Dimension-free limits of SGD for two-layers neural networks

(and some applications)

Bruno Loureiro
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Based on
arXiv: 2202.00293,
2302.05882, 2305.18502

Statistical Physics and Machine Learning back together again
08.08.2023

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In collaboration with

Luca Arnaboldi
(EPFL)

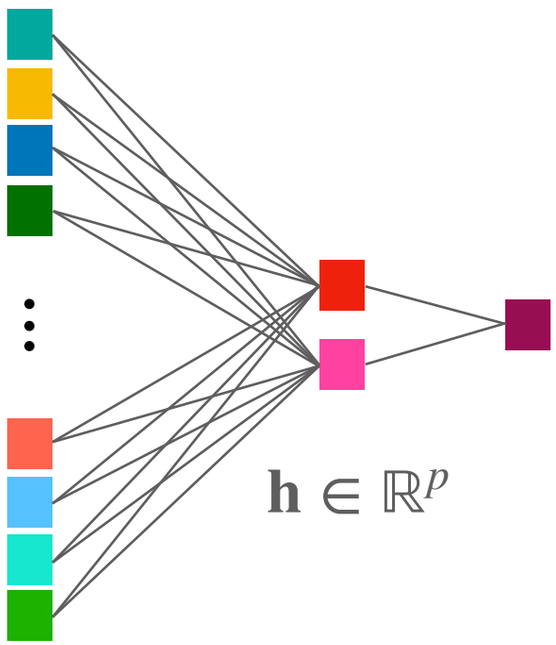
Rodrigo Veiga
(EPFL)

Ludovic Stéphan
(EPFL)

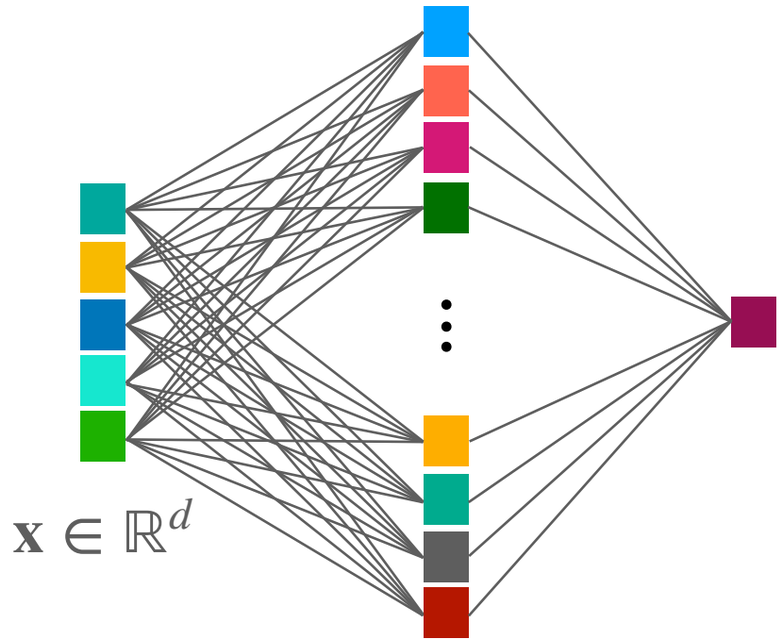
Lenka Zdeborová
(EPFL)

Florent Krzakala
(EPFL)

Narrow networks



Wide networks



$\frac{p}{d}$

$p \ll d$

???

$p \gg d$

(Saad & Solla)

[Saad & Solla '95;
Goldt et al. '19;
Ben Arous, Gheissari,
Jagannath '21, '22]

(Mean-field limit)

[Mei, Montanari, Nguyen 18';
Chizat, Bach 18';
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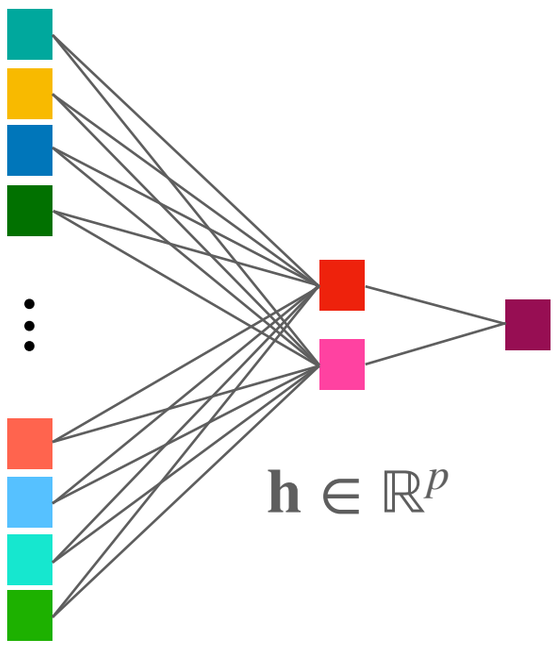

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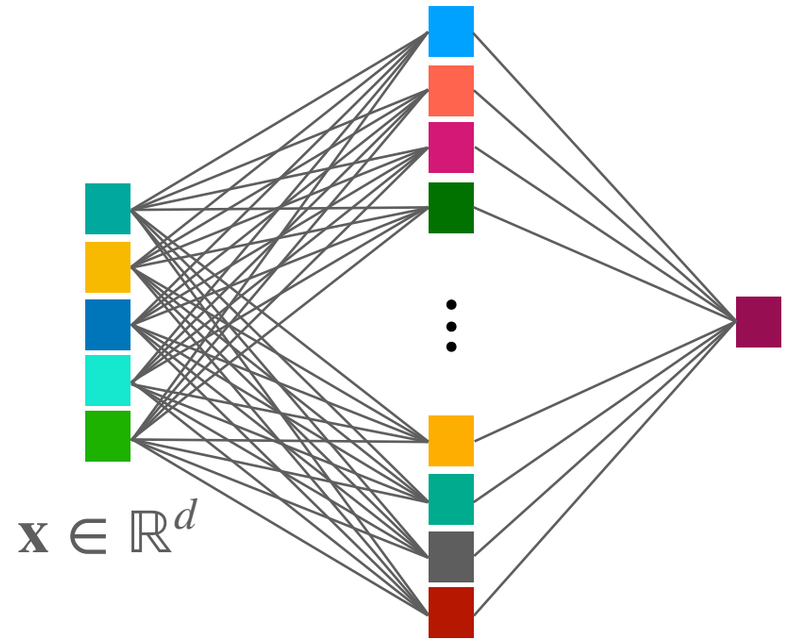

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$\frac{p}{d}$

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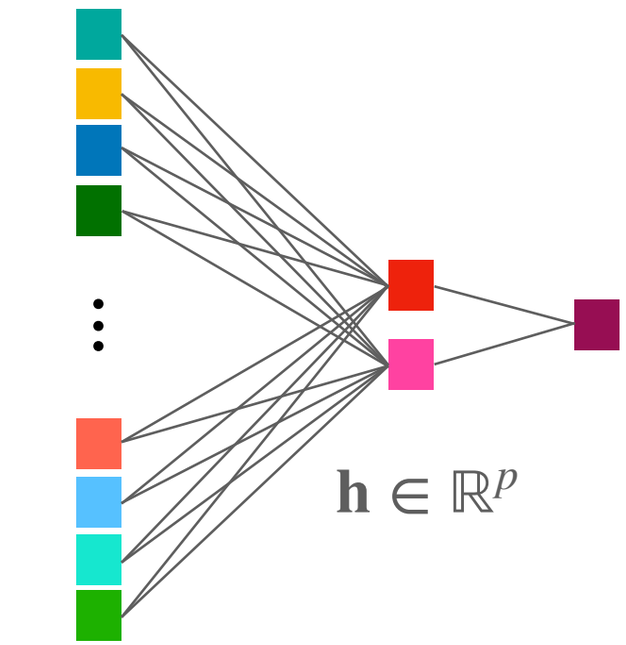
[Mei, **Misiakiewicz**, Montanari '19;
Abbe, Adsera, **Misiakiewicz** '22, '23;
Hajjar, Chizat '22;
Berthier, Montanari, Zhou '23]

Narrow networks



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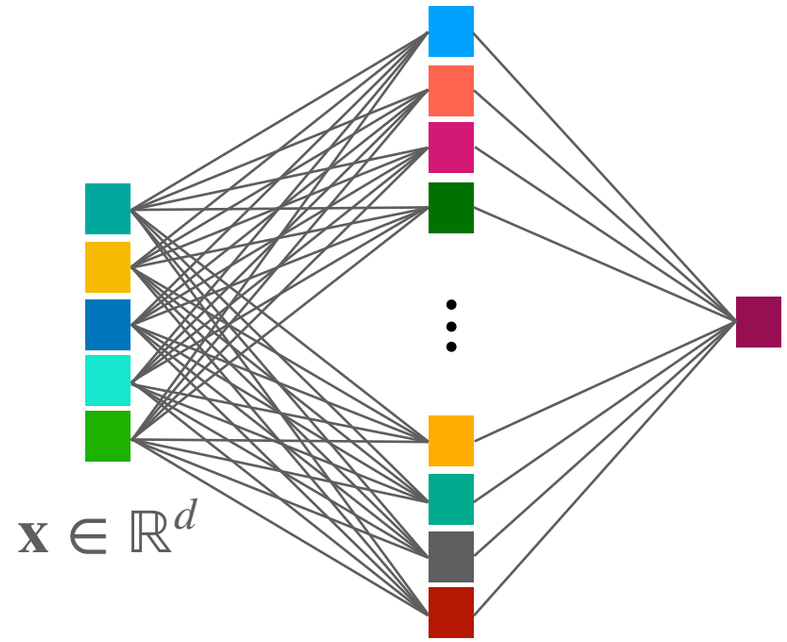

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[Mei, Montanari, Nguyen 18';
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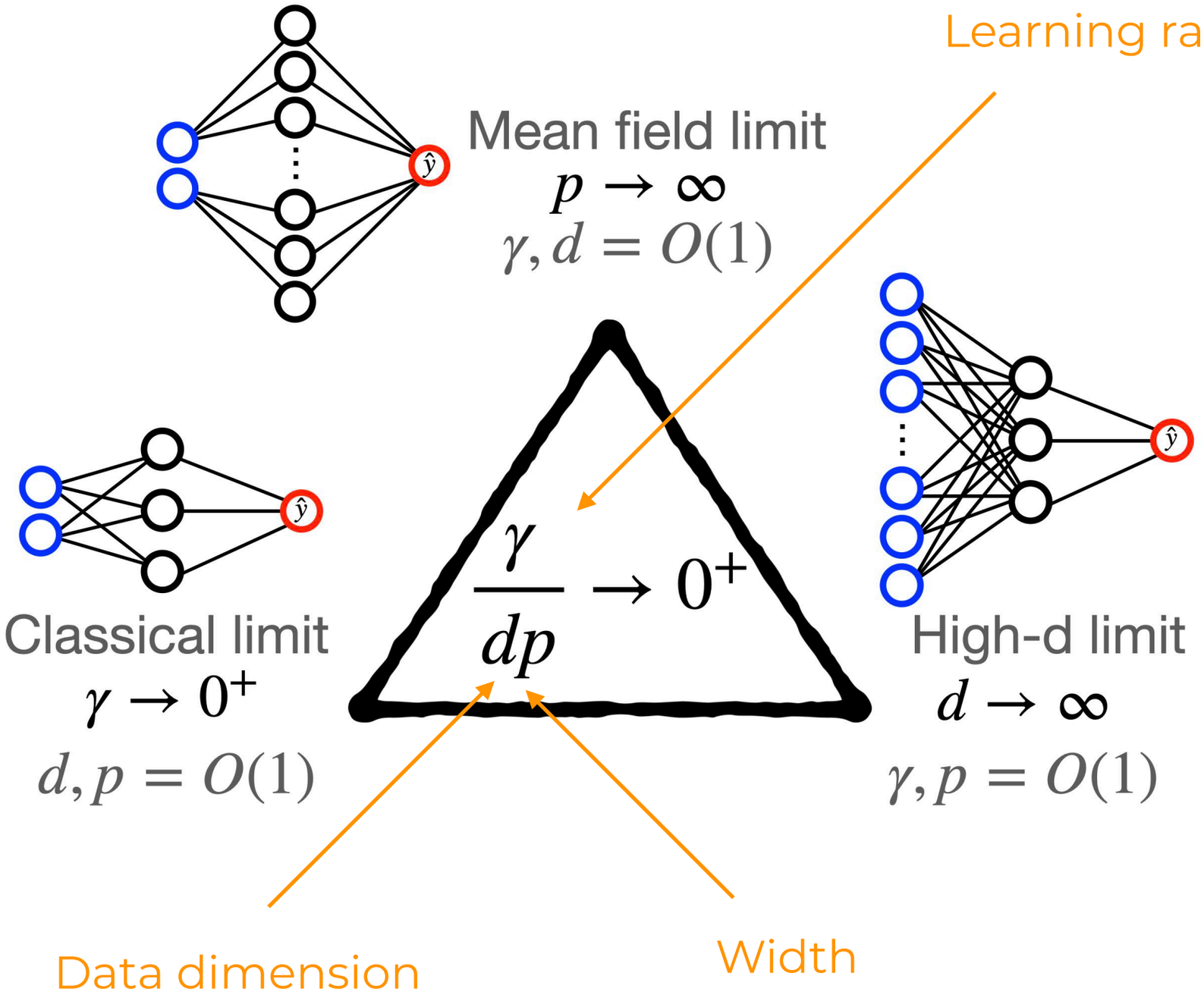
$\frac{p}{d}$

???

This work

[**Veiga et al. '22**;
Arnaboldi et al. '23]

SPOILER ALERT



Empirical risk minimisation

Let $(x^\nu, y^\nu)_{\nu\in[n]} \in \mathbb{R}^d \times \mathbb{R}$ ind. sampled from ρ .

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Want: Function $\hat{y} = f_\Theta(x)$ that "generalises" well, i.e.

minimise $$\mathscr{R}(\Theta) = \frac{1}{2}\mathbb{E}_{(x,y)\sim\rho}\left[\left(y - f_\Theta(x)\right)^2\right]$$

Population Risk

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☹ Problem: in practice, does't know ρ. So instead...

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Population Risk

Problem: in practice, does't know ρ. So instead...

minimise $$\hat{\mathscr{R}}_n(\Theta) = \frac{1}{2n}\sum_{\nu\in[n]}\left(y^\nu - f_\Theta(x^\nu)\right)^2$$

Empirical Risk

Algorithm: SGD

Algorithm: Let $b_k \subset [n]$ be mini-batch.

$$\Theta^{k+1} = \Theta^k - \gamma_k \nabla_{\Theta^k} \hat{\mathscr{R}}_{b_k}\left(\Theta^k\right)$$

$$\hat{\mathscr{R}}_b(\Theta) = \frac{1}{2|b|} \sum_{\nu \in b} \left(y^\nu - f_\Theta(x^\nu)\right)^2$$

mini-batch

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$$b_k = [n], \quad \forall k$$

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mini-batch

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$\gamma \to 0^+$ at fixed d, p:

$$\dot{\Theta}(t) = -\nabla_\Theta \hat{\mathscr{R}}_n\left(\Theta(t)\right)$$

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b_k independent

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[Robbins & Monro 51']

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[Robbins & Monro 51']

Another look at SGD

Rewrite SGD:

$$\Theta^{k+1} = \Theta^k - \gamma_k \nabla_{\Theta^k} \mathscr{R}\left(\Theta^k\right) + \gamma_k \varepsilon^k$$

GD on population

Effective Noise

Where:

$$\varepsilon^k = \nabla_{\Theta^k}\left[\mathscr{R}\left(\Theta^k\right) - \hat{\mathscr{R}}_{B_k}\left(\Theta^k\right)\right]$$

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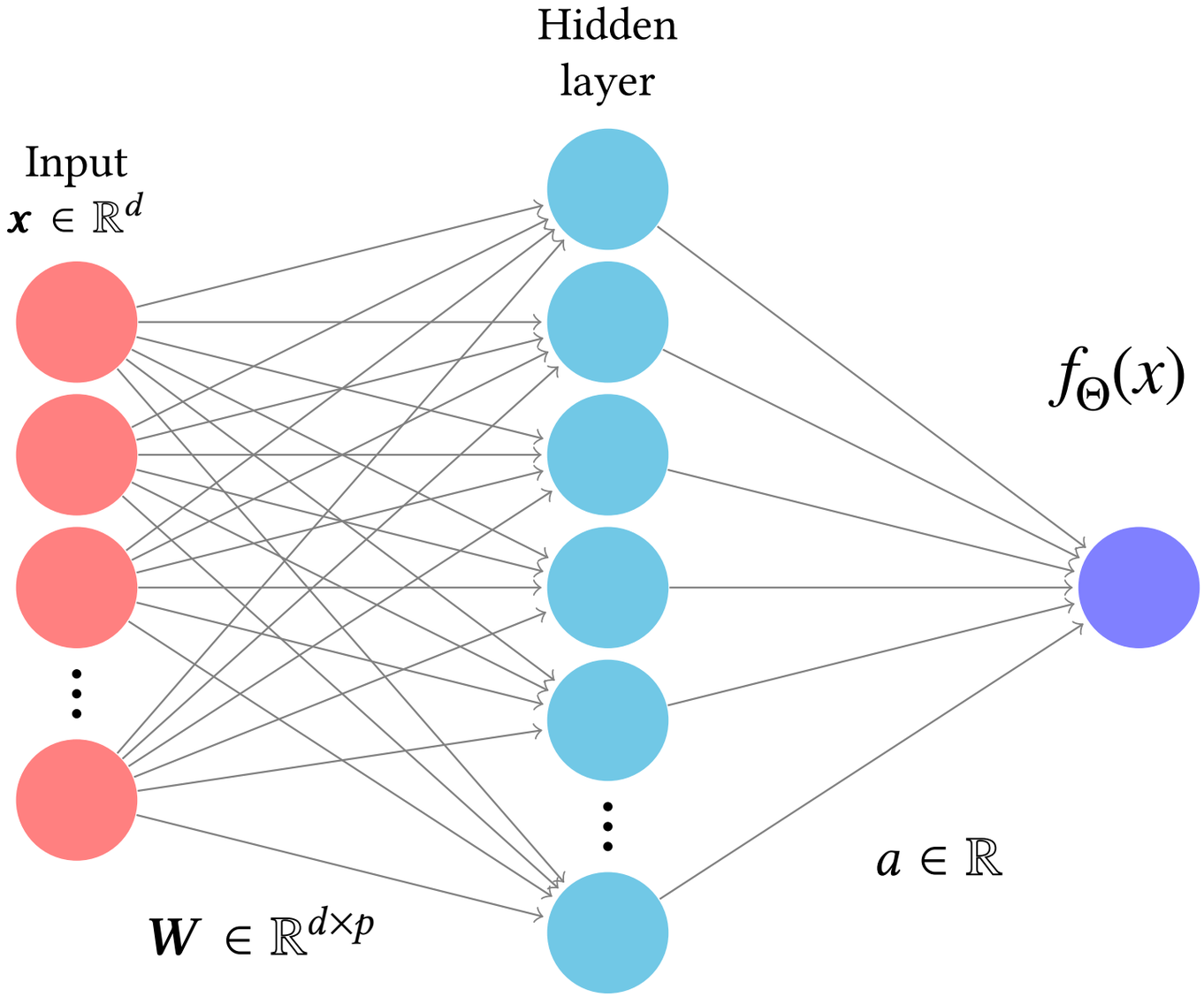
🤔 Question: How to characterise this?

Two-layer neural networks

Let $(\mathbf{x}^\nu, y^\nu) \in \mathbb{R}^d \times \mathbb{R}$ denote $\nu = 1, \cdots, n$ i.i.d. samples from p

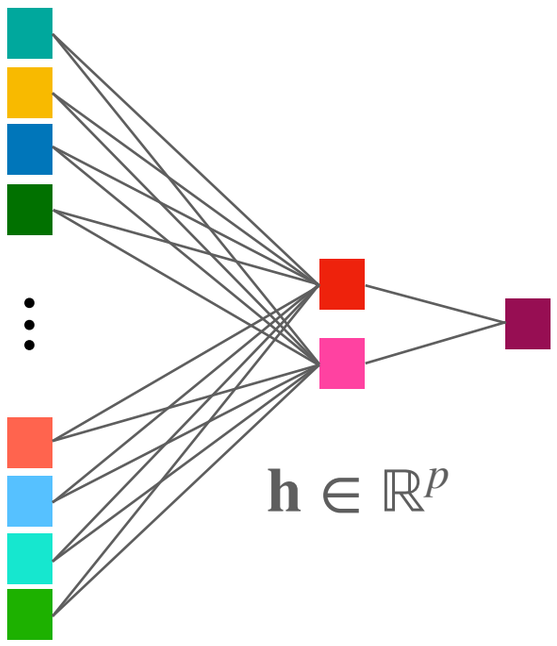


$$f_\Theta(x) = \sum_{i=1}^{p} a_i \sigma(w_i^\top x)$$

$$\Theta \equiv (\mathbf{a}, \mathbf{W}) \in \mathbb{R}^p \times \mathbb{R}^{p \times d}$$

What is known?

Narrow networks

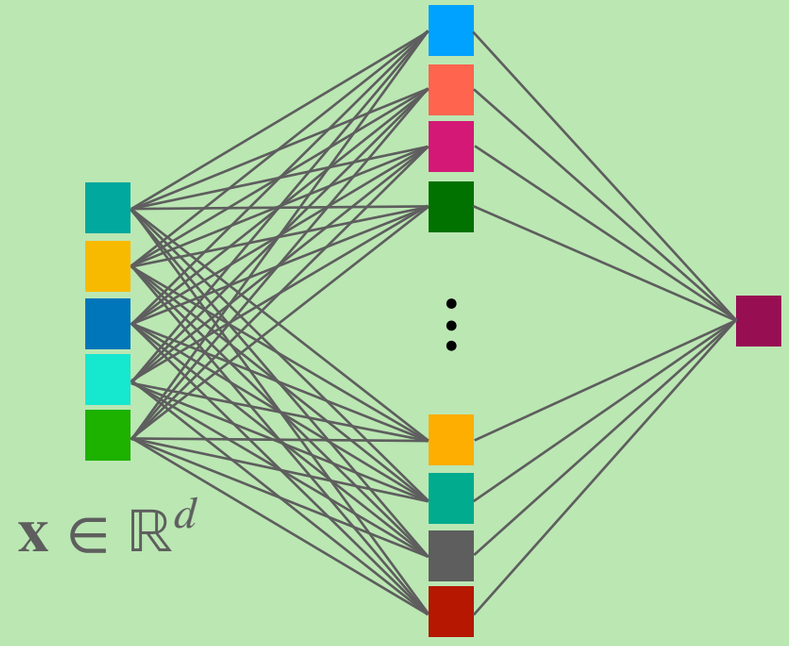


$p \ll d$

(Saad & Solla)

[Saad & Solla '95;
Goldt et al. '19;
Ben Arous, Gheissari,
Jagannath '21, '22]

Wide networks



$p \gg d$

(Mean-field limit)

[Mei, Montanari, Nguyen 18';
Chizat, Bach 18';
Rotskoff, **Vanden-Eijnden** 18';
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$\frac{p}{d}$

Mean-field limit

On the Global Convergence of Gradient Descent for Over-parameterized Models using Optimal Transport

Lénaïc Chizat
INRIA, ENS, PSL Research University
Paris, France
lenaic.chizat@inria.fr

Francis Bach
INRIA, ENS, PSL Research University
Paris, France
francis.bach@inria.fr

TRAINABILITY AND ACCURACY OF NEURAL NETWORKS: AN INTERACTING PARTICLE SYSTEM APPROACH

GRANT M. ROTSKOFF AND ERIC VANDEN-EIJNDEN

Mean field analysis of neural networks: A central limit theorem

Justin Sirignano[a,*], Konstantinos Spiliopoulos[b,1]

A mean field view of the landscape of two-layer neural networks

Song Mei[a], Andrea Montanari[b,c,1], and Phan-Minh Nguyen[b]

Mean-field limit

Idea: Define empirical density of weights:

$$\rho_p^{\nu}(\Theta) = \frac{1}{p}\sum_{i=1}^{p}\delta(\theta - \theta_i^{\nu}) \qquad\qquad \theta_i = (a_i, w_i) \in \mathbb{R}^{d+1}$$

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The risk is linear in $\hat{\rho}_p$!

$$\mathscr{R}(\Theta) = \mathbb{E}\left(y - \int \hat{\rho}_p(\mathrm{d}a, \mathrm{d}w) a\sigma(w \cdot x)\right)^2$$

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Show that, at fixed d and $\gamma_k \ll 1/d$:

One-pass SGD $\xrightarrow{p \to \infty}$ $\partial_t \rho_t = \gamma \nabla_\theta\left(\rho_t \nabla_\theta \mathscr{C}(\theta; \rho_t)\right)$

"Mean-field" limit

[Mei, Montanari, Nguyen 18'; Chizat, Bach 18'; Rotskoff, Vanden-Eijnden 18'; Sirignano, Spiliopoulos 18']

Global convergence

From [Chizat, Bach 21', arXiv: 2110.08084]

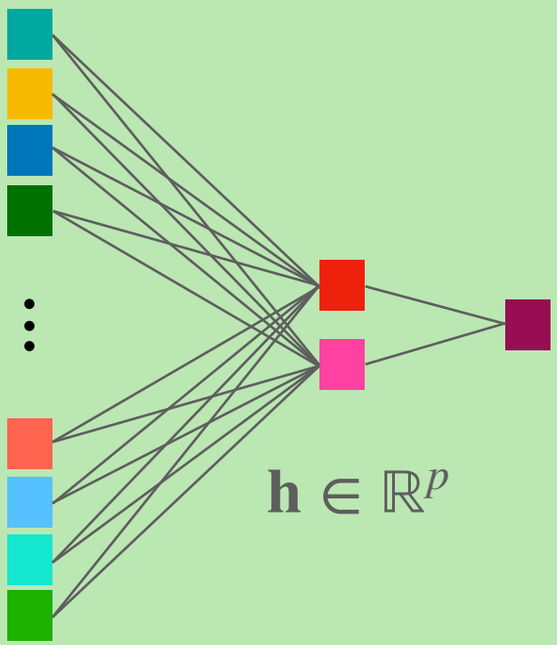
Theorem 2 (Informal) *If the support of the initial distribution includes all directions in* $\mathbb{R}^{d+1}$, *and if the function* Ψ *is positively 2-homogeneous then if the Wasserstein gradient flow weakly converges to a distribution, it can only be to a global optimum of* F.

From qualitative to quantitative results? Our result states that for infinitely many particles, we can only converge to a global optimum (note that we cannot show that the flow always converges). However, it is only a qualitative result in comparison with what is known for convex optimization problems in Section 2.2:

- This is only for $m = +\infty$, and we cannot provide an estimation of the number of particles needed to approximate the mean field regime that is not exponential in t (see such results e.g. in [28]).
- We cannot provide an estimation of the performance as the function of time, that would provide an upper bound on the running time complexity.

[Mei, Montanari, Nguyen 18'; Chizat, Bach 18'; Rotskoff, Vanden-Eijnden 18'; Sirignano, Spiliopoulos 18']

Narrow networks



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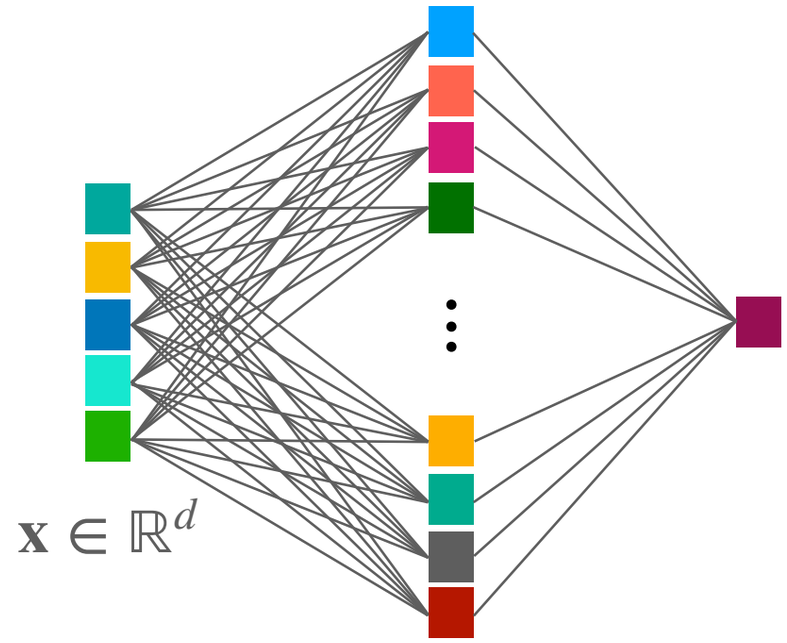

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$\frac{p}{d}$

Narrow networks

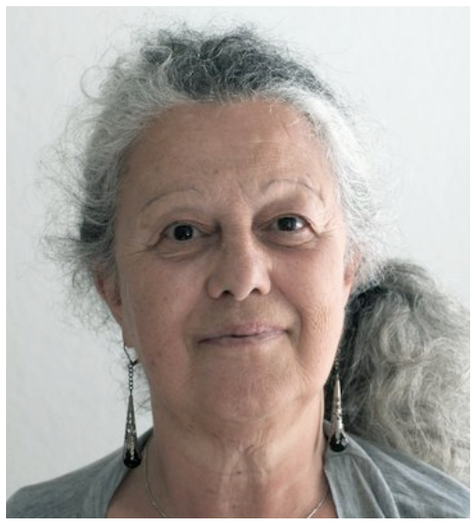
VOLUME 74, NUMBER 21 PHYSICAL REVIEW LETTERS 22 MAY 1995

Exact Solution for On-Line Learning in Multilayer Neural Networks

David Saad[1] and Sara A. Solla[2]
[1]*Department of Physics, University of Edinburgh, King's Buildings, Mayfield Road, Edinburgh EH9 3JZ, United Kingdom*
[2]*CONNECT, The Niels Bohr Institute, Blegdamsdvej 17, Copenhagen 2100, Denmark*
(Received 14 October 1994)

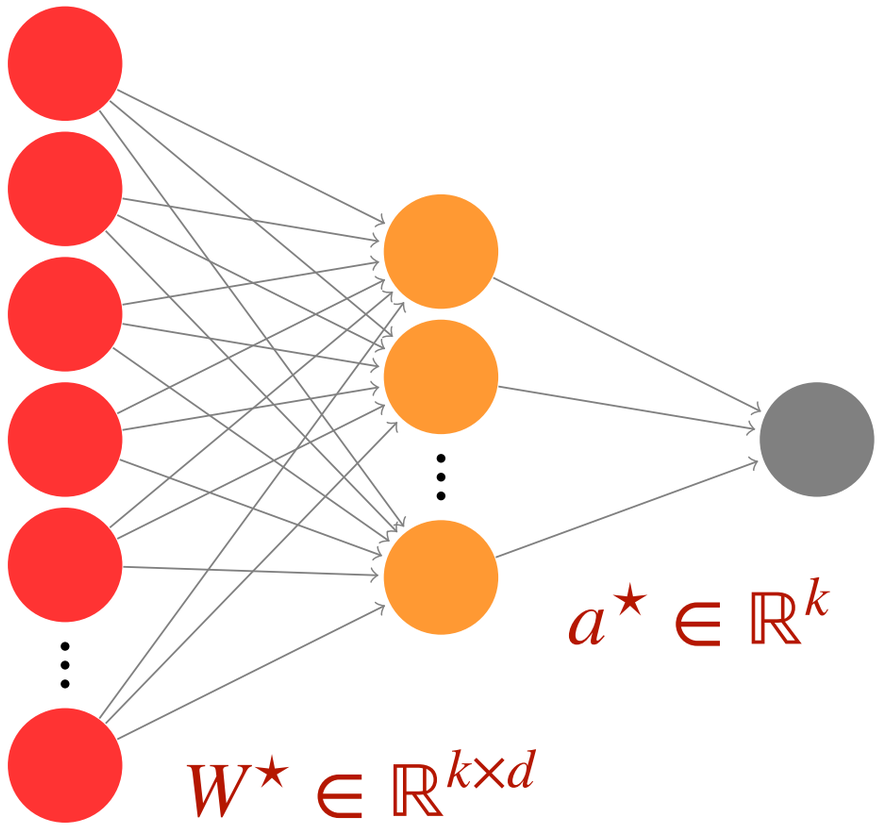
We present an analytic solution to the problem of on-line gradient-descent learning for two-layer neural networks with an arbitrary number of hidden units in both teacher and student networks.

PACS numbers: 87.10.+e, 02.50.–r, 05.20.–y



Teacher-student setting

Teacher network



$$x^\nu \sim \mathcal{N}(0, I_d) \qquad z^\nu \sim \mathcal{N}(0,1)$$

$$y^\nu = f_{W*}(x^\nu) + \sqrt{\Delta} z^\nu$$

$$f_{\Theta*}(x) = \frac{1}{k}\sum_{r=1}^{k} a_r^\star \sigma(w_r^{*\top} x)$$

Teacher-student setting

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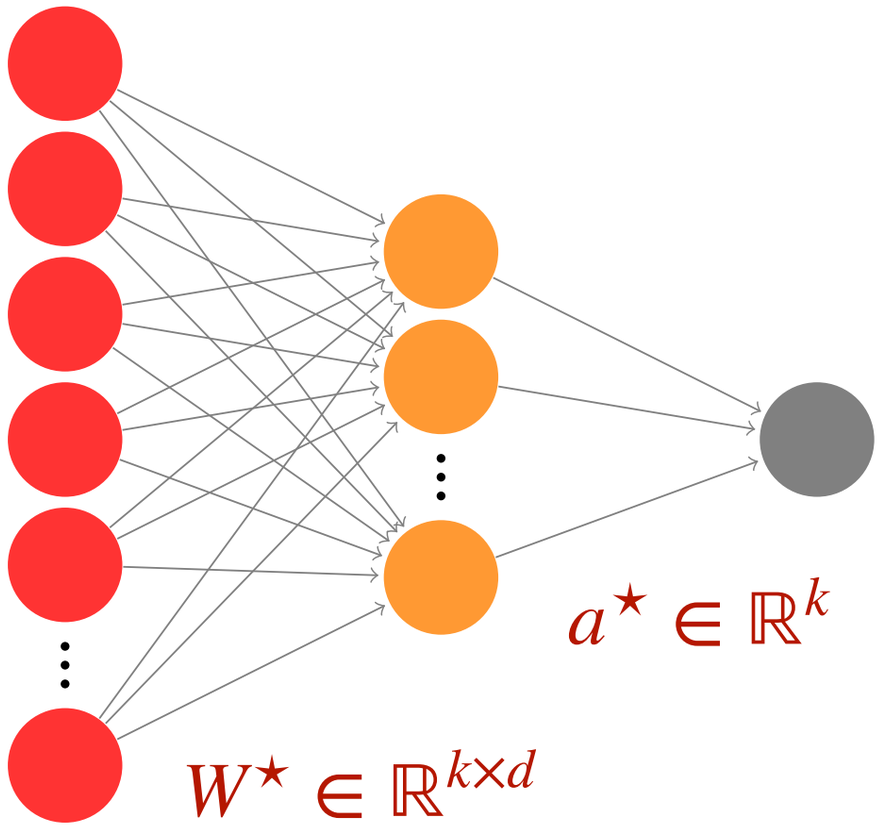
Teacher network



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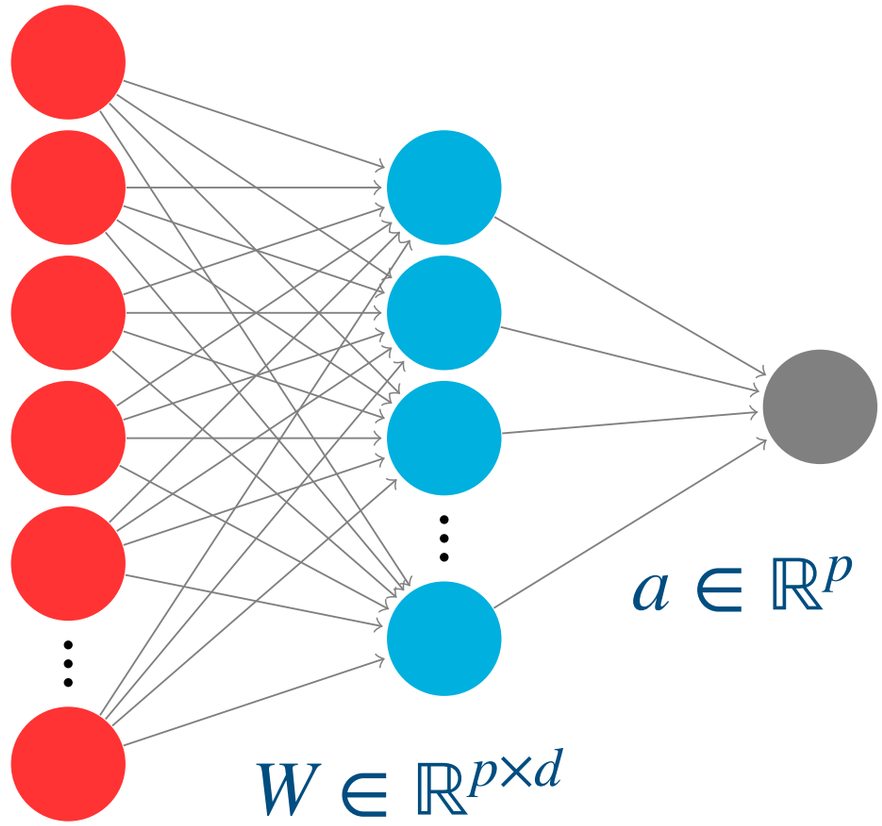
Student network



$$f_\Theta(x) = \frac{1}{p} \sum_{i=1}^{p} a_i \sigma(w_i^\top x)$$

Sufficient statistics

Goal: track population error exactly throughout the dynamics

$$\mathscr{R}(a^{\nu}, w^{\nu}) = \frac{1}{2}\mathbb{E}_{\mathbf{x}\sim\mathcal{N}(0,\mathrm{I_d})}\left[\left(\frac{1}{k}\sum_{r=1}^{k} a_r^{\star}\sigma(w_r^{*\top}x) - \frac{1}{p}\sum_{i=1}^{p} a_i^{\nu}\sigma(w_i^{\nu\top}x)\right)^2\right] + \frac{\Delta}{2}$$

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$$\mathscr{R}(a^\nu, w^\nu) = \frac{1}{2}\mathbb{E}_{(\lambda^{\star\nu}, \lambda^\nu)\sim\mathcal{N}(0,\Omega^\nu)}\left[\left(\frac{1}{k}\sum_{r=1}^{k} a_r^\star \sigma(\lambda_r^{*\nu}) - \frac{1}{p}\sum_{i=1}^{p} a_i \sigma(\lambda_i^\nu)\right)^2\right] + \frac{\Delta}{2}$$

Where:

$$\Omega^\nu = \begin{pmatrix} P & M^\nu \\ M^{\nu\top} & Q^\nu \end{pmatrix} \in \mathbb{R}^{(k+p)\times(k+p)}$$

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Key idea:

One-pass SGD $\longrightarrow$

$$a^{\nu+1} = \psi_1(a^\nu, \Omega^\nu)$$
$$\Omega^{\nu+1} = \psi_2(a^\nu, \Omega^\nu)$$

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Key idea:

One-pass SGD

$$\begin{aligned} a^{\nu+1} &= \psi_1(a^\nu, \Omega^\nu) \\ \Omega^{\nu+1} &= \psi_2(a^\nu, \Omega^\nu) \end{aligned} \xrightarrow{d\to\infty} \begin{aligned} \frac{\mathrm{d}\bar{a}(t)}{\mathrm{d}t} &= \bar{\psi}_1(\bar{a}(t), \bar{\Omega}(t)) \\ \frac{\mathrm{d}\bar{\Omega}(t)}{\mathrm{d}t} &= \bar{\psi}_2(\bar{a}(t), \bar{\Omega}(t)) \end{aligned}$$

[Saad & Solla '95; Goldt et al. '19]

Can we go beyond $d \to \infty$?

Setting

One-pass SGD for two-layer neural networks in the teacher-student setting.

Architecture: $$f_\Theta(x) = \frac{1}{p}\sum_{i=1}^{p} a_i \sigma(w_i \cdot x)$$

Data model: $$y^\nu = \frac{1}{k}\sum_{r=1}^{k} a_r^\star \sigma(w_r^\star \cdot x^\nu) + \sqrt{\Delta} z^\nu \qquad x^\nu \sim \mathcal{N}(0, I_d) \qquad z^\nu \sim \mathcal{N}(0,1)$$

Algorithm: $$\Theta^{\nu+1} = \Theta^\nu - \gamma_\nu \nabla_{\Theta^\nu} (y^\nu - f_{\Theta^\nu}(x^\nu))^2$$

Focus on realisable case $p \geq k$.

Taking a closer look

Looking more closely...

$$\Omega^{\nu+1} = \Omega^{\nu} + \delta t_{\nu}\ \psi(\Omega^{\nu})$$

$$M^{\nu+1} - M^{\nu} = \frac{\gamma}{dp}\ \psi^{M}_{GF}(\Omega^{\nu})$$

$$Q^{\nu+1} - Q^{\nu} = \frac{\gamma}{dp}\ \psi^{Q}_{GF}(\Omega^{\nu}) + \frac{\gamma^2}{dp^2}\ \psi_{noise}(\Omega^{\nu})$$

Taking a closer look

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$$M^{\nu+1} - M^{\nu} = \frac{\gamma}{dp}\ \psi_{GF}^{M}(\Omega^{\nu})$$

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Population gradient

Noise

Main theoretical result

Define step-size $\delta t = \frac{\gamma}{dp}$ and $M(t), Q(t)$ such that:

$$M(\nu\delta t) = M^{\nu} \qquad\qquad Q(\nu\delta t) = Q^{\nu}$$

Main theoretical result

Define step-size $\delta t = \frac{\gamma}{dp}$ and $\Omega(t)$ such that:

$$\Omega(\nu\delta t) = \Omega^{\nu}$$

Theorem [Veiga, Stephan, BL, Krzakala, Zdeborová '22]

Then $\forall 0 \leq \nu \leq \left\lfloor \frac{n}{\delta t} \right\rfloor$:

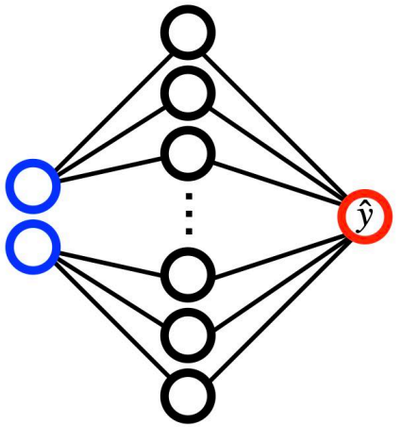
$$\mathbb{E}\,||\,\Omega^{\nu} - \bar{\Omega}(\nu\delta t)\,||_{\infty} \leq e^{C\nu\delta t}\sqrt{\frac{\gamma}{dp}}$$

Where $\bar{\Omega}(t) = \mathbb{E}[\Omega(t)]$ is the solution of an ODE:

$$\frac{\mathrm{d}\bar{\Omega}(\mathrm{t})}{\mathrm{dt}} = \mathbb{E}\left[\psi(\bar{\Omega}(t))\right]$$

Generalises [**Goldt et al**. '19], builds upon [Wang, Hu, **Lu** '18]

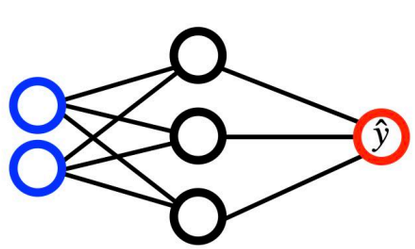
The different regimes



Mean field limit

$$p \to \infty$$

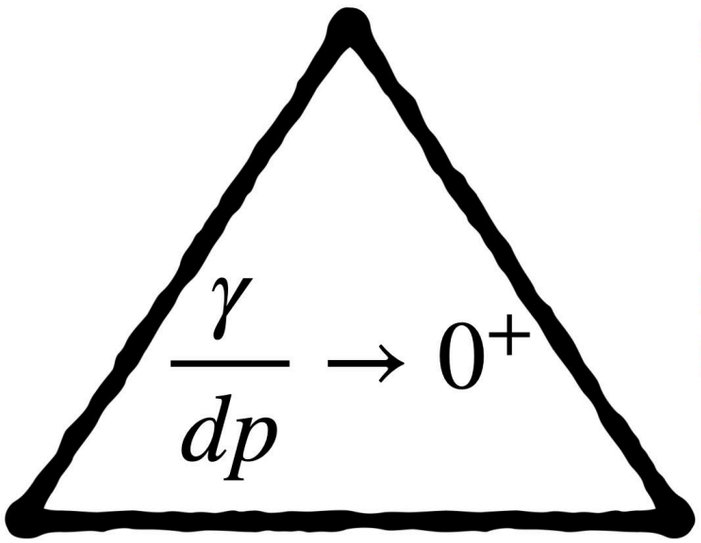
$$\gamma, d = O(1)$$

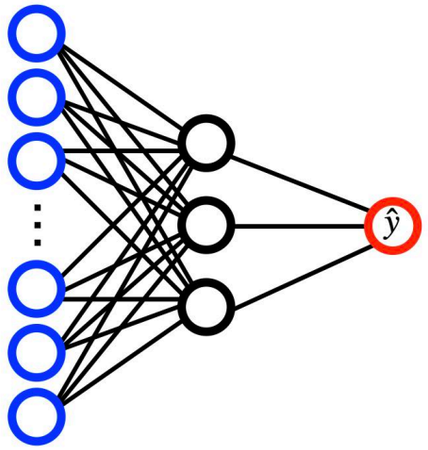


Classical limit

$$\gamma \to 0^+$$

$$d, p = O(1)$$





High-d limit

$$d \to \infty$$

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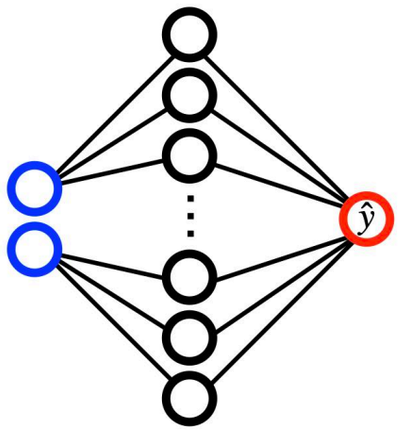
The different regimes



Mean field limit
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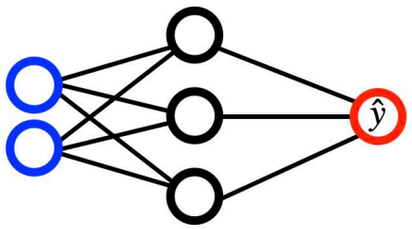

Classical limit
$\gamma \to 0^+$
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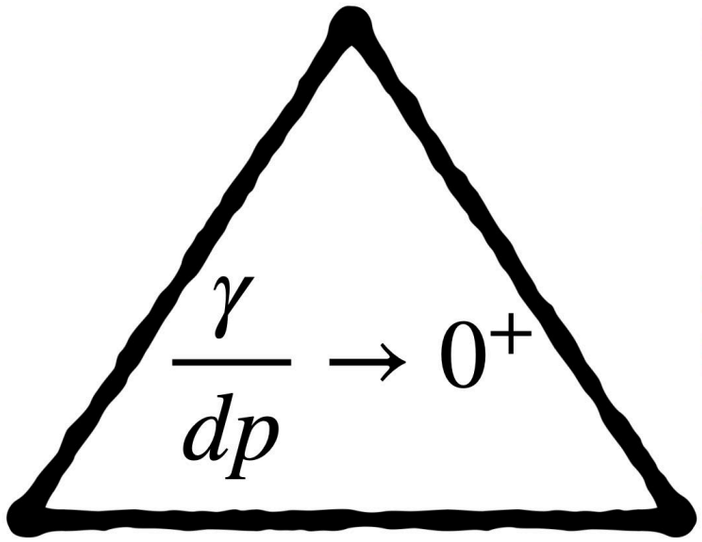

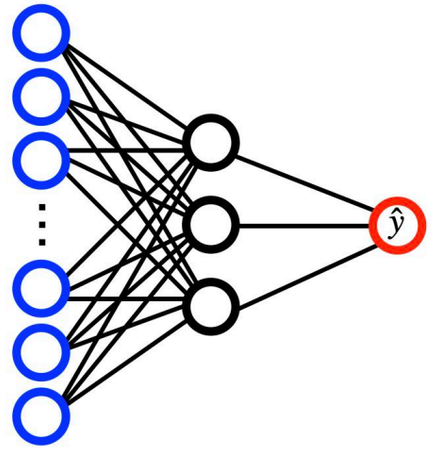

High-d limit
$d \to \infty$
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$$\dot{M}(t) = \psi^M_{\mathrm{GF}}(\bar{M}(t), \bar{Q}(t))$$

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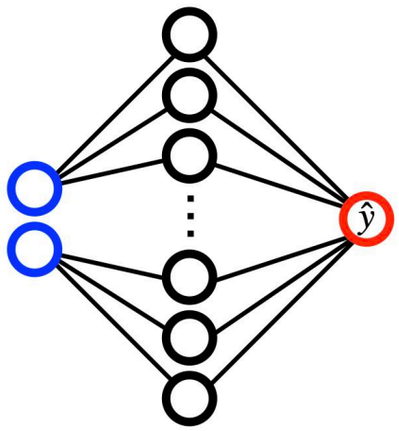
The different regimes



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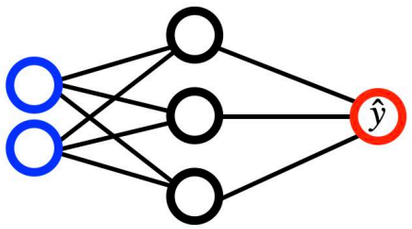

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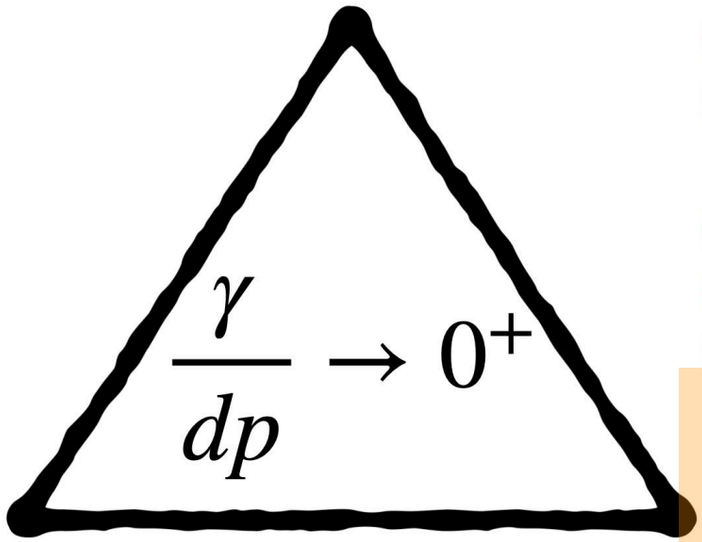

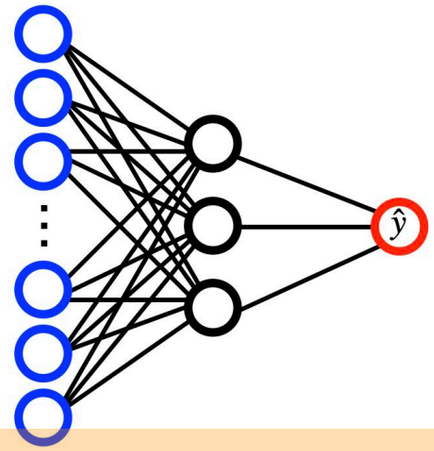

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$$\dot{M}(t) = \psi^M_{\mathrm{GF}}(\bar{M}(t), \bar{Q}(t))$$

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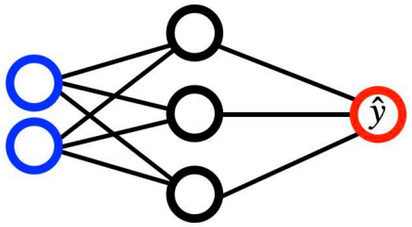
Classical regime



Classical limit

$$\gamma \to 0^+$$

$$d, p = O(1)$$

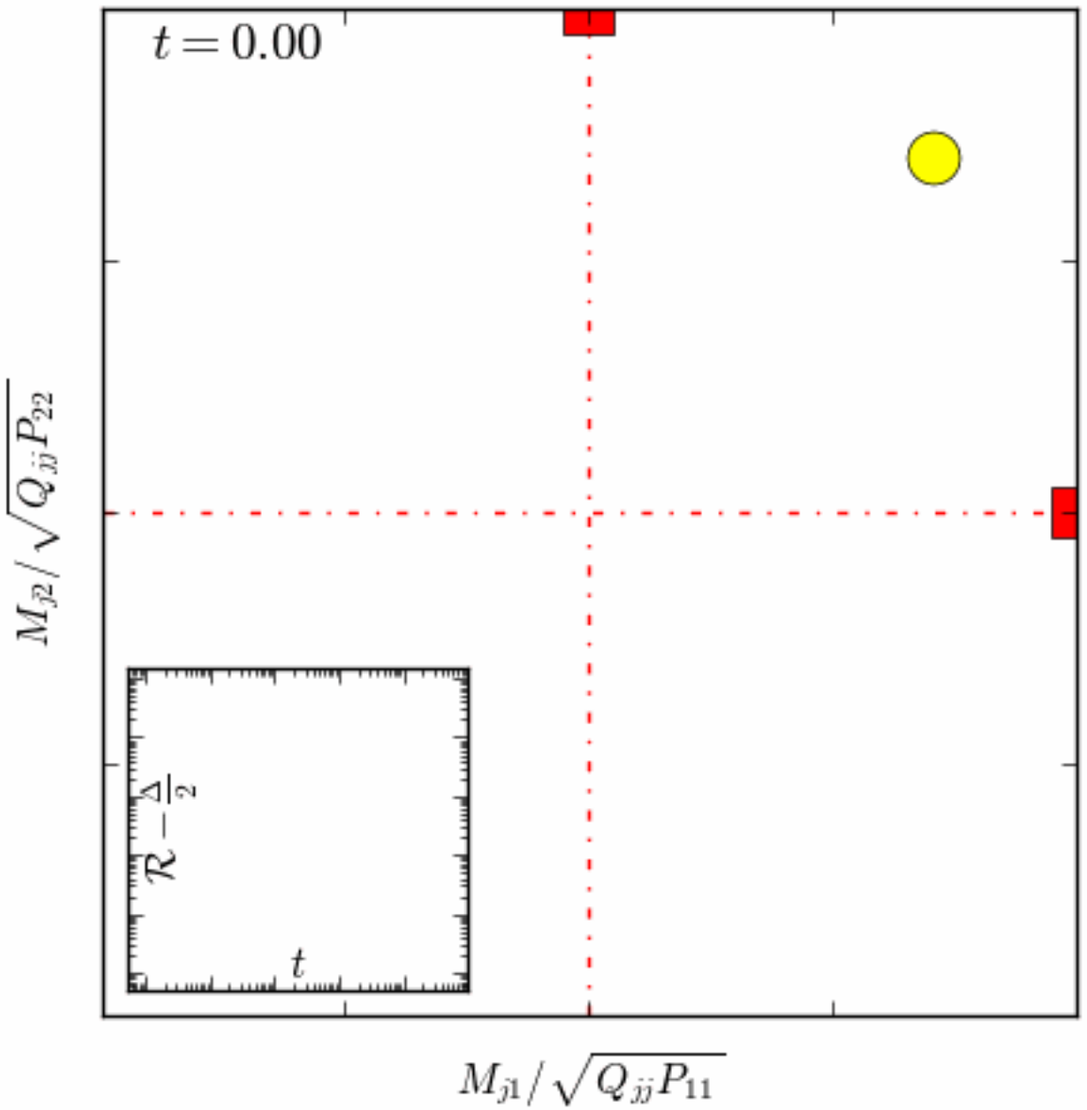
$$k = 2$$

$$p = 10$$

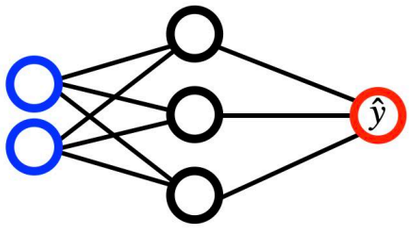
$$\Delta = 10^{-3}$$

$$\gamma = 5 \times 10^{-2}$$

$$\sigma = \sigma_\star = \mathrm{erf}$$



Classical regime



Classical limit

$$\gamma \to 0^+$$

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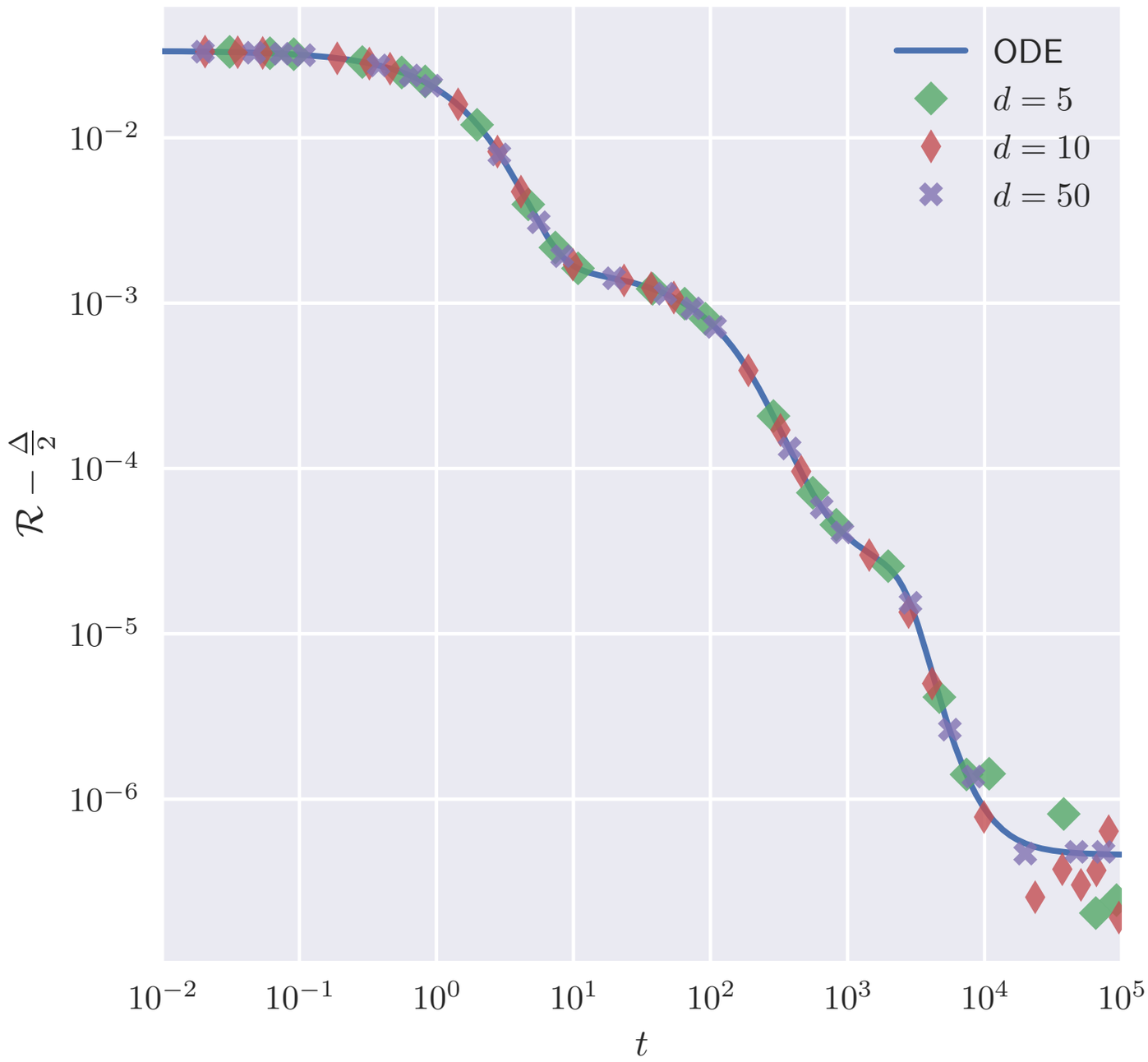
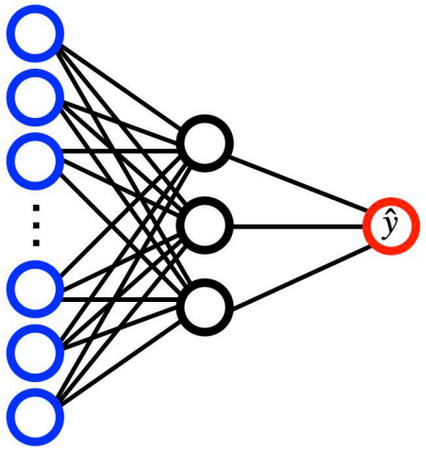


High-dimensional regime [Saad & Solla '95]



High-d limit

$$d \to \infty$$

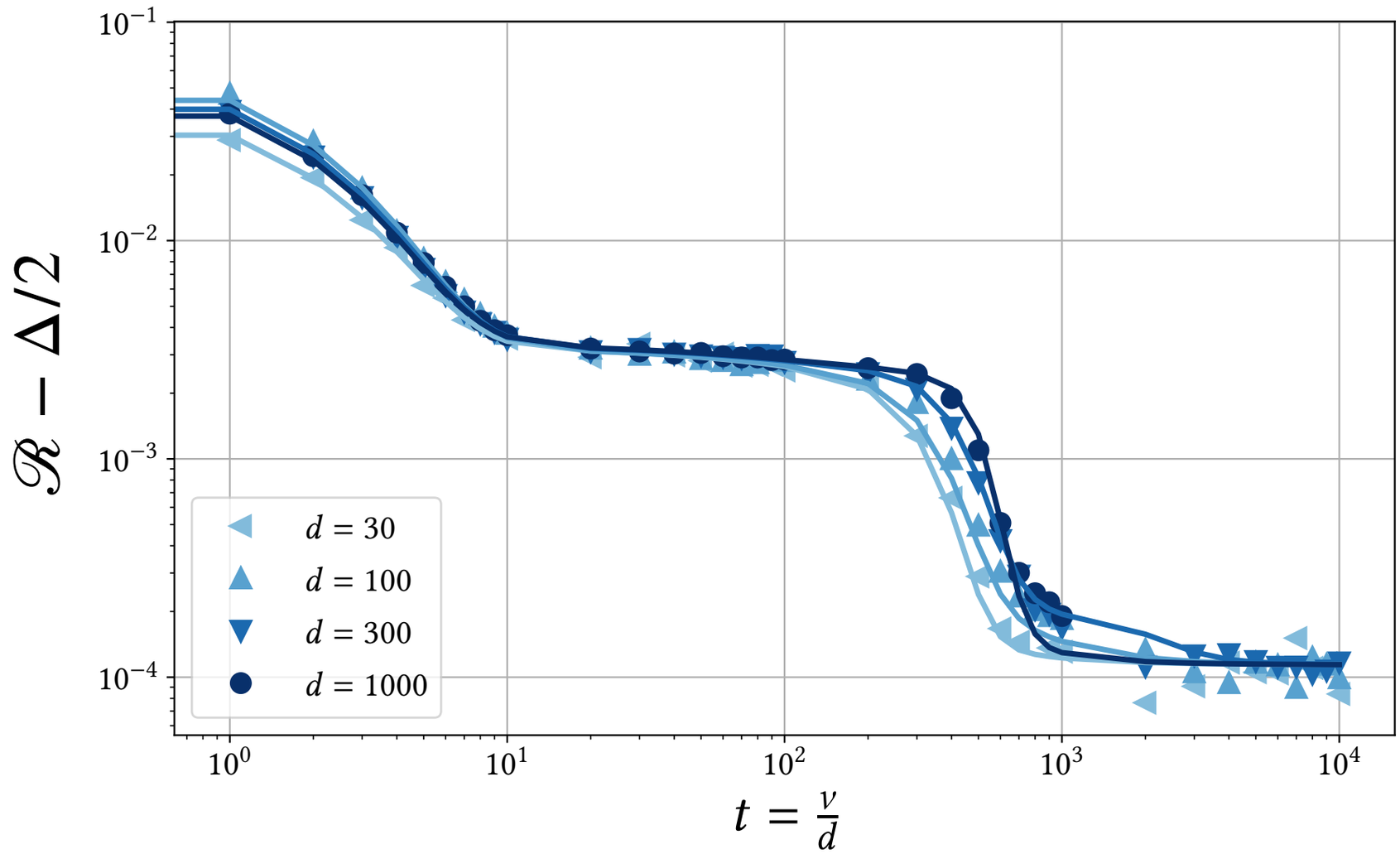
$$\gamma, p = O(1)$$

$$k = 4 \quad p = 8$$

$$\Delta = 10^{-3}$$

$$\gamma = 0.1$$

$$\sigma = \sigma_\star = \mathrm{erf}$$



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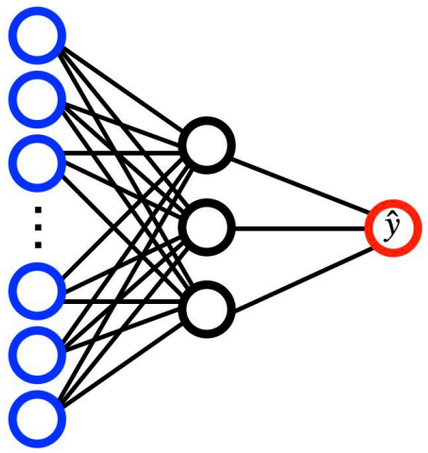

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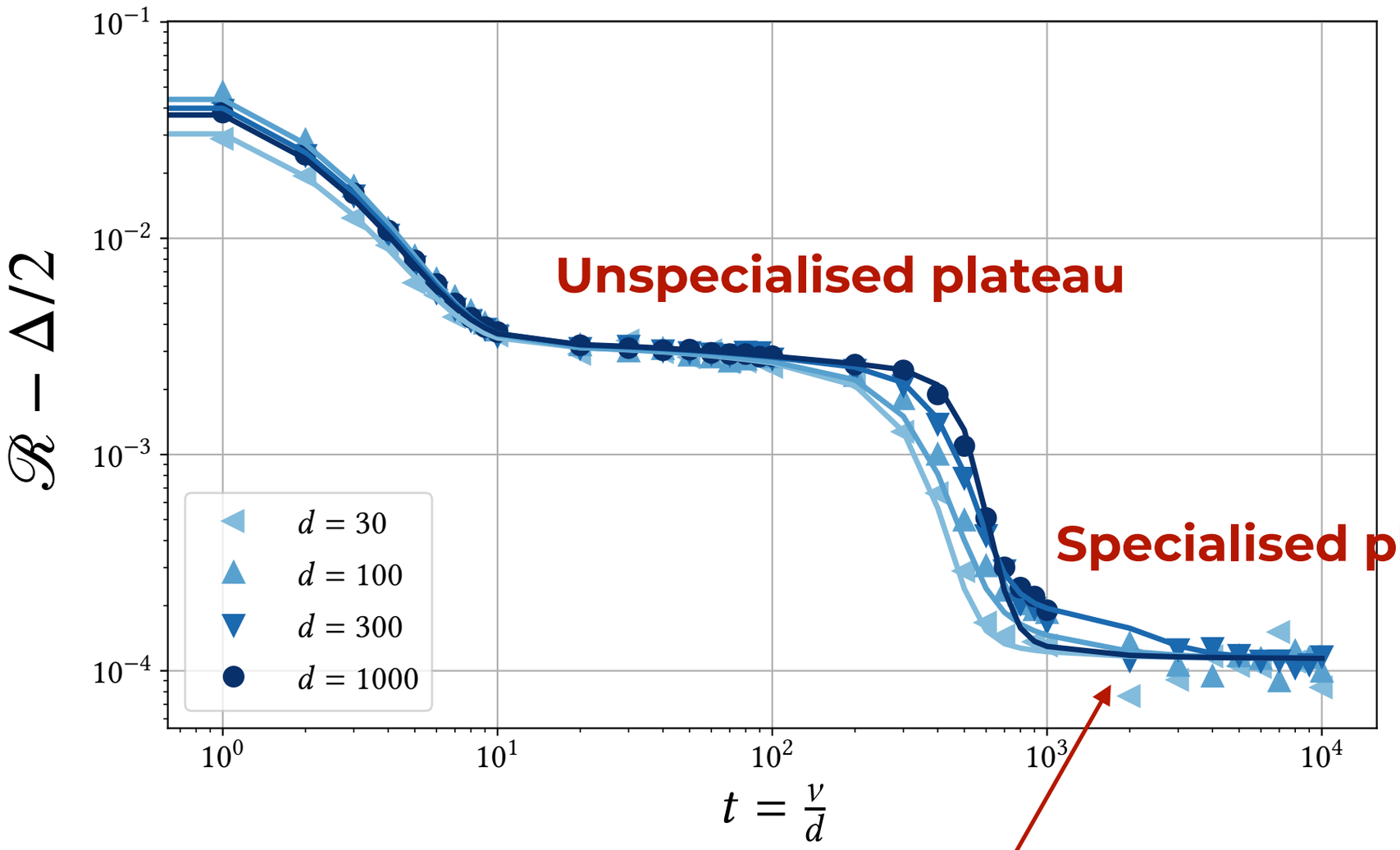
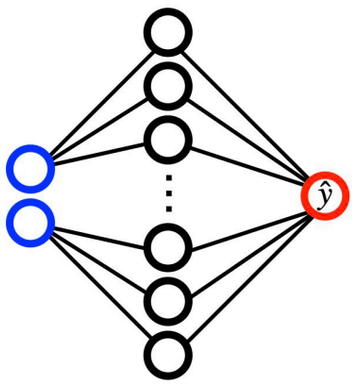


Mean-field regime



Mean field limit

$p \to \infty$

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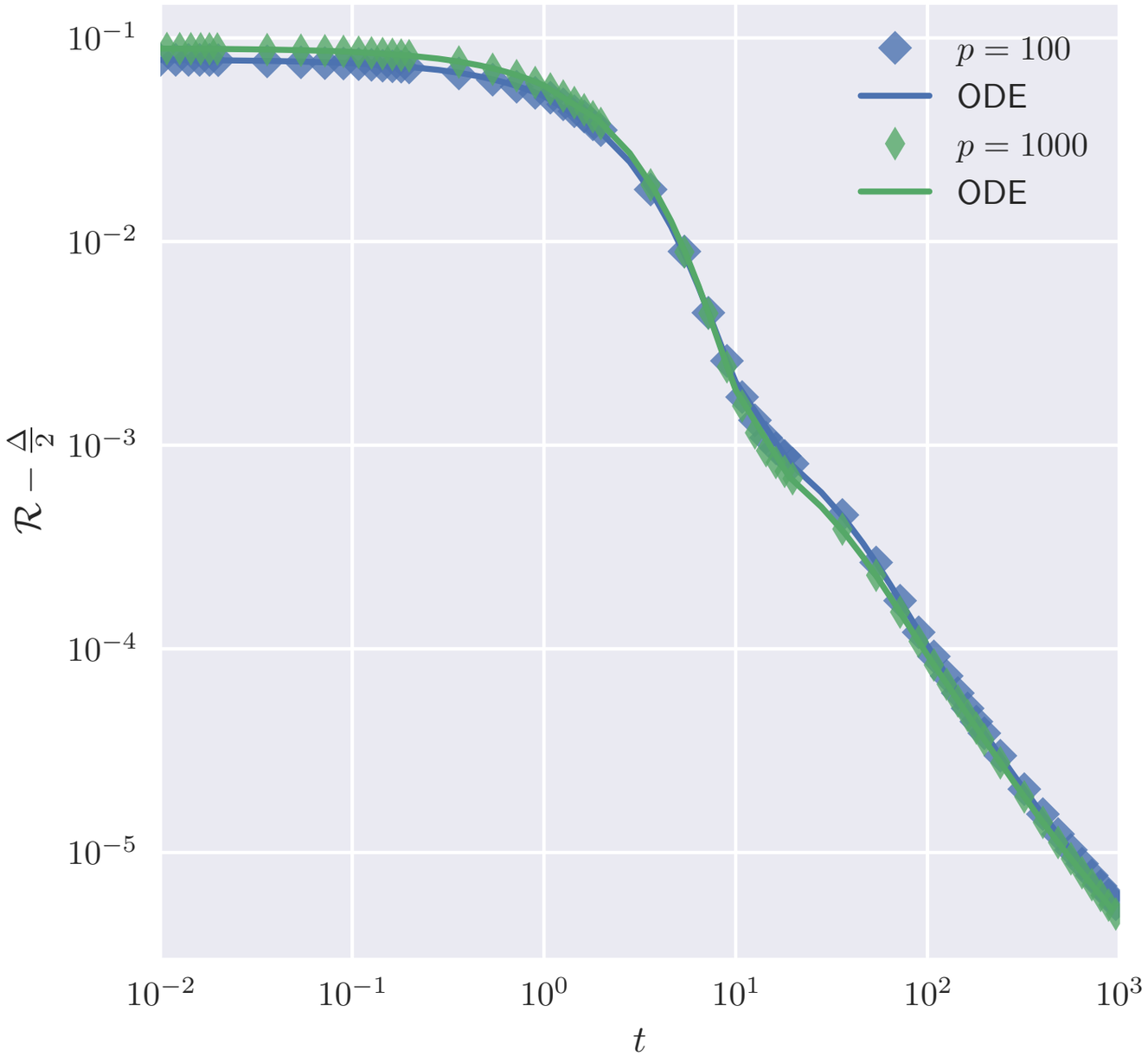
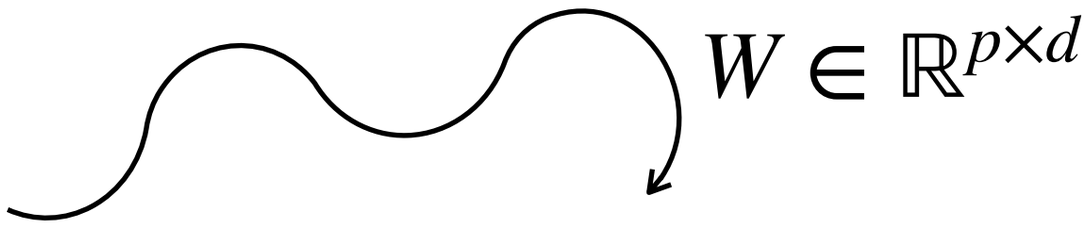


Mean-field regime

🤔 But $Q \in \mathbb{R}^{p \times p}$!!!

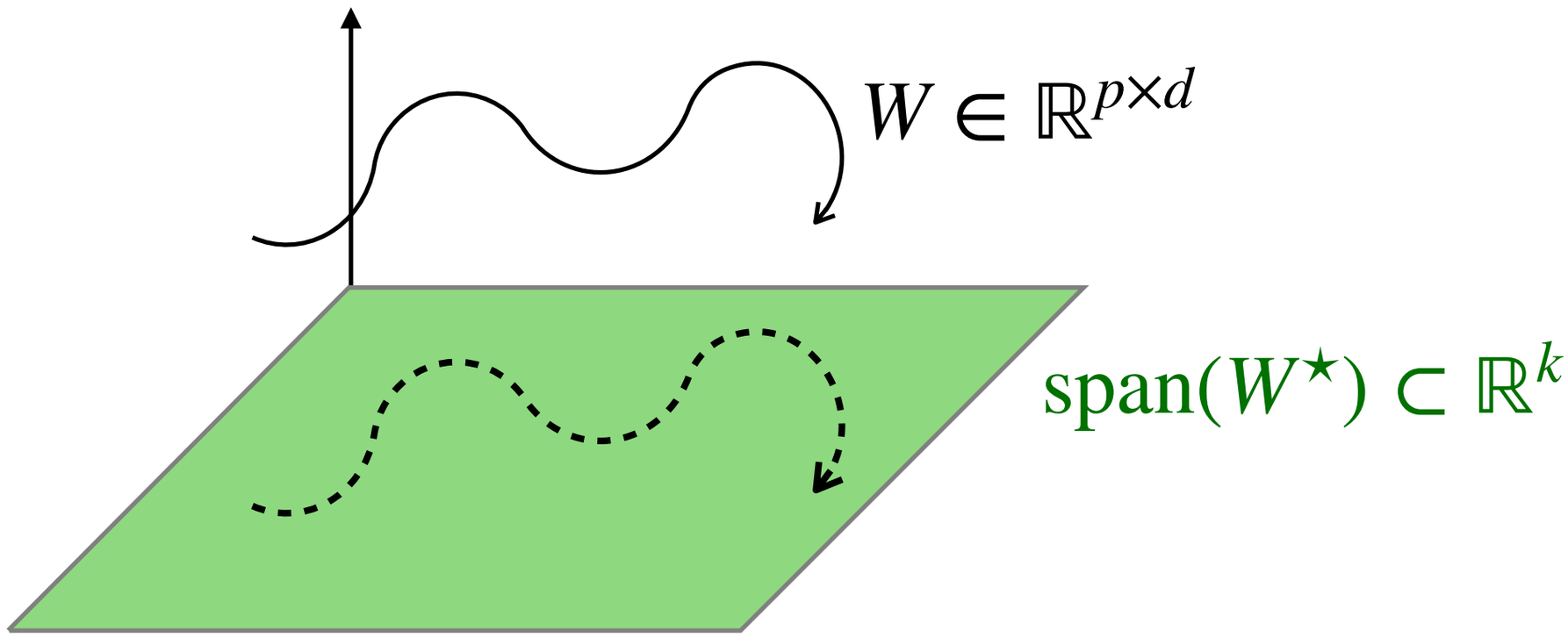


Mean-field regime

🤔 But $Q \in \mathbb{R}^{p \times p}$!!!

$$W = MP^{-1}W^\star + W^\perp$$

Teacher subspace

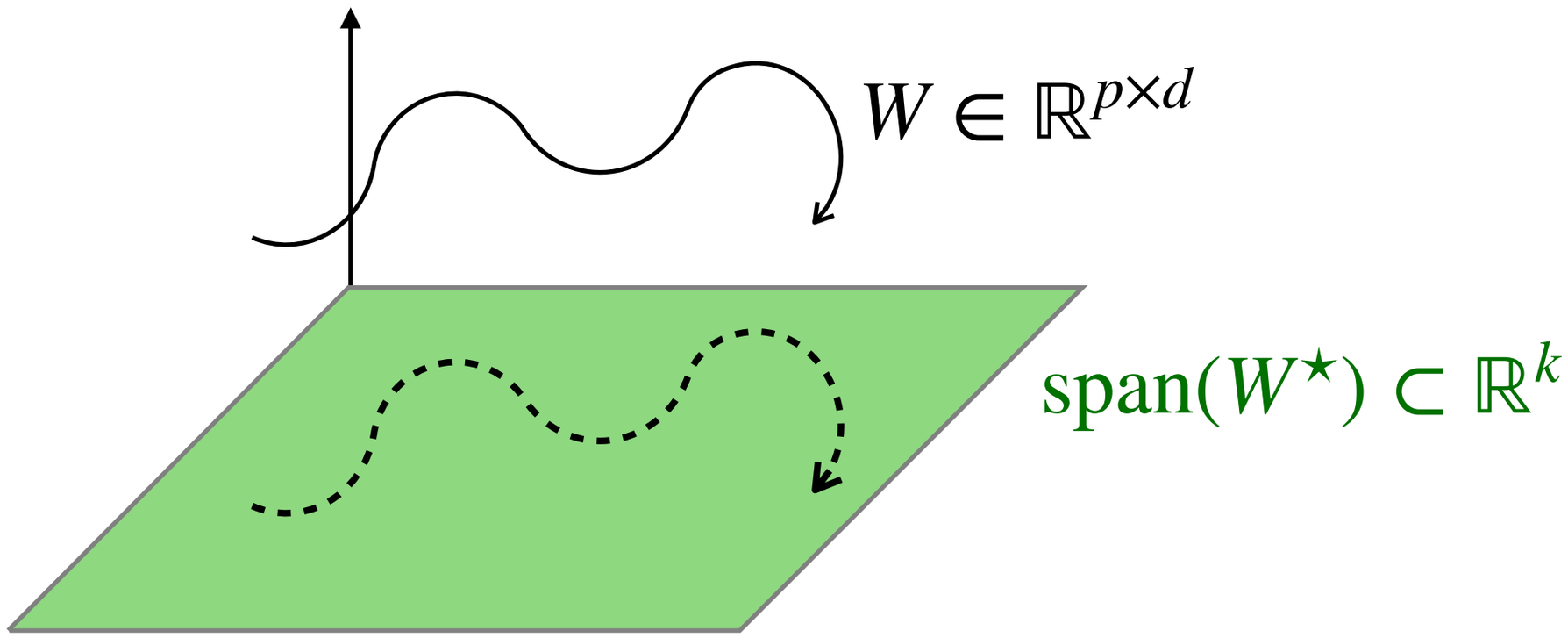


Mean-field regime

🤔 But $Q \in \mathbb{R}^{p \times p}$!!!

$$W = \underbrace{MP^{-1}W^\star}_{\text{Teacher subspace}} + W^\perp \xrightarrow[p \to \infty]{} Q \approx MPM^\top + D_{\sqrt{q^\perp}} \Xi D_{\sqrt{q^\perp}}$$

$$\Xi \sim \mathbb{S}^{d-k-1}$$

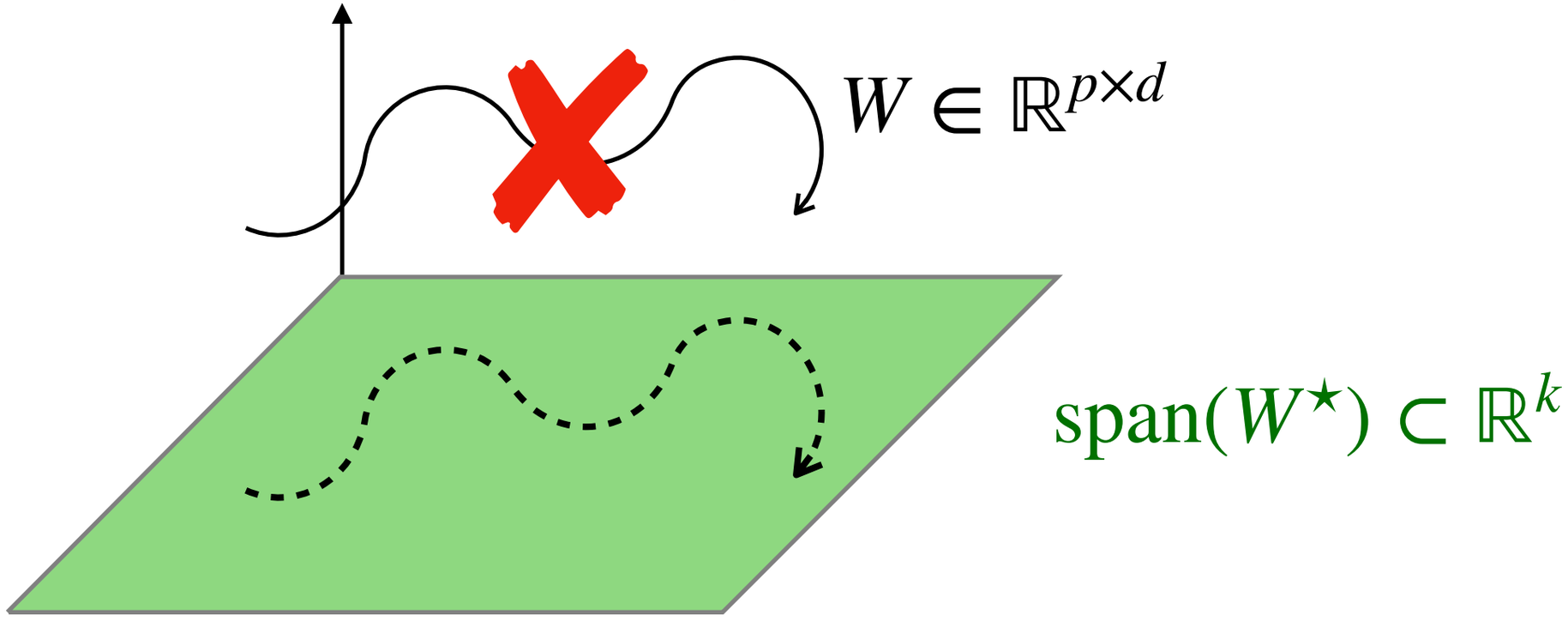


Mean-field + high-d

Theorem [Arnaboldi, Stephan, BL, Krzakala '23]

$$\mathbb{E}\,||\,Q(t) - MP^{-1}M^{\mathsf{T}} + \mathrm{diag}(Q^{\perp})\,||_{\infty} \leq e^{Ct}\left(p^{-1/2} + d^{-1/2}\right)$$

Suppressed in $1/\sqrt{d}$



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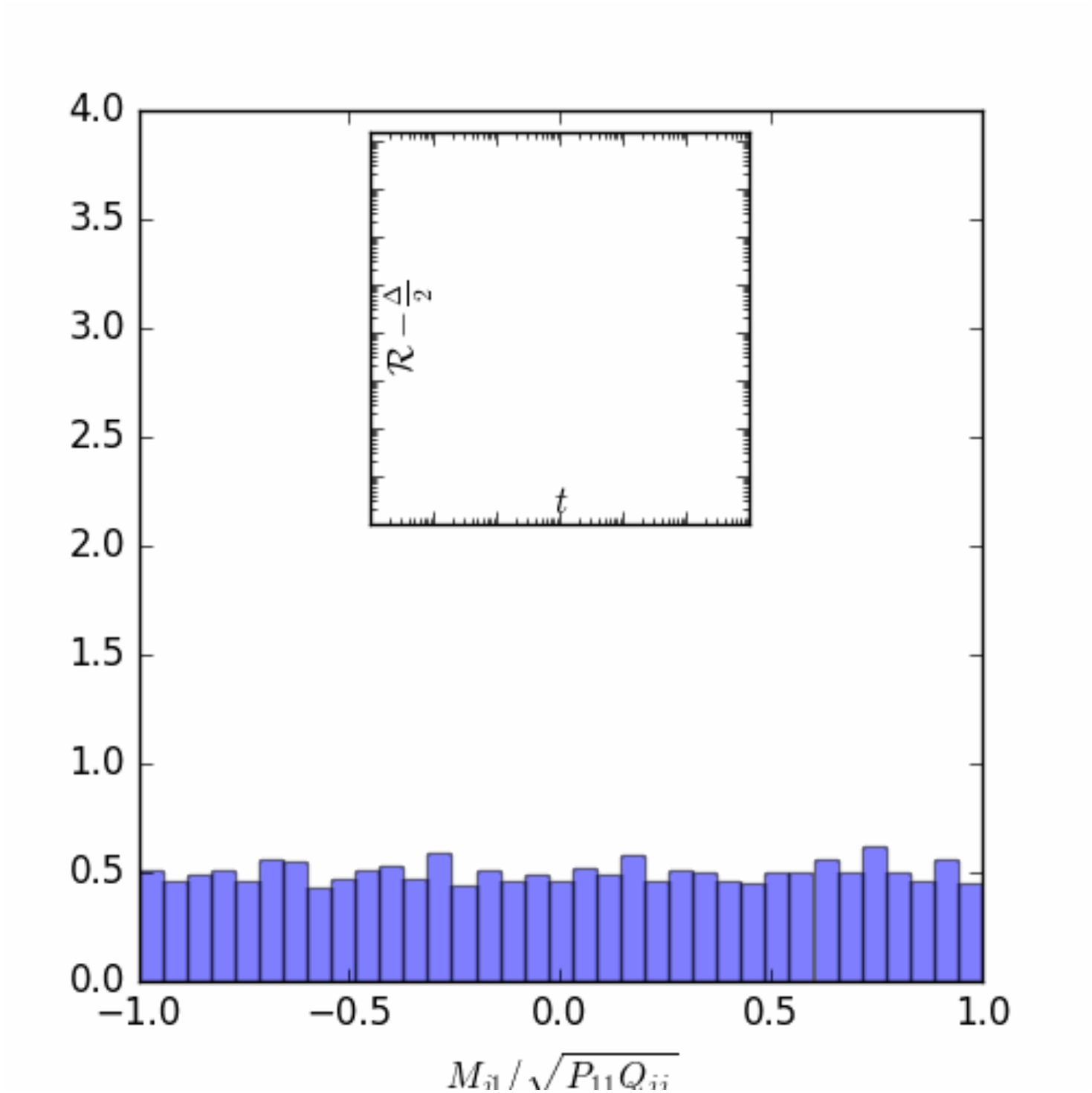
This implies MF-like PDE for the sufficient statistics:

$$\hat{\mu}_t(m,q) = \frac{1}{p}\sum_{i=1}^{p} \delta(m - m_i(t))\delta(q - Q^{\perp}_{ii}(t))$$

$$\partial_t \hat{\mu}_p(m,q) = \nabla_{(m,q)} \cdot (\hat{\mu}_t \varphi(\,\cdot\,, \hat{\mu}_t))$$

Mean-field and high-d



But what can we do with these equations?

Single-index models

"Simple case" $k = 1$ $\qquad y^\nu = \sigma_\star(w^{\star\top} x^\nu)$

- $p = 1, \sigma_\star = \sigma$: information exponent [Ben Arous, Gheissari, Jagannath '21]

$$n = O(1) \qquad \kappa = 1$$

$$n = O(d \log d) \qquad \kappa = 2$$ [Chen et al. '19; Tan, Vershynin '19]

$$n = O(d^{k-1}) \qquad \kappa \geq 2$$

See also: Joan's talk for beyond Gaussian data
Alex's on landscape smoothening

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- $p \to \infty$: Symmetric targets [Hajjar & Chizat '22]

Staircase functions
Leap complexity [Abbe, Adsera, Misiakiewicz '22, '23]

$\sigma_\star \neq \sigma, \kappa = 1$ [Berthier, Montanari, Zhou '23]

See also: Ludovic's and Joan's for multi-index target

Single-index models

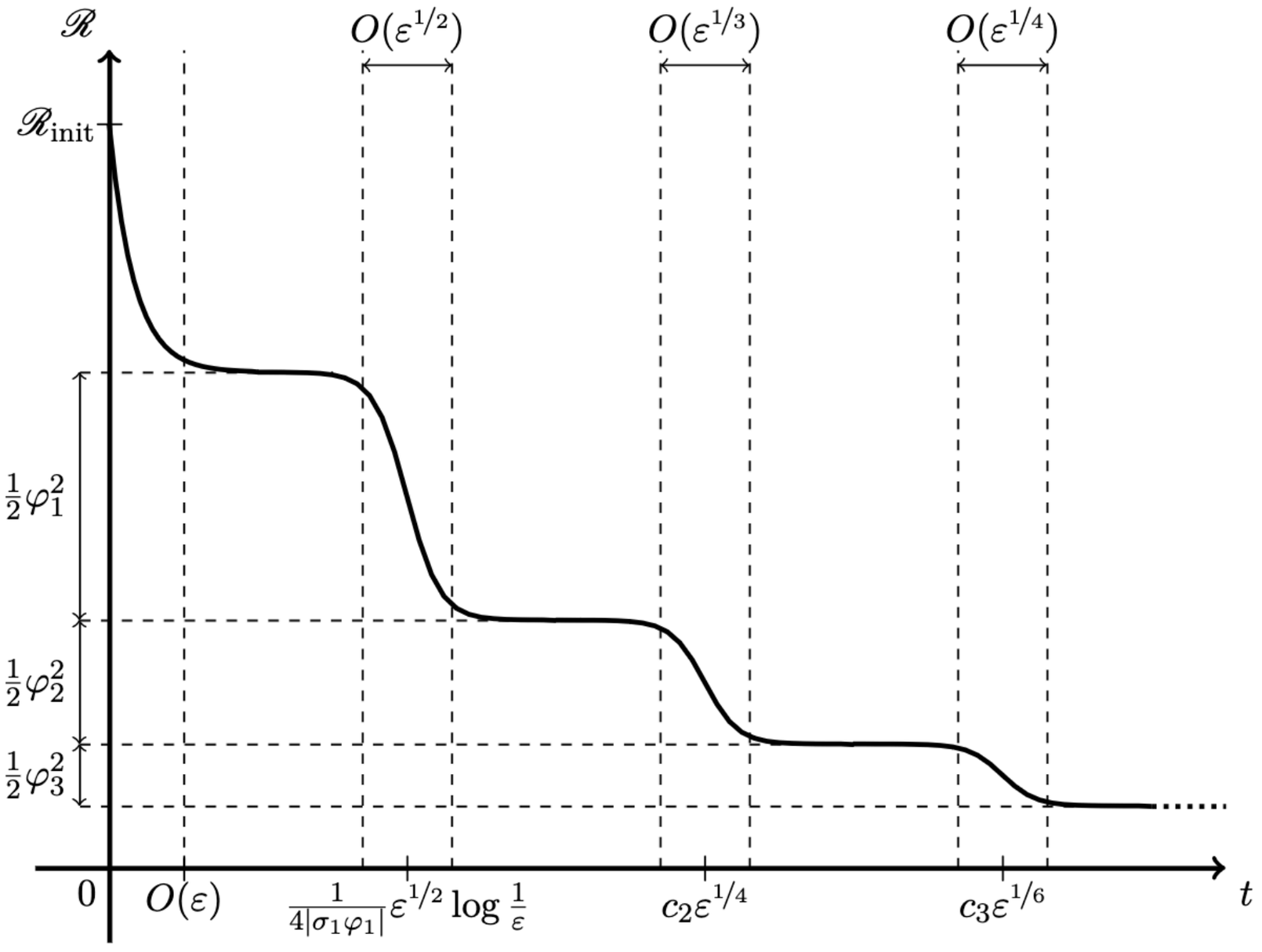
[Berthier, Montanari, Zhou '23]

$$\gamma_a = \varepsilon\gamma$$

$$y^\nu = \sigma_\star(w^{\star\top} x^\nu)$$

$$f_\Theta(x) = \int \rho(da, dw) a\sigma(w^\top x)$$

$(\sigma_\star, \sigma)$ "standard"
$(\kappa = 1)$



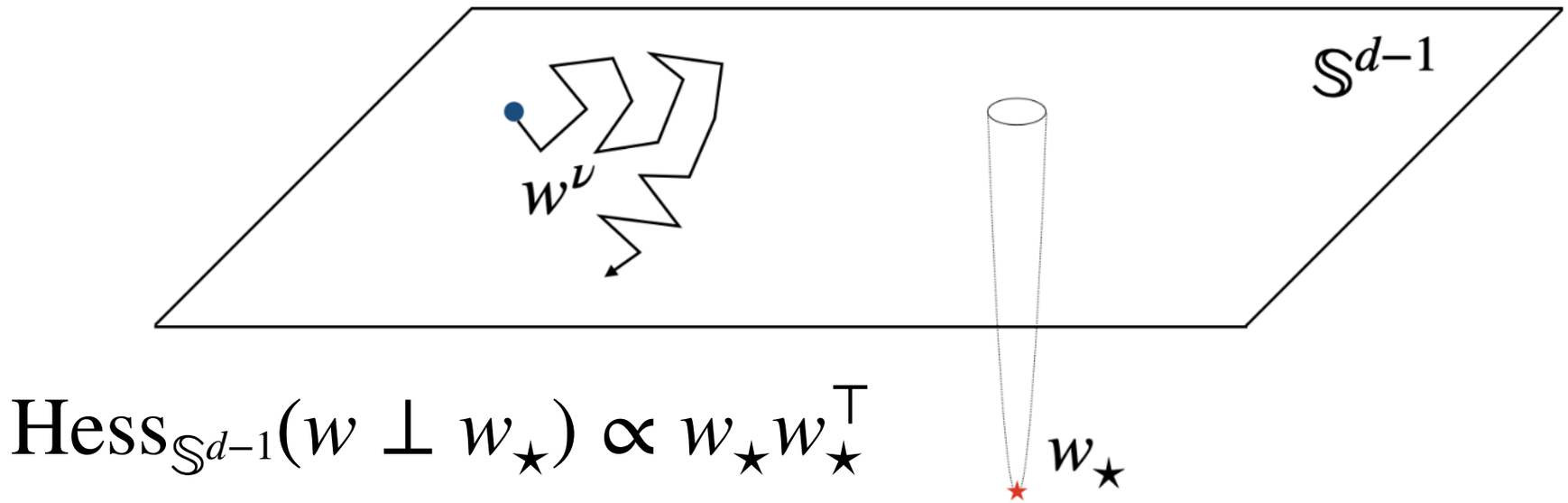
What about $\kappa > 1$?

Phase retrieval

$$y^\nu = (w^{\star\top} x^\nu)^2 \qquad f_\Theta(x) = \frac{1}{p}\sum_{i=1}^{p} (w_i^\top x^\nu)^2 \qquad w^\star, w_i \sim \mathbb{S}^{d-1}$$

Phase retrieval

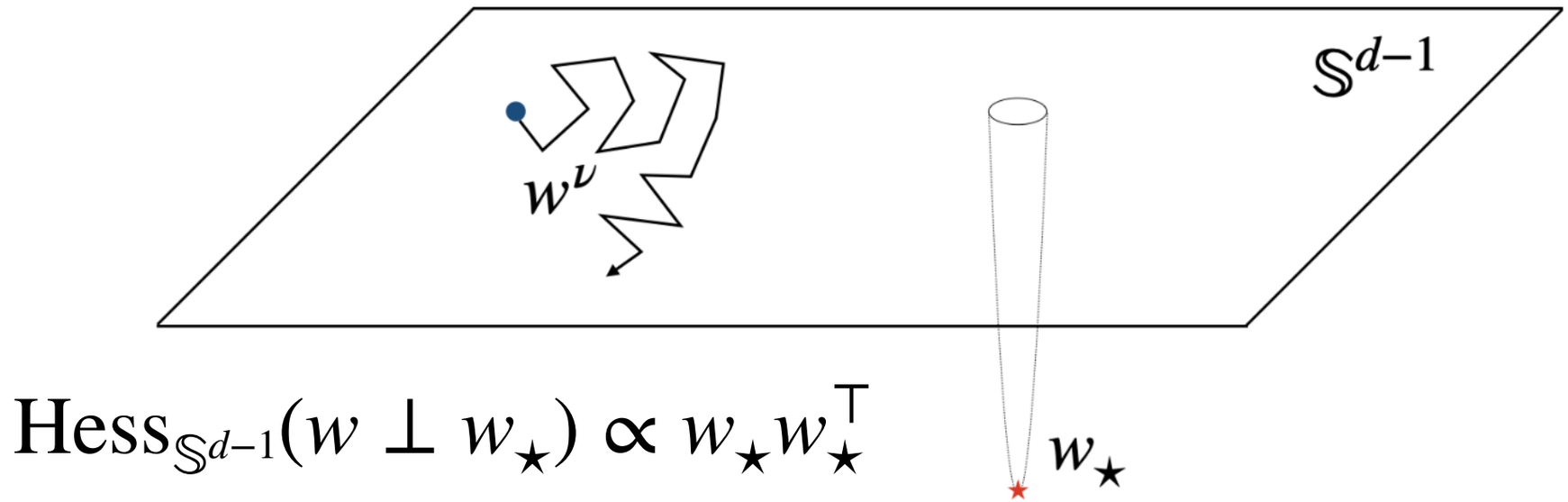
$$y^\nu = (w^{\star\top} x^\nu)^2 \qquad f_\Theta(x) = \frac{1}{p}\sum_{i=1}^{p} (w_i^\top x^\nu)^2 \qquad w^\star, w_i \sim \mathbb{S}^{d-1}$$



$$\mathrm{Hess}_{\mathbb{S}^{d-1}}(w \perp w_\star) \propto w_\star w_\star^\top$$

Phase retrieval

$$y^\nu = (w^{\star\top} x^\nu)^2 \qquad f_\Theta(x) = \frac{1}{p}\sum_{i=1}^{p} (w_i^\top x^\nu)^2 \qquad w^\star, w_i \sim \mathbb{S}^{d-1}$$



$$\mathrm{Hess}_{\mathbb{S}^{d-1}}(w \perp w_\star) \propto w_\star w_\star^\top$$

Questions:

- Know $n = O(d \log d)$, but constants? [Chen et al. '19; Tan, Vershynin '19]
- Does $p \to \infty$ helps? [Mannelli, Vanden-Eijnden, Zdeborová '20]
- Does SGD noise matters? [Ben Arous, Gheissari, Jagannath '22]

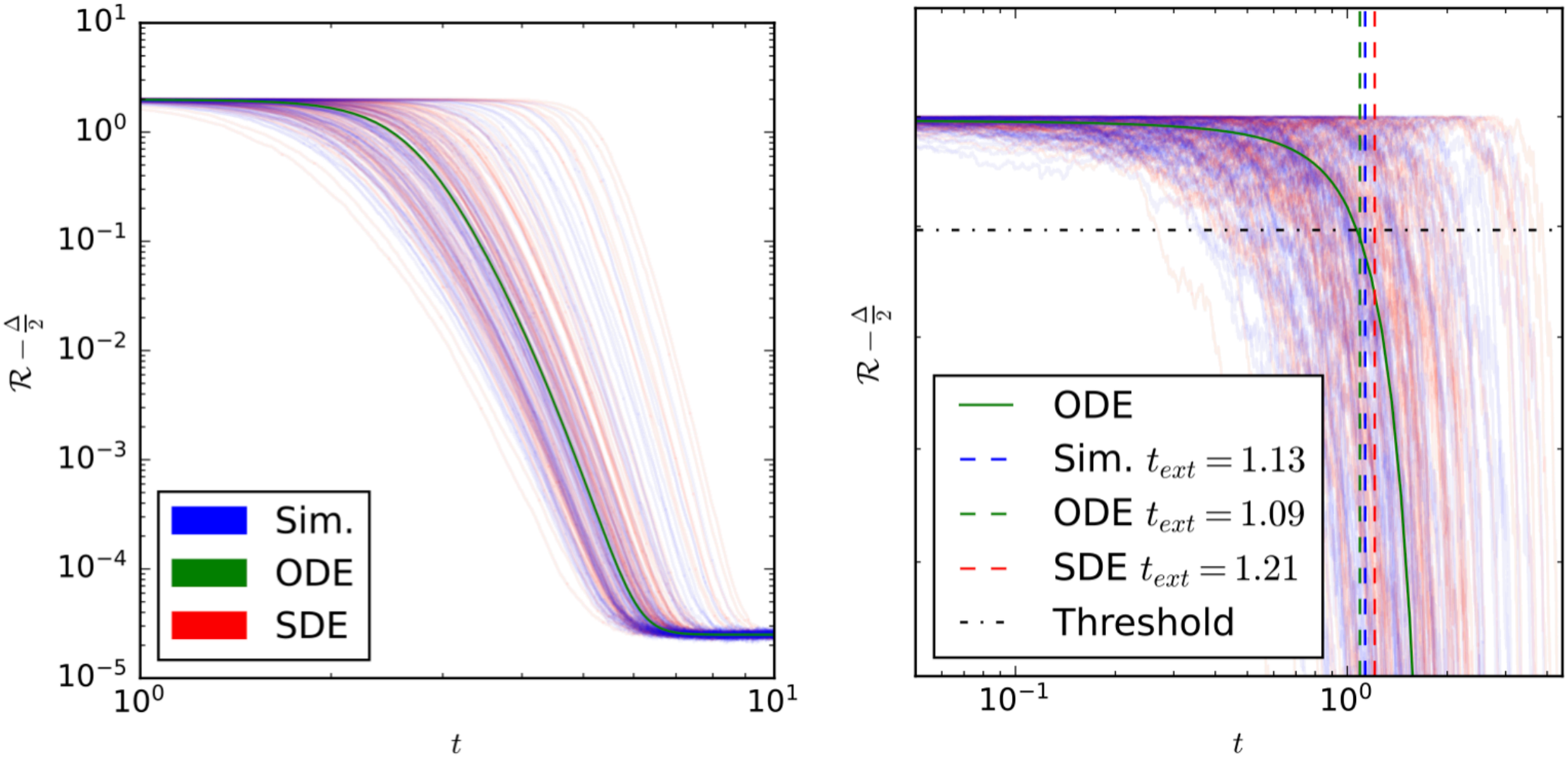
Does noise matter?

Random initial condition: $w(t=0) \sim \mathrm{Uni}(\mathbb{S}^{d-1})$ $\qquad d = 3000$

ODE: $\dot{m}(t) = \bar{\psi}(m(t))$

SDE: $\mathrm{d}m_t = \bar{\psi}(m_t)\mathrm{d}t + \Sigma_t^{1/2}\mathrm{d}B_t$

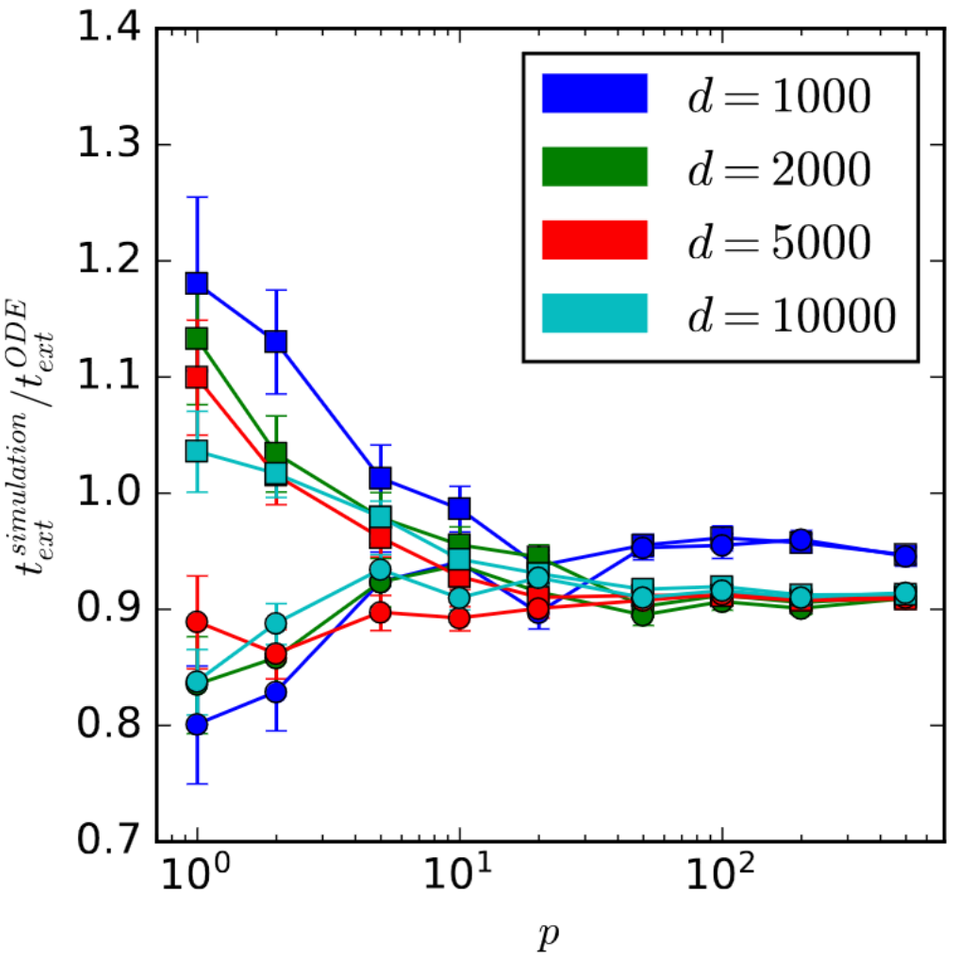
[Ben Arous, Gheissari, Jagannath '22]



[Arnaboldi, Krzakala, BL, Stephan 2023]

Does width matter?

Random initial condition: $w(t=0) \sim \mathrm{Uni}(\mathbb{S}^{d-1})$



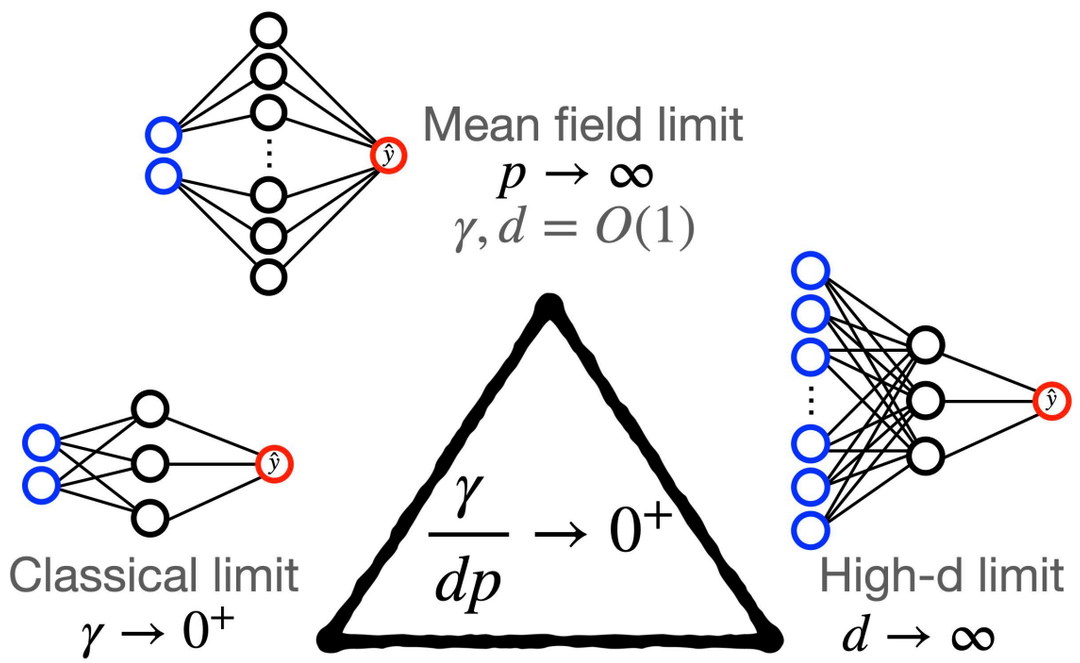
$$t_{\text{ext}}^{(\text{anl})} = \frac{\log\left[\frac{T(p+1)d + (p+1)(1-T)}{2p}\right]}{8\left[1 - \frac{\gamma}{p}\left(1 + \frac{1}{p} + \frac{4}{p^2} + \frac{\Delta}{2}\right)\right]}$$

$$t_{\text{ext}}^{(\text{qnc})} = \mathbb{E}_{\mu_0,\tau_0\sim\mathscr{P}_p^d}\left[\frac{\log\left[\frac{Tp(p+1)d + (2\mu_0 p - \tau_0)(1-T)}{2\mu_0 p}\right]}{8\left[1 - \frac{\gamma}{p}\left(1 + \frac{1}{p} + \frac{4}{p^2} + \frac{\Delta}{2}\right)\right]}\right]$$

$$\mathscr{P}_p^d \equiv \left(d\sum_{j=1}^{p}(u_j\cdot v)^2, 2d\sum_{j=1}^{p}\sum_{l=j+1}^{p}(u_j\cdot u_l)^2\right) \qquad v, u_j \sim \mathbb{S}^{d-1}$$

[Arnaboldi, Krzakala, BL, Stephan 2023]

Take aways



- Low-dimensional reductions of SGD dynamics for 2-layer NN
- Statistical Physics and mean-field limit back together (again)
- SGD noise and overparametrisation not always help you escape mediocrity