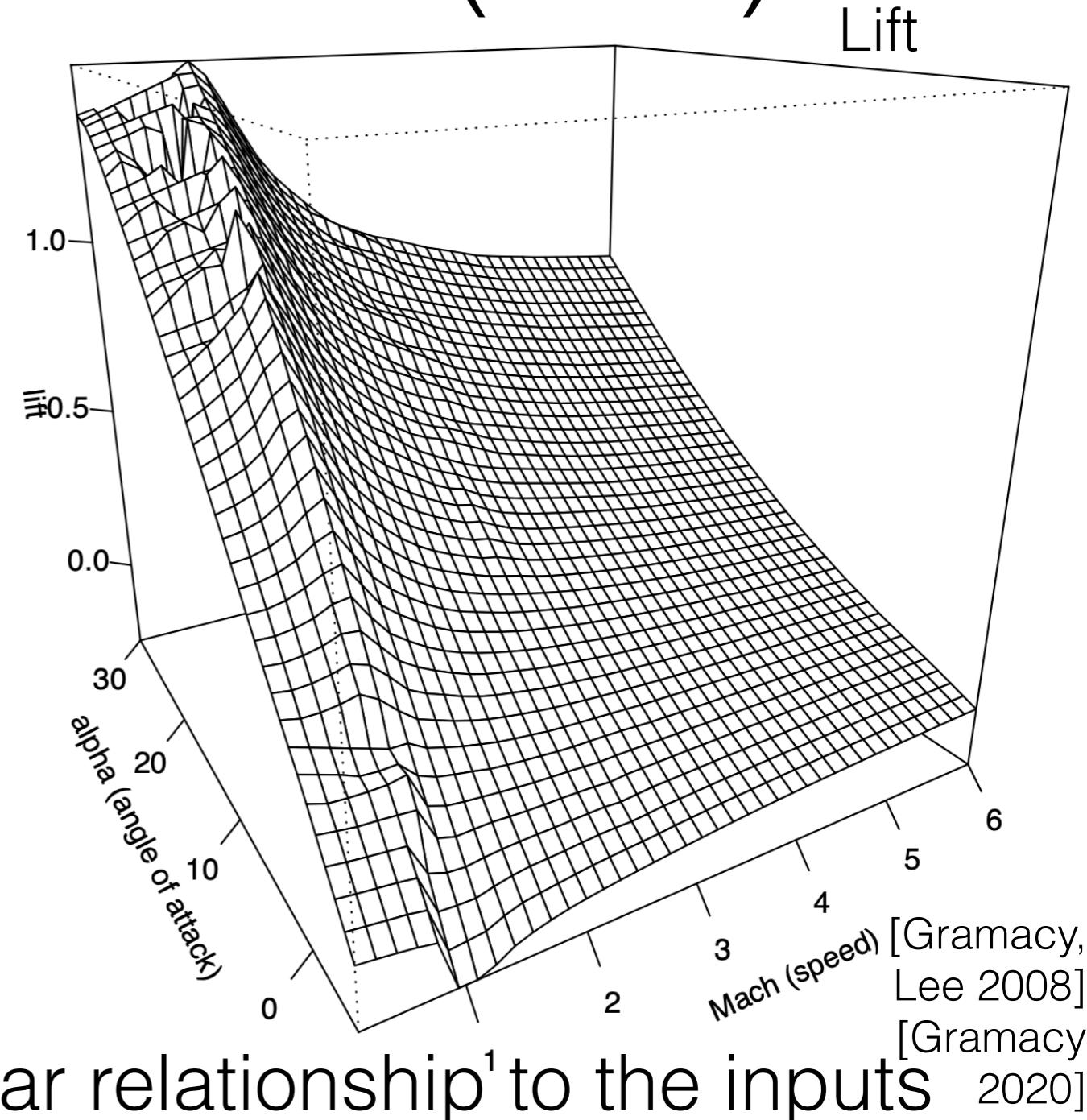
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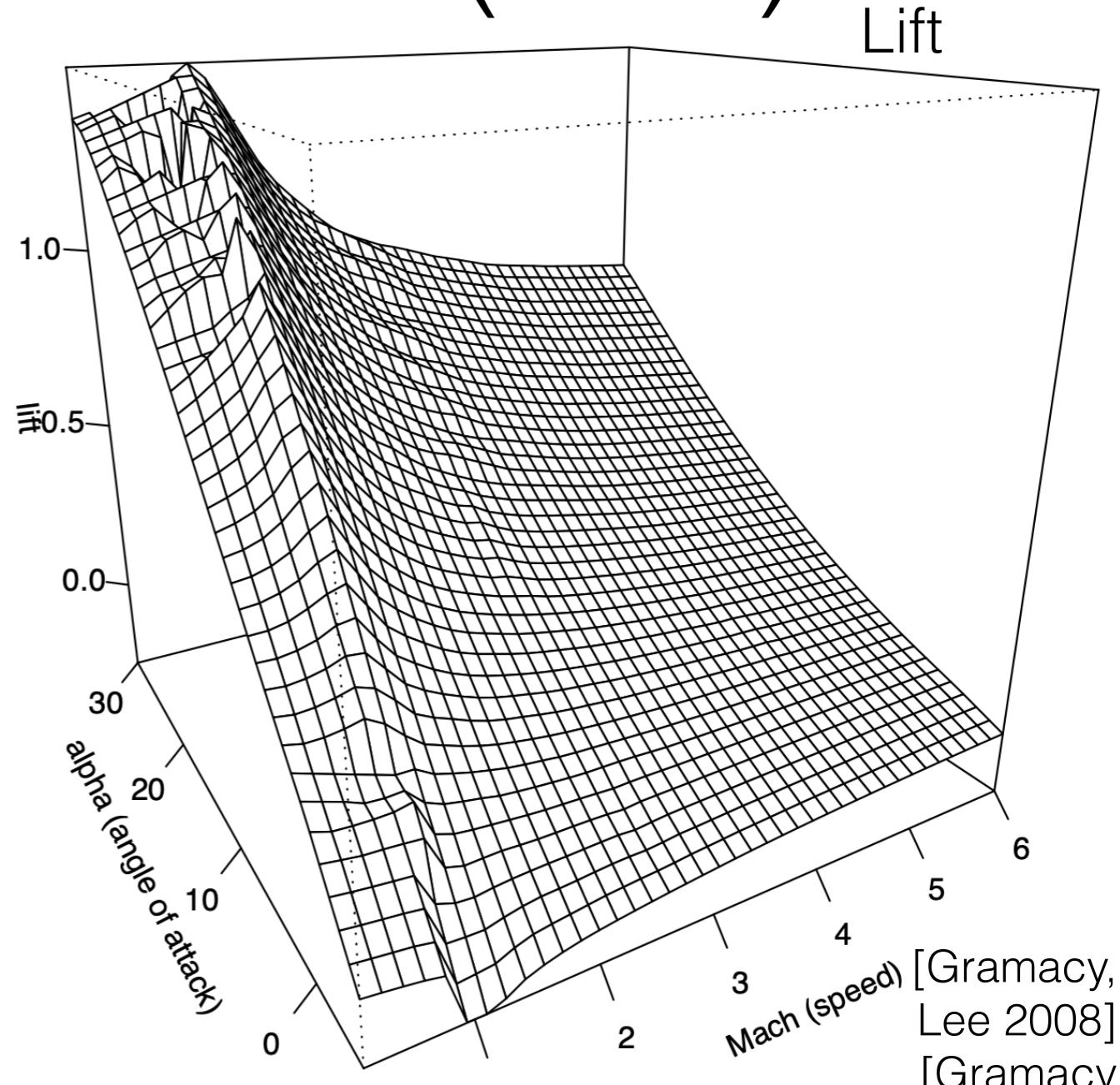
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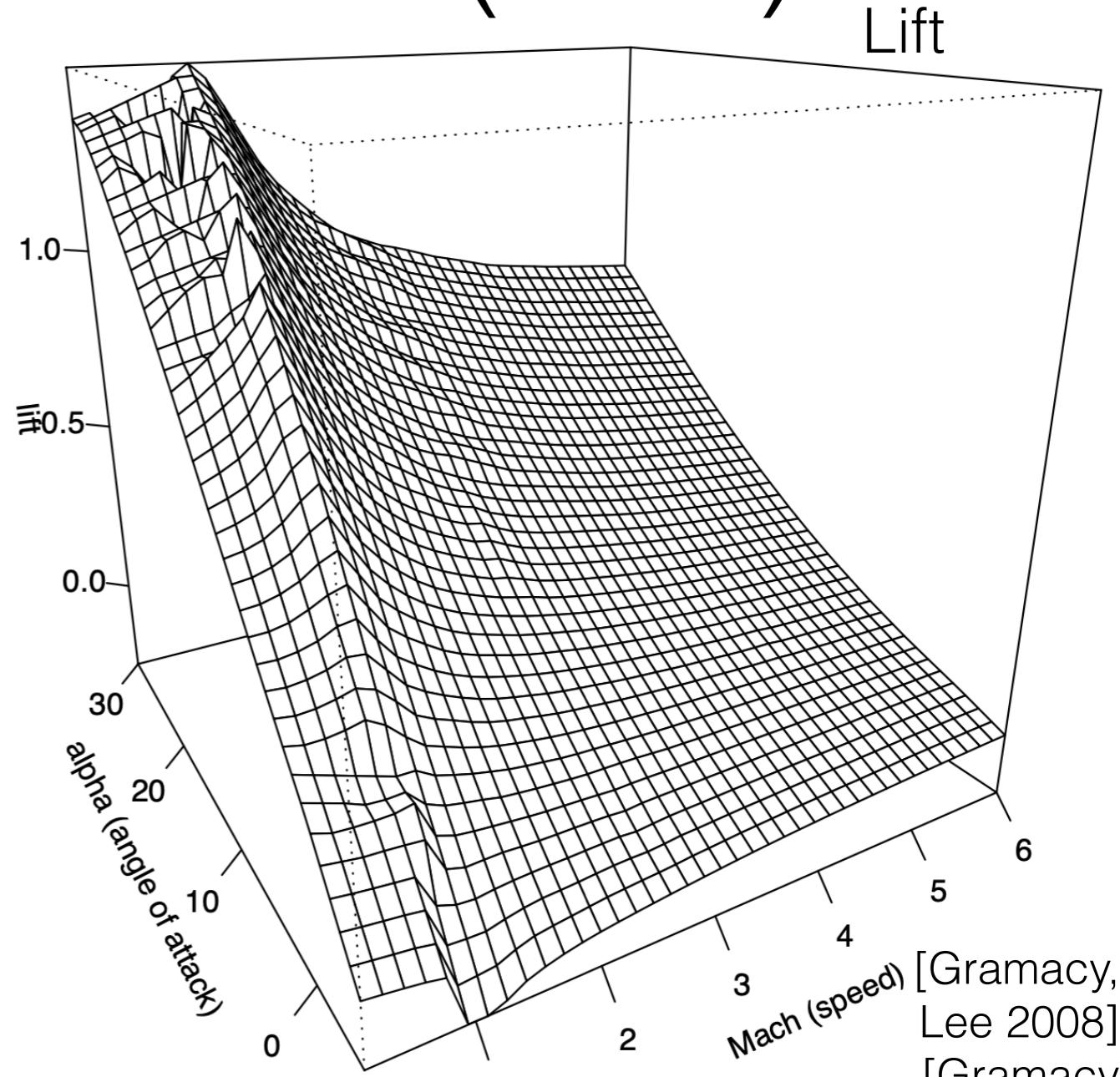
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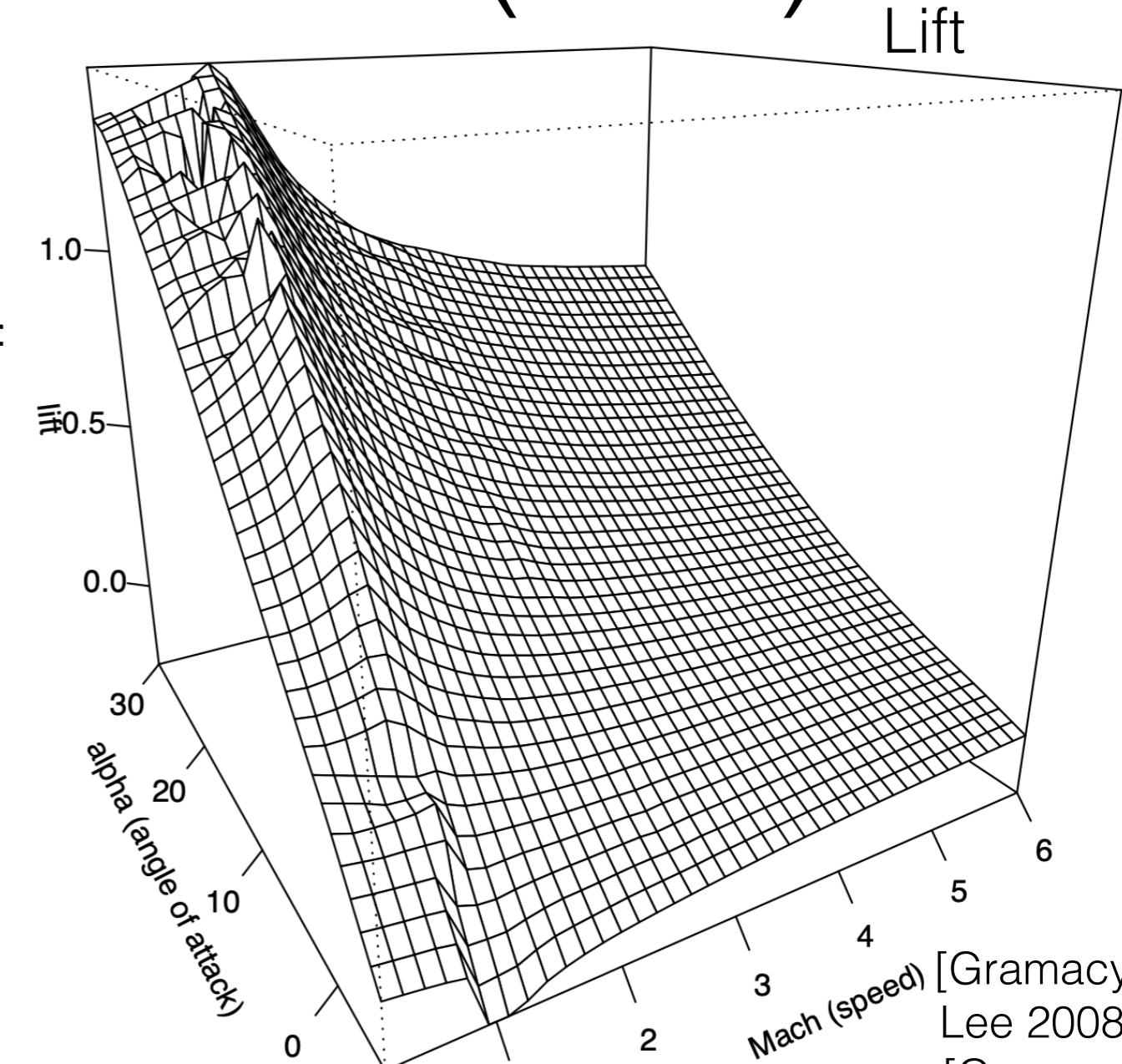
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[Snoek et al 2012, 2015; Garnett 2023]

One more example: learn (& optimize) performance in machine learning as a function of tuning parameters

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- Goal:
 - Learn the mechanism behind standard GPs to identify benefits and pitfalls

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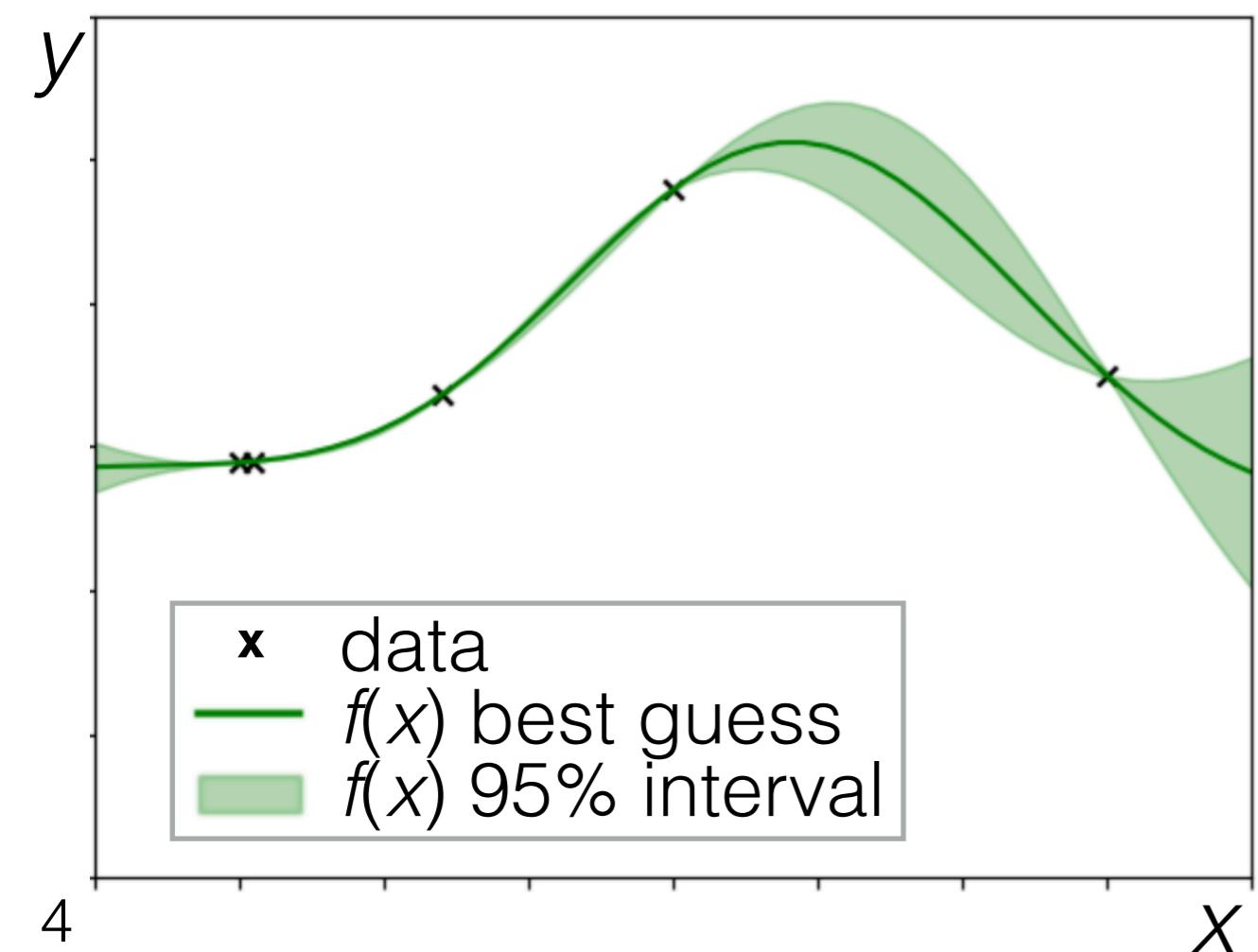


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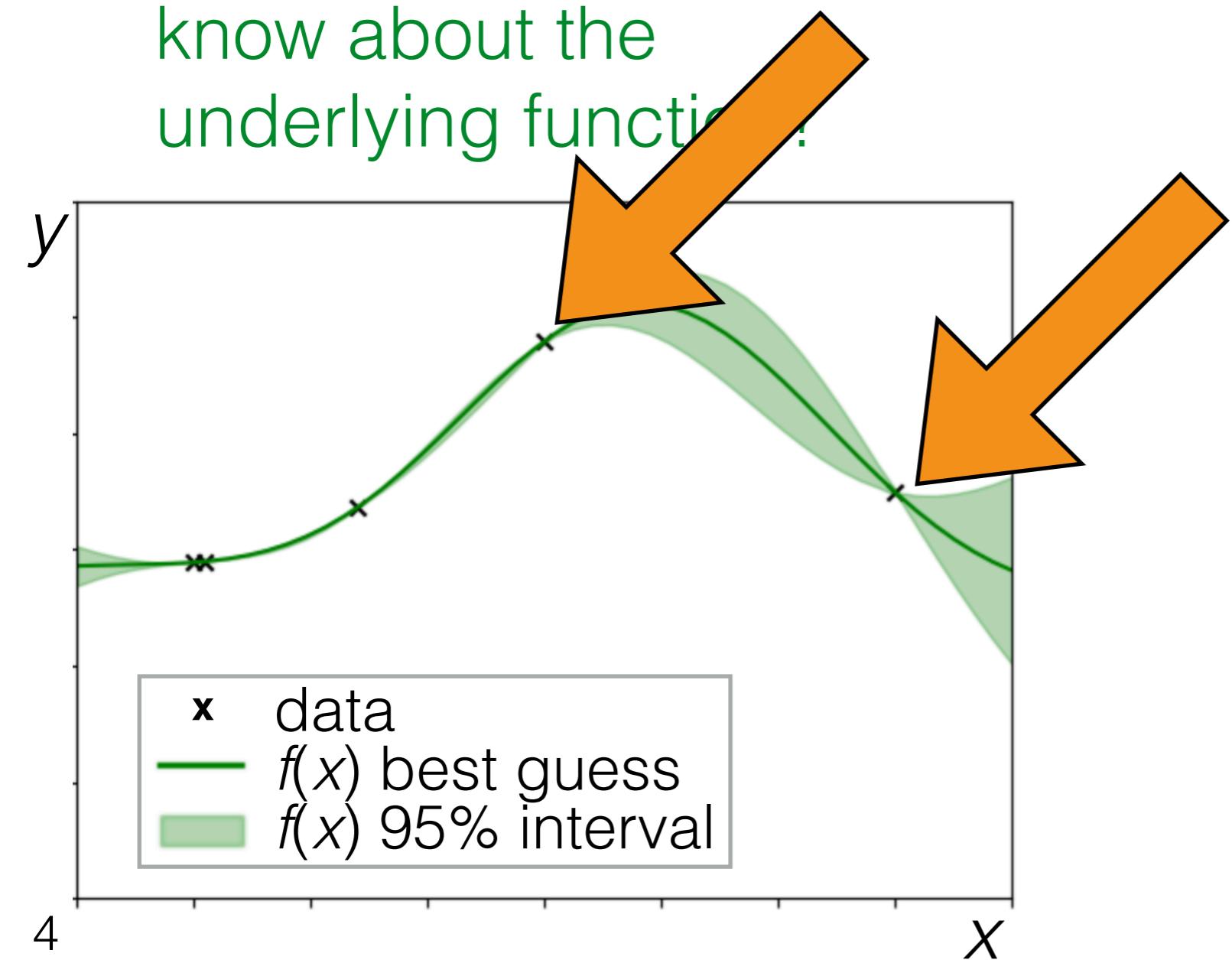
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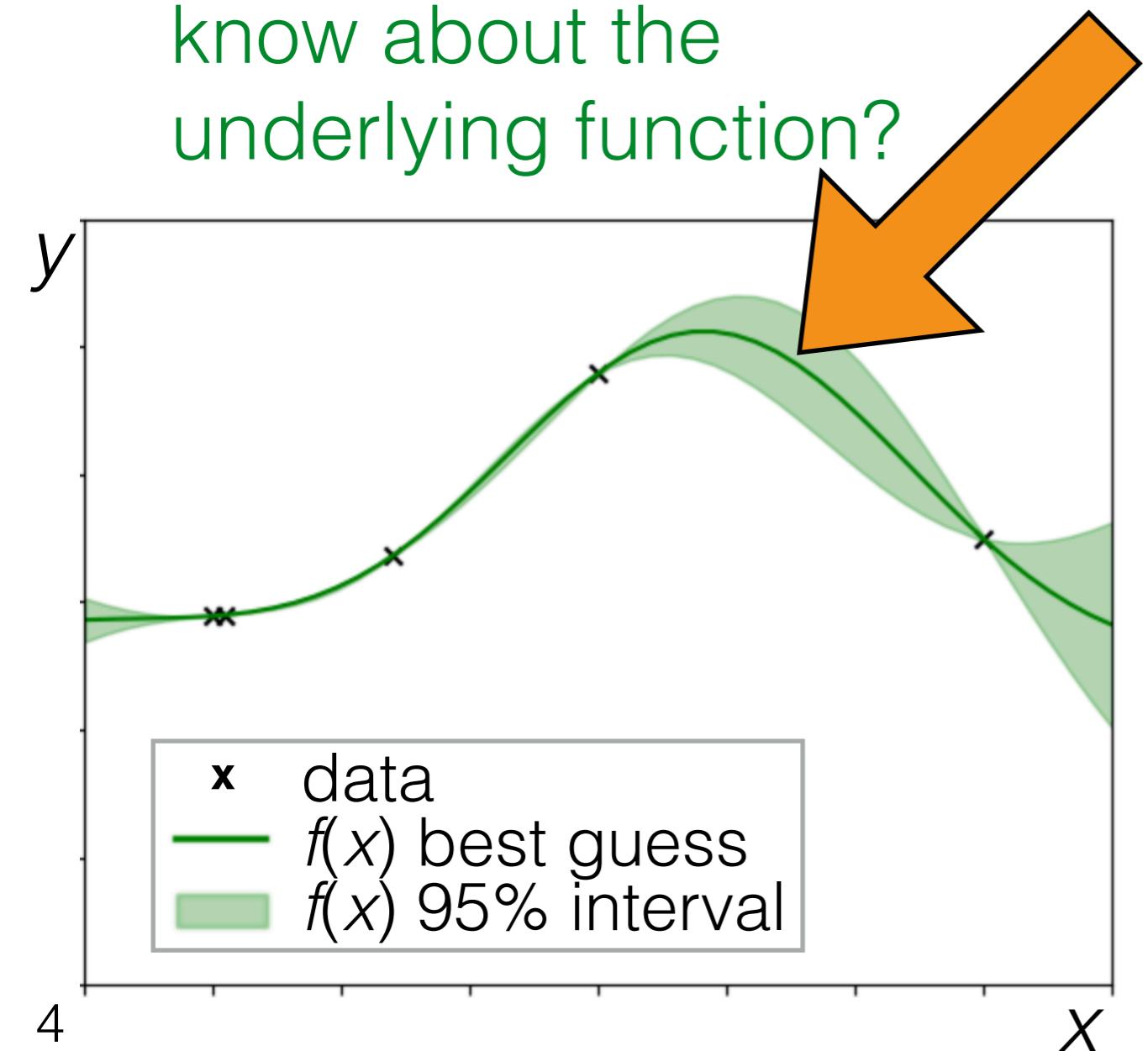
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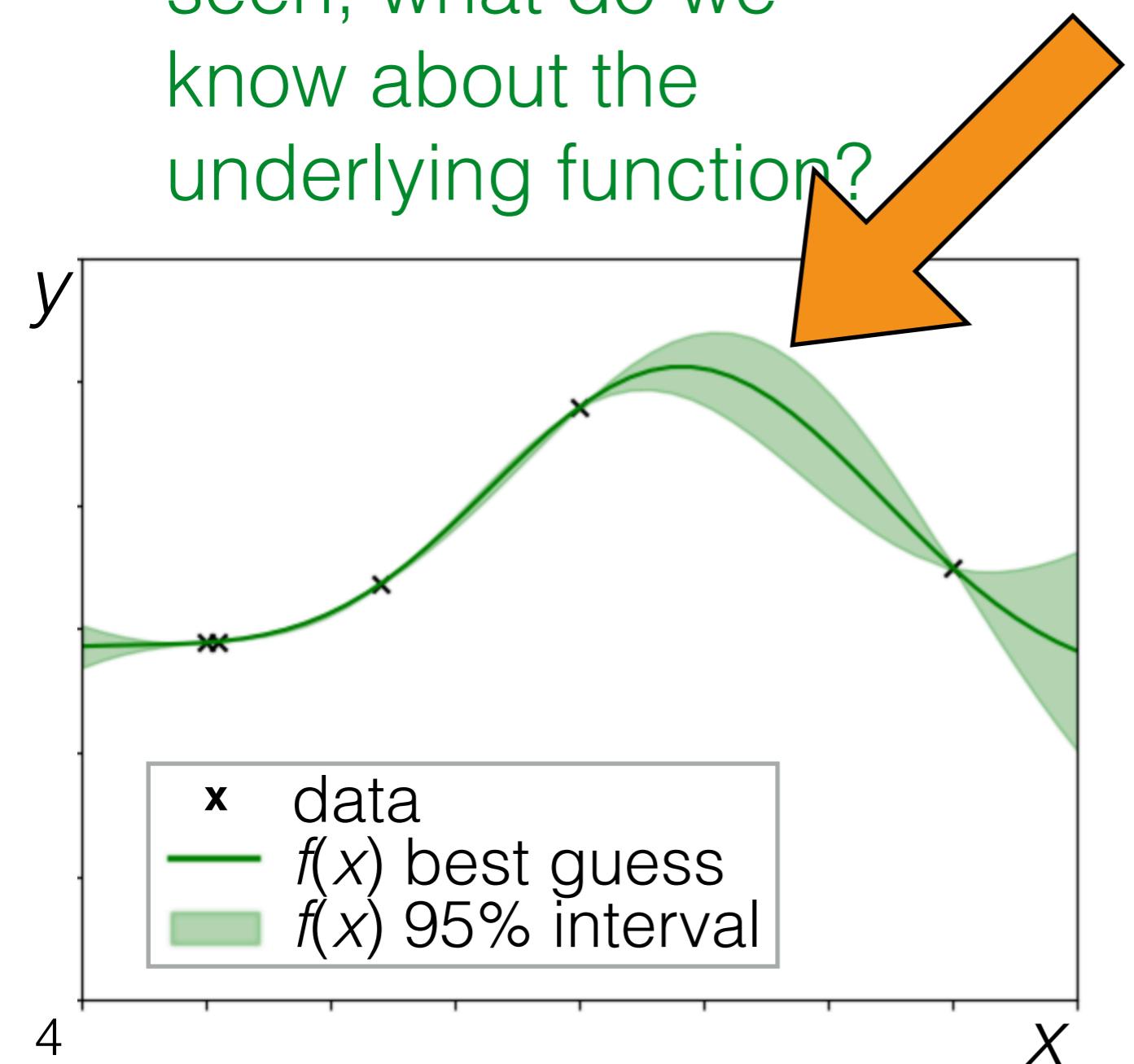
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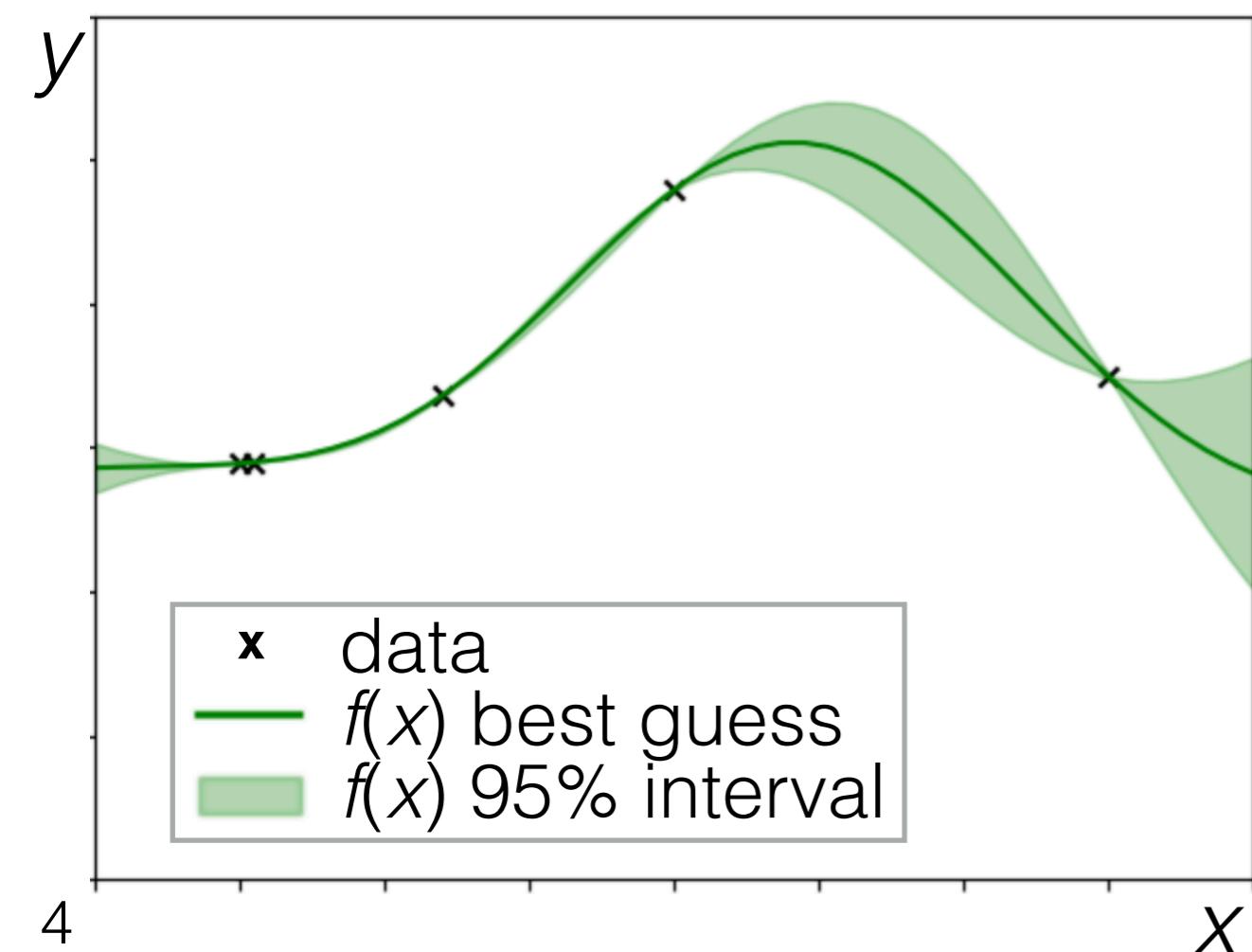
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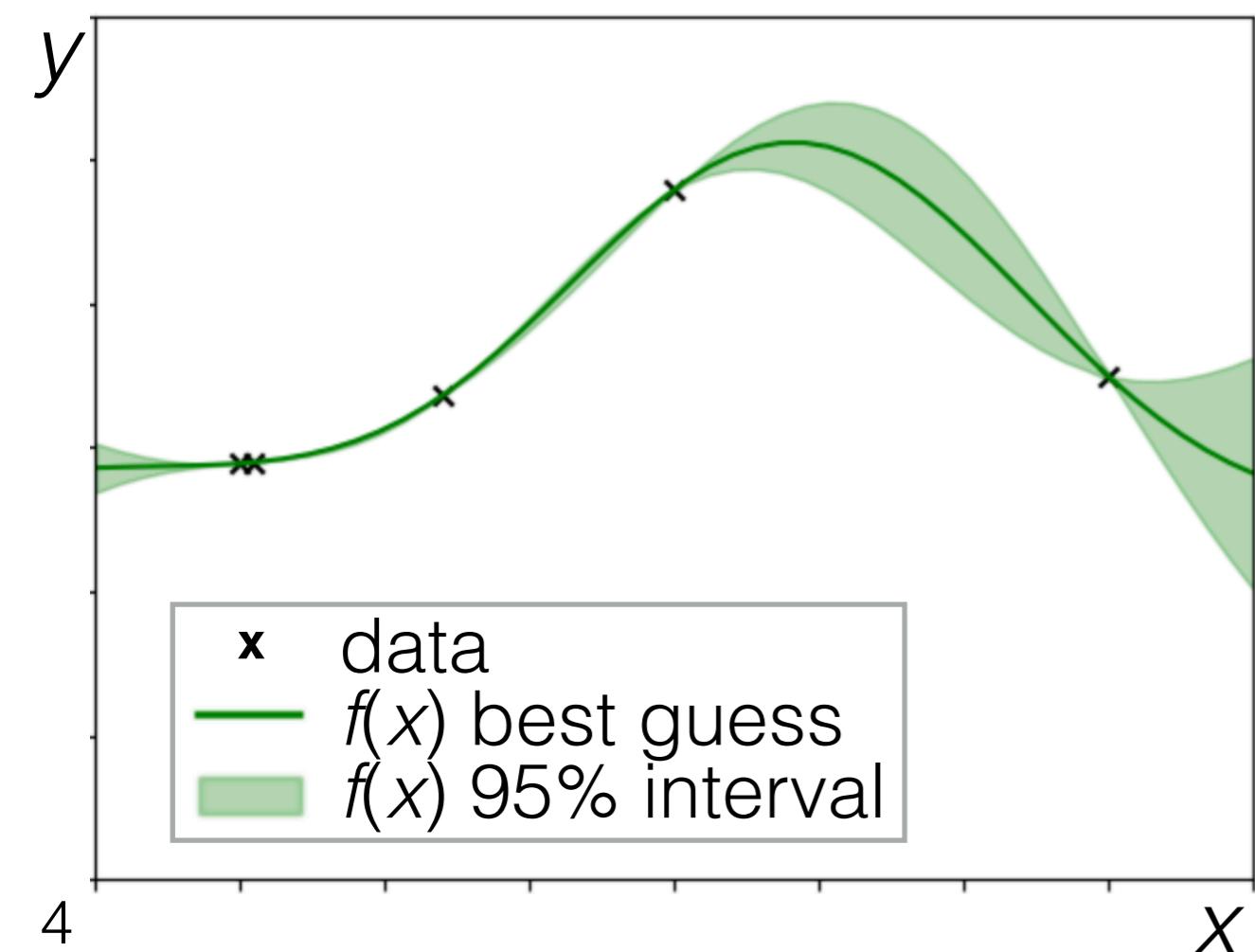


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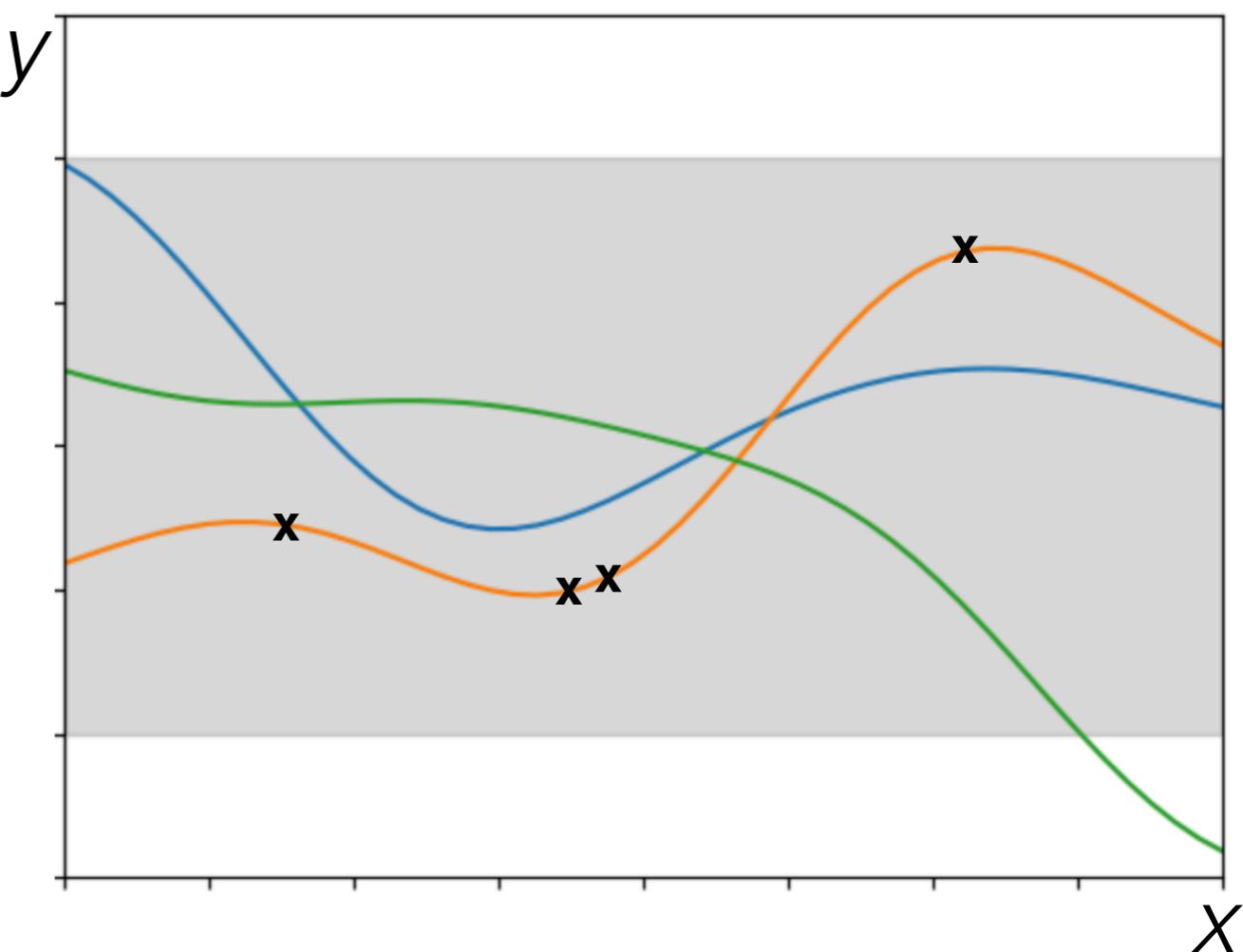
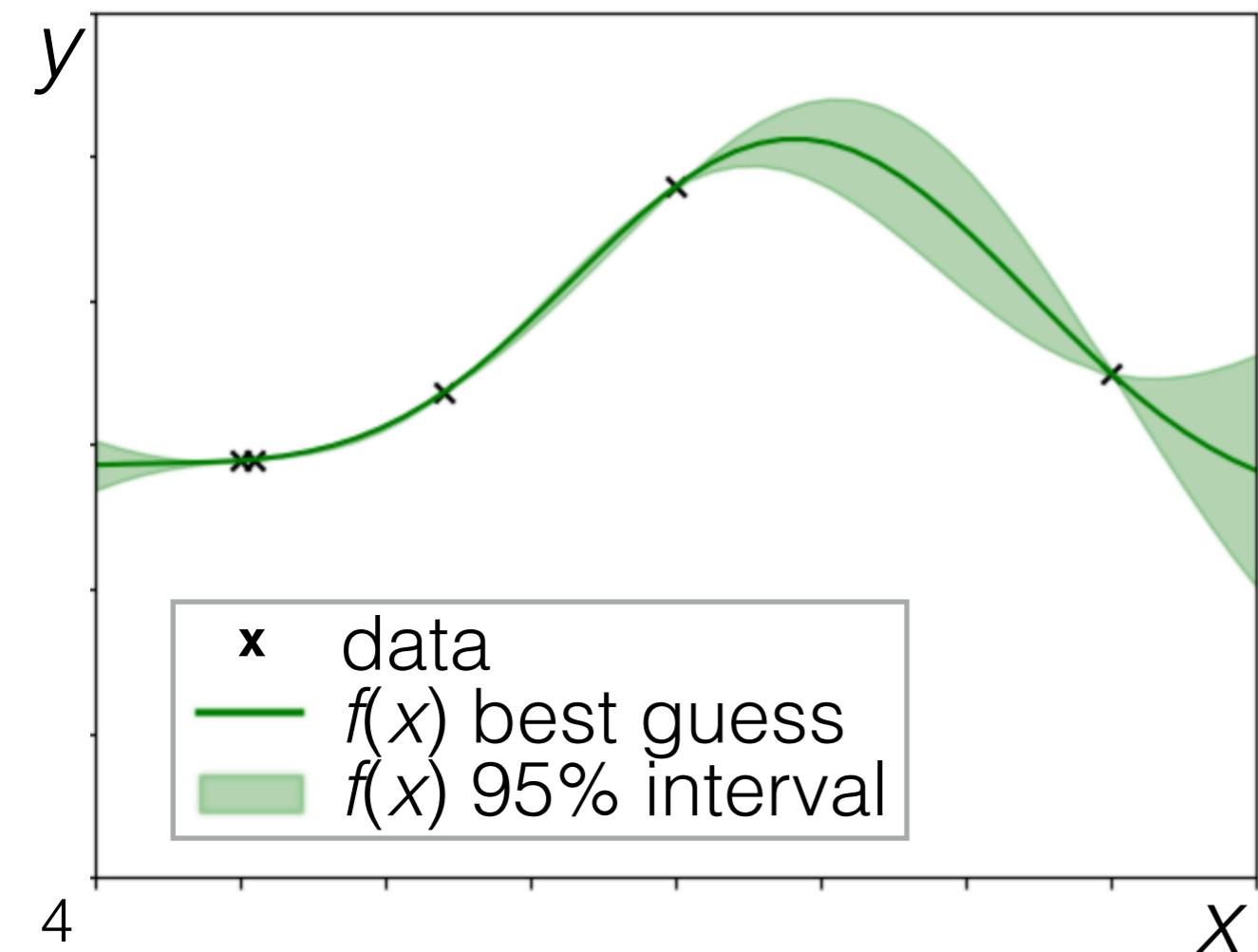


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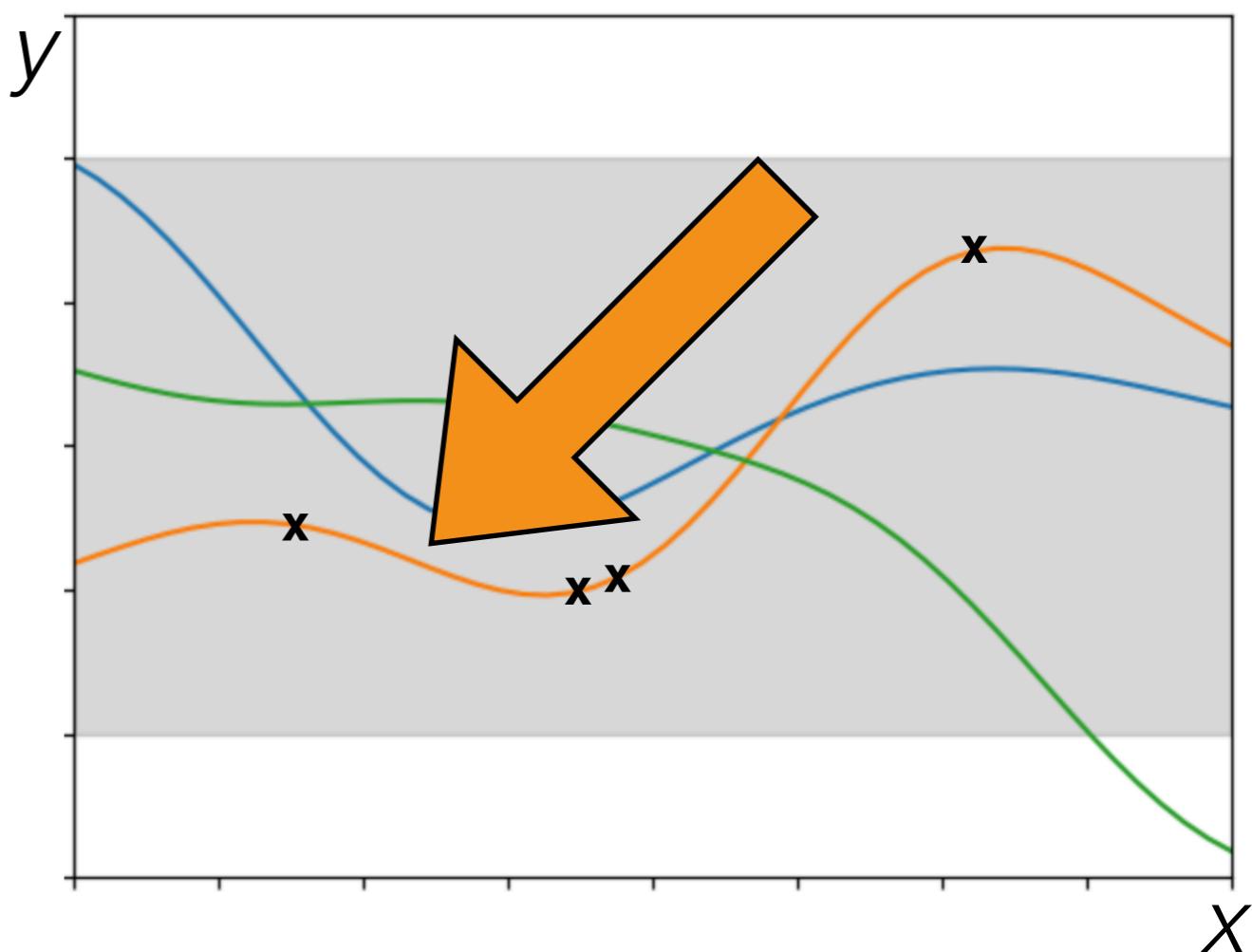
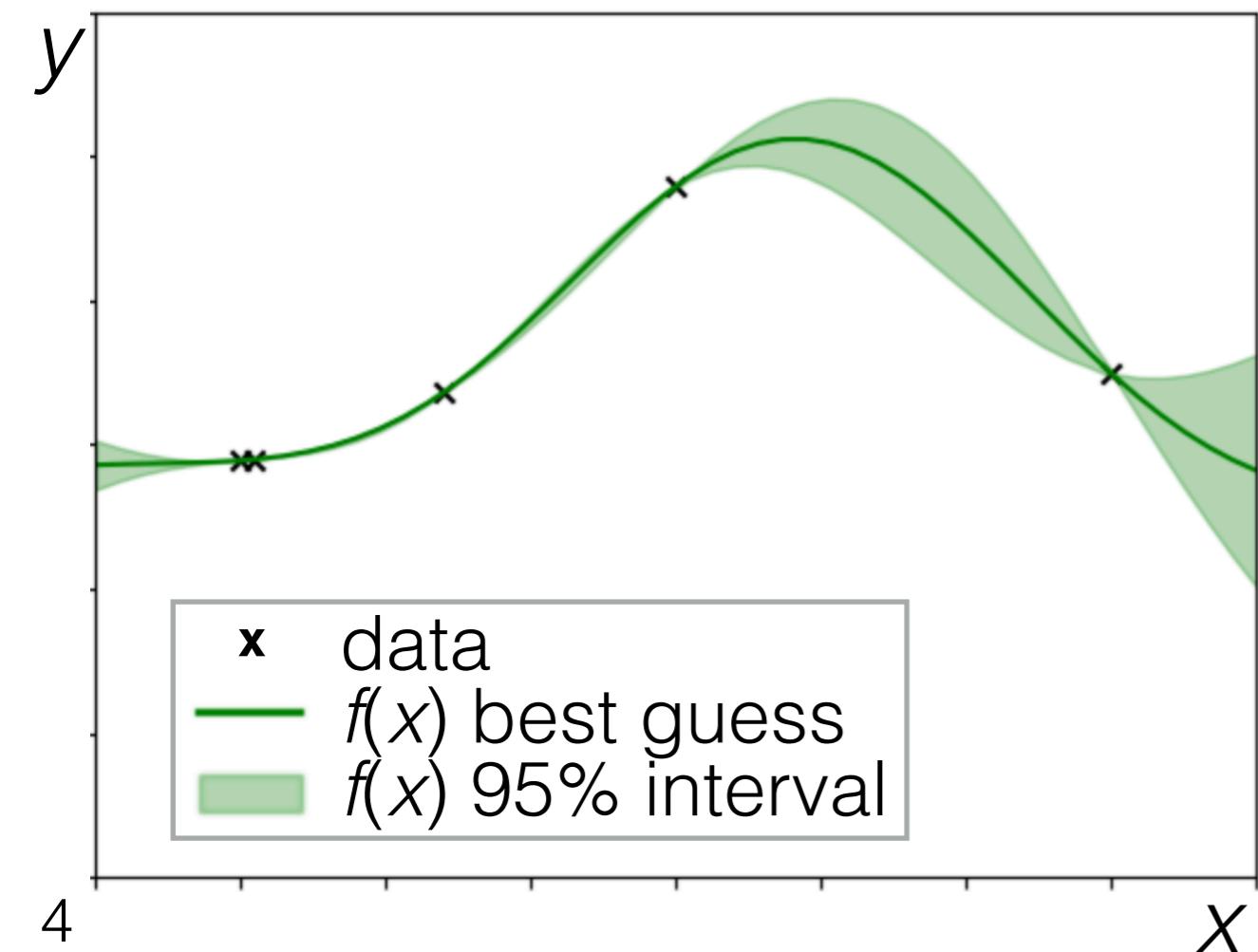


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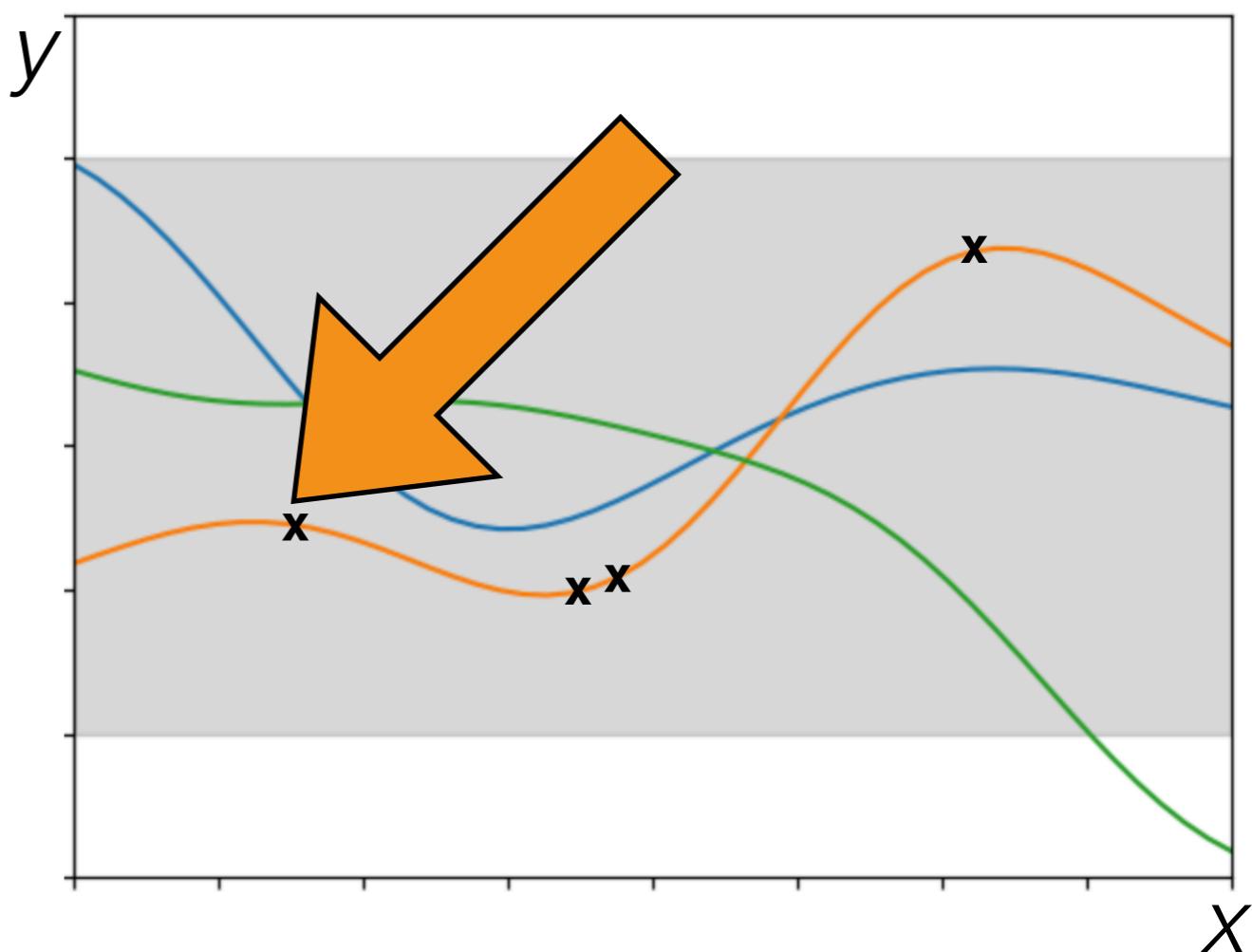
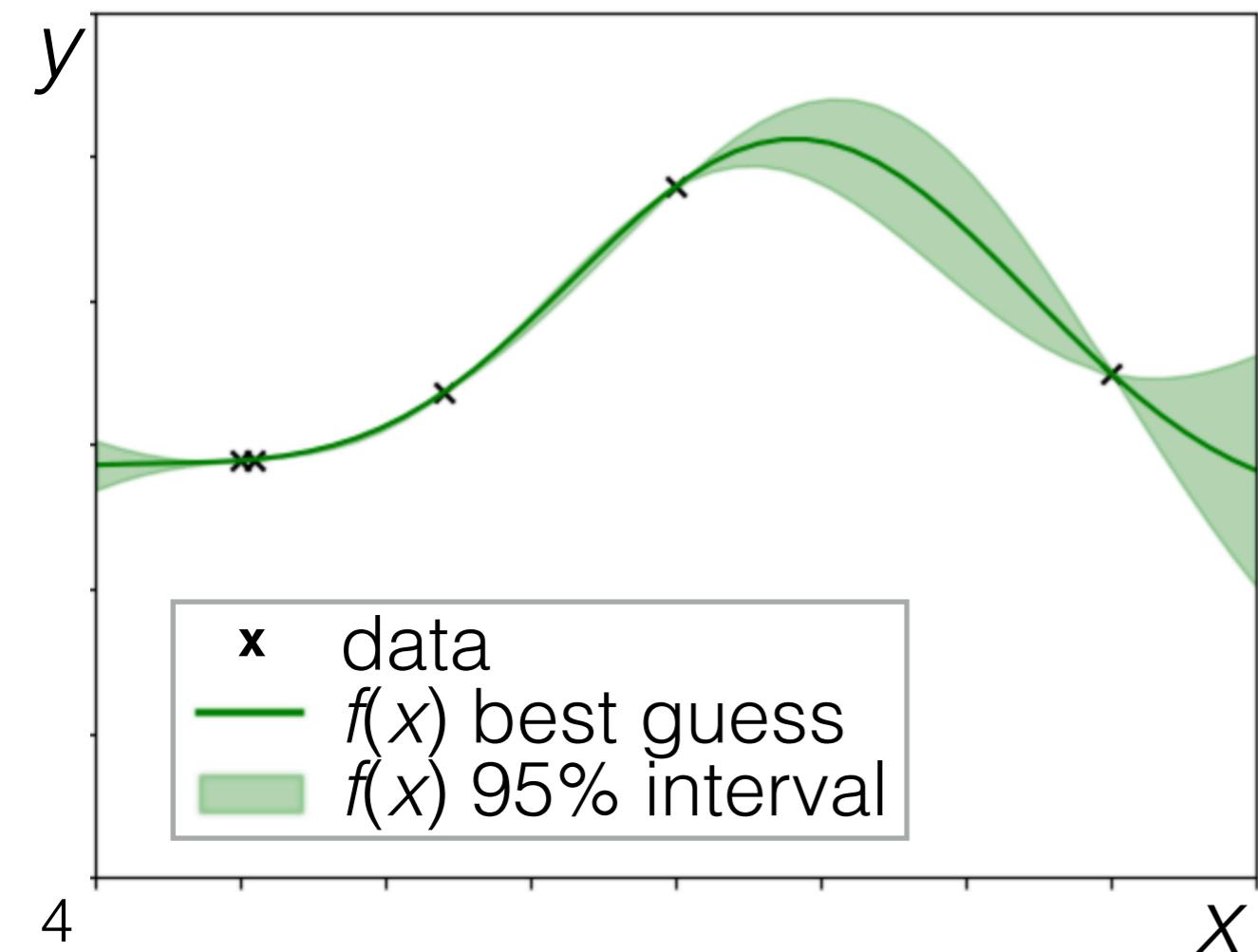


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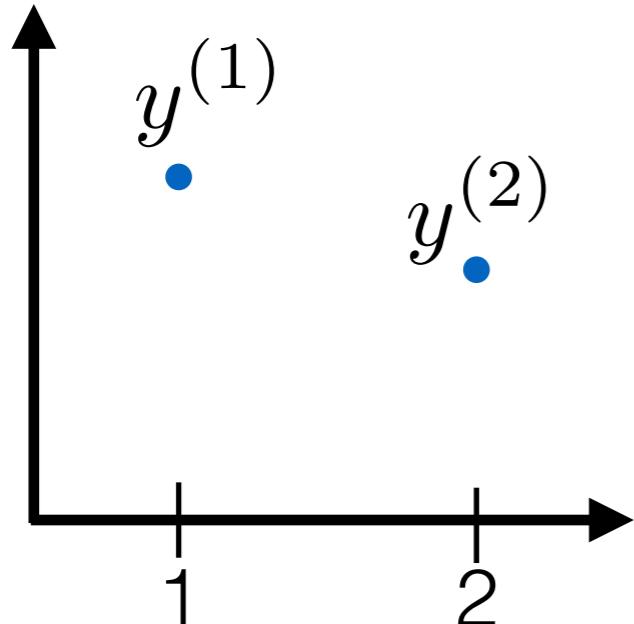
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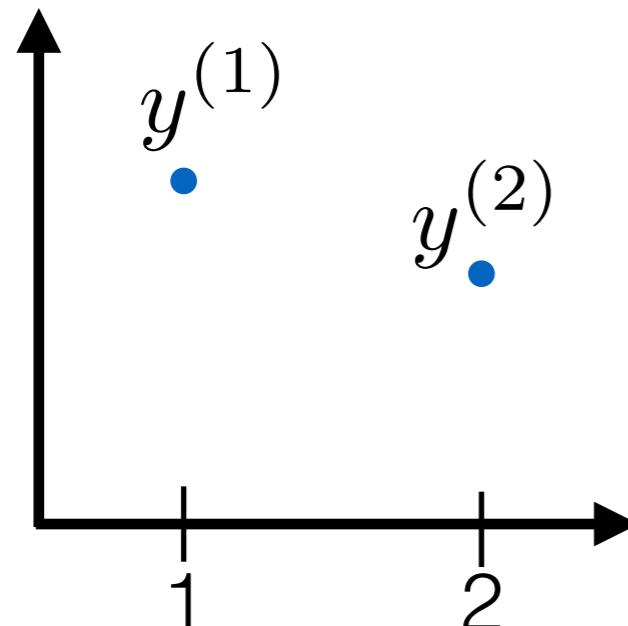
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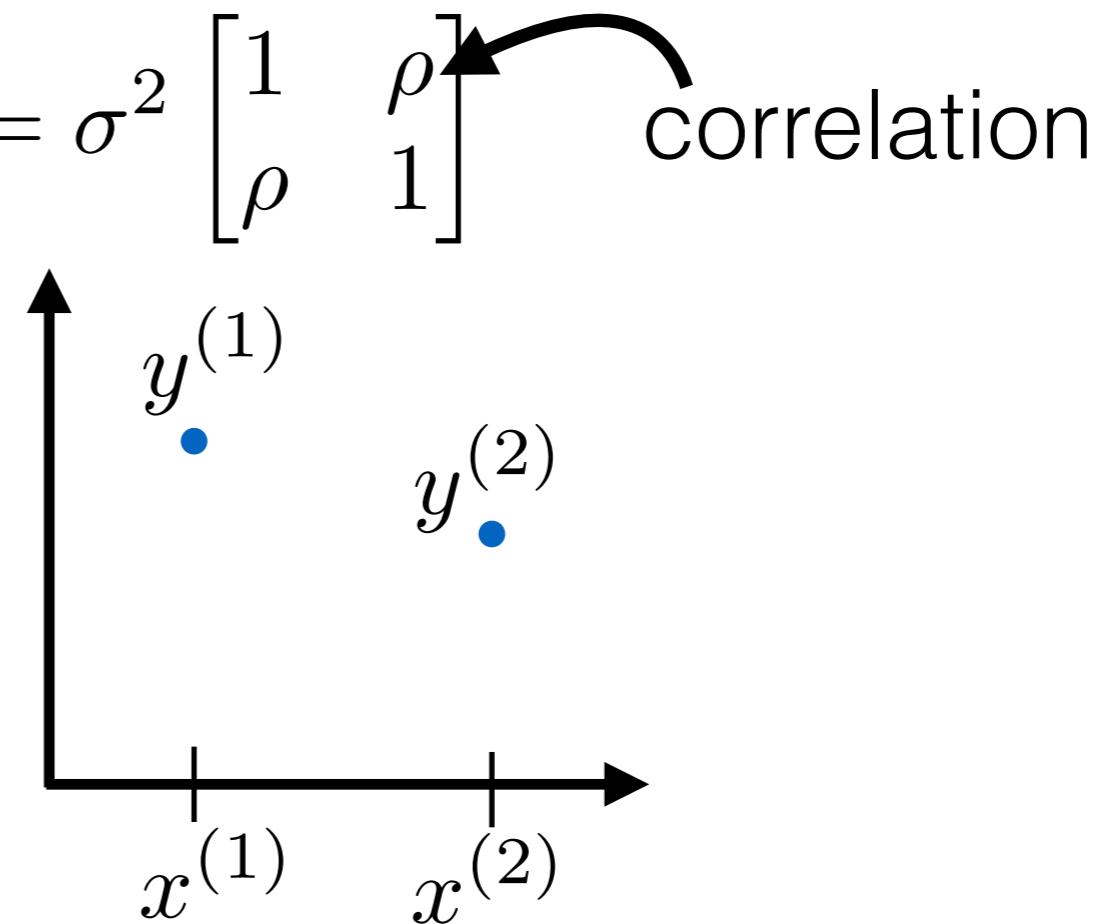
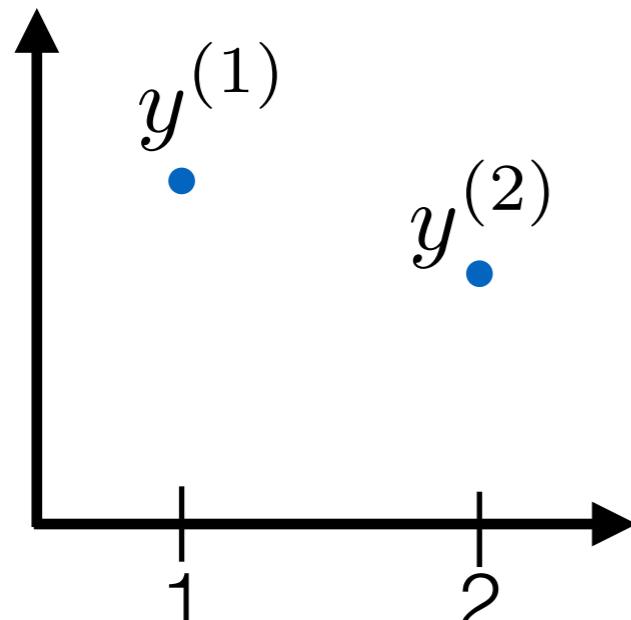


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correlation

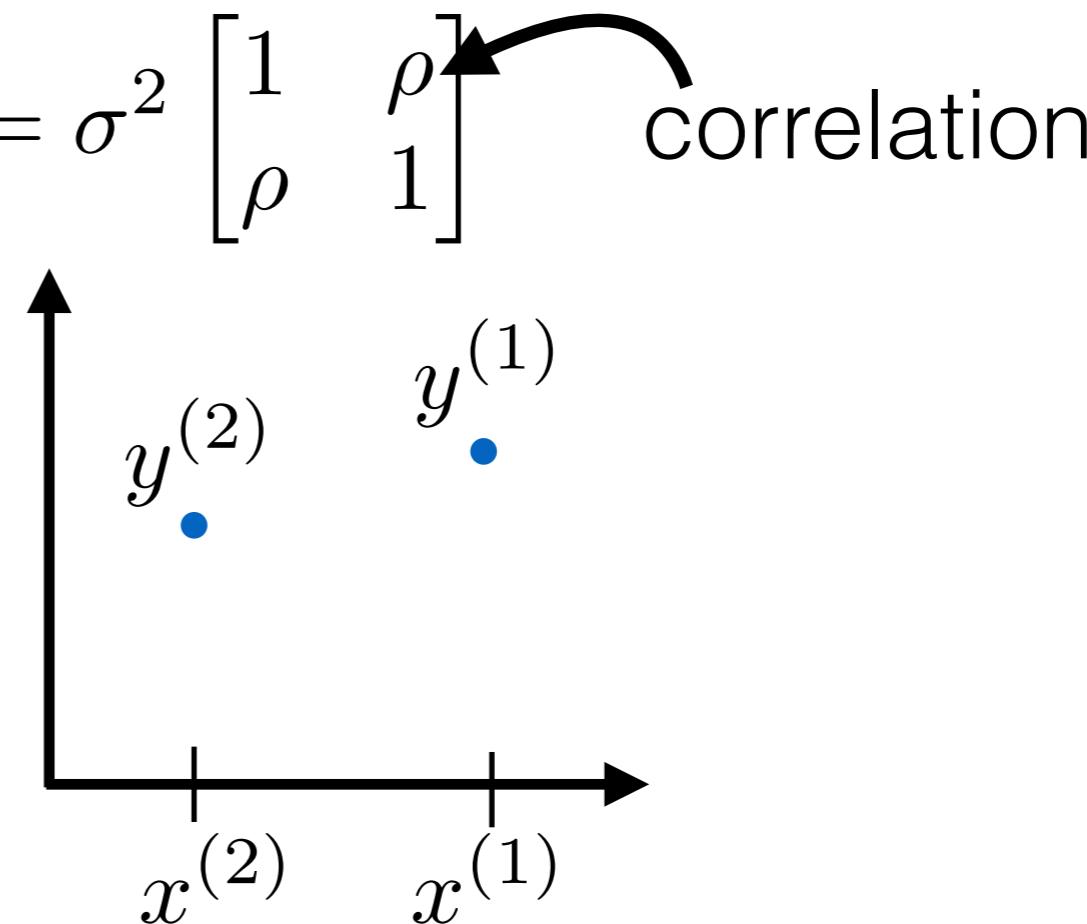
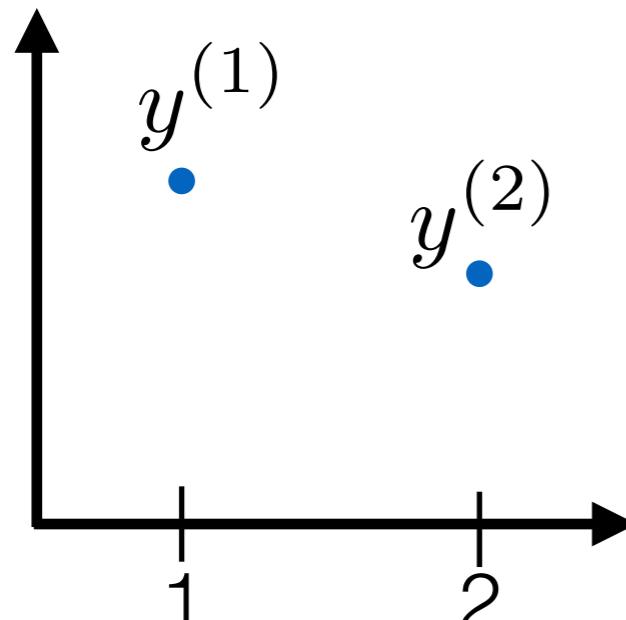
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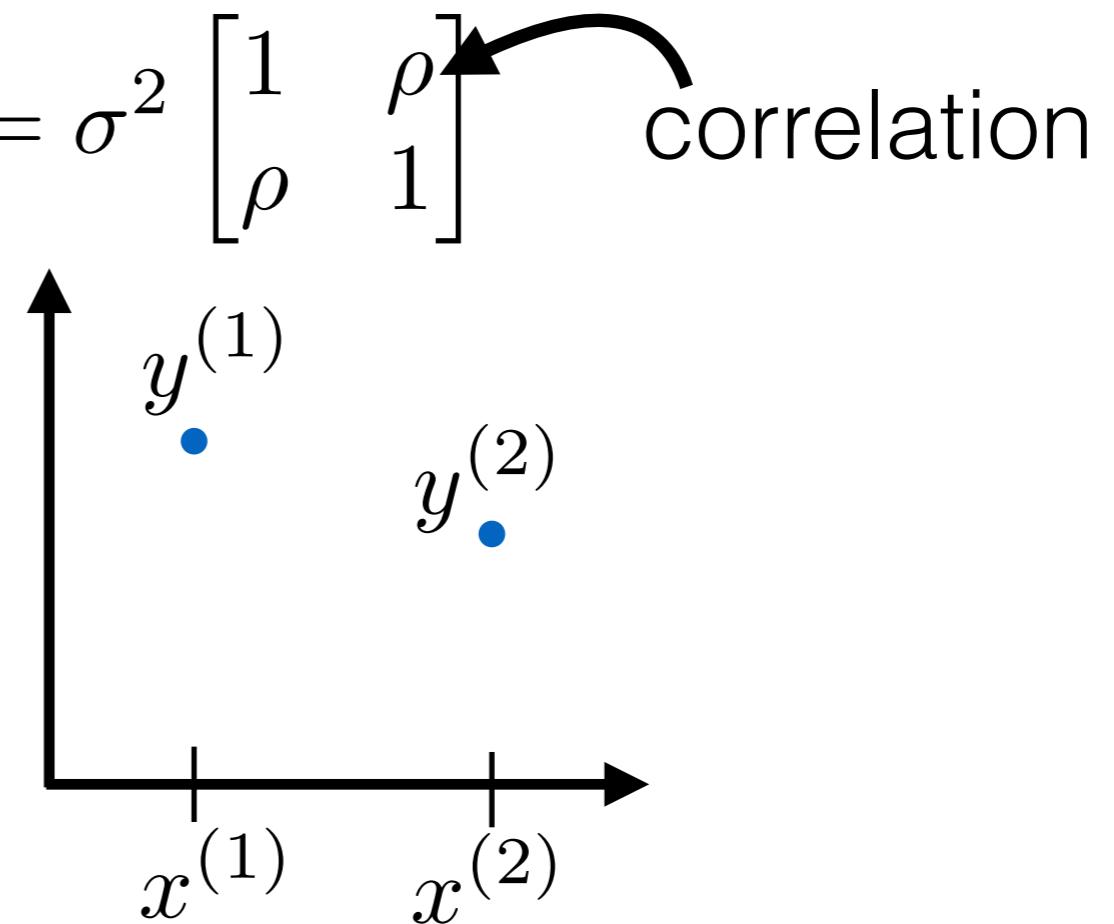
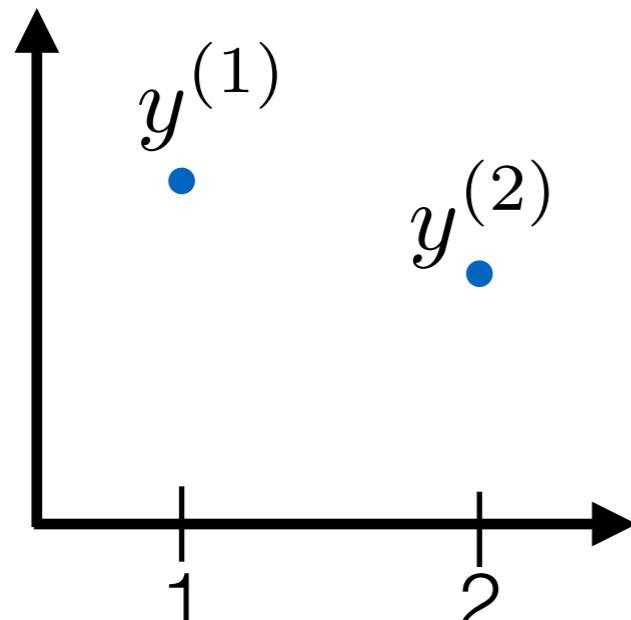
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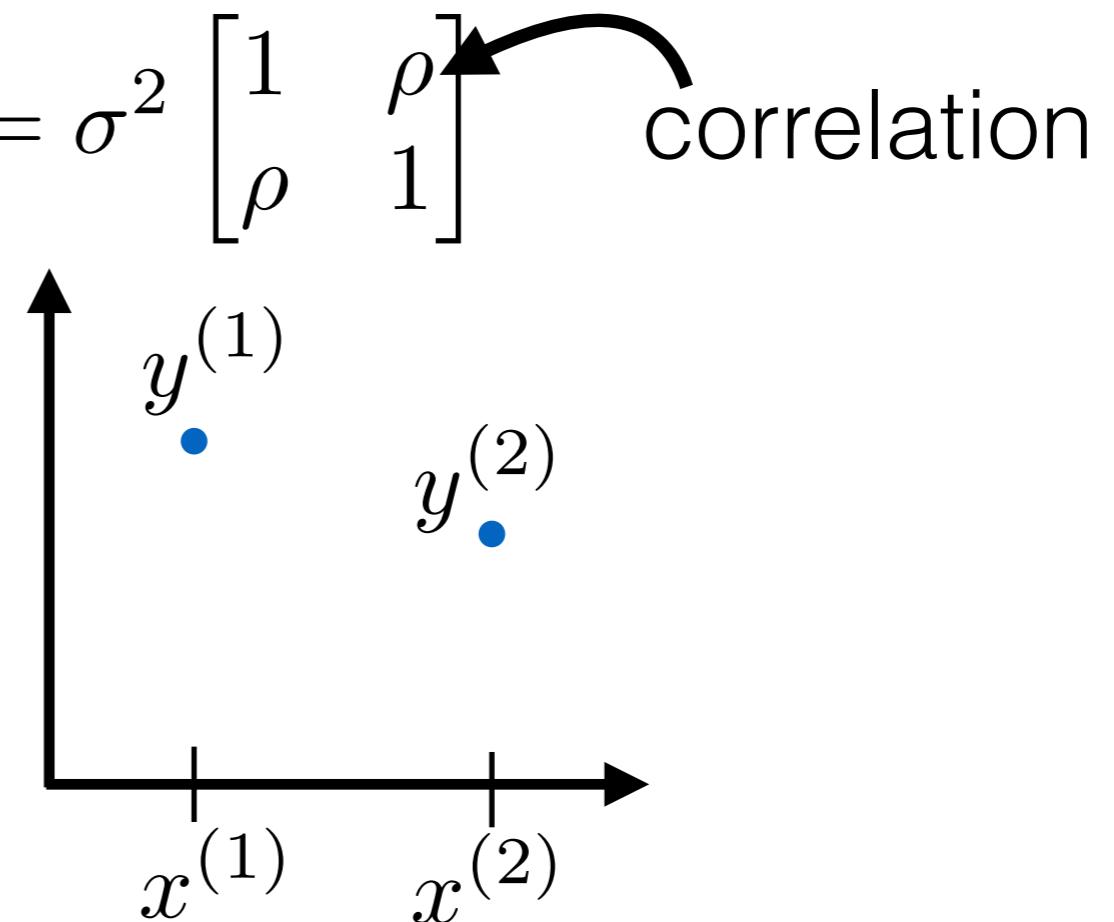
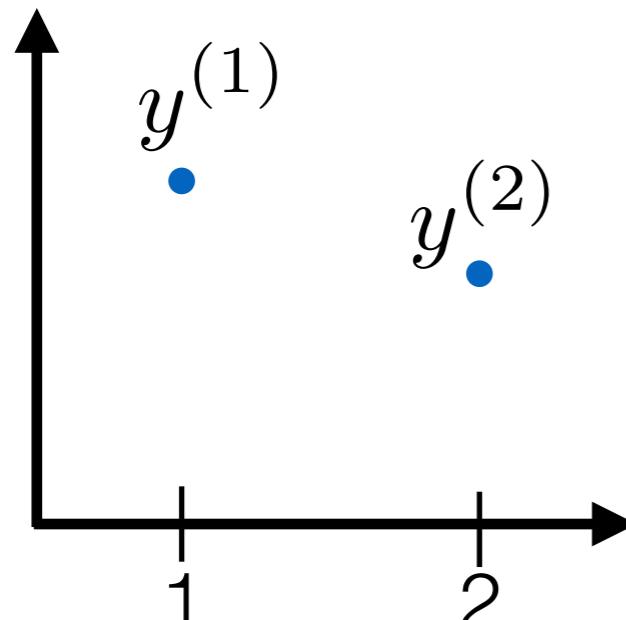
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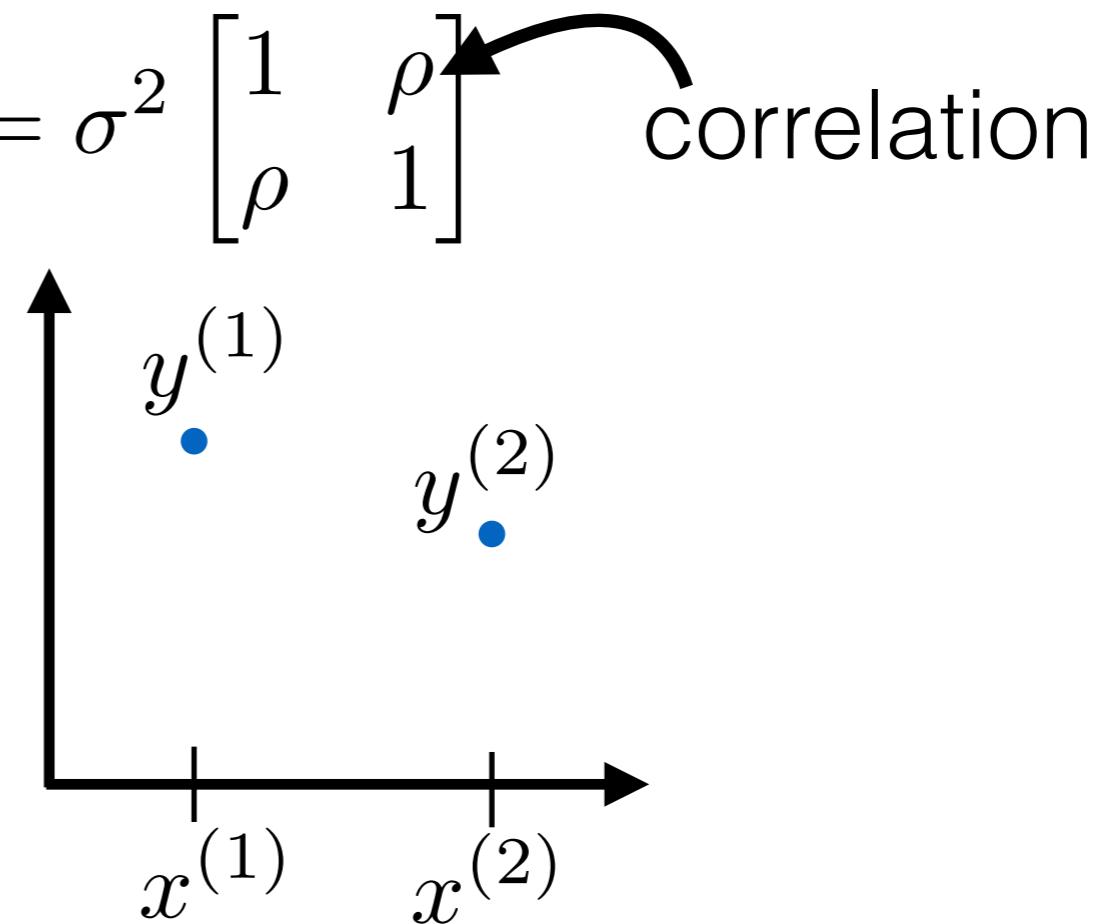
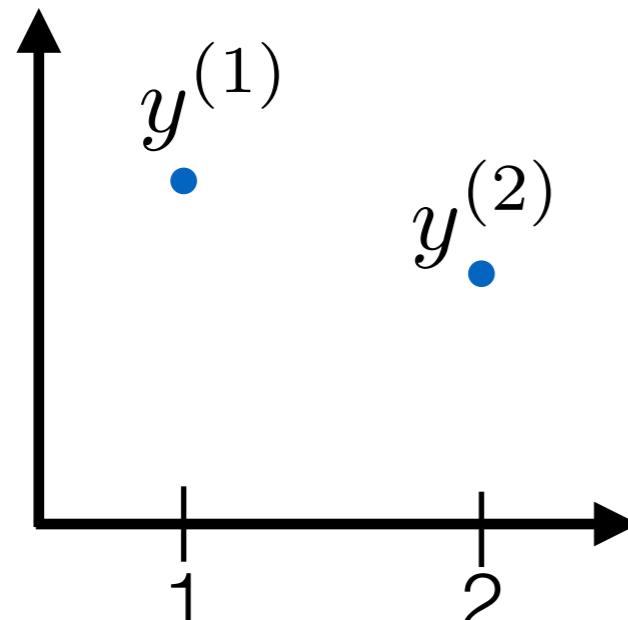
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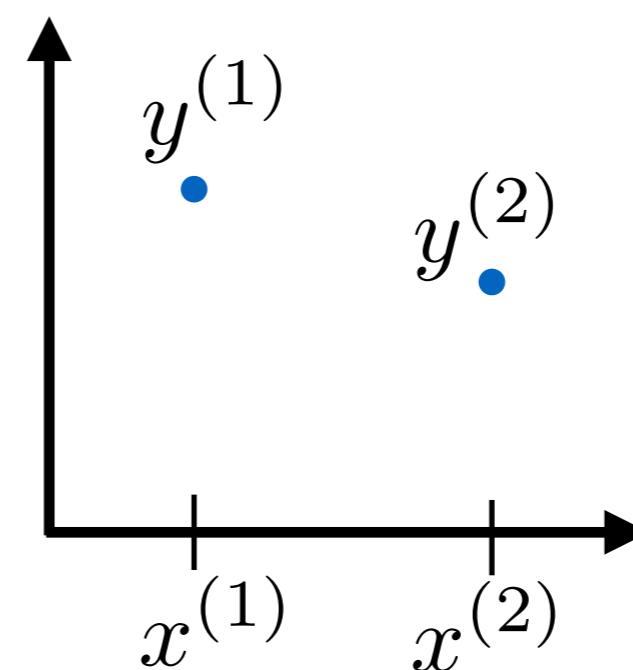
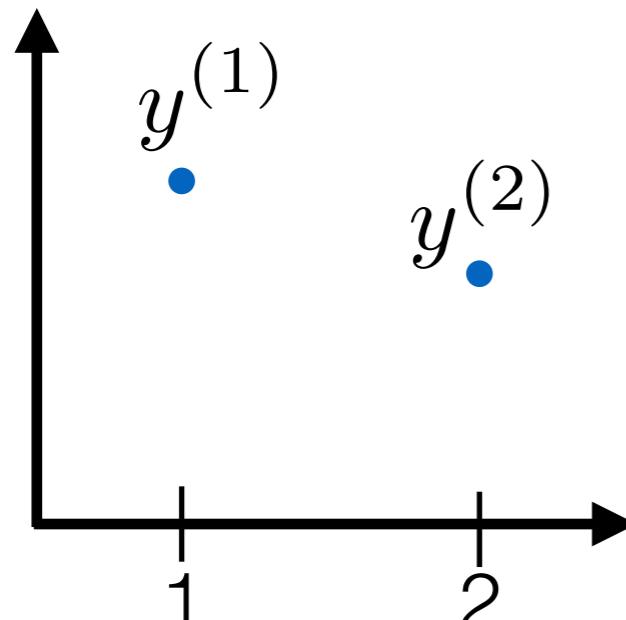
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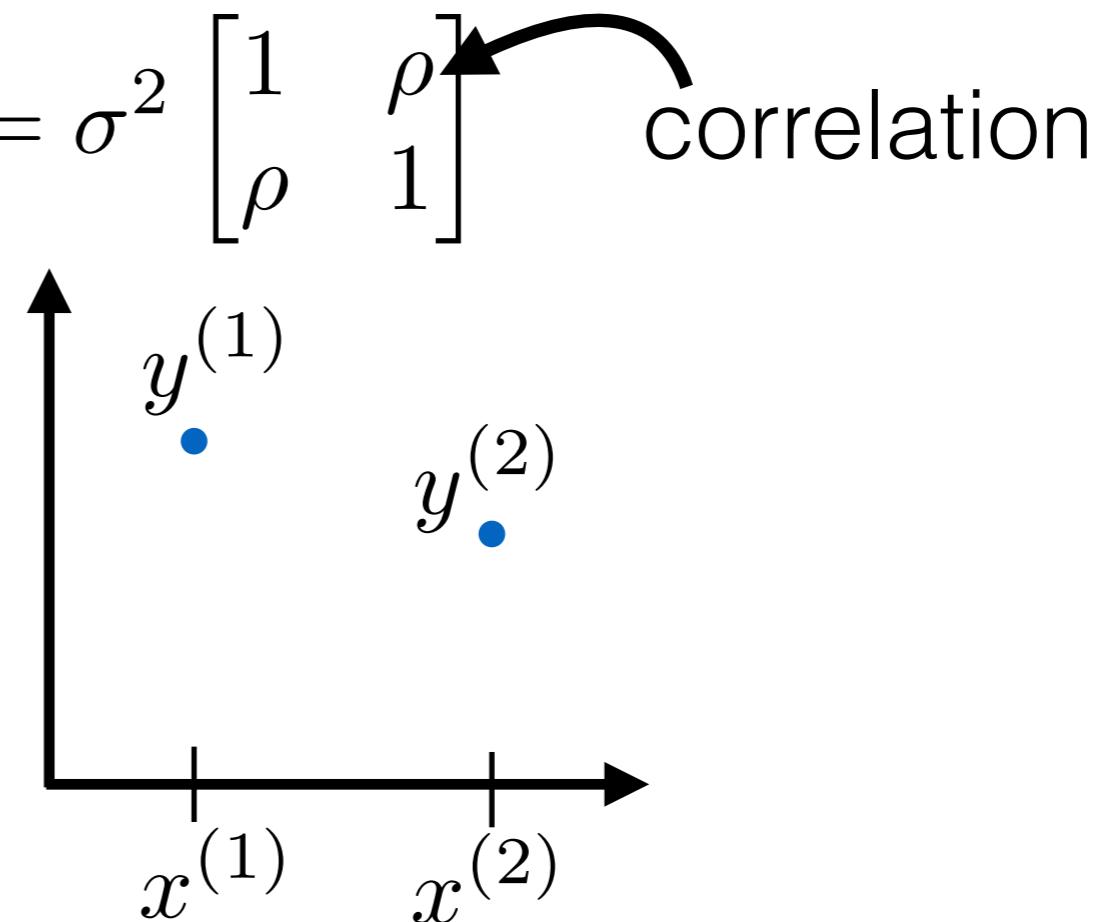
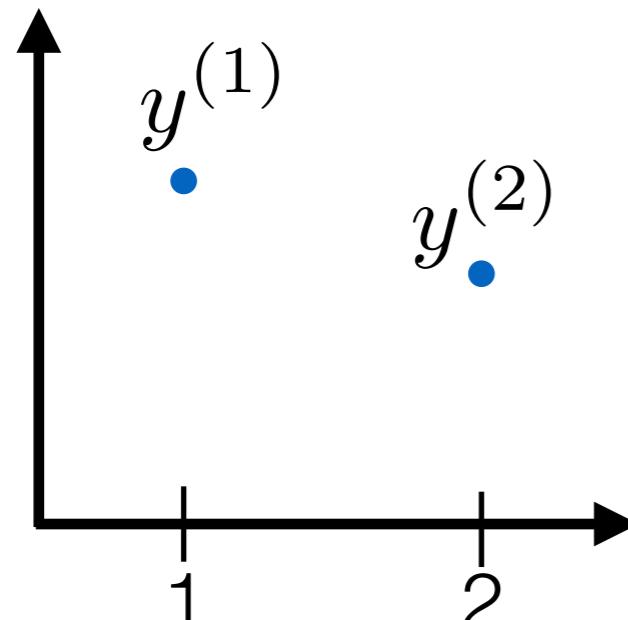
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 - Where the correlation goes to 1 as the x 's get close

Multivariate Gaussian using locations

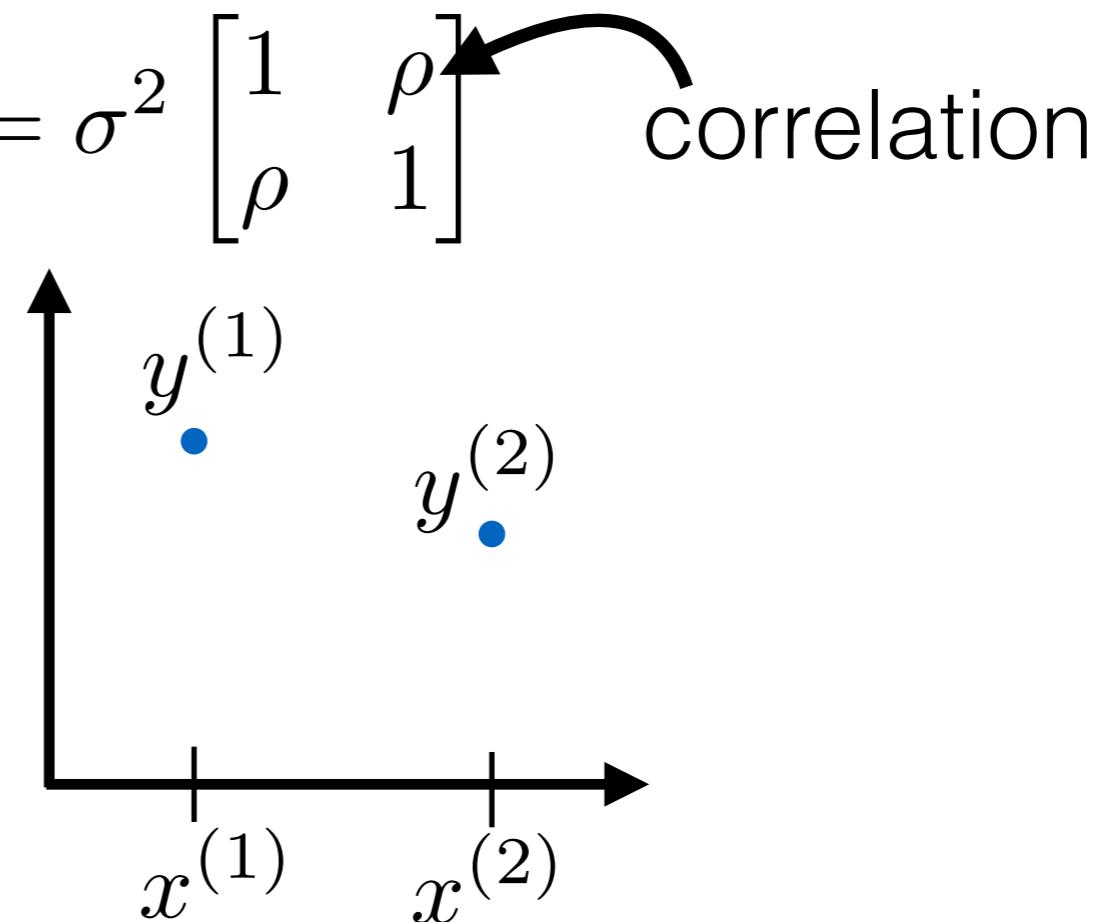
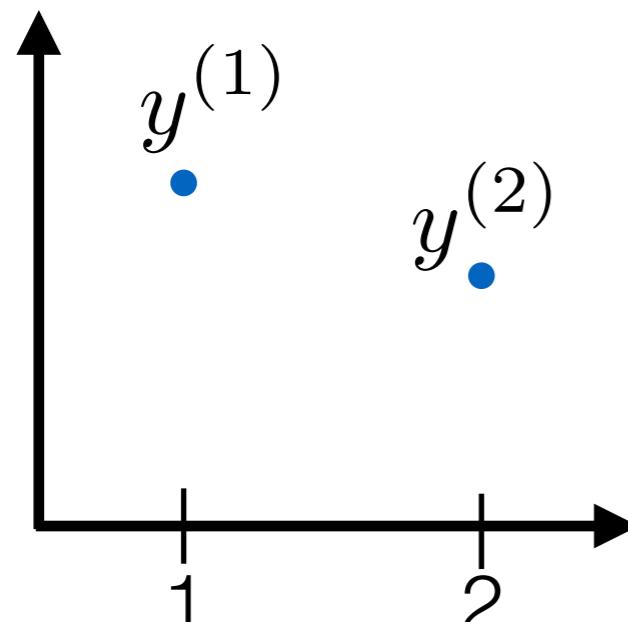
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We just drew random functions from a type of
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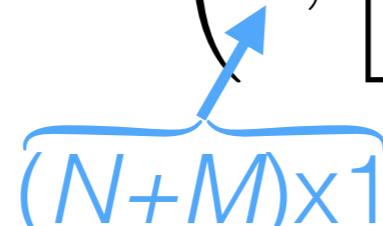
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Inference about unknowns given data

- Let X collect the N “training” data points (indexed 1 to N)
- Let X' collect the M “test” data points
 - Where we want to evaluate the function
 - Indexed $N+1$ to $N+M$
- $K(X, X')$ is the $N \times M$ matrix with (n,m) entry $k(x^{(n)}, x^{(N+m)})$
- Then by our model

$$\begin{matrix} N \times 1 \\ M \times 1 \end{matrix} \begin{bmatrix} f(X) \\ f(X') \end{bmatrix} \sim \mathcal{N} \left(\mathbf{0}, \begin{bmatrix} K(X, X) & K(X, X') \\ K(X', X) & K(X', X') \end{bmatrix} \right)$$

$\underbrace{(N+M) \times 1}_{\text{f}(X)}$ $\underbrace{(N+M) \times (N+M)}_{K(X, X')}$

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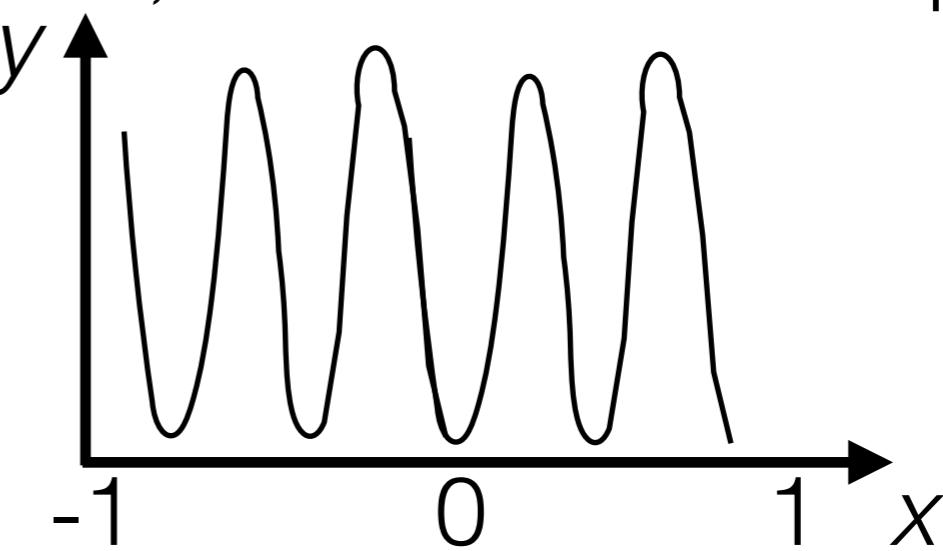
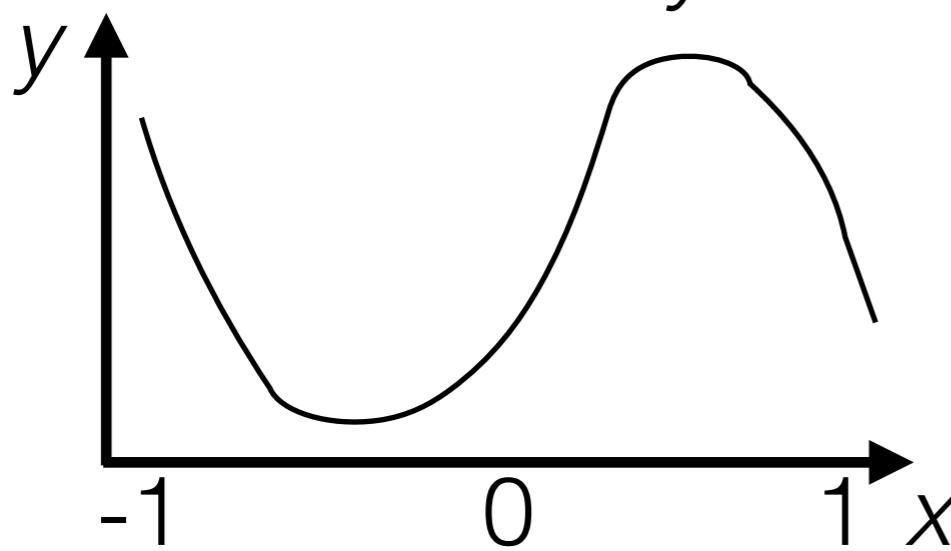
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Goal:

- Learn the mechanism behind standard GPs to identify benefits and pitfalls

Resources

<http://www.tamarabroderick.com/tutorials.html>

- Rasmussen and Williams 2006. *Gaussian Processes for Machine Learning*. <https://gaussianprocess.org/gpml/>
 - Chapters 1, 2, 4, 5
- Gramacy 2020. *Surrogates: Gaussian process modeling, design and optimization for the applied sciences*.
<https://bookdown.org/rbg/surrogates/>
- Garnett 2023. *Bayesian Optimization*. <https://bayesoptbook.com/>
- Software options include:
 - scikit-learn, GPy, GPflow, GPyTorch
- My setup for this tutorial: pip install X
 - X = jupyterlab, notebook, numpy, matplotlib, scikit-learn

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