

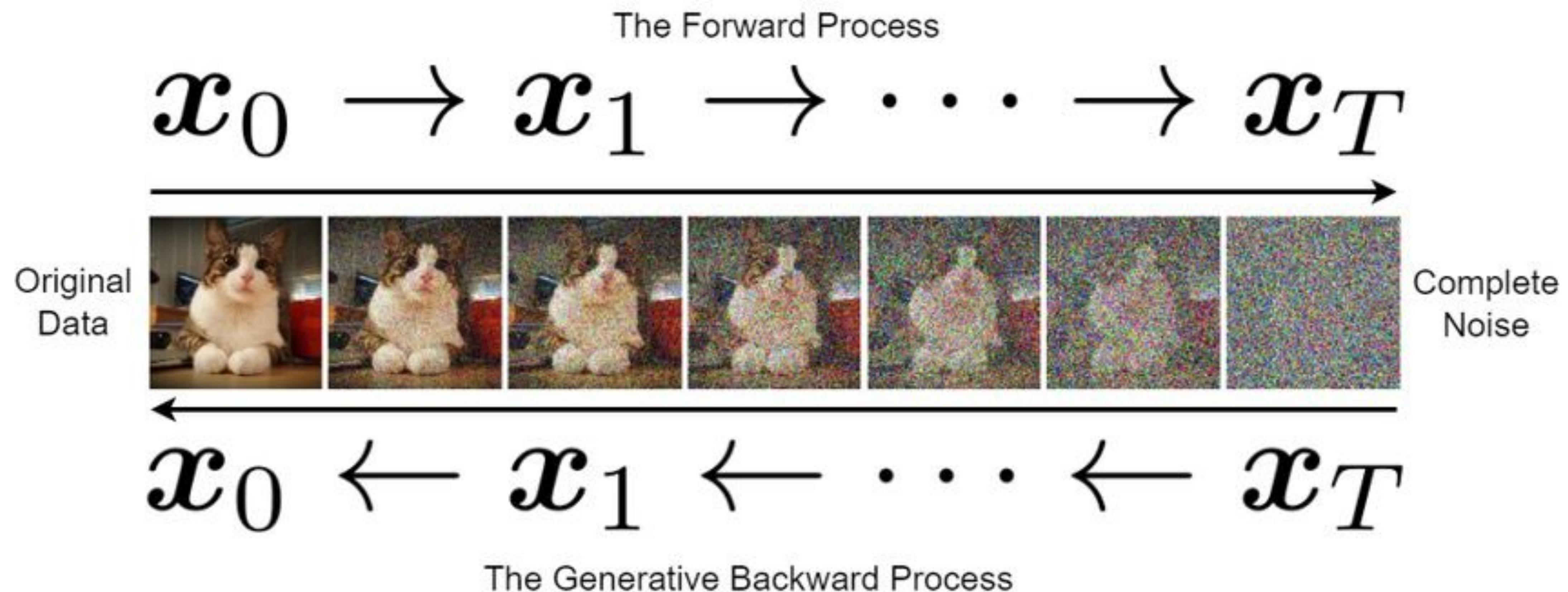
# **A solvable model of Generative Diffusion and the memorization phenomenon**

**Leonardo Bandera**

# Agenda

- Diffusion Sampling and problem statement
- Understanding training dynamics: the original setting
- First line of research: towards a more realistic architecture
- Second line of research: structured data

# Generative Diffusion

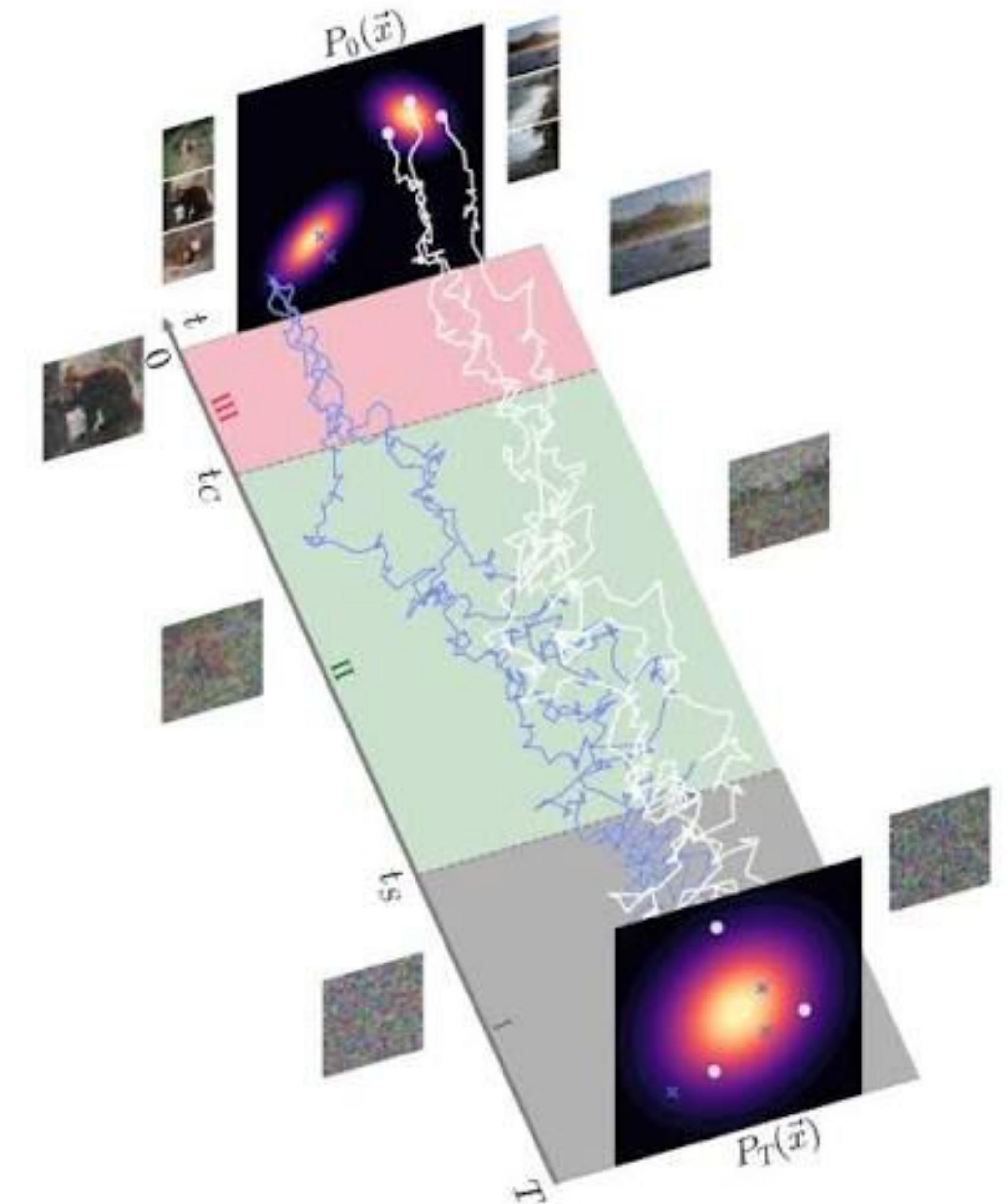


# Score-based Diffusion

- Forward process:  $\frac{dx}{dt} = -x(t) + \eta(t)$
- Reversed process:  $\frac{dx}{d\tau} = x(\tau) + 2 \nabla \log P_\tau(x) + \tilde{\eta}(\tau)$
- The score  $S(x, t) = \nabla \log P_t(x)$  is unknown... we learn it!

$$\mathcal{L}_\lambda(\theta) = \frac{1}{n} \sum_{\mu=1}^n \mathbb{E}_{t \sim Q(t)} \mathbb{E}_{\xi \sim \mathcal{N}(0, \mathbb{I}_d)} \| \hat{S}^\theta(x_t^\mu(\xi), t) + \frac{\xi}{\sqrt{\Delta_t}} \|_2^2$$

# Problem: sampling with the empirical loss minimizer leads to memorization!



Giulio Biroli, Tony Bonnaire, Valentin de Bortoli, and Marc Mézard.  
Dynamical regimes of diffusion models. Nature Communications,  
15(1):9957, nov 2024

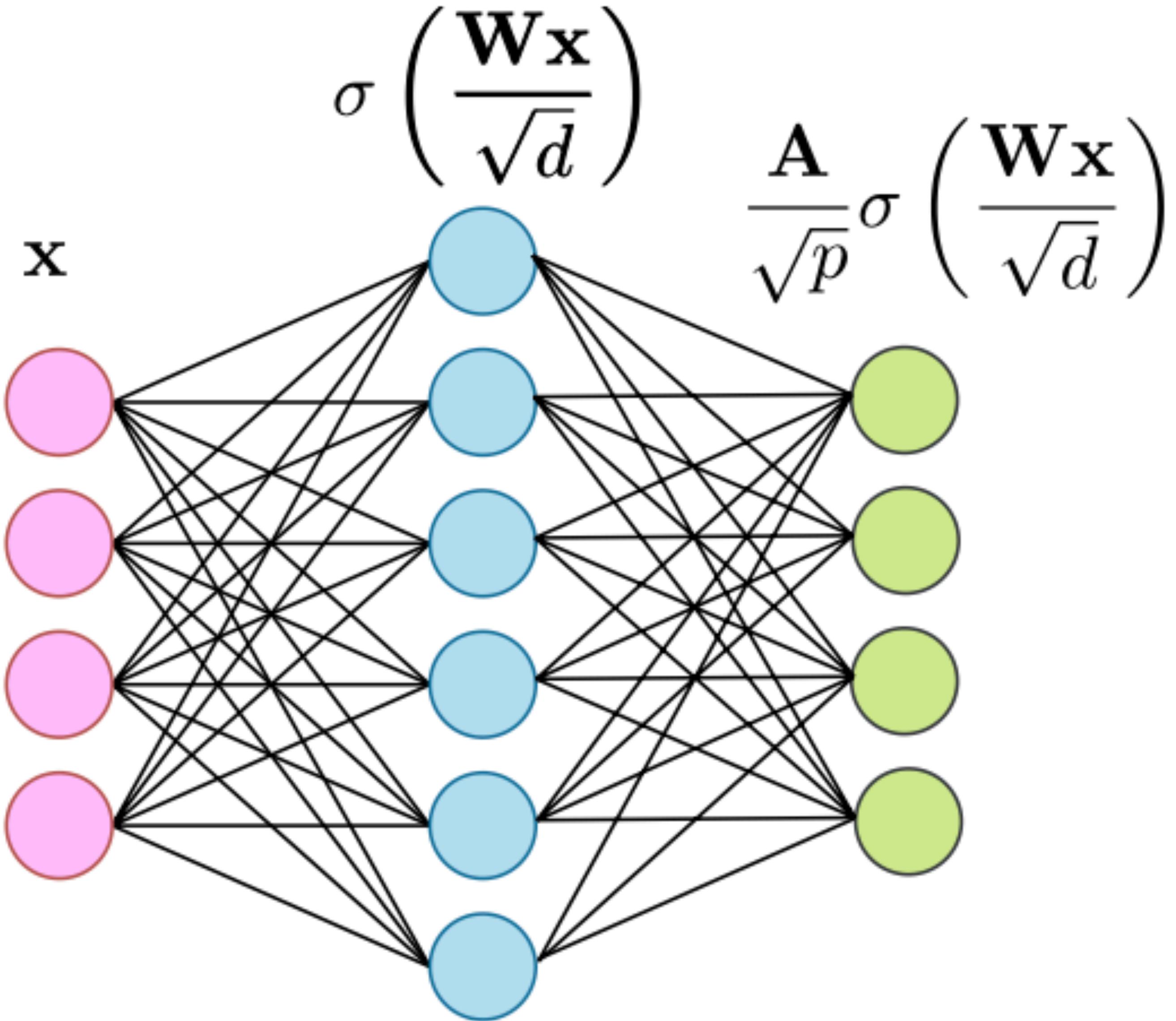
# Why real diffusion systems avoid this degeneracy?

- Architectural constraints
- Training dynamics

# The original setting

Gaussian data

One RFNN per time



## Gradient Flow

$$\dot{A}(\tau) = -2\Delta_t \frac{d}{p} AU - \frac{2d\sqrt{\Delta_t}}{\sqrt{p}} V^\top$$

where

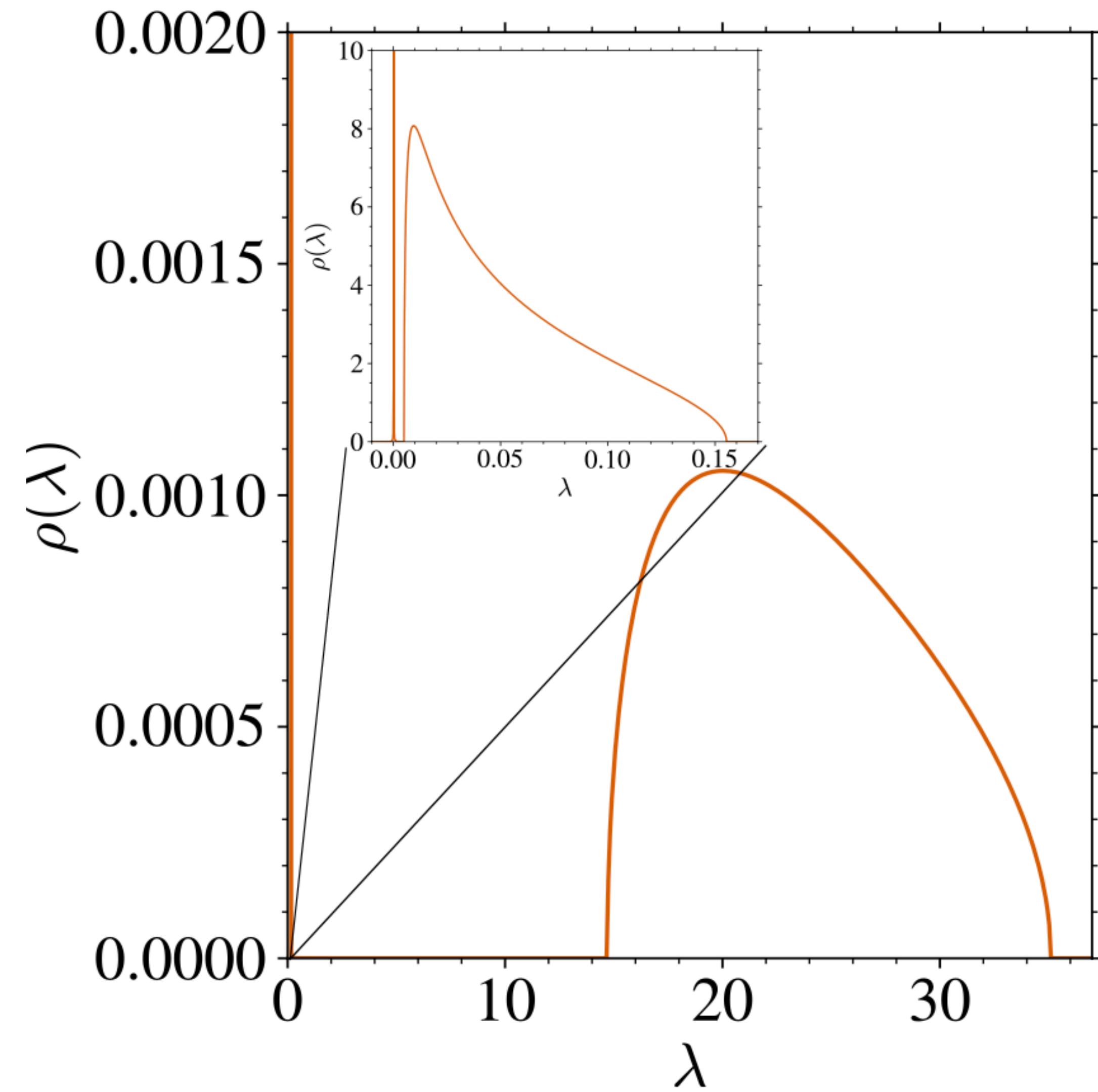
$$U = \frac{1}{n} \sum_{\nu=1}^n \mathbb{E}_\xi [\sigma(\frac{Wx_t^\nu(\xi)}{\sqrt{d}})\sigma(\frac{Wx_t^\nu(\xi)}{\sqrt{d}})^\top]$$

The timescales of the training dynamics are given by the inverse eigenvalues of the matrix  $\Delta_t \frac{d}{p} U$  !

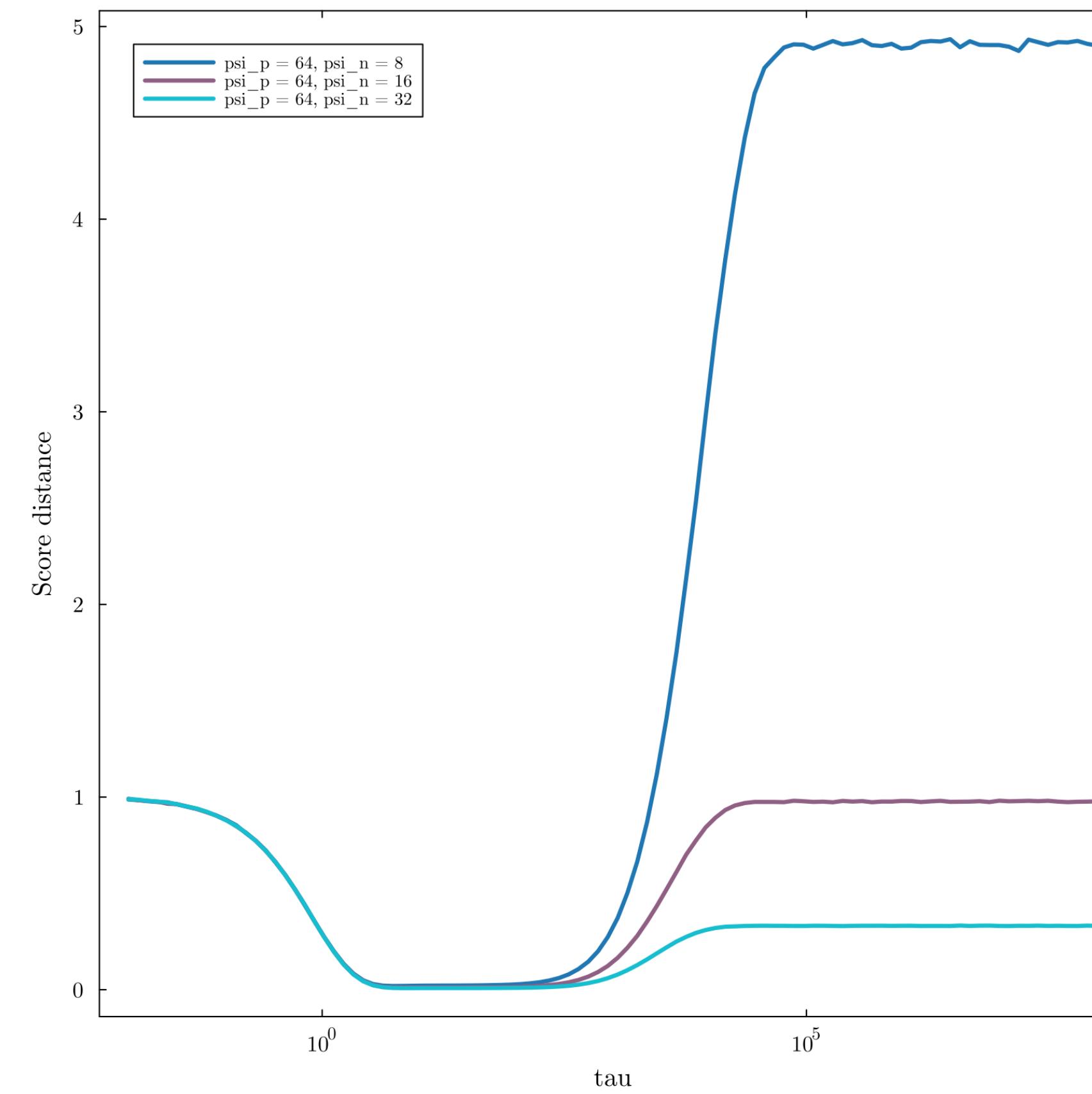
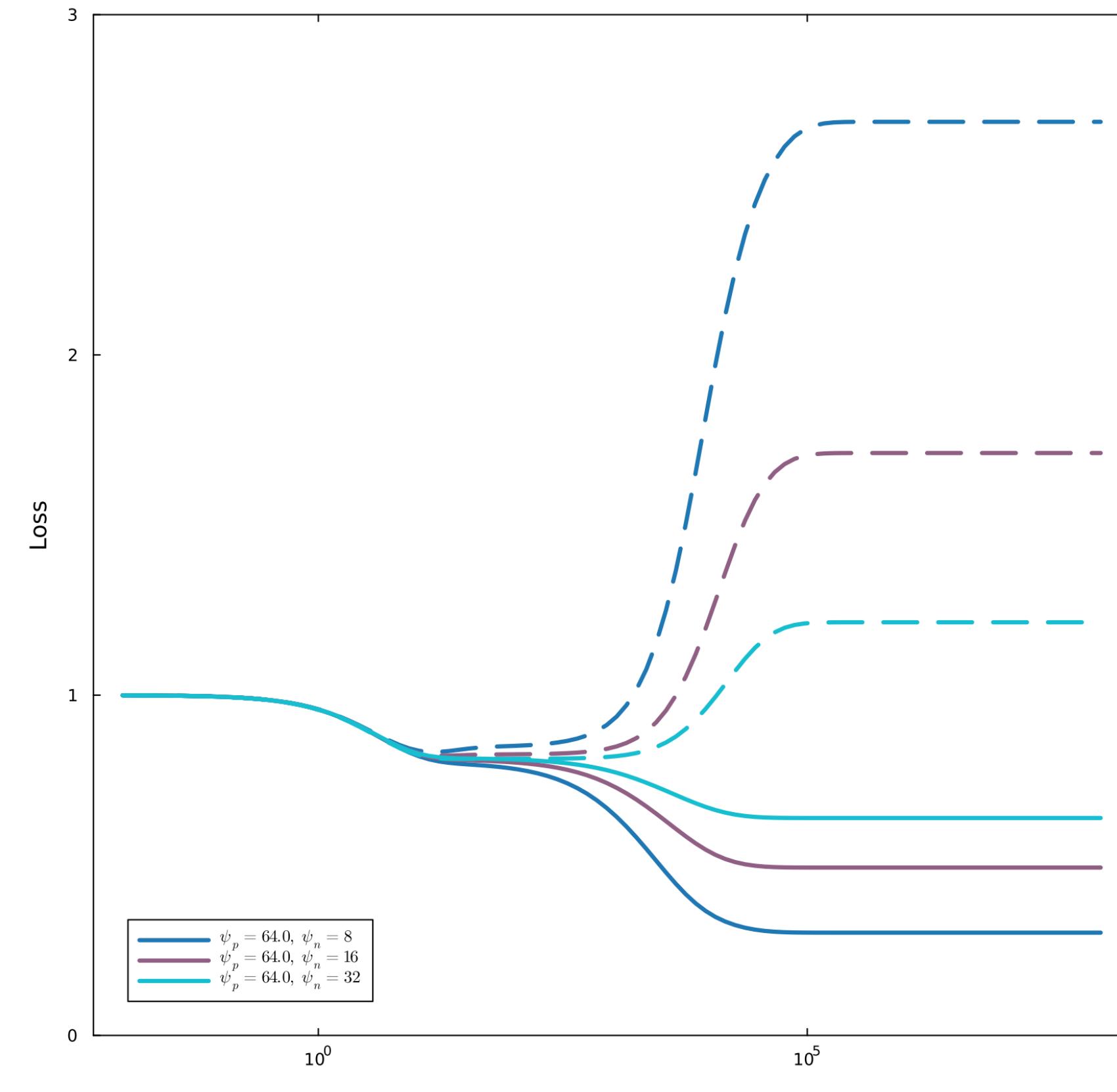
# $U$ spectrum

- Stieltjes transform
- GEP
- Replica

***Two bulks!***



**What's happening at the metrics at the timescales associated to the bulks?**

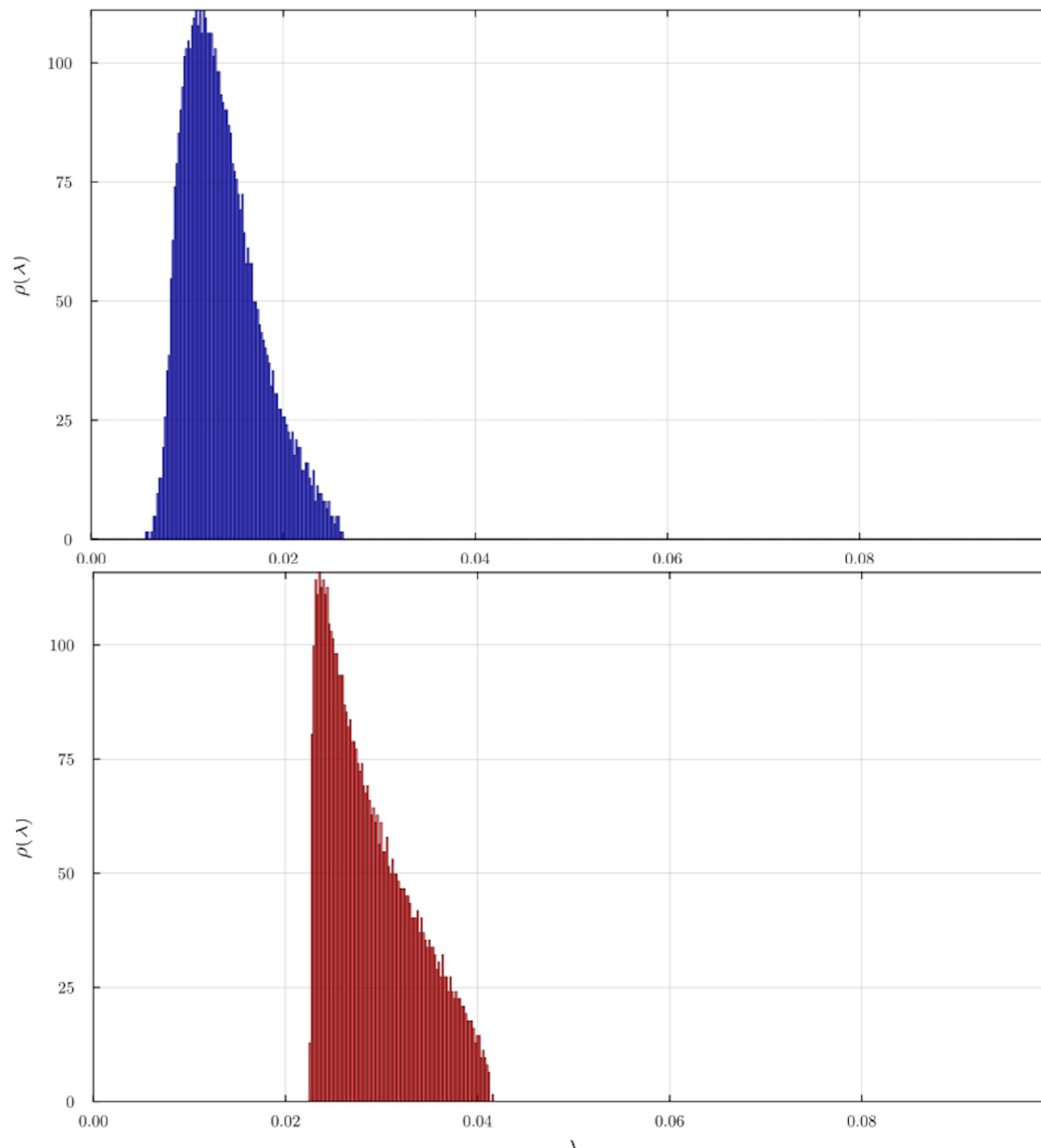
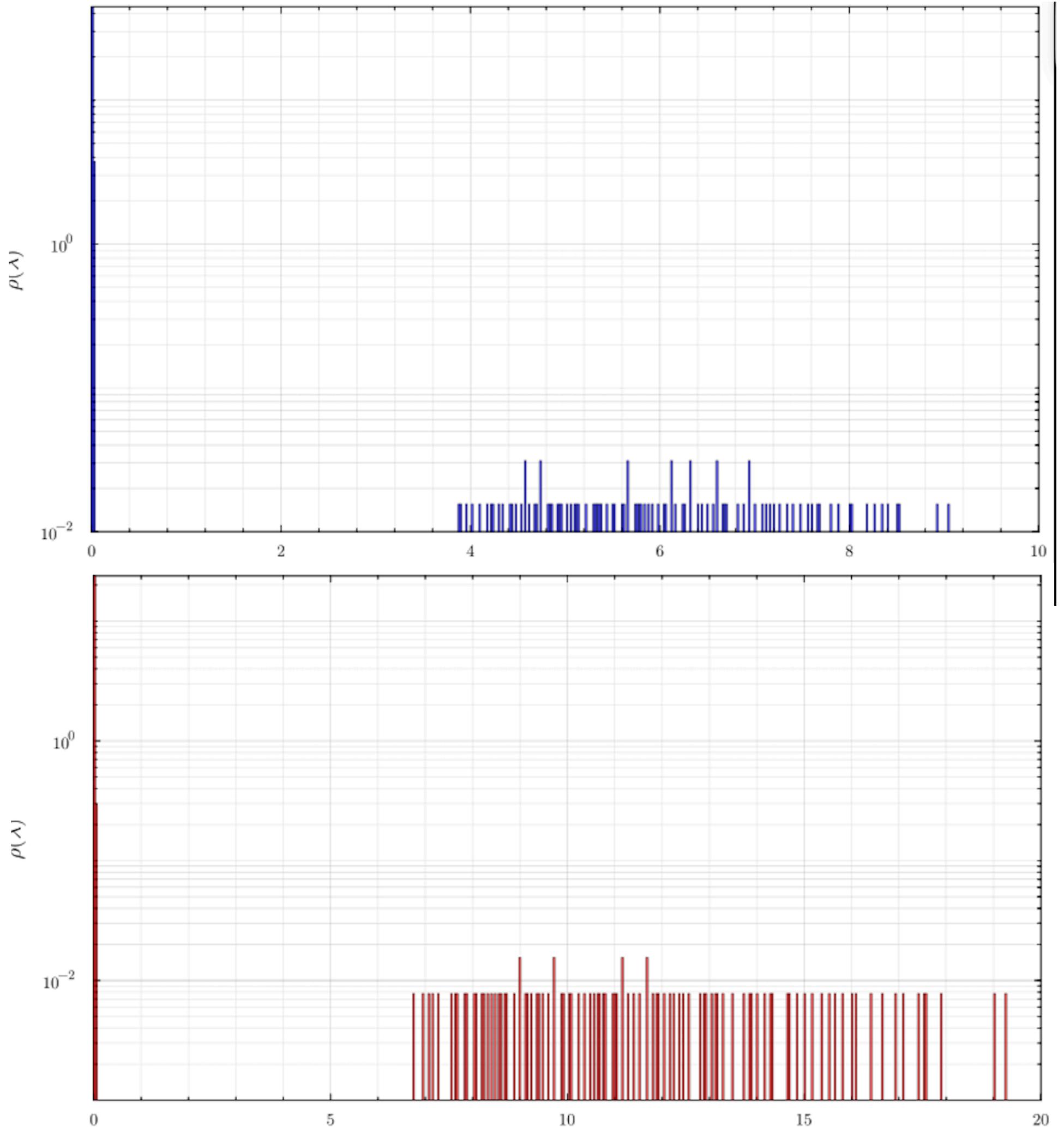


# Time Integrated RFNN

$$S_A(x, t) = \alpha_t \frac{A}{\sqrt{p}} \sigma \left( \frac{Wx}{\sqrt{d}} + tb \right) + \beta_t x$$

$$\mathcal{L}(A, \{x_t^\nu\}) = \frac{1}{n} \sum_{\nu=1}^n \frac{1}{d} \mathbb{E}_{\xi, t} \| \sqrt{\Delta_t} S_A(x_t^\nu(\xi), t) + \xi \|_2^2$$

- Same phenomenology
- Time integration brakes GEP: we cannot compute  $U$  spectrum!



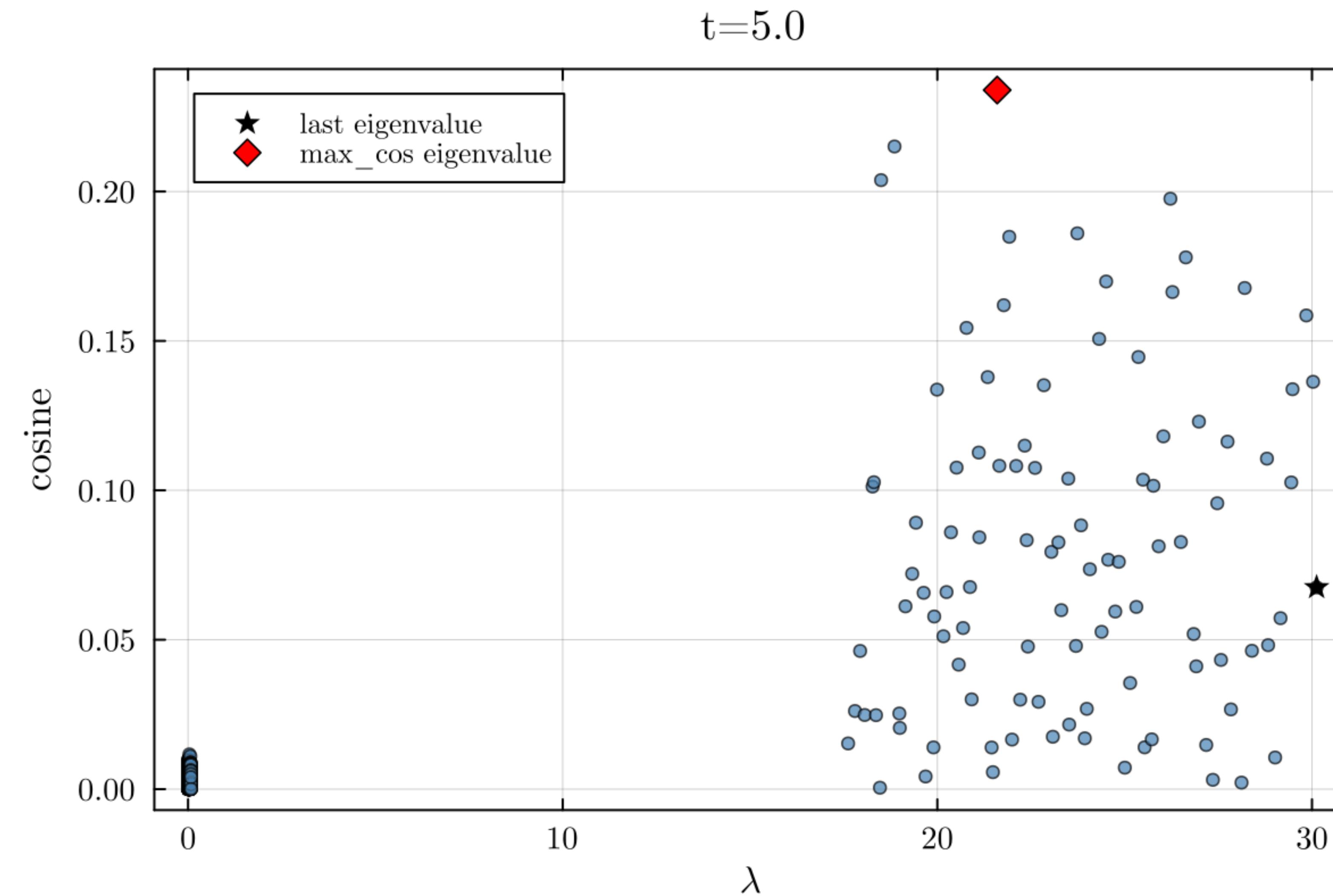
# MoG Data

$$P_0 = \frac{1}{2} \mathcal{N}(\mathbf{m}, \sigma_x^2 \mathbb{I}_d) + \frac{1}{2} \mathcal{N}(-\mathbf{m}, \sigma_x^2 \mathbb{I}_d)$$

or equivalently

$$\mathbf{x}^\mu = c^\mu \mathbf{m} + \sigma_x z^\mu$$

# Phenomenology: $U$ spectrum BBP transition



# GEP holds!

- $U_{GEP}$  for MoG data is  $U_{GEP}$  for gaussian data plus rank-1 terms: the bulks are the same!
- We must focus on the outlier...

Brandon Livio Annesi, Dario Bocchi, and Chiara Cammarota. Overparametrization

bends the landscape: Bbp transitions at initialization in simple neural networks.

We need to compute this:

$$\overline{G}_{ij} = \lim_{n \rightarrow 0} \mathbb{E}_x \int \prod_{a=1}^n d\psi^a \exp \left[ -\frac{1}{2} \sum_a (\psi^a)^T (z \mathbb{I}_N - U) \psi^a \right] \psi_i^1 \psi_j^1$$

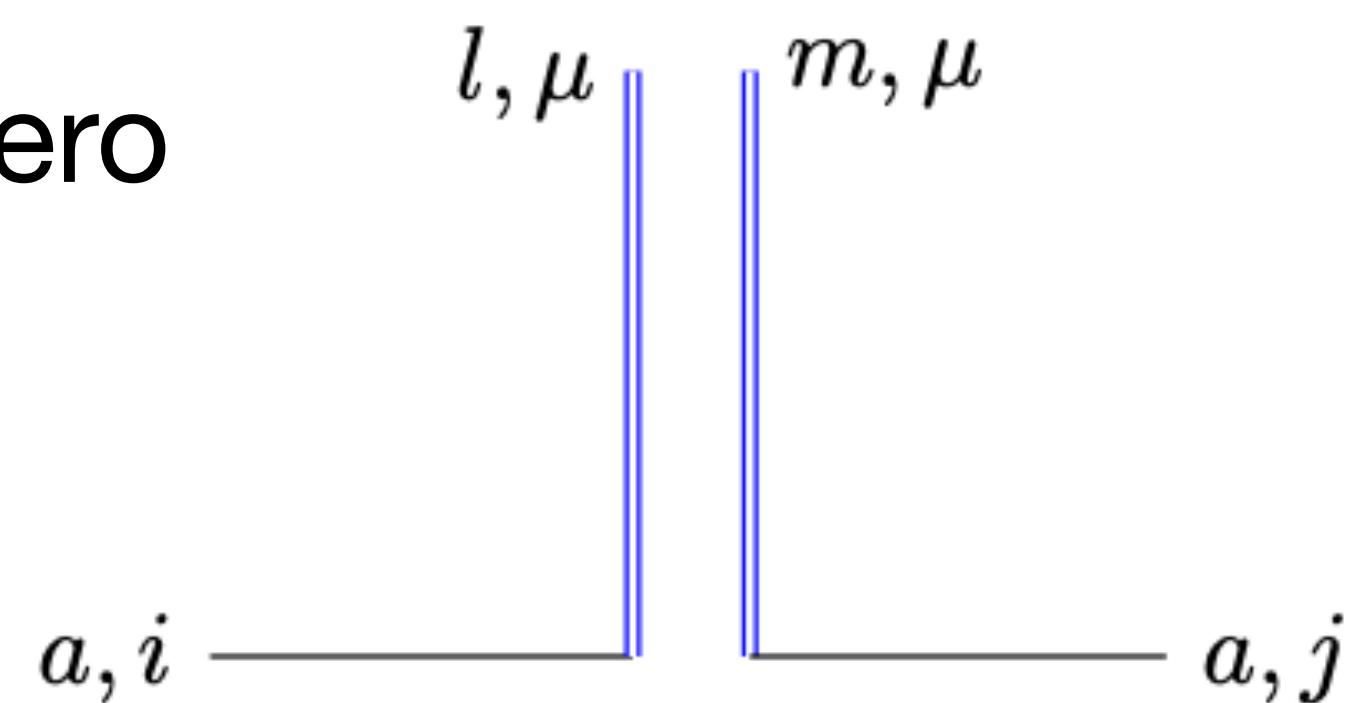
## It's a matter of gaussian averages!

- Wick theorem to reduce averages over many fields to averages of pairs
- Feynman diagrams to keep track of all possible pairings and interactions between different gaussian fields

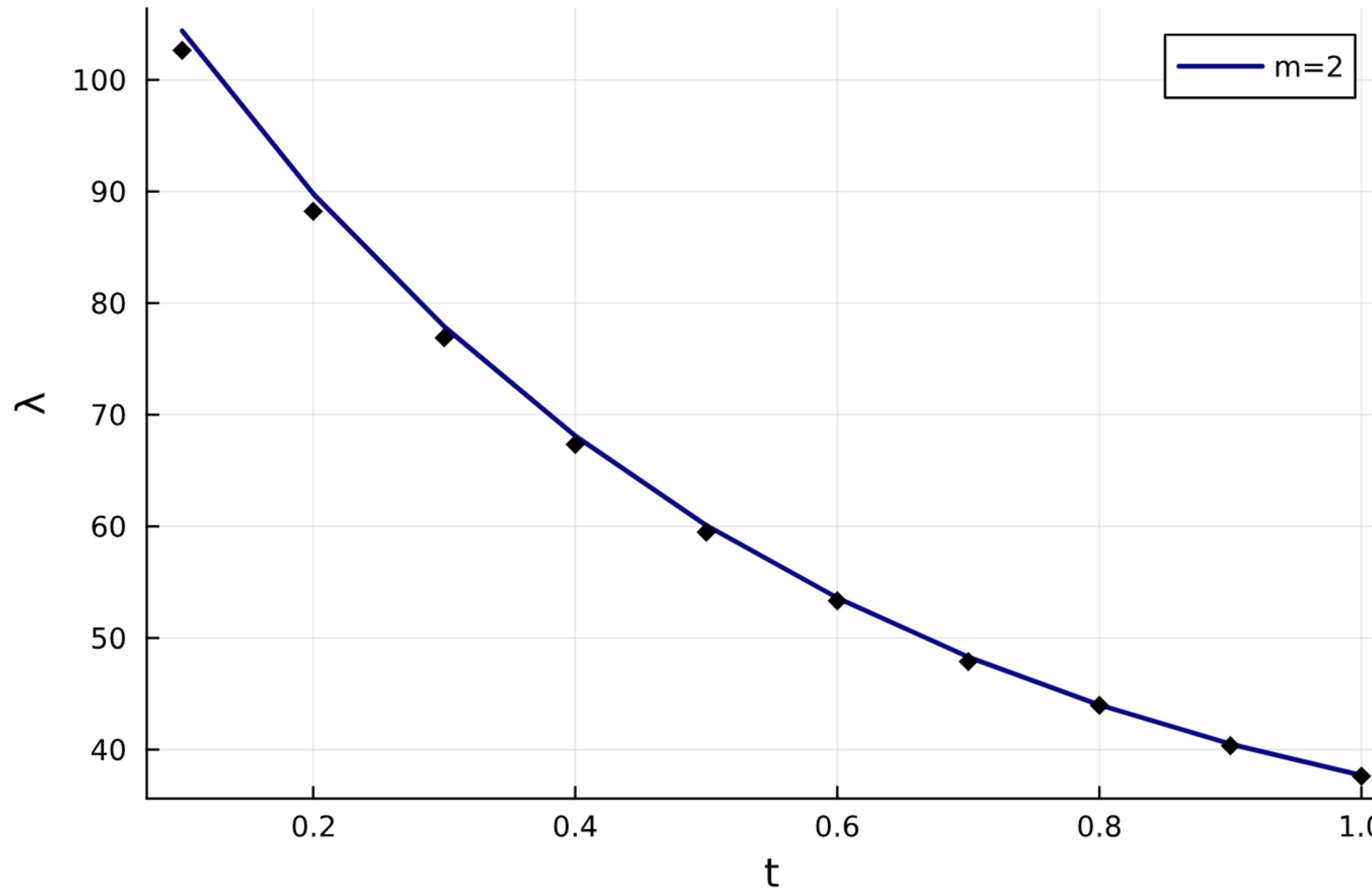
$$\Sigma_{ij}^b = \sum_{\mu l} i - \overset{l}{\mu} j + \sum_{\mu, l, m, n, k} i - \overset{l}{\mu} \underset{\bar{G}_{kn}^b}{\circlearrowleft} \overset{m}{\mu} \underset{k}{n} \underset{n}{\mu} j + \sum_{\mu, l, m, n, k} i - \overset{l}{\mu} \underset{\bar{G}_{kn}^b}{\circlearrowleft} \overset{m}{\mu} \underset{k}{n} \underset{\bar{G}_{pr}^b}{\circlearrowleft} \overset{q}{\mu} \underset{r}{p} \underset{p}{\mu} j + \dots$$

We get to a self-consistent equation for  $\bar{G}_{ij}$ :

- solving it gives the bulks
- the condition for the outlier is setting a denominator to zero



## Solutions for the outlier equation



## ***This is interesting at two levels:***

- *Diffusion dynamics*: what's happening at trajectories at transition time?
- *Training dynamics*: what's happening at the training metrics at the timescale associated to the outlier?

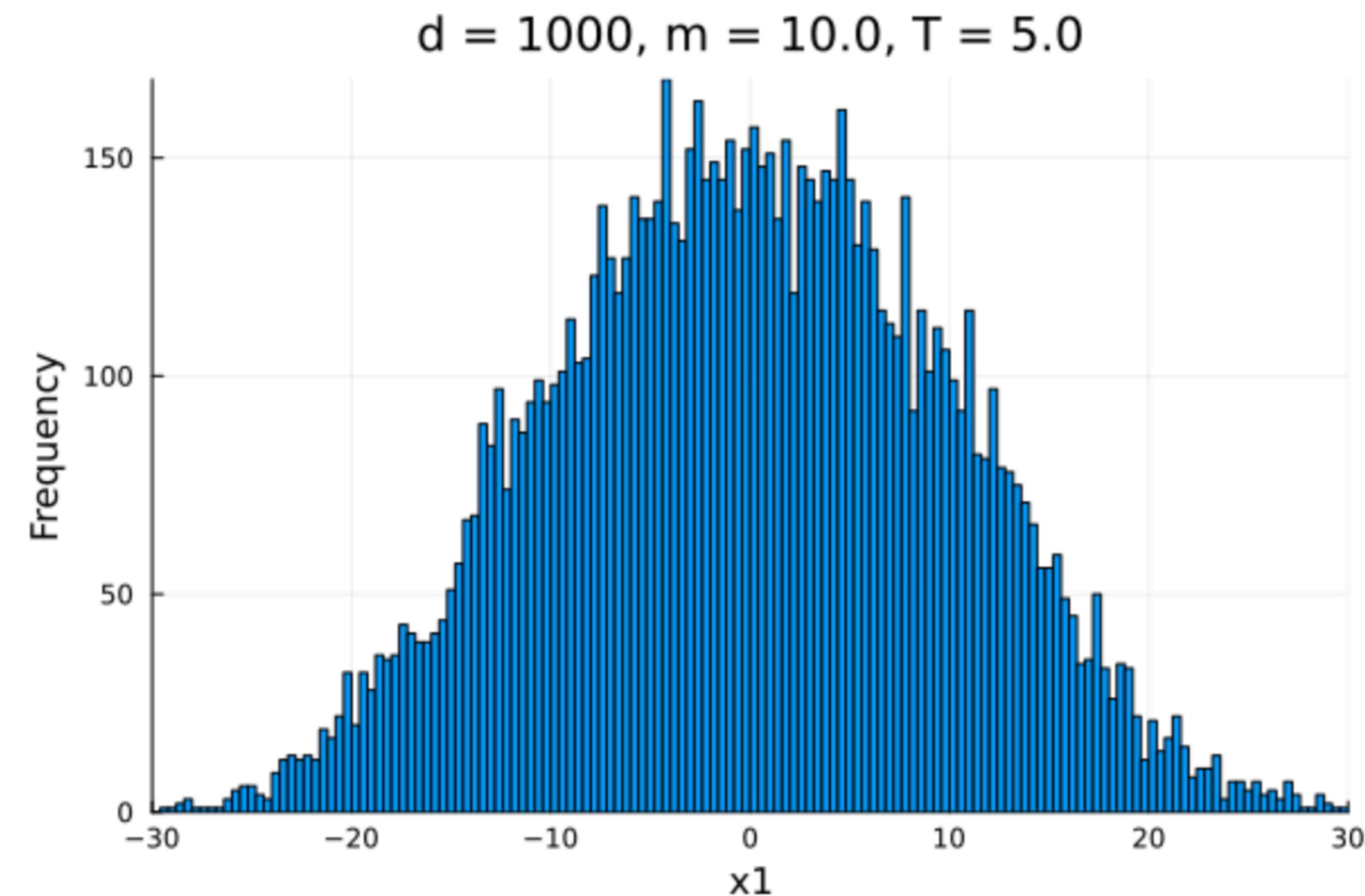
**But...  
...**

**... a legit doubt:**

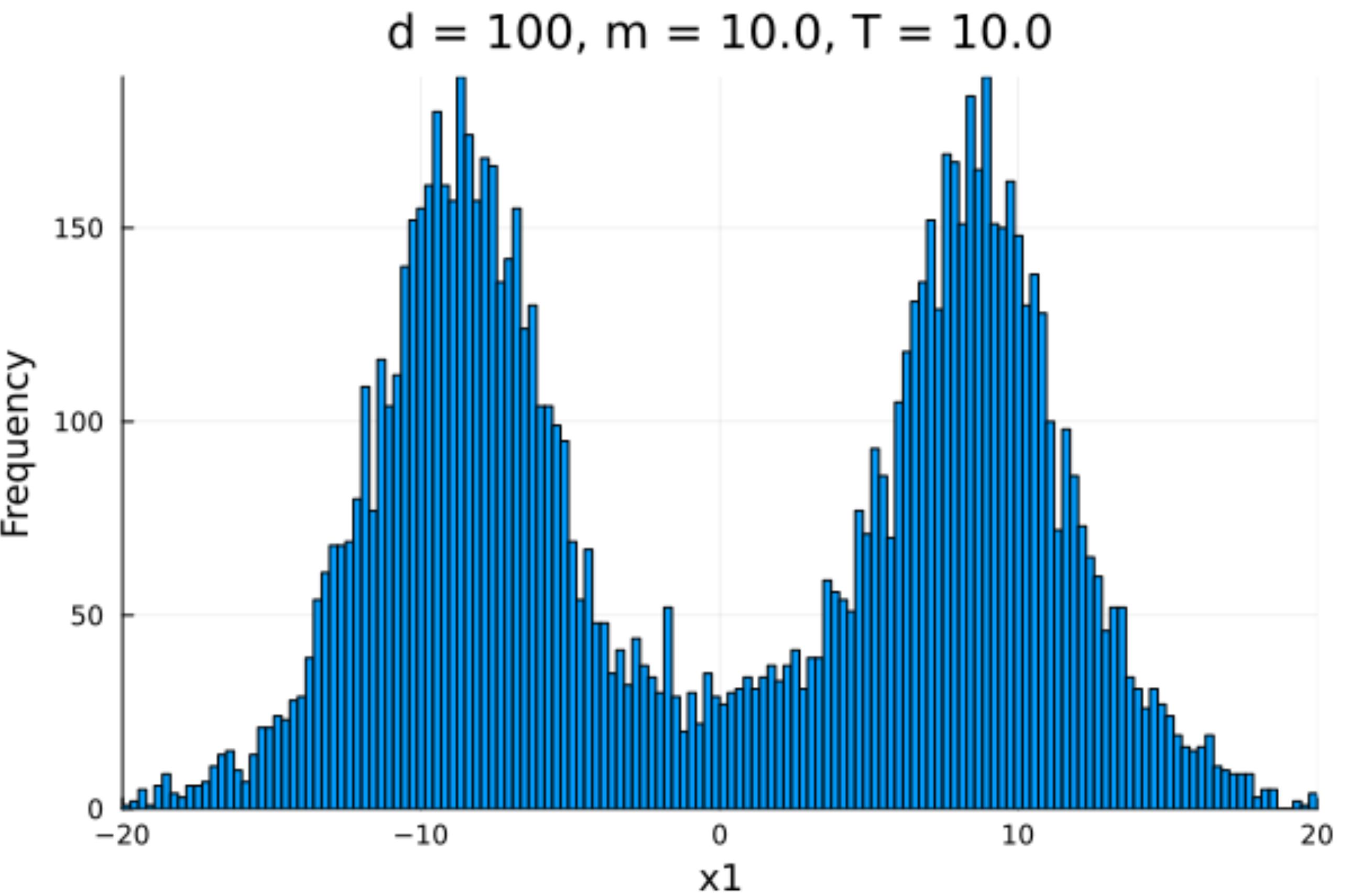
**Can RFNN learn  
a mixture?**

# It depends on the Gaussians separation!

If  $\| \mathbf{m} \| \sim \mathcal{O}(1)$  the random features score is approximately linear, so the backward process can at most produce a gaussian distribution!



If  $\| \mathbf{m} \| \sim \mathcal{O}(\sqrt{d})$  the random features score is non linear, and we can sample effectively from a mixture.



# Conclusions

The behavior of the dominant eigenvalue reveals the point (in terms of  $t$  and  $\tau$ ) at which the diffusion process becomes sensitive to the informative direction.

- ***Non-separated regime:*** the process cannot recover the bimodal structure and diffusion collapses to a single component whose variance aligns with the signal direction
- ***Well-separated regime:*** the process recovers the multimodal structure and separates the modes