

Gaussian Processes for Regression: Models, Algorithms, and Applications

Tamara Broderick
Associate Professor
MIT

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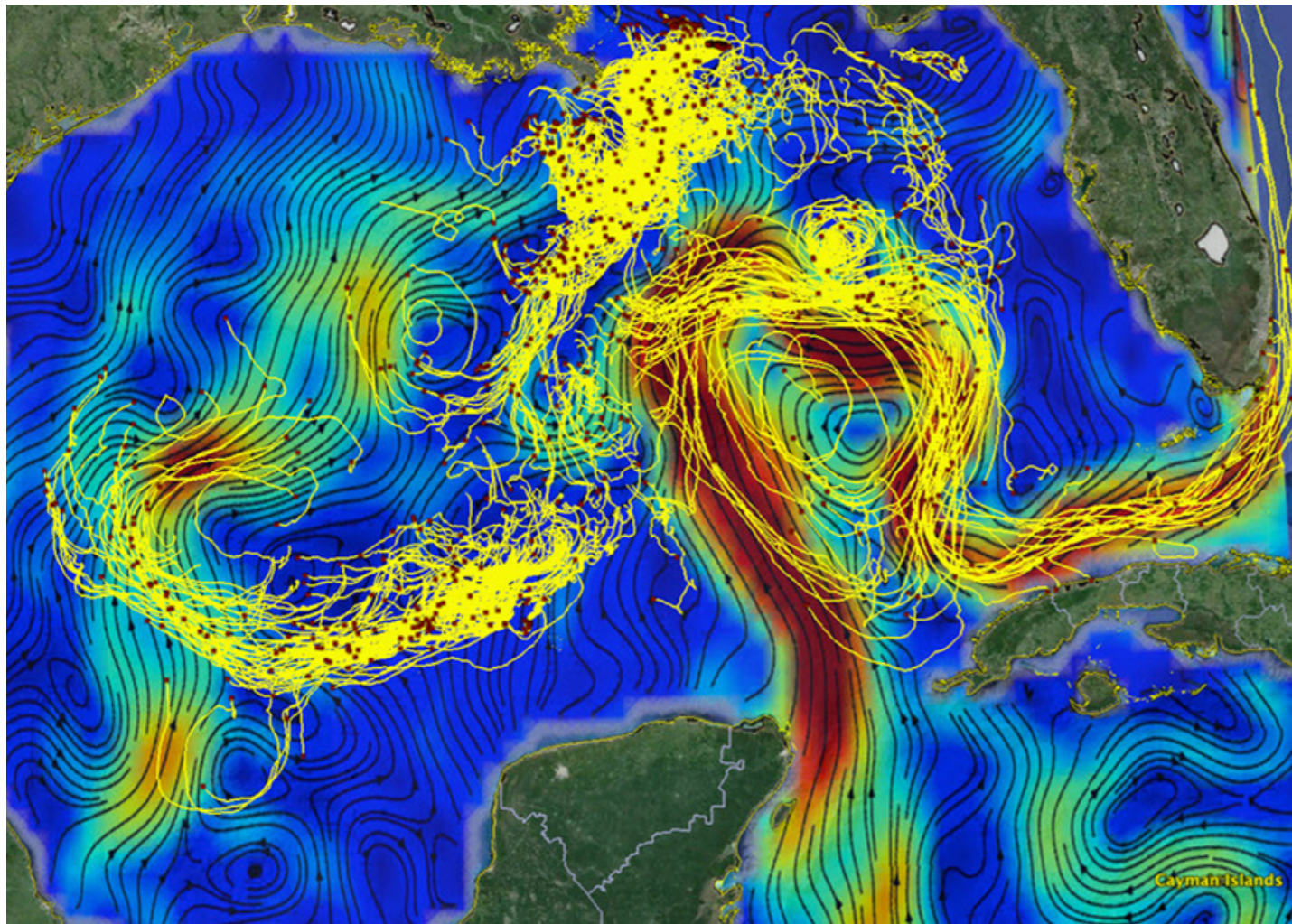
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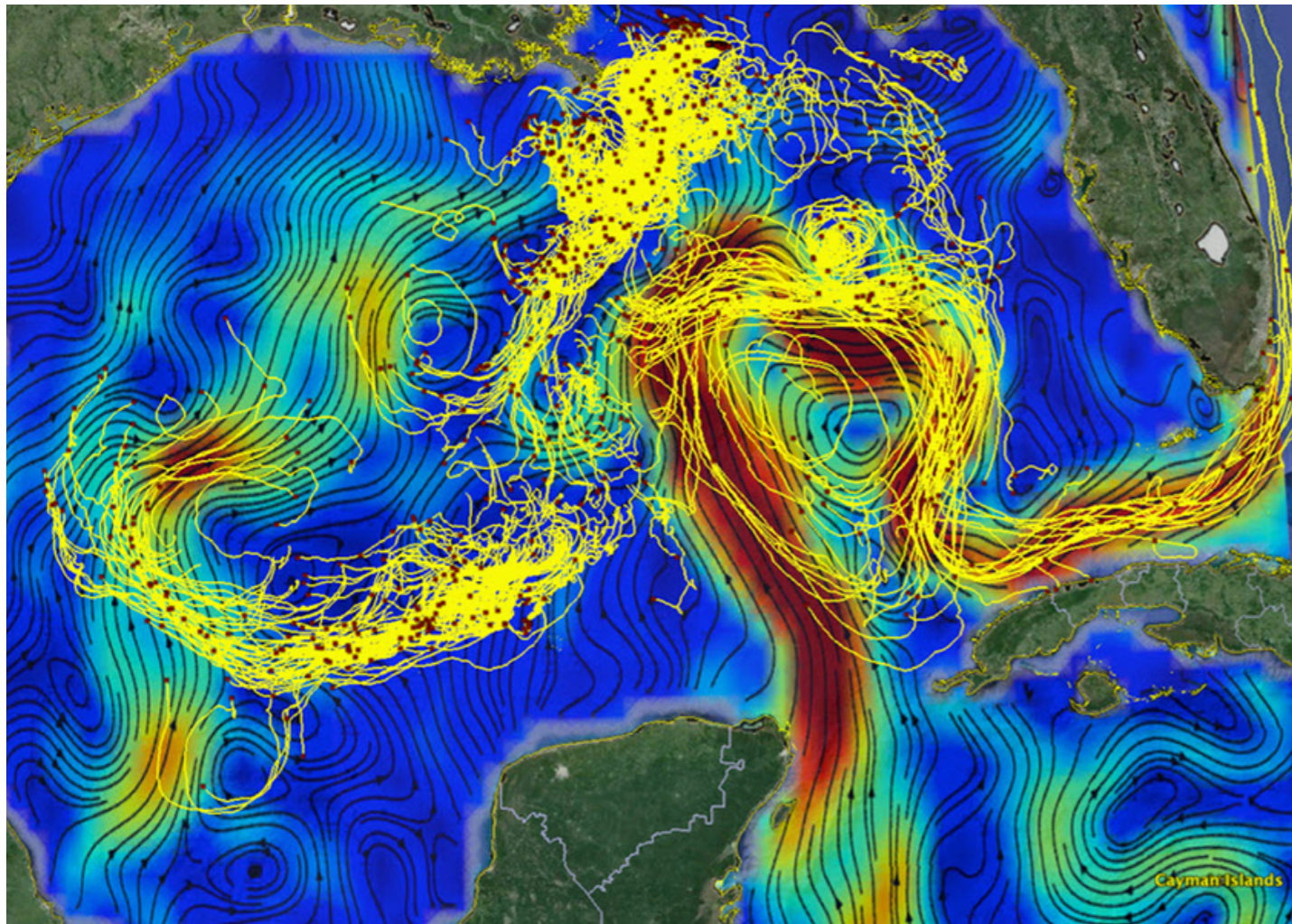


Example:

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

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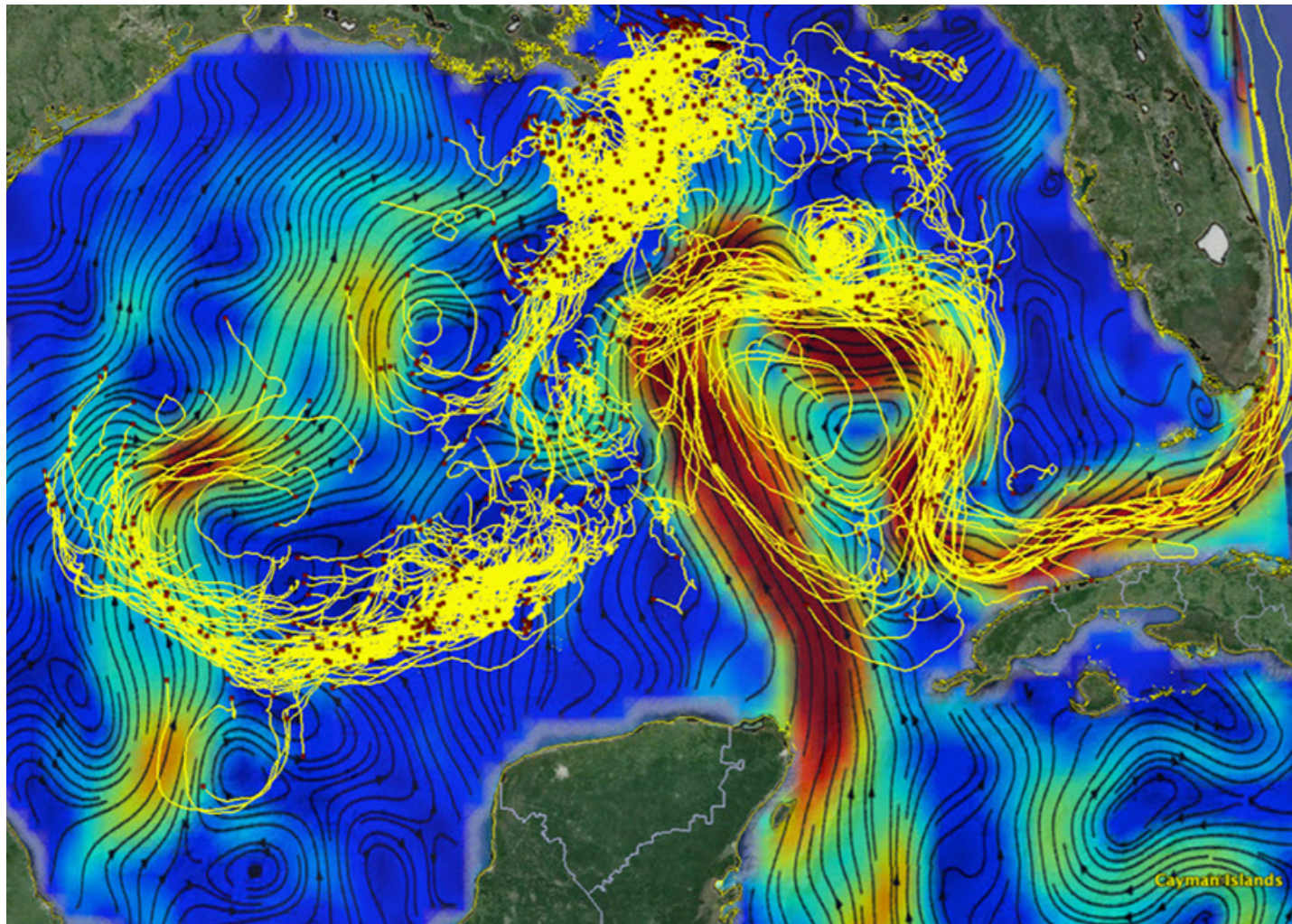
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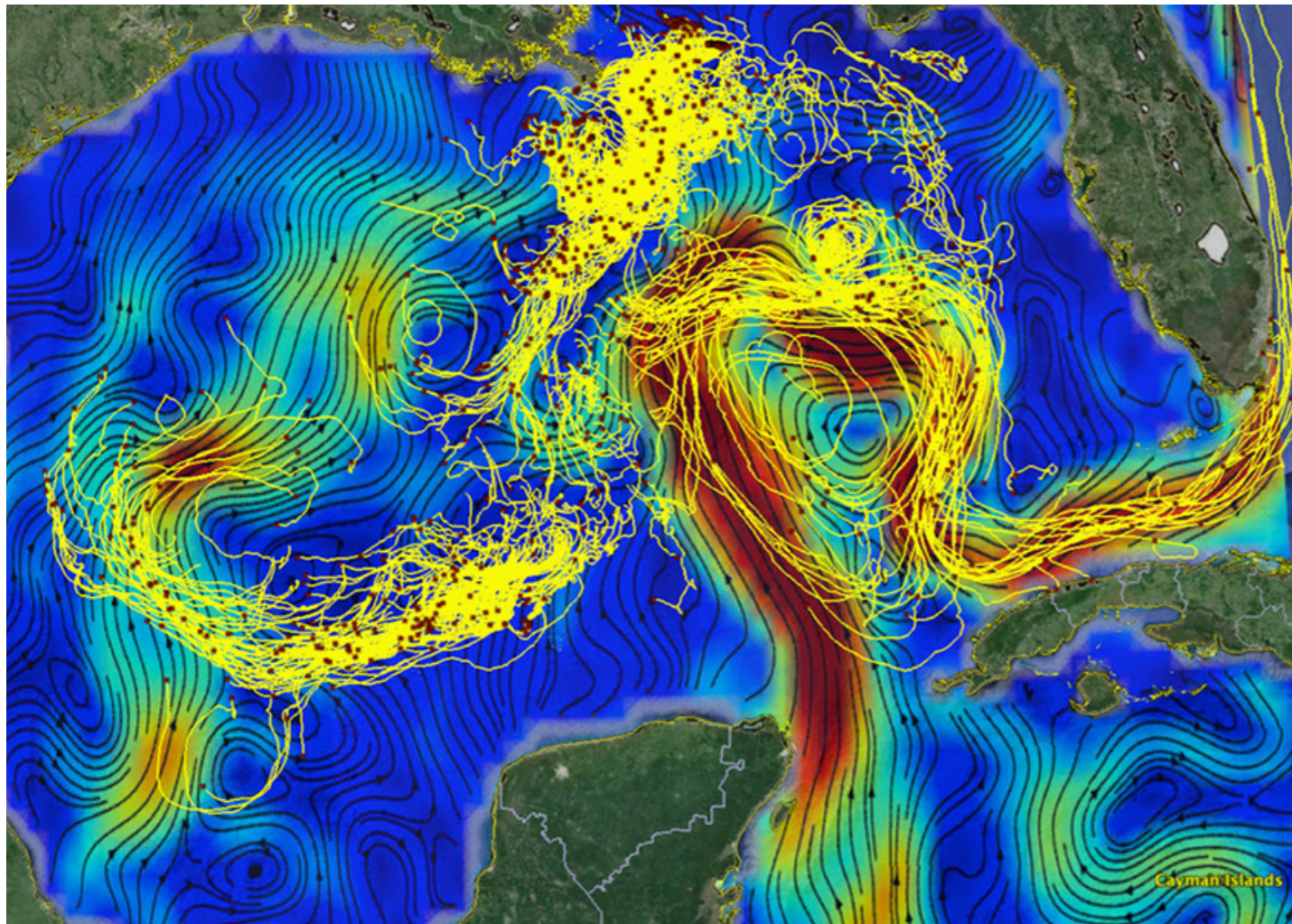
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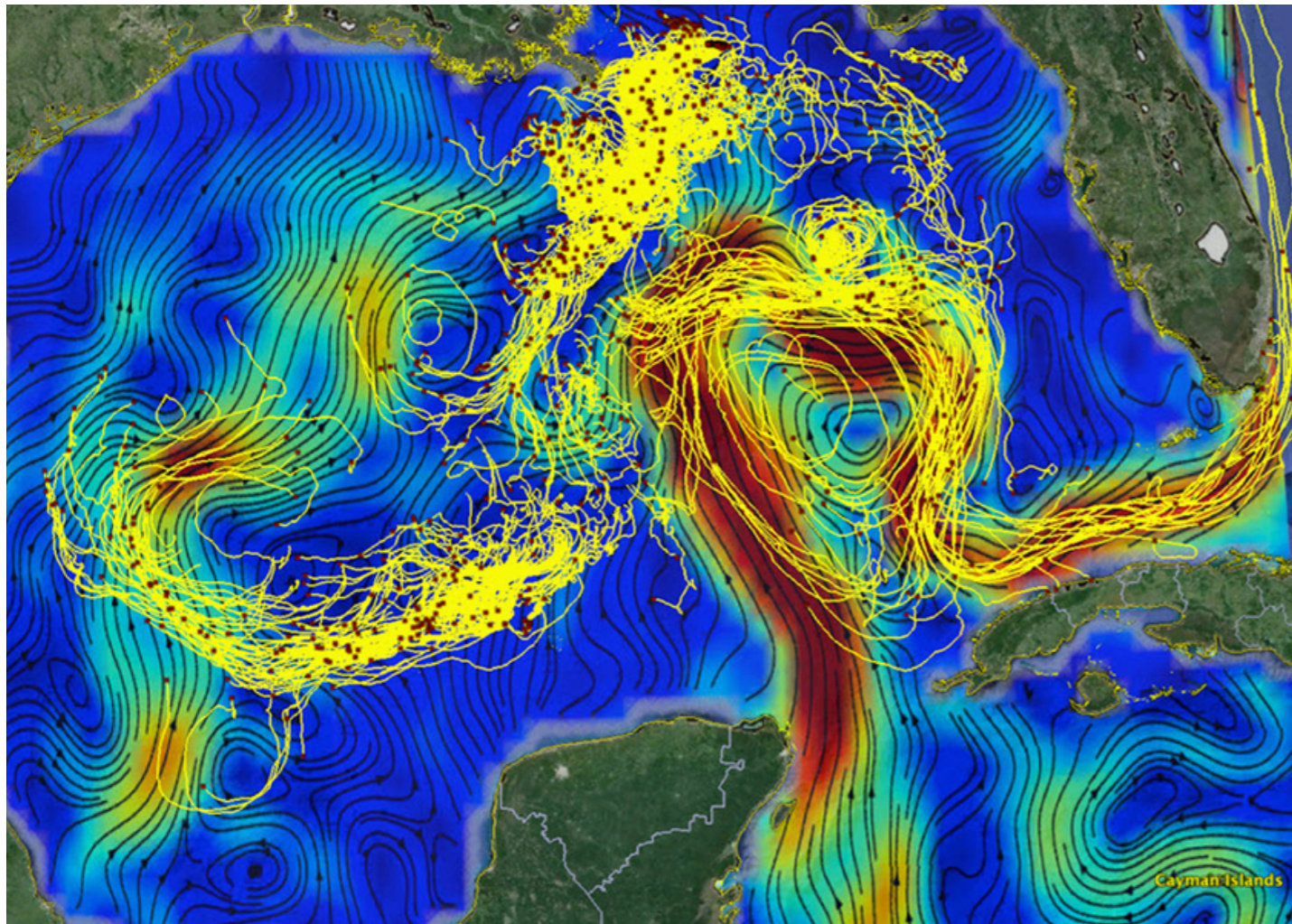
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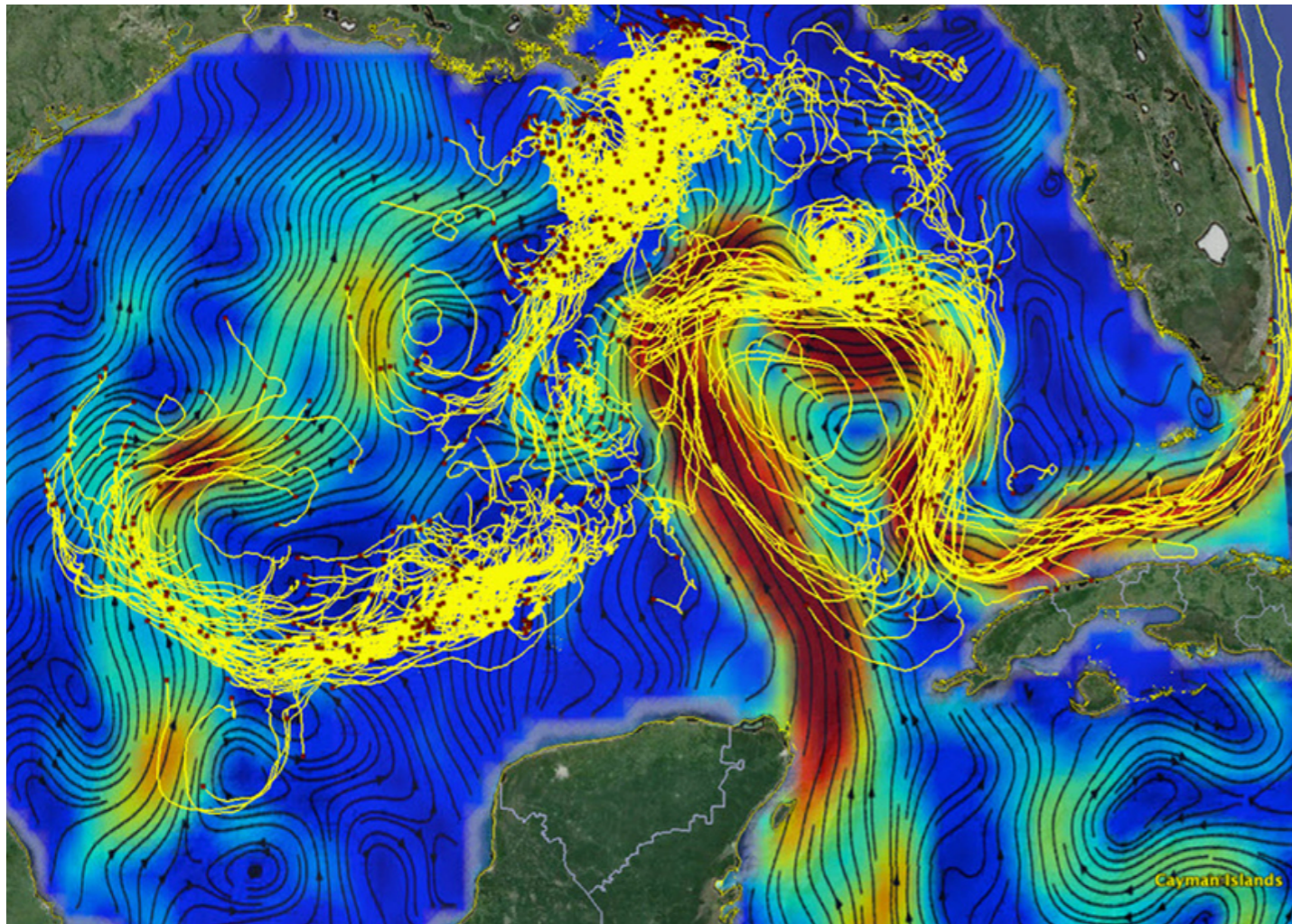
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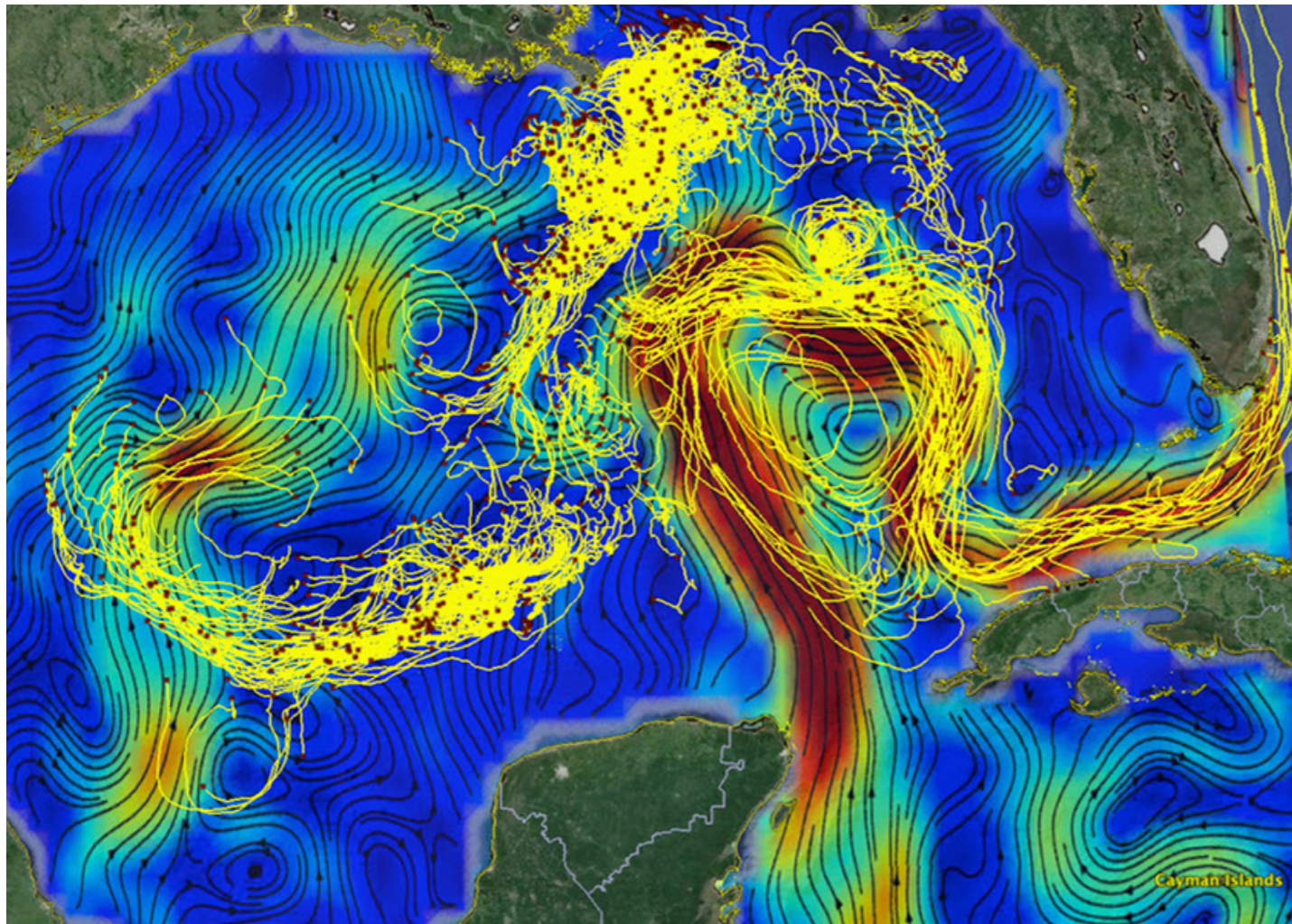
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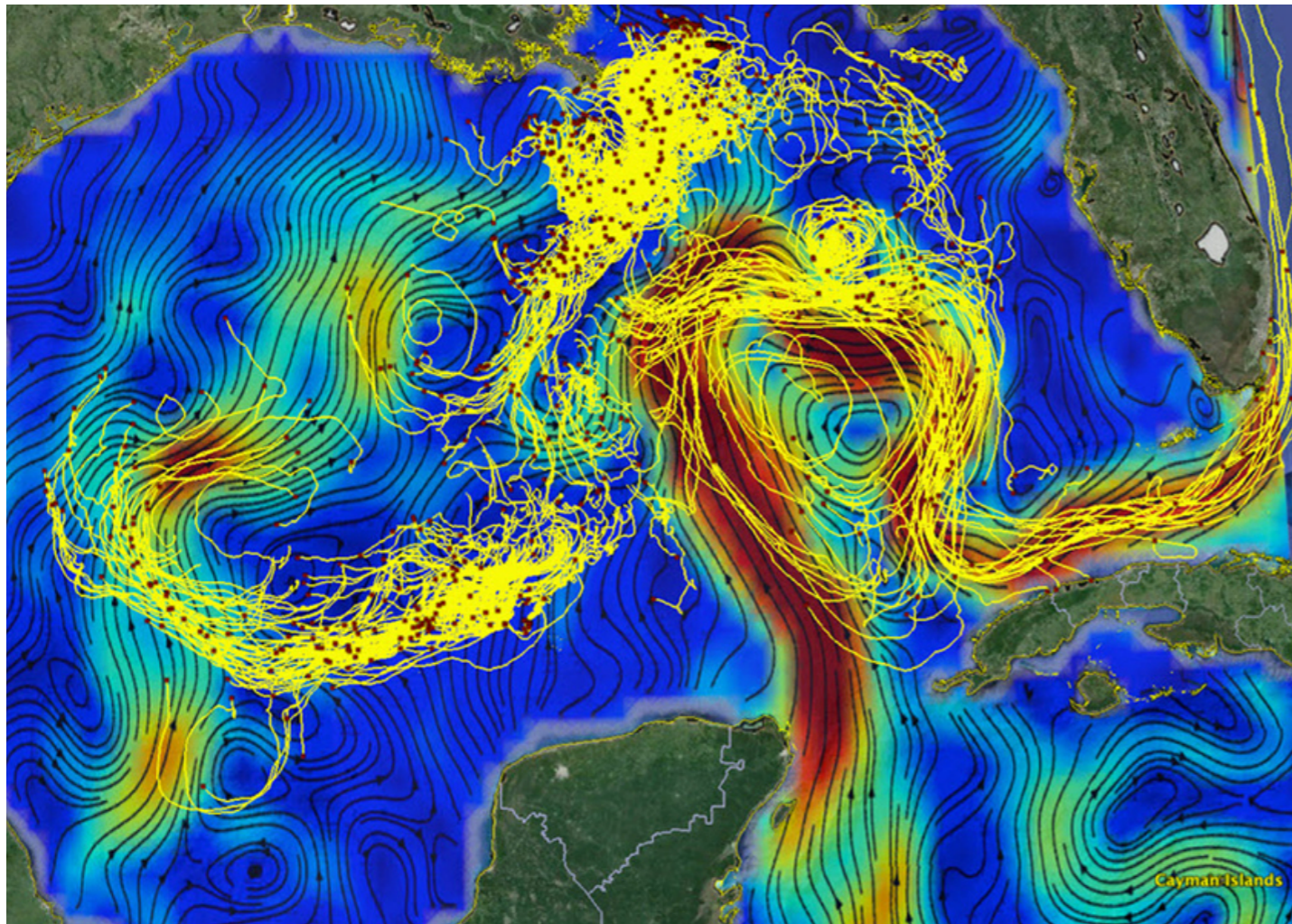
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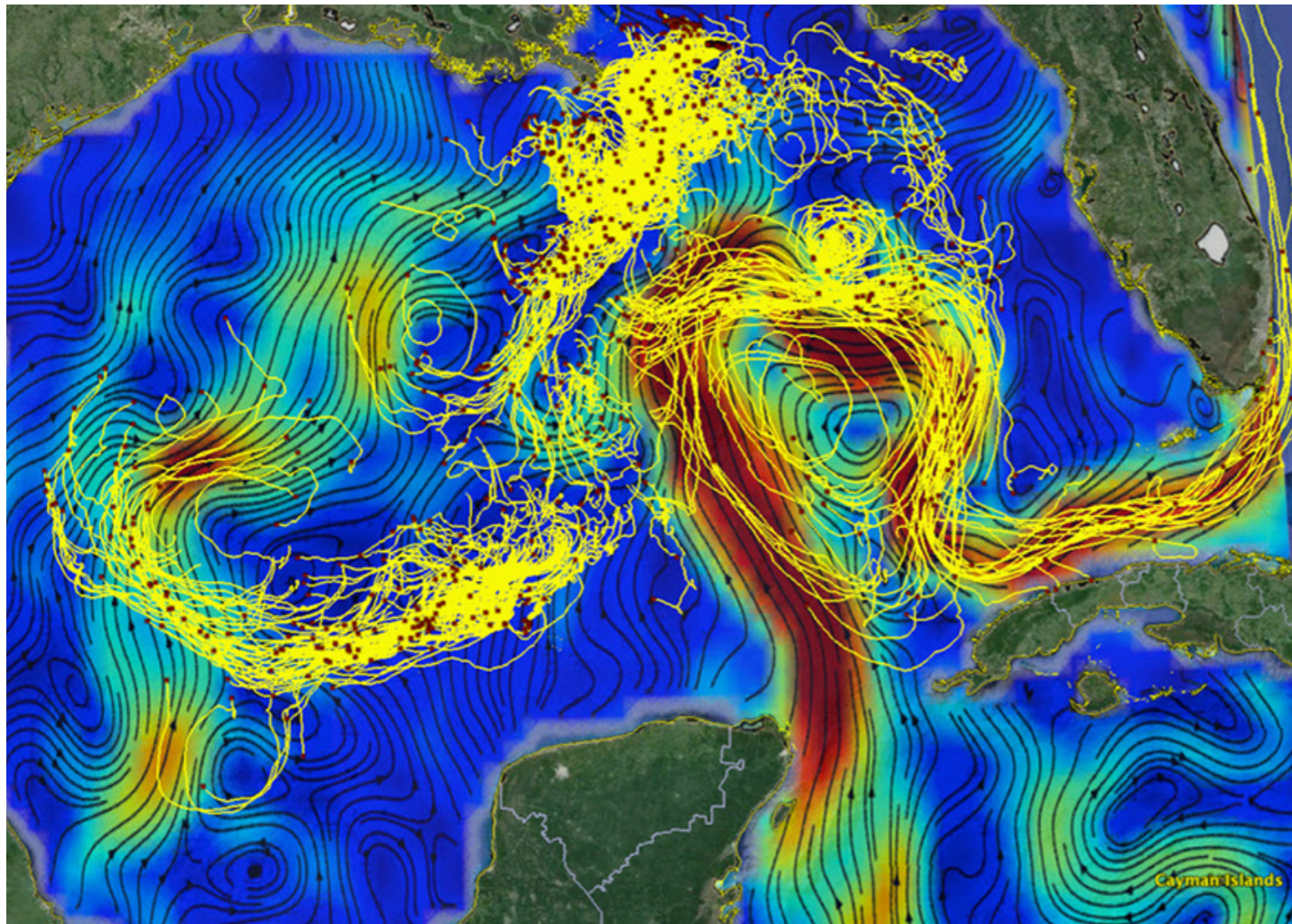
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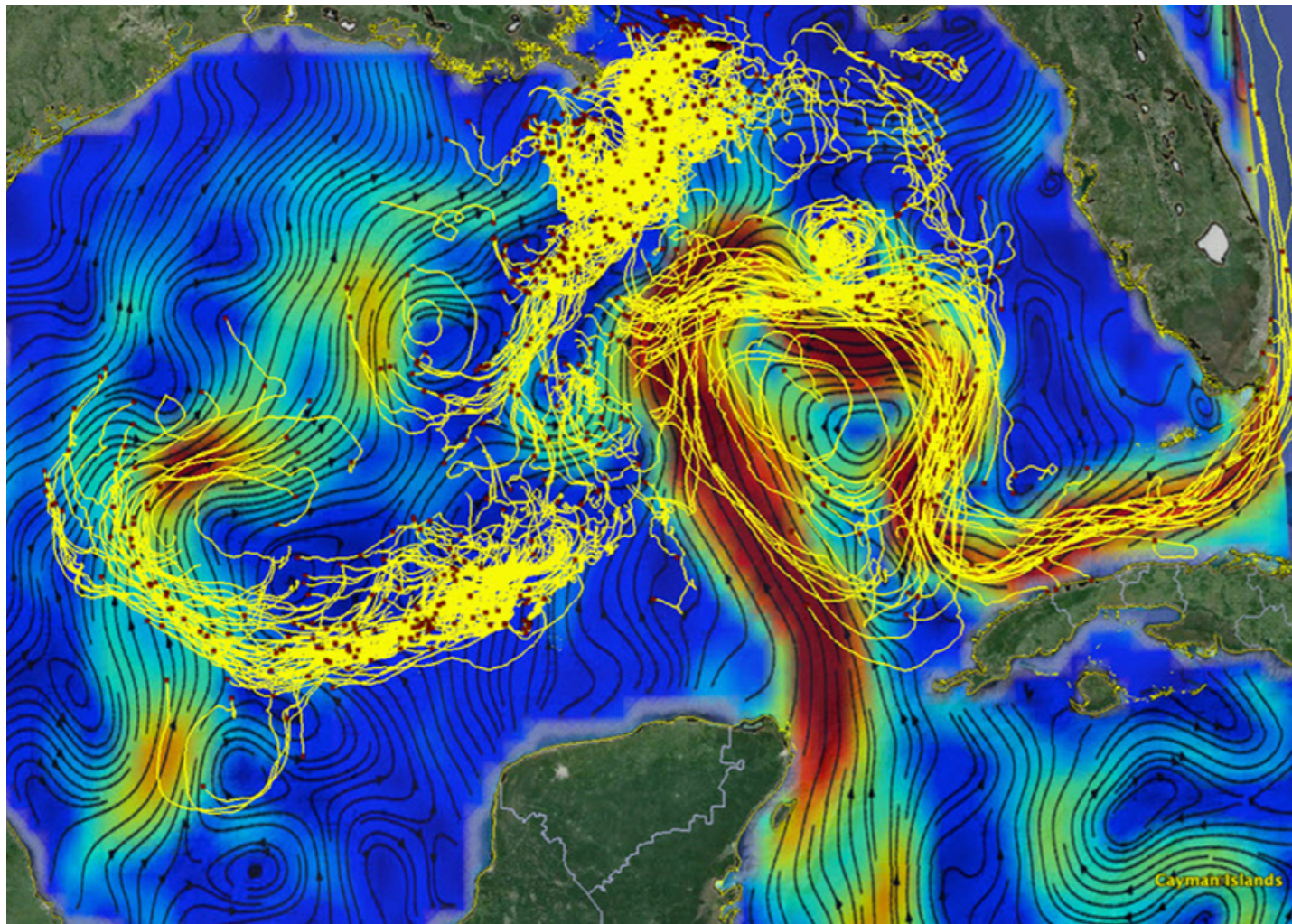
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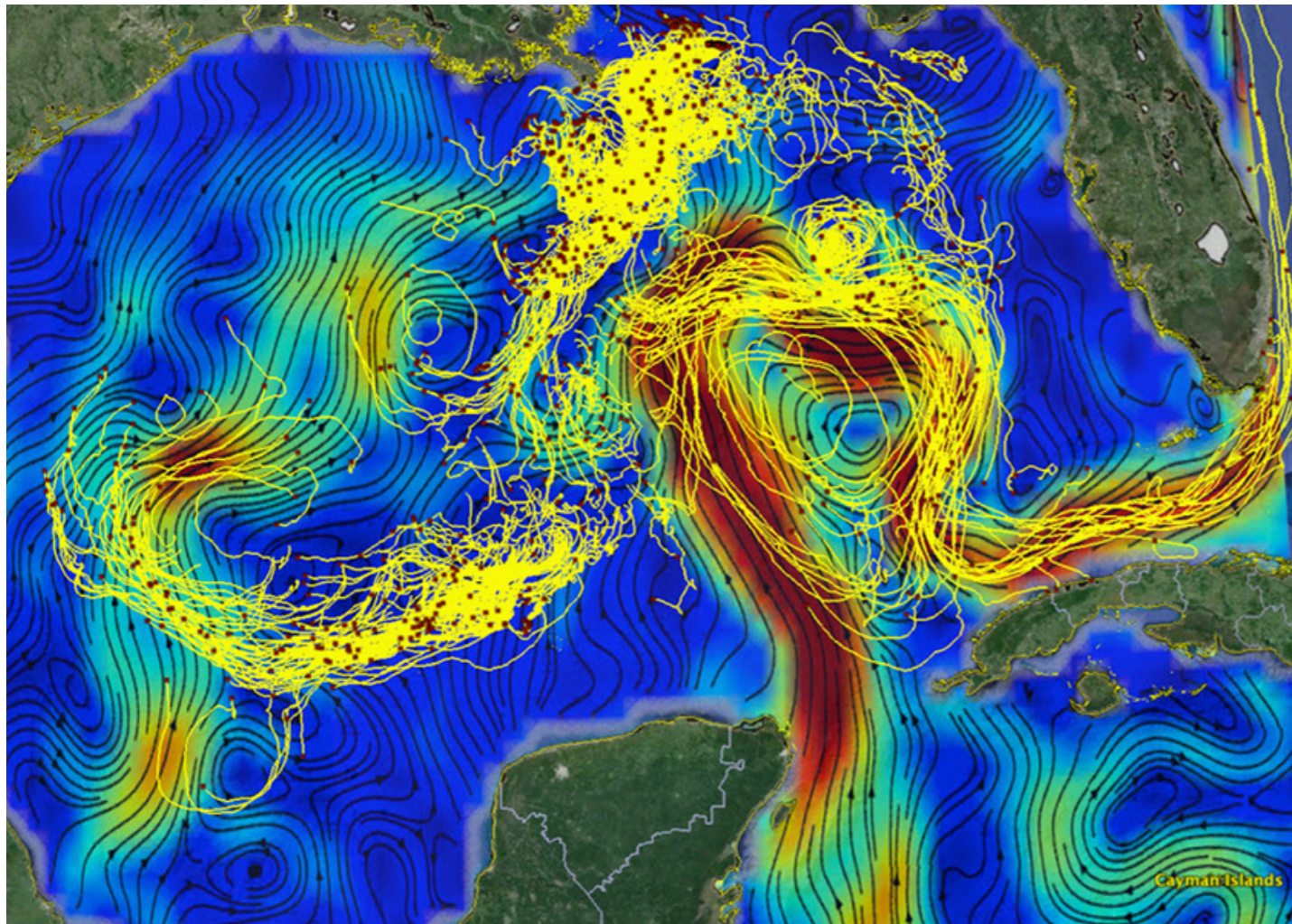
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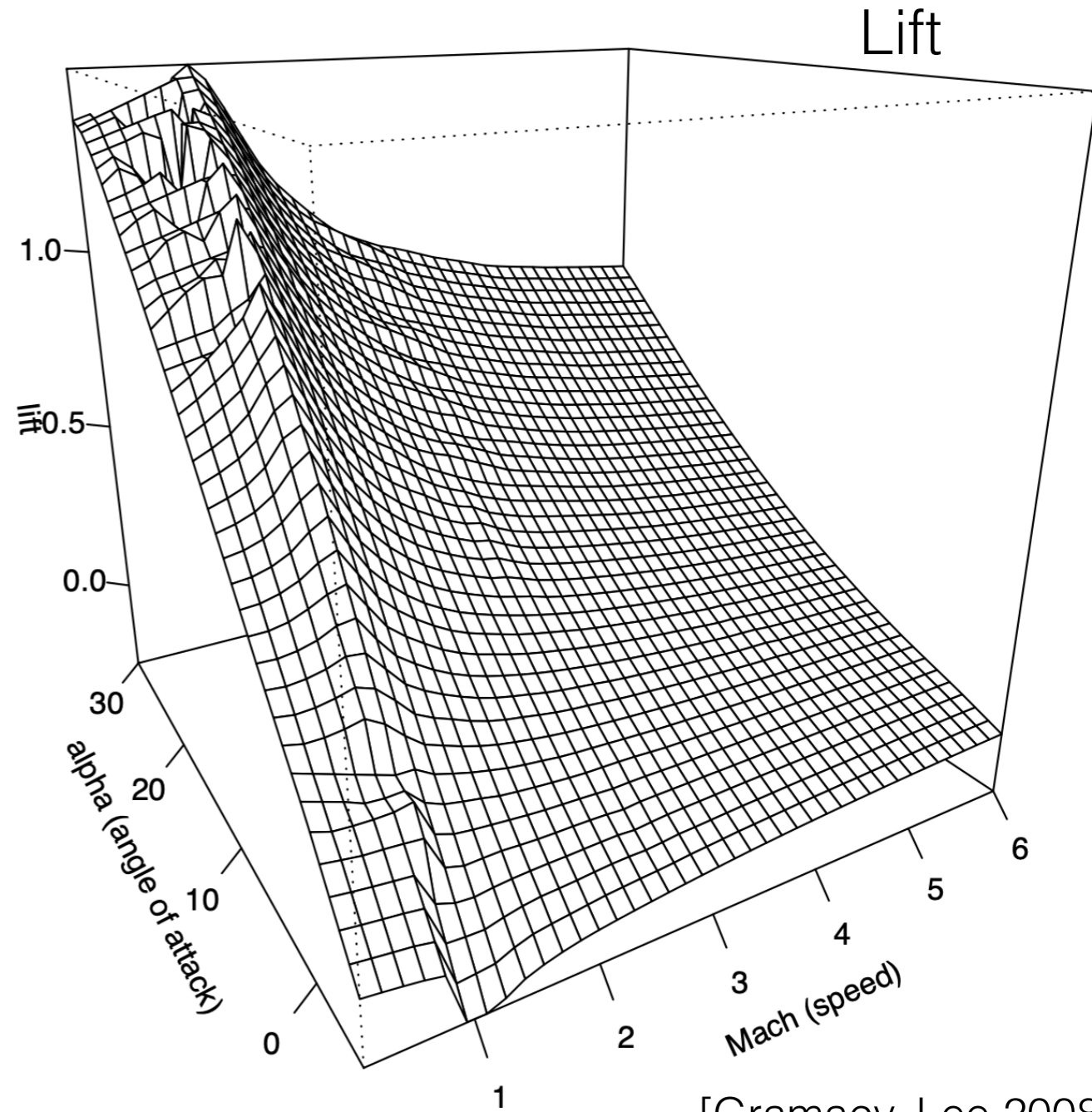
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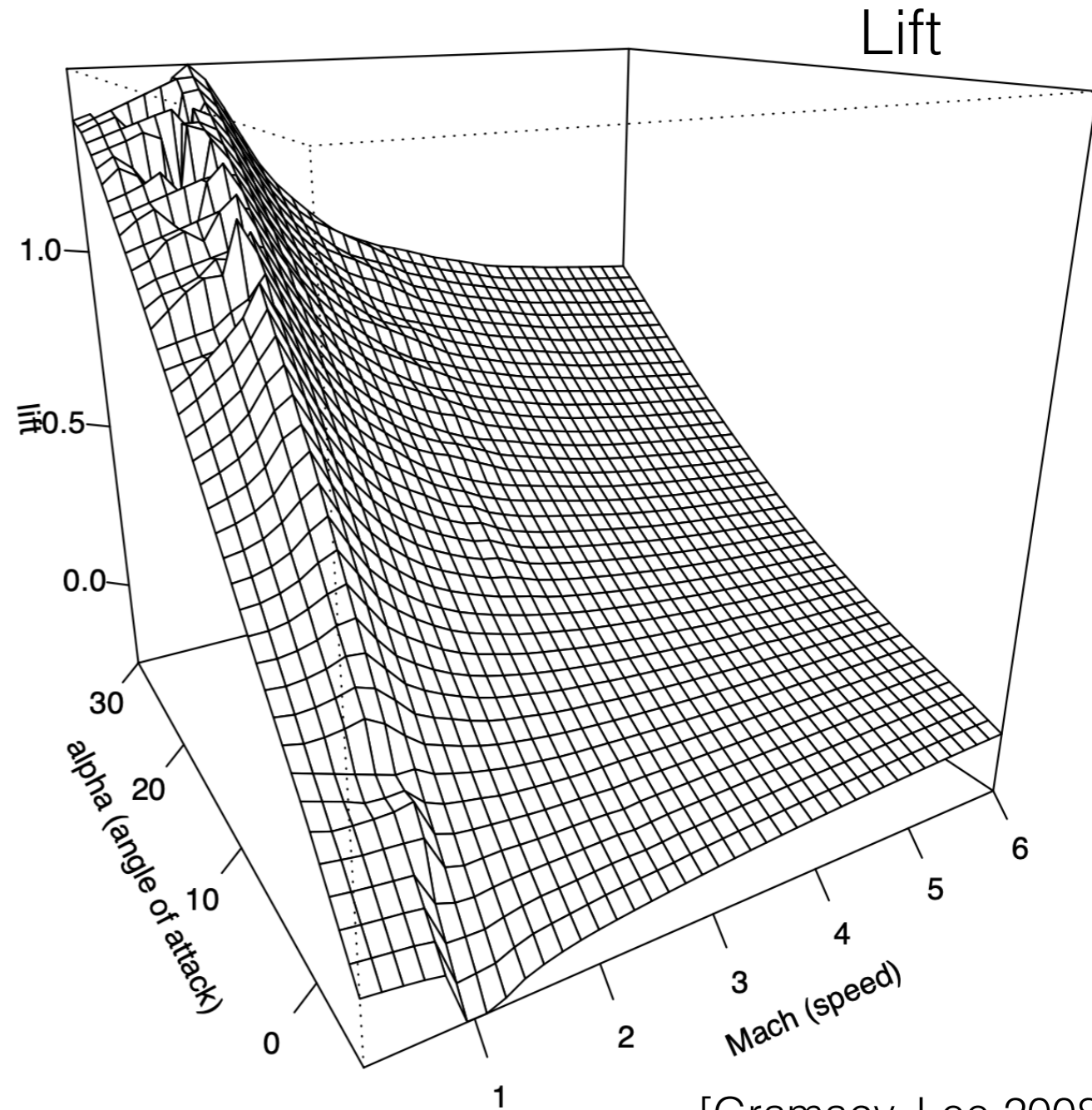
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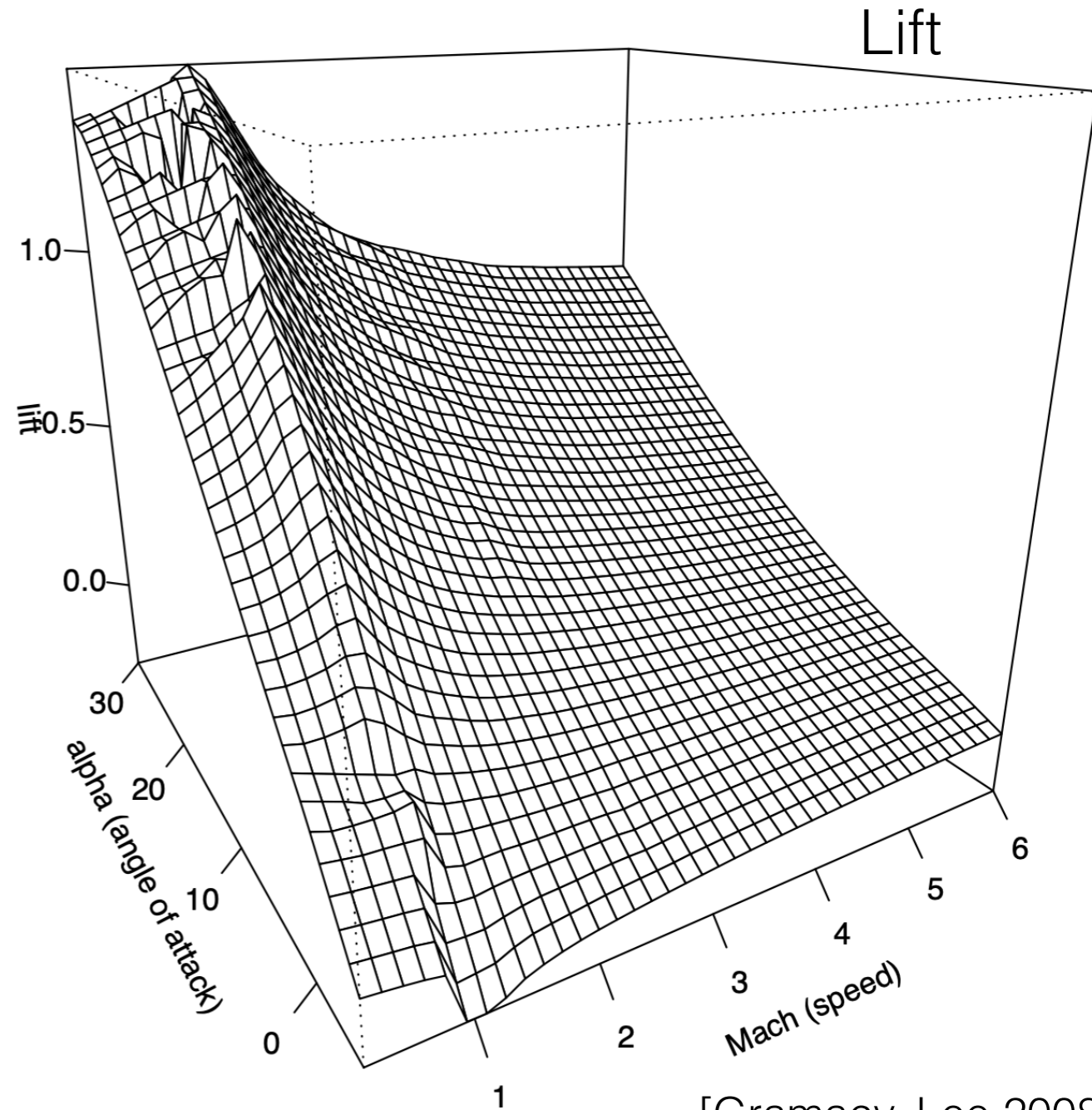
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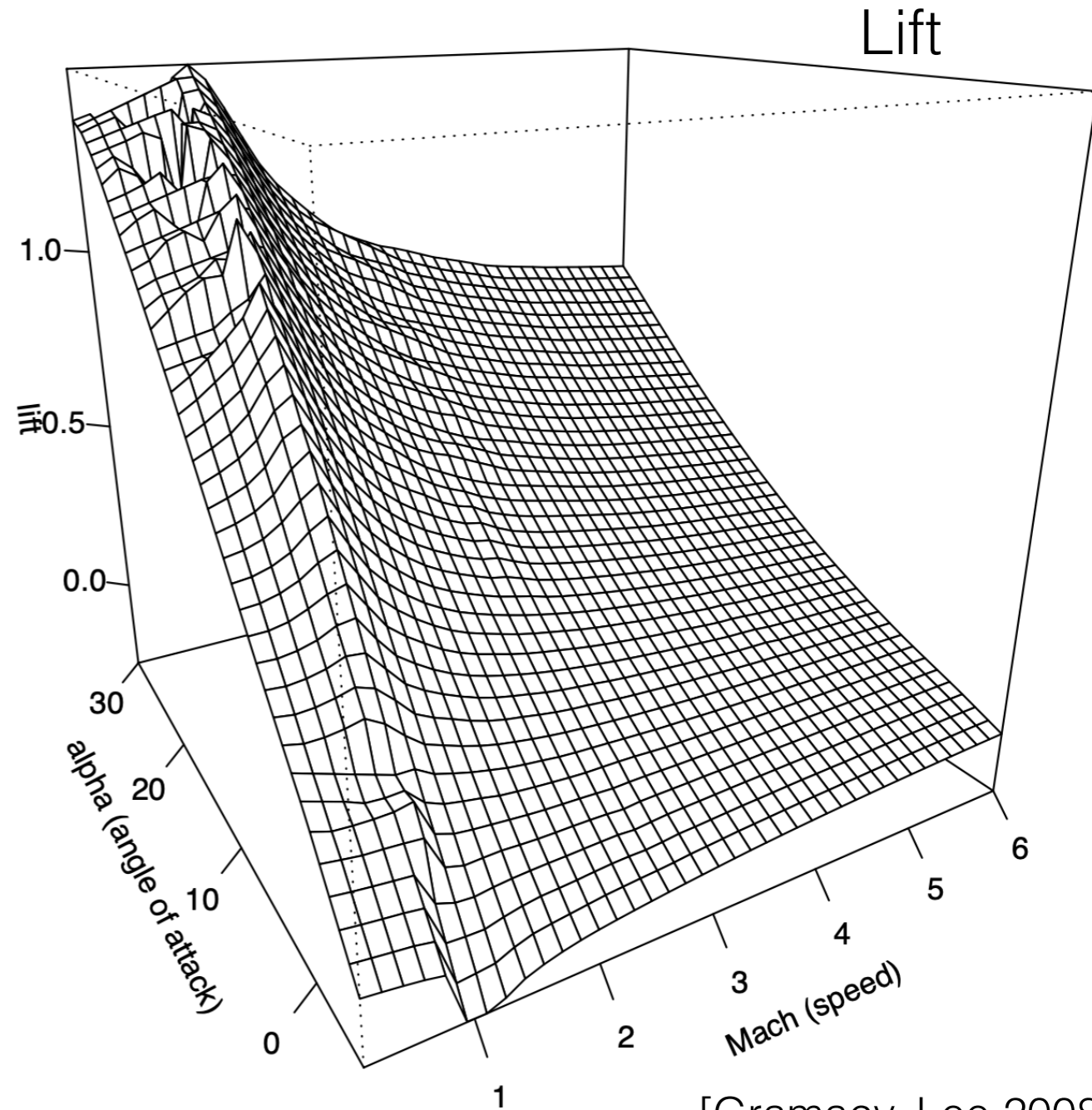
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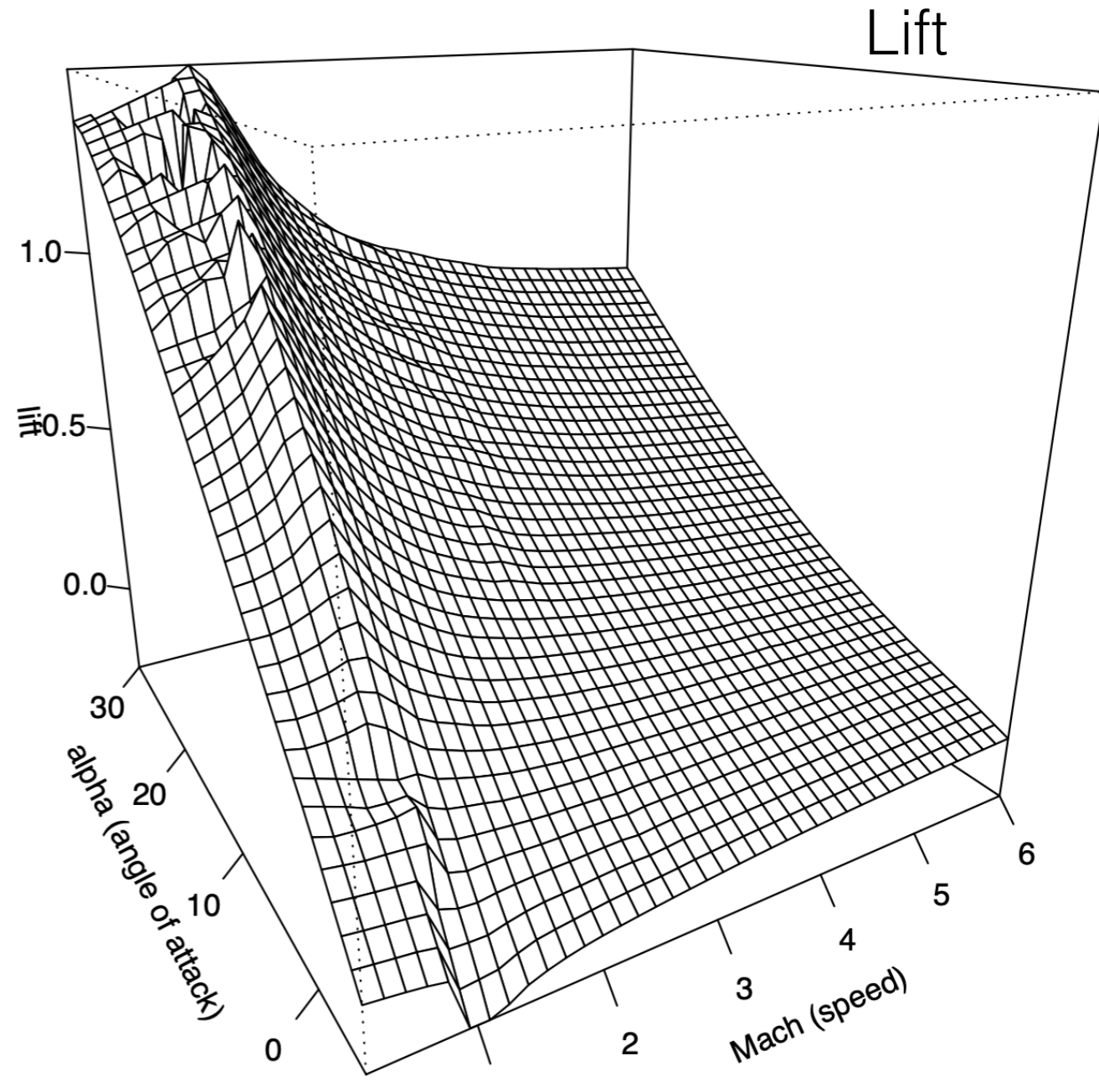
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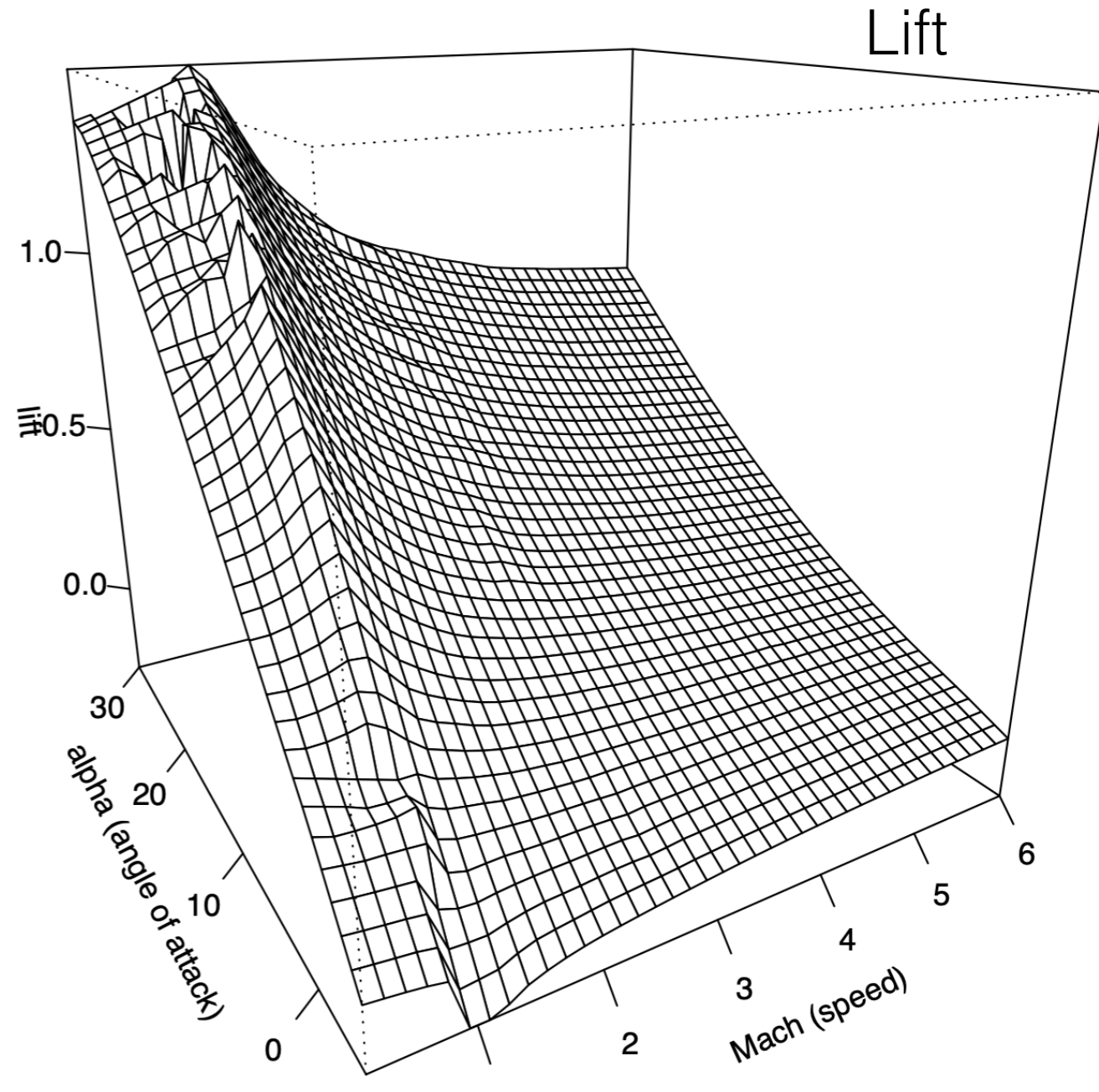
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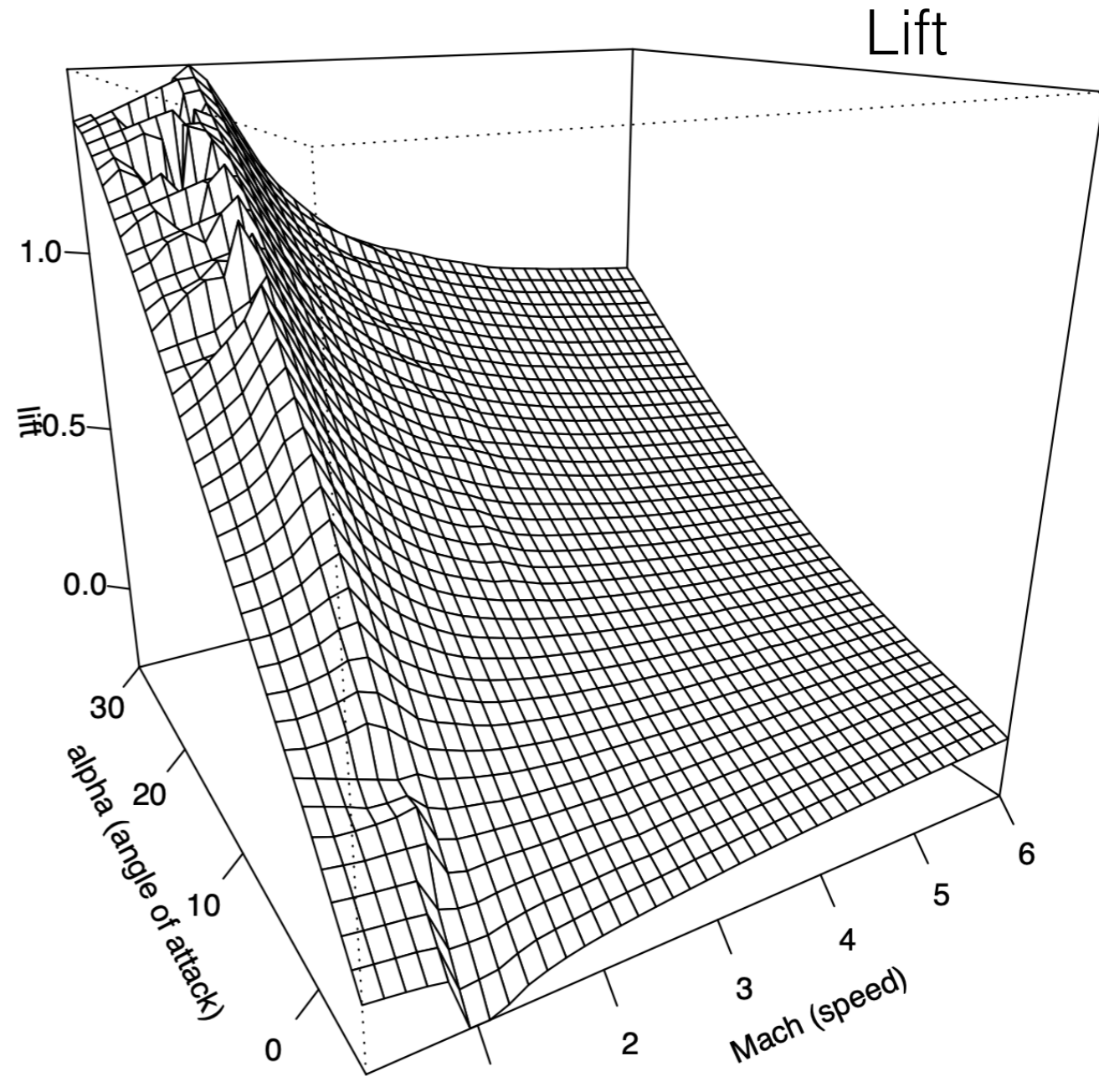
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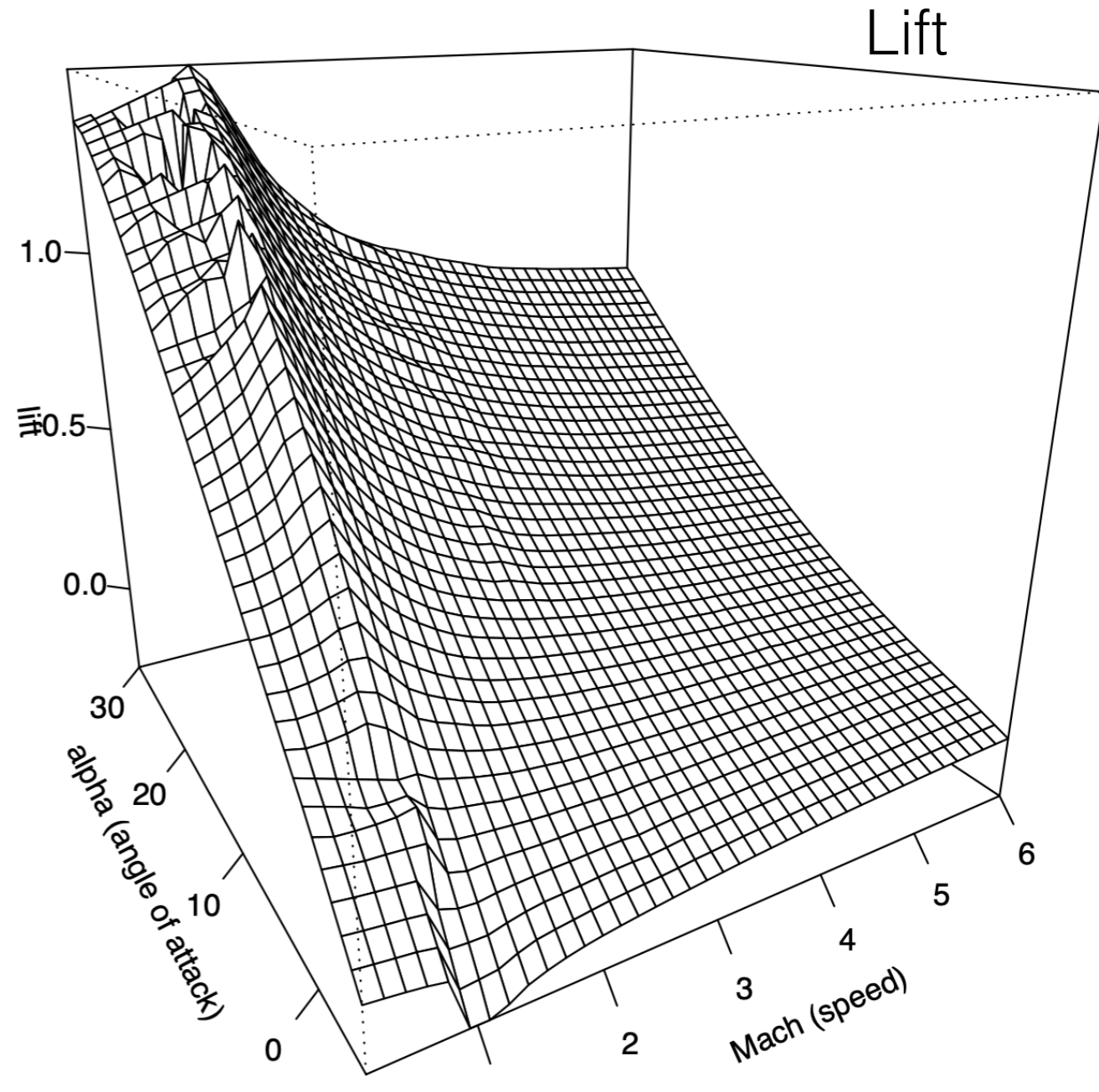
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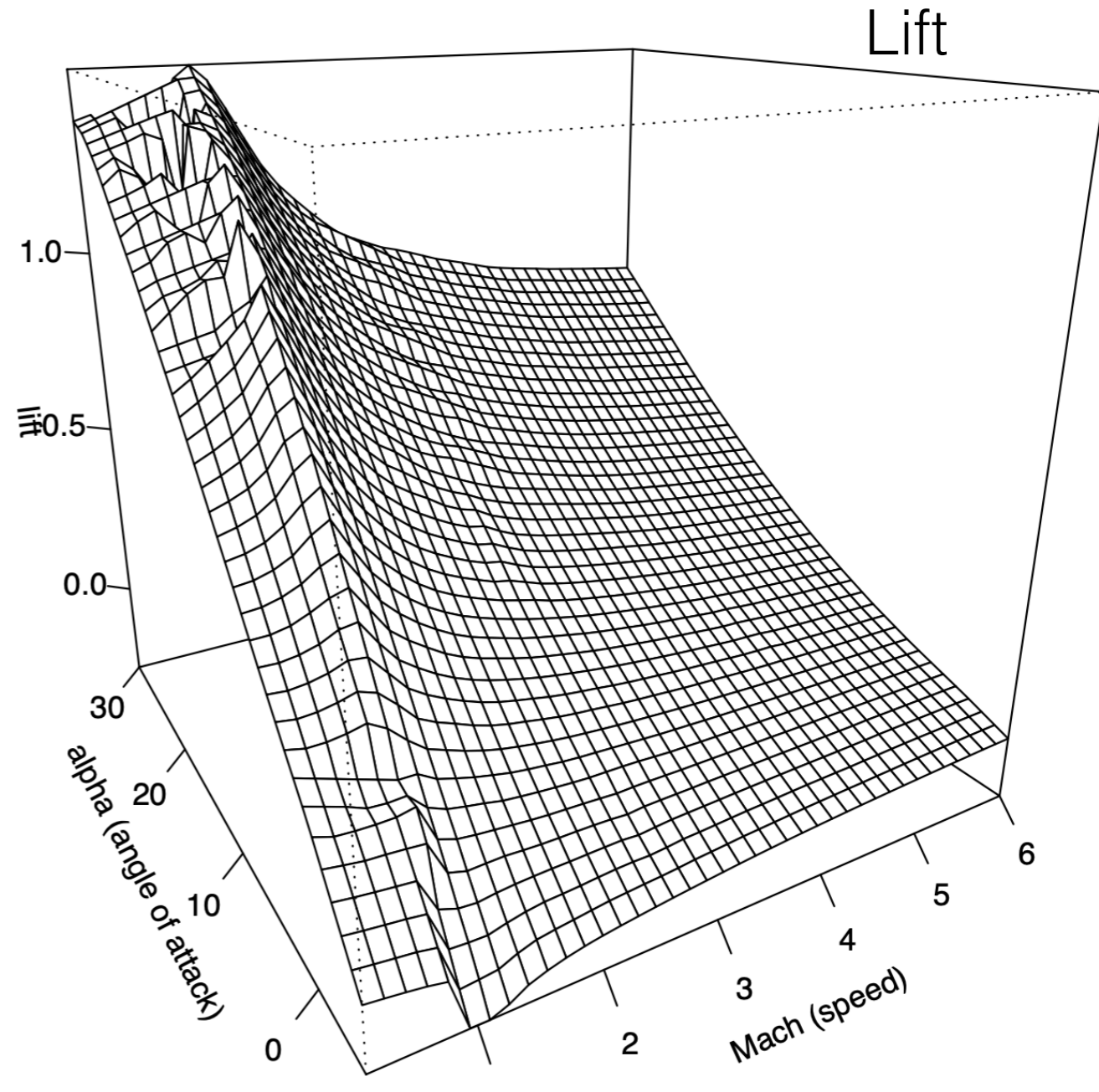
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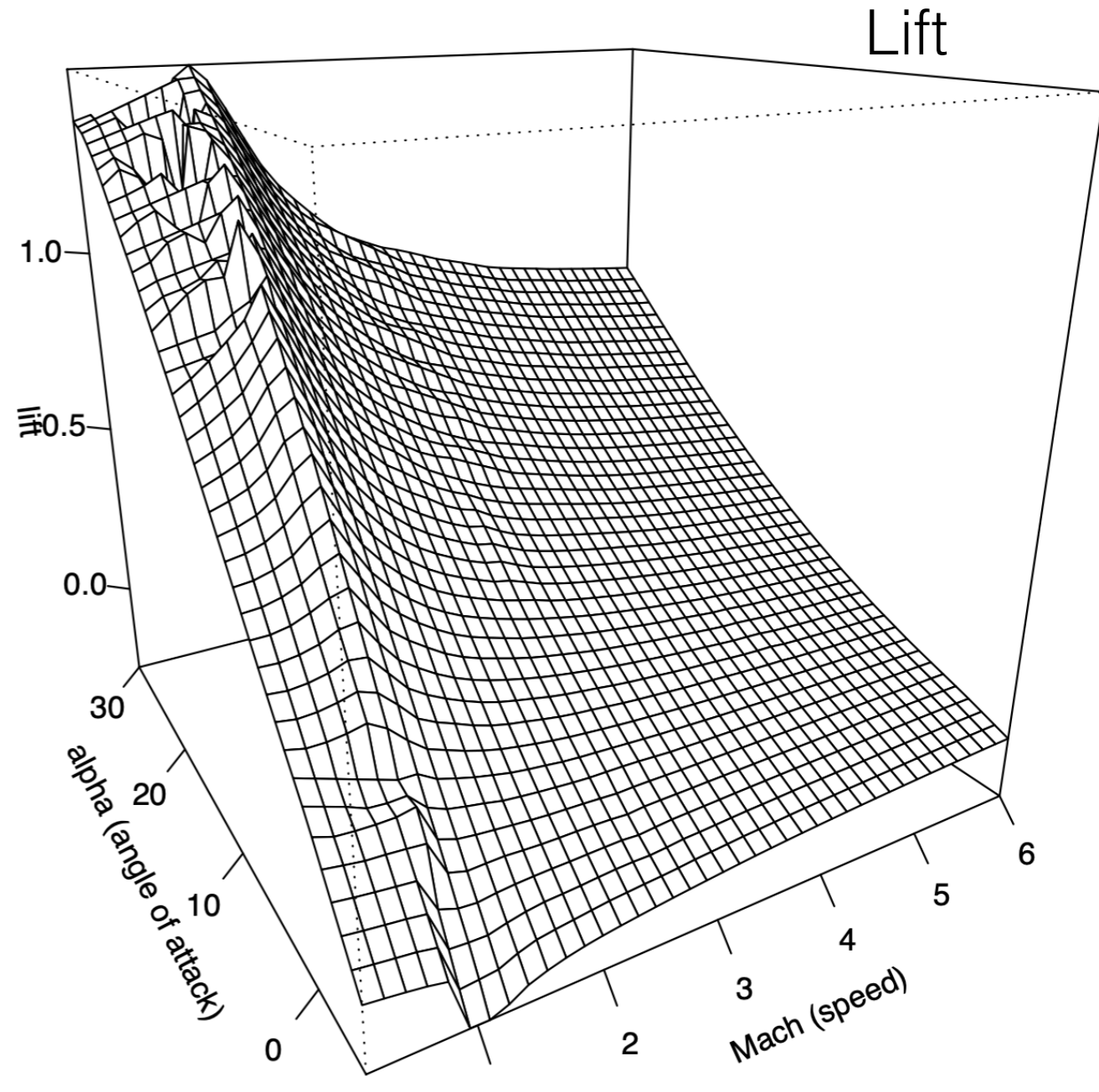
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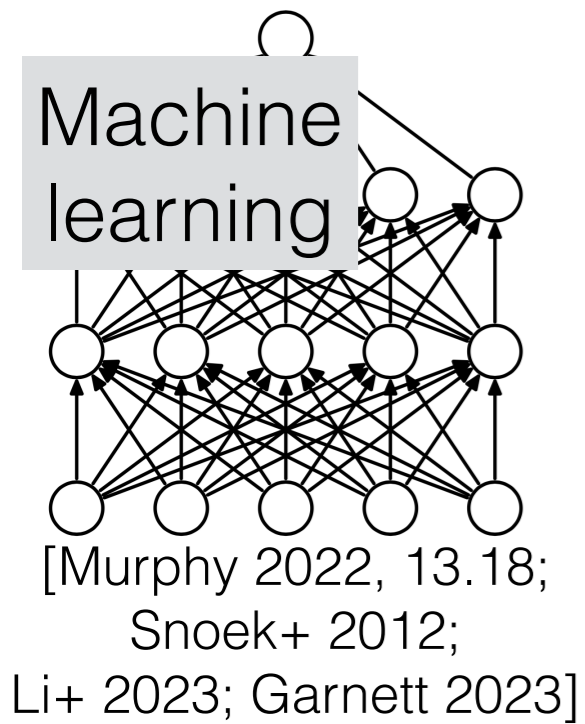
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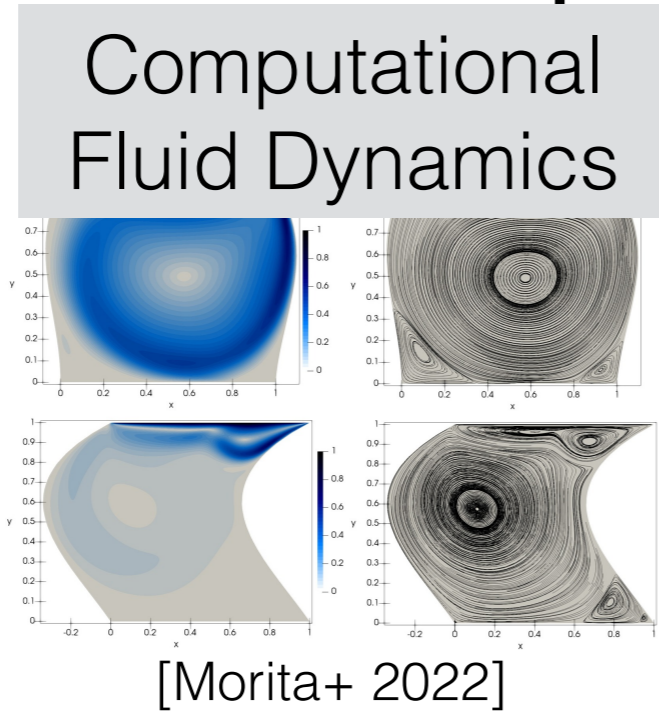
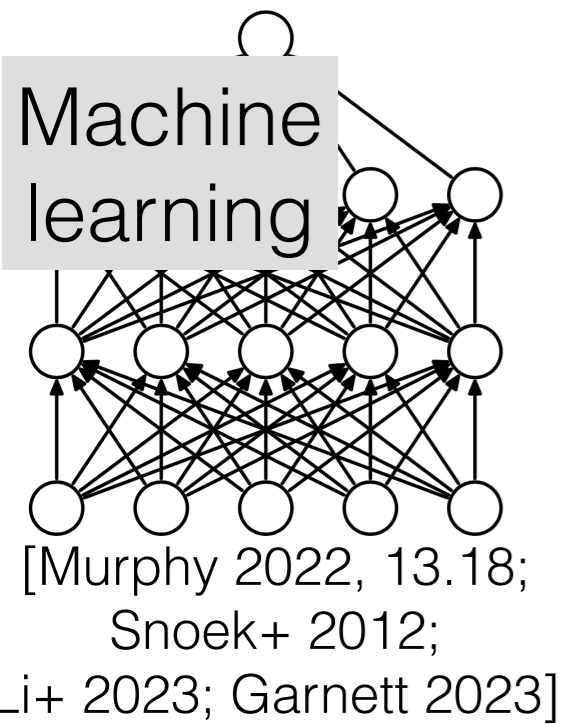
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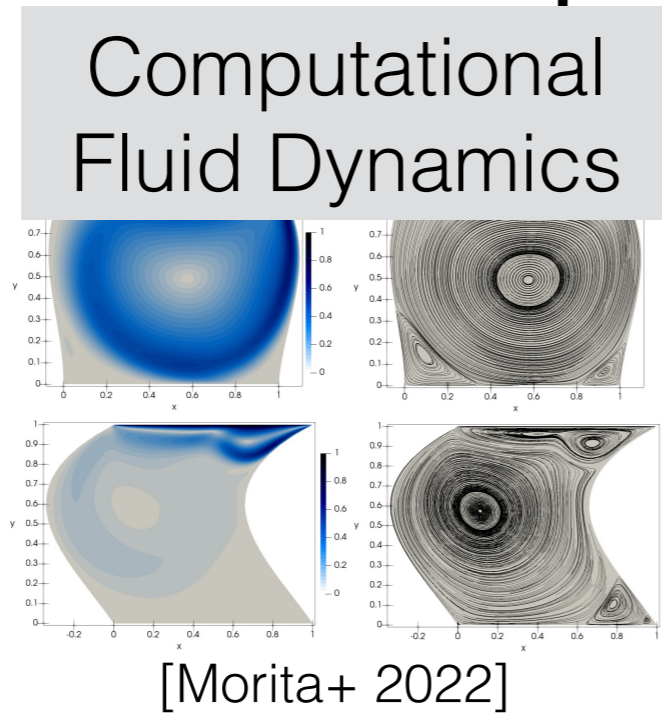
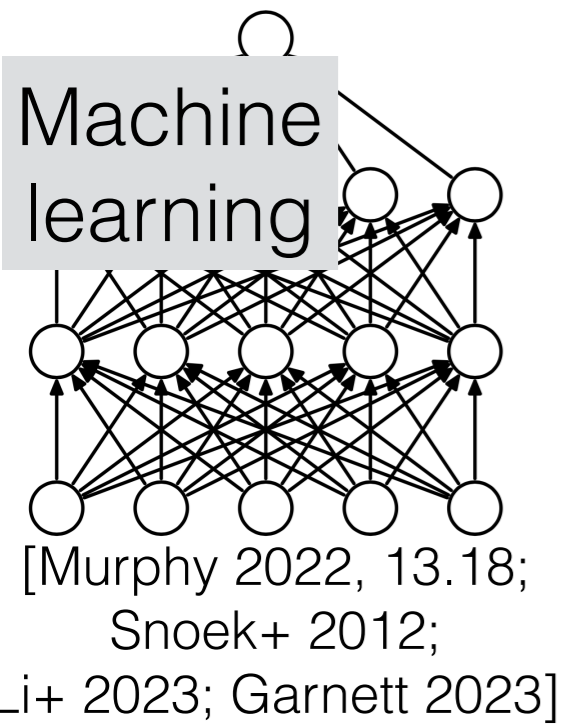
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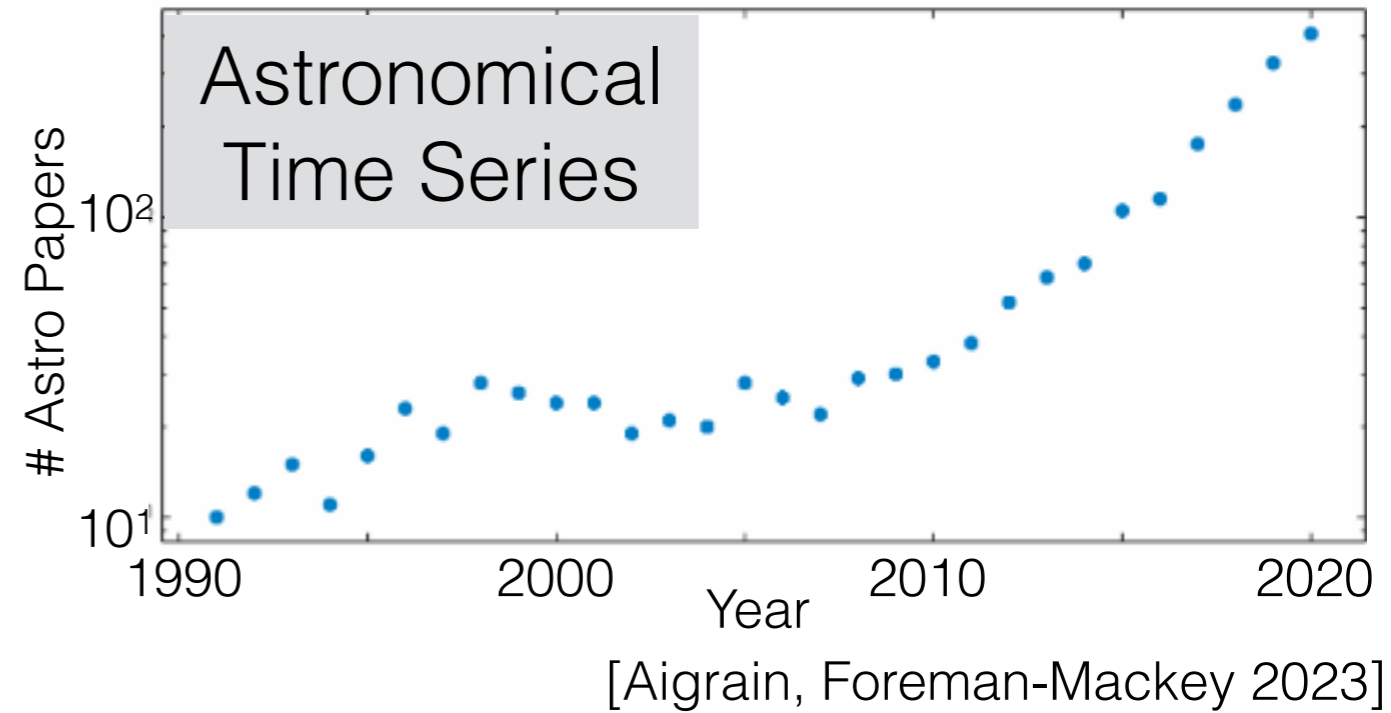
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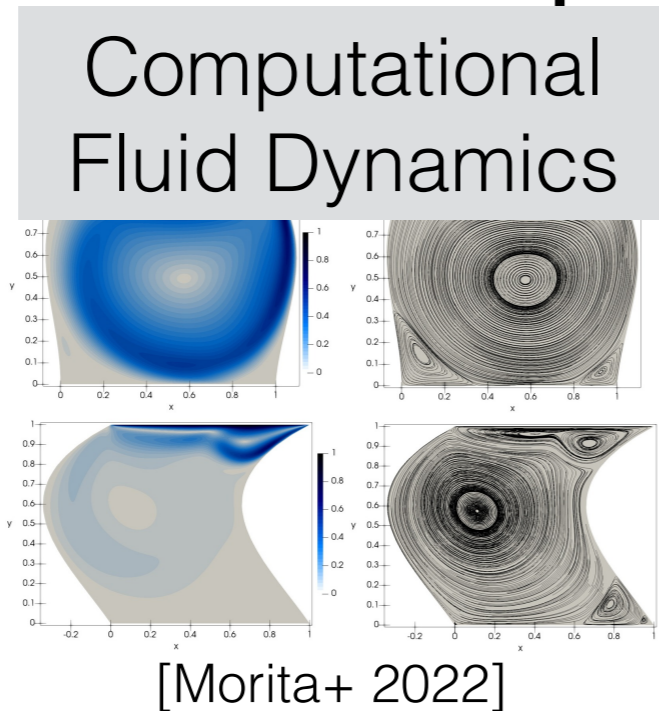
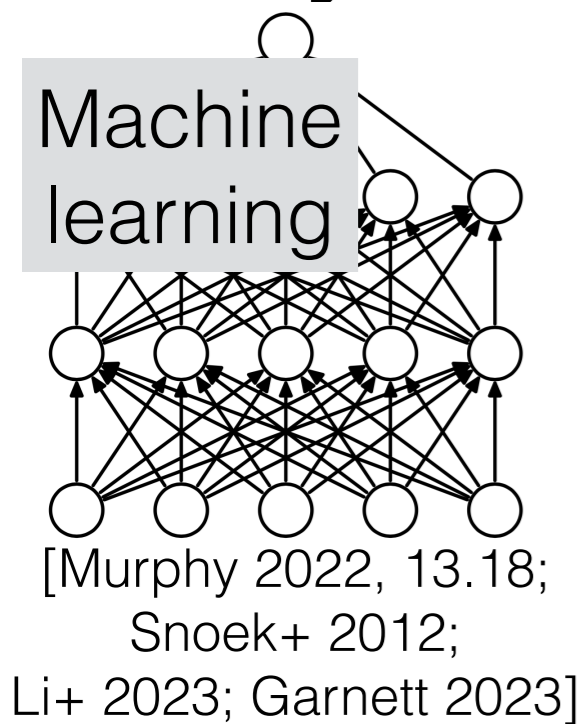
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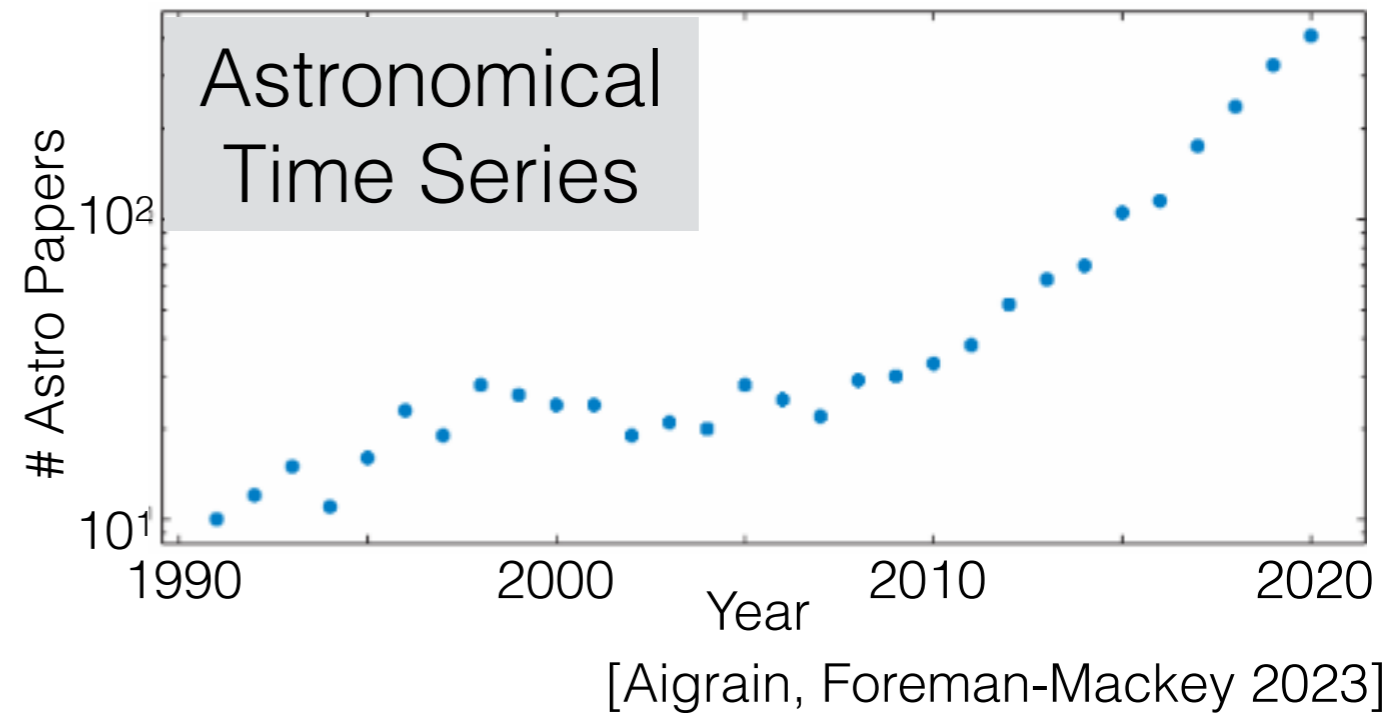
Astrophysics Data System search for “Gaussian process”



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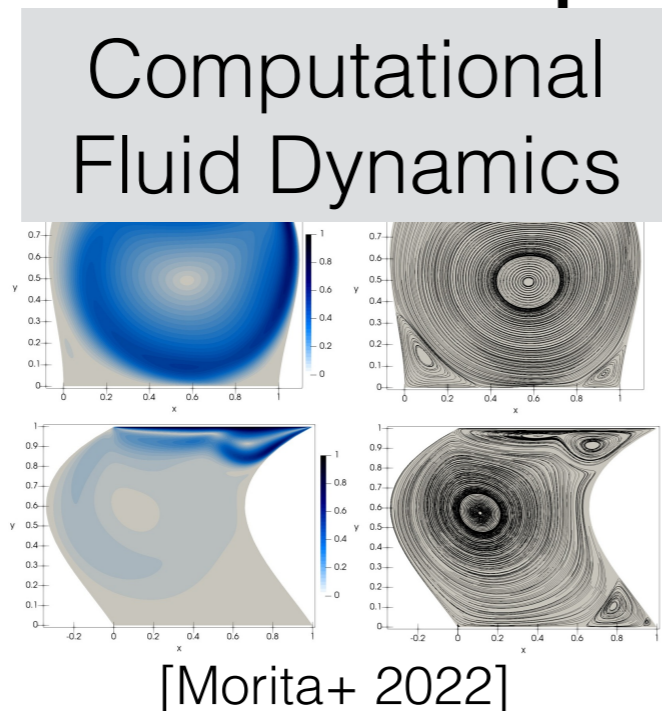
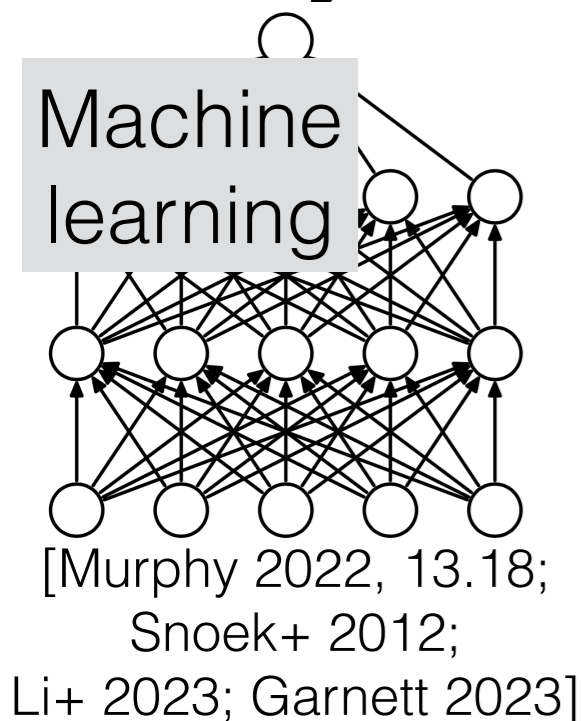


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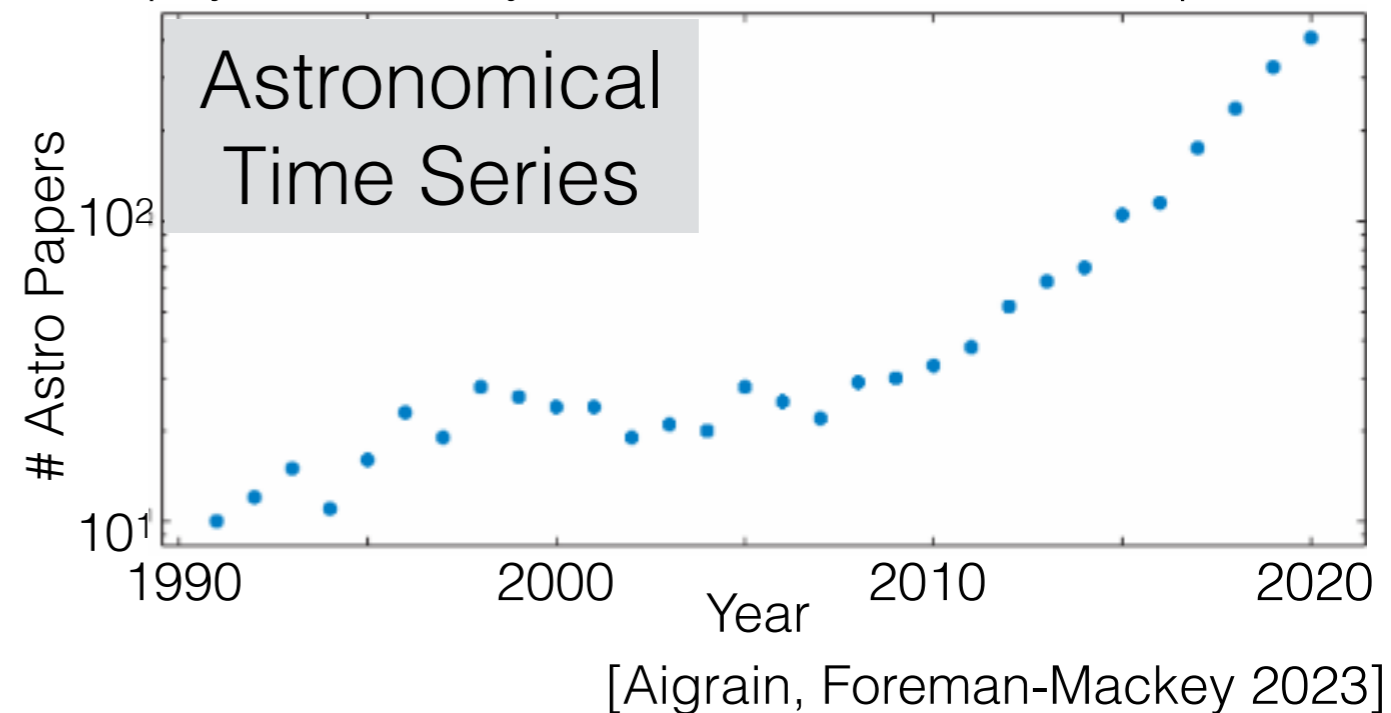


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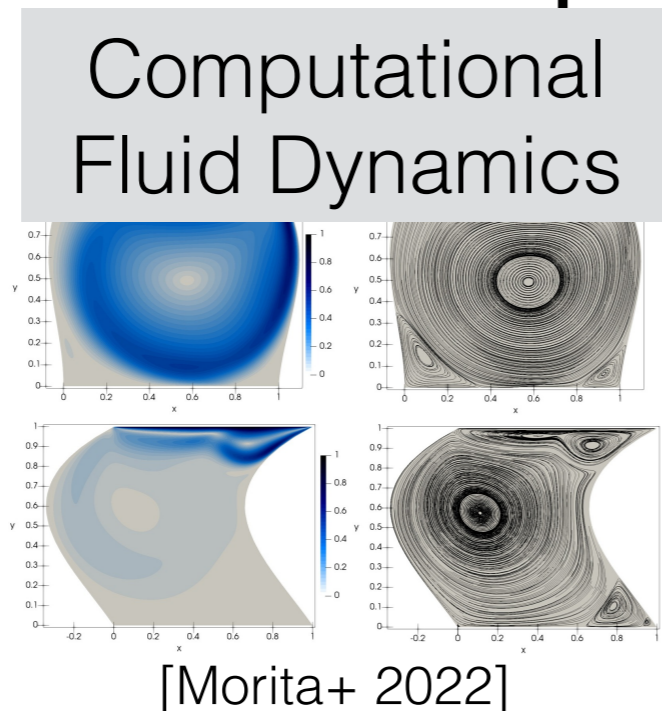
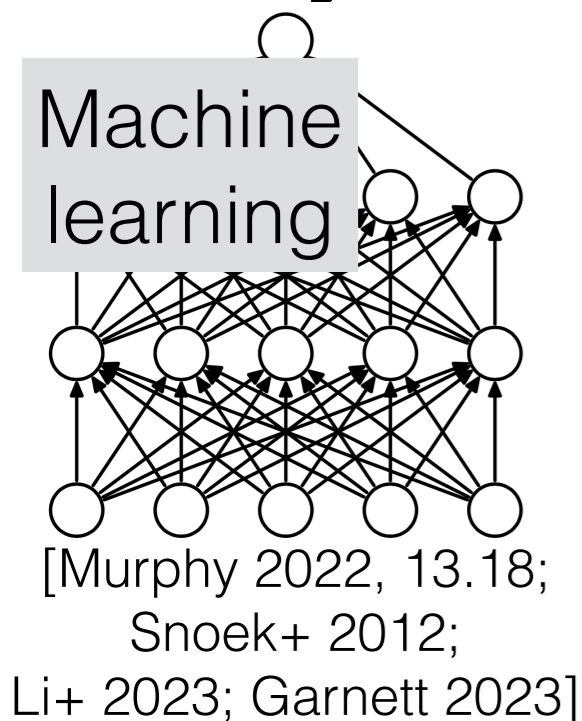
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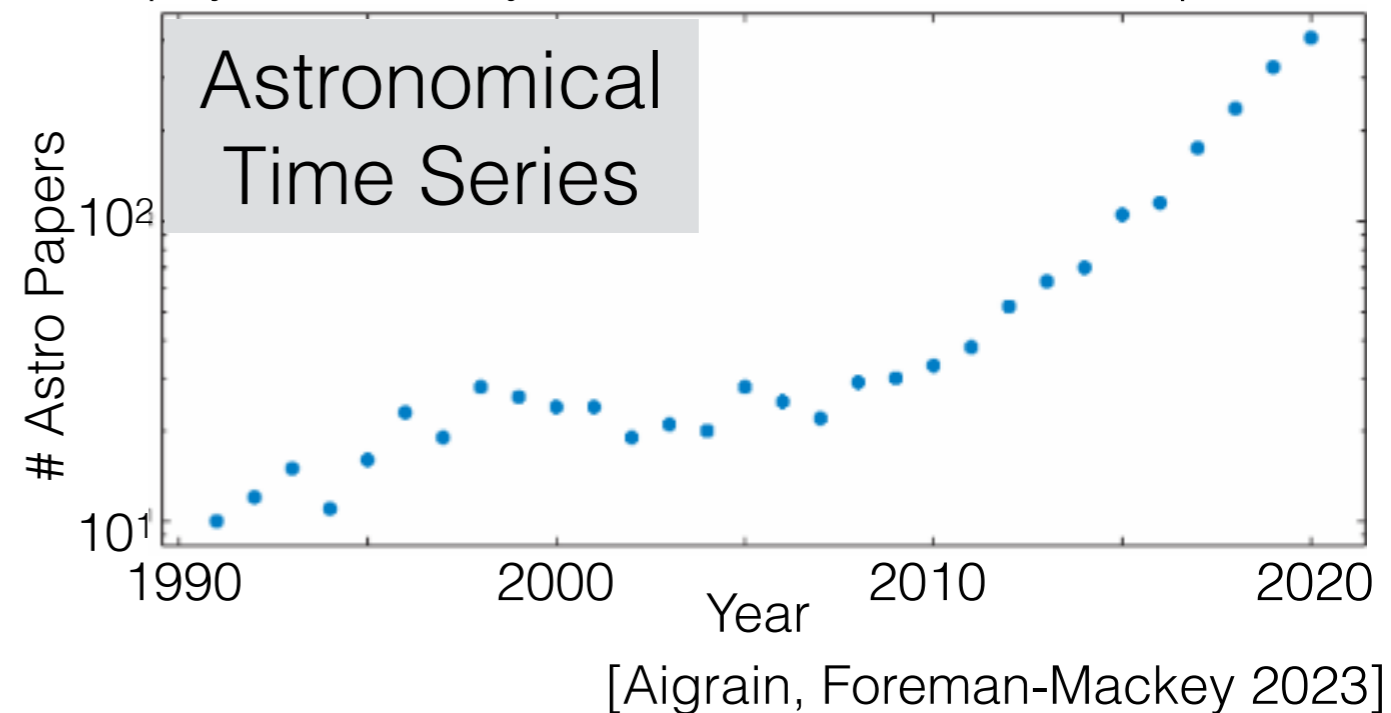
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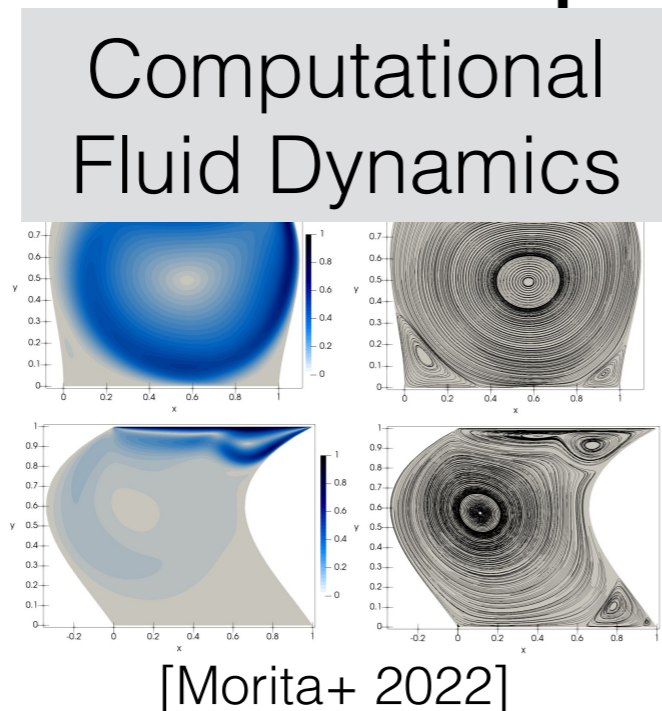
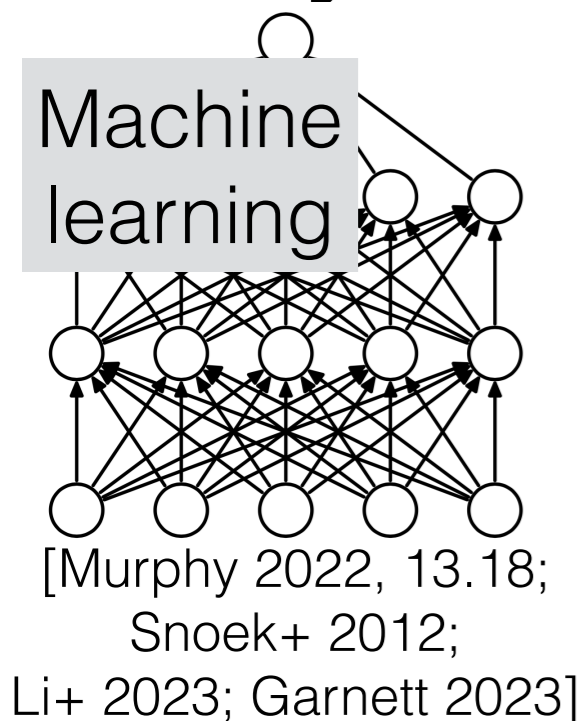
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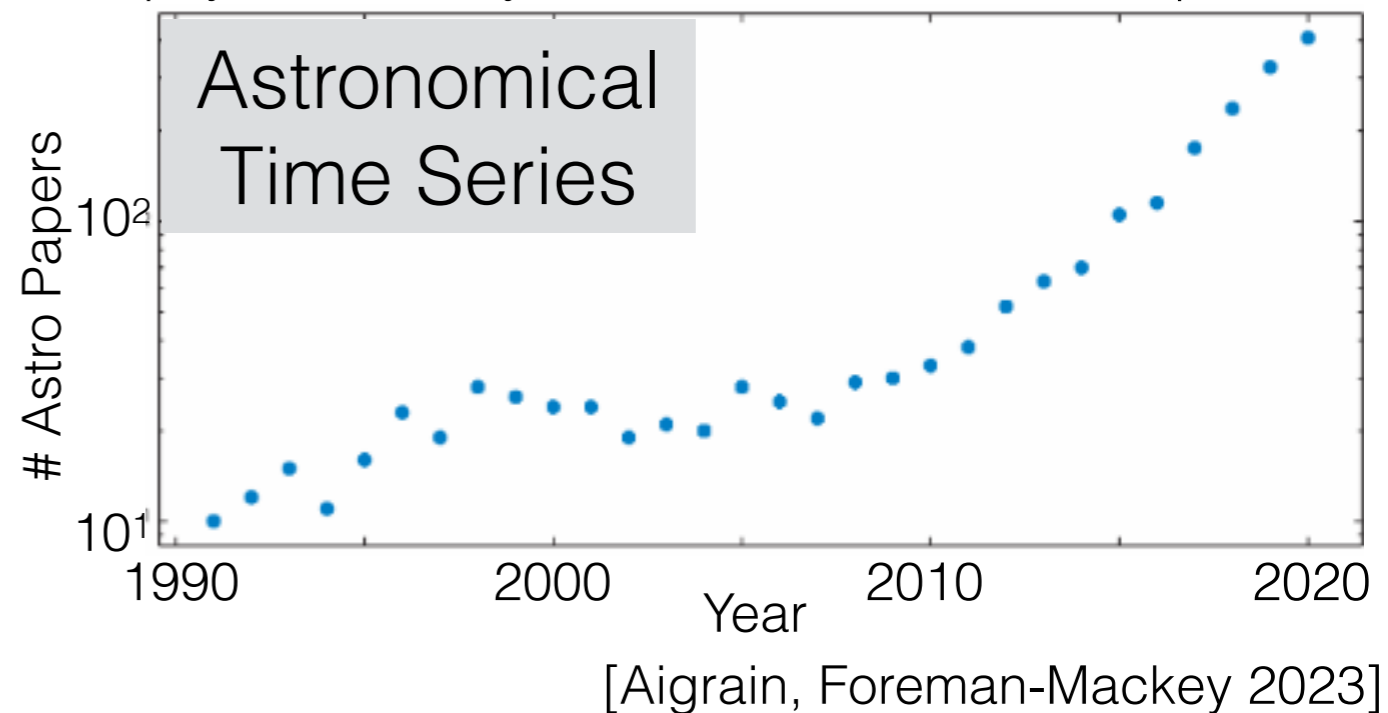
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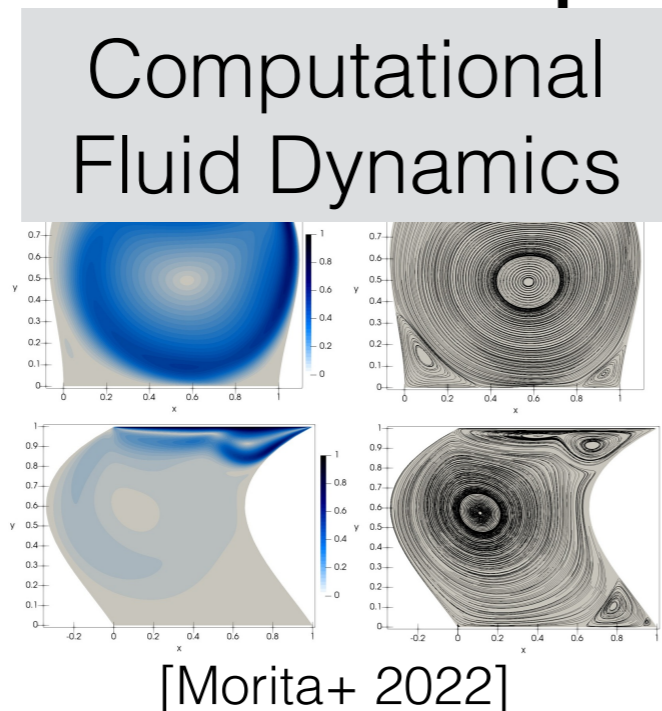
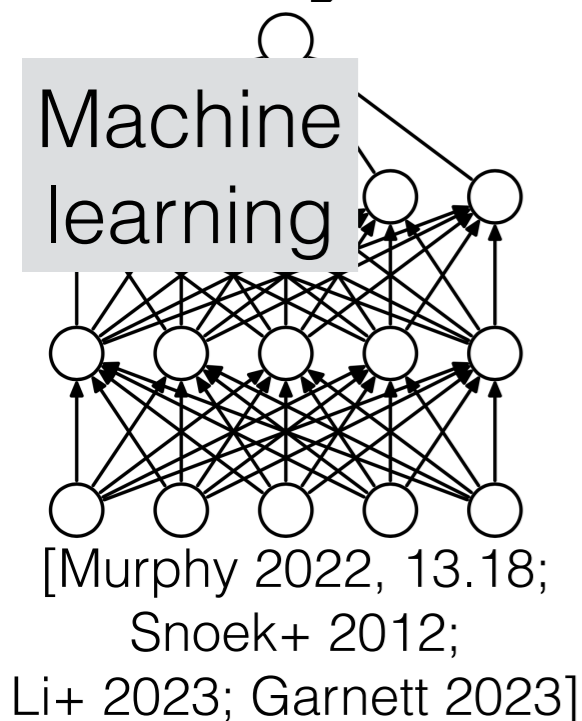
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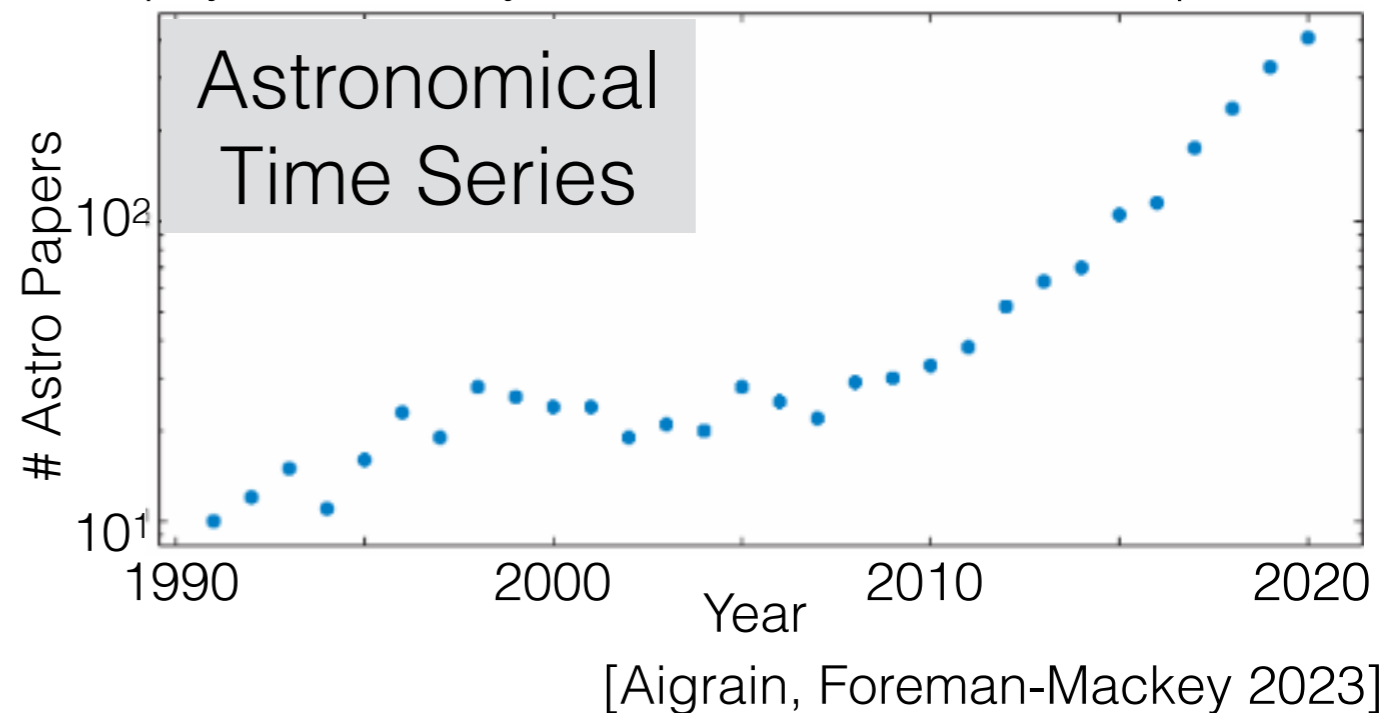
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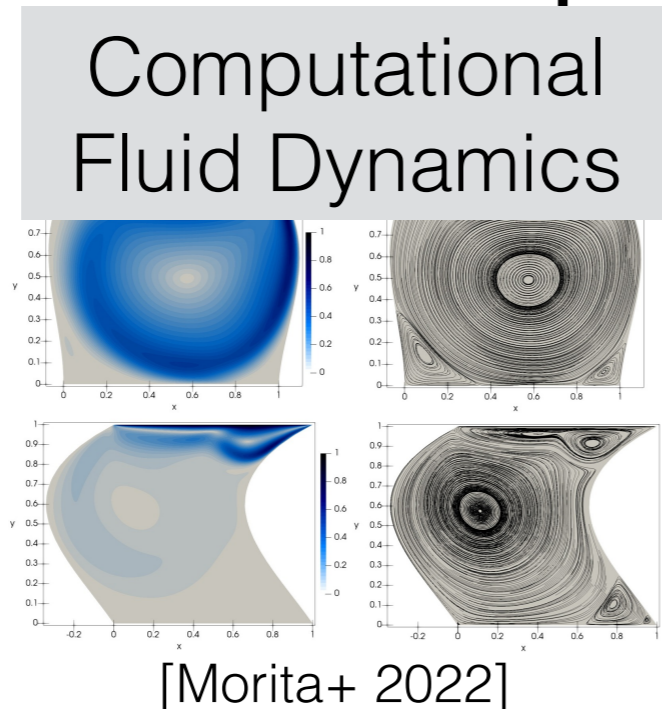
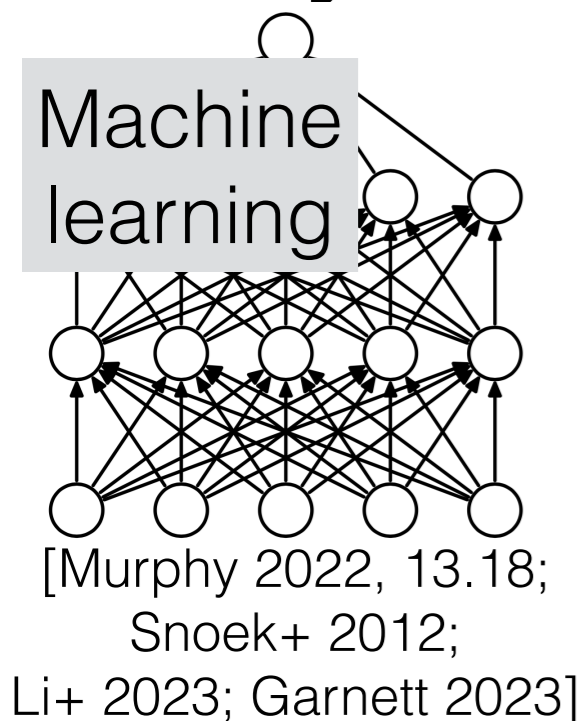
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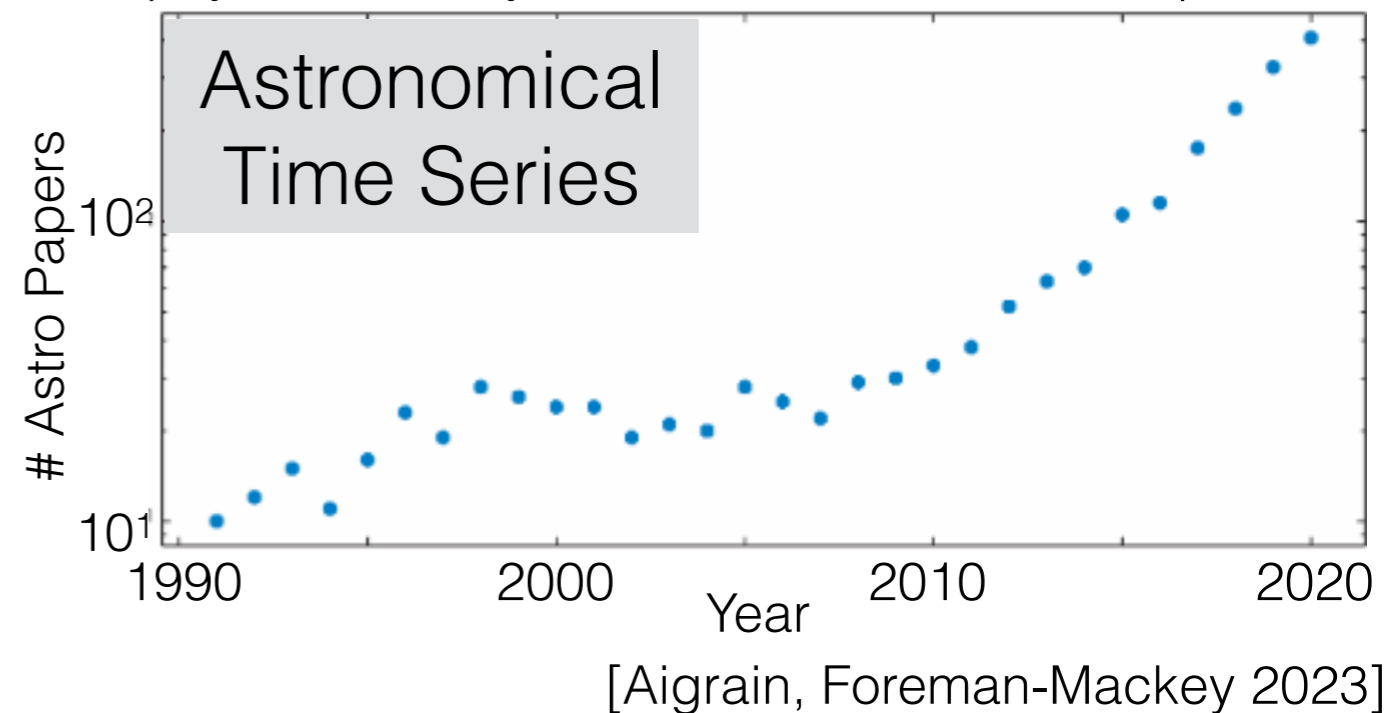
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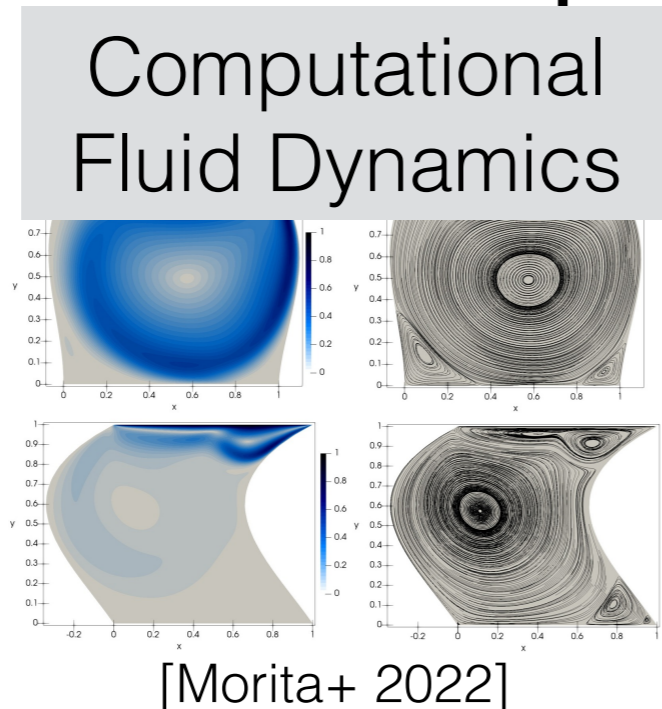
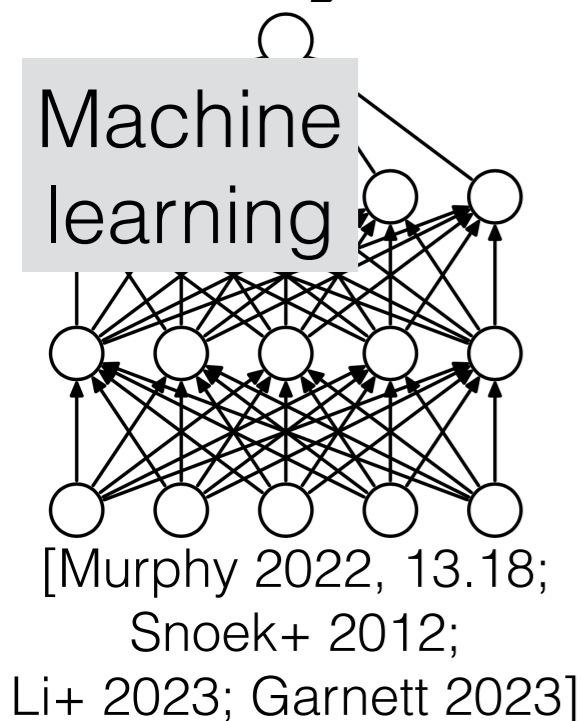


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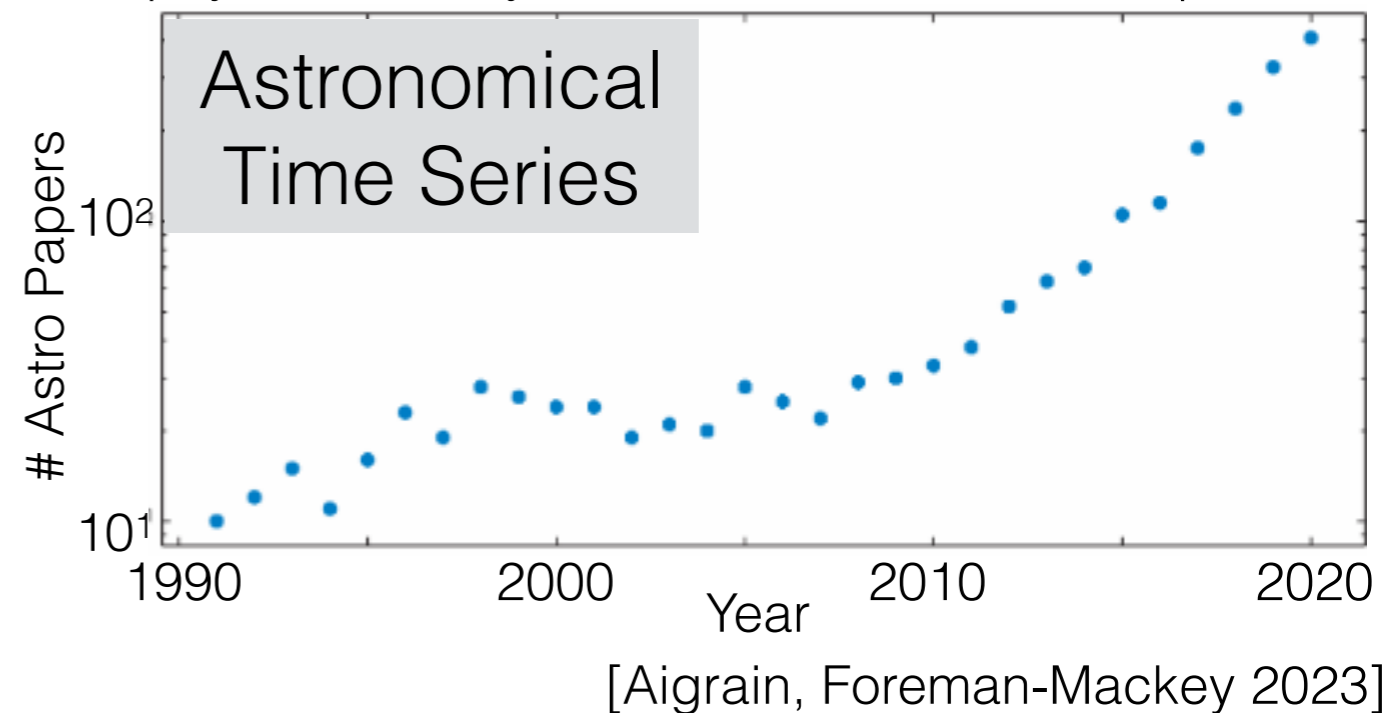
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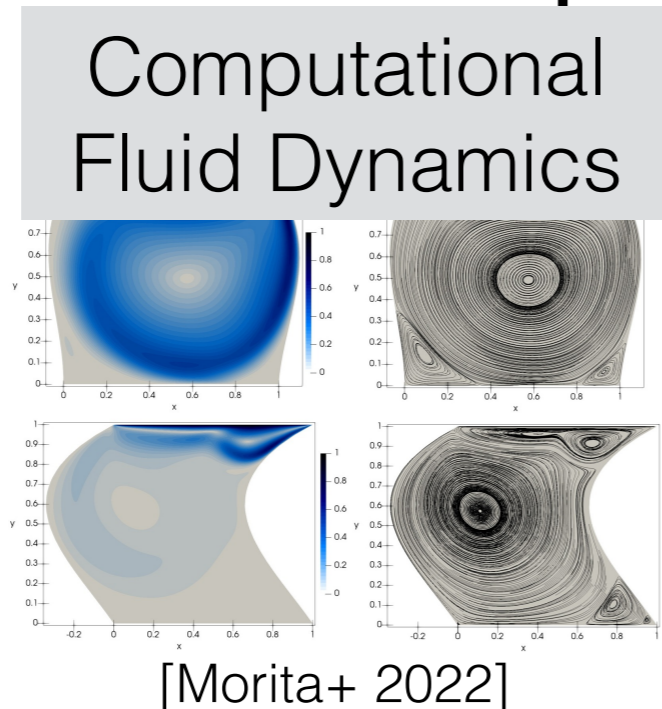
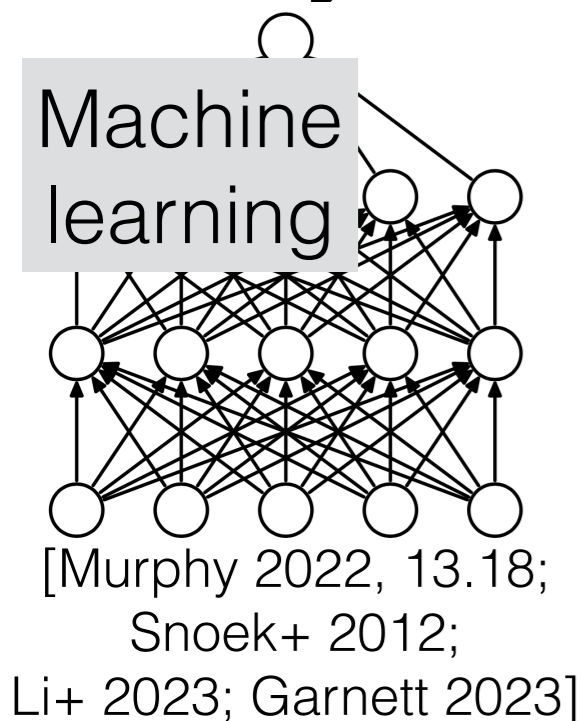


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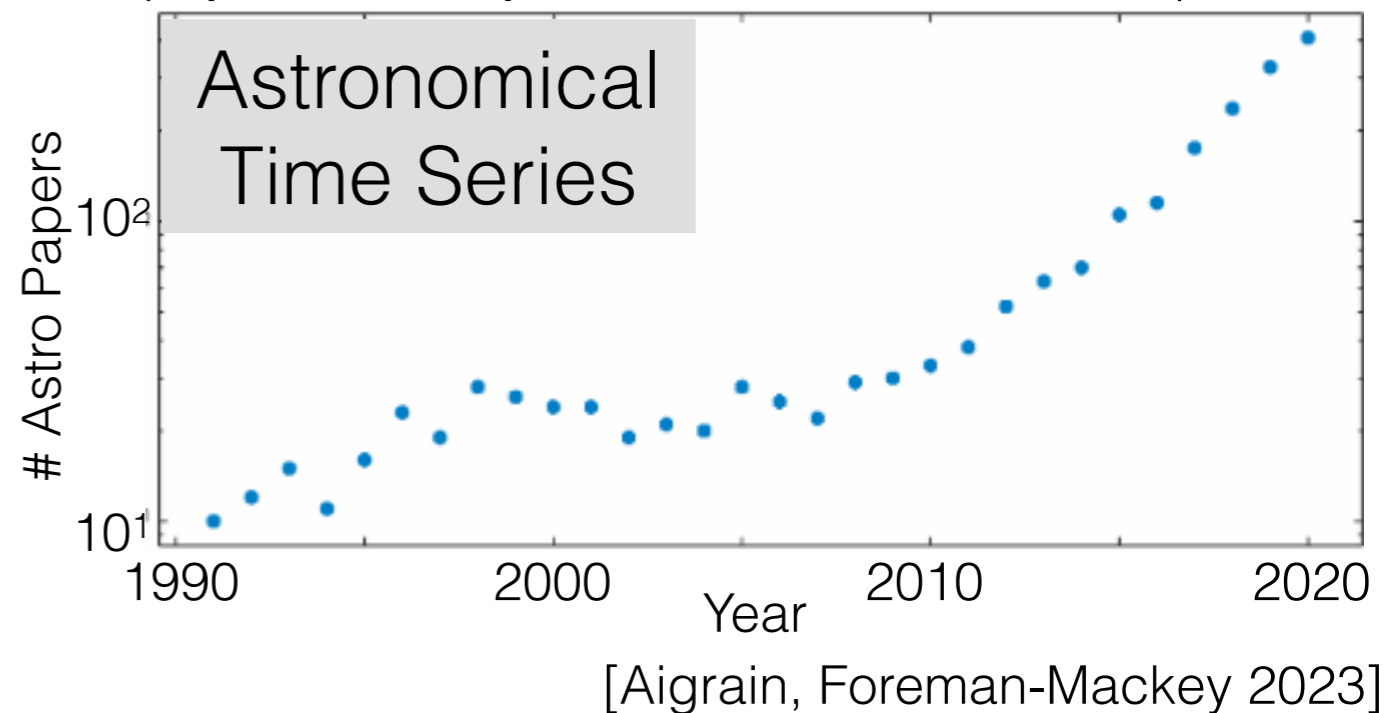
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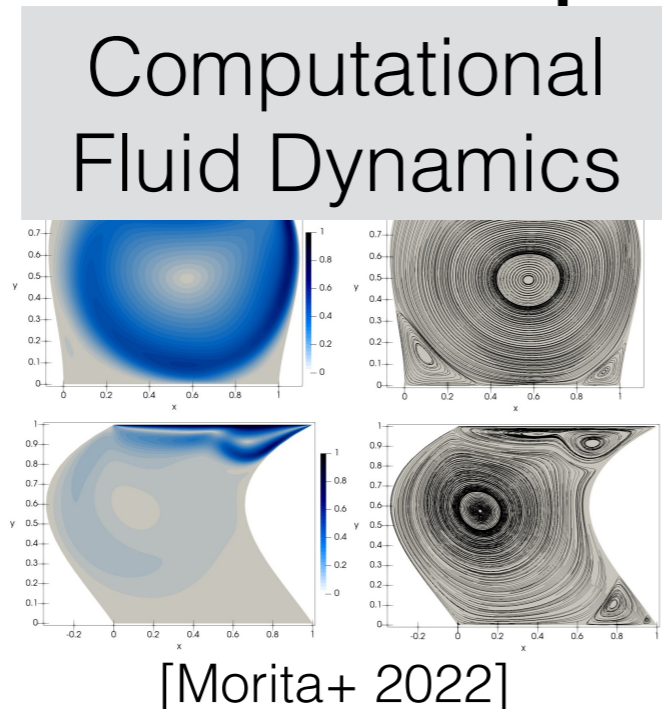
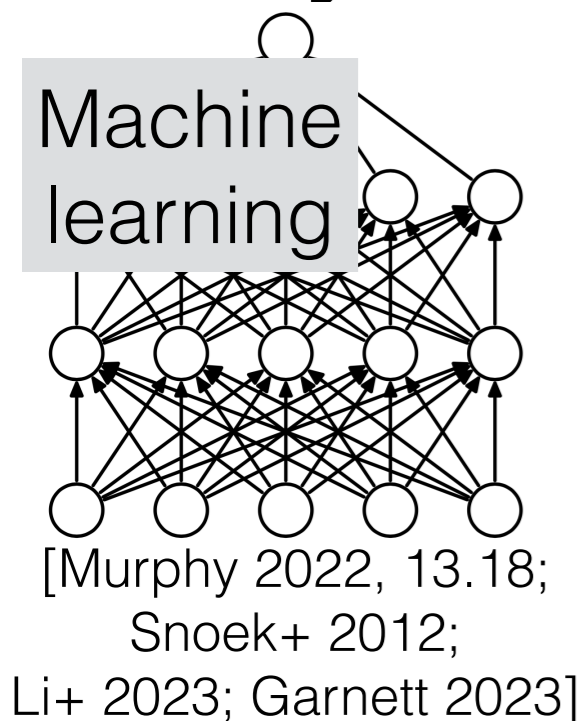


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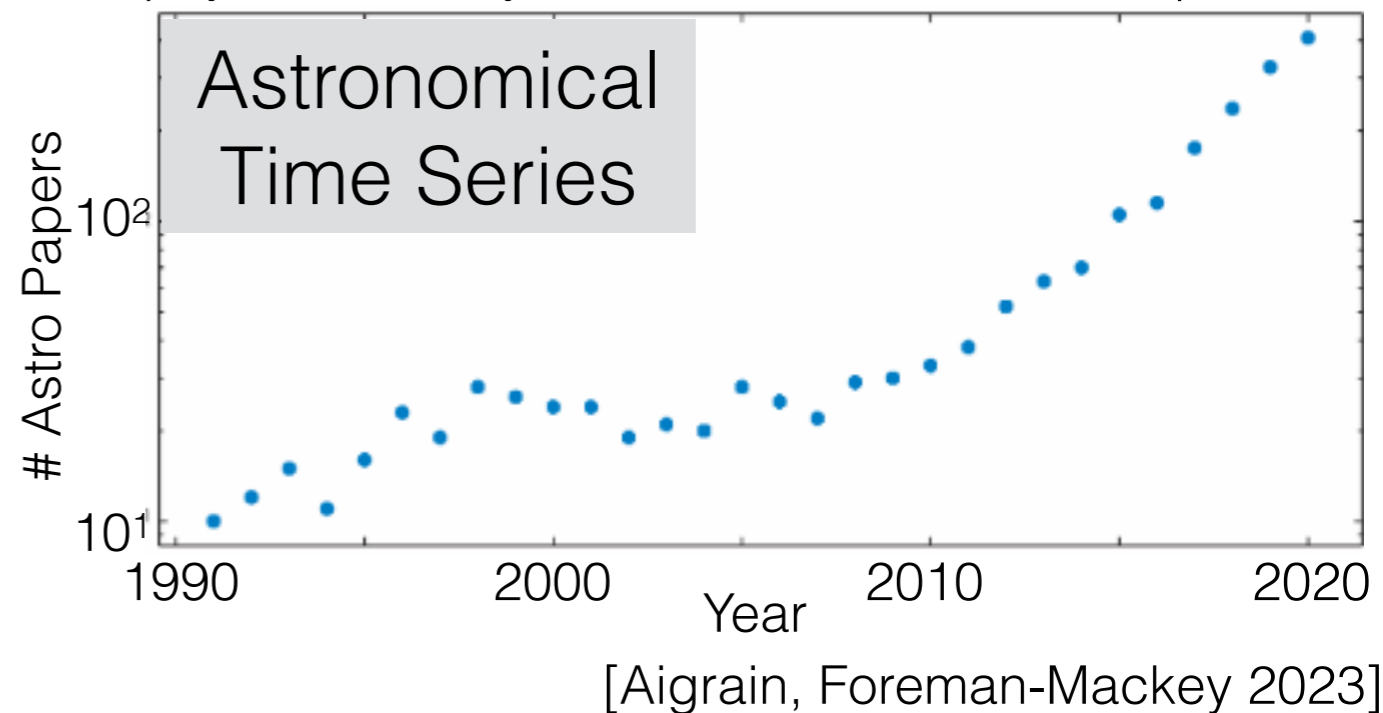
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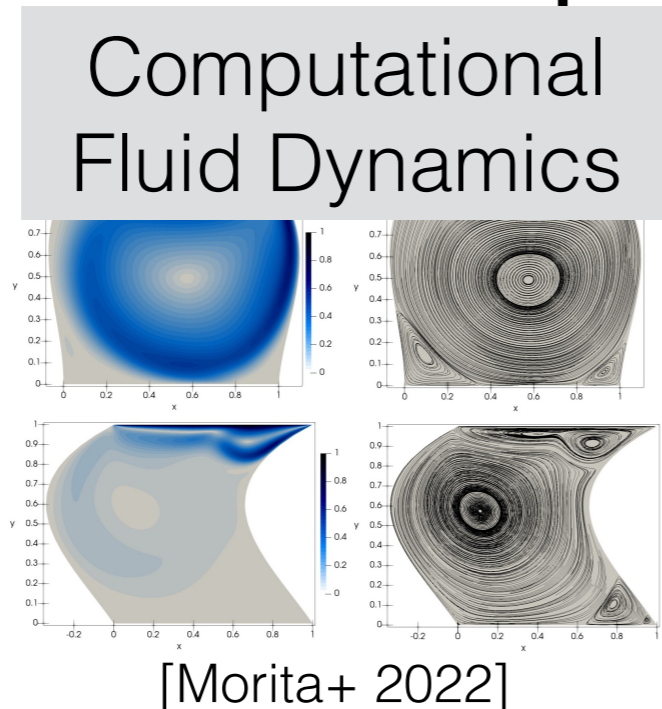
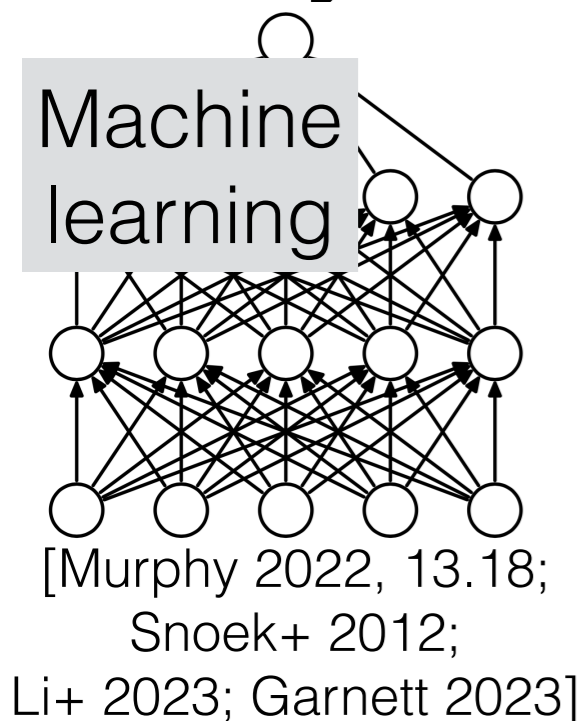


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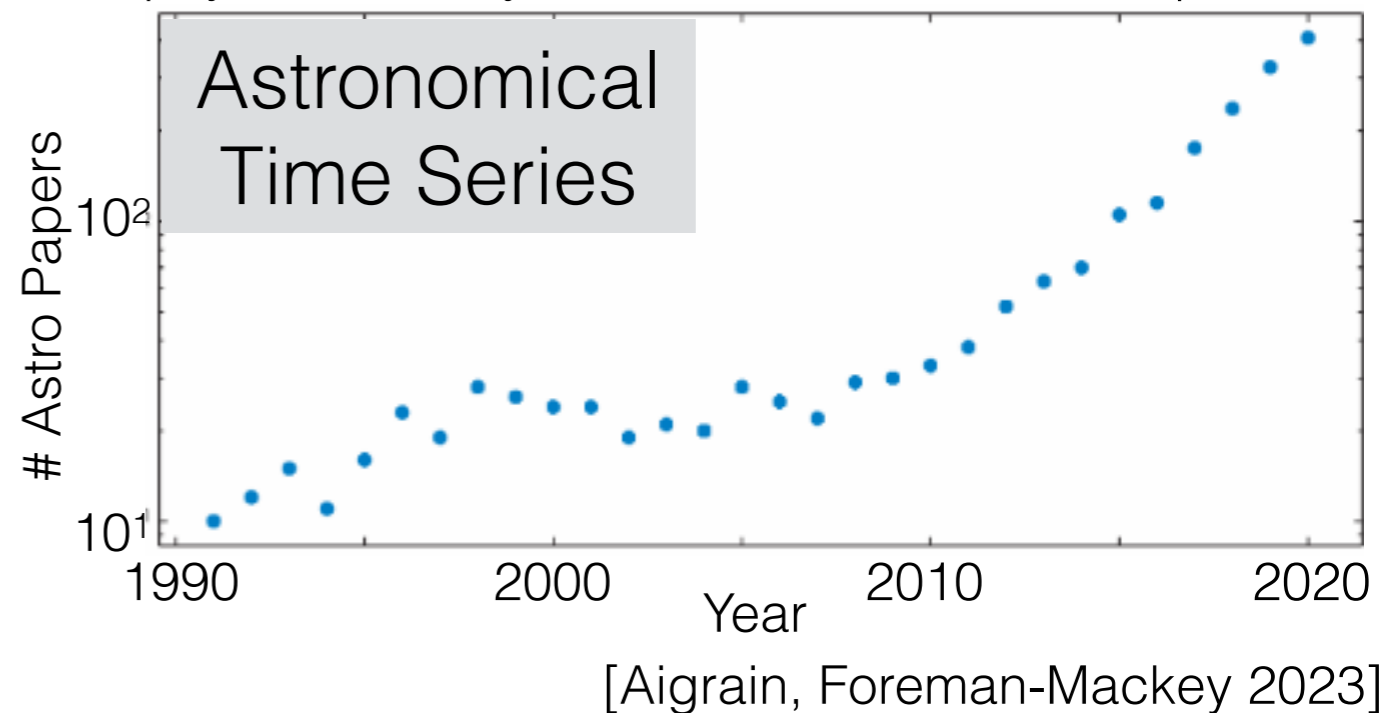
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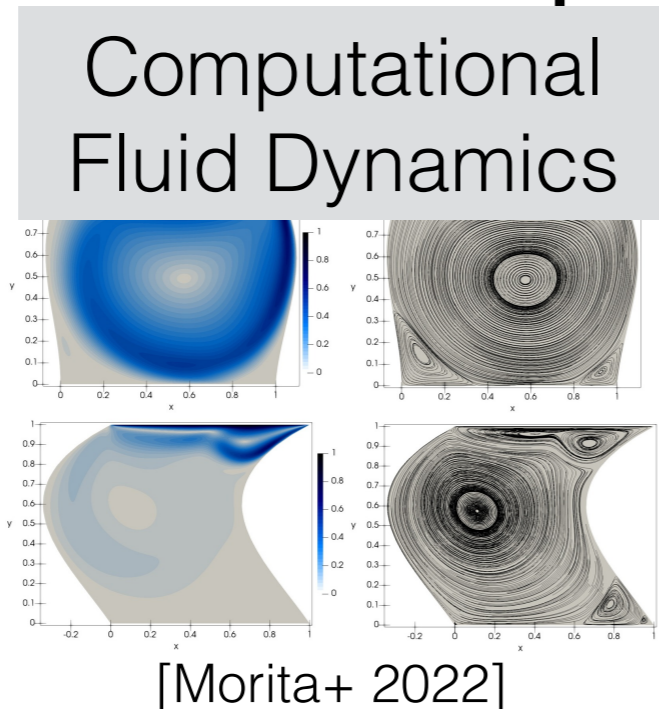
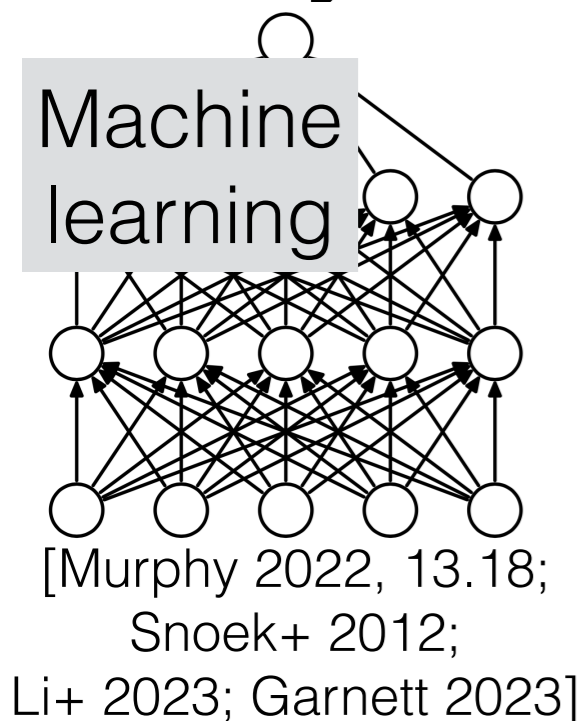
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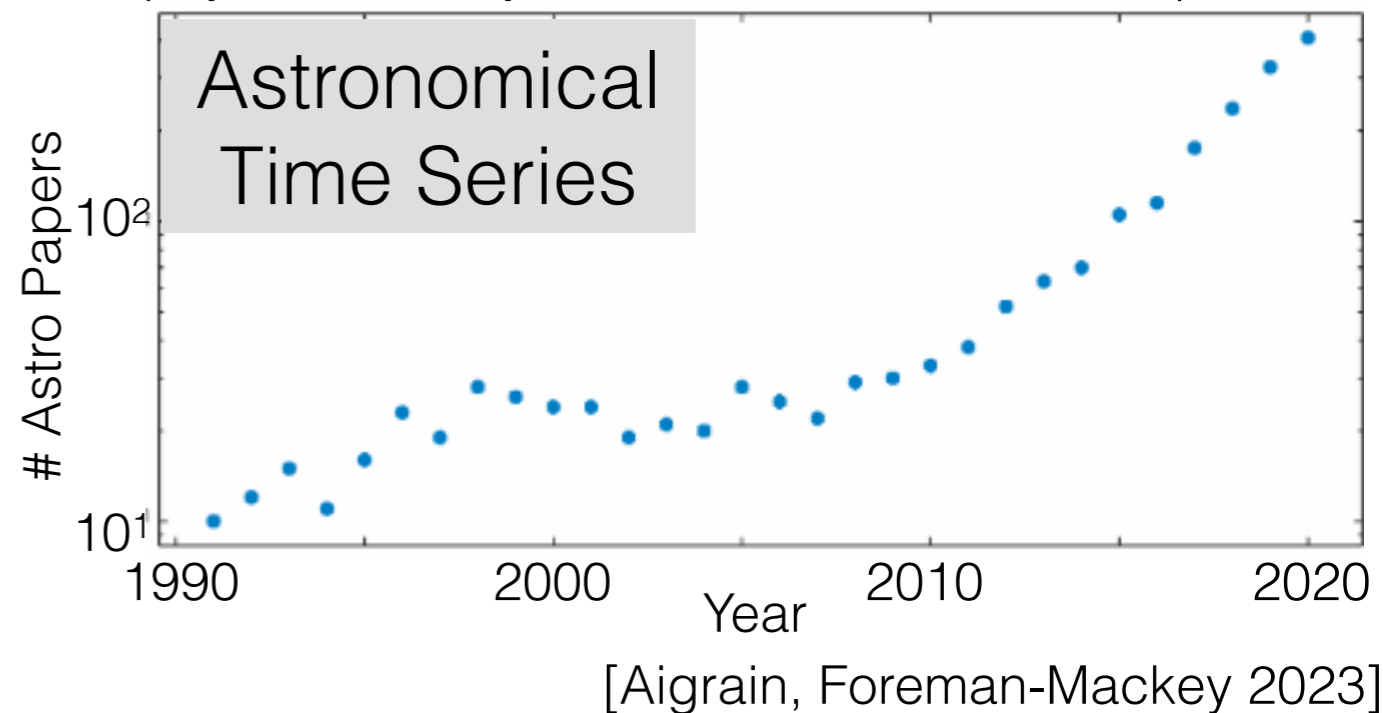
Bonus benefits: • Ease of use (software, tuning) • Supports optimization of outcome • Predictions & uncertainties over derivatives & integrals • Module in more-complex methods

Why Gaussian processes?

see also “kriging,”
“optimal
interpolation (OI)”



Astrophysics Data System search for “Gaussian process”



A recurring motif:

- We'd like to estimate a potentially nonlinear but smooth function of a handful of inputs
- We have access to sparse (possibly noisy) observations of the function
- We'd like to quantify our uncertainty

Bonus benefits: • Ease of use (software, tuning) • Supports optimization of outcome • Predictions & uncertainties over derivatives & integrals • Module in more-complex methods

Roadmap

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- A Bayesian approach

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- What is a Gaussian process?

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- Goals:
 - Learn the mechanism behind standard GPs to identify benefits and pitfalls
 - Learn the skills to be responsible users of standard GPs (transferable to other ML/AI methods)


A Bayesian approach

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

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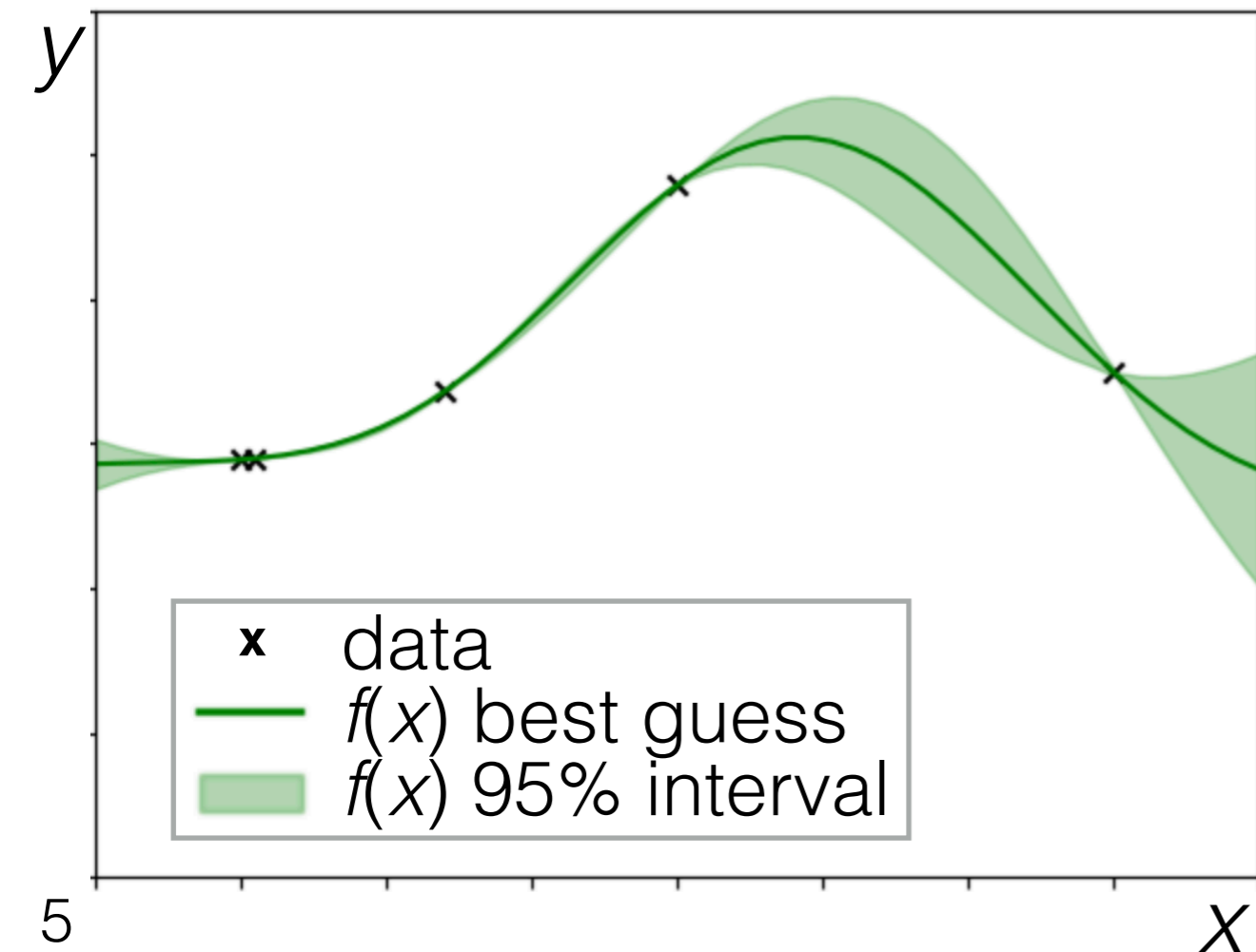


Given the data we've seen, what do we know about the underlying function?

A Bayesian approach

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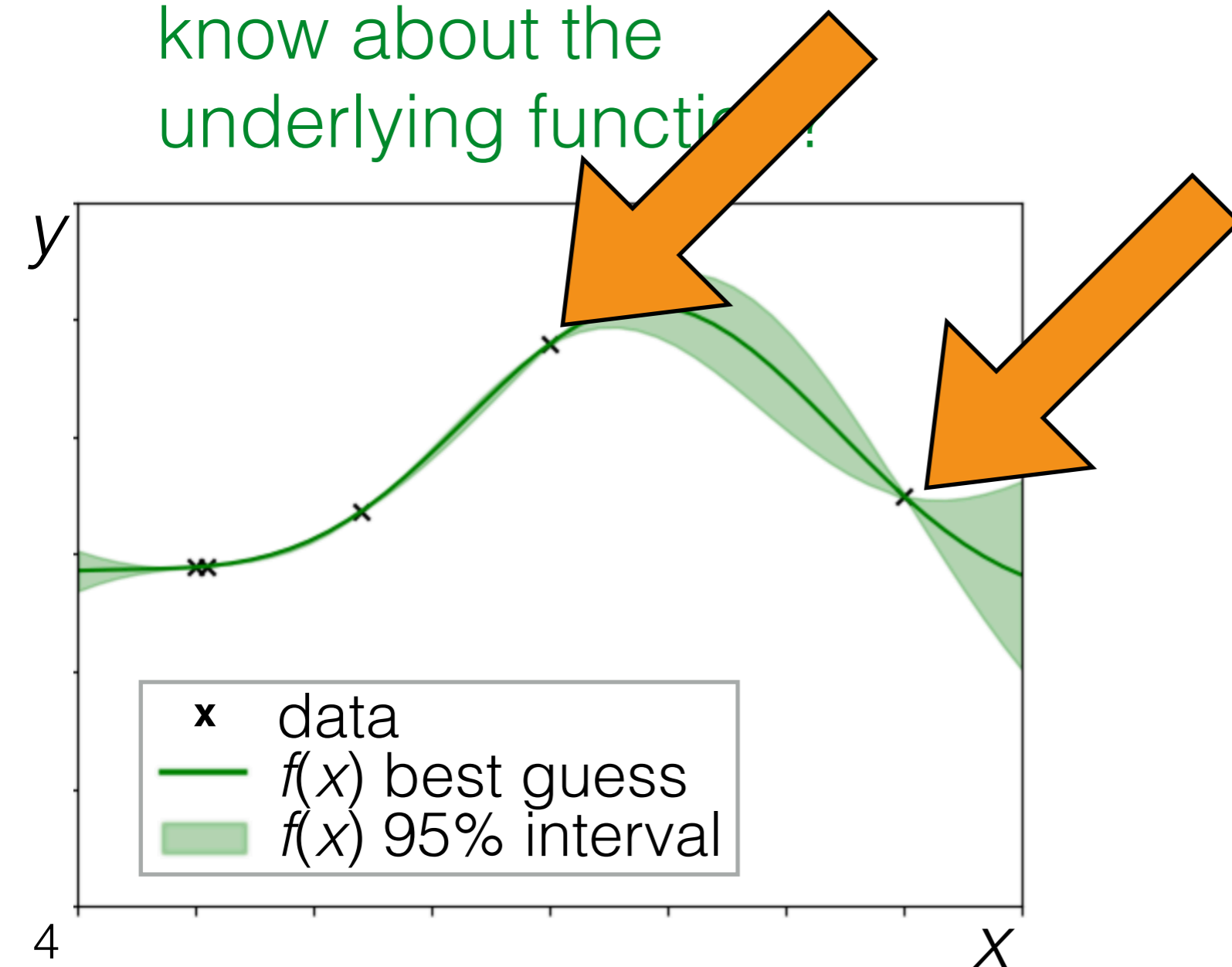
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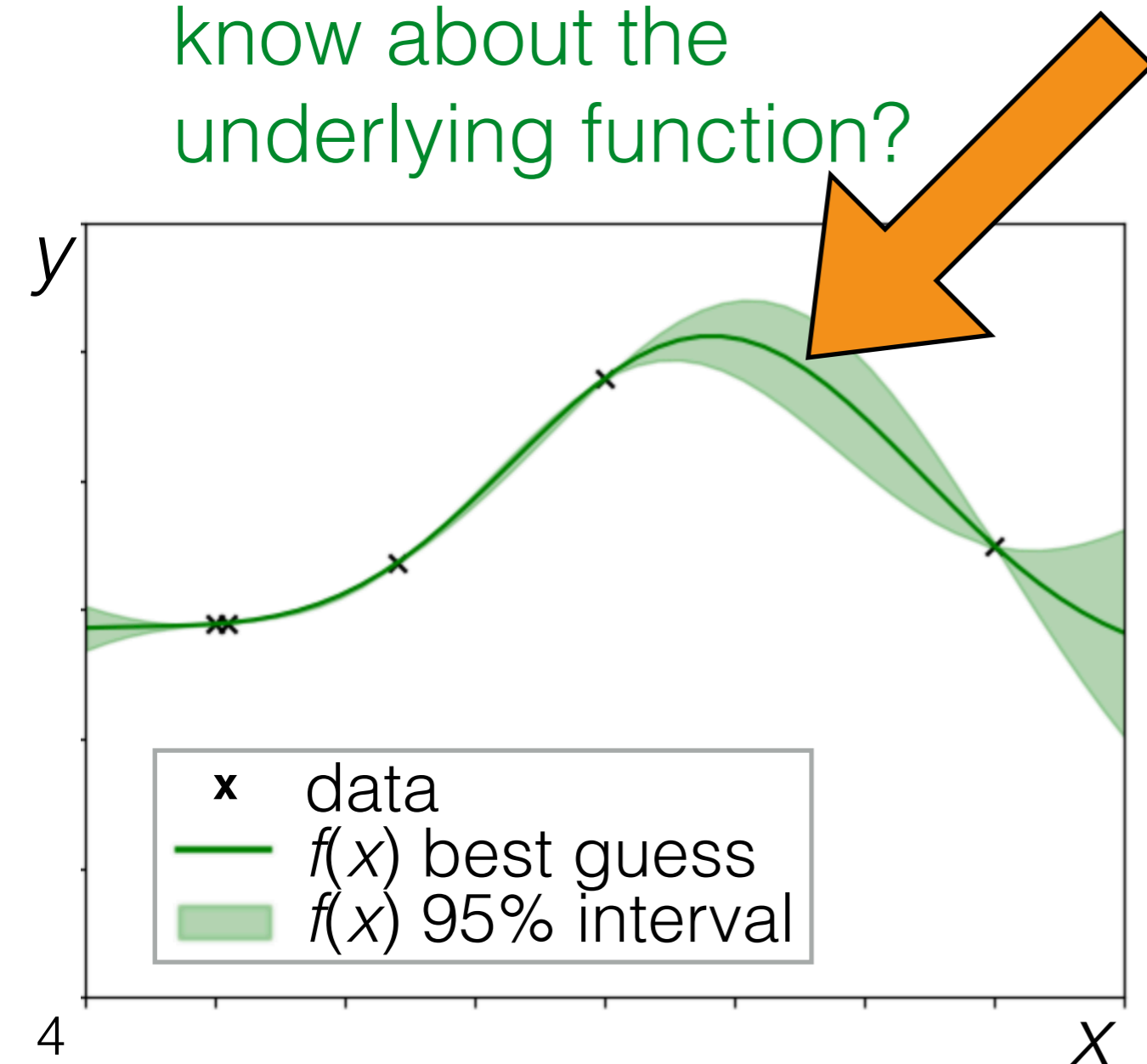
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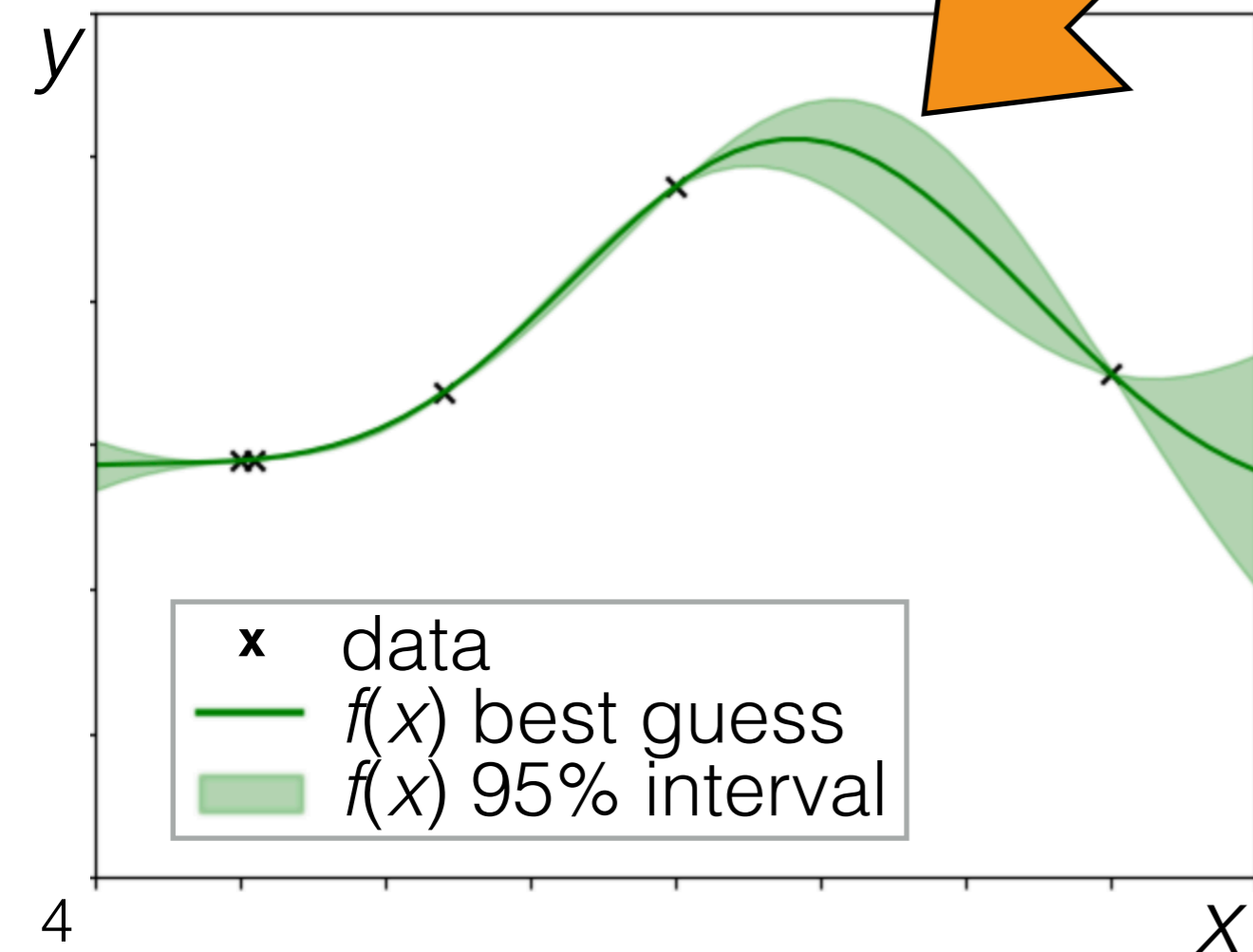
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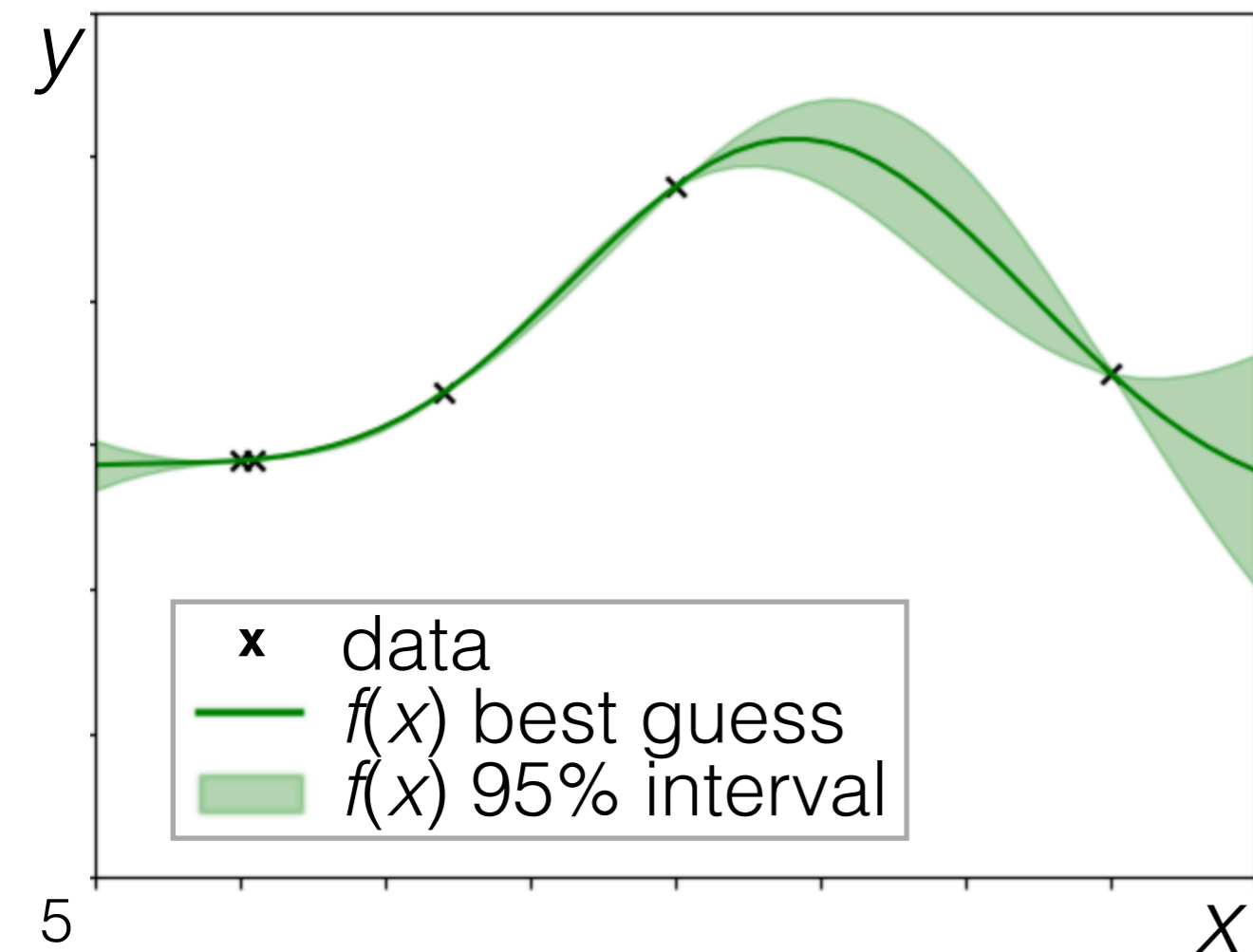
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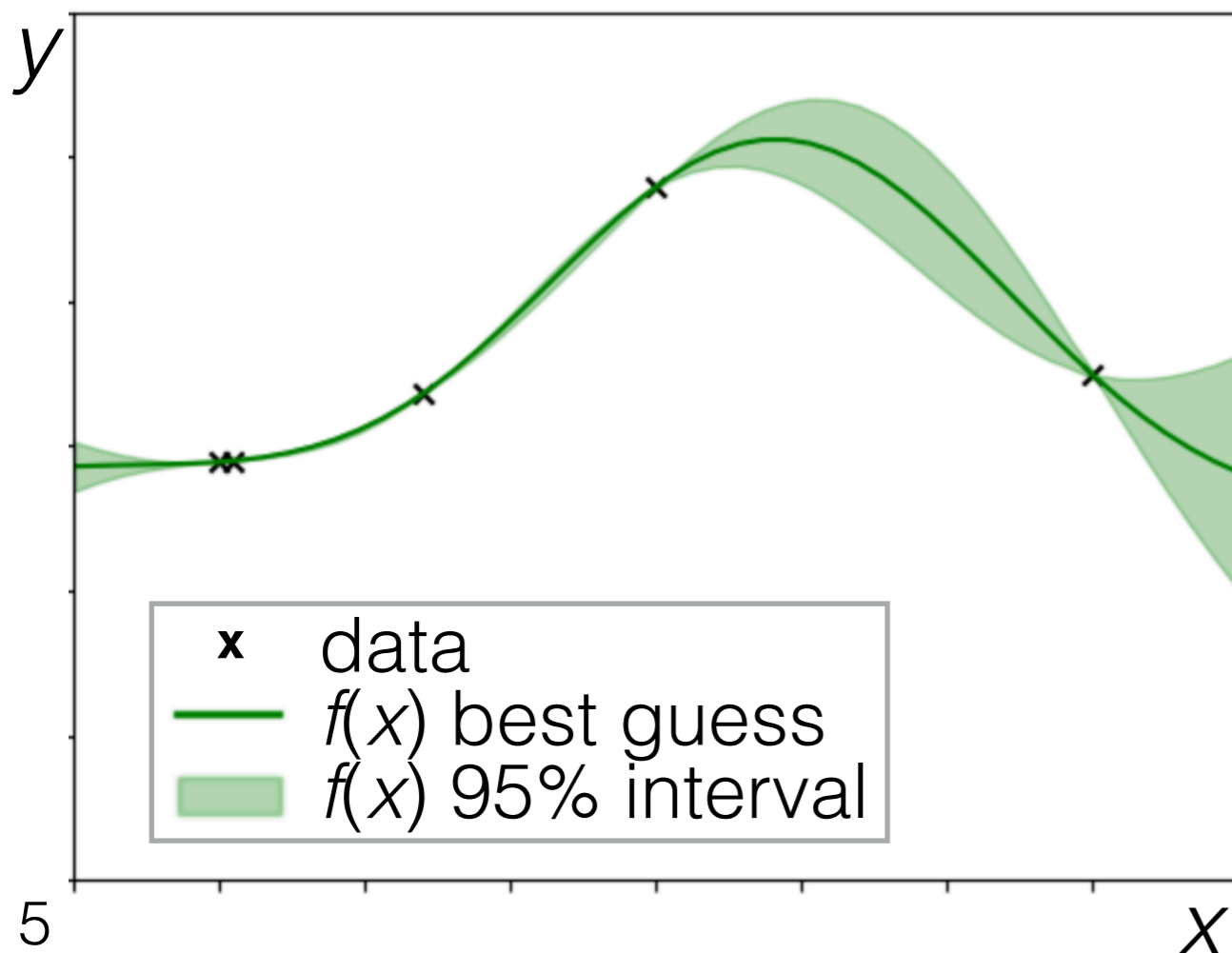


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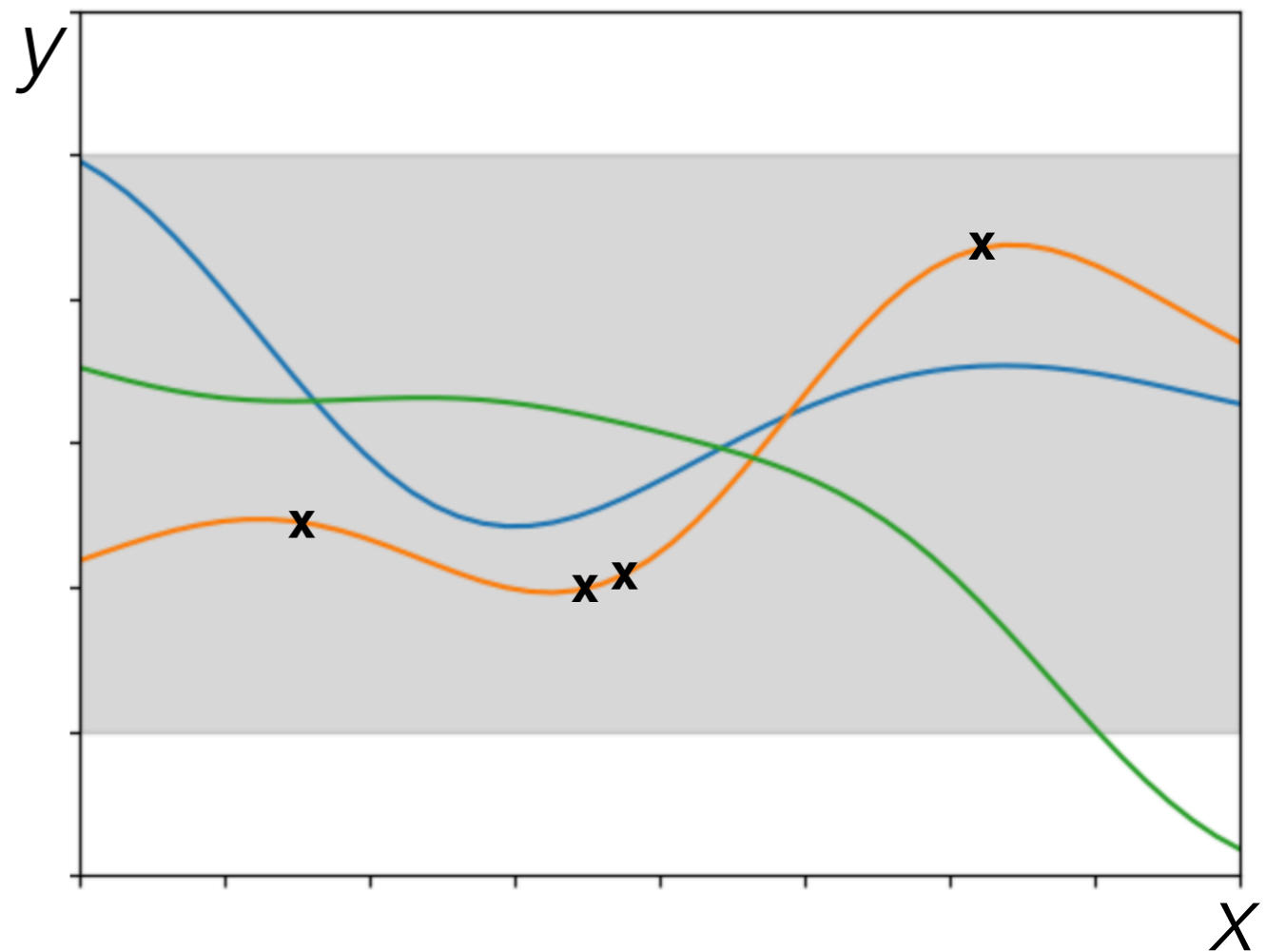
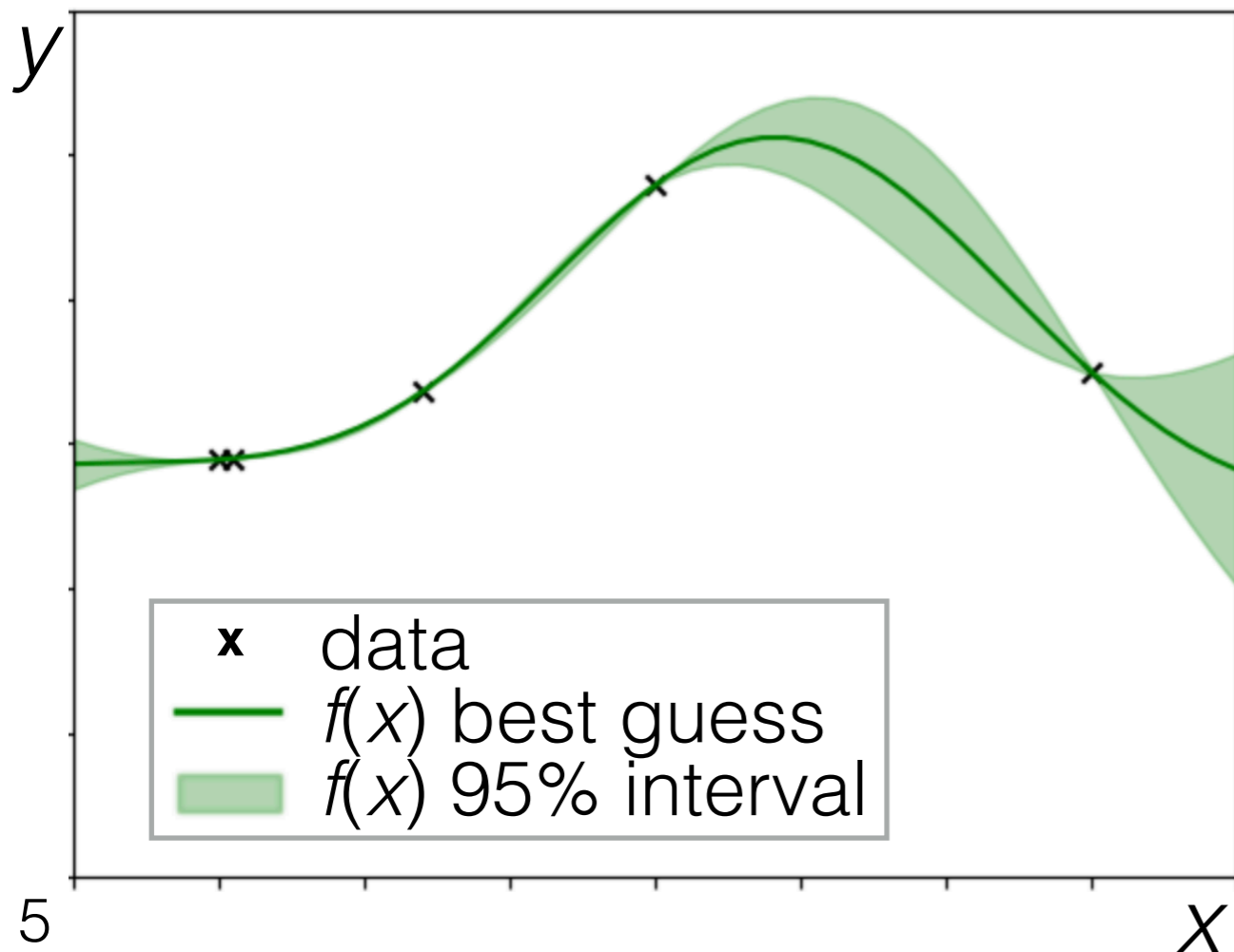


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Univariate Gaussian distribution review

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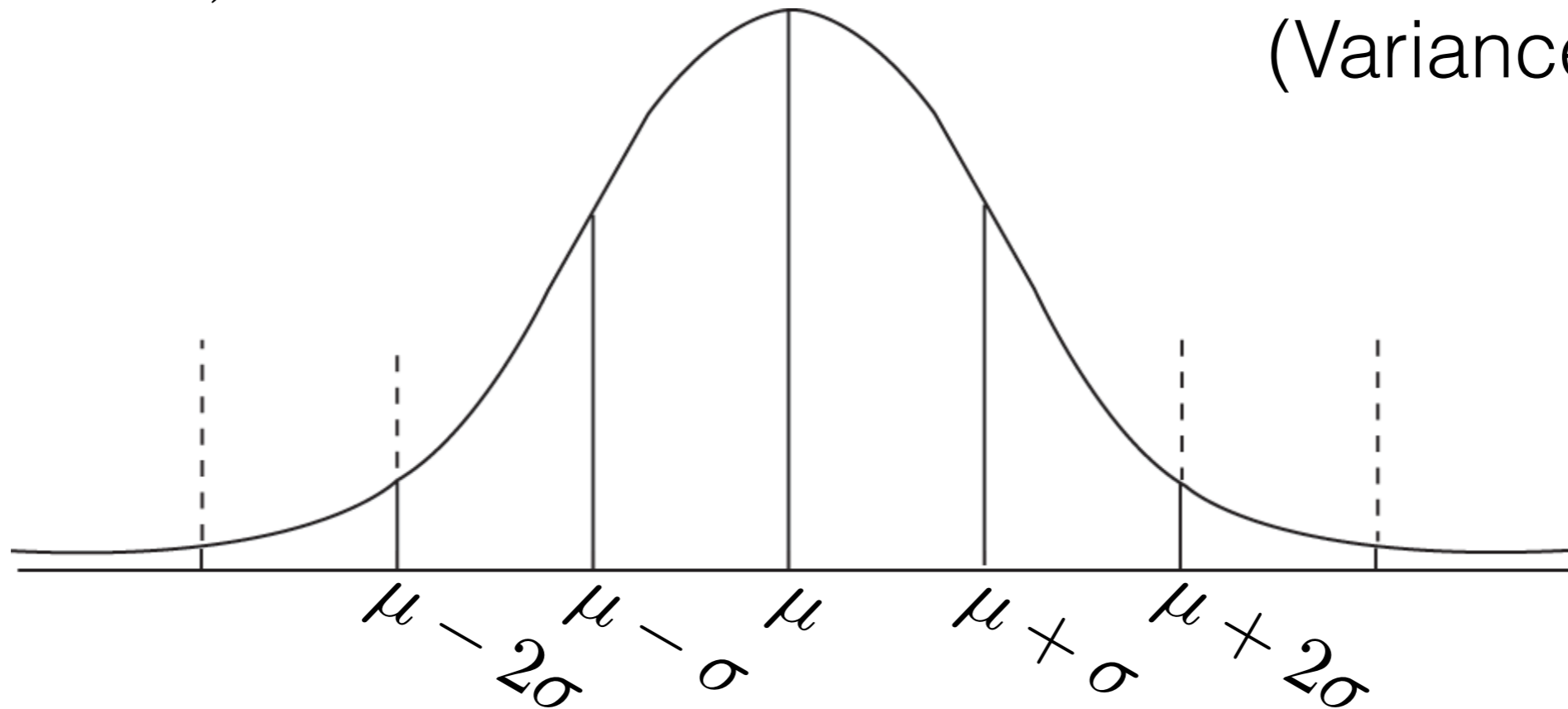
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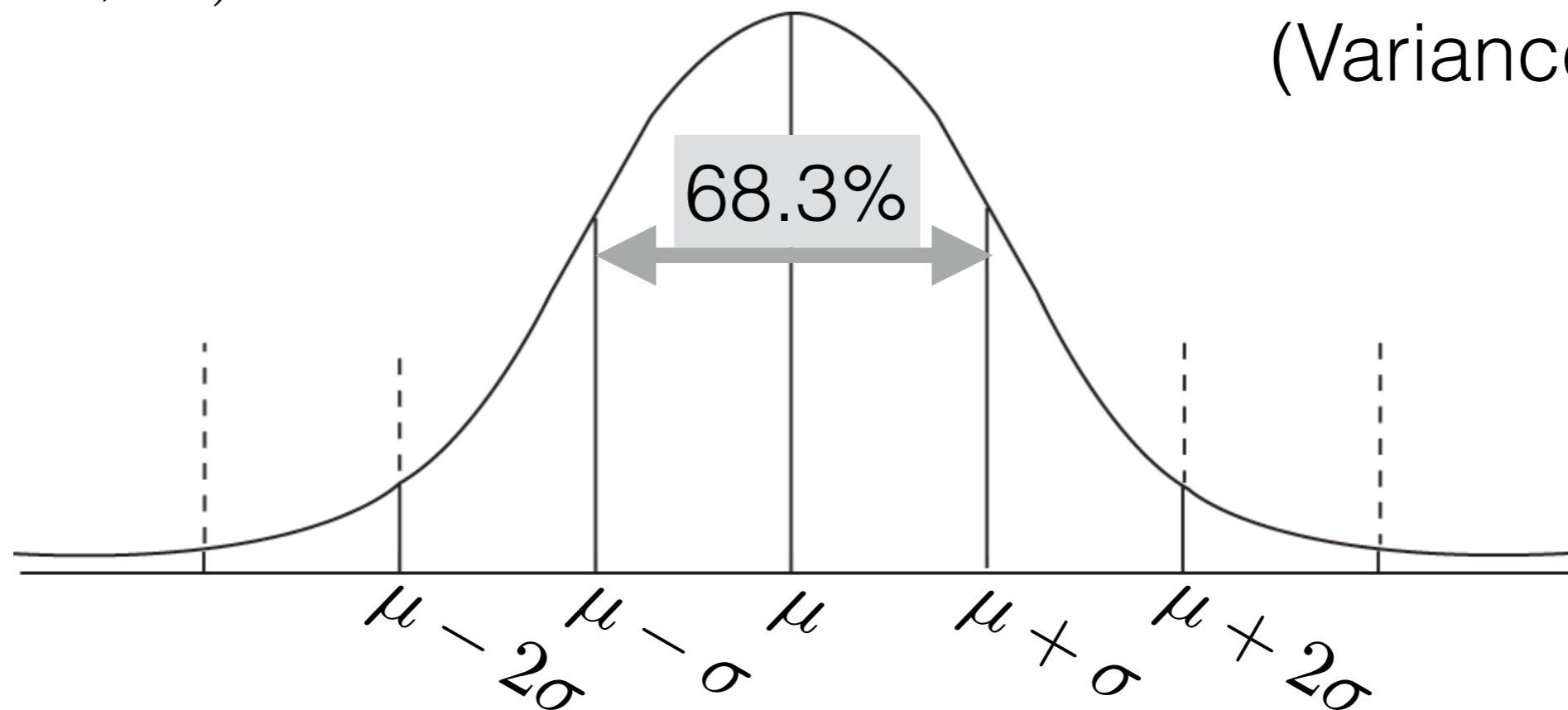
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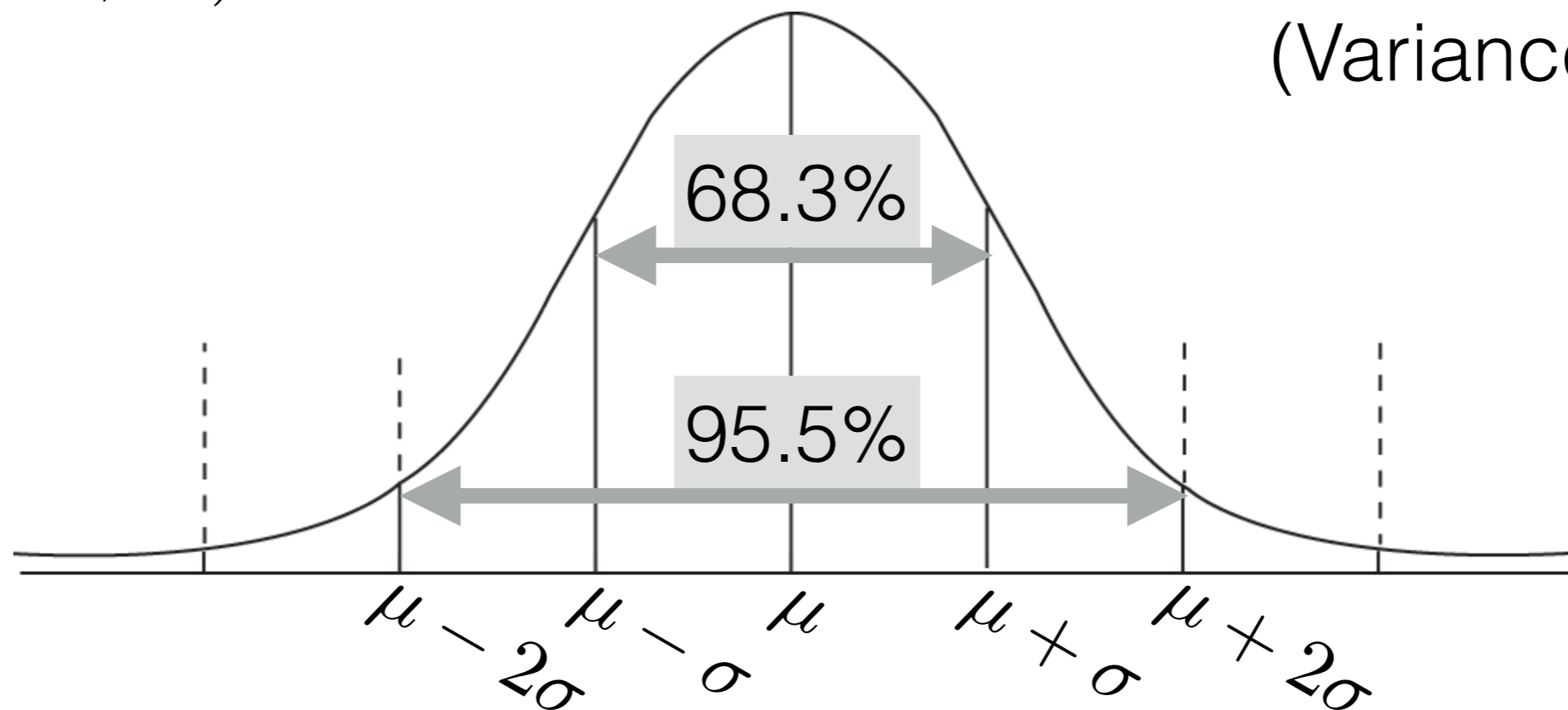
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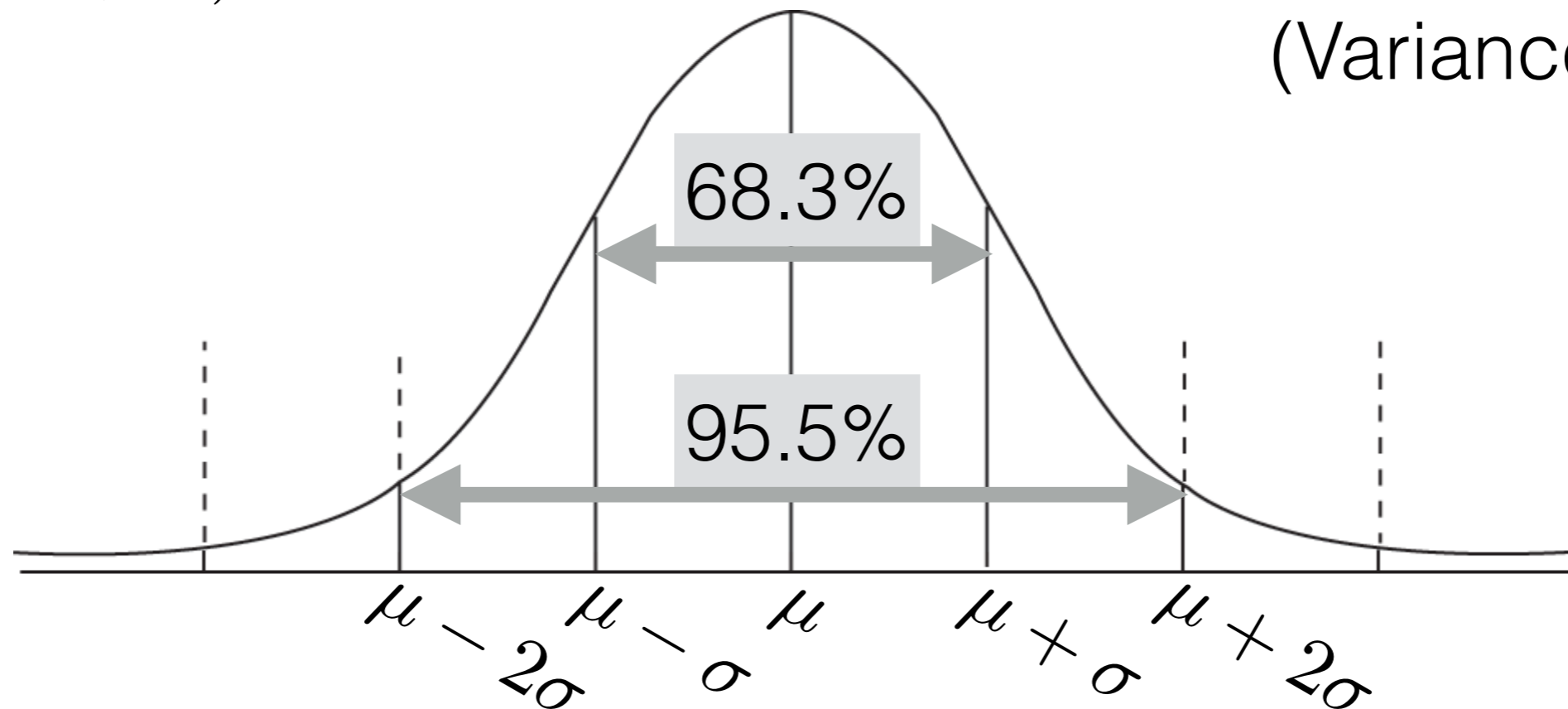
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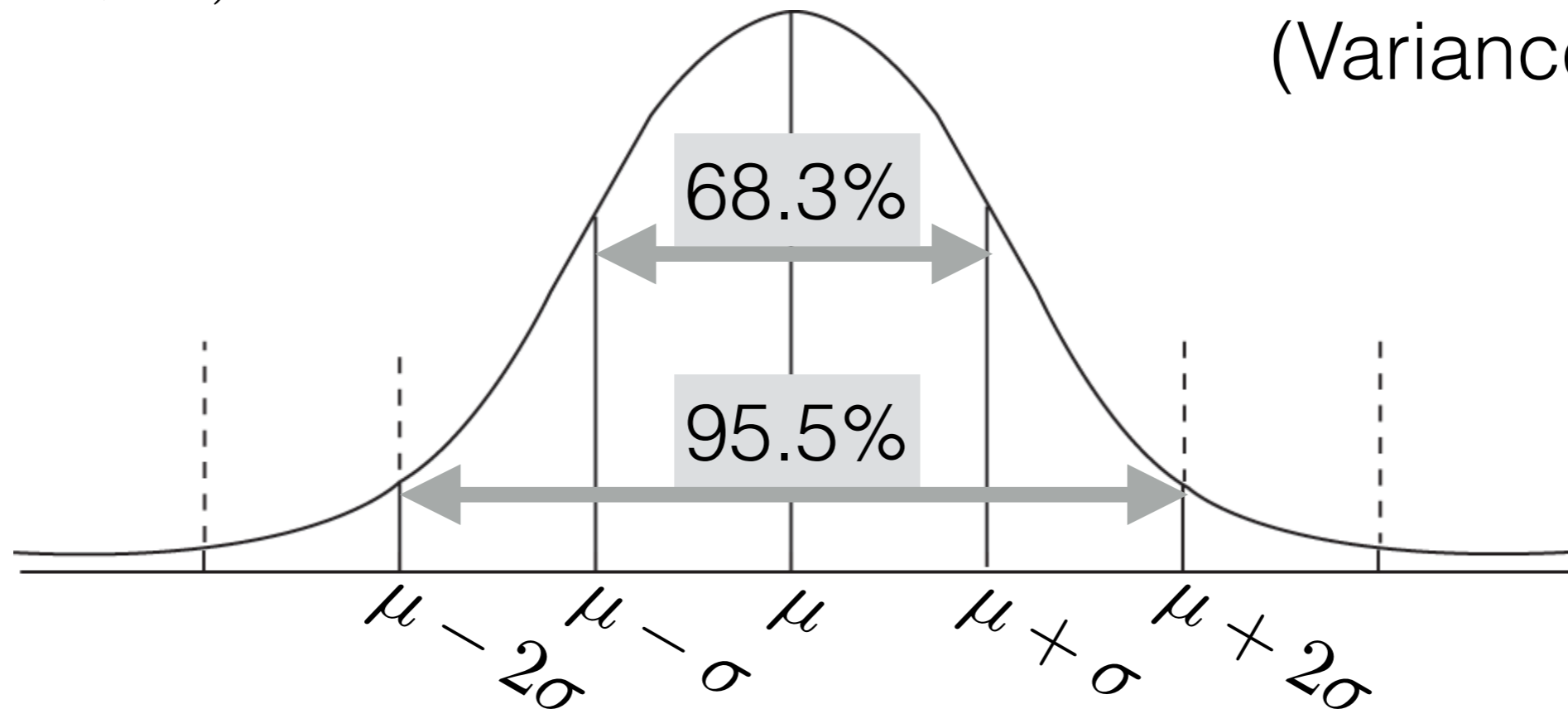


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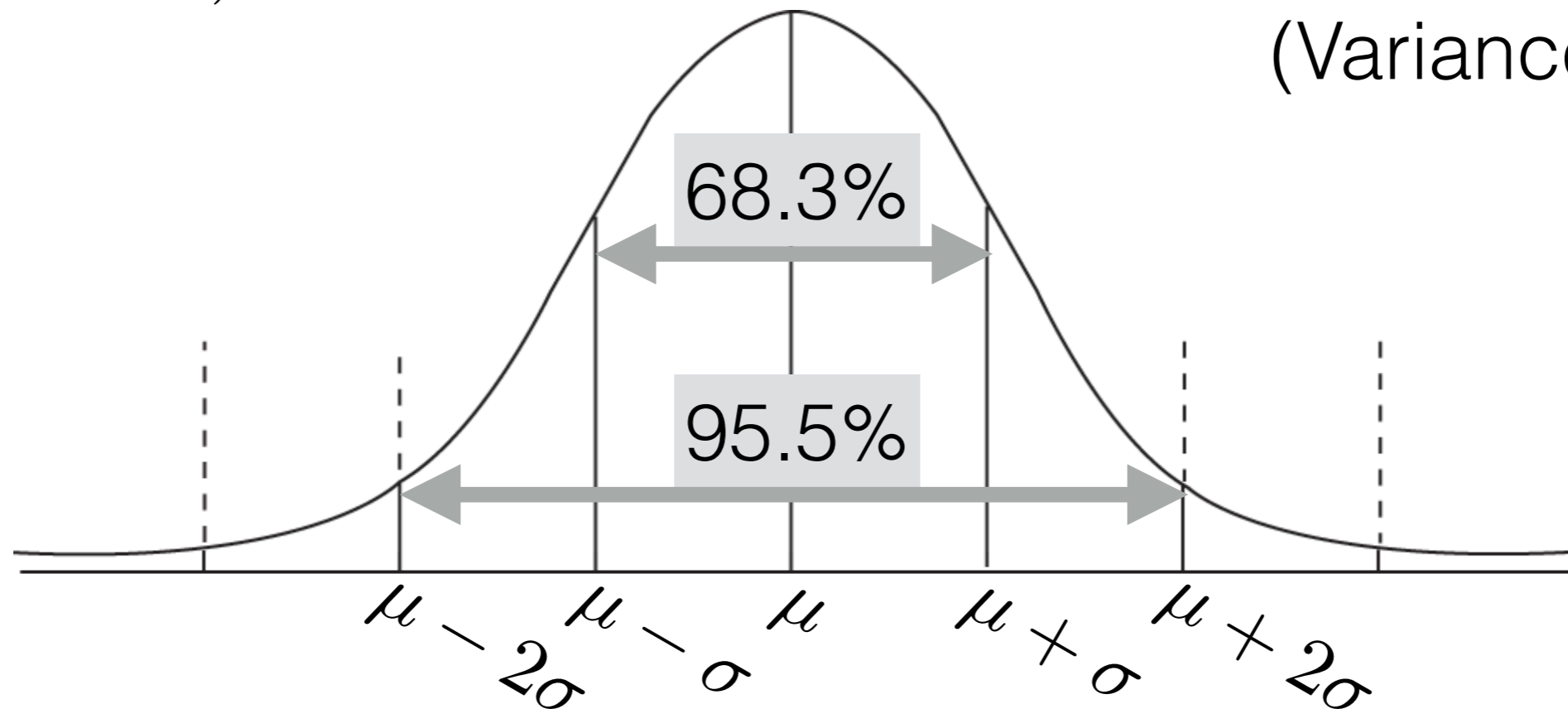


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- If $Y \sim \mathcal{N}(0, 1)$, then $Y + \mu \sim \mathcal{N}(\mu, 1)$

$$\sigma Y \sim \mathcal{N}(0, \sigma^2)$$

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 - y & the mean μ are real-valued vectors with dimension M
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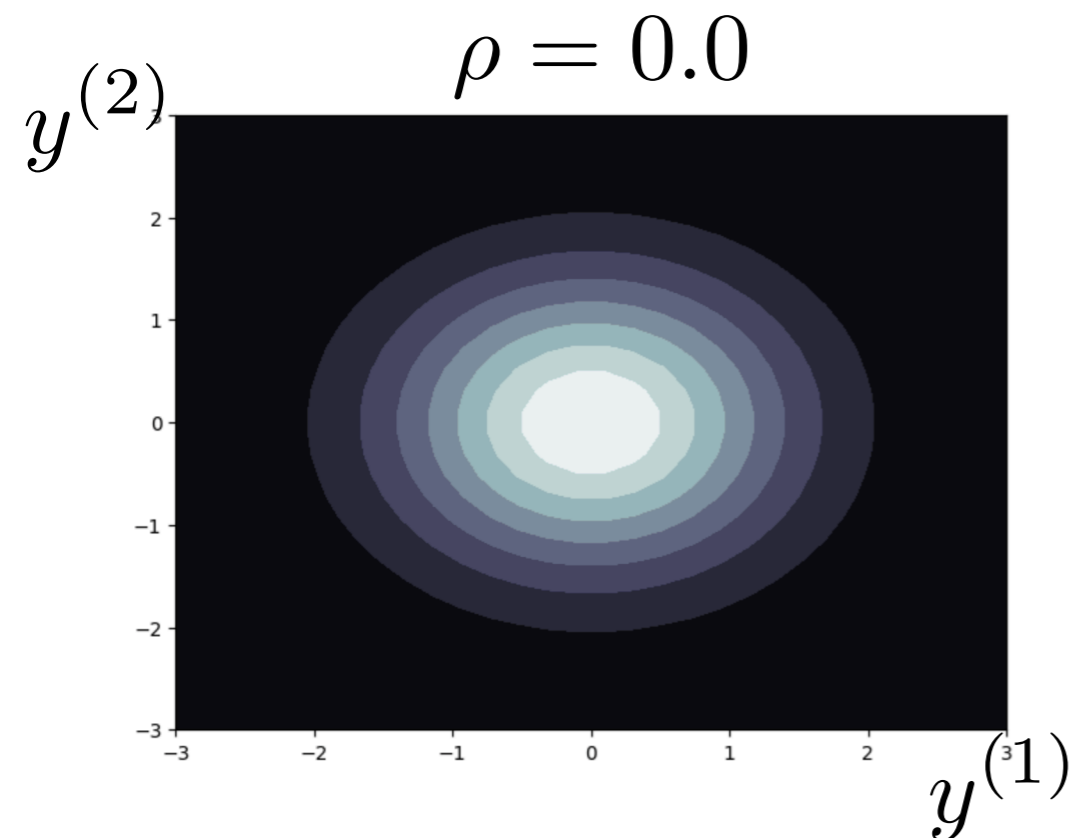
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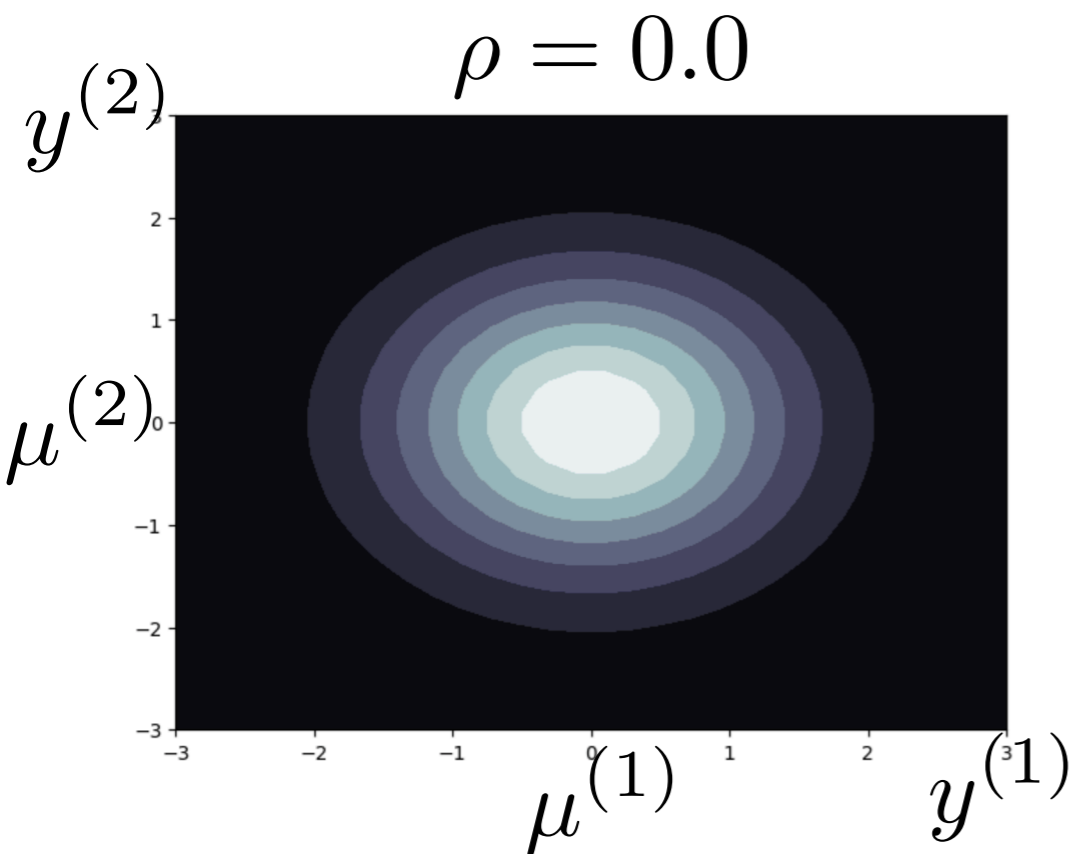
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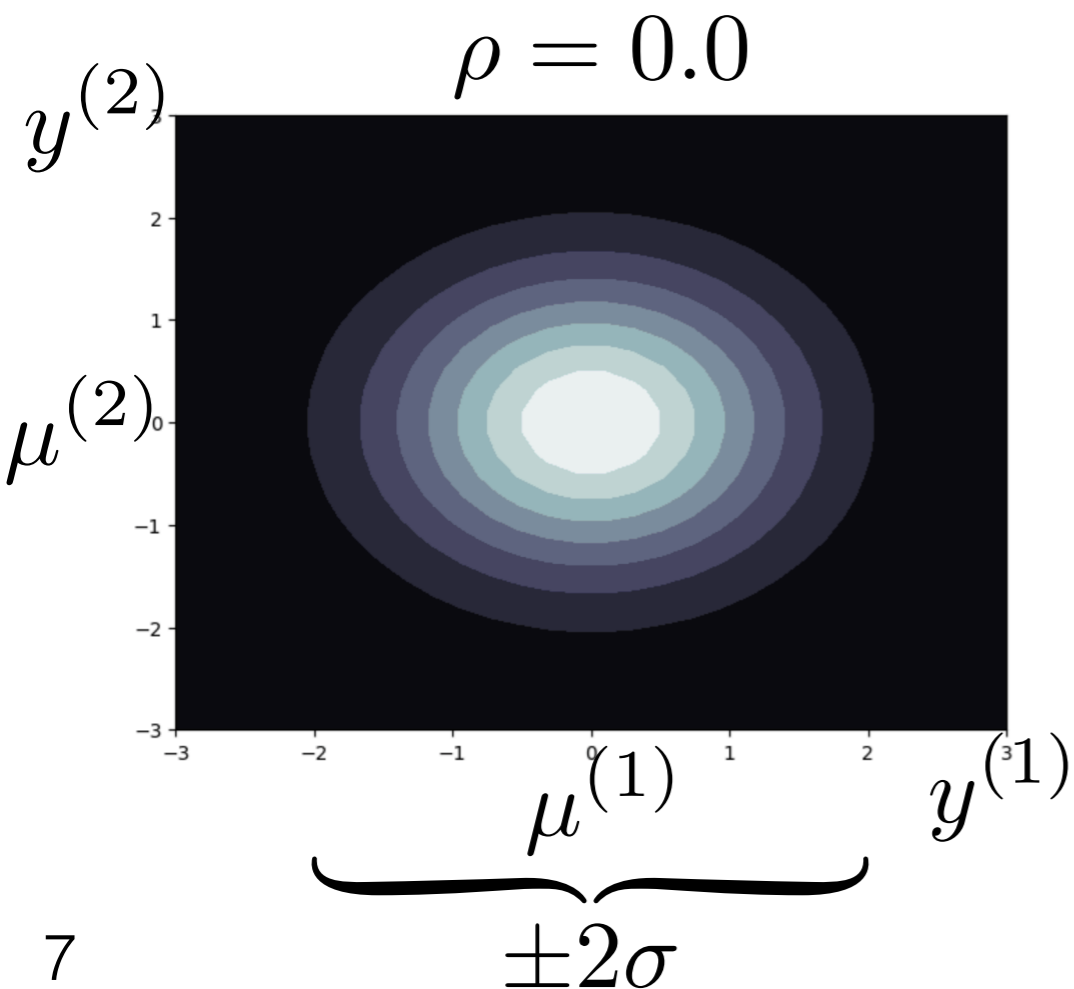
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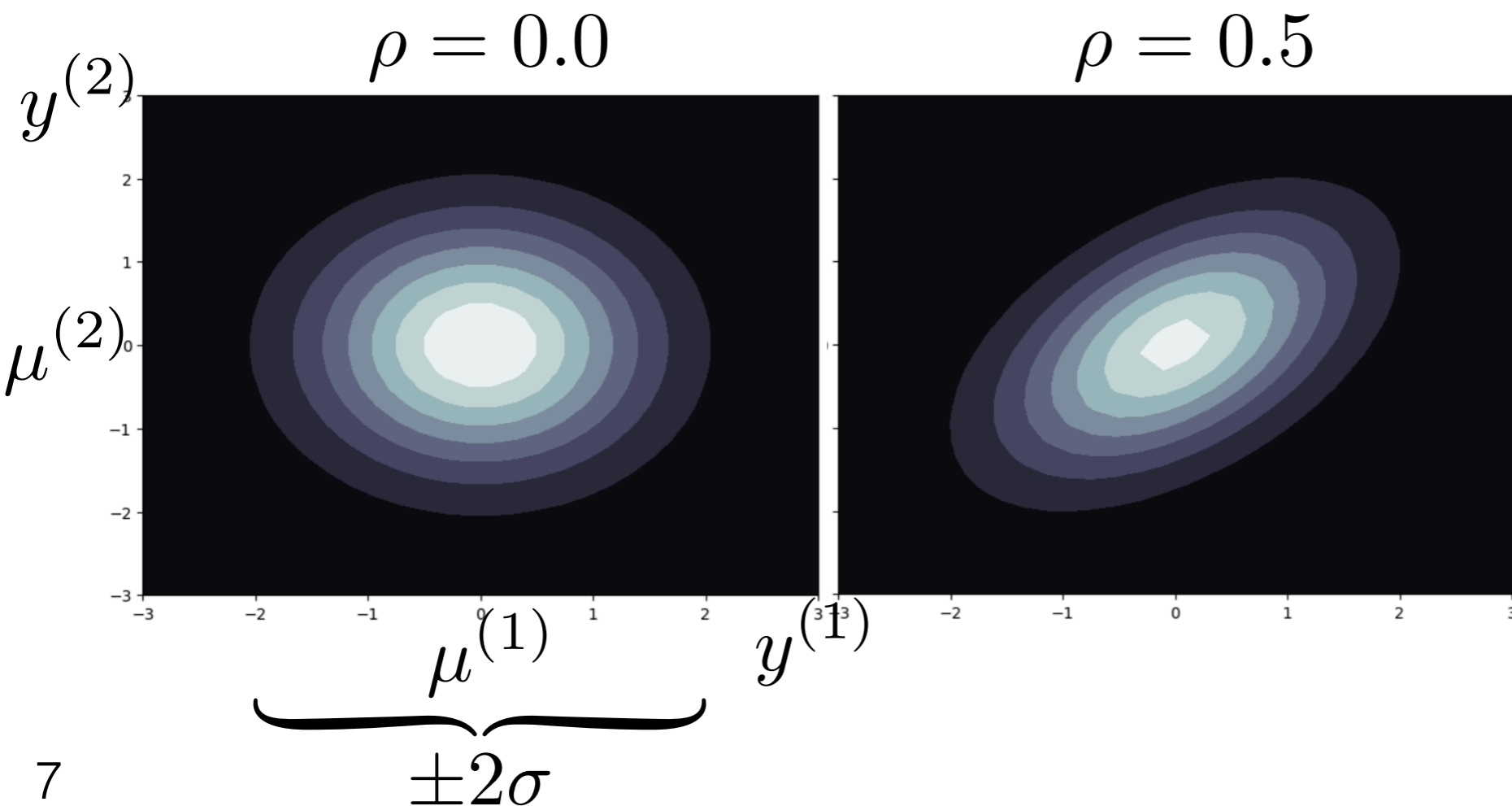
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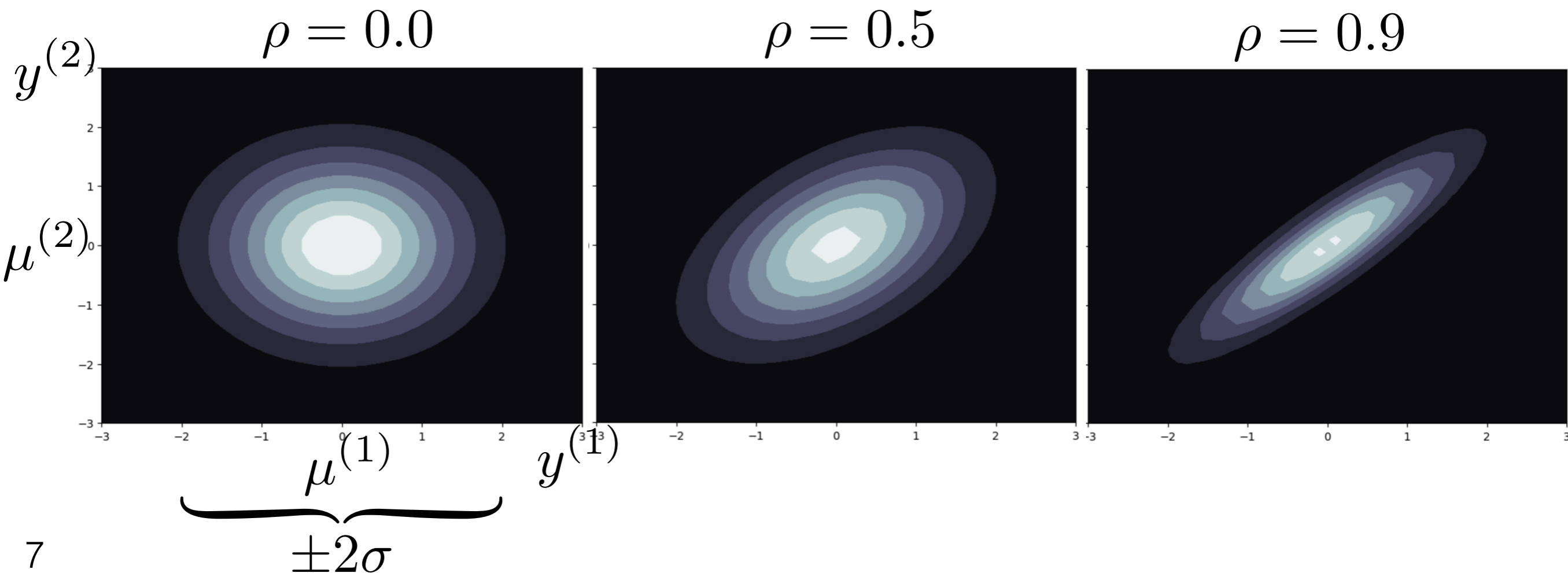
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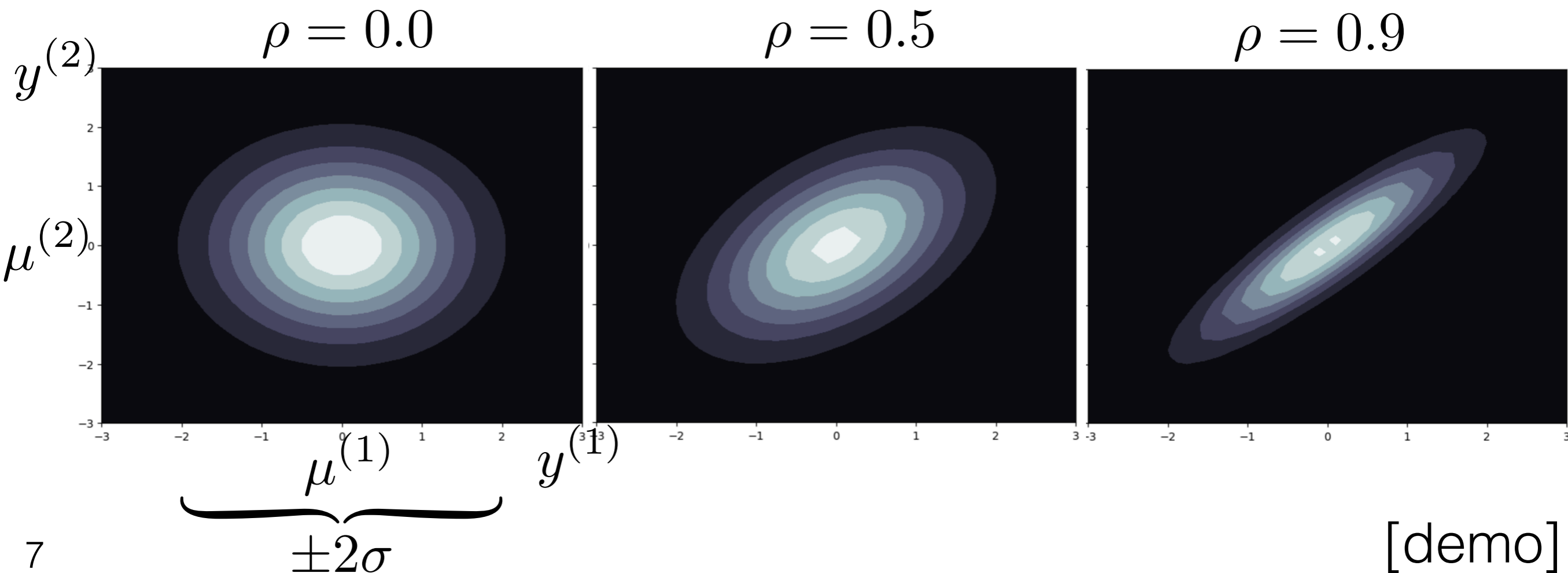
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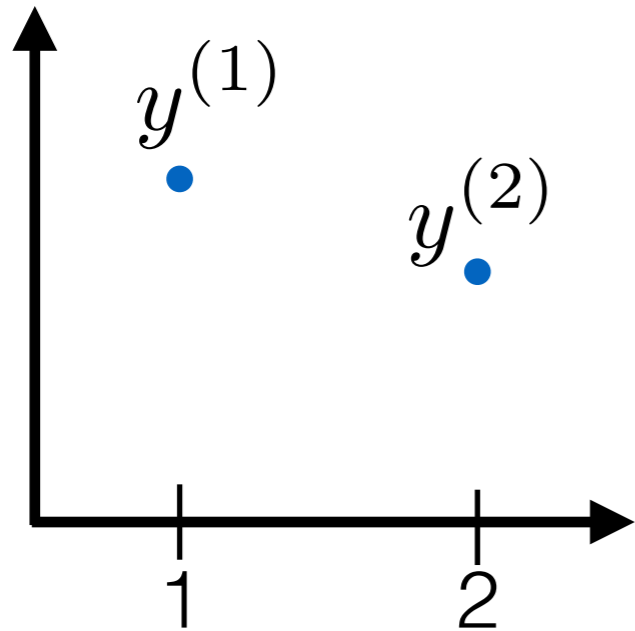
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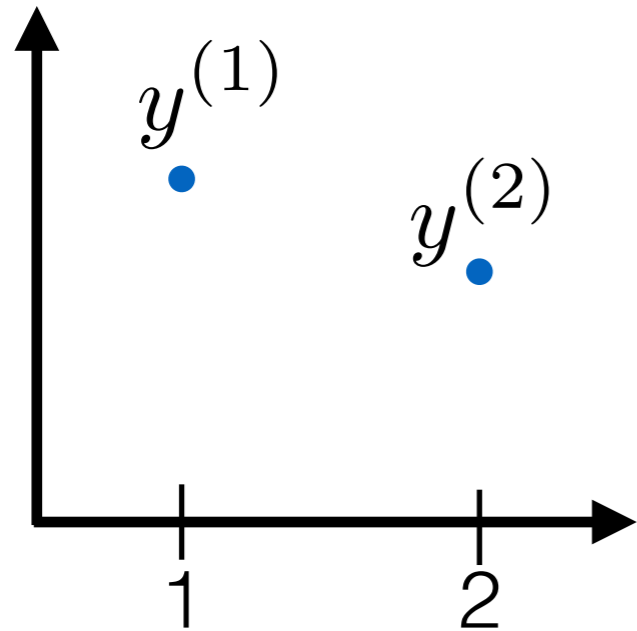
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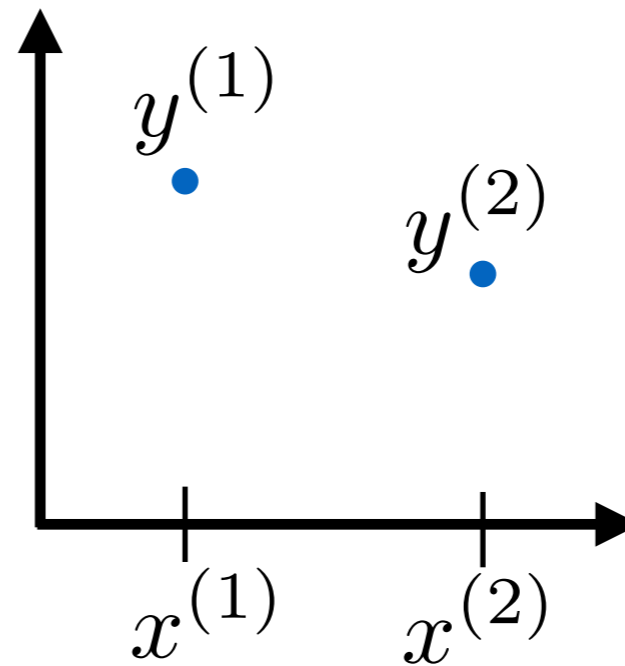
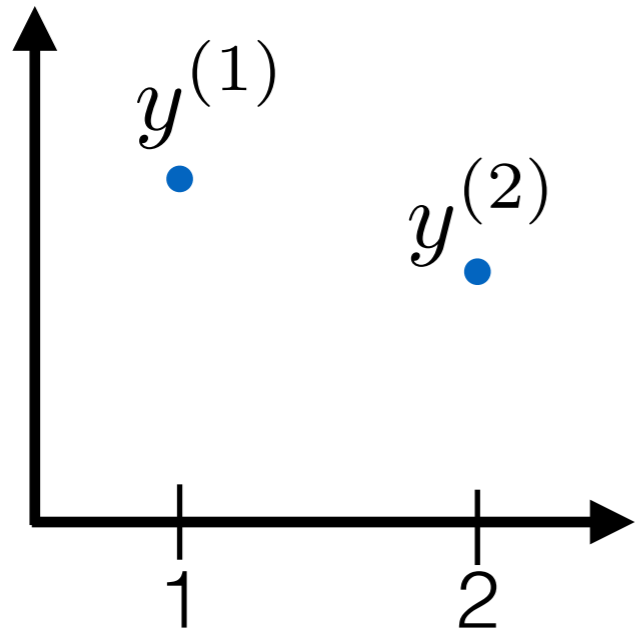
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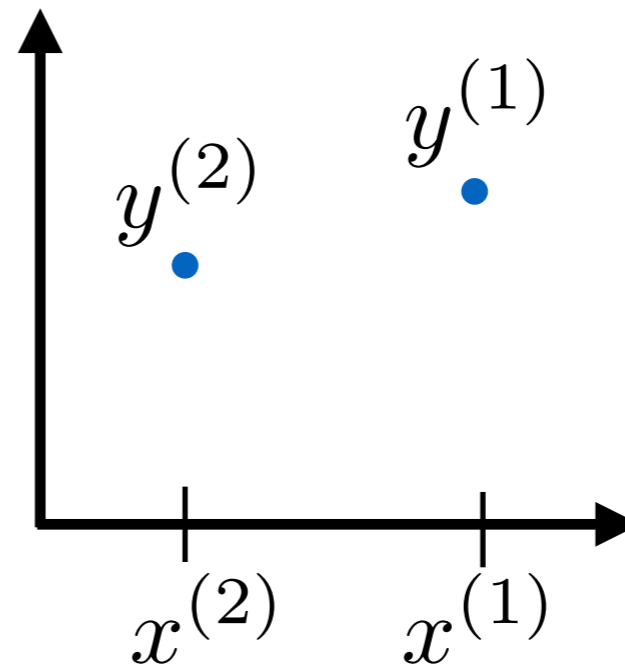
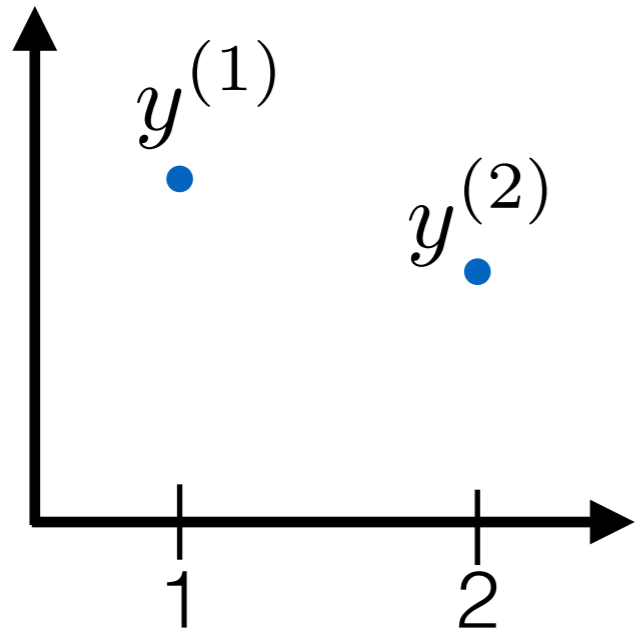
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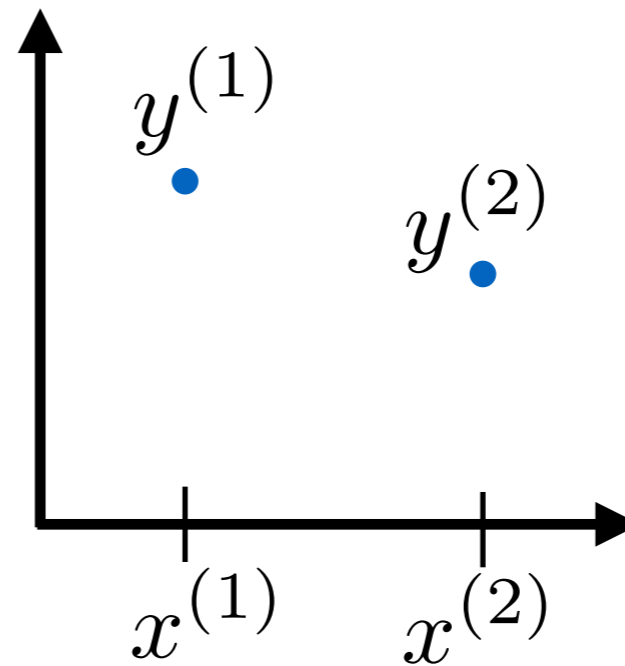
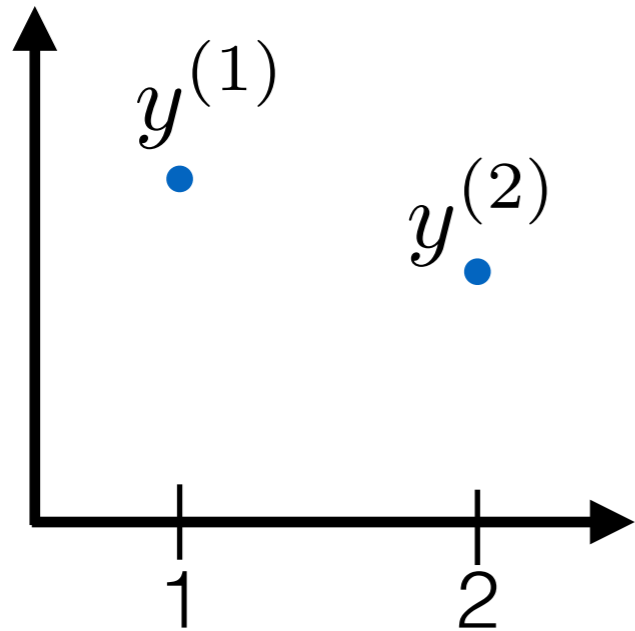
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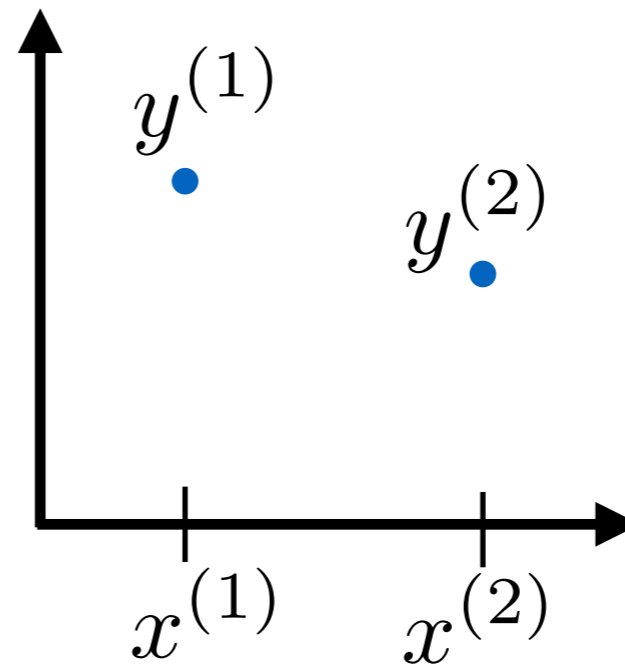
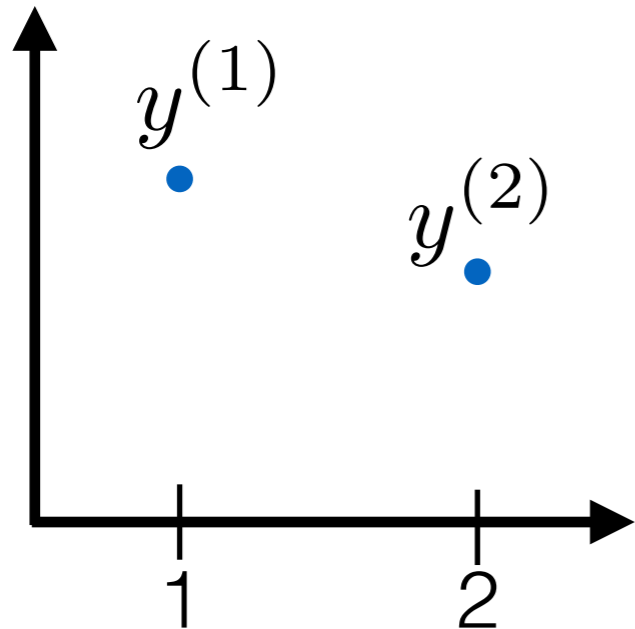
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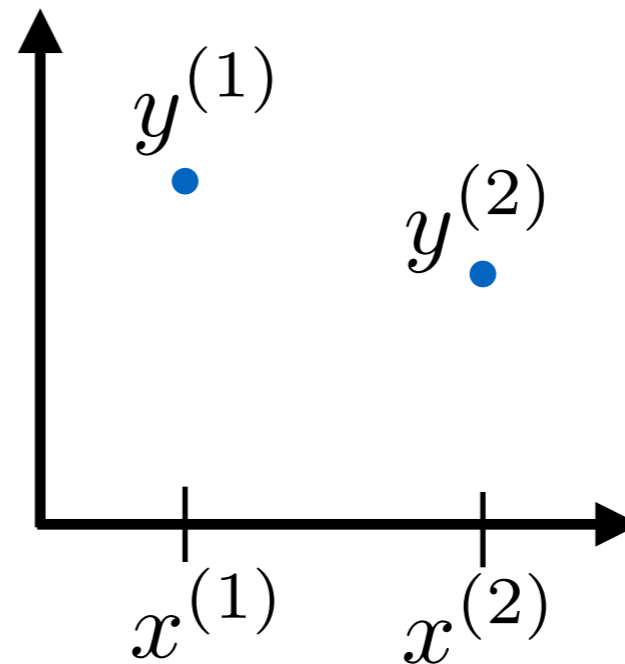
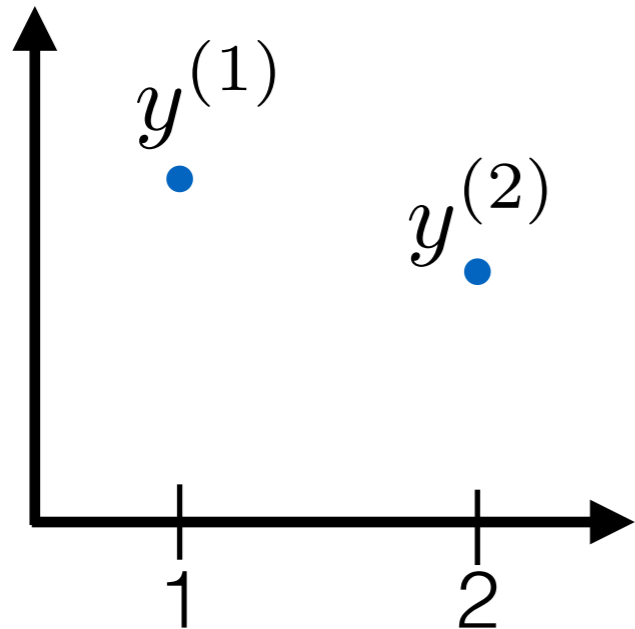
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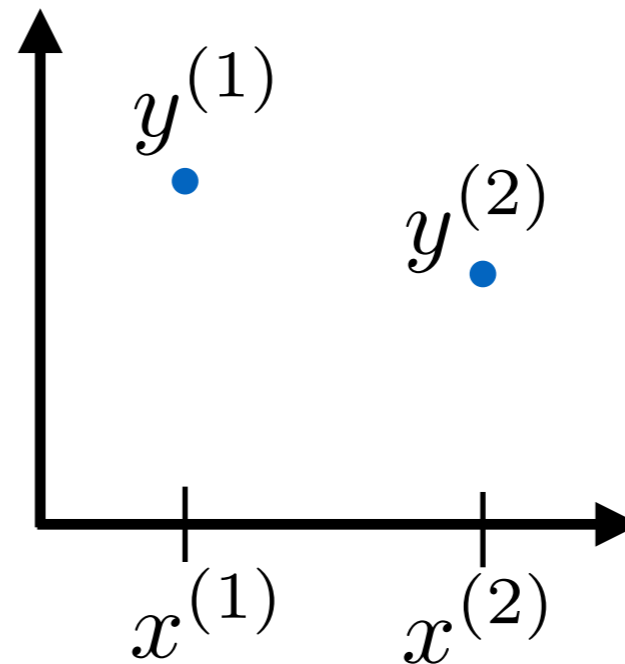
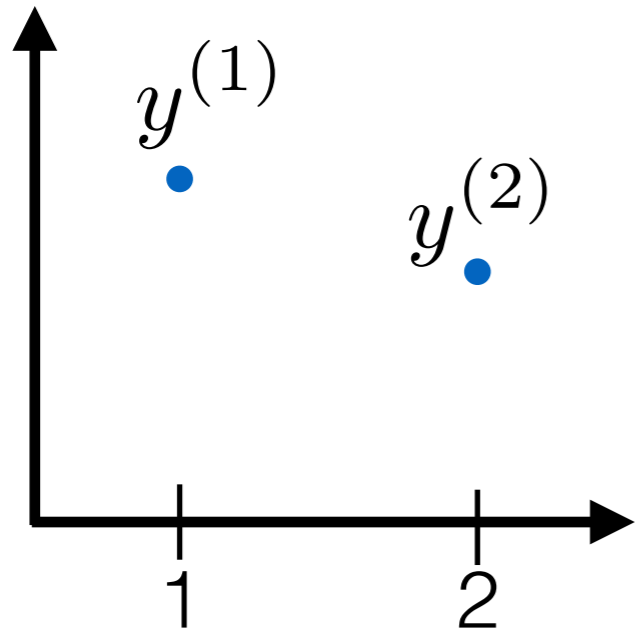
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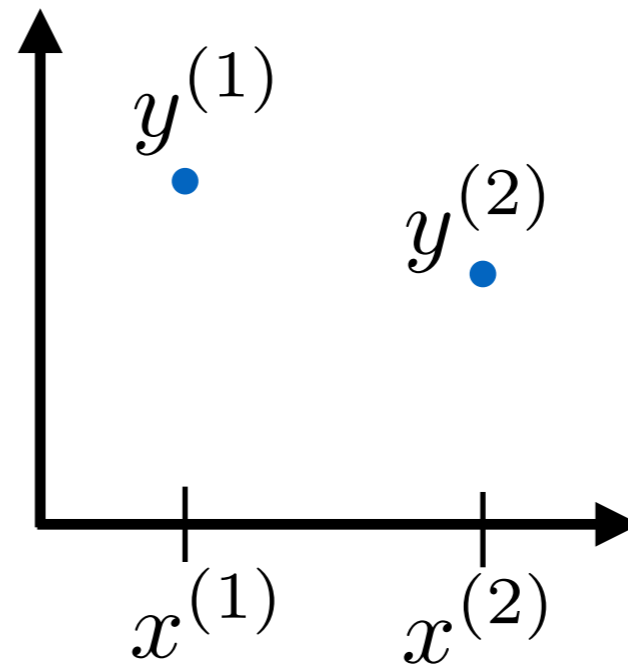
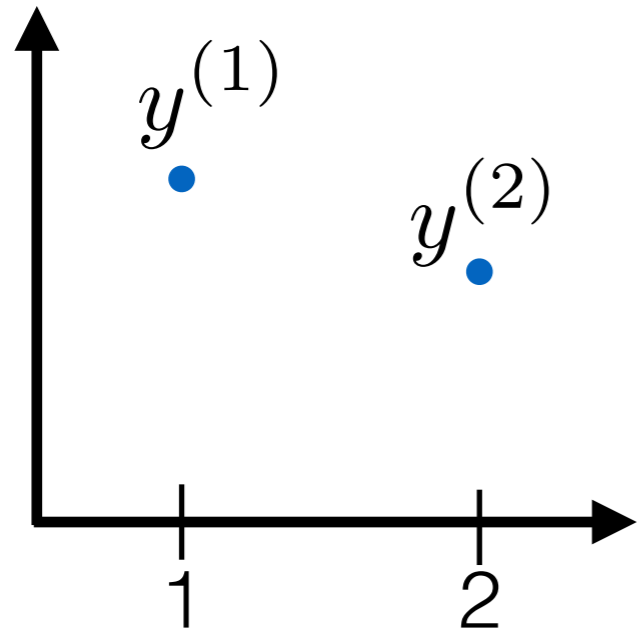
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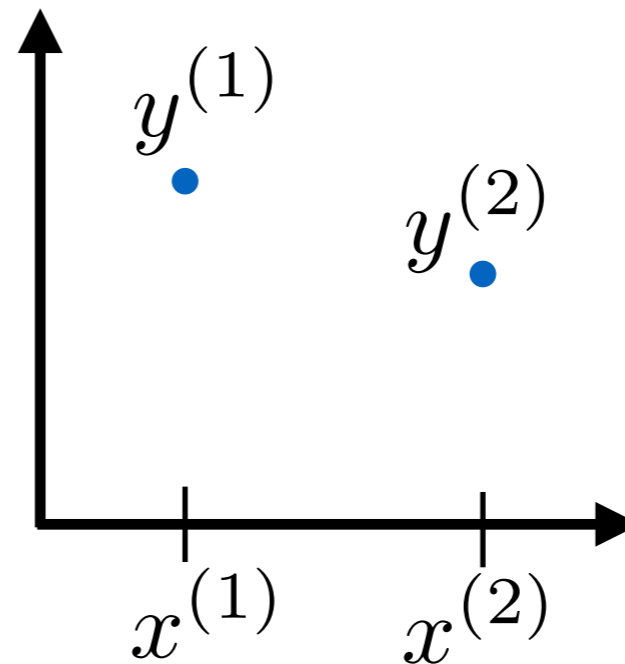
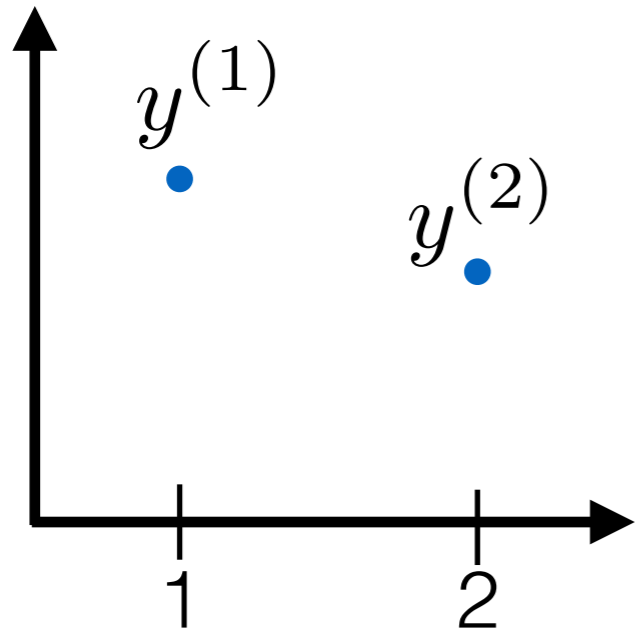
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$$K_{m,m'} = \sigma^2 \rho(|x^{(m)} - x^{(m')}|)$$

Multivariate Gaussian using locations

- Next: Similar setup but an M -dimensional Gaussian instead of just 2 dimensions

- We have M locations (need not be in order):

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

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- Let's try $\rho(\Delta) = \exp(-\frac{1}{2}\Delta^2)$

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 - Check: $\rho(0) = ?$

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- Check: $\rho(0) = 1$, $\rho(\Delta)$ is ? as Δ increases

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[demo1, demo2]

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[demo1, demo2]

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We just drew random functions from a type of Gaussian
process that is very commonly used in practice!