

Gaussian Processes for Regression: Models, Algorithms, and Applications

Tamara Broderick
Associate Professor
MIT

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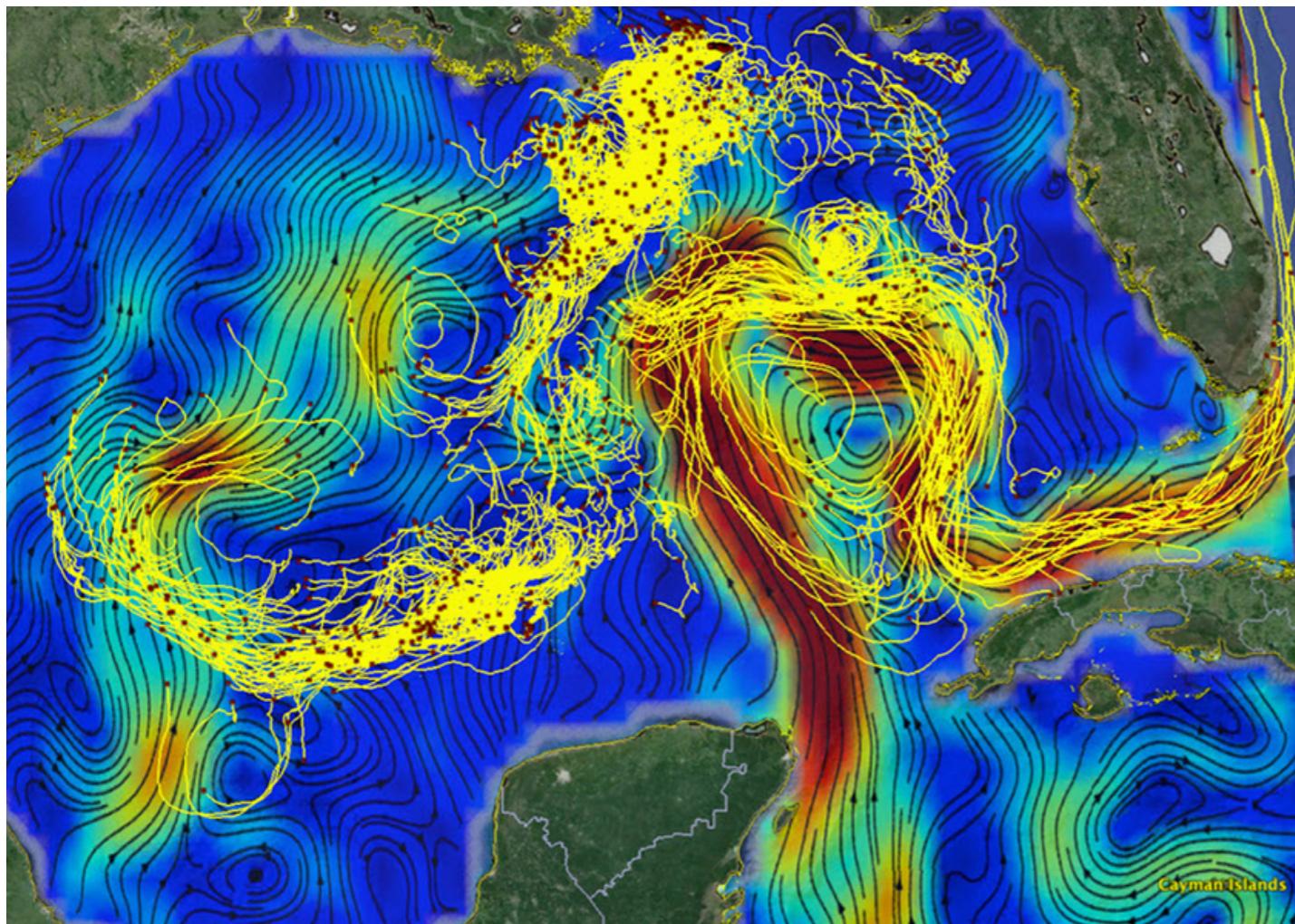
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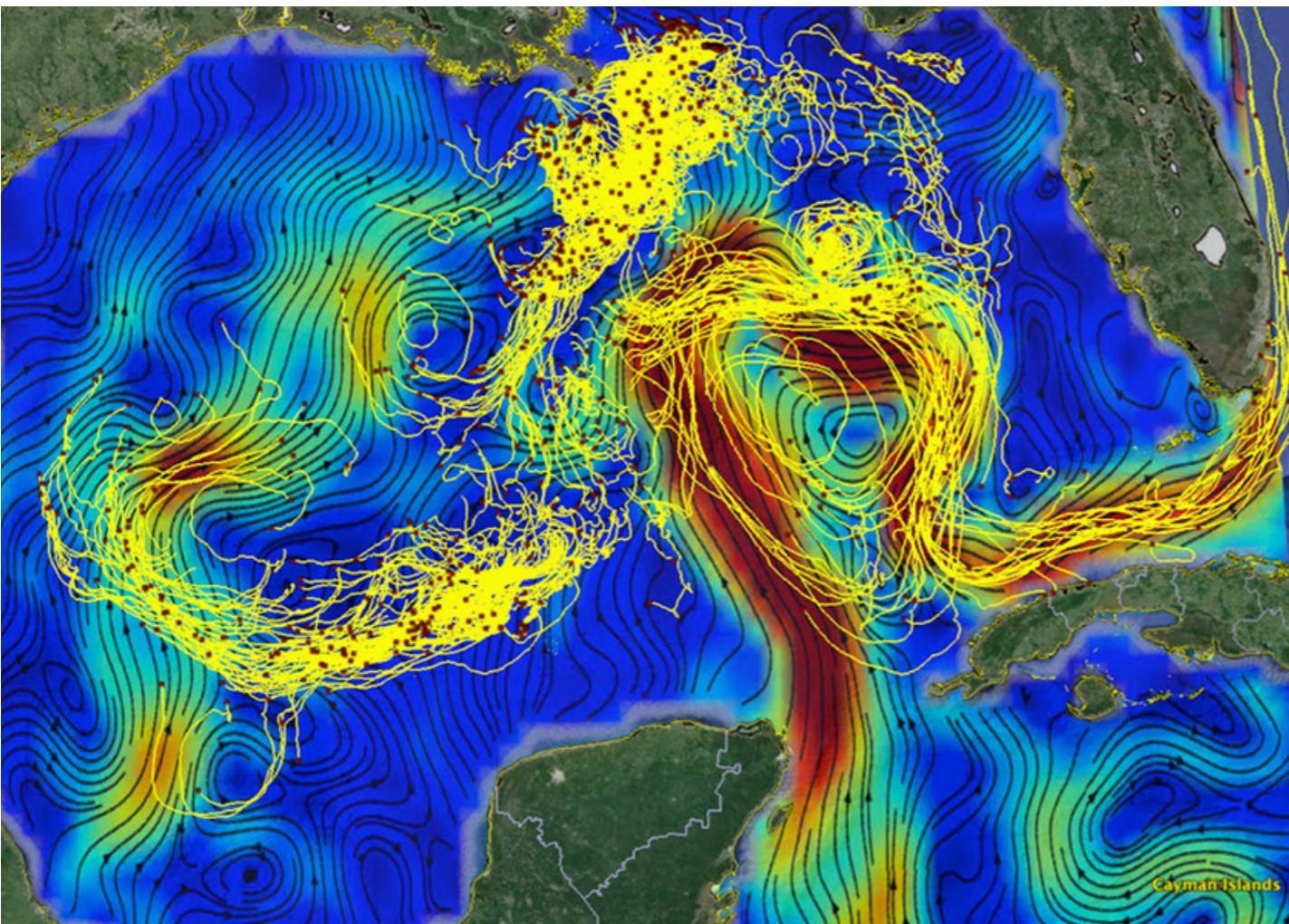


Example:

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

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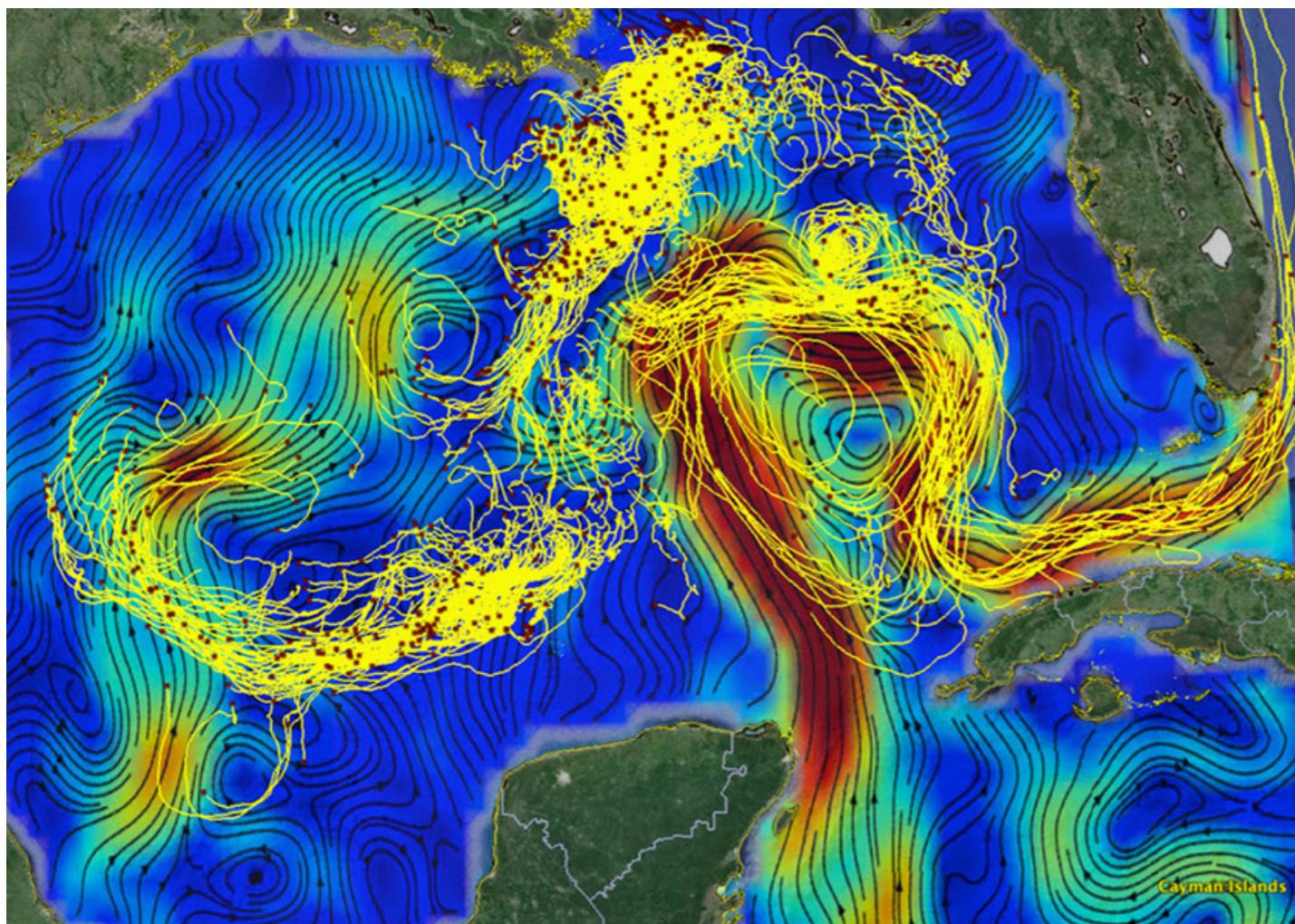
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- The ocean current (velocity vector field) varies by space & time

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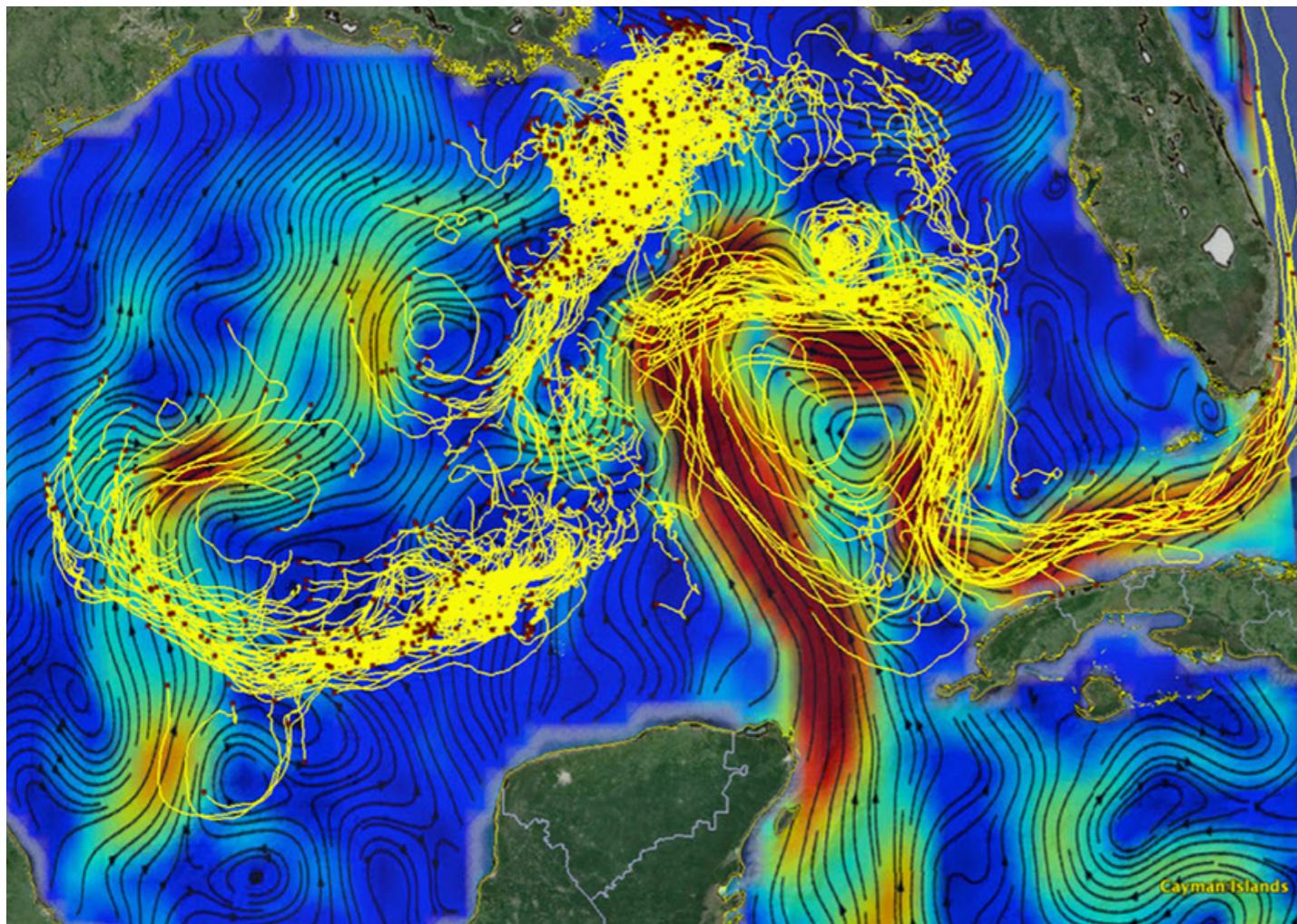
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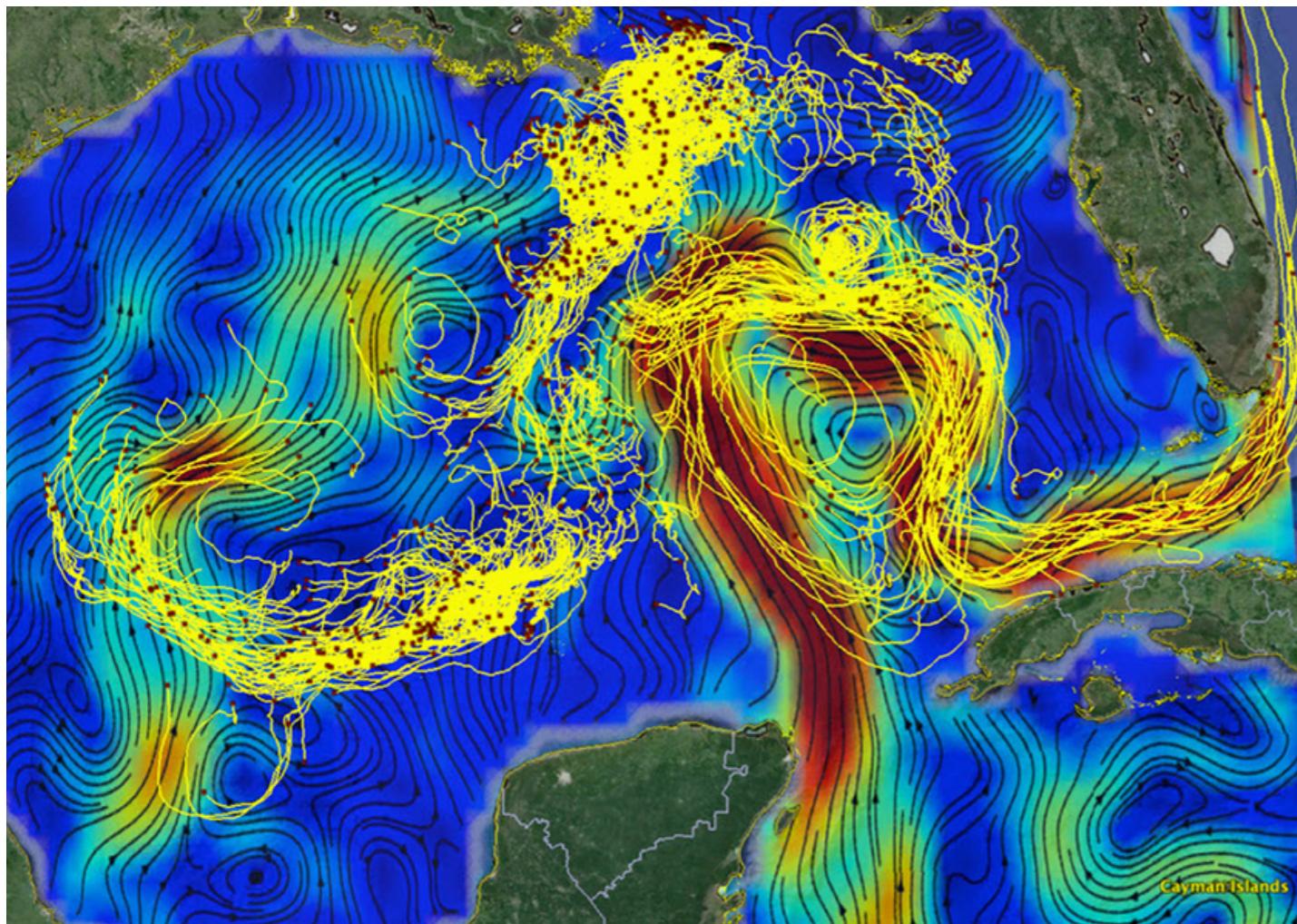
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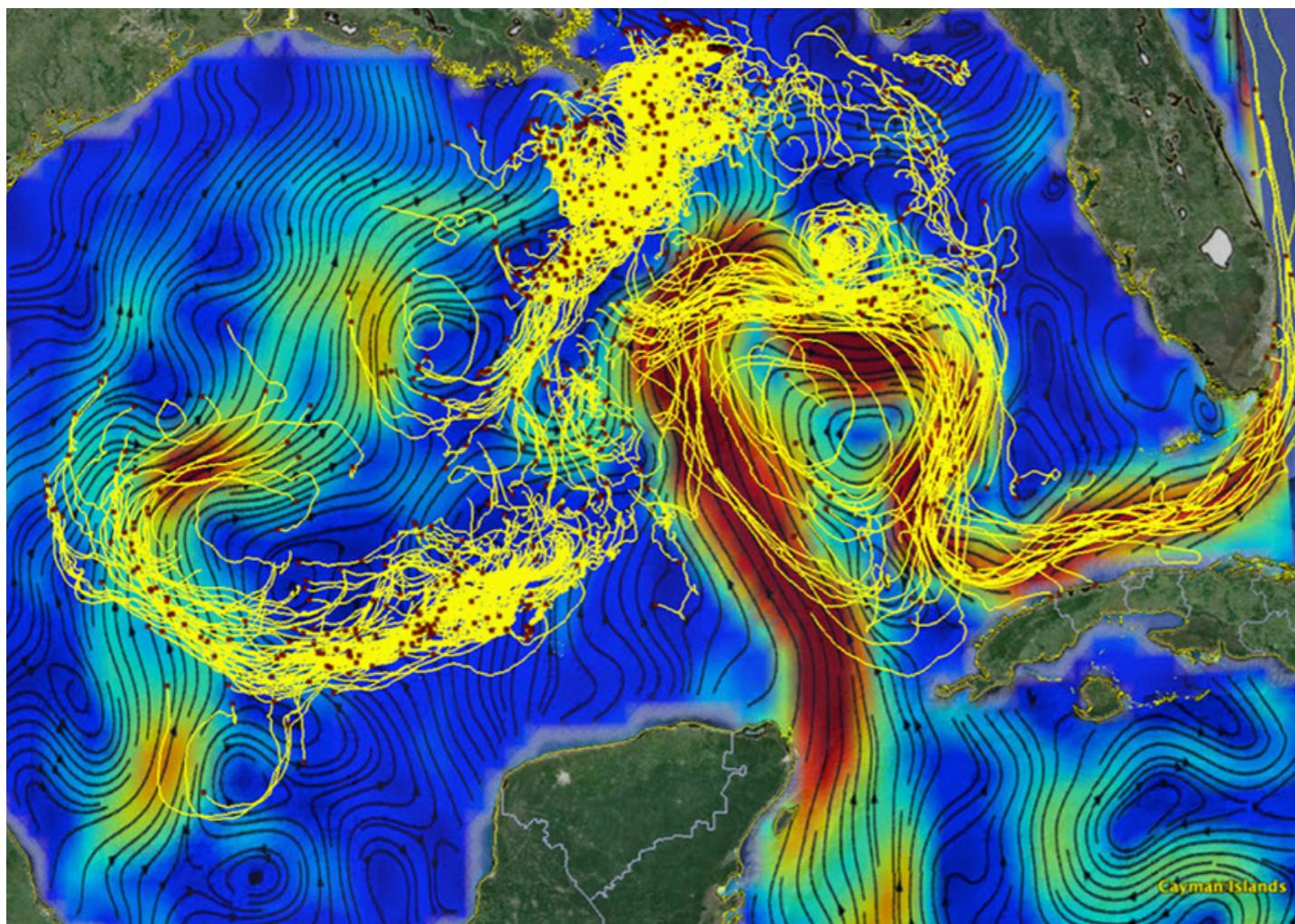
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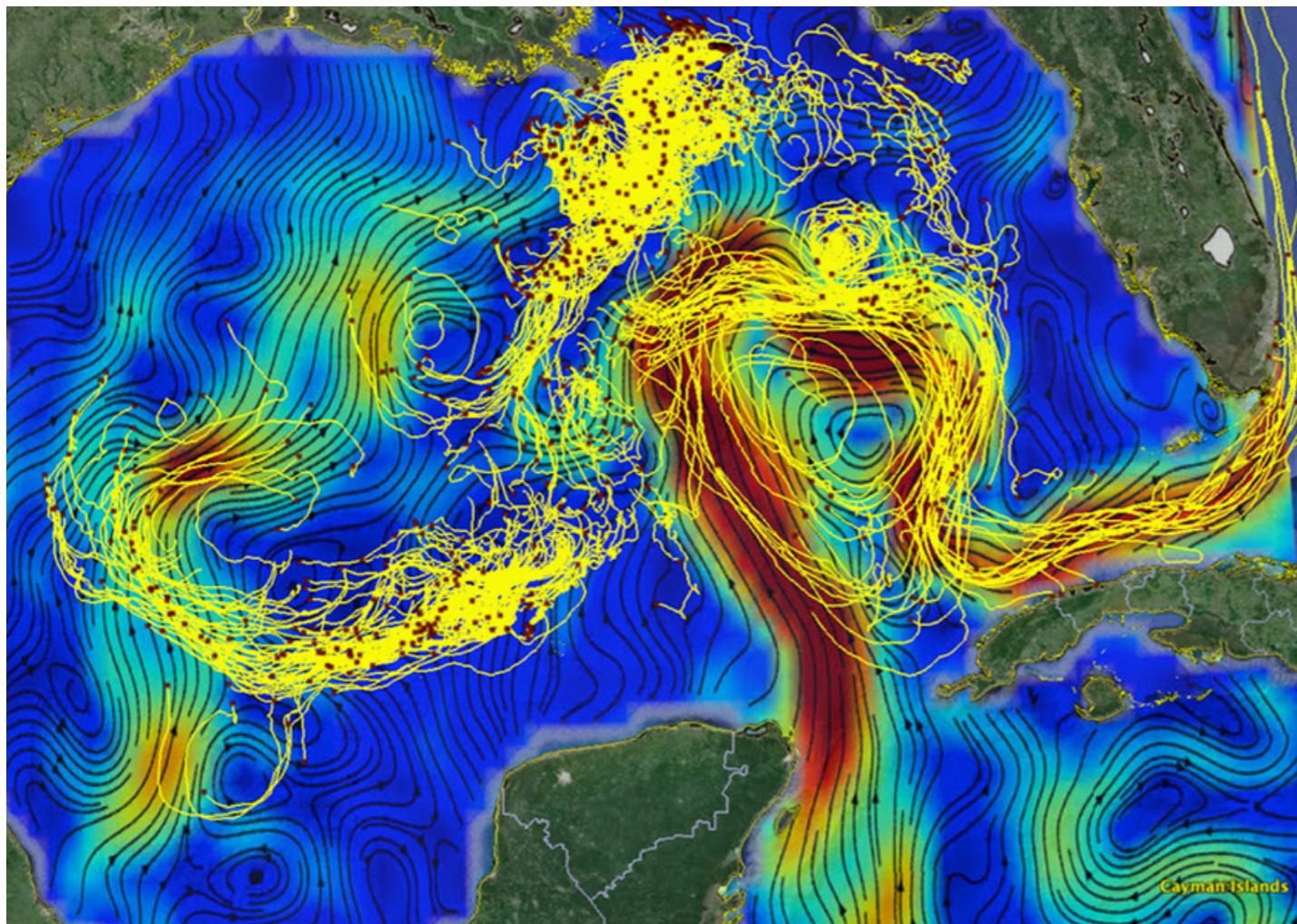
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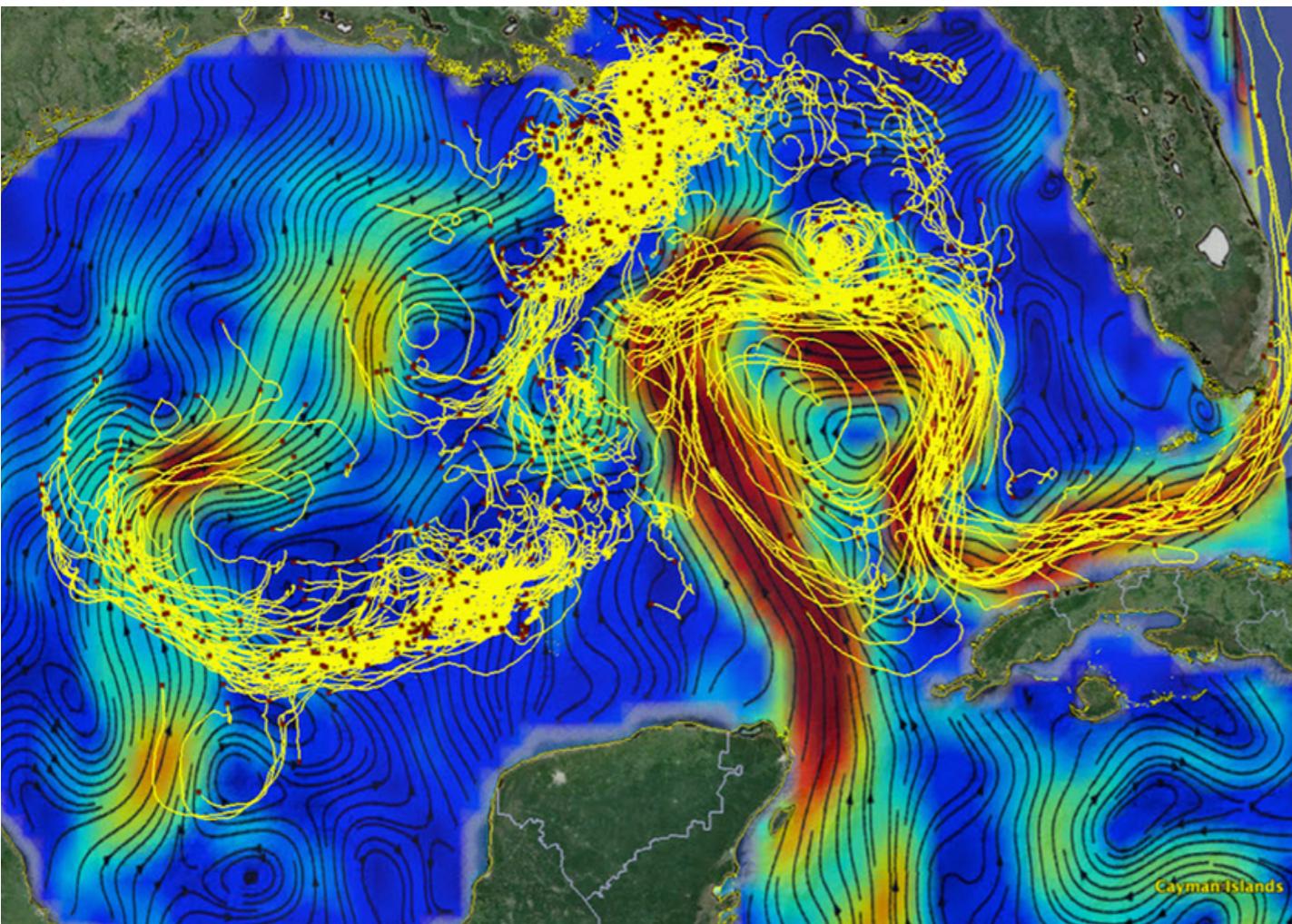
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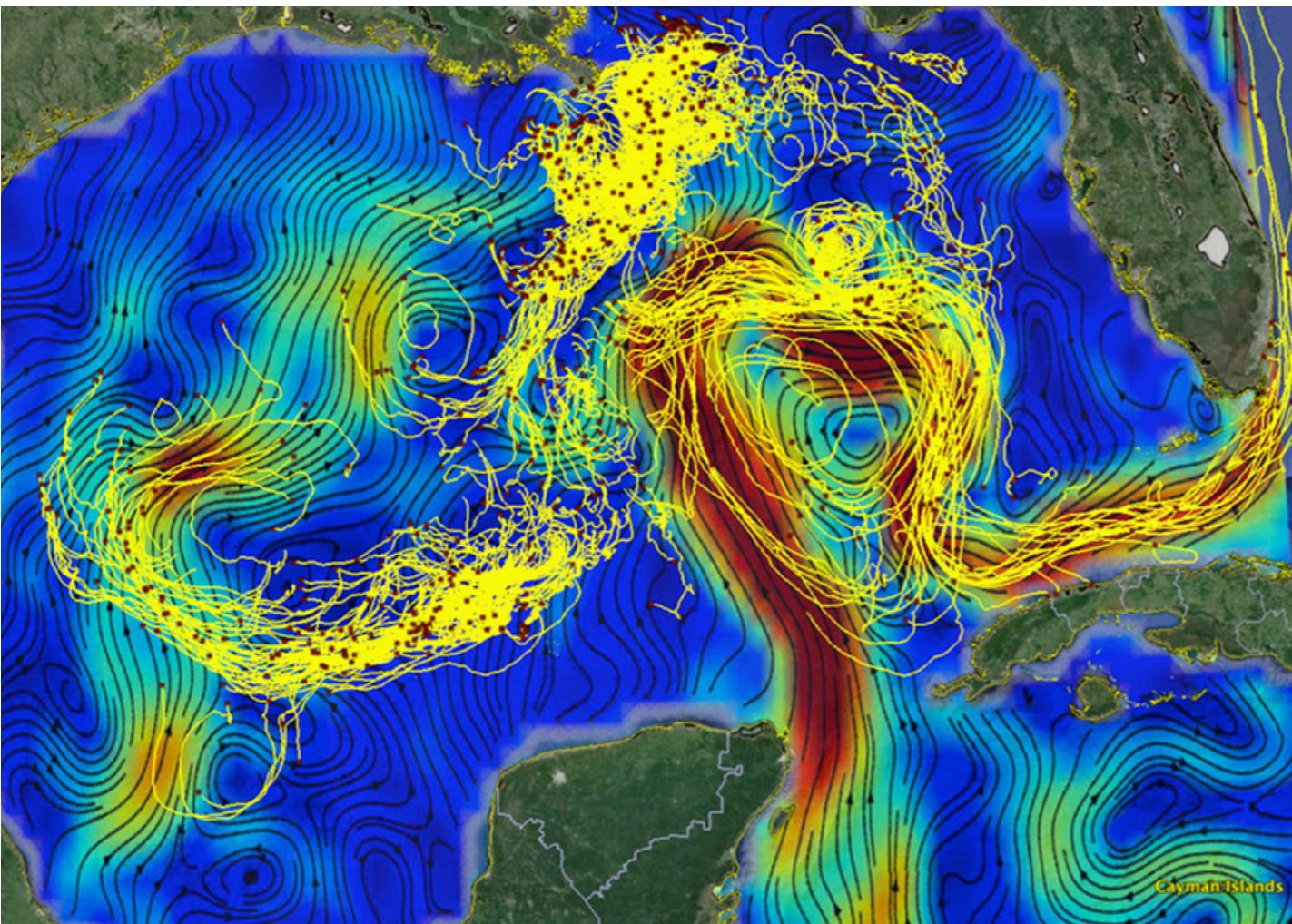
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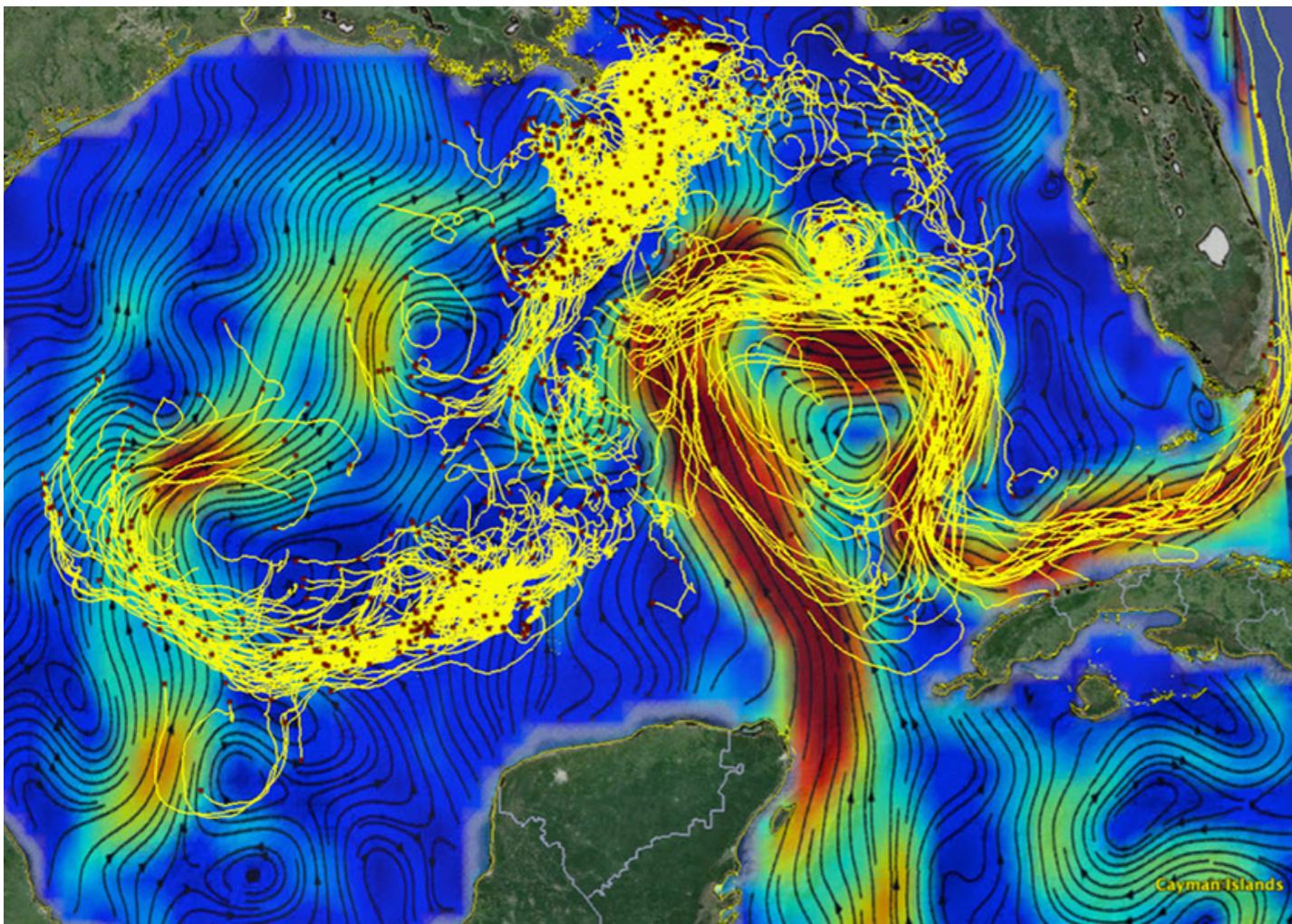
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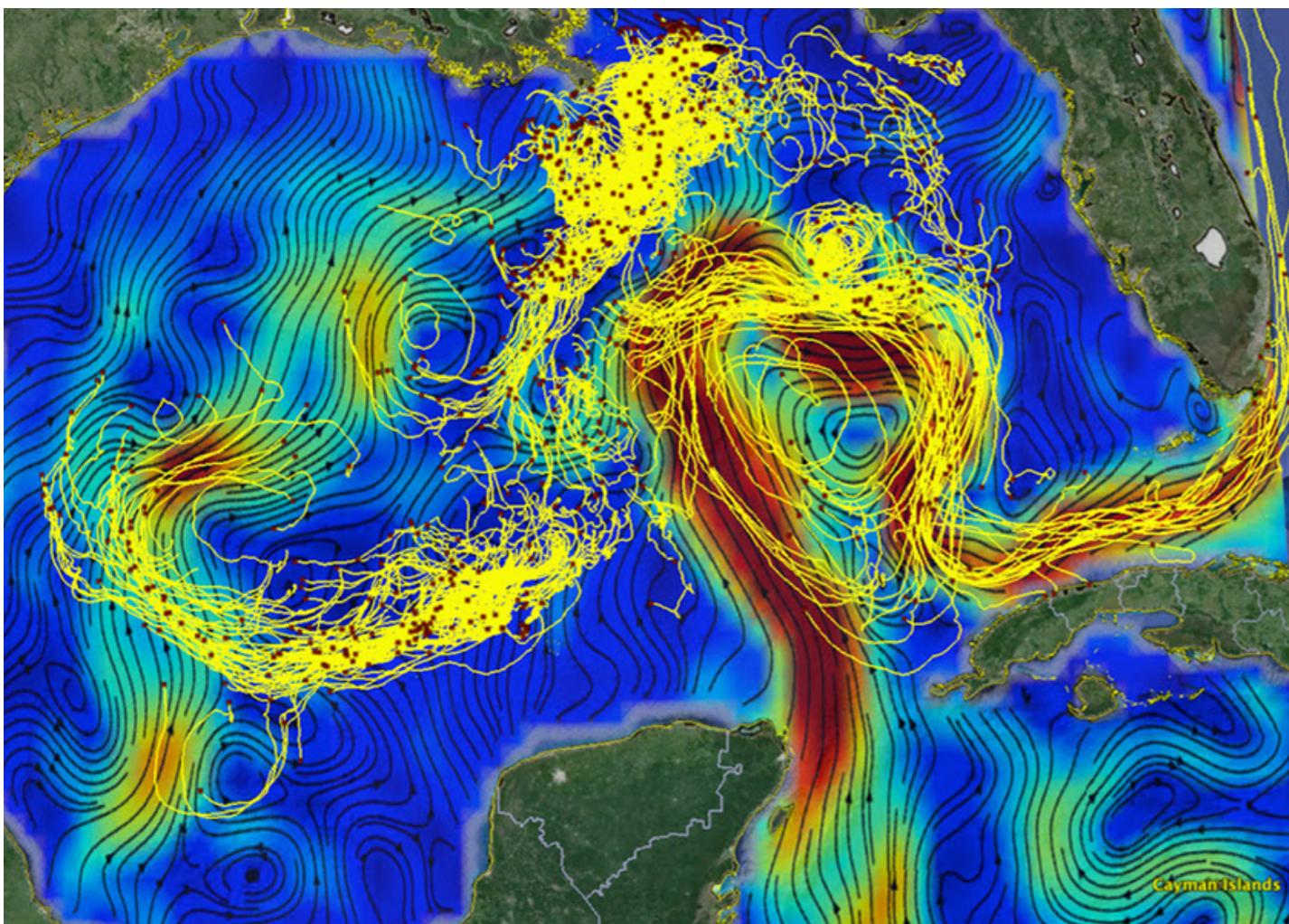
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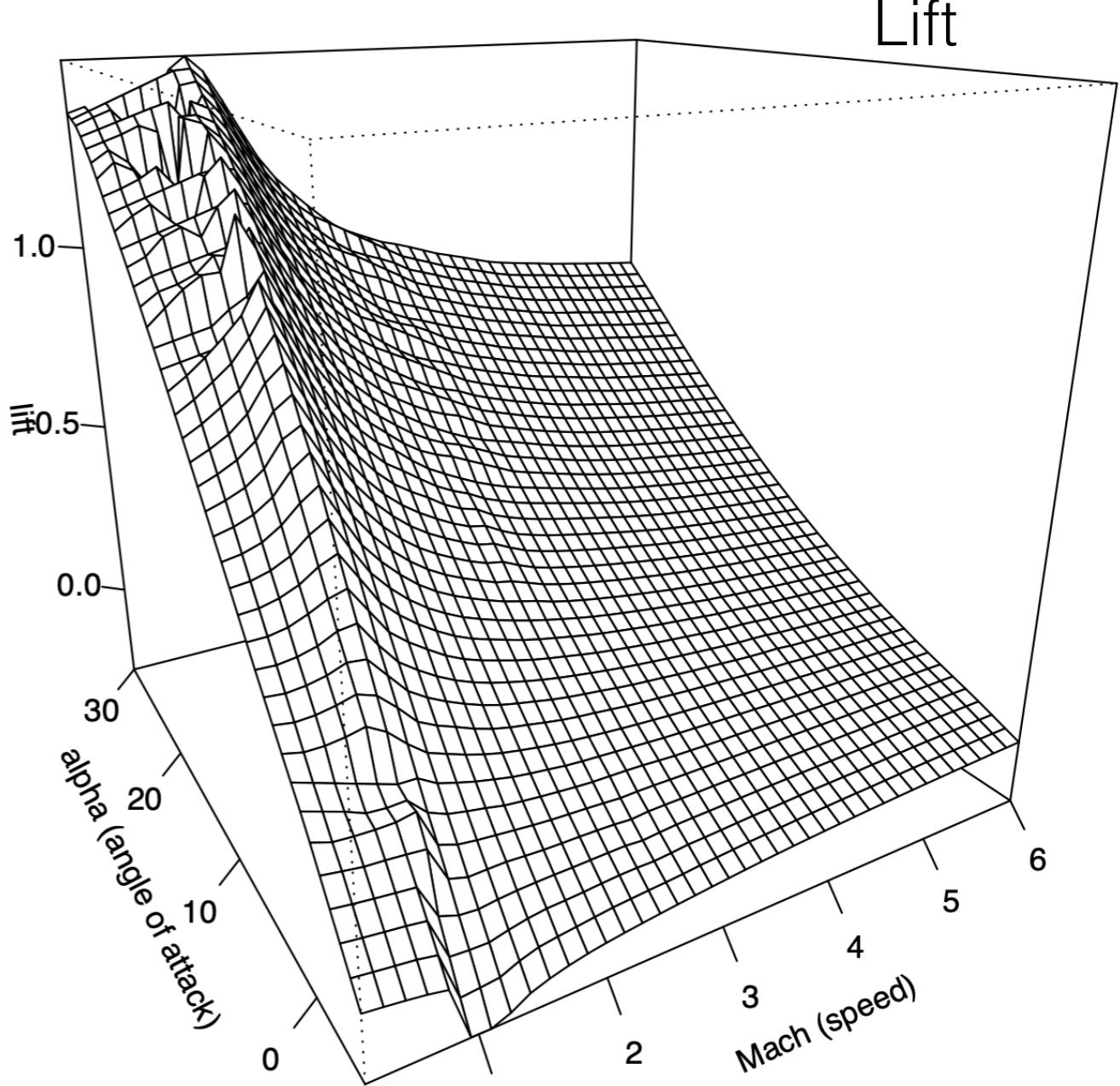
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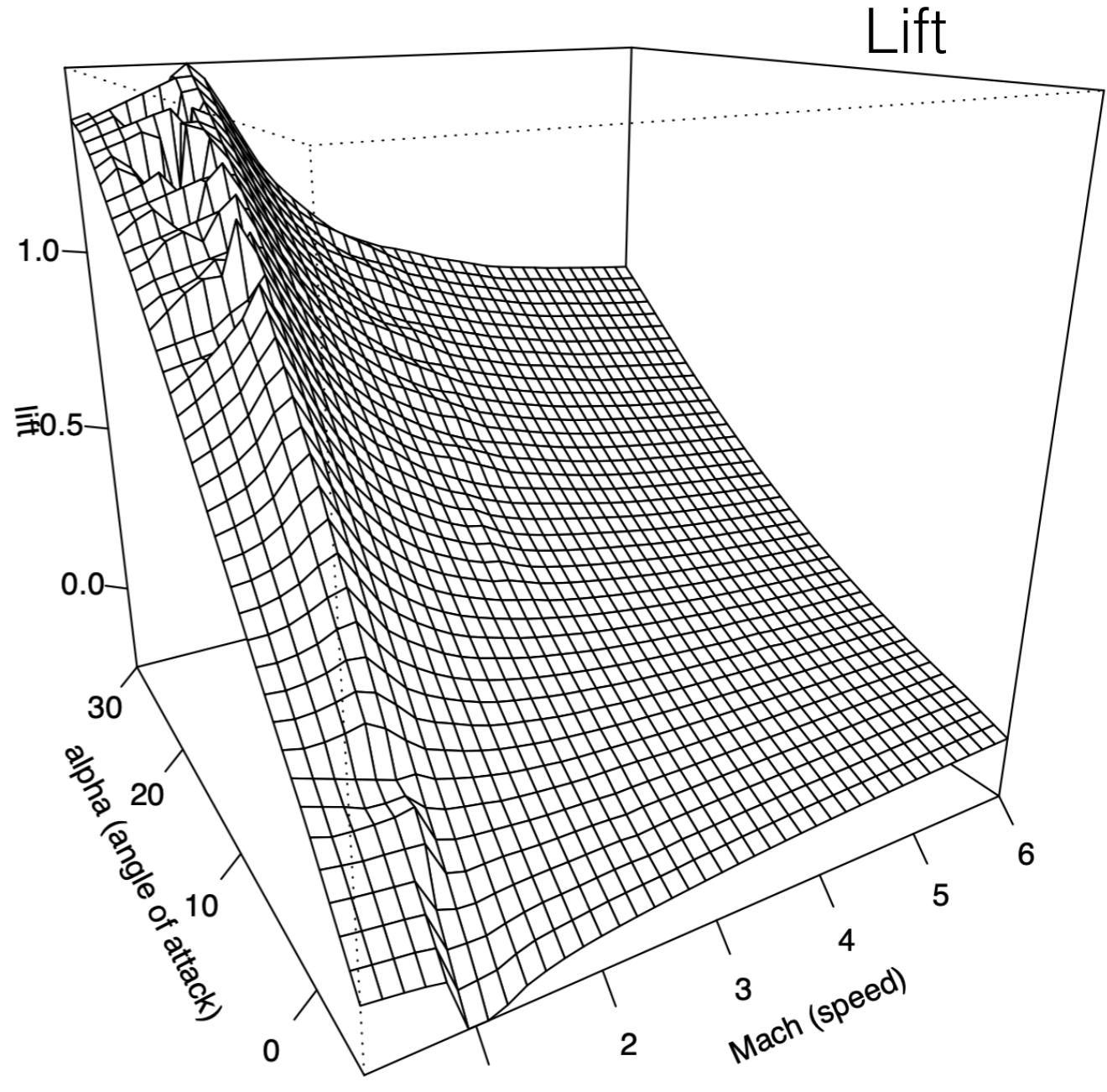
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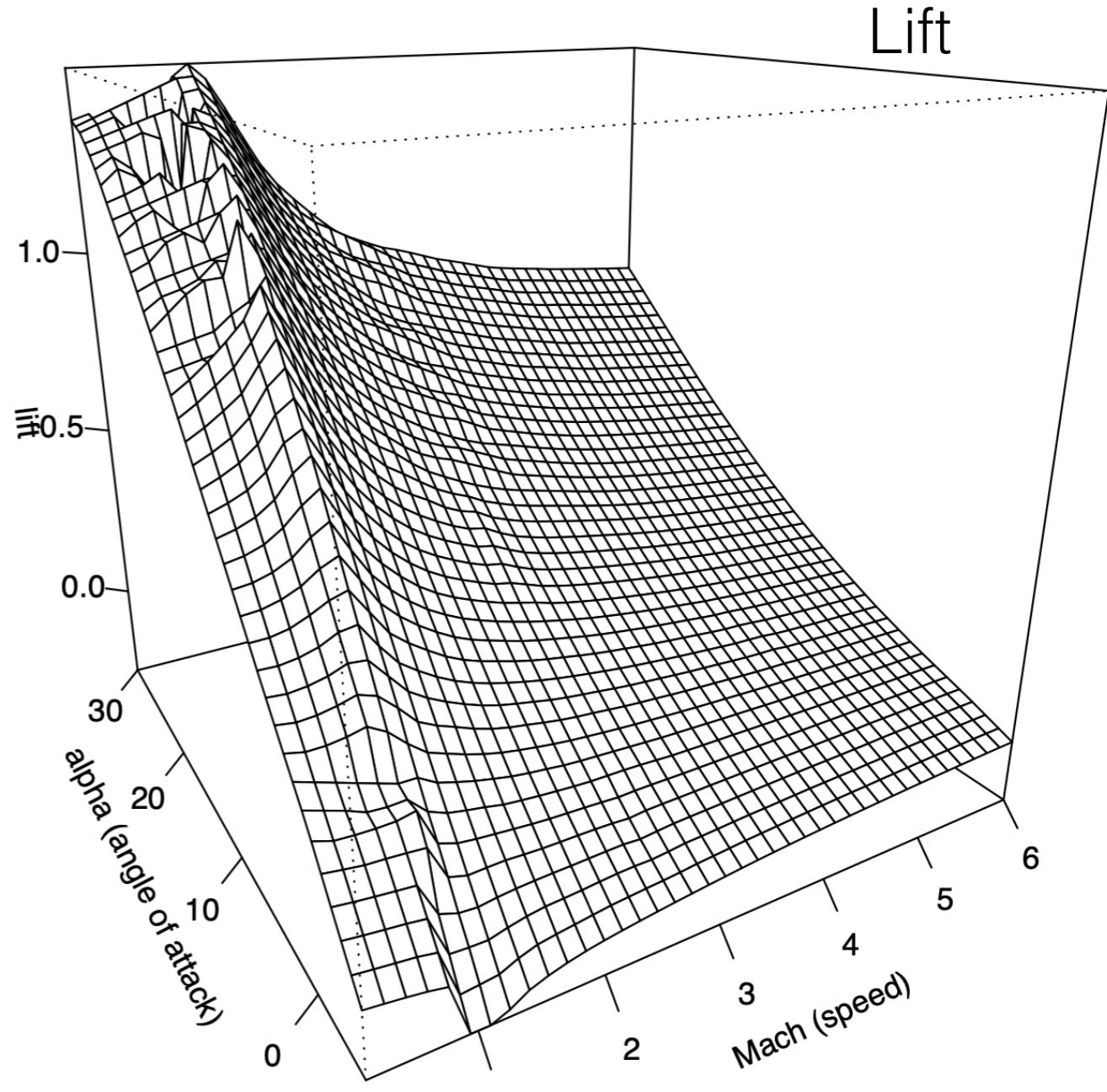
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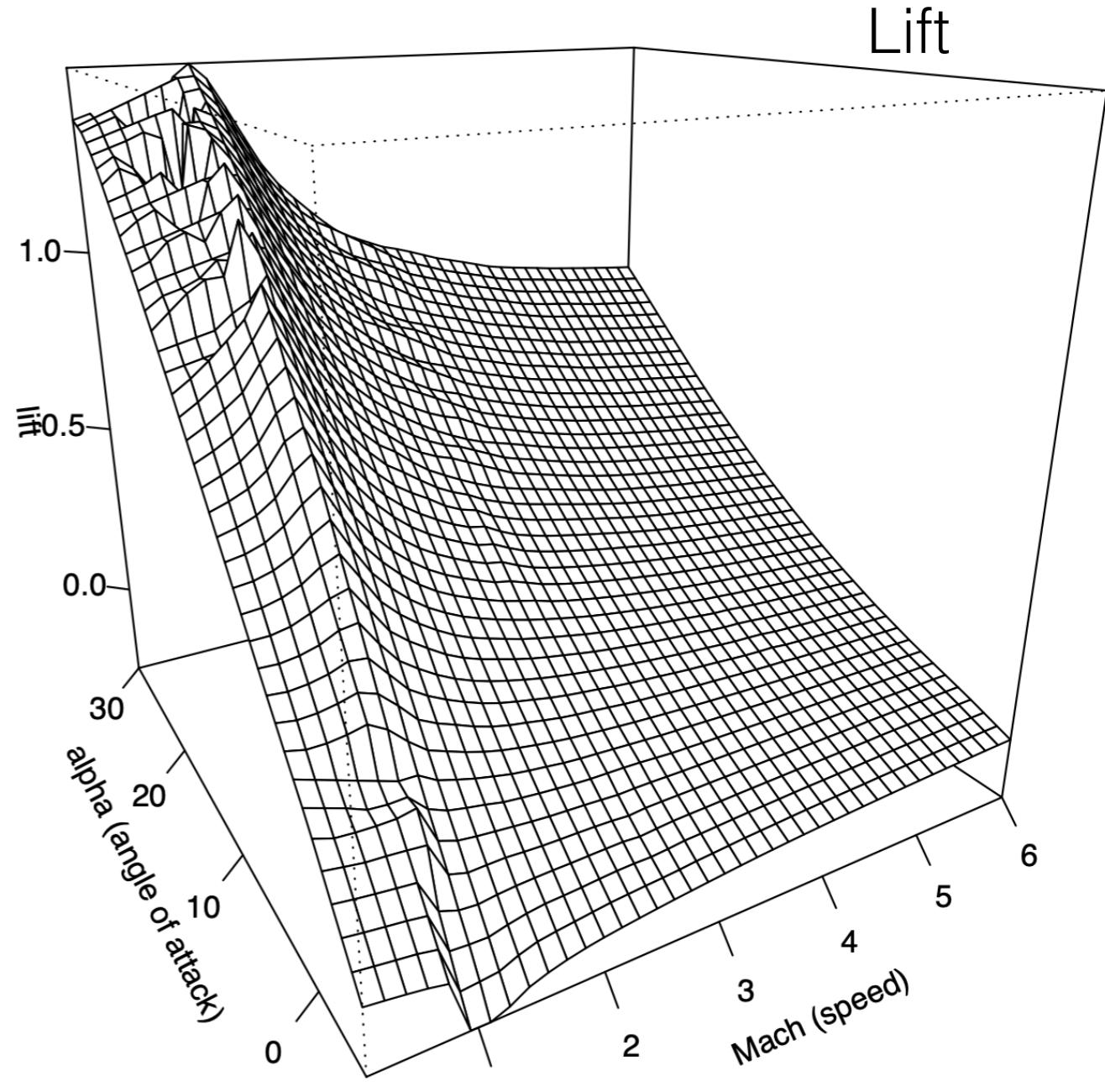
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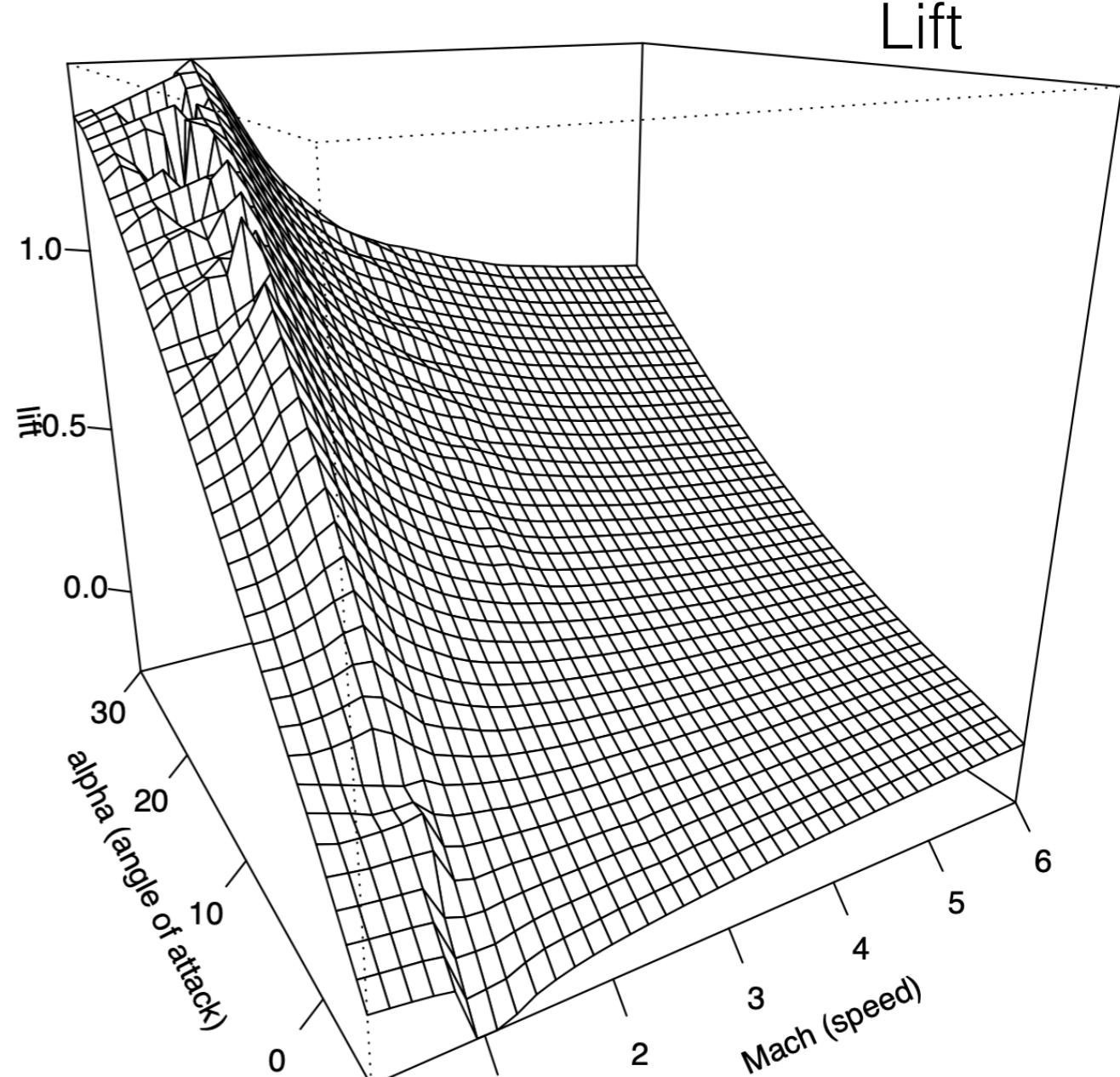
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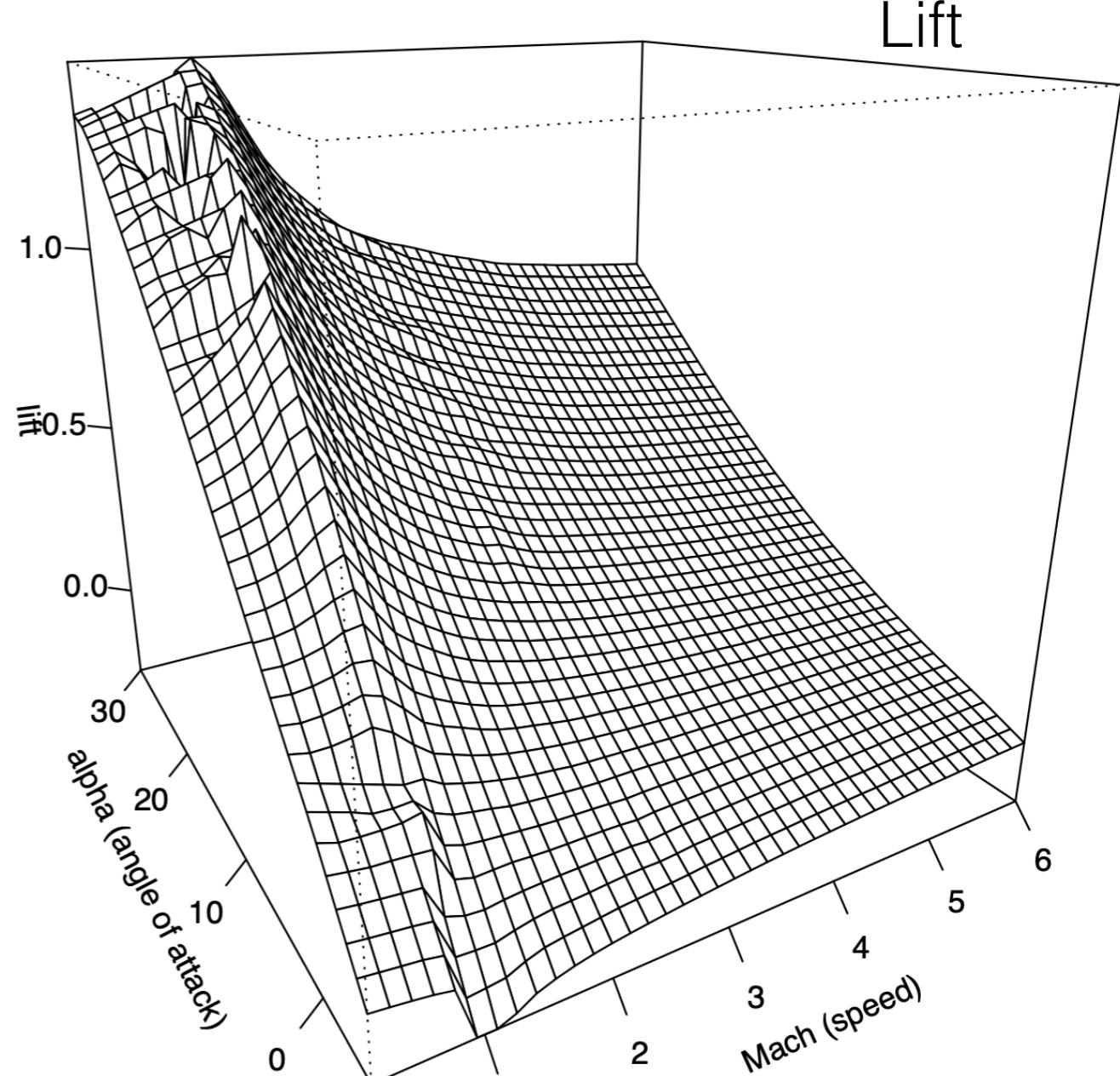
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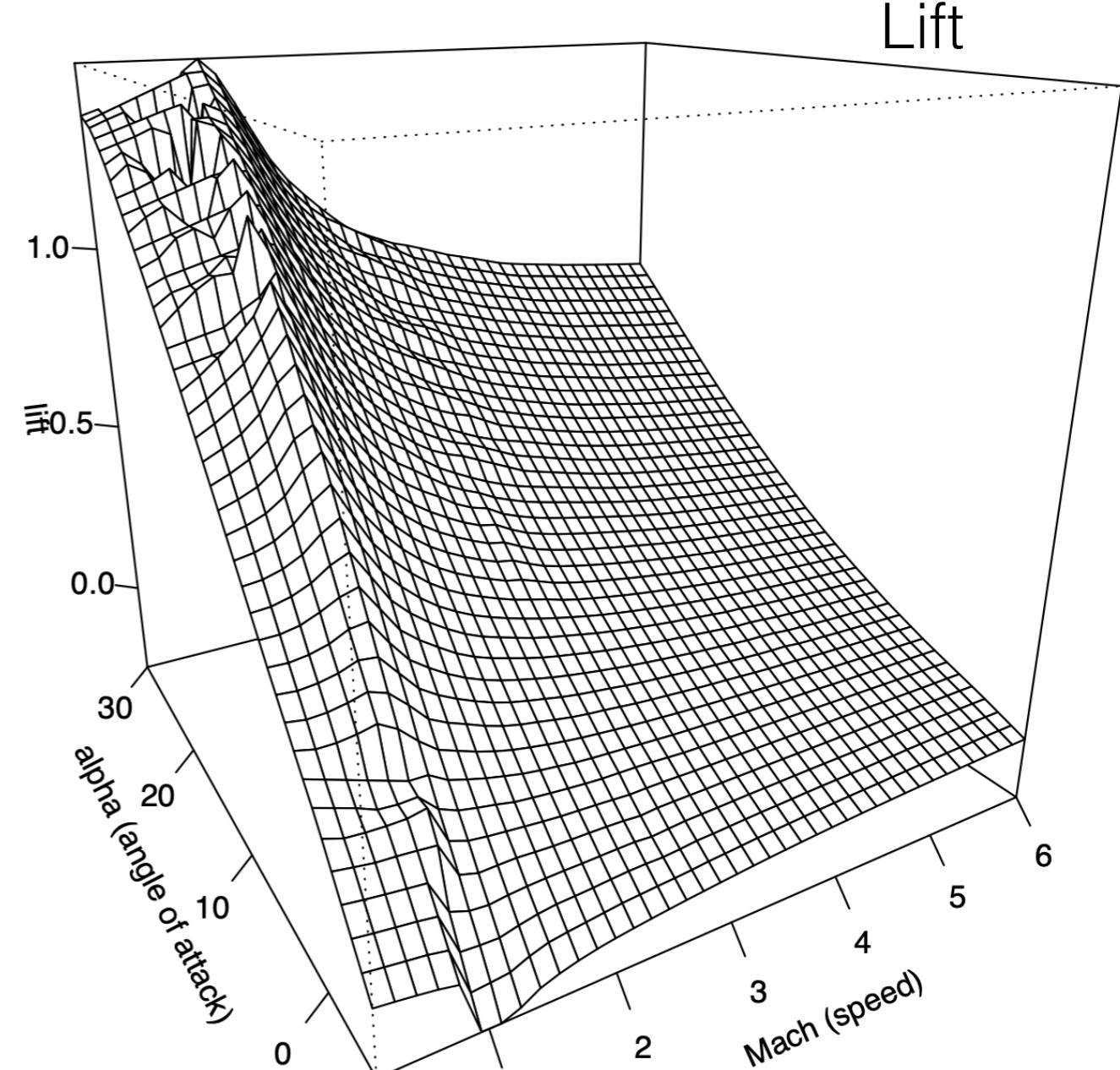
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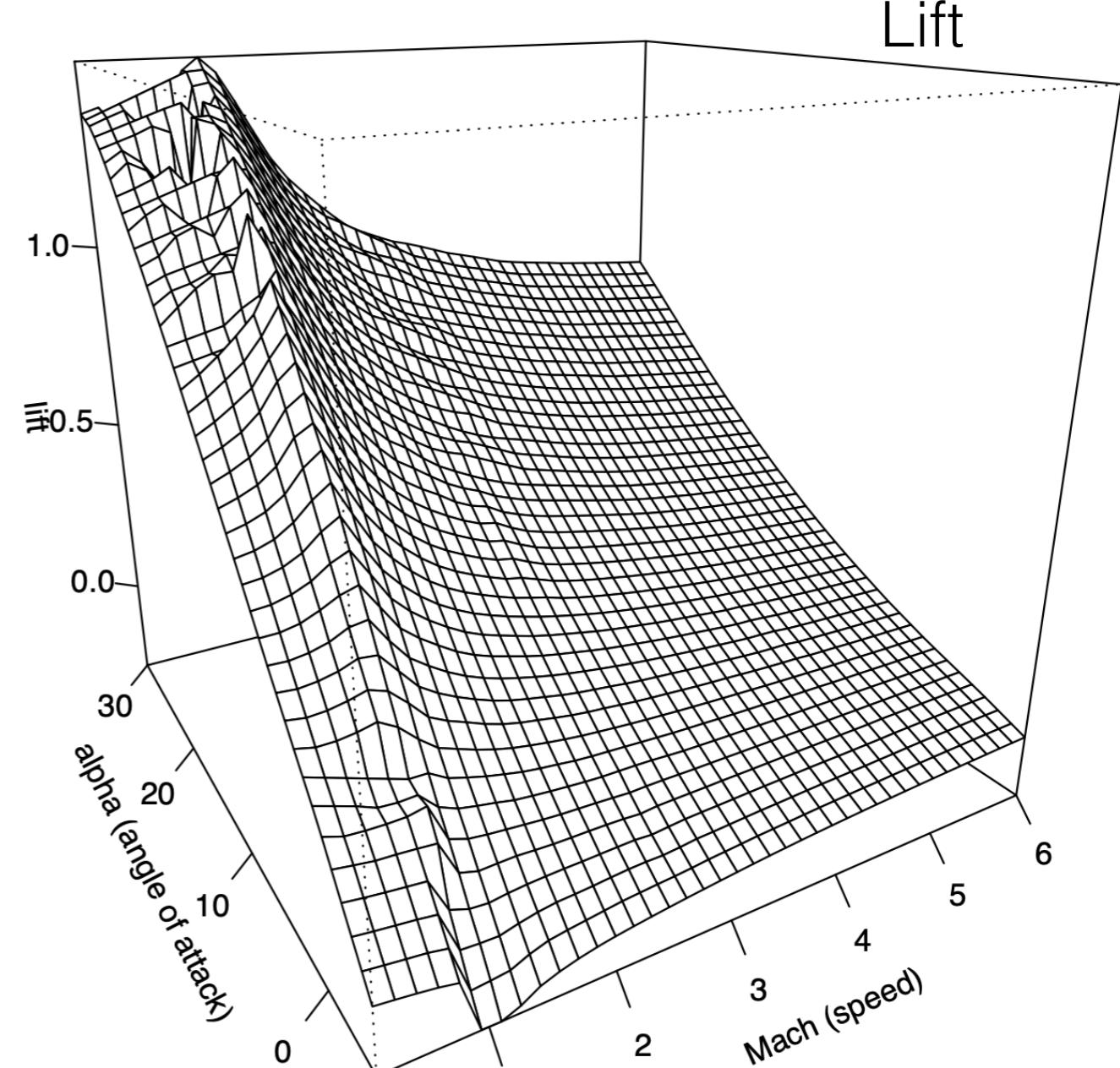
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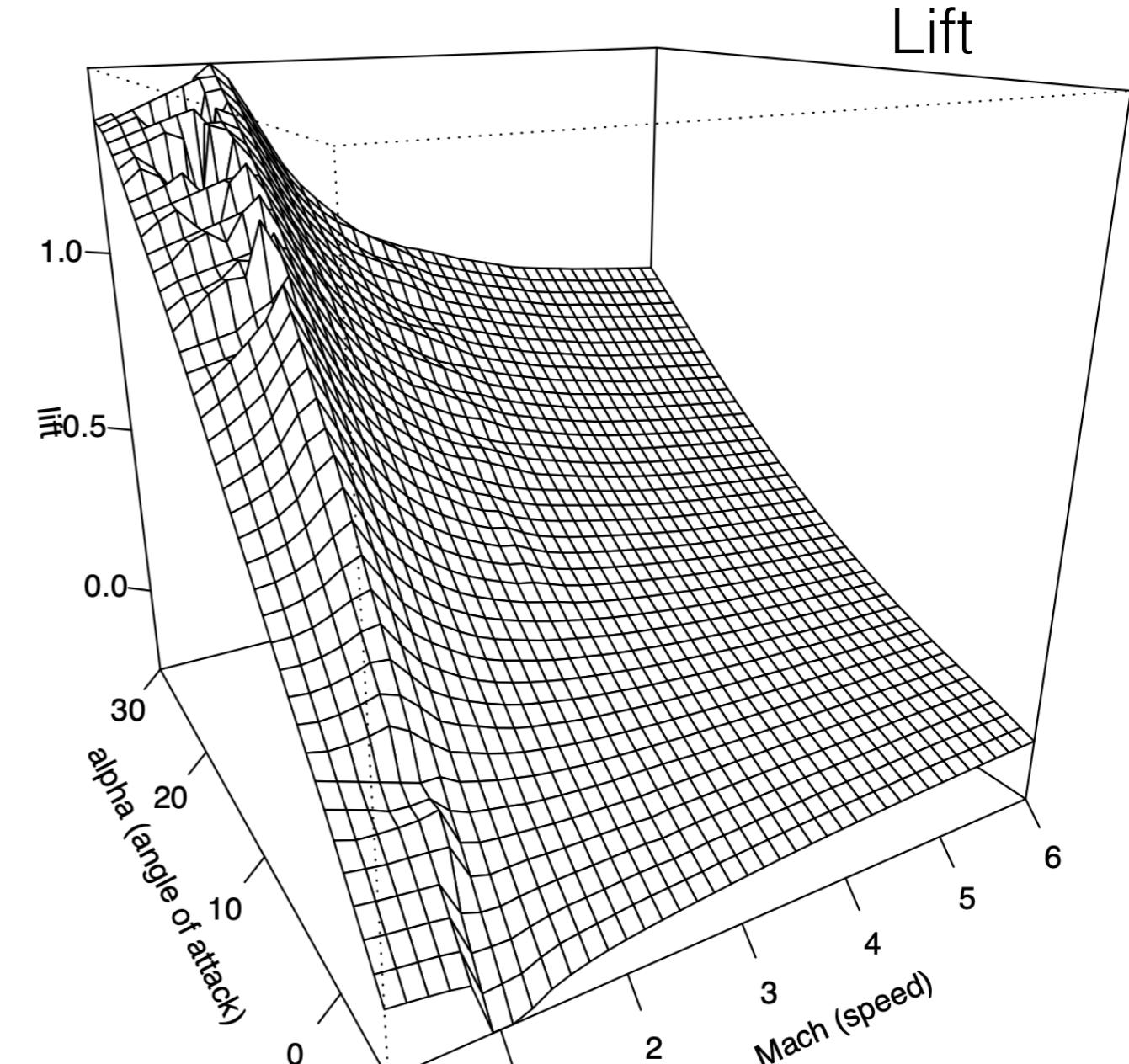
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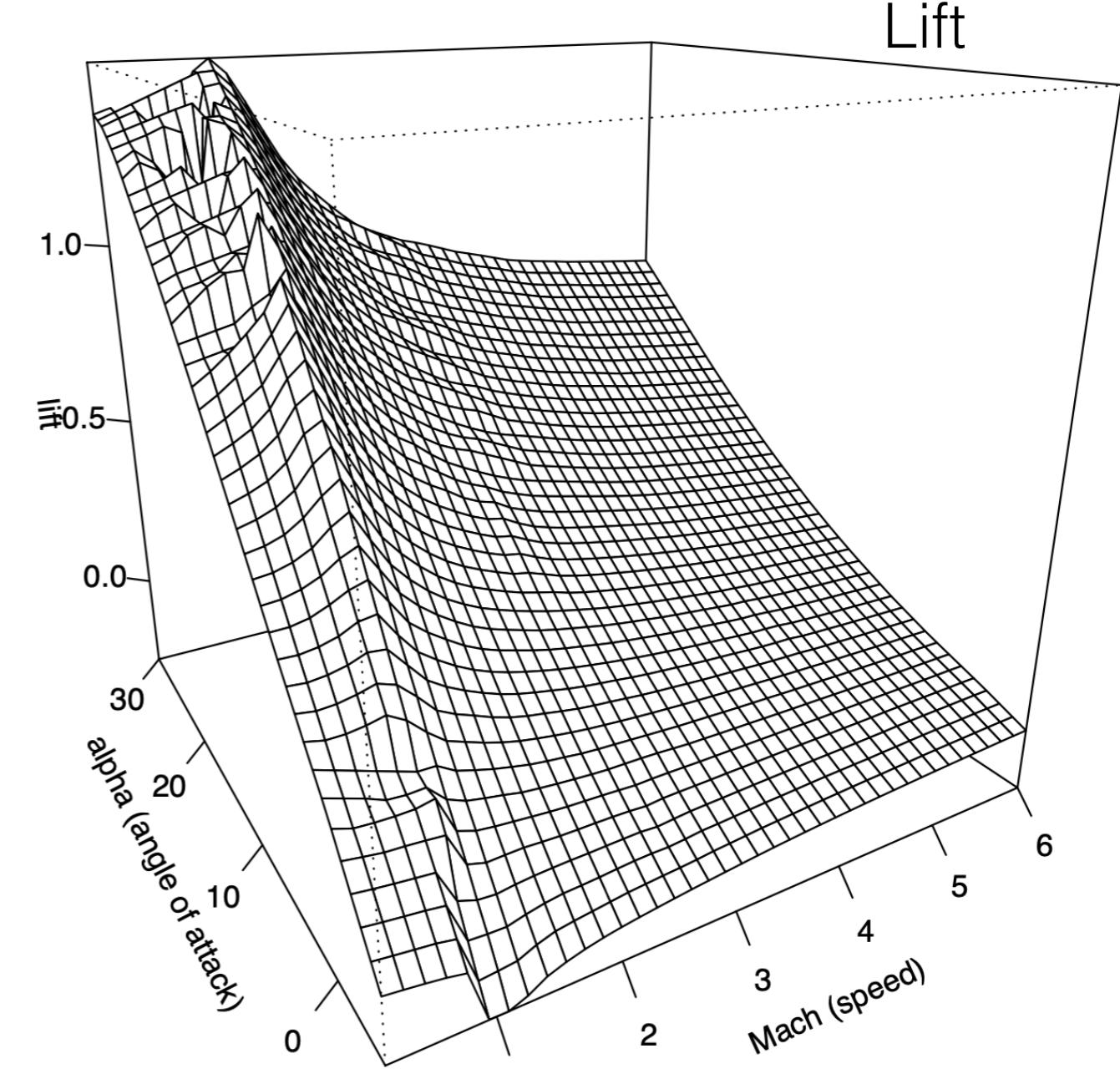
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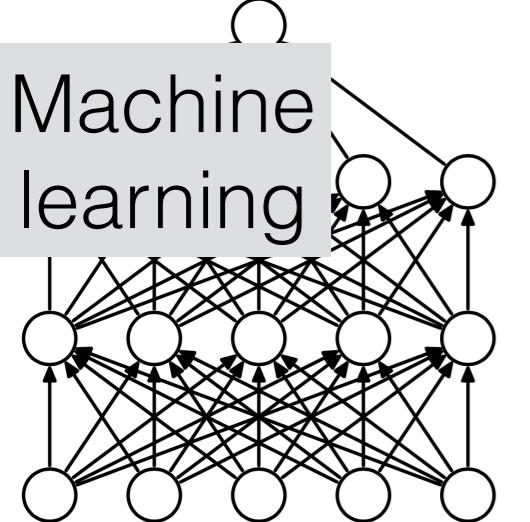
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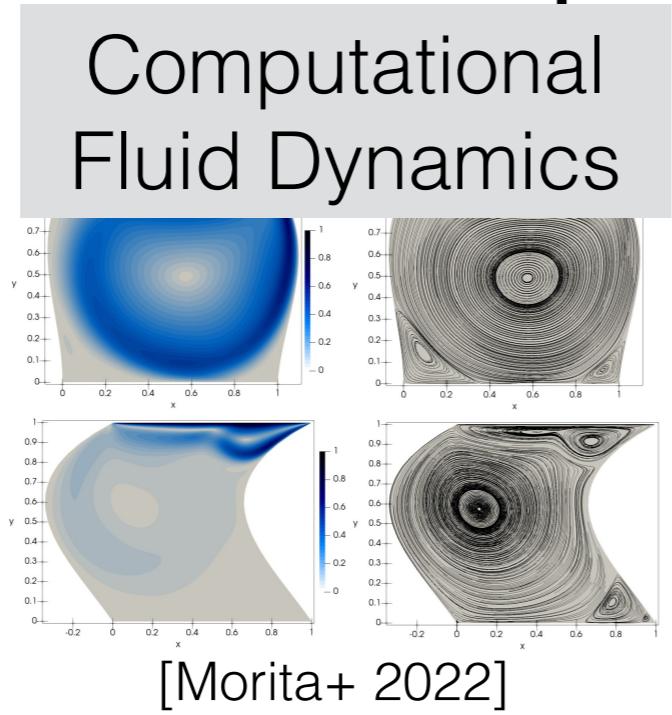
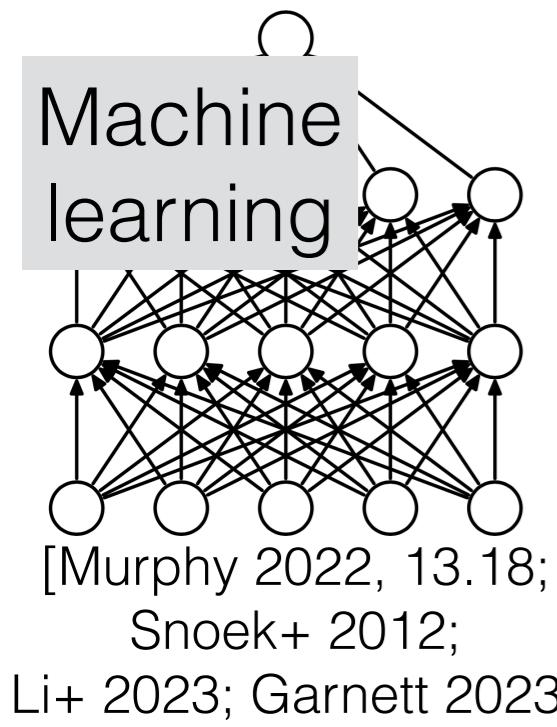
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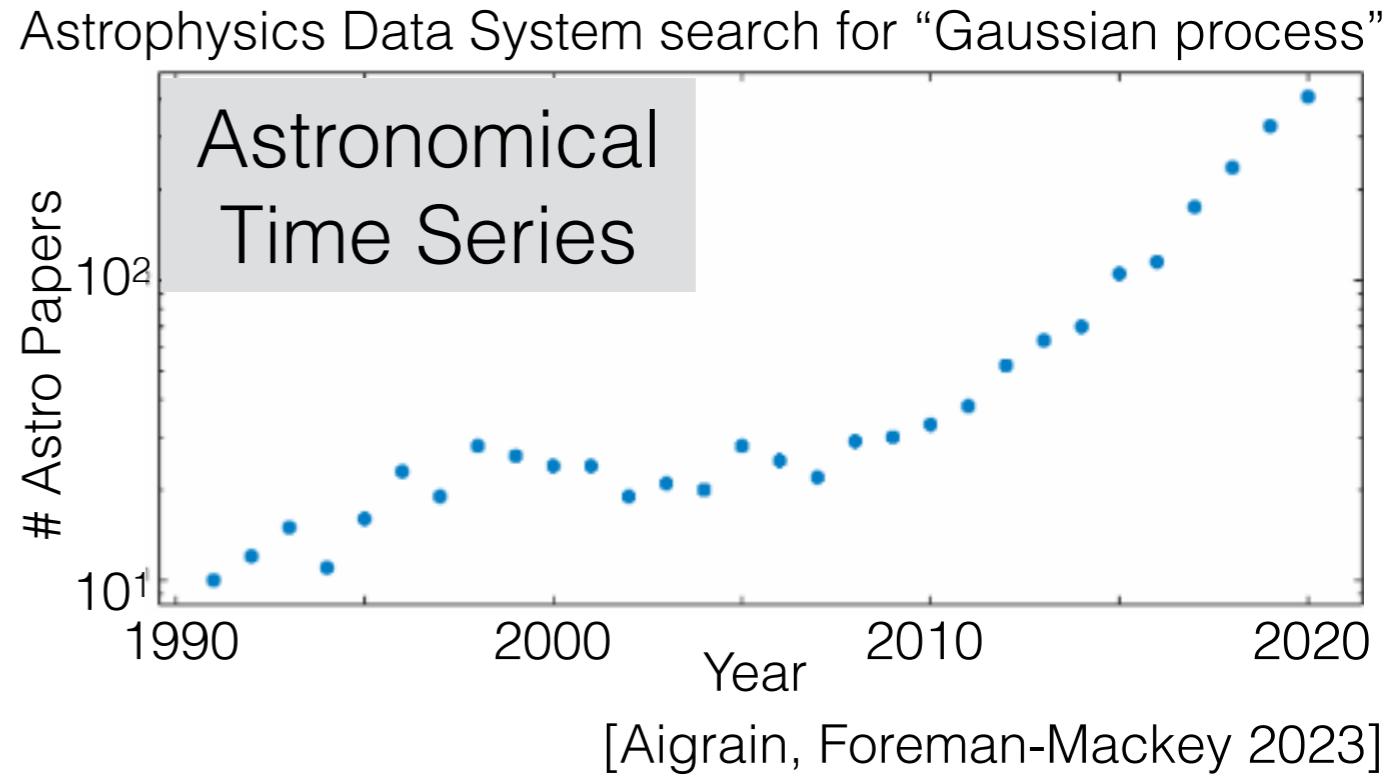
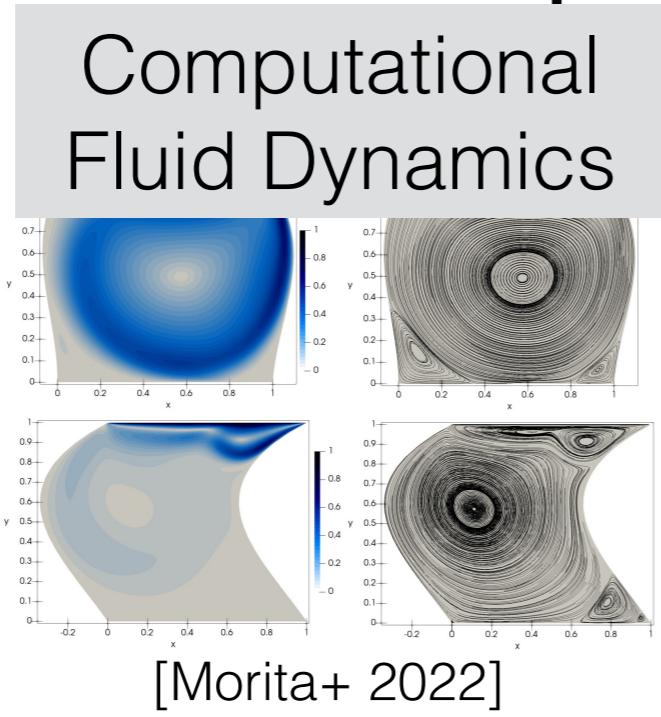
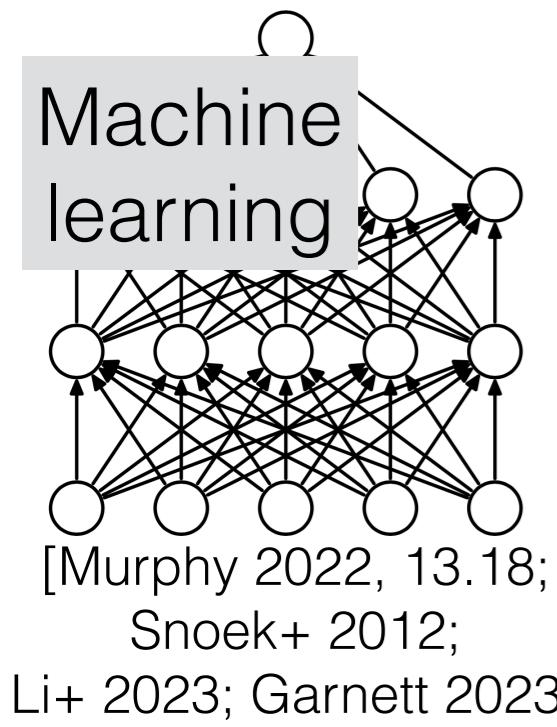


[Murphy 2022, 13.18;
Snoek+ 2012;
Li+ 2023; Garnett 2023]

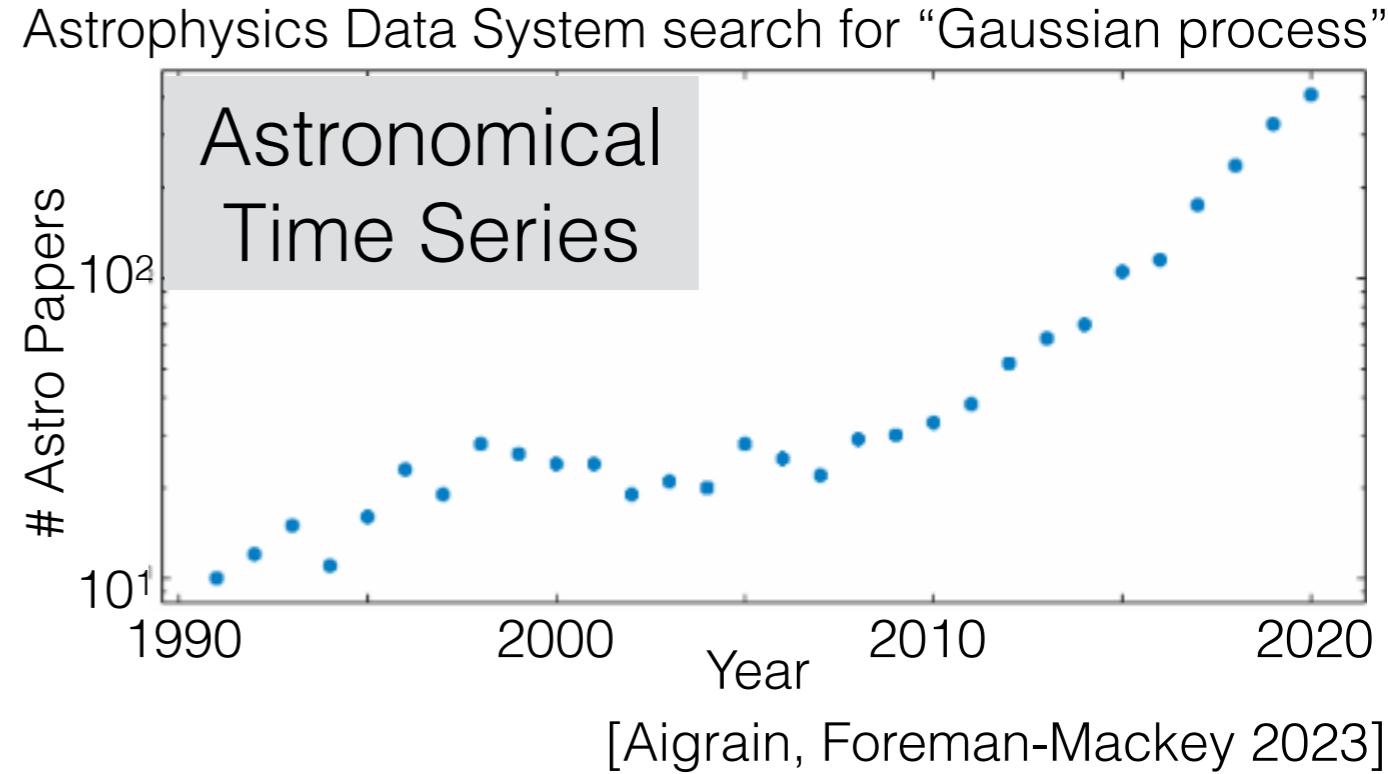
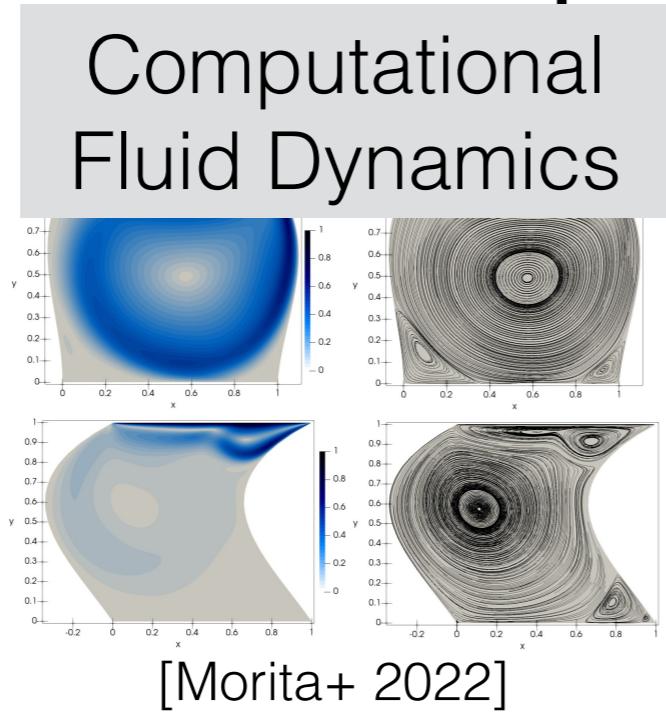
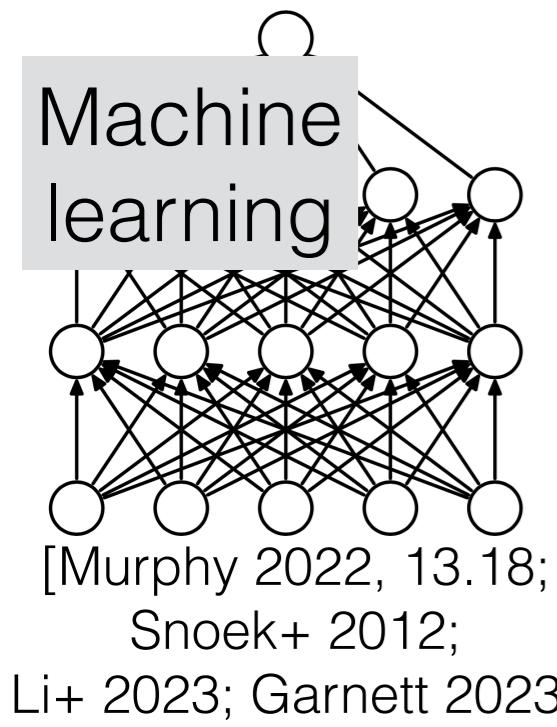
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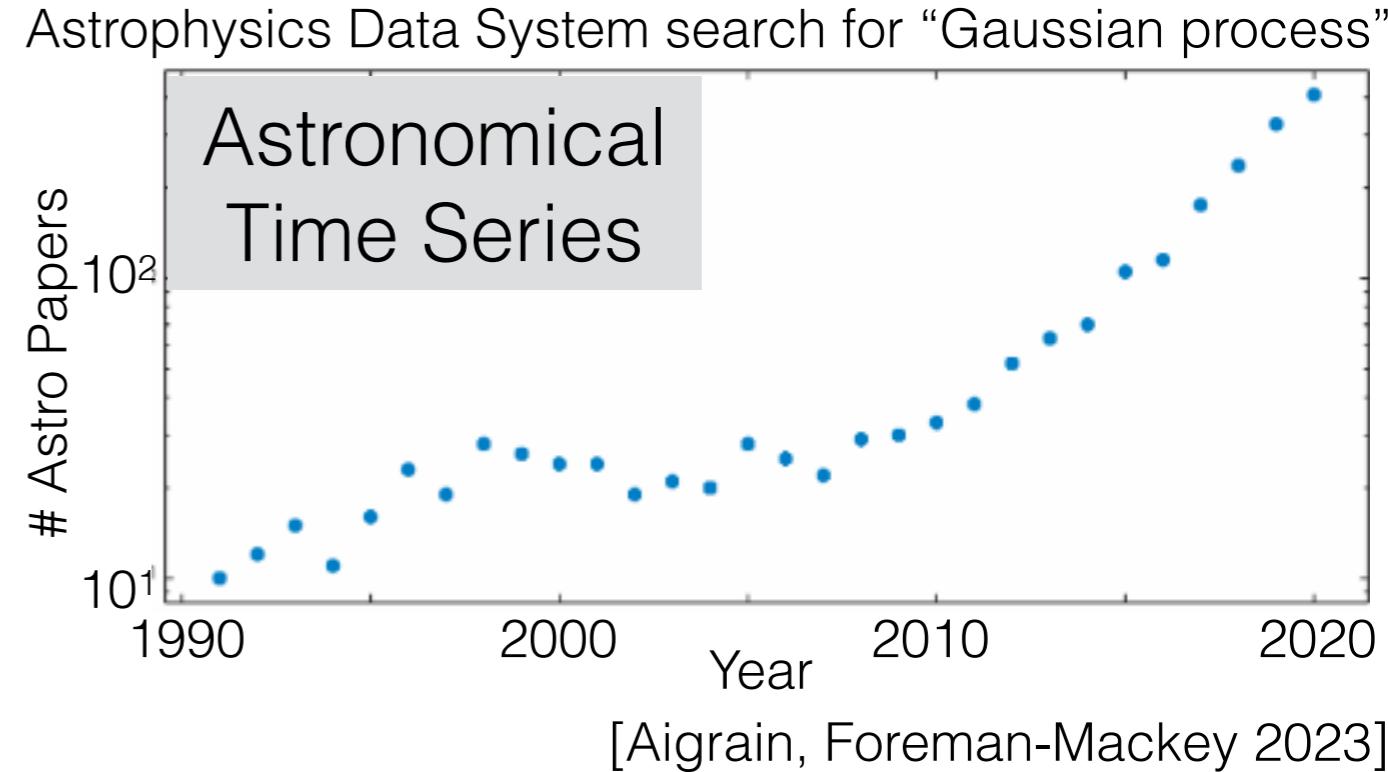
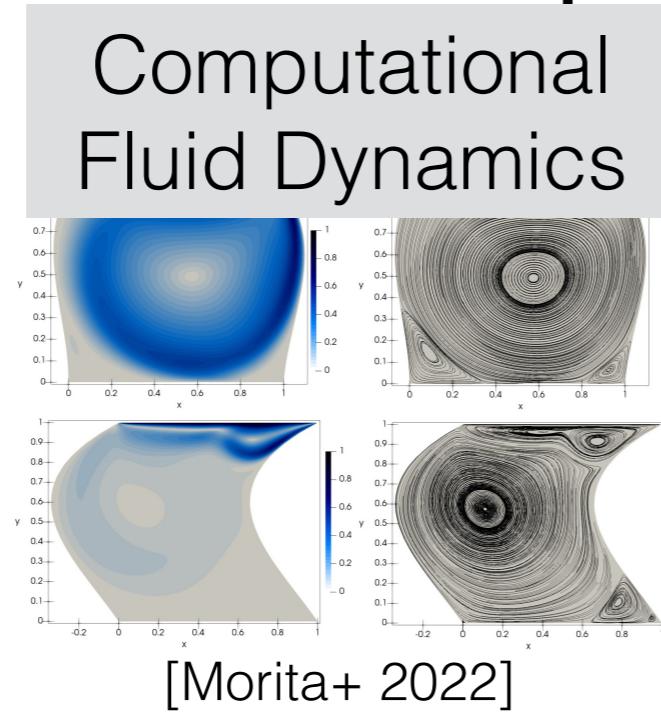
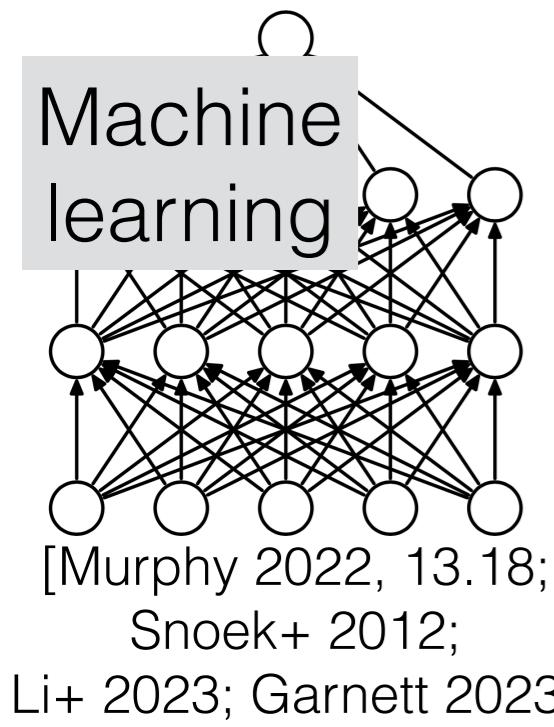


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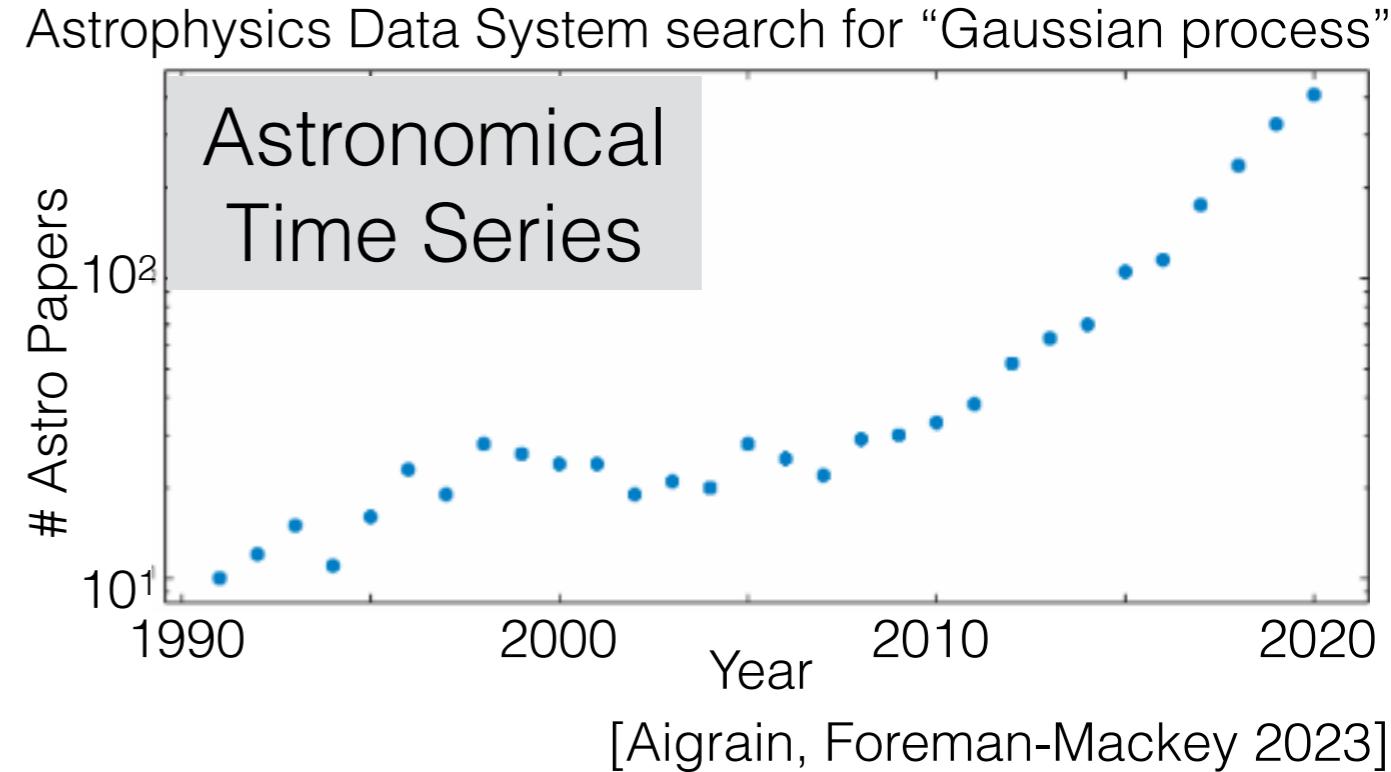
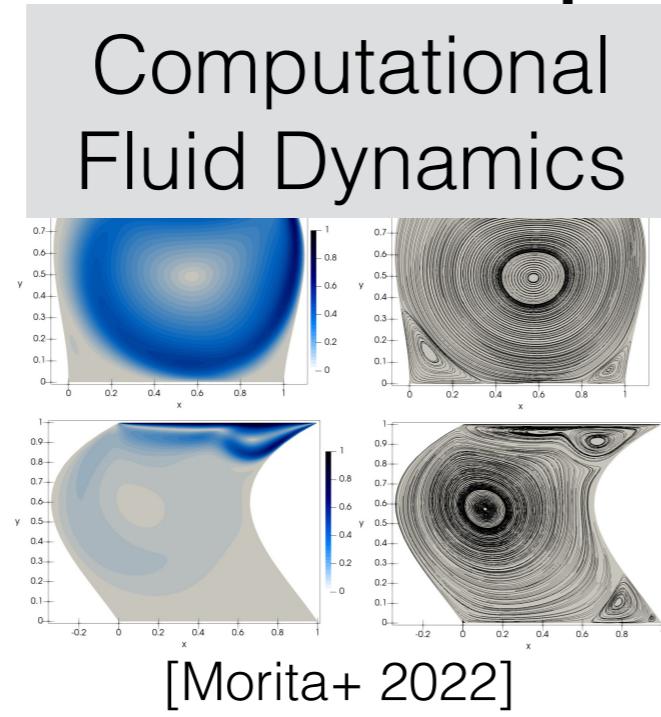
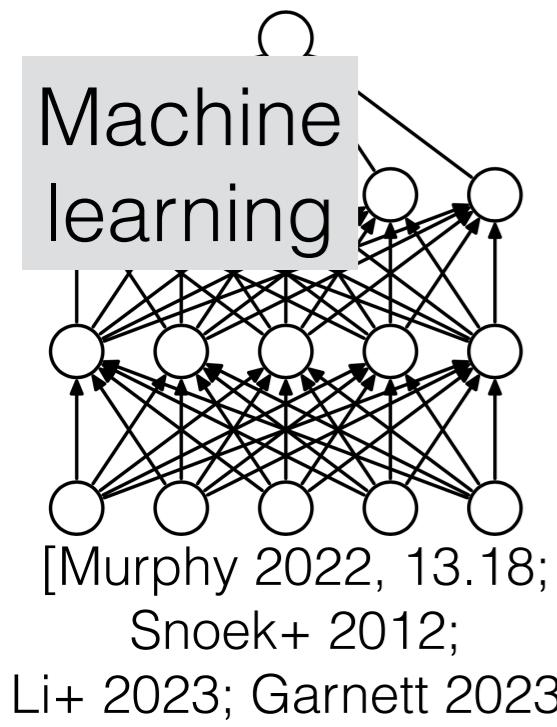
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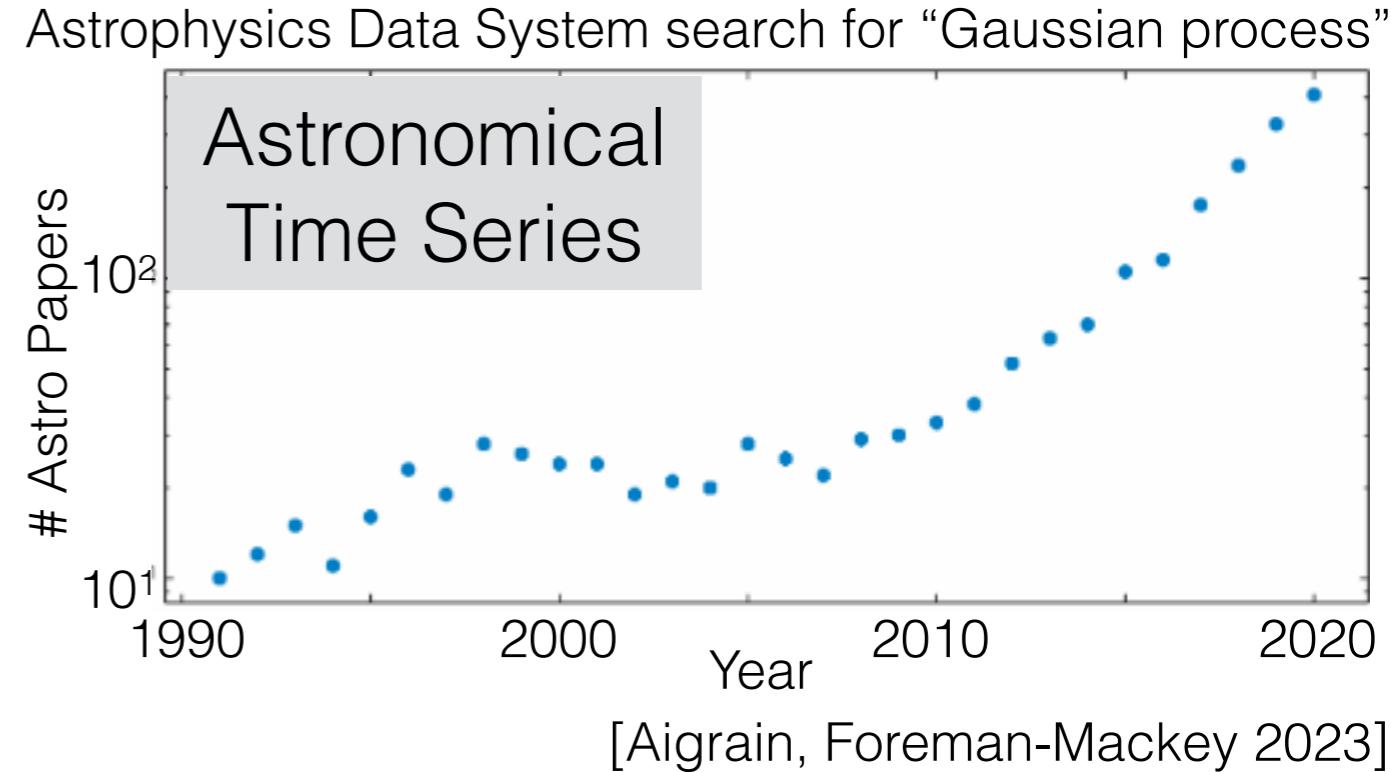
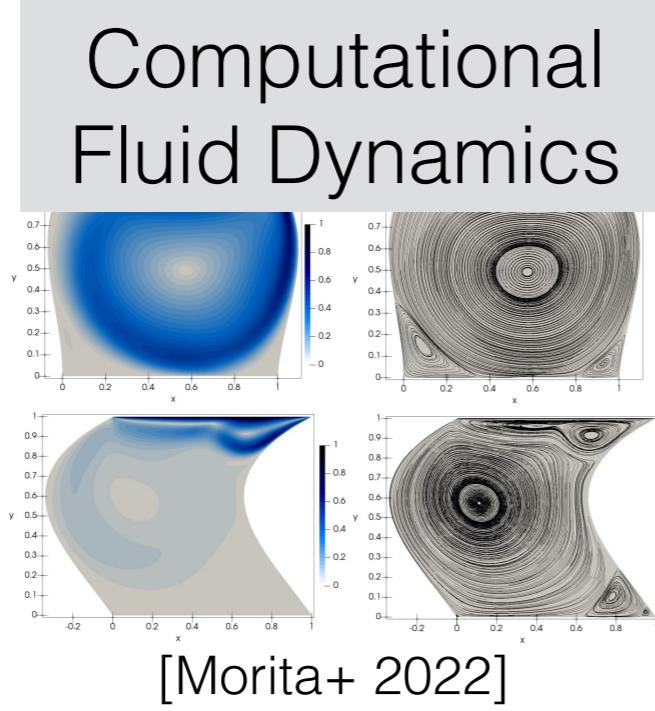
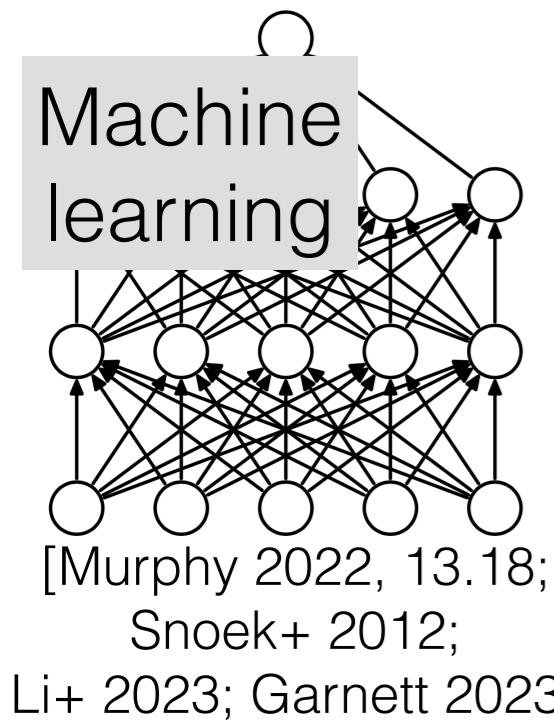
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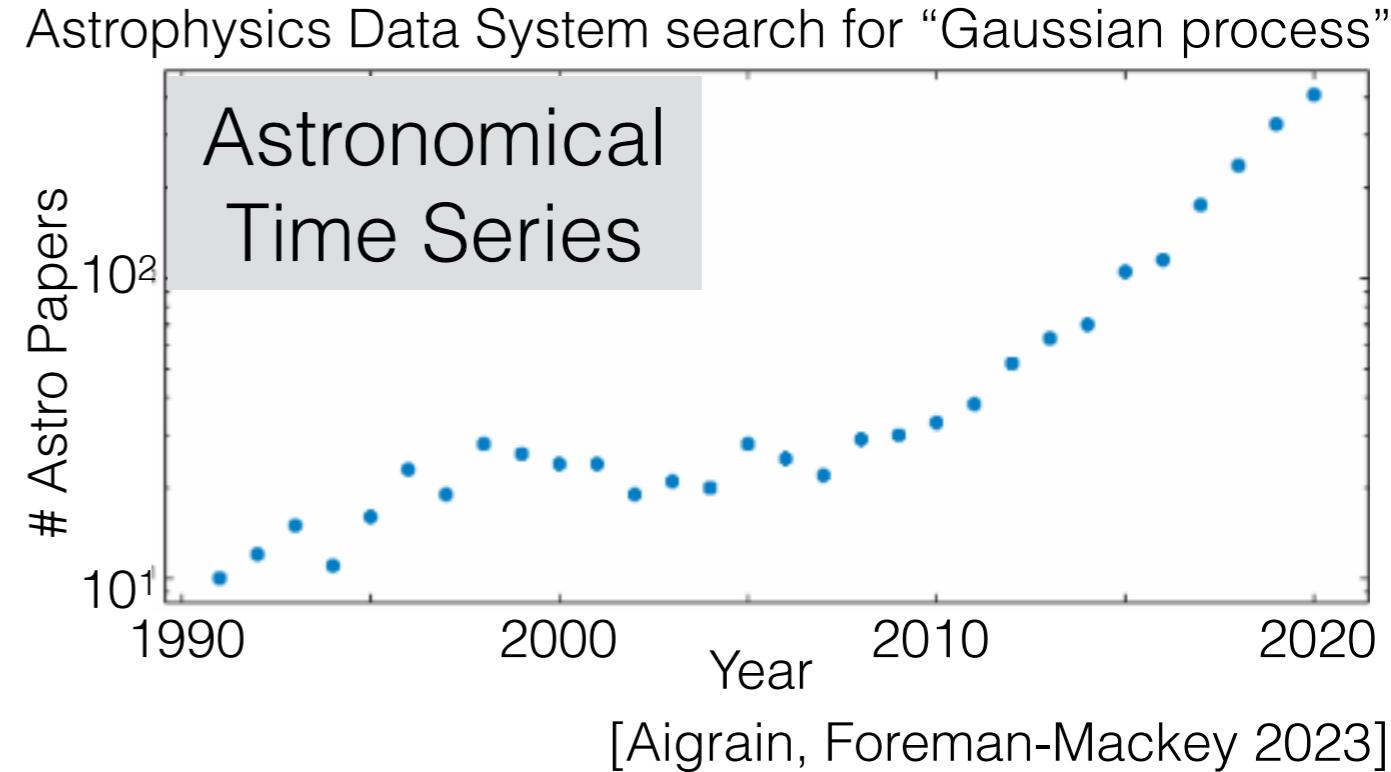
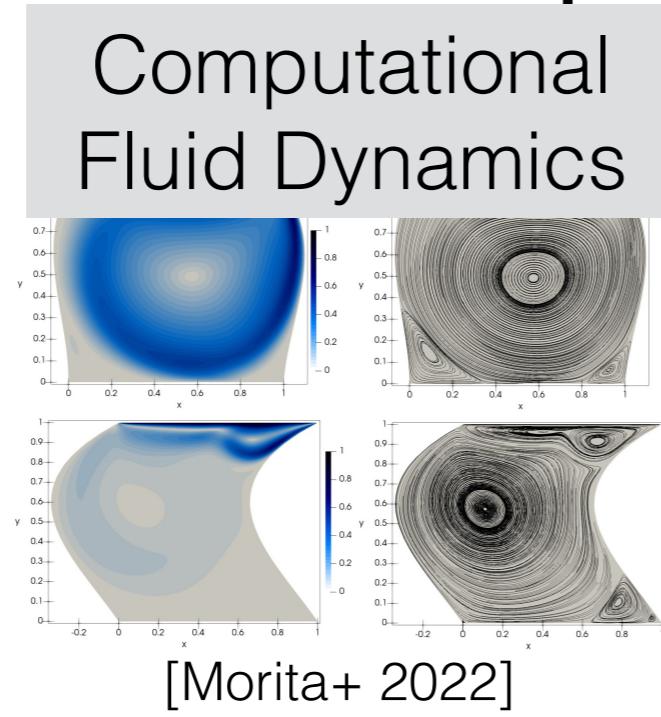
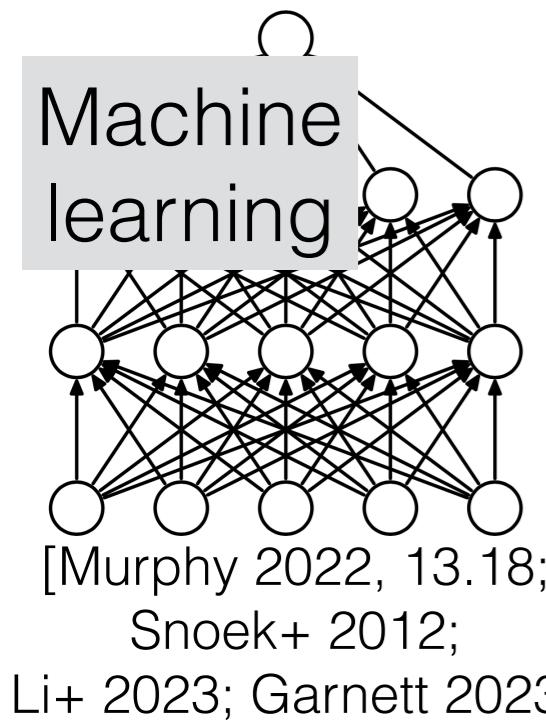
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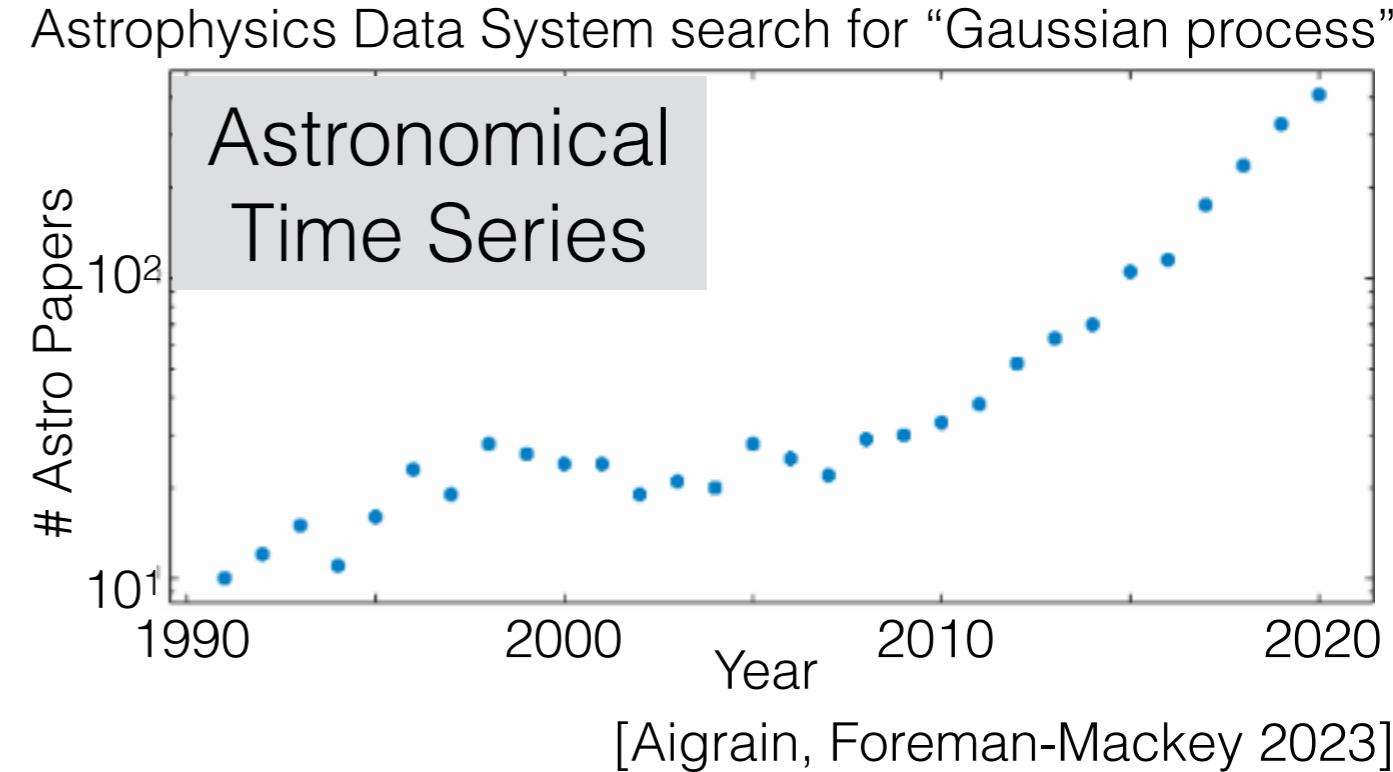
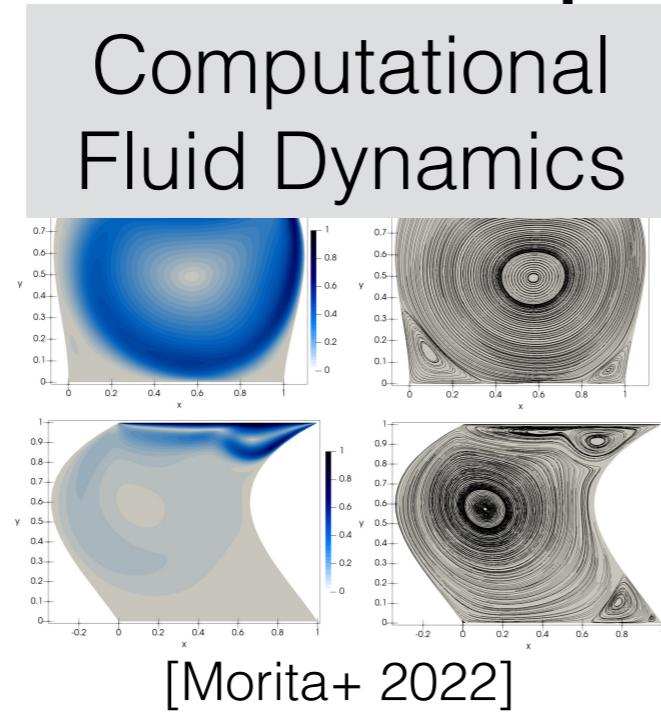
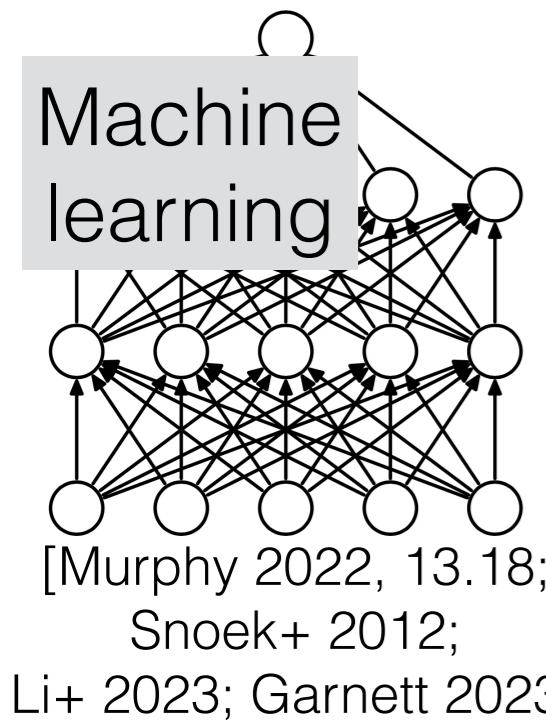
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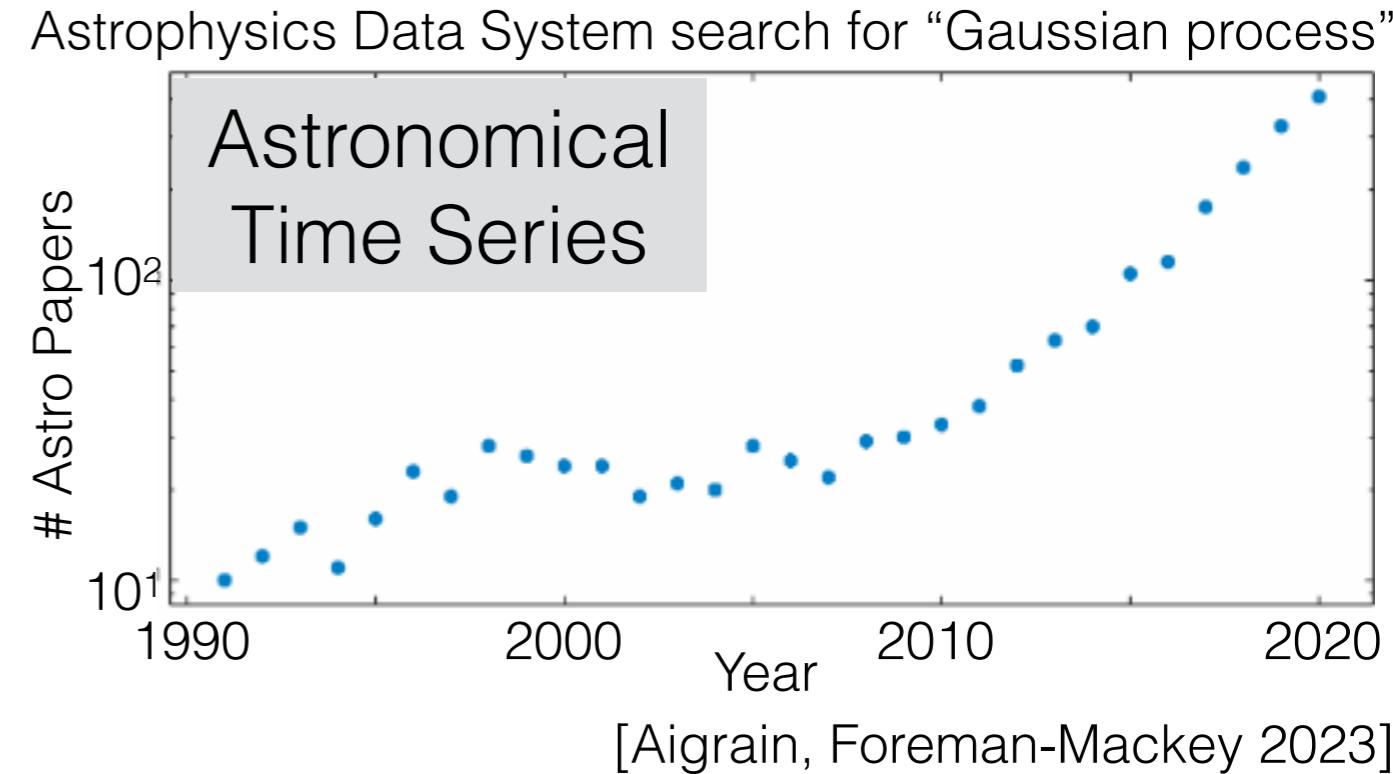
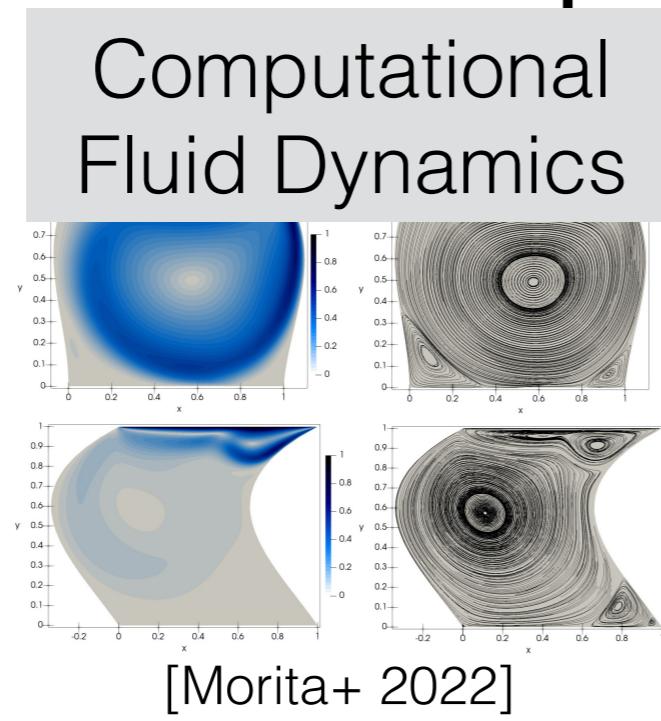
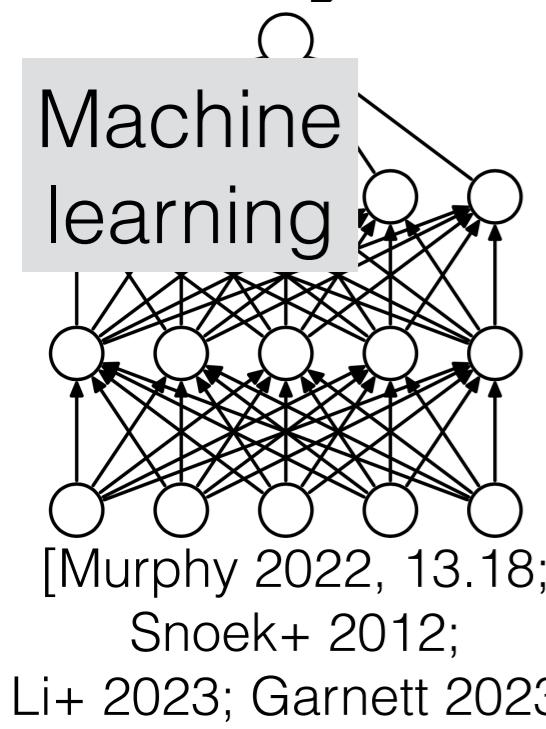


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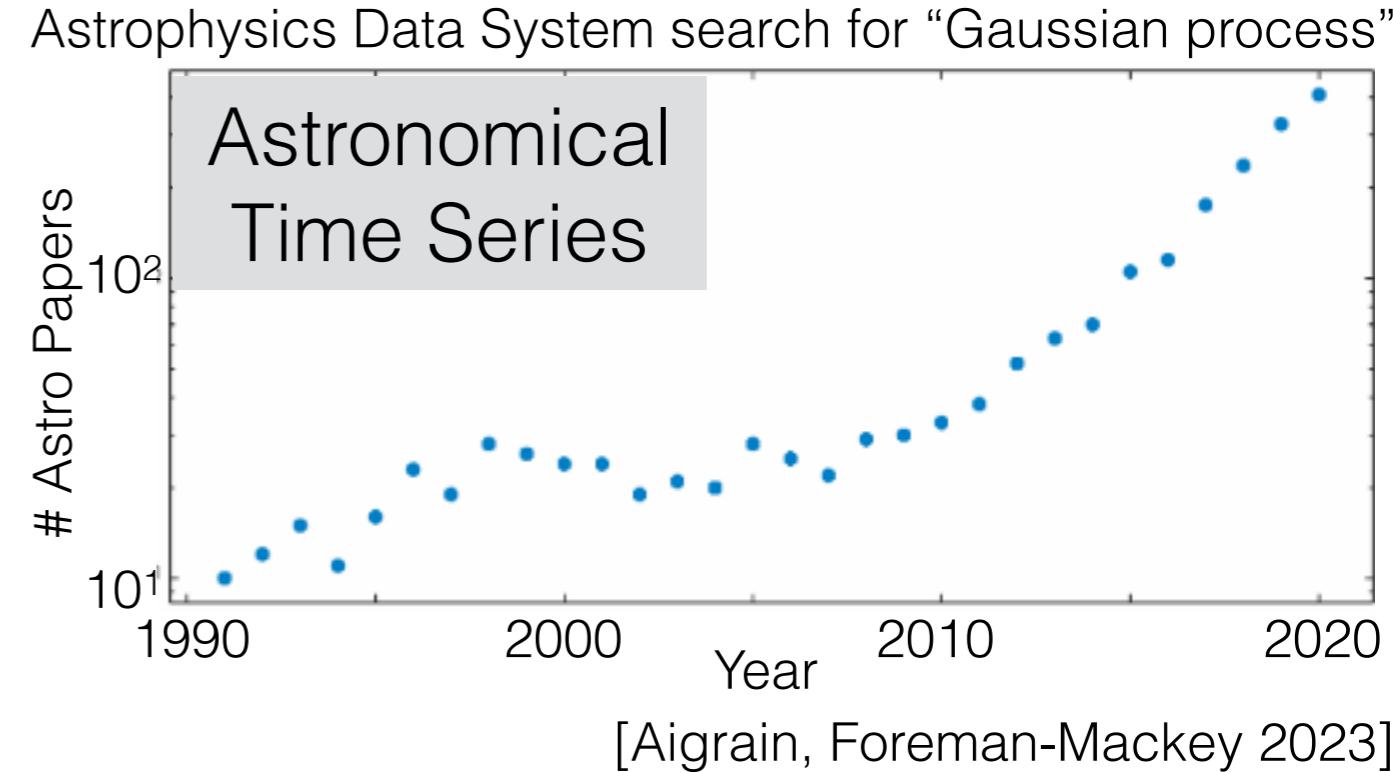
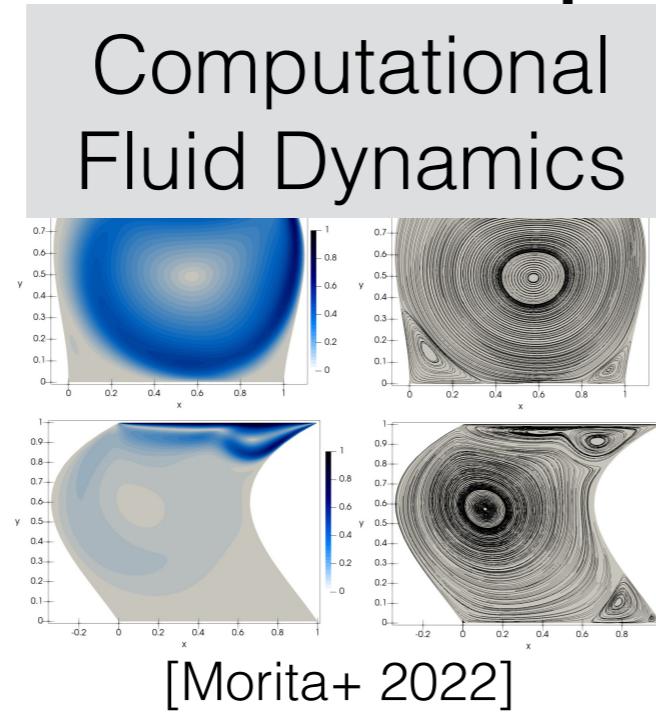
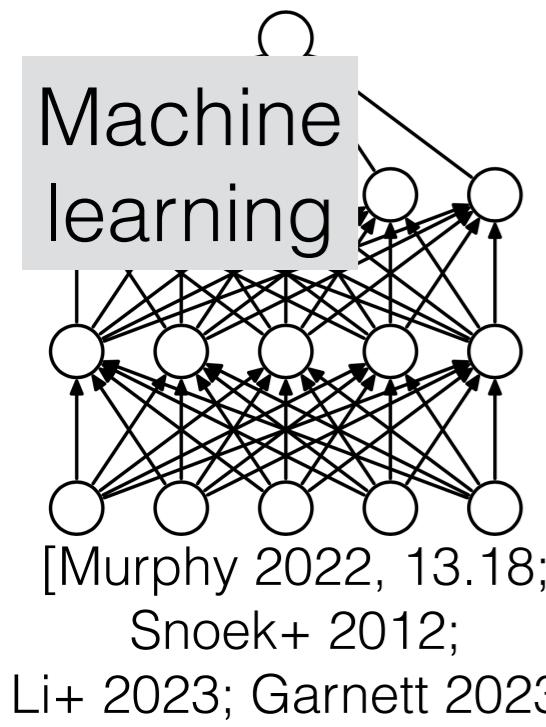


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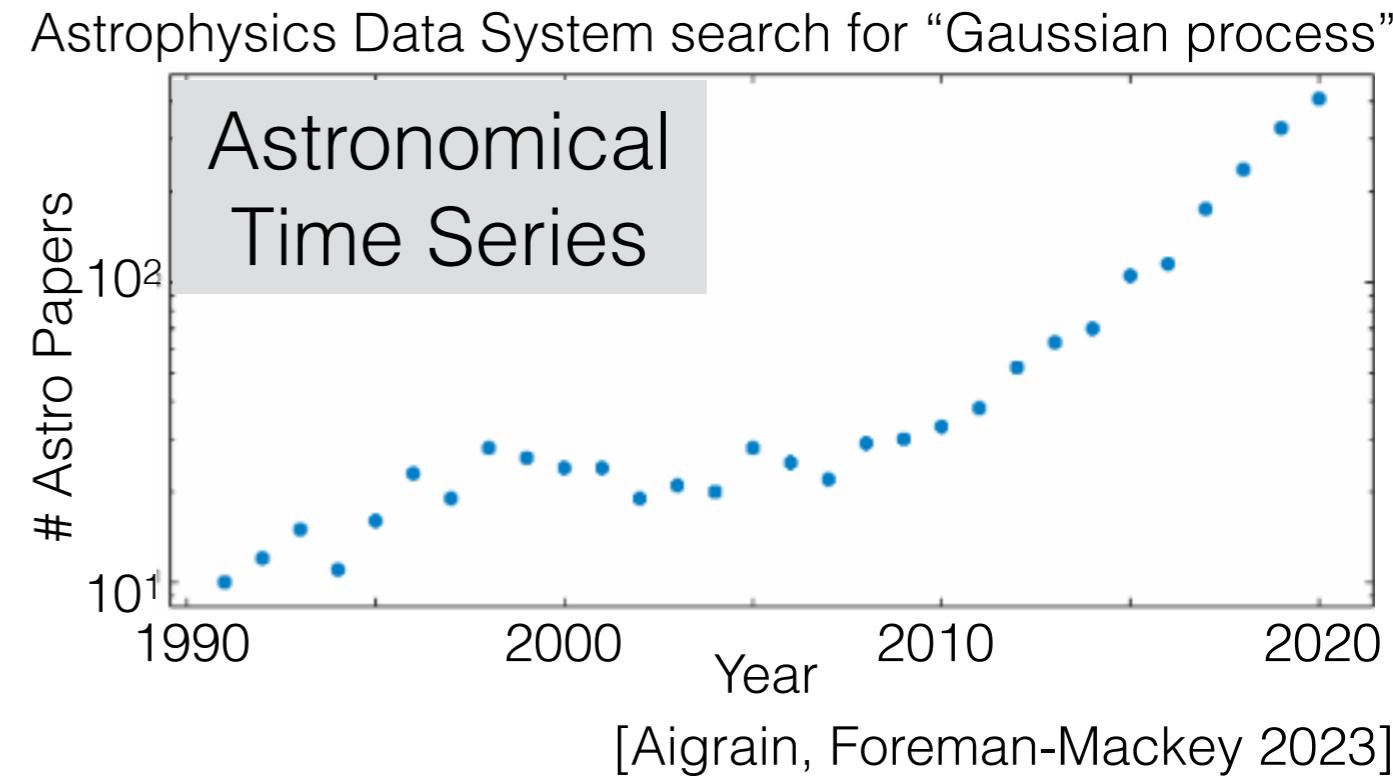
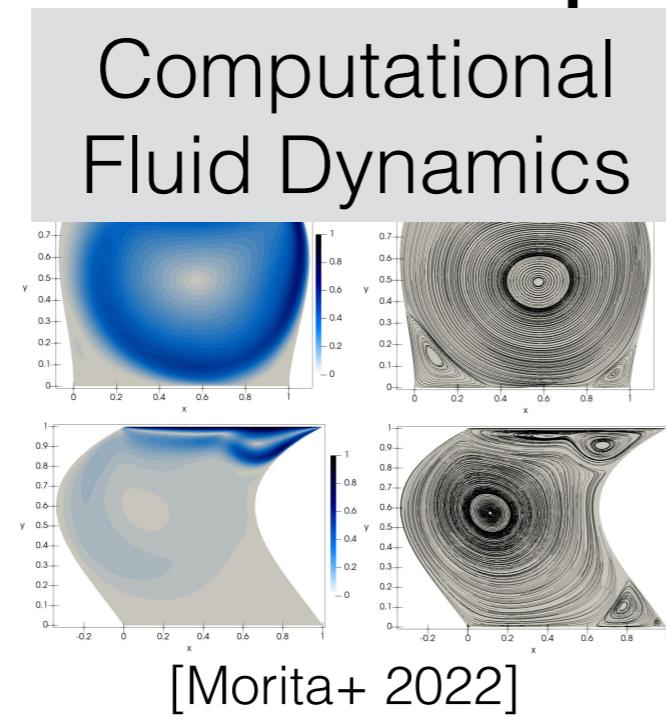
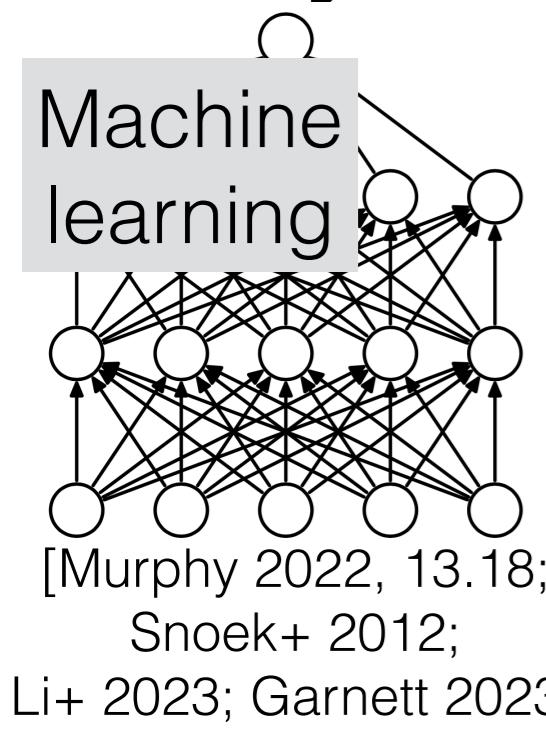


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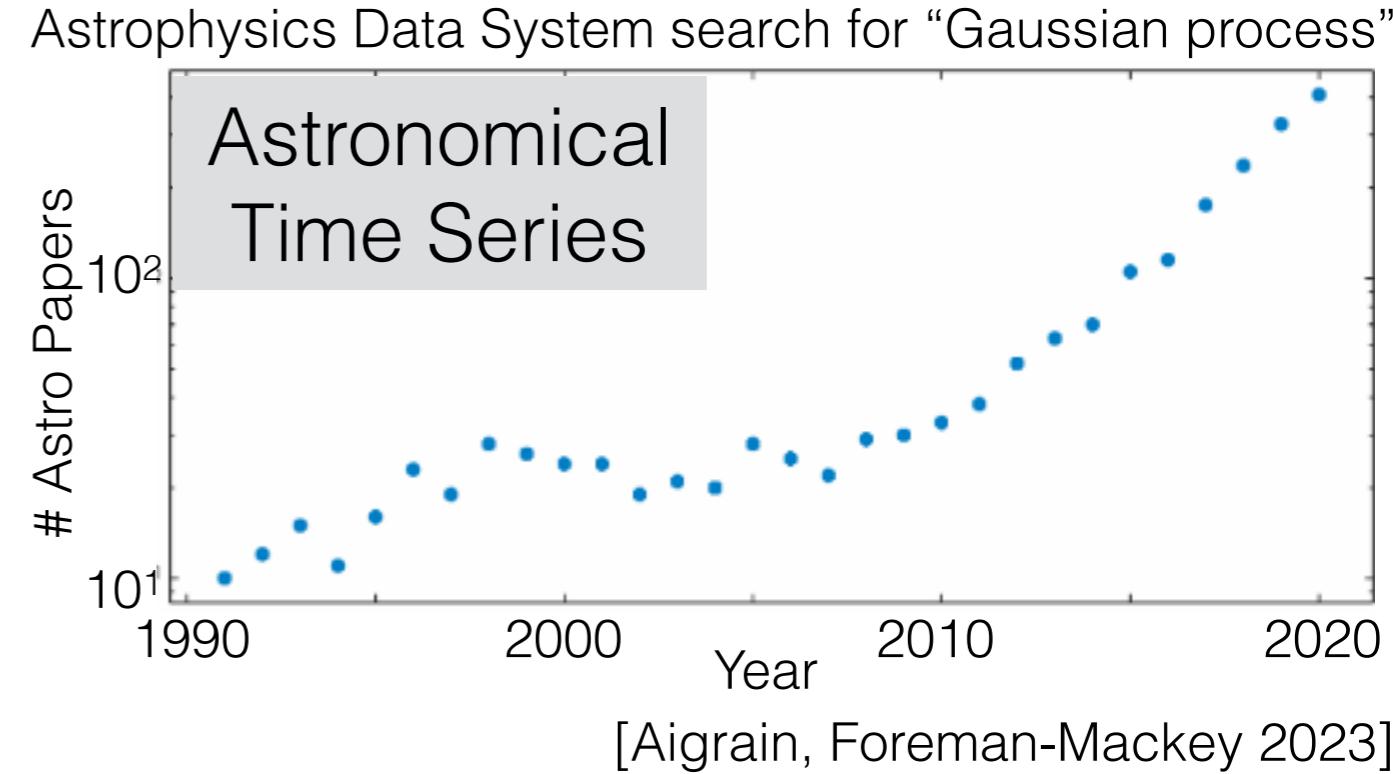
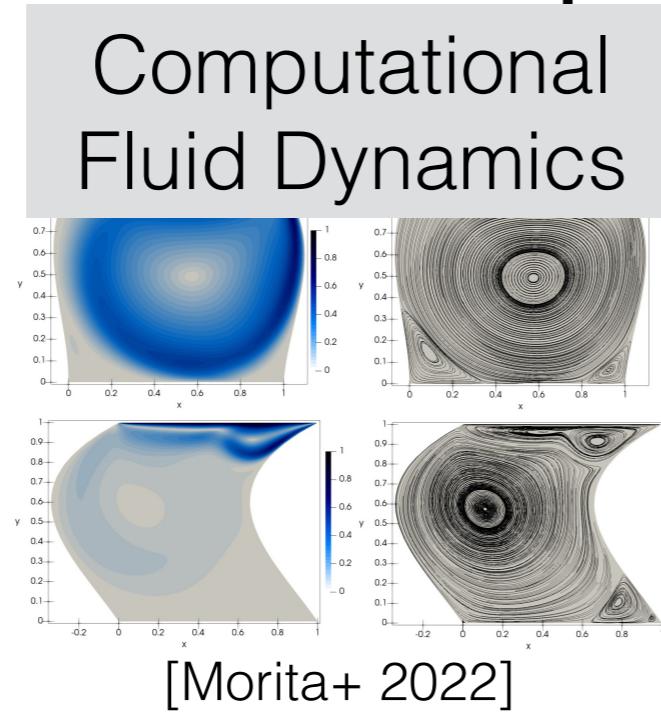
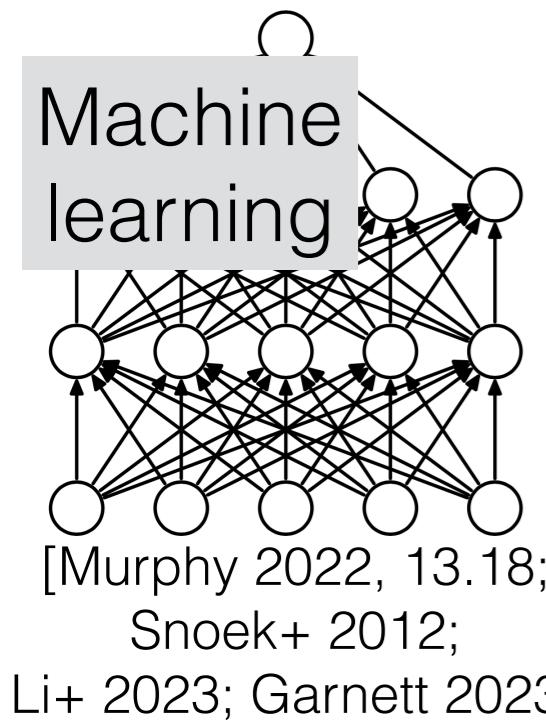
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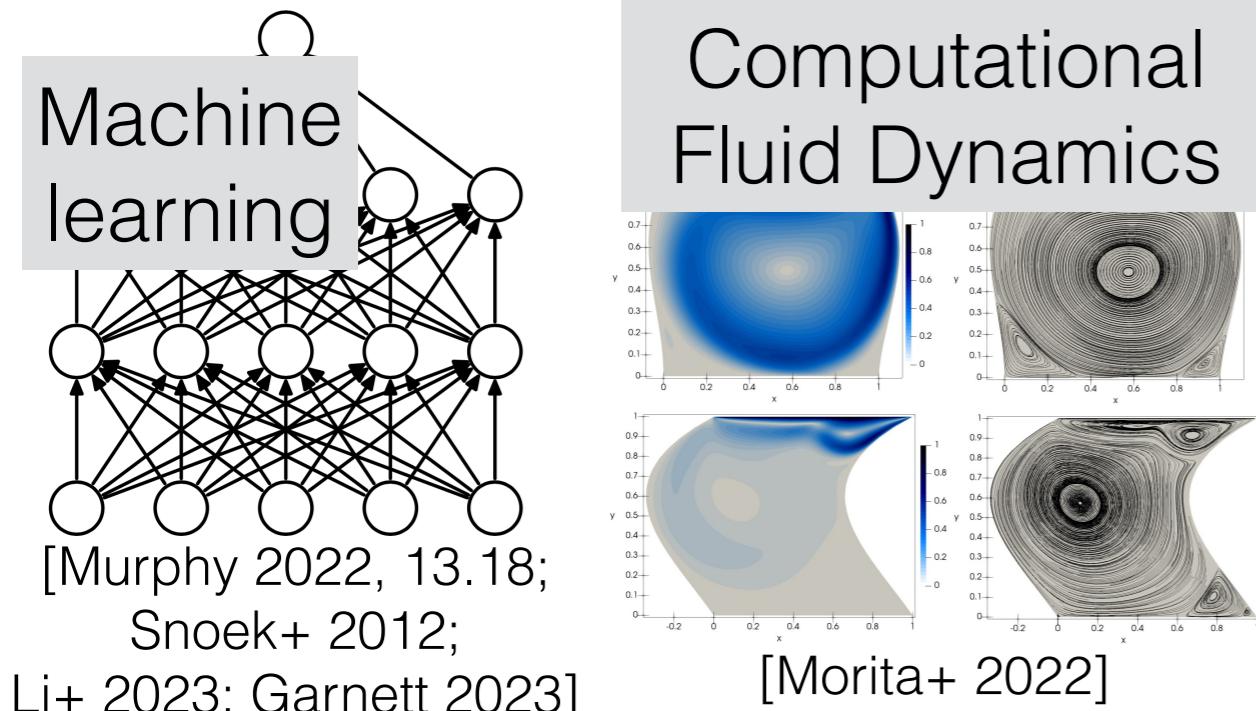
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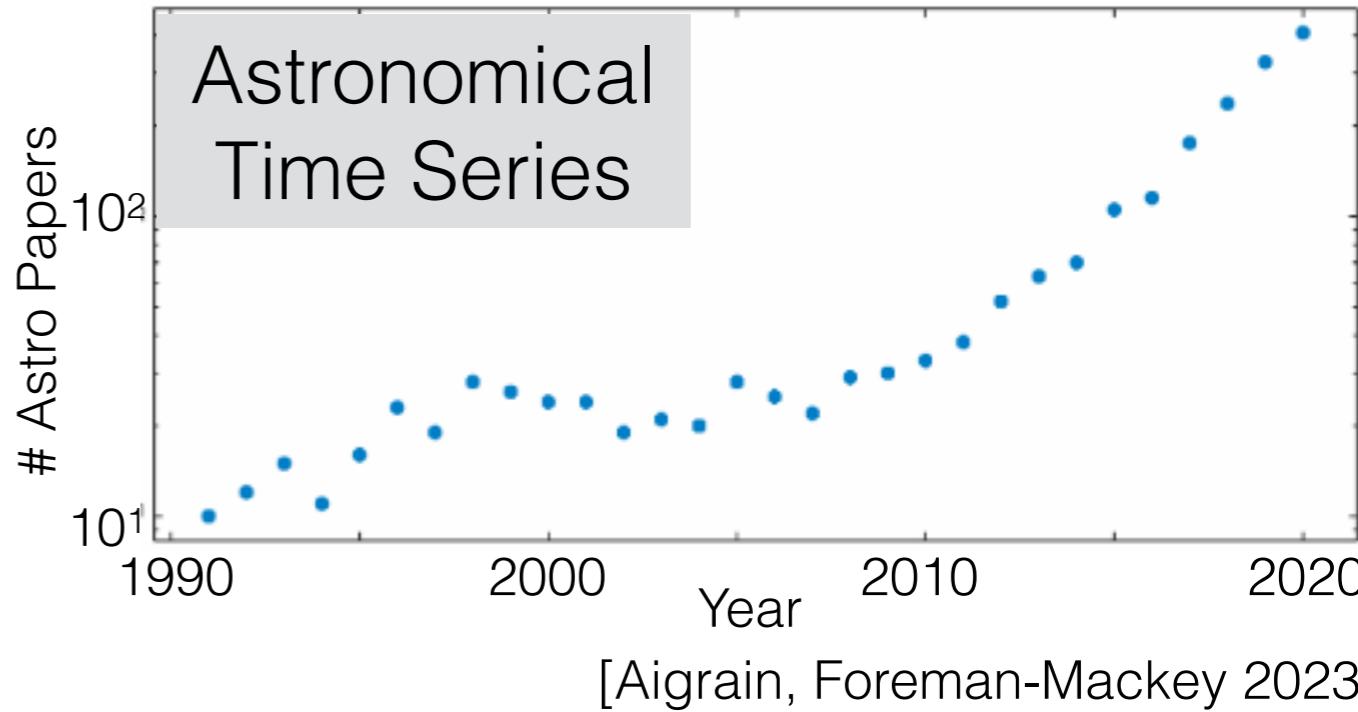
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- Predictions & uncertainties over derivatives & integrals
- Module in more-complex methods

Why Gaussian processes?

see also “kriging,”
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Astrophysics Data System search for “Gaussian process”



[Aigrain, Foreman-Mackey 2023]

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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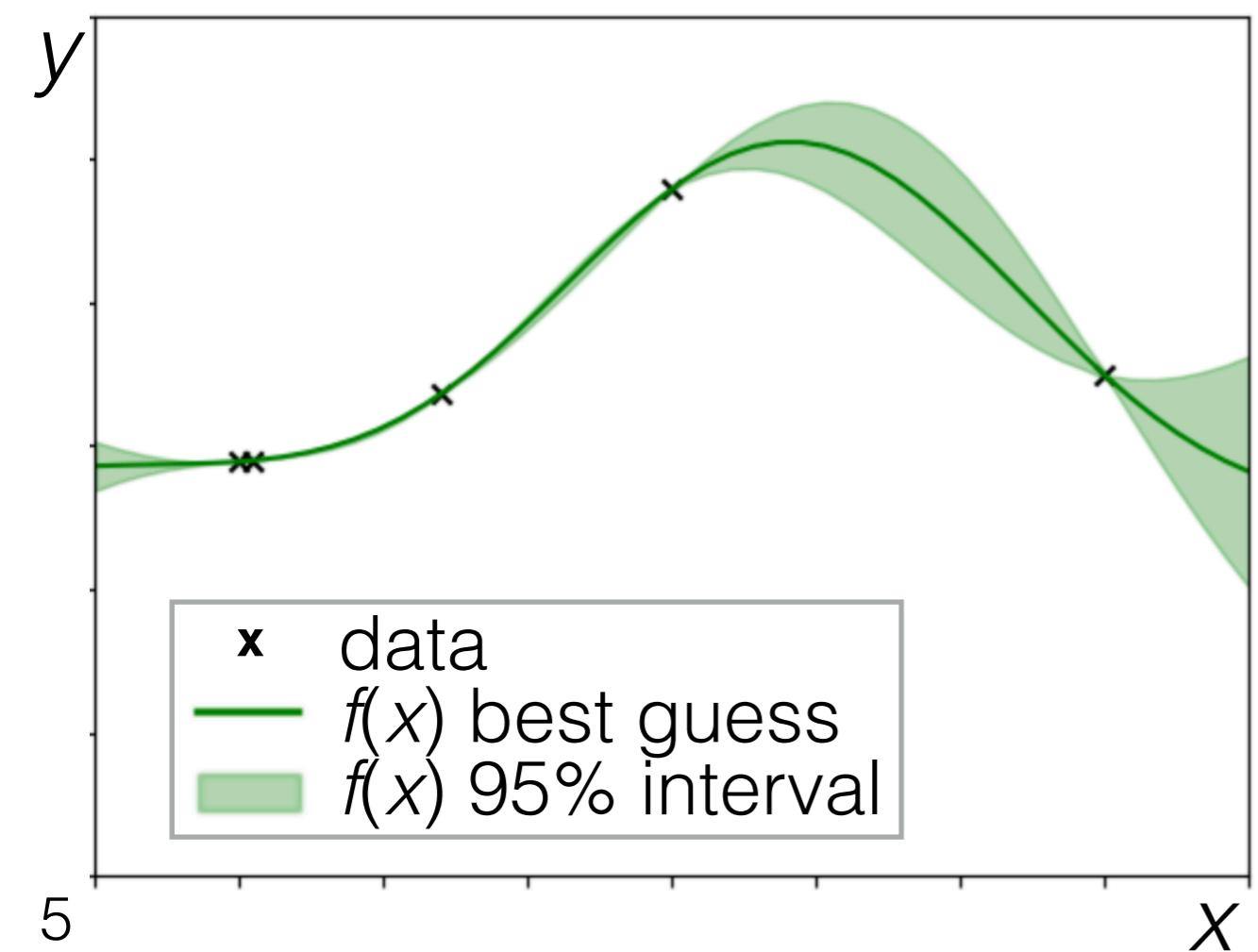


Given the data we've seen, what do we know about the underlying function?

A Bayesian approach

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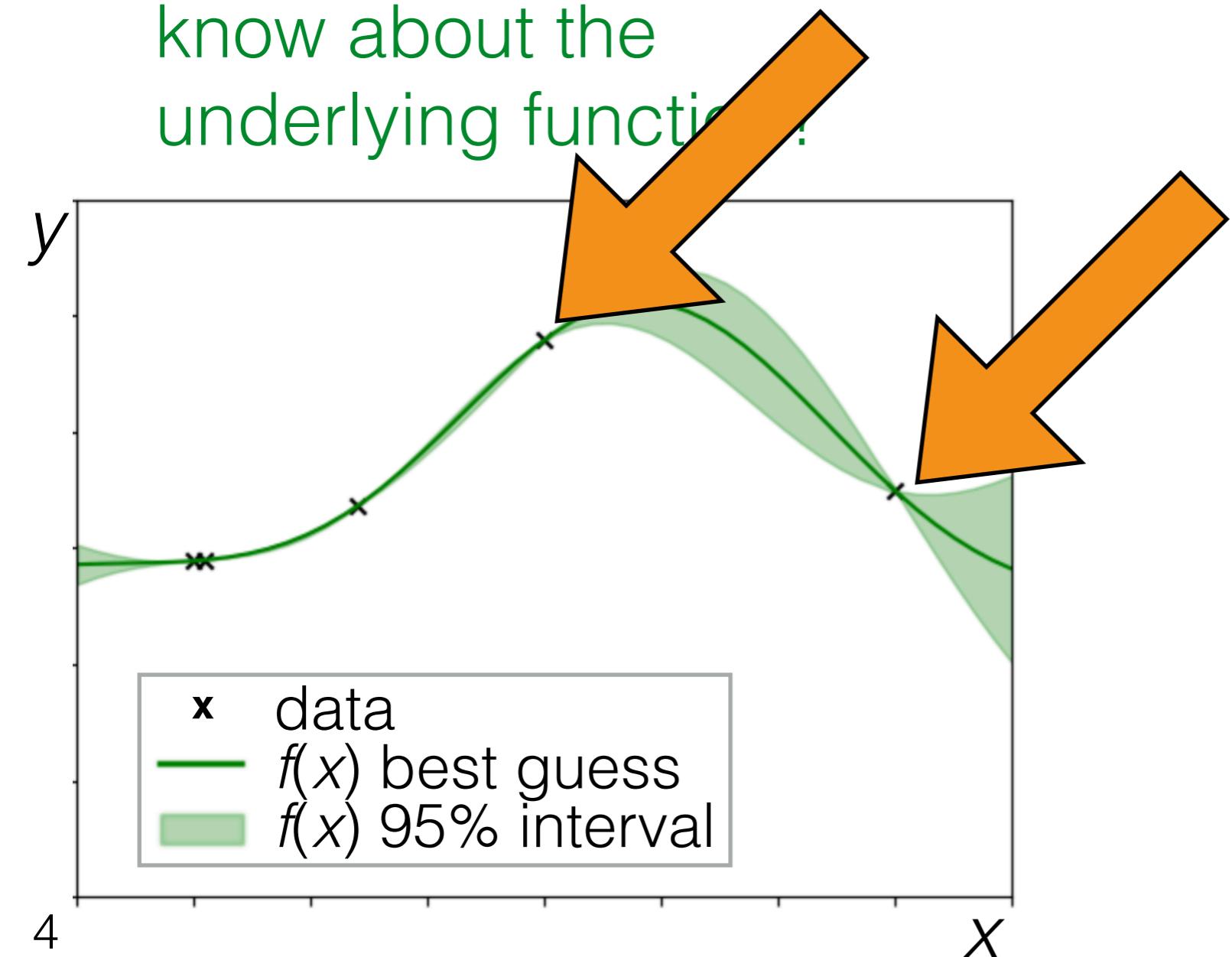
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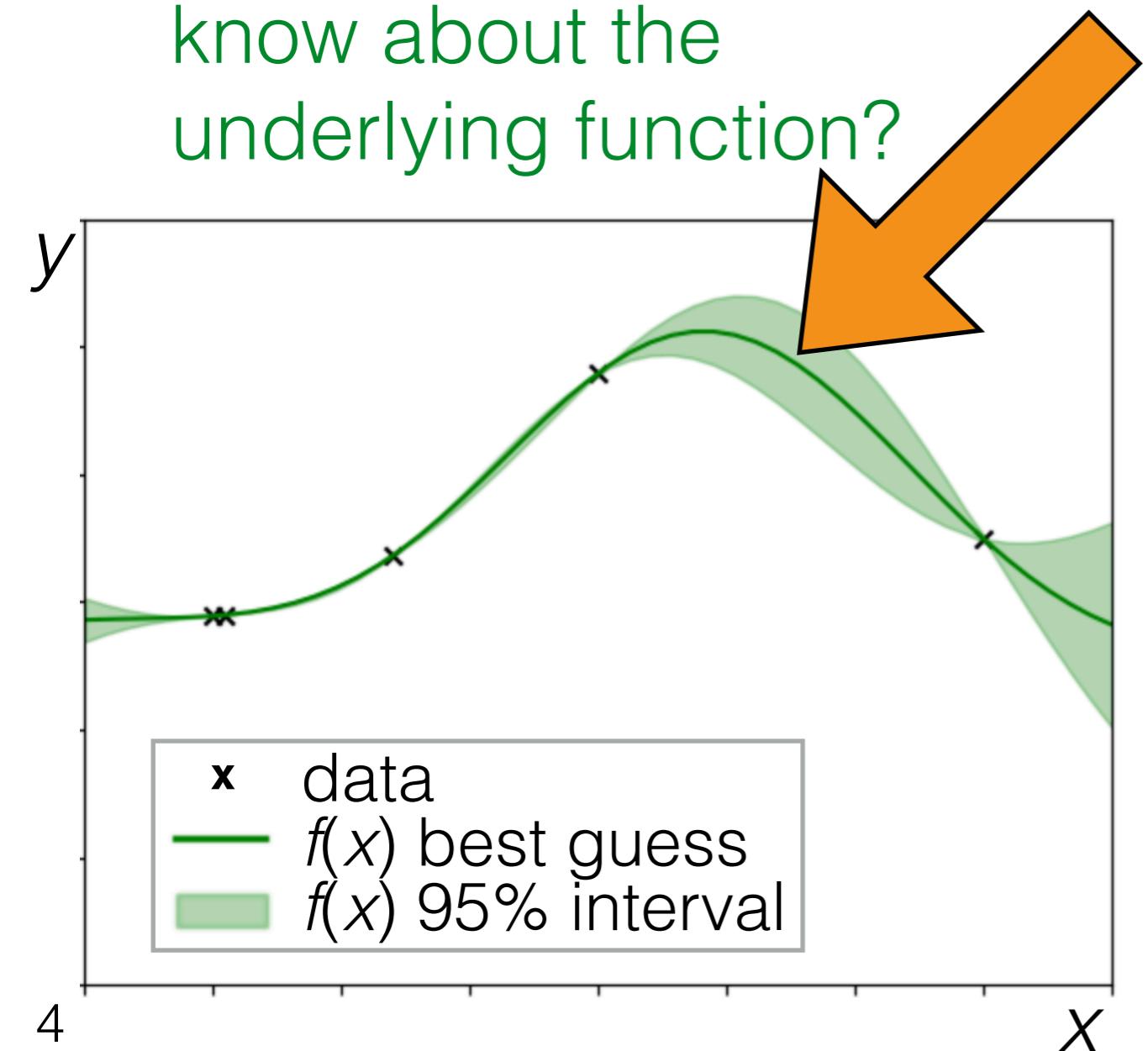
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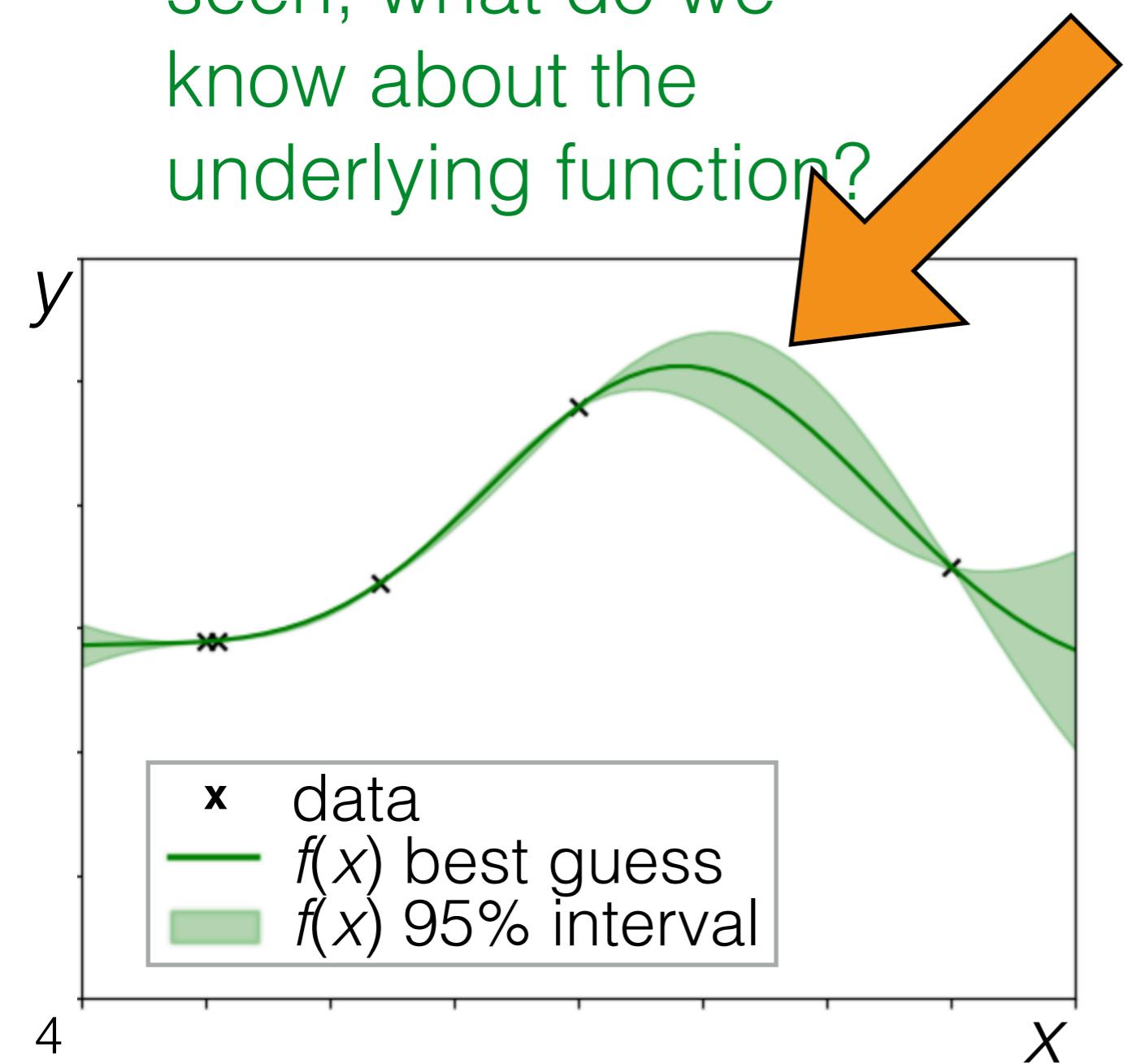
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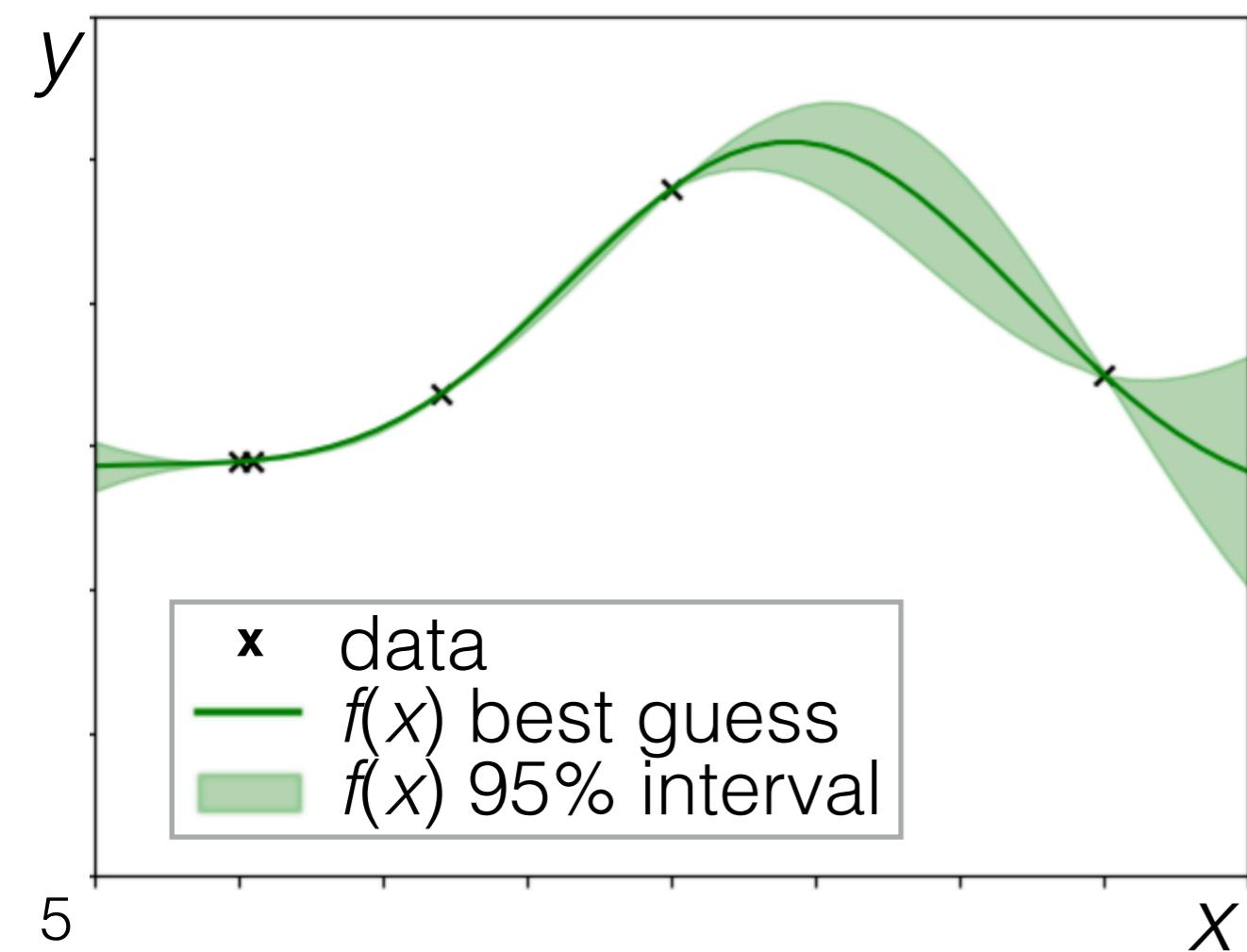
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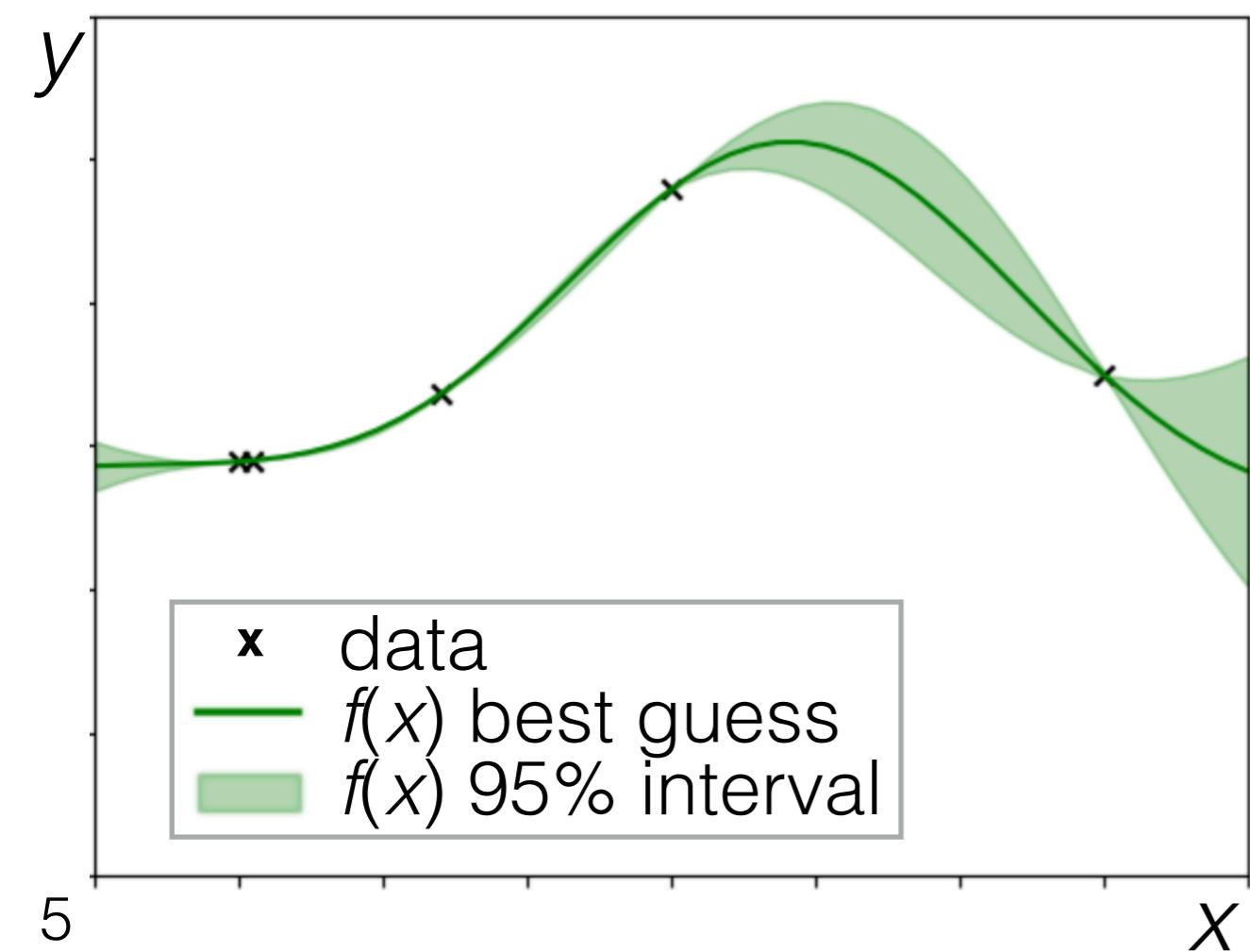


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A (statistical) model that can generate functions and data of interest

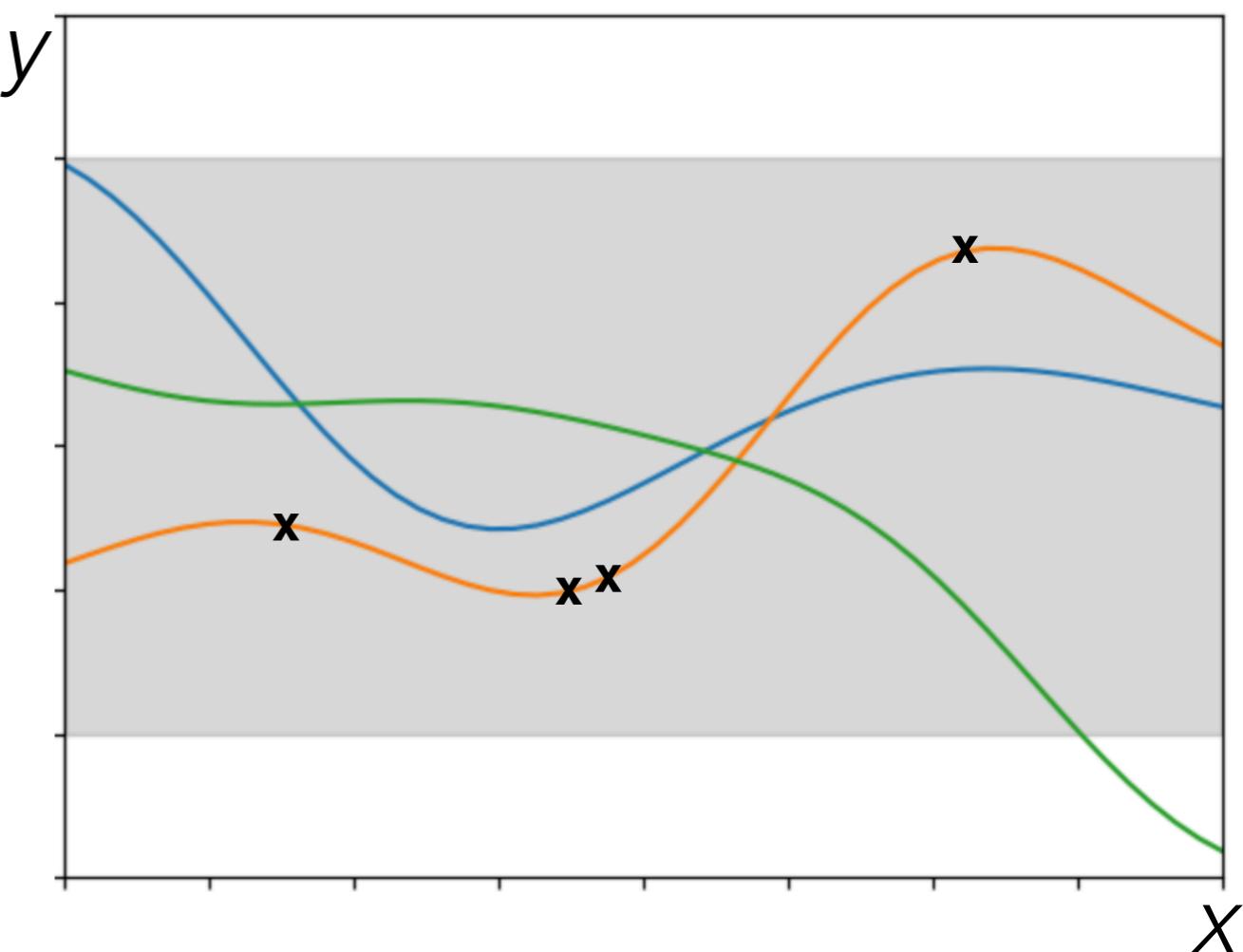
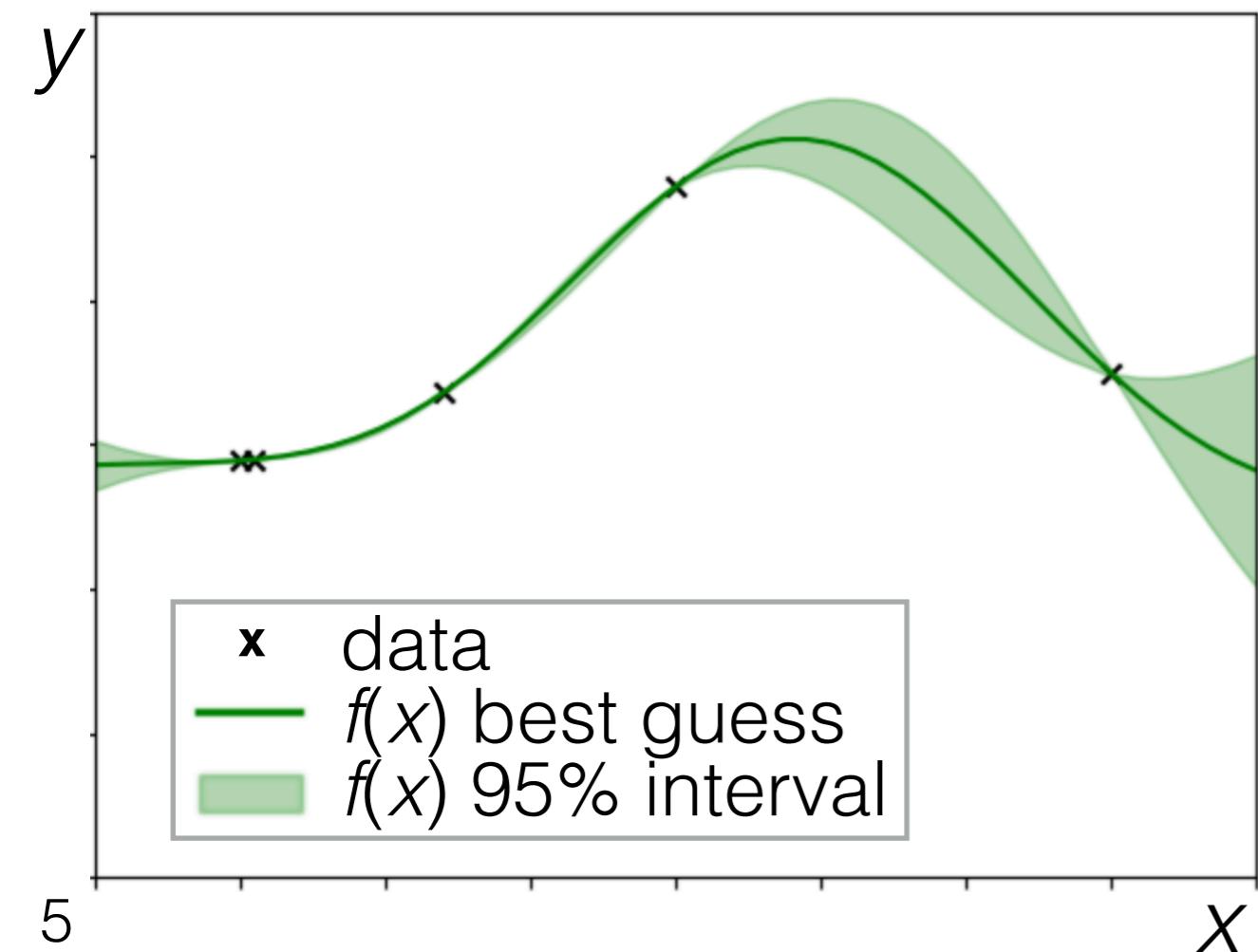


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Univariate Gaussian distribution review

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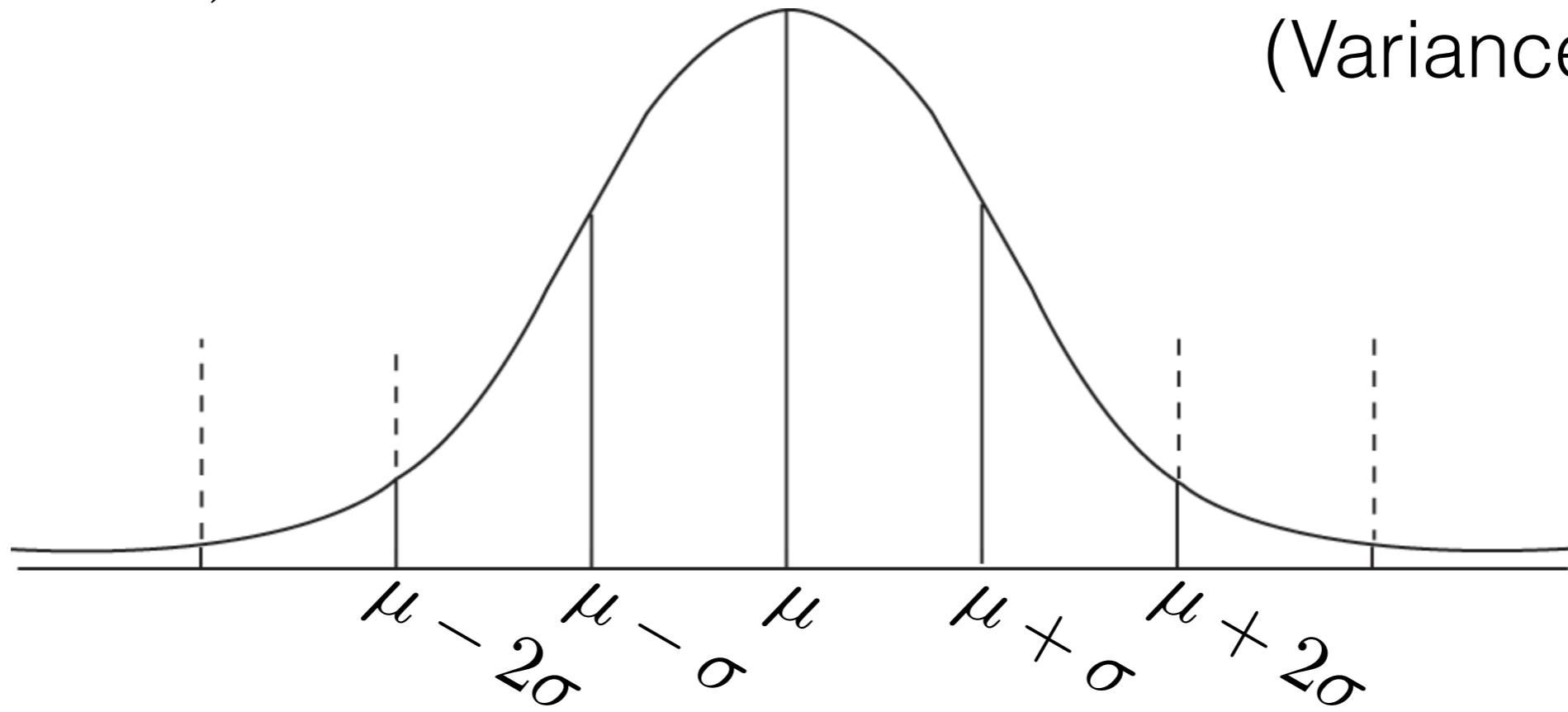
$$\mathcal{N}(y|\mu, \sigma^2) = (2\pi\sigma^2)^{-1/2} \exp\left[\frac{-(y-\mu)^2}{\sigma^2}\right]$$

Mean $\mu \in (-\infty, \infty)$
Standard deviation $\sigma \in (0, \infty)$
(Variance σ^2)
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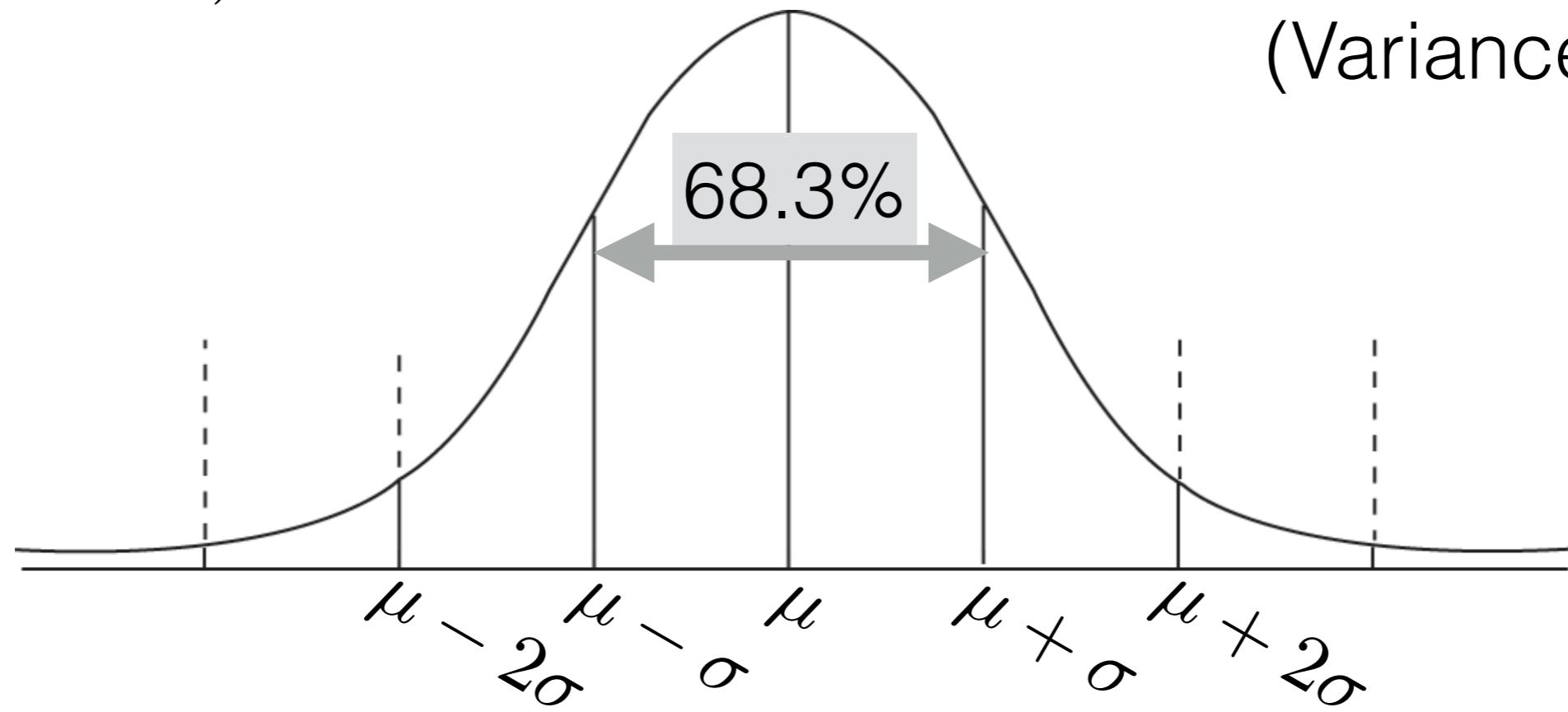
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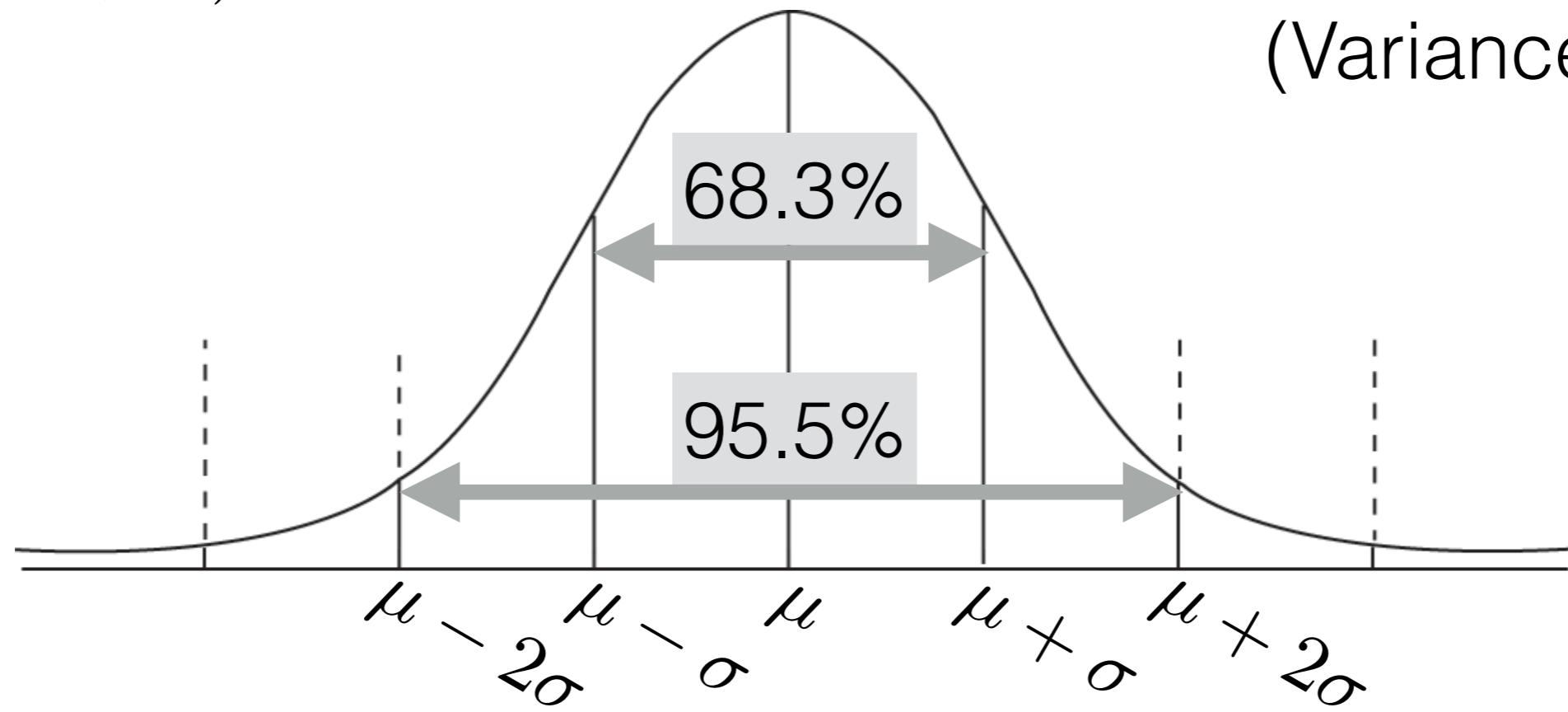
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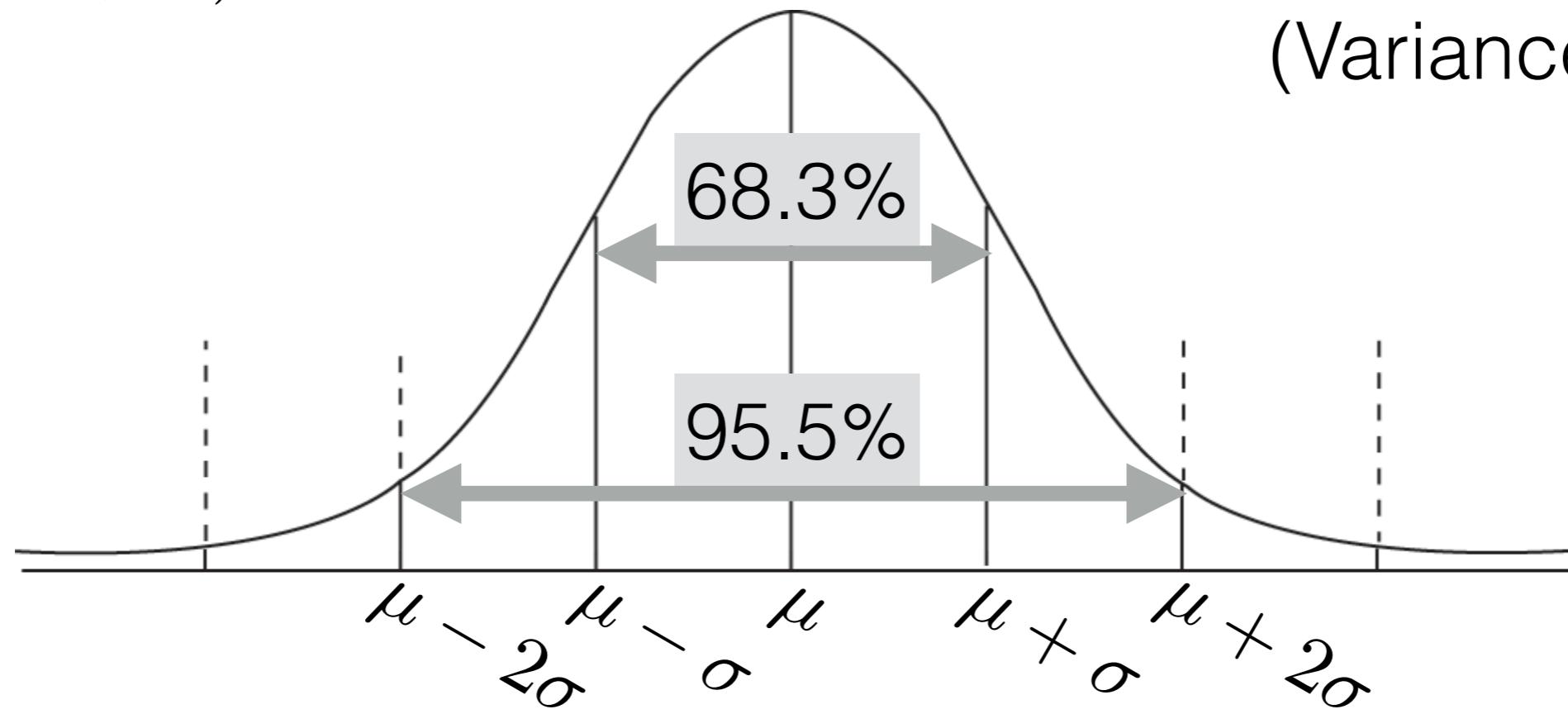
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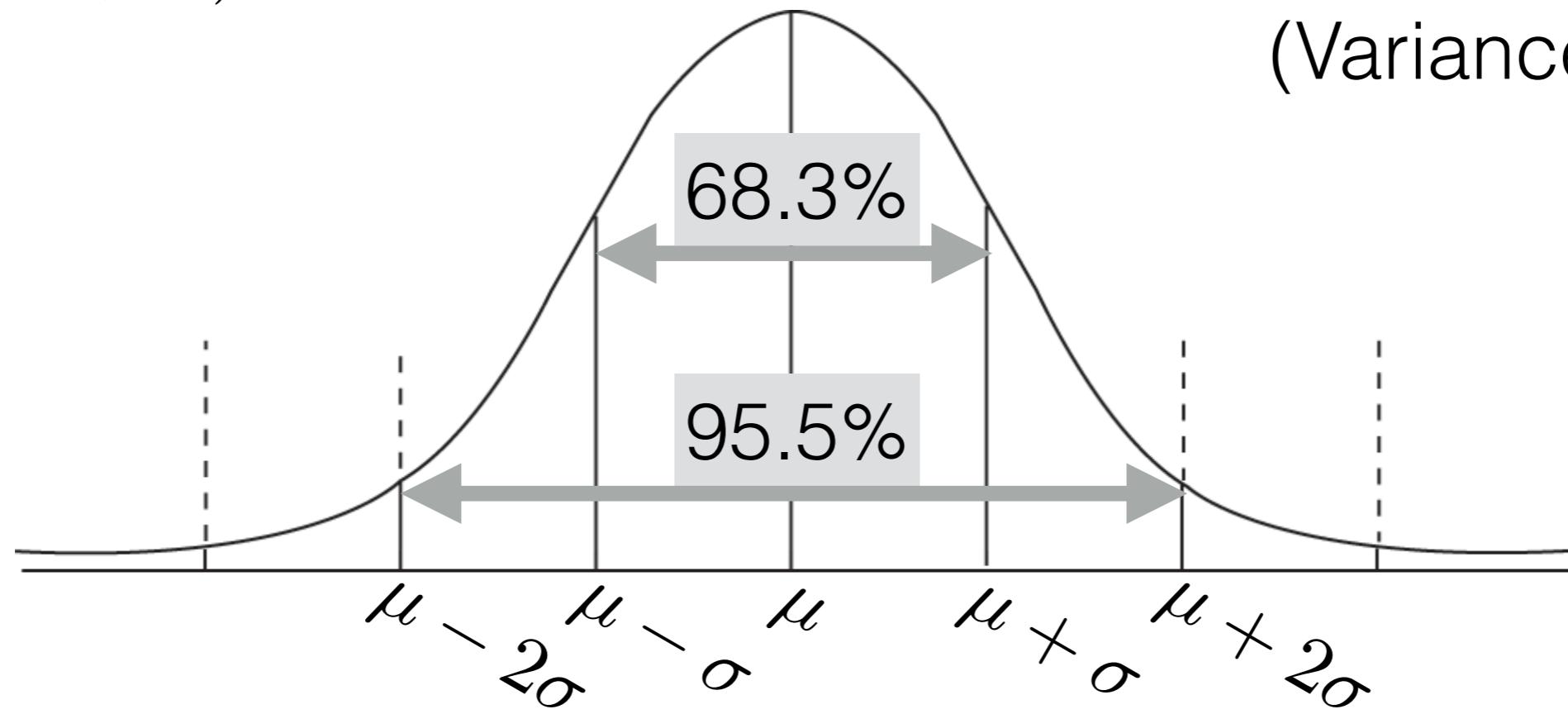


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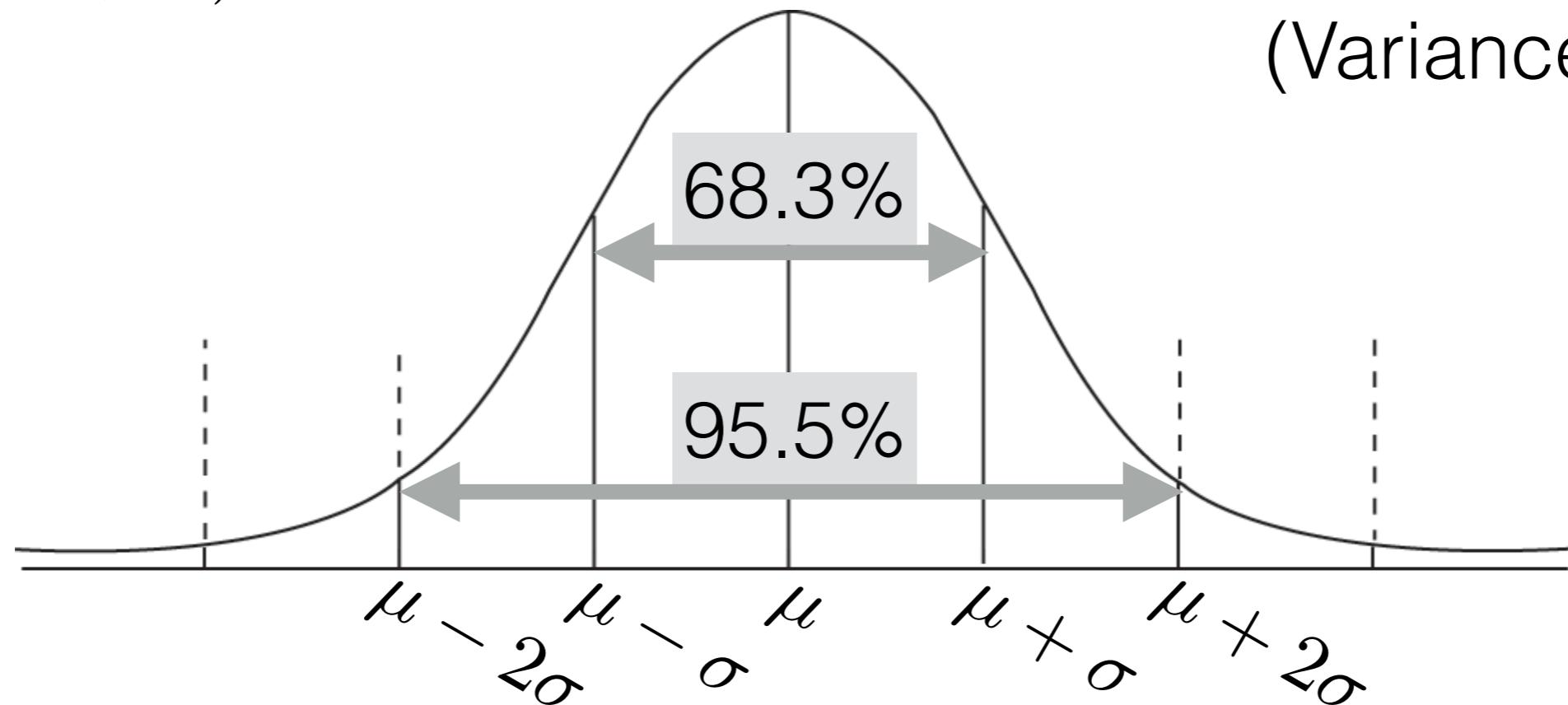


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- About 95% of the mass falls within 2 standard deviations of the mean [demo]
- If $Y \sim \mathcal{N}(0, 1)$, then $Y + \mu \sim \mathcal{N}(\mu, 1)$

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

Multivariate Gaussian review

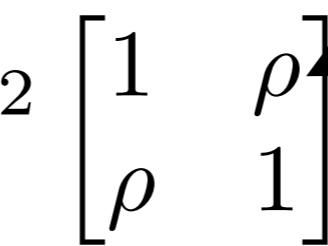
Multivariate Gaussian review

- General form: $\mathcal{N}(y|\mu, K)$ with
 - y & the mean μ are real-valued vectors with dimension M
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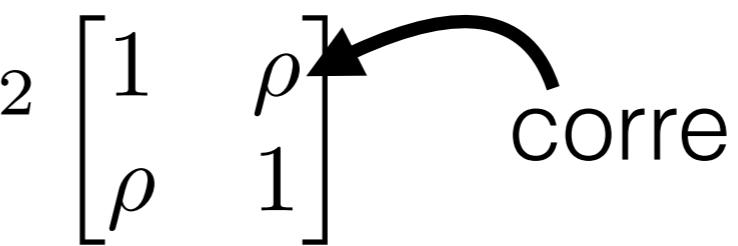
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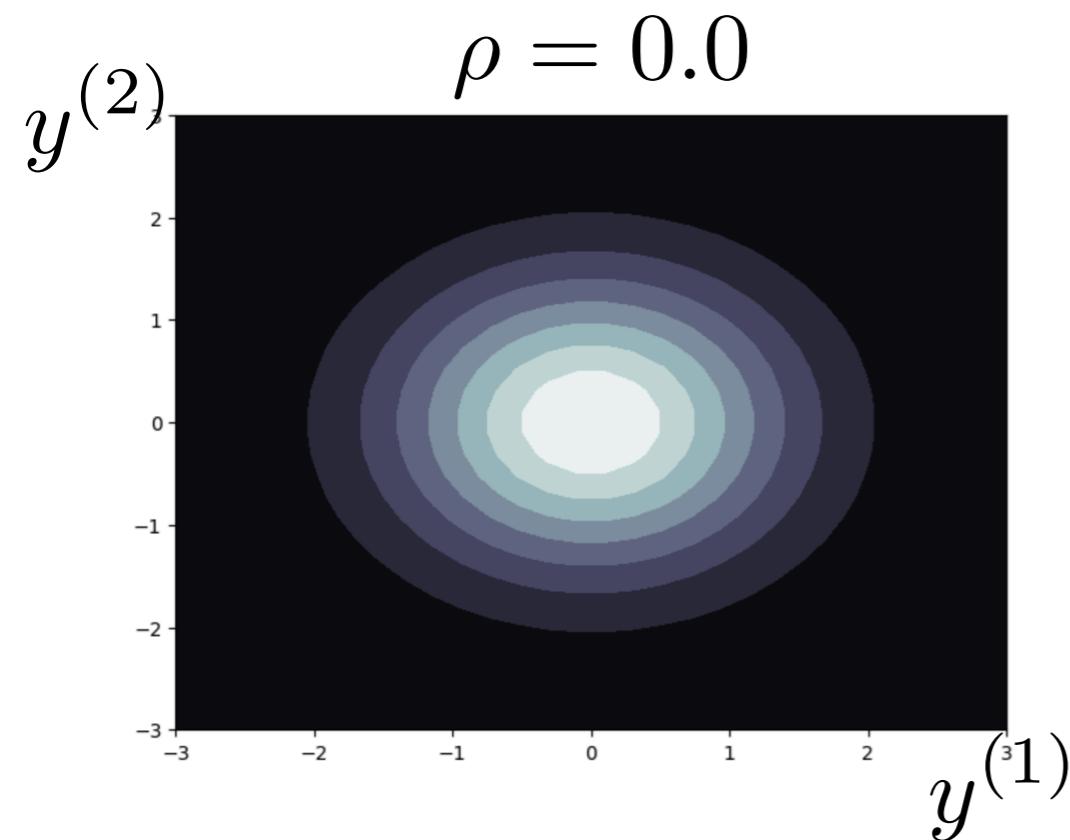
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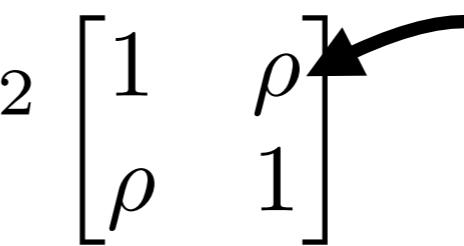
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- Let's also assume $K = \sigma^2 \begin{bmatrix} 1 & \rho \\ \rho & 1 \end{bmatrix}$  correlation

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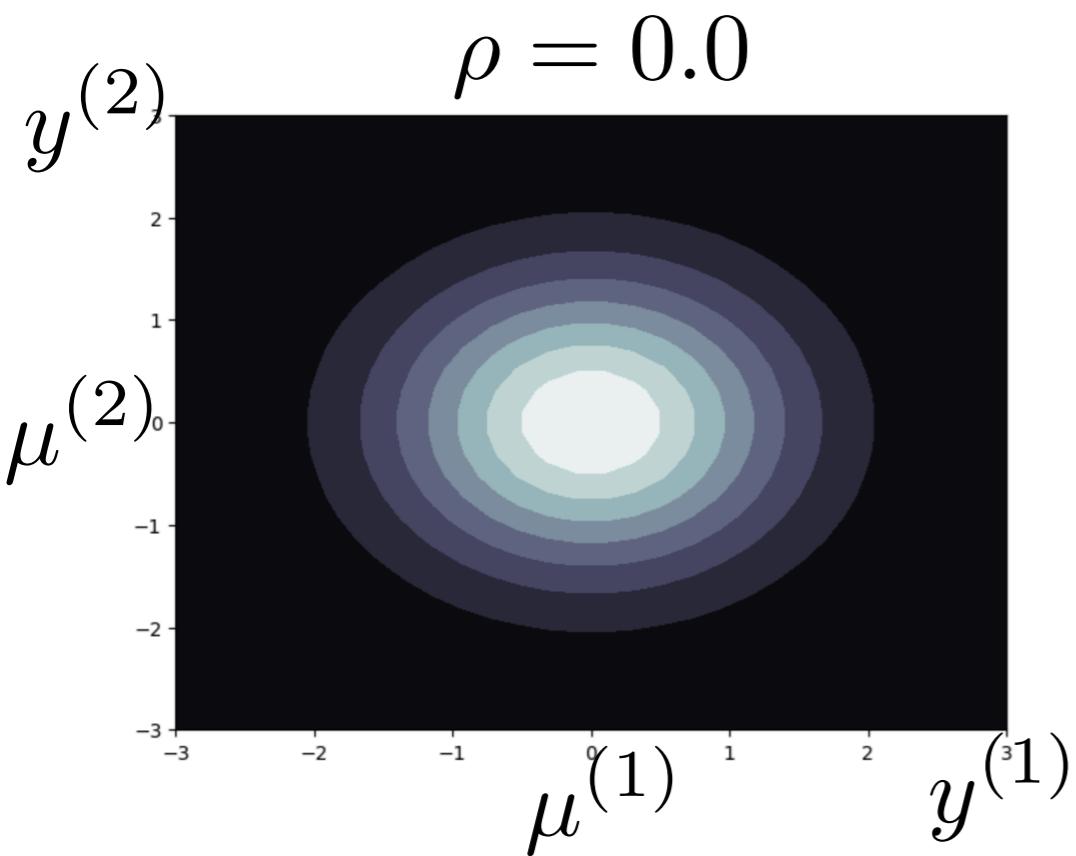
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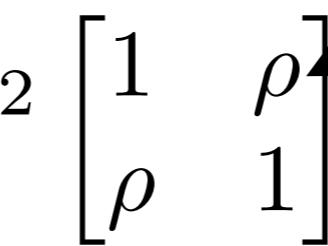
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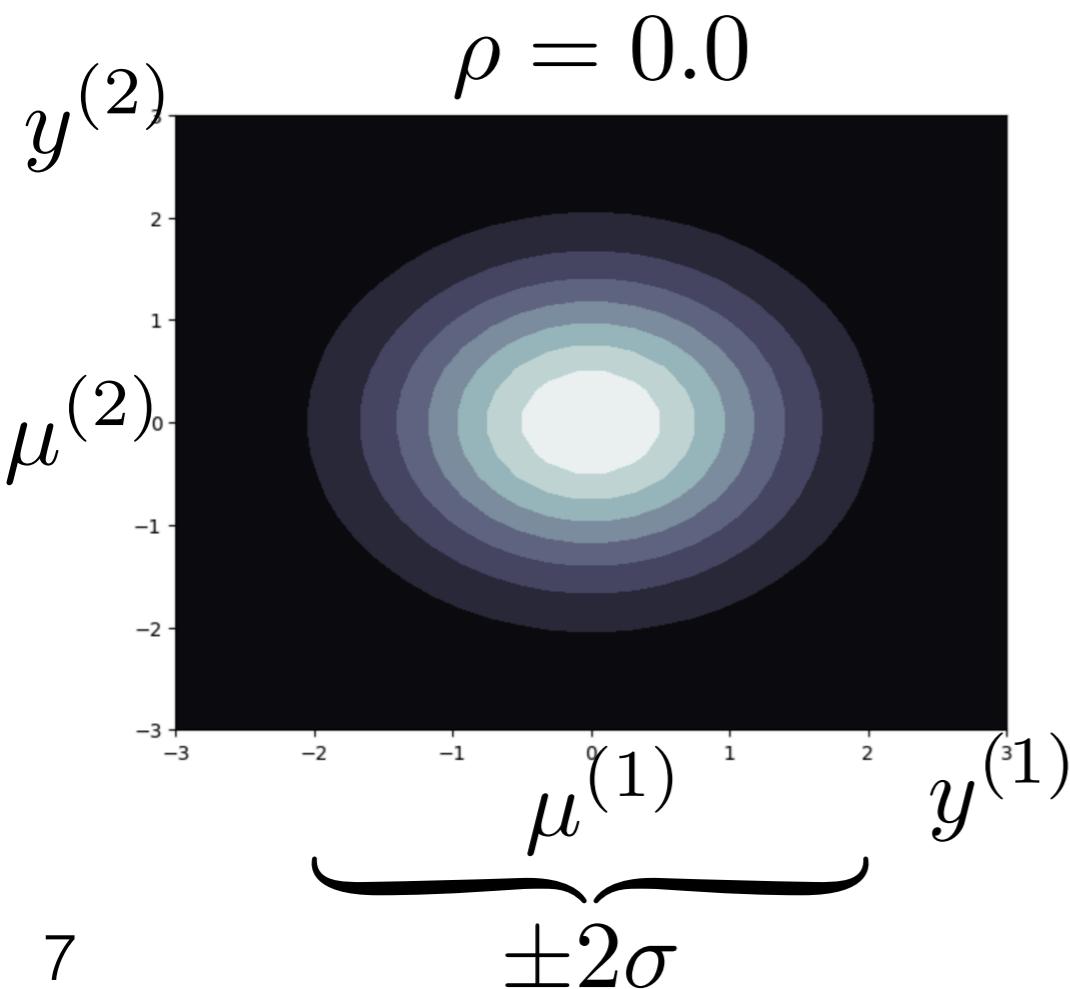
A diagram showing a 2D Gaussian distribution centered at the origin. The horizontal axis is labeled $\mu^{(1)}$ and the vertical axis is labeled $\mu^{(2)}$. Concentric ellipses are centered at the origin, representing the probability density function. A curved arrow points from the label "correlation" to the off-diagonal element ρ in the covariance matrix.



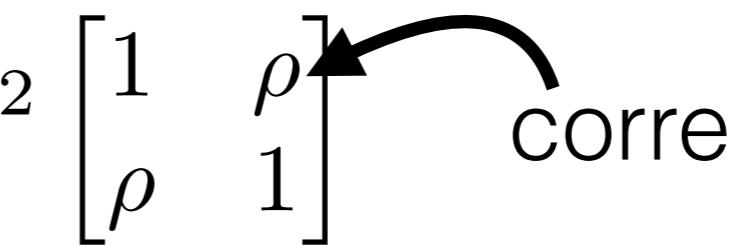
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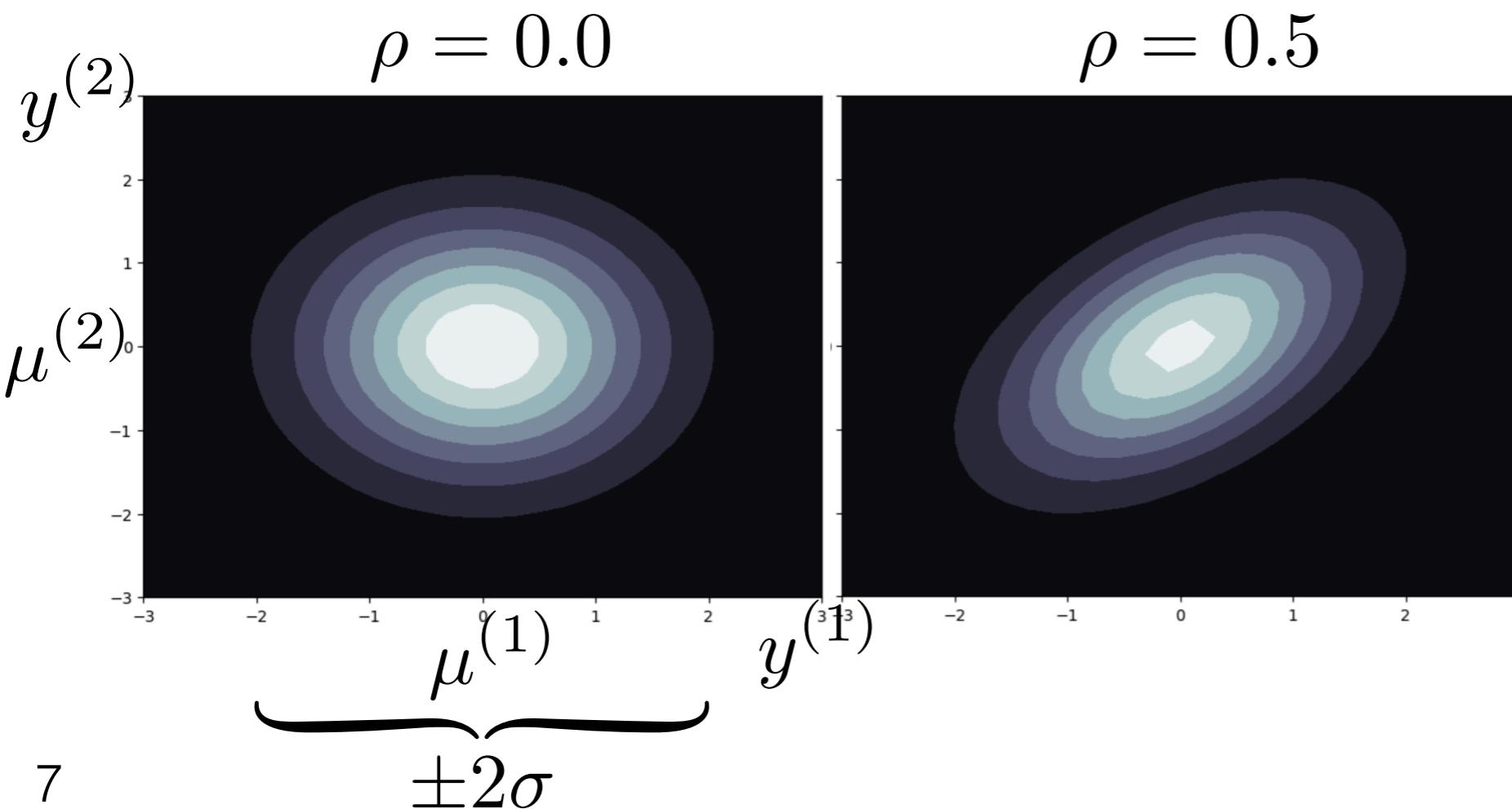
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A 2D plot of a bivariate Gaussian distribution. The horizontal axis is labeled $y^{(1)}$ and the vertical axis is labeled $y^{(2)}$. The mean vector μ is at the center of the distribution. Concentric ellipses represent the standard deviation $\pm 2\sigma$. A curved arrow points from the label "correlation" to the off-diagonal element ρ in the covariance matrix.

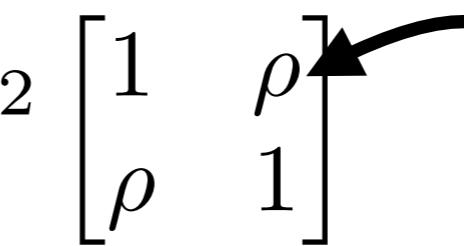


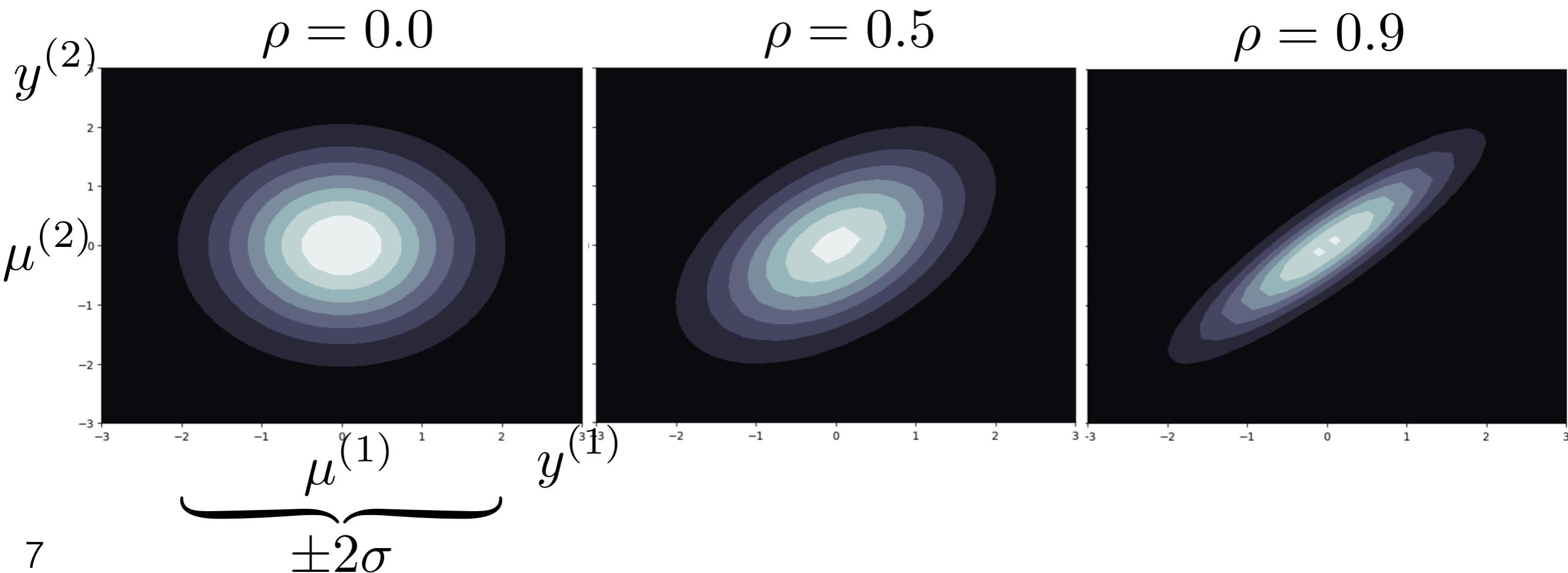
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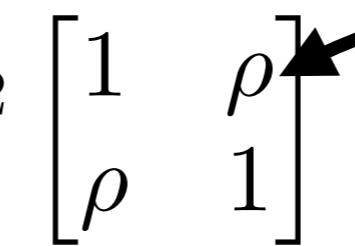


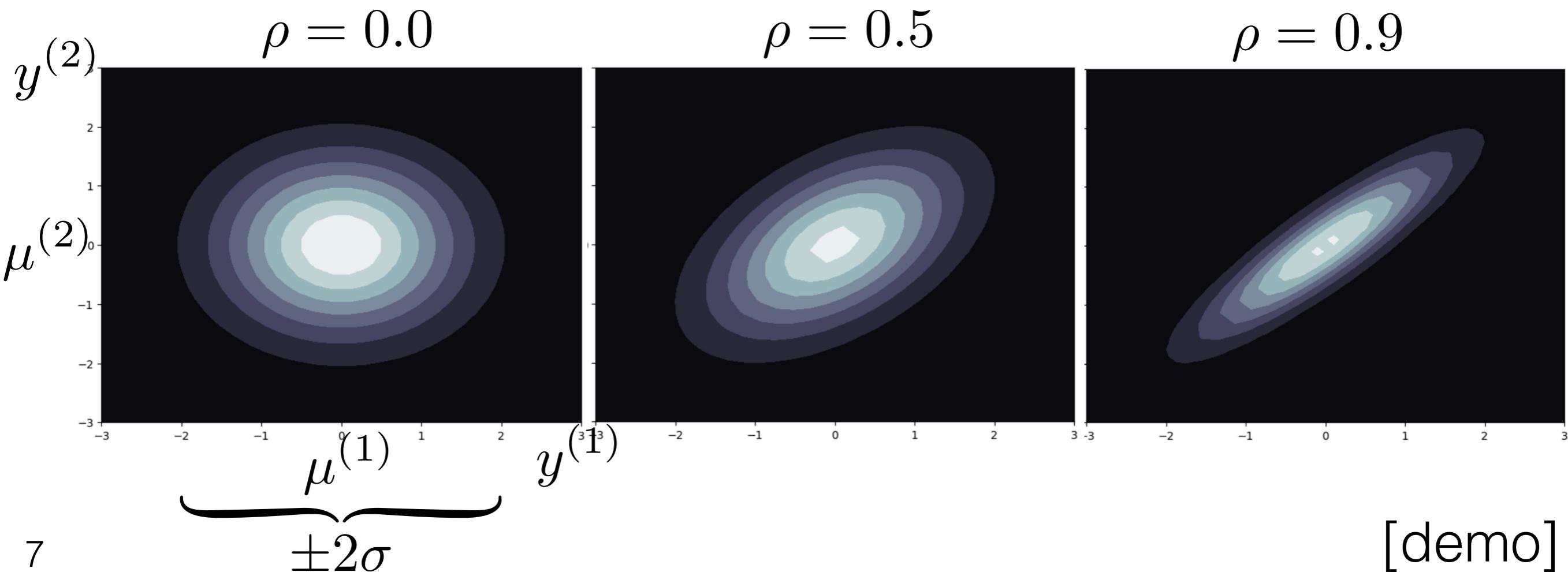
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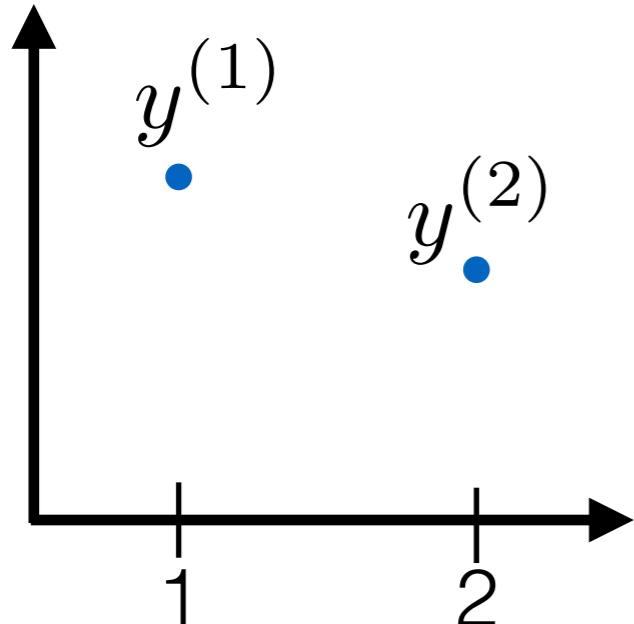
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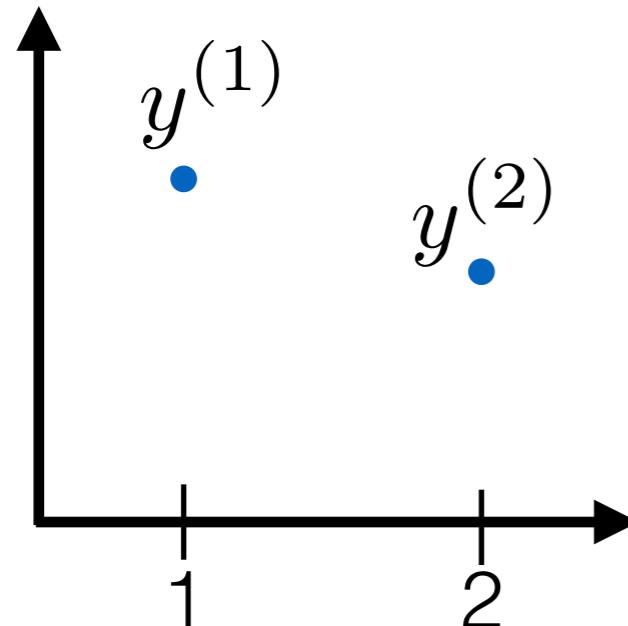
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Multivariate Gaussian using locations

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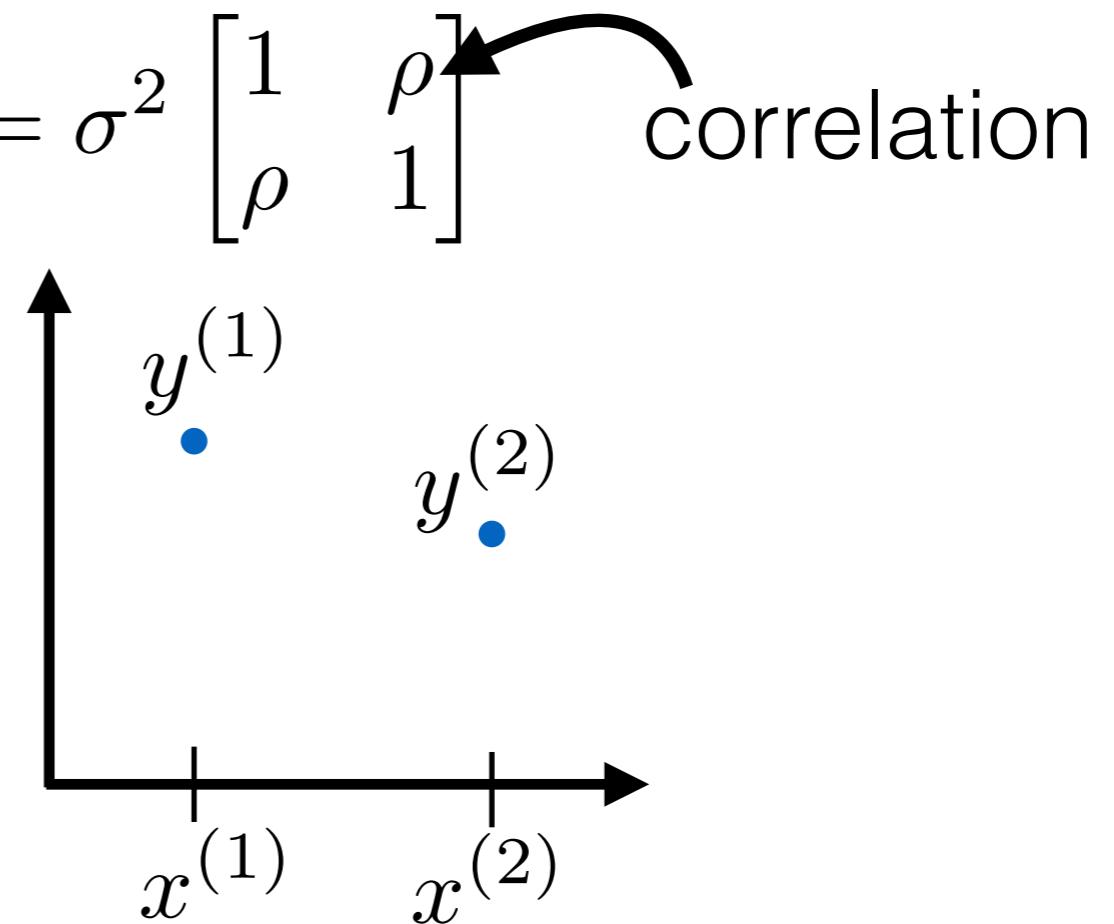
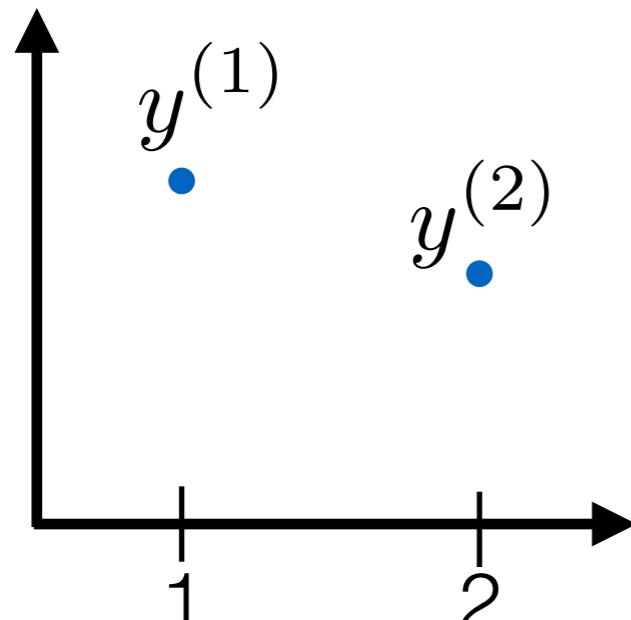


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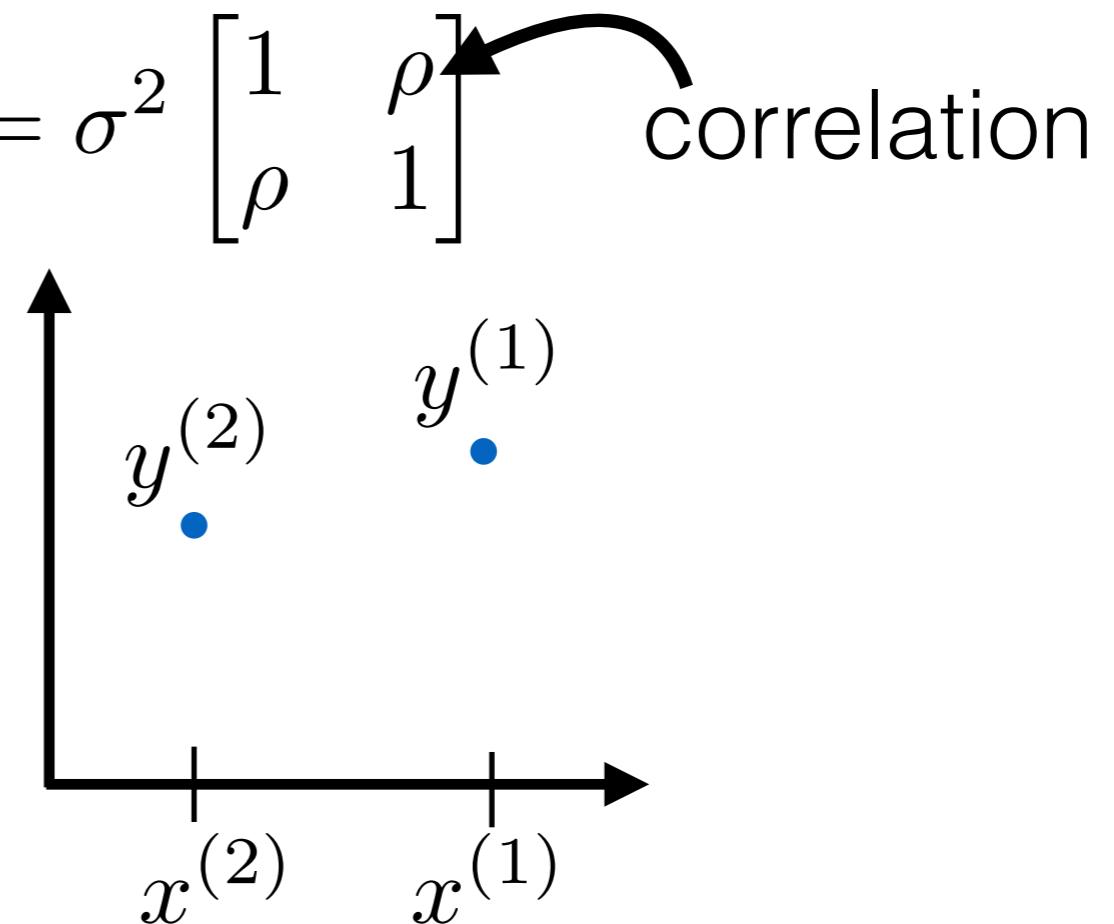
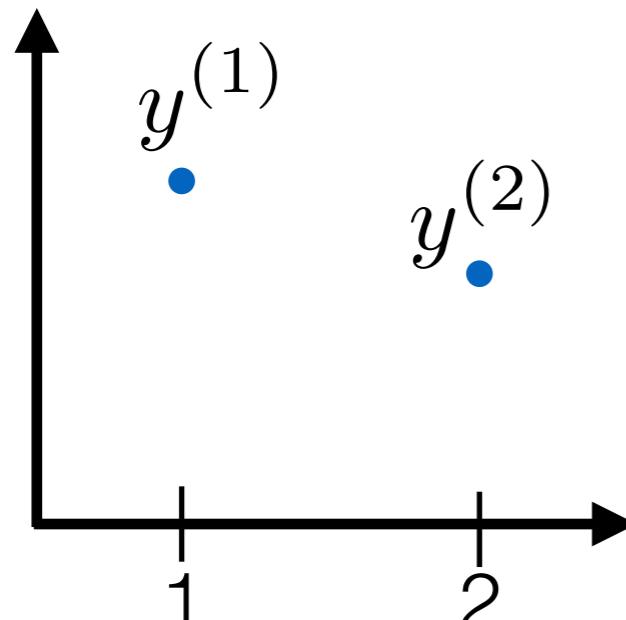
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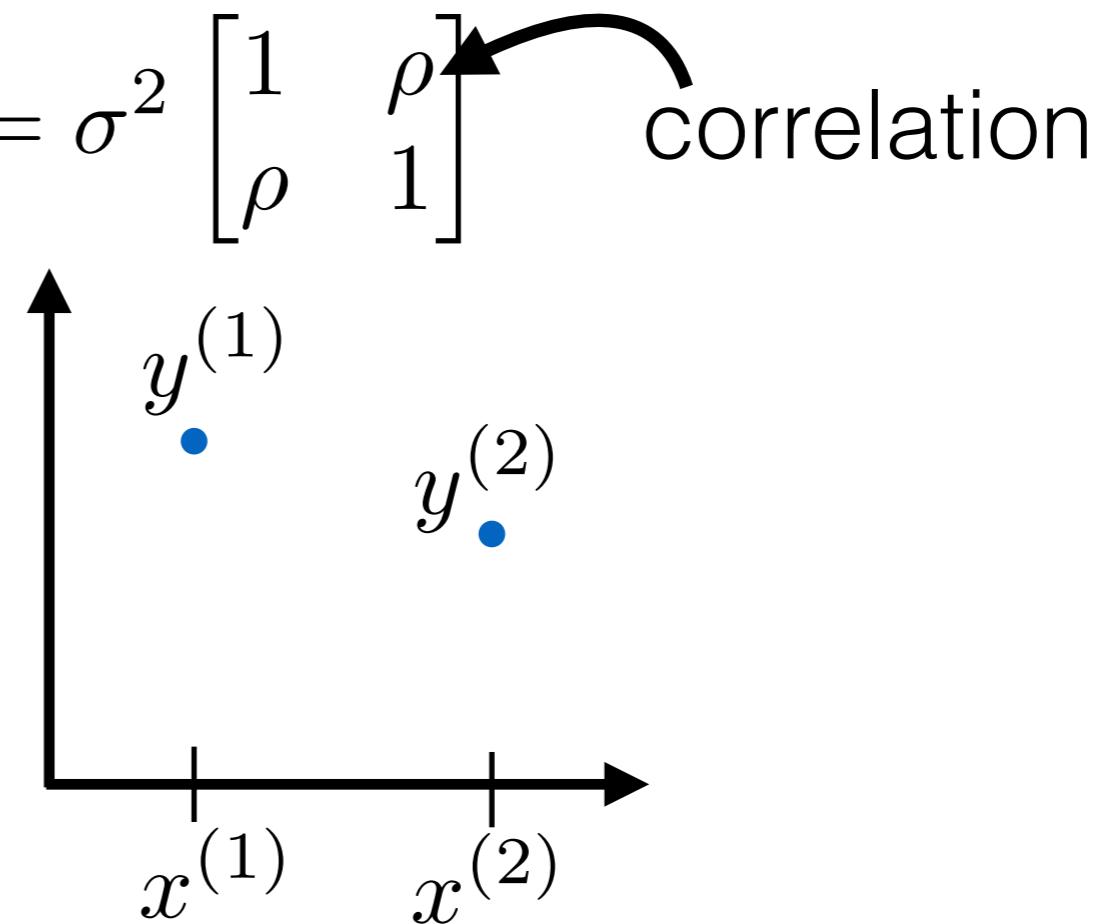
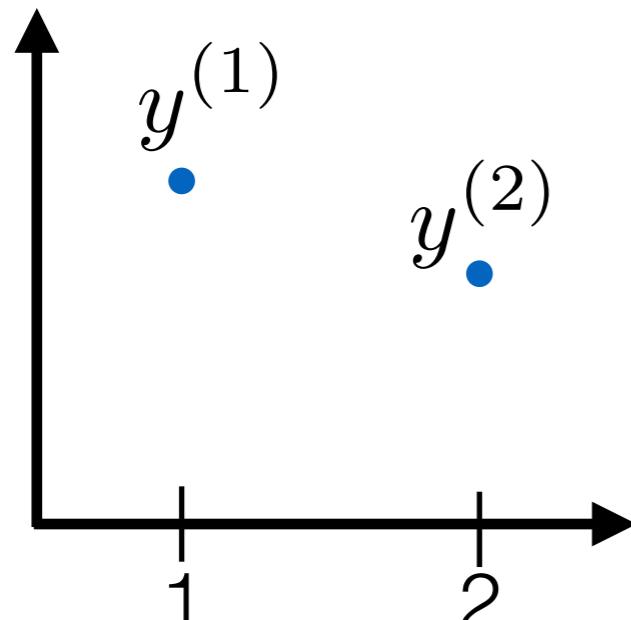
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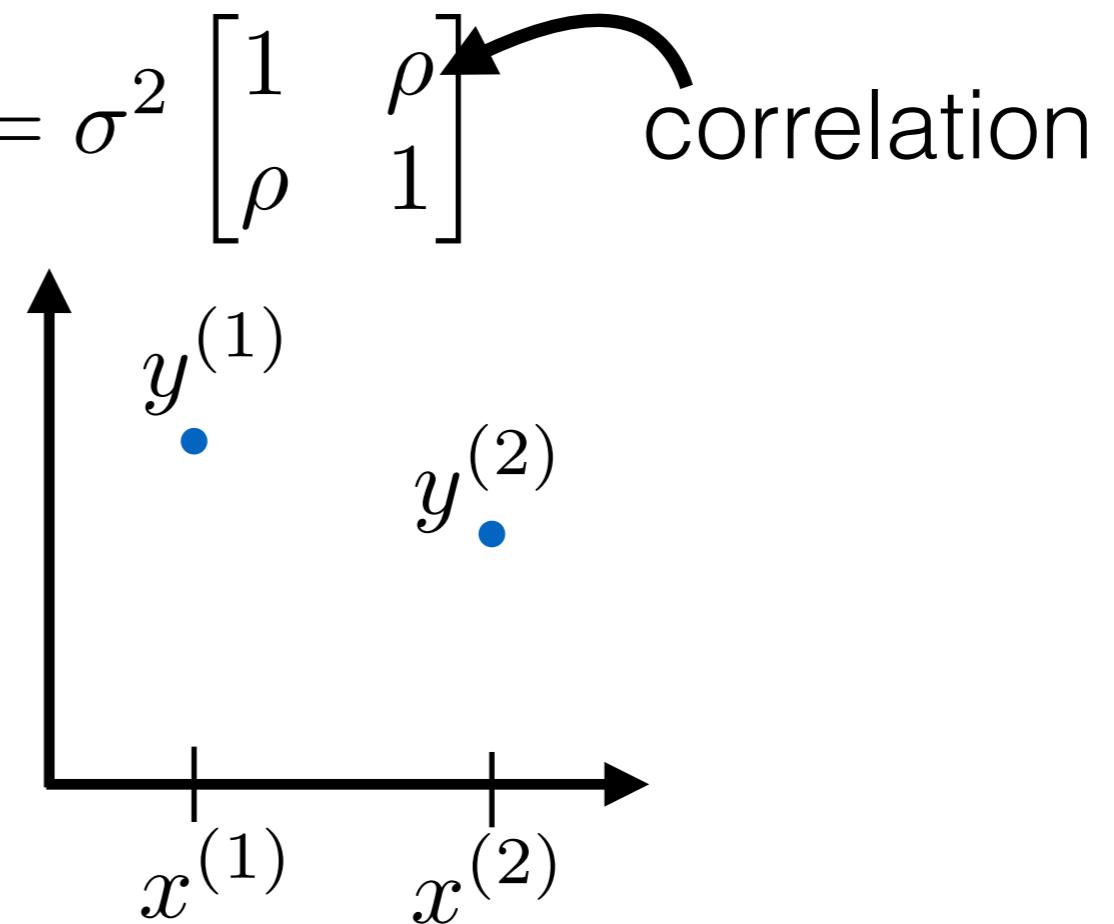
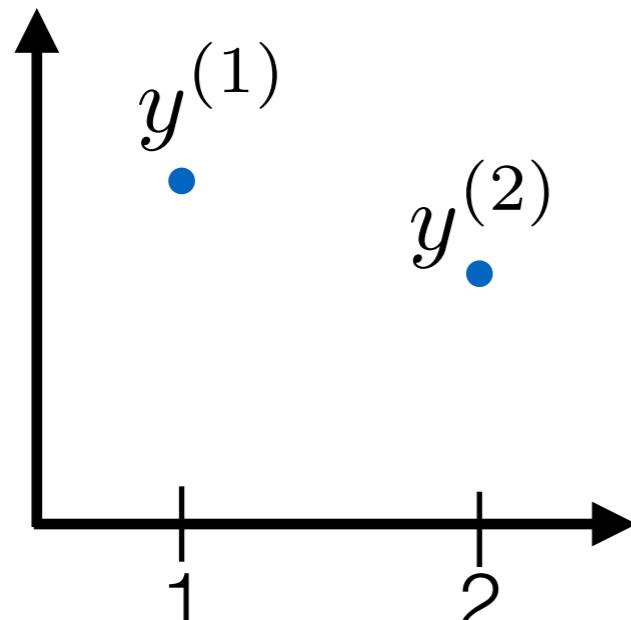
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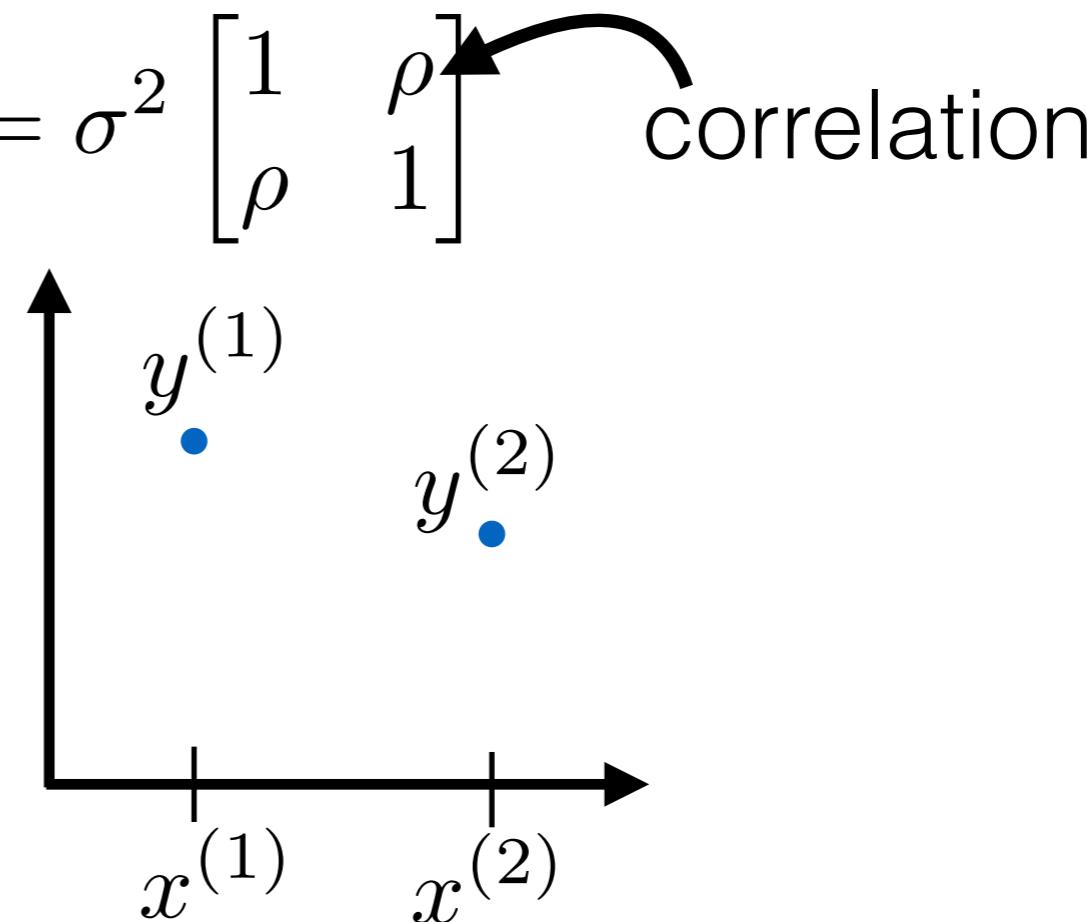
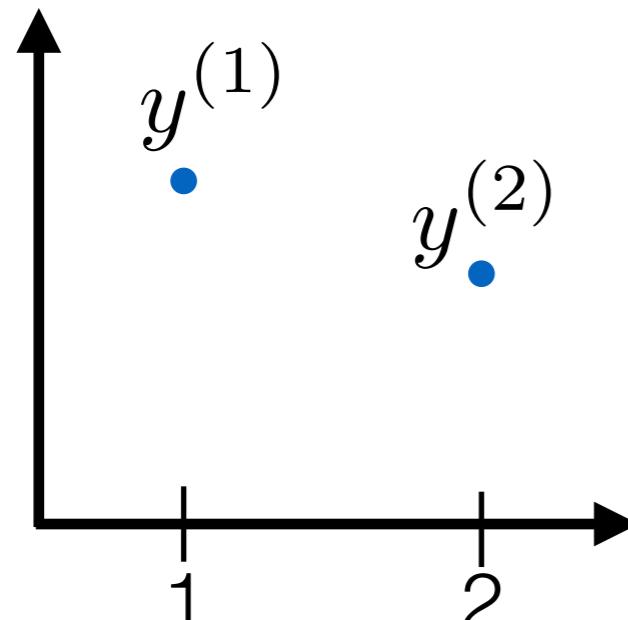
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- What if we let the correlation depend on the x 's?

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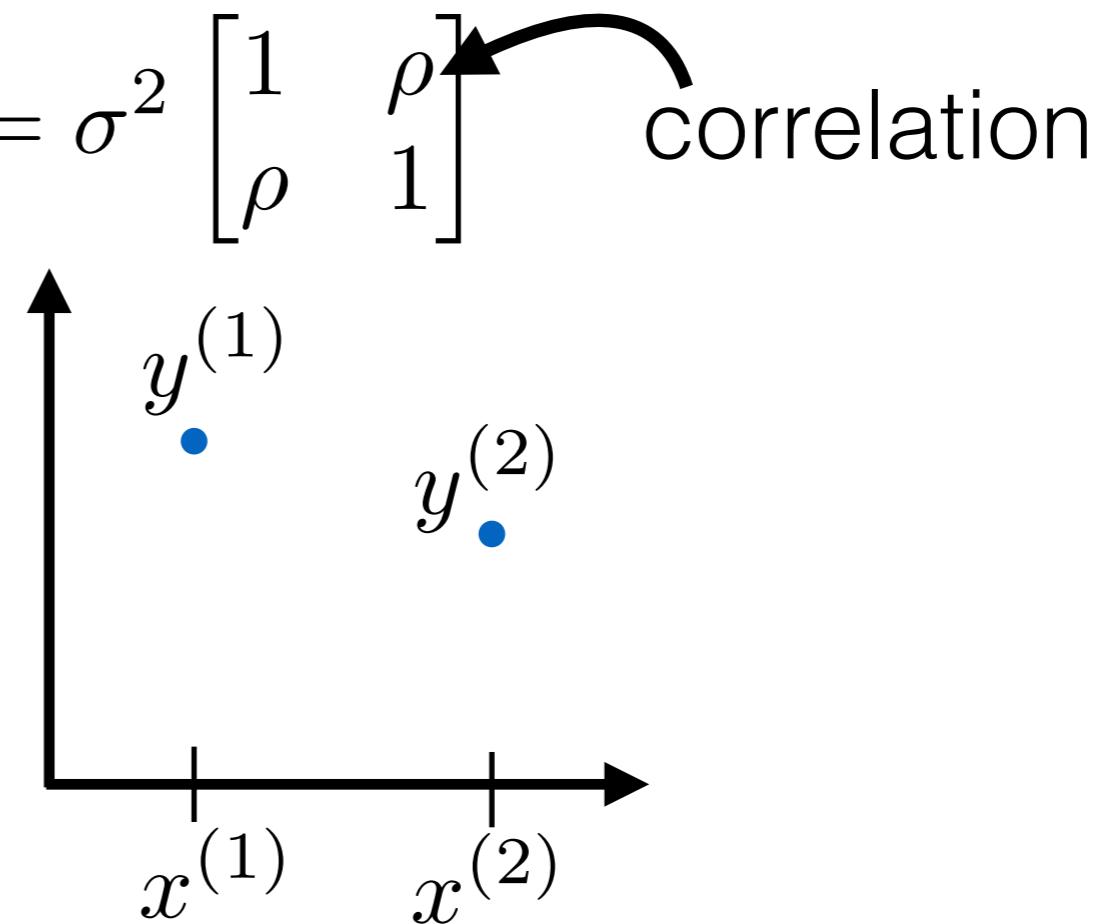
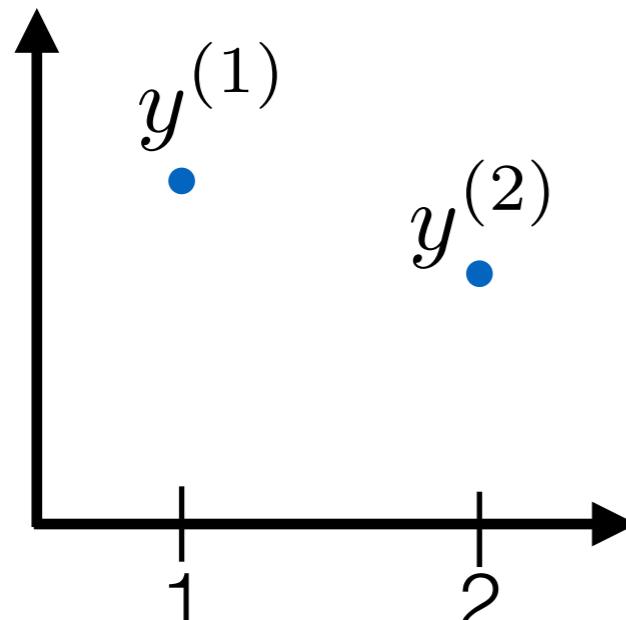
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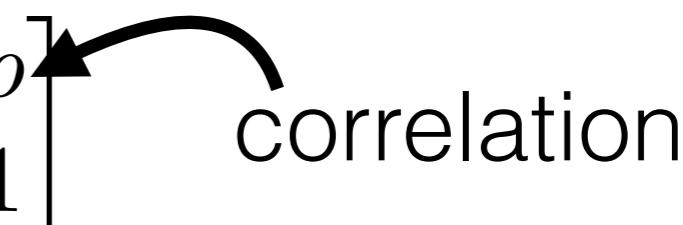
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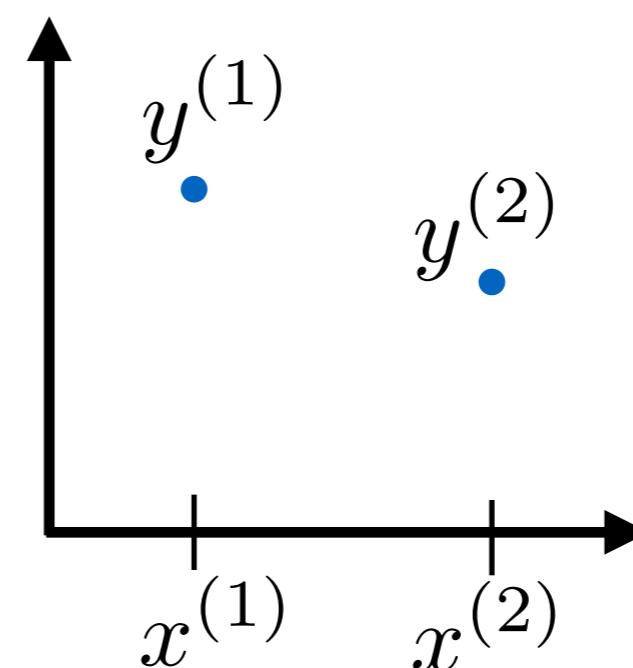
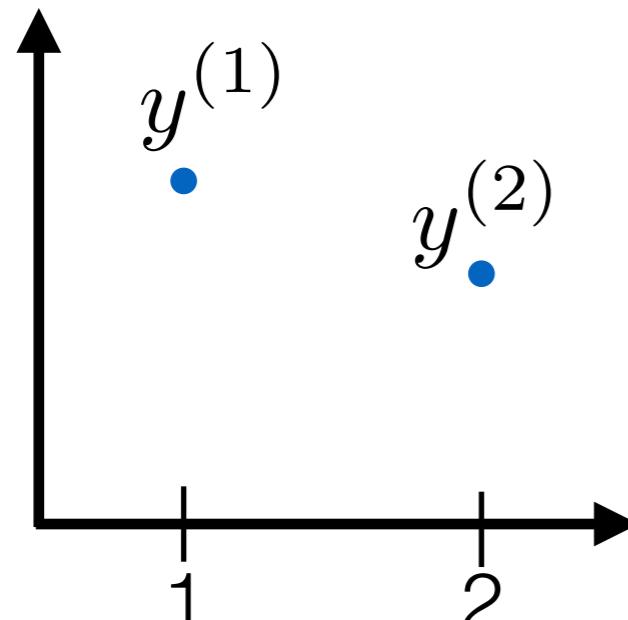
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Multivariate Gaussian using locations

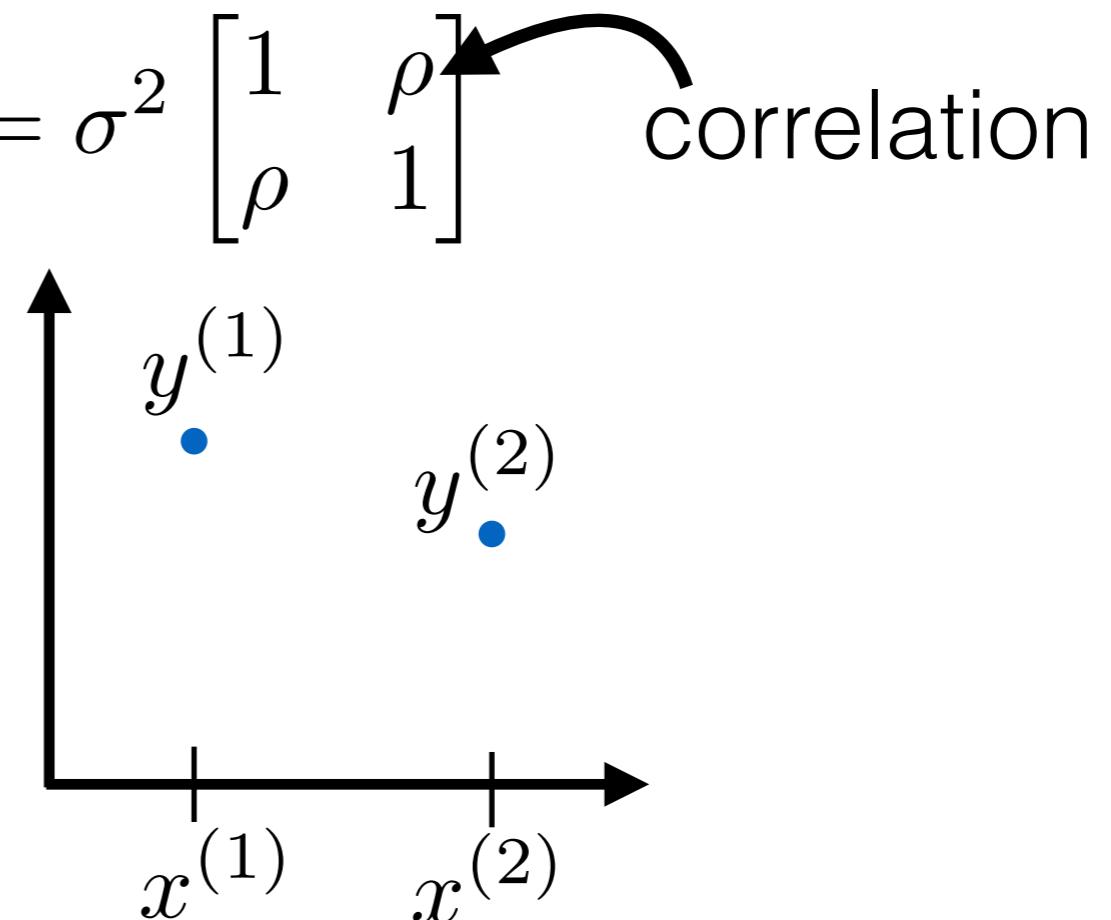
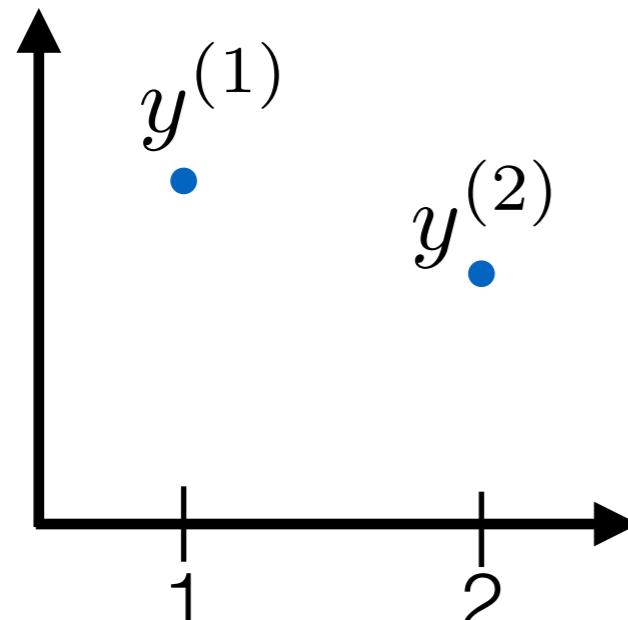
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 - And goes to 0 as the x 's get far

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- With $\mu = [0, 0]^\top$ and $K = \sigma^2 \begin{bmatrix} 1 & \rho \\ \rho & 1 \end{bmatrix}$



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 - Let $\rho = \rho(|x^{(1)} - x^{(2)}|)$
 - Where the correlation goes to 1 as the x 's get close
 - And goes to 0 as the x 's get far

Multivariate Gaussian using locations

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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!