



Wonders of high-dimensions: the maths and physics of ML

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Part III

Two layer neural networks in the rich regime

SGD dynamics of two-layer NNs

Recall from last lecture...

Assuming that $a_{0,i} = O(1)$ and introducing a scaling:

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

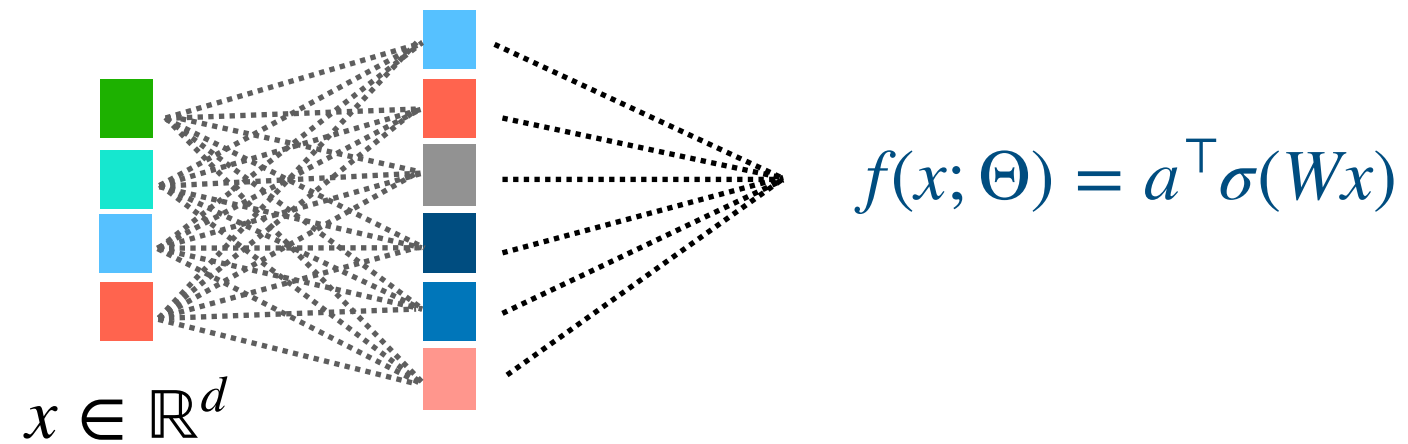
It can be shown that for $p \gg 1$: [\[Chizat, Oyallon & Bach '19\]](#)

$$\mathbb{E}[\kappa(\Theta_0)] \lesssim \frac{1}{\sqrt{p}} + \frac{1}{p\alpha(p)}$$

Which means $f(x; \Theta) \approx \bar{f}_{\text{lin}}(x; \Theta_0)$ if $p\alpha(p) \rightarrow \infty$ as $p \rightarrow \infty$

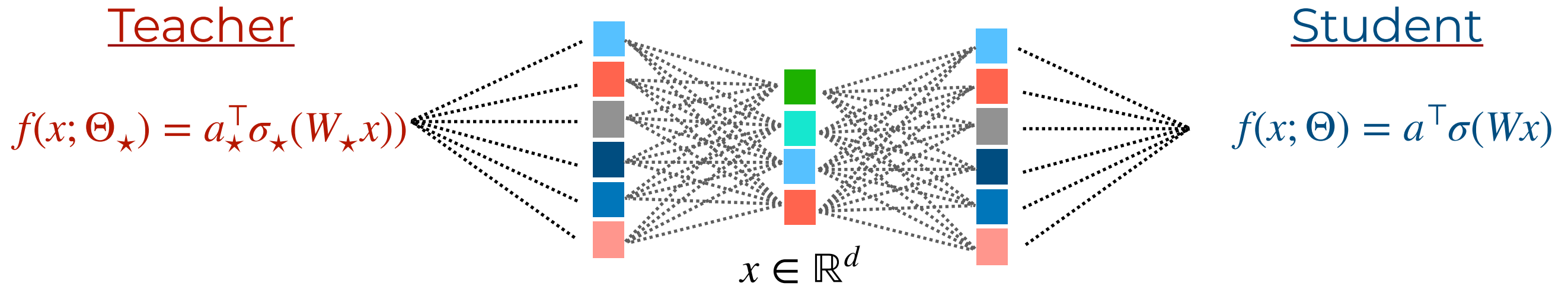
a.k.a. “lazy” regime

Teacher-student setup



Hypothesis: $f(x; \Theta) = \frac{1}{p} \sum_{i=1}^p a_i \sigma(w_i^\top x)$

Teacher-student setup



Hypothesis:

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

Data: $(x^{\nu}, y^{\nu})_{\nu \in [n]} \in \mathbb{R}^d \times \mathcal{Y}$ generated as:

$$y^{\nu} = \frac{1}{k} \sum_{r=1}^k a_{\star, r} \sigma(w_{\star}^{\top} x^{\nu}) + \sqrt{\Delta} z^{\nu}$$

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

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

Algorithm: SGD

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

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

$$\hat{\mathcal{R}}_b(\Theta) = \frac{1}{2|b|} \sum_{\nu \in b} (y^\nu - f(x^\nu; \Theta))^2$$

mini-batch

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Gradient descent (GD)

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

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

$$\dot{\Theta}(t) = - \nabla_{\Theta} \hat{\mathcal{R}}_n(\Theta(t))$$

Algorithm: SGD

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One-pass SGD

b_k independent

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Another look at SGD

Rewrite SGD:

$$\Theta^{k+1} = \underbrace{\Theta^k - \gamma_k \nabla_{\Theta^k} \mathcal{R}(\Theta^k)}_{\text{GD on population}} + \underbrace{\gamma_k \varepsilon^k}_{\text{Effective Noise}}$$

Where:

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

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Question: How to characterise this?

Summary of setting

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

Architecture:

$$f(x; \Theta) = \frac{1}{p} \sum_{i=1}^p a_i \sigma(w_i \cdot x)$$

Data model:

$$y^\nu = \frac{1}{k} \sum_{r=1}^k a_r^\star \sigma(w_r^\star \cdot x^\nu) + \sqrt{\Delta} z^\nu \quad \begin{array}{l} x^\nu \sim \mathcal{N}(0, I_d) \\ z^\nu \sim \mathcal{N}(0, 1) \end{array}$$

Algorithm:

$$\Theta^{\nu+1} = \Theta^\nu - \gamma_\nu \nabla_{\Theta^\nu} (y^\nu - f(x^\nu; \Theta^\nu))^2$$

Sufficient statistics

Goal: track population error exactly throughout the dynamics

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

Sufficient statistics

Goal: track population error exactly throughout the dynamics

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

Where:

$$\Omega^\nu = \frac{1}{d} \begin{pmatrix} W_{\star} W_{\star}^{\top} & W_{\star} W^{\nu \top} \\ W^{\nu} W_{\star}^{\top} & W^{\nu} W^{\nu \top} \end{pmatrix} = \begin{pmatrix} P & M^\nu \\ M^{\nu \top} & Q^\nu \end{pmatrix} \in \mathbb{R}^{(k+p) \times (k+p)}$$

Sufficient statistics

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Key idea:

$$\text{One-pass SGD} \longrightarrow \Omega^{\nu+1} = \psi(\Omega^\nu)$$

Tracking overlaps

Starting point: one-pass SGD

$$\Theta^{\nu+1} = \Theta^{\nu} - \frac{\gamma_{\nu}}{2} \nabla_{\Theta^{\nu}} (y^{\nu} - f(x^{\nu}; \Theta^{\nu}))^2$$

Tracking overlaps

Starting point: one-pass SGD

$$\begin{aligned}\Theta^{\nu+1} &= \Theta^{\nu} - \frac{\gamma_{\nu}}{2} \nabla_{\Theta^{\nu}} (y^{\nu} - f(x^{\nu}; \Theta^{\nu}))^2 \\ &= \Theta^{\nu} + \gamma_{\nu} (y^{\nu} - f(x^{\nu}; \Theta^{\nu})) \nabla_{\Theta^{\nu}} f(x^{\nu}; \Theta^{\nu})\end{aligned}$$

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But:

$$\nabla_{a_i} f(x; \Theta) = \frac{1}{p} \sigma(w_i^{\top} x)$$

$$\nabla_{w_i} f(x; \Theta) = \frac{1}{p} a_i \sigma'(w_i^{\top} x) x$$

Tracking overlaps

Starting point: one-pass SGD

$$a_i^{\nu+1} = a_i^\nu + \frac{\gamma_\nu}{p} \mathcal{E}^\nu \sigma(w_i^{\nu\top} x^\nu)$$

$$w_i^{\nu+1} = w_i^\nu + \frac{\gamma_\nu}{p} \mathcal{E}^\nu a_i \sigma'(w_i^{\nu\top} x^\nu) x^\nu$$

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Goal: Go from this to equation for Ω^ν

Tracking overlaps

Starting point: one-pass SGD

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Goal: Go from this to equation for Ω^ν

$$\mathcal{E}^\nu = (y^\nu - f(x^\nu; \Theta^\nu))$$

$$= \left(\frac{1}{k} \sum_{r=1}^k a_{\star,r} \sigma_{\star}(w_{\star,r}^\top x^\nu) - \sqrt{\Delta} z^\nu - \frac{1}{p} \sum_{i=1}^p a_i^\nu \sigma(w_i^{\nu\top} x^\nu) \right)$$

Tracking overlaps

Starting point: one-pass SGD

$$a_i^{\nu+1} = a_i^\nu + \frac{\gamma_\nu}{p} \mathcal{E}^\nu \sigma(\lambda_i^\nu)$$

$$w_i^{\nu+1} = w_i^\nu + \frac{\gamma_\nu}{p} \mathcal{E}^\nu a_i \sigma'(\lambda_i^\nu) x^\nu$$

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Tracking overlaps

$$w_i^{\nu+1} = w_i^\nu + \frac{\gamma_\nu}{p} \mathcal{E}^\nu a_i \sigma'(\lambda_i^\nu) x^\nu$$

Equation for $M^\nu = \frac{1}{d} W_\star W^{\nu\top}$:

Tracking overlaps

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Equation for $M^\nu = \frac{1}{d} W_\star W^{\nu\top}$:

$$w_{\star,r}^\top w_i^{\nu+1} = w_{\star,r}^\top w_i^\nu + \frac{\gamma_\nu}{p} \mathcal{E}^\nu a_i \sigma'(\lambda_i^\nu) w_{\star,r}^\top x^\nu$$

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$$M_{ri}^{\nu+1} = M_{ri}^\nu + \frac{\gamma_\nu}{dp} \mathcal{E}^\nu a_i \sigma'(\lambda_i^\nu) \lambda_{\star,r}^\nu$$

Tracking overlaps

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Equation for $Q^\nu = \frac{1}{d} W^\nu W^{\nu\top}$:

$$w_j^{\nu+1\top} w_i^{\nu+1} = w_j^{\nu+1\top} \left(w_i^\nu + \frac{\gamma_\nu}{p} \mathcal{E}^\nu a_i \sigma'(\lambda_i^\nu) x^\nu \right)$$

Tracking overlaps

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Tracking overlaps

$$w_i^{\nu+1} = w_i^\nu + \frac{\gamma_\nu}{p} \mathcal{E}^\nu a_i \sigma'(\lambda_i^\nu) x^\nu$$

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Equation for $Q^\nu = \frac{1}{d} W^\nu W^{\nu\top}$:

$$Q_{ji}^{\nu+1} = Q_{ji}^\nu + \frac{\gamma_\nu}{dp} \left(\mathcal{E}^\nu \sigma'(\lambda_j^\nu) \lambda_i^\nu + \mathcal{E}^\nu \sigma'(\lambda_i^\nu) \lambda_j^\nu \right) \\ + \frac{\gamma_\nu^2}{dp^2} (\mathcal{E}^\nu)^2 \sigma'(\lambda_i^\nu) \sigma'(\lambda_j^\nu) \|x^\nu\|_2^2$$

Tracking overlaps: summary

$$w_i^{\nu+1} = w_i^\nu + \frac{\gamma_\nu}{p} \mathcal{E}^\nu a_i \sigma'(\lambda_i^\nu) x^\nu$$

Stochastic process
in $\mathbb{R}^{p \times d}$



$$M_{ri}^{\nu+1} - M_{ri}^\nu = \frac{\gamma_\nu}{dp} \Psi_M^{(\text{GF})}(M, Q)$$

$$Q_{ji}^{\nu+1} - Q_{ji}^\nu = \frac{\gamma_\nu}{dp} \Psi_Q^{(\text{GF})}(M, Q) + \frac{\gamma_\nu^2}{dp^2} \Psi_Q^{(\text{var})}(M, Q)$$

Stochastic process
in $\mathbb{R}^{p(p+k)}$

Concentration result

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

$$M(\nu\delta t) = M^\nu$$

$$Q(\nu\delta t) = Q^\nu$$

Concentration result

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

$$M(\nu\delta t) = M^\nu \quad Q(\nu\delta t) = Q^\nu$$

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

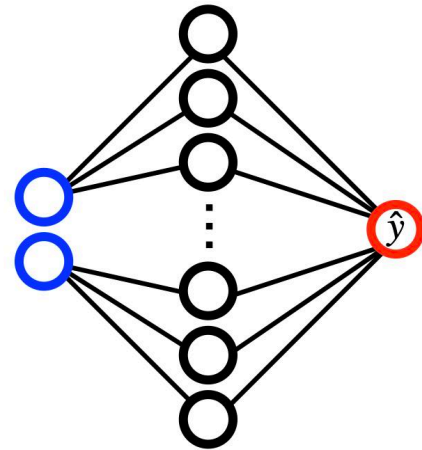
Then $\forall 0 \leq \nu \leq \left\lfloor \frac{n}{\delta t} \right\rfloor$:

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

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

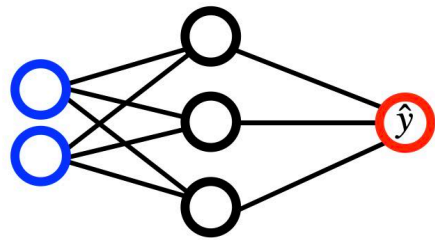
$$\frac{d\bar{\Omega}(t)}{dt} = \mathbb{E} \left[\psi(\bar{\Omega}(t)) \right]$$

The different limiting regimes



Mean field limit

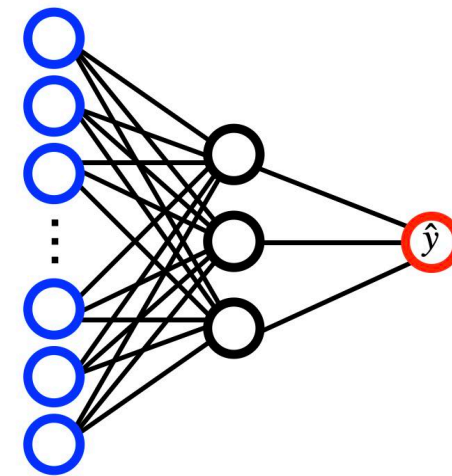
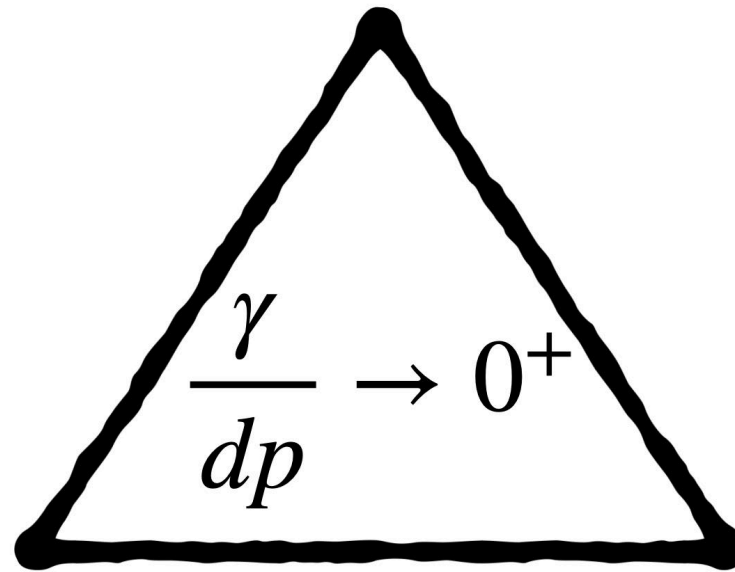
$$p \rightarrow \infty$$
$$\gamma, d = O(1)$$



Classical limit

$$\gamma \rightarrow 0^+$$

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

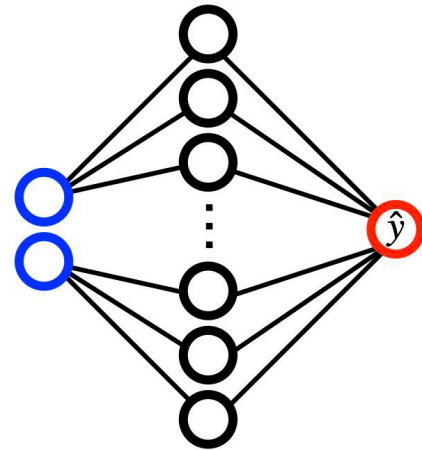


High-d limit

$$d \rightarrow \infty$$

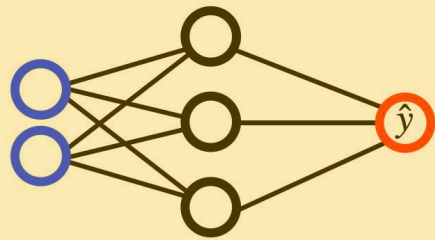
$$\gamma, p = O(1)$$

The different limiting regimes



Mean field limit

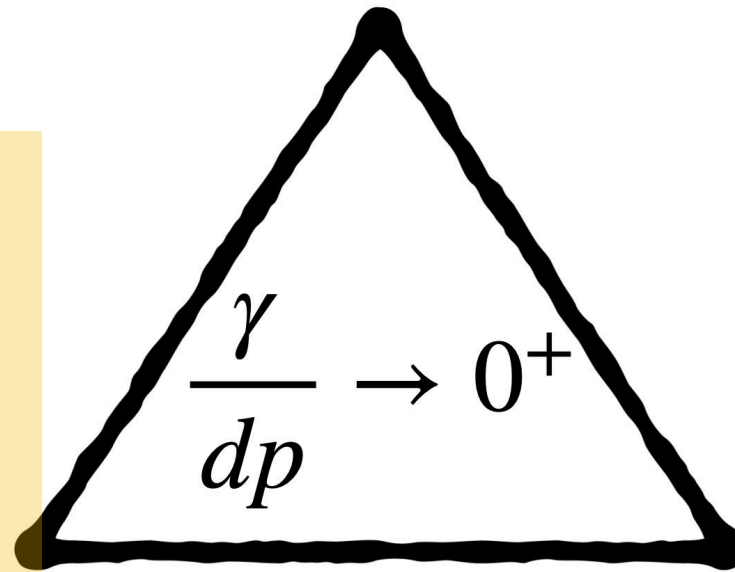
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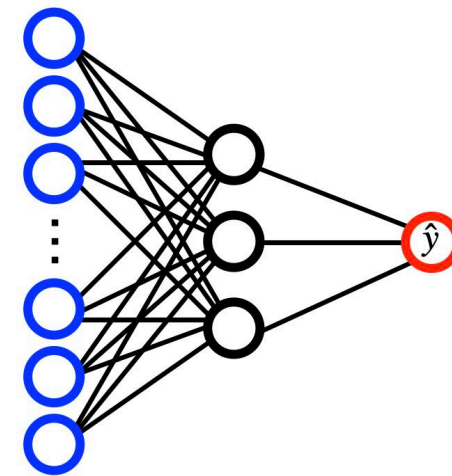
Classical limit

$$\gamma \rightarrow 0^+$$

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



$$\frac{\gamma}{dp} \rightarrow 0^+$$

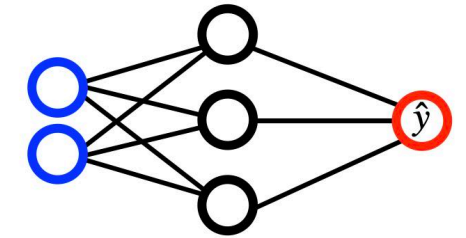


High-d limit

$$d \rightarrow \infty$$

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

Classical regime



Classical limit

$$\gamma \rightarrow 0^+$$

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$$\Theta^{\nu+1} = \Theta^{\nu} - \frac{\gamma_{\nu}}{2} \nabla_{\Theta^{\nu}} (y^{\nu} - f(x^{\nu}; \Theta^{\nu}))^2$$

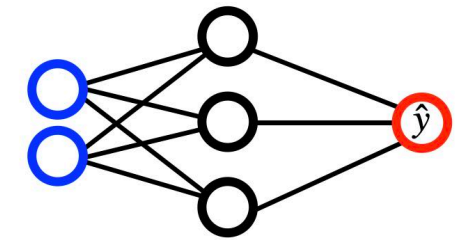


$$\gamma \rightarrow 0^+$$

[Robins & Monro '51]

$$\dot{\Theta}(t) = -\frac{1}{2} \nabla_{\Theta} \mathbb{E}_{(x,y)} [(y - f(x; \Theta(t)))^2]$$

Classical regime



Classical limit

$$\gamma \rightarrow 0^+$$

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

$$\Theta^{\nu+1} = \Theta^{\nu} - \frac{\gamma_{\nu}}{2} \nabla_{\Theta^{\nu}} (y^{\nu} - f(x^{\nu}; \Theta^{\nu}))^2$$

\downarrow $\gamma \rightarrow 0^+$
[Robins & Monro '51]

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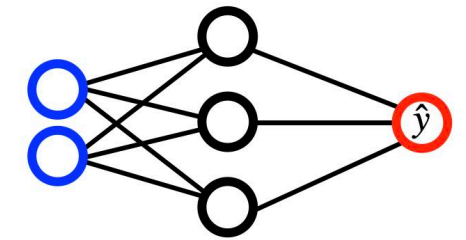
Subleading in γ

$$\Theta^{k+1} = \Theta^k - \gamma_k \nabla_{\Theta^k} \mathcal{R}(\Theta^k) + \gamma_k \epsilon^k$$

GD on population

Effective Noise

Classical regime



Classical limit

$$\gamma \rightarrow 0^+$$

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

$$\Theta^{\nu+1} = \Theta^{\nu} - \frac{\gamma_{\nu}}{2} \nabla_{\Theta^{\nu}} (y^{\nu} - f(x^{\nu}; \Theta^{\nu}))^2$$



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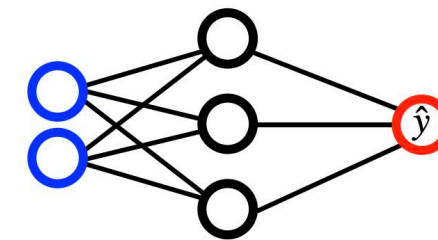
[Robins & Monro '51]

$$\dot{\Theta}(t) = -\frac{1}{2} \nabla_{\Theta} \mathbb{E}_{(x,y)} [(y - f(x; \Theta(t)))^2]$$

$$\dot{M}_{ri}(t) = \mathbb{E}[\Psi_M^{(\text{GF})}(\bar{M}, \bar{Q})]$$

$$\dot{Q}_{ji}(t) = \mathbb{E}[\Psi_Q^{(\text{GF})}(\bar{M}, \bar{Q})]$$

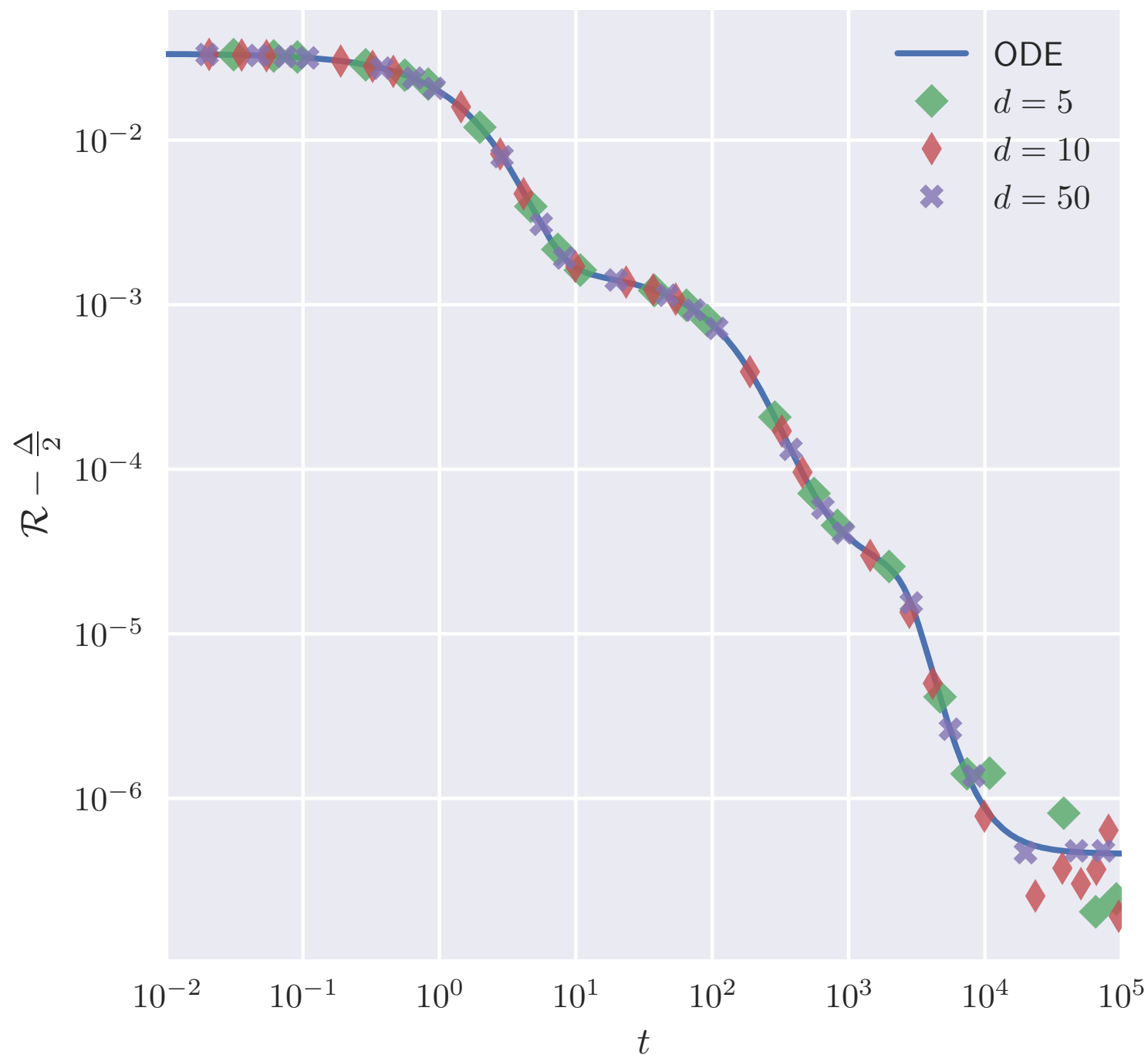
Classical regime



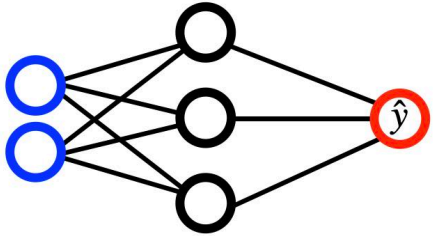
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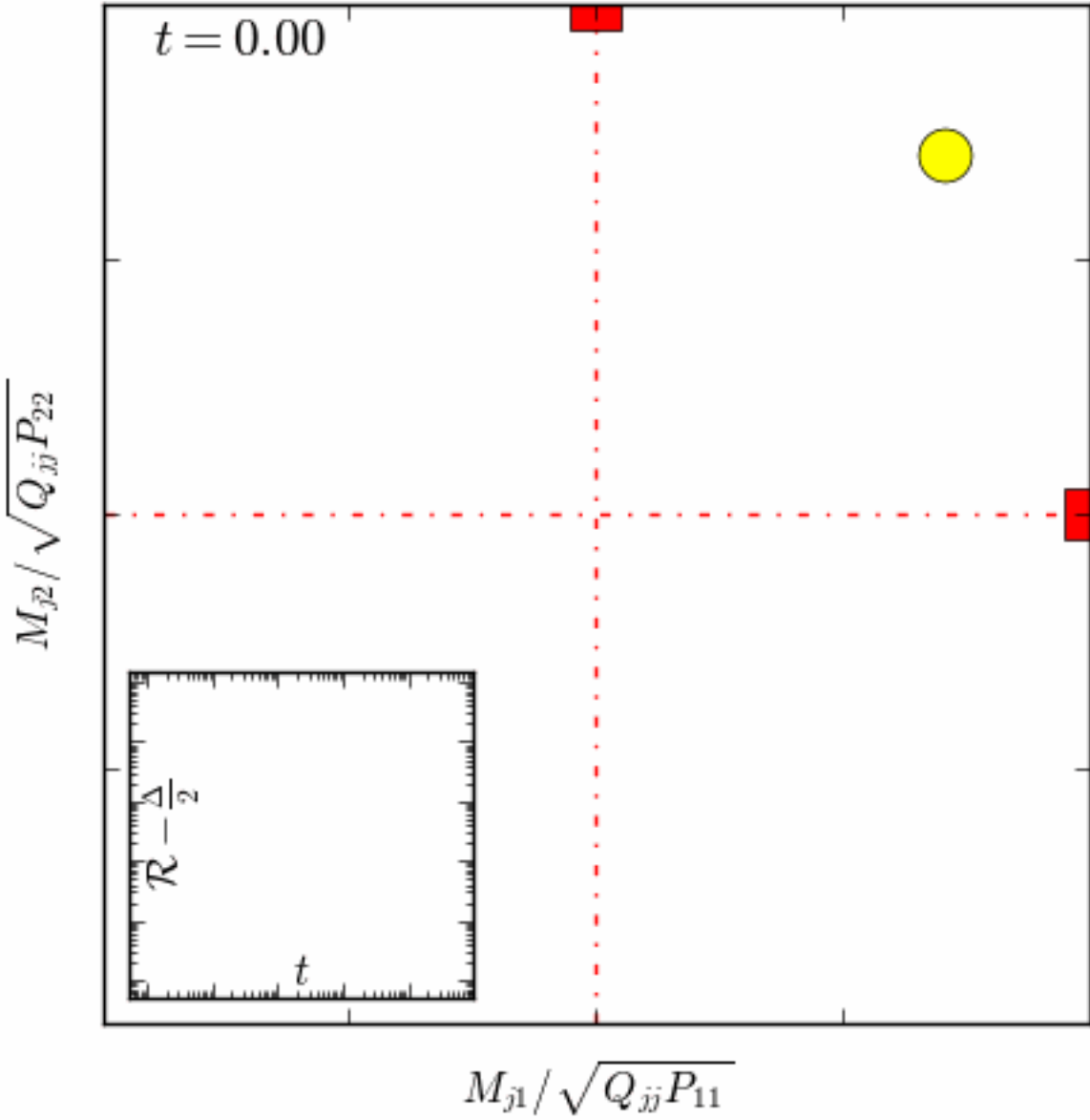
Classical regime



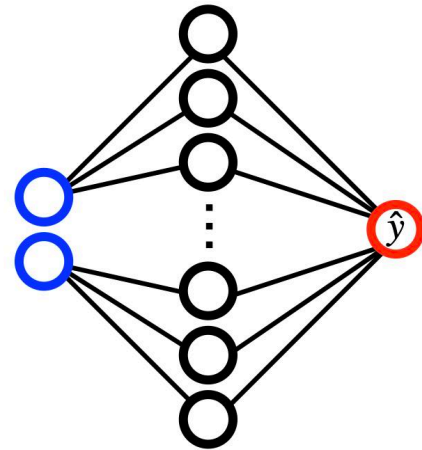
Classical limit

$$\gamma \rightarrow 0^+$$

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

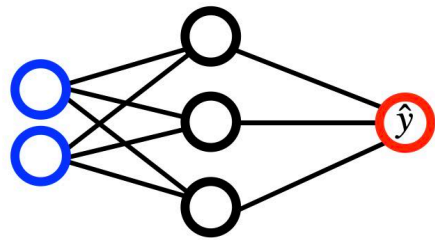


The different limiting regimes



Mean field limit

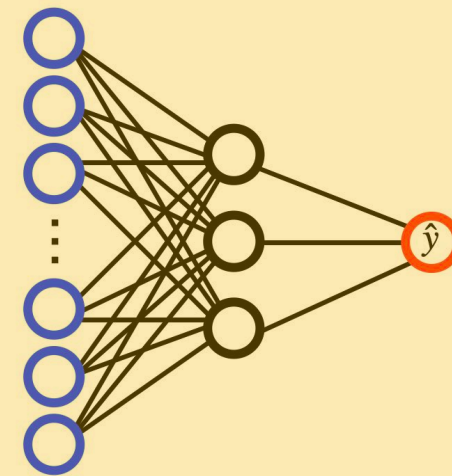
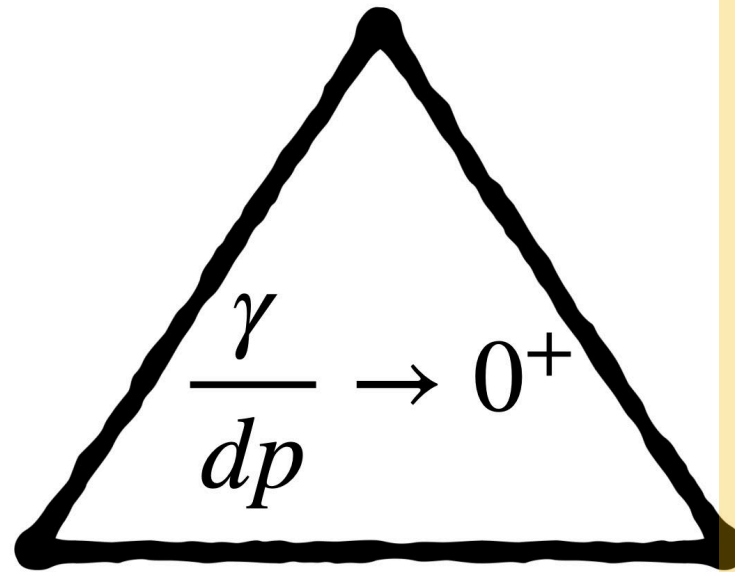
$$p \rightarrow \infty$$
$$\gamma, d = O(1)$$



Classical limit

$$\gamma \rightarrow 0^+$$

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



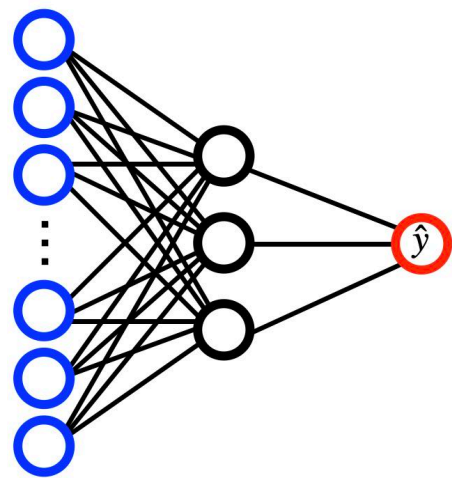
High-d limit

$$d \rightarrow \infty$$

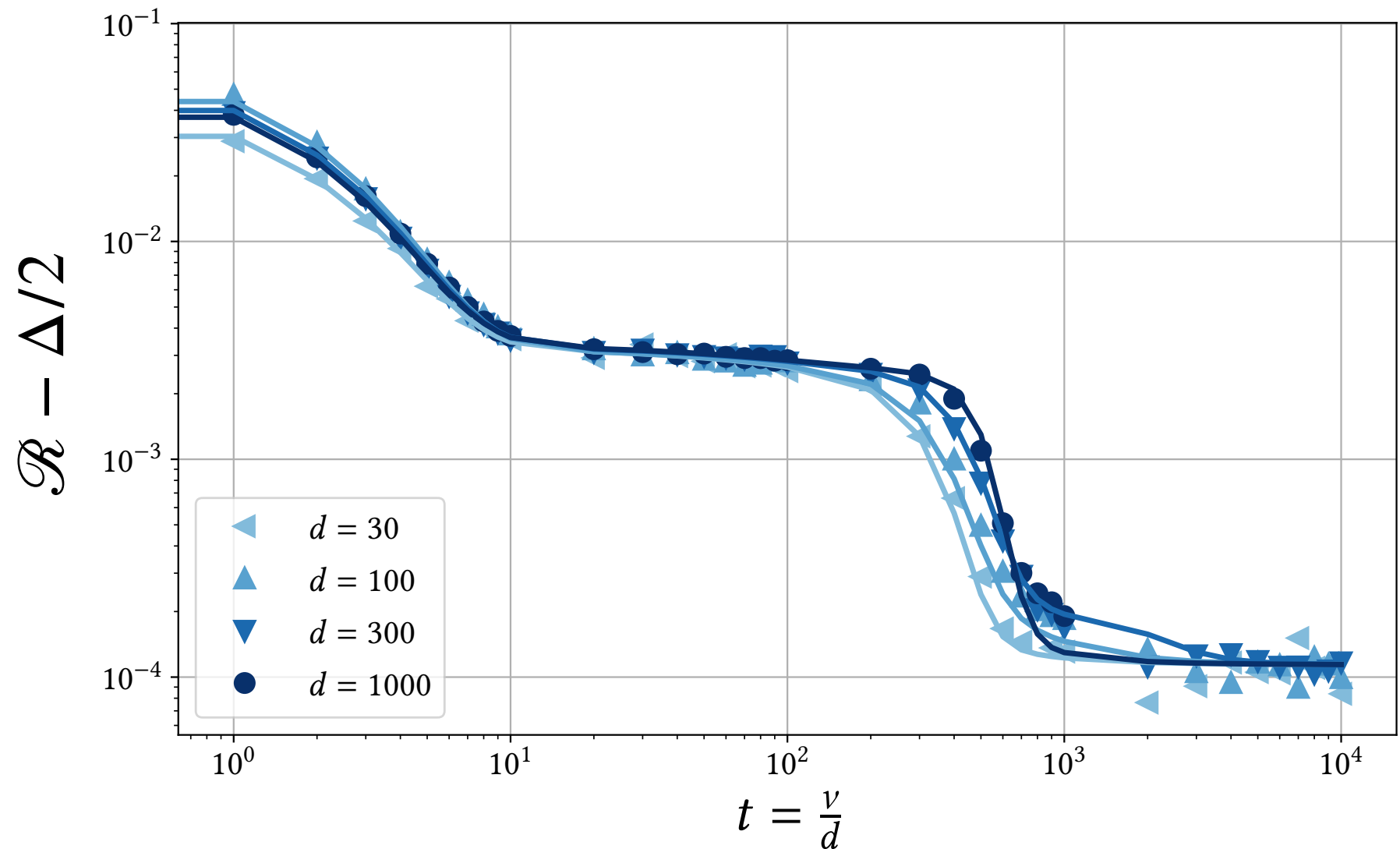
$$\gamma, p = O(1)$$

High-dimensional regime

[Saad & Solla '95]



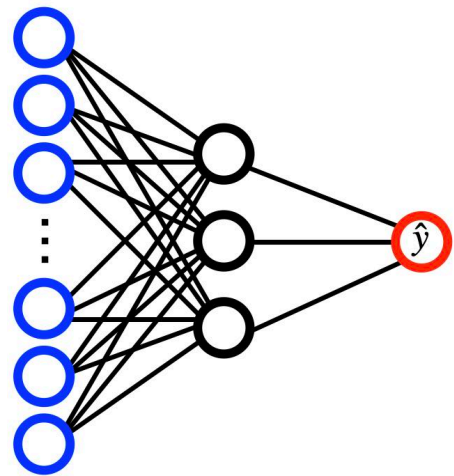
High-d limit
 $d \rightarrow \infty$
 $\gamma, p = O(1)$



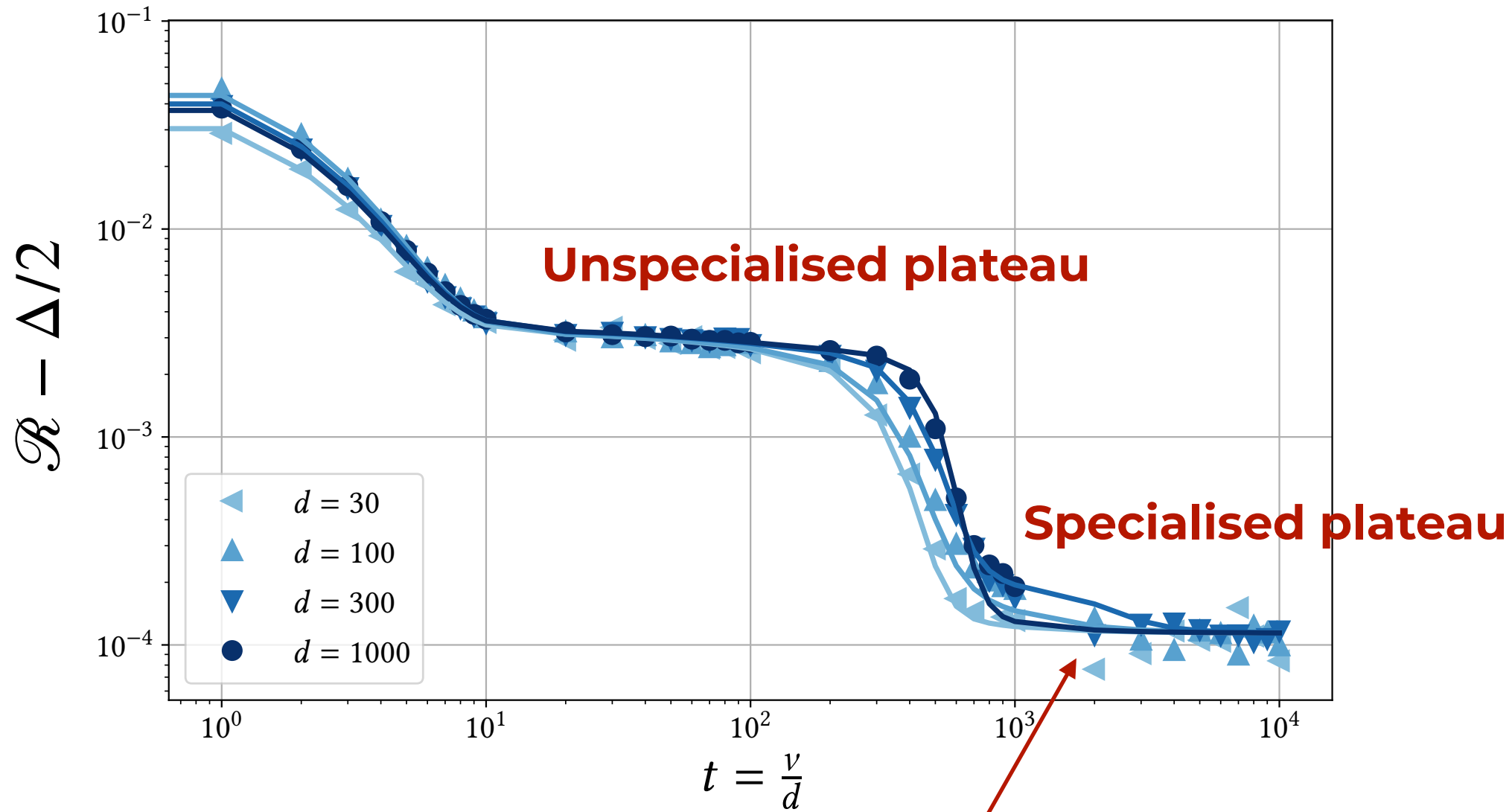
$$\begin{aligned}\dot{\bar{M}}_{ri}(t) &= \mathbb{E}[\Psi_M^{(\text{GF})}(\bar{M}, \bar{Q})] \\ \dot{\bar{Q}}_{ji}(t) &= \mathbb{E}[\Psi_Q^{(\text{GF})}(\bar{M}, \bar{Q})] + \frac{\gamma}{p} \mathbb{E}[\Psi_Q^{\text{var}}(\bar{M}, \bar{Q})]\end{aligned}$$

High-dimensional regime

[Saad & Solla '95]

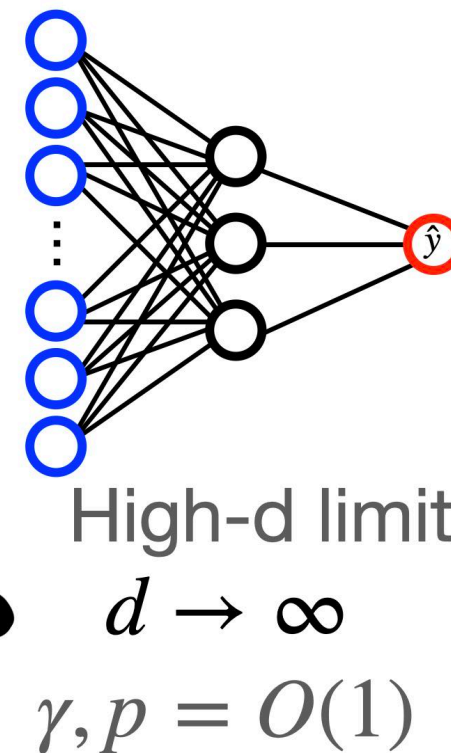
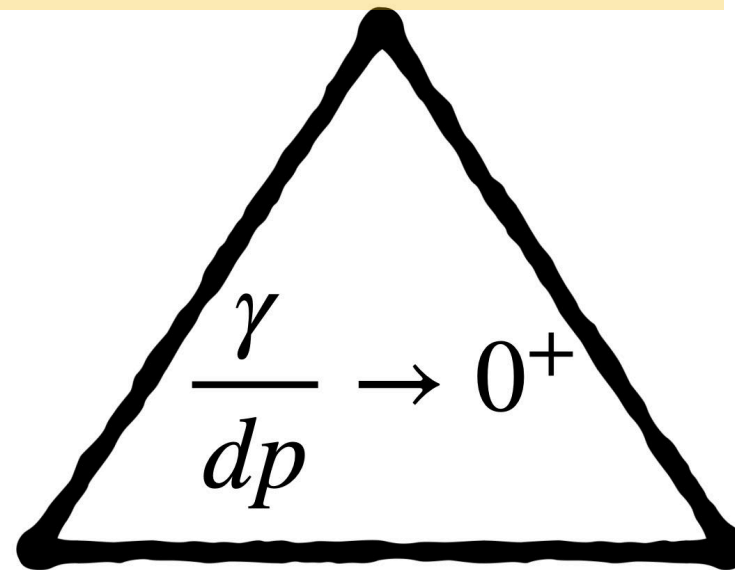
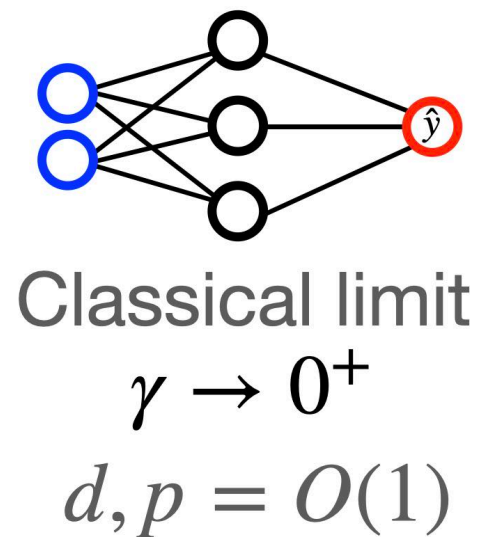
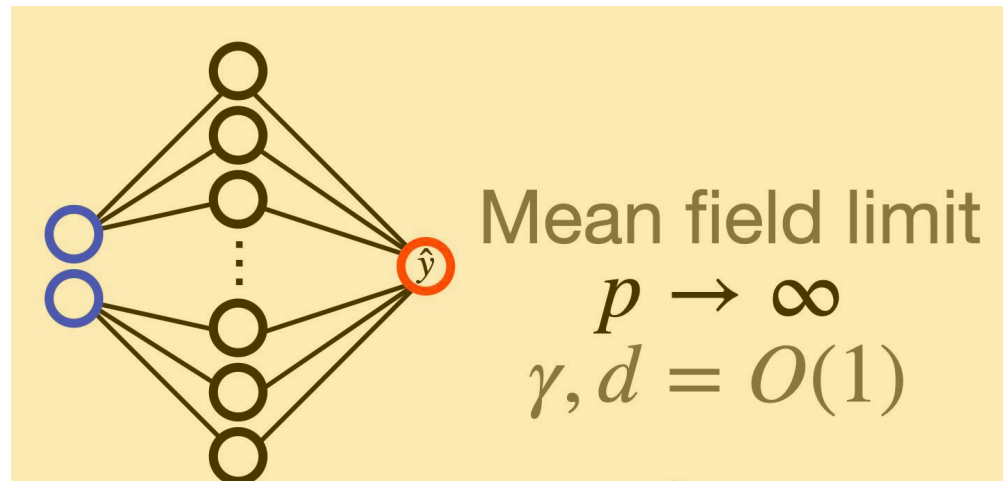


High-d limit
 $d \rightarrow \infty$
 $\gamma, p = O(1)$

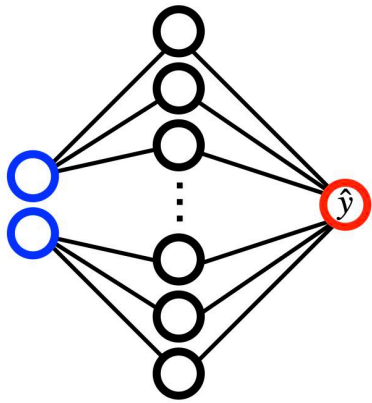


$$\mathcal{R}_{\infty} - \Delta/2 \propto \gamma \Delta$$

The different limiting regimes

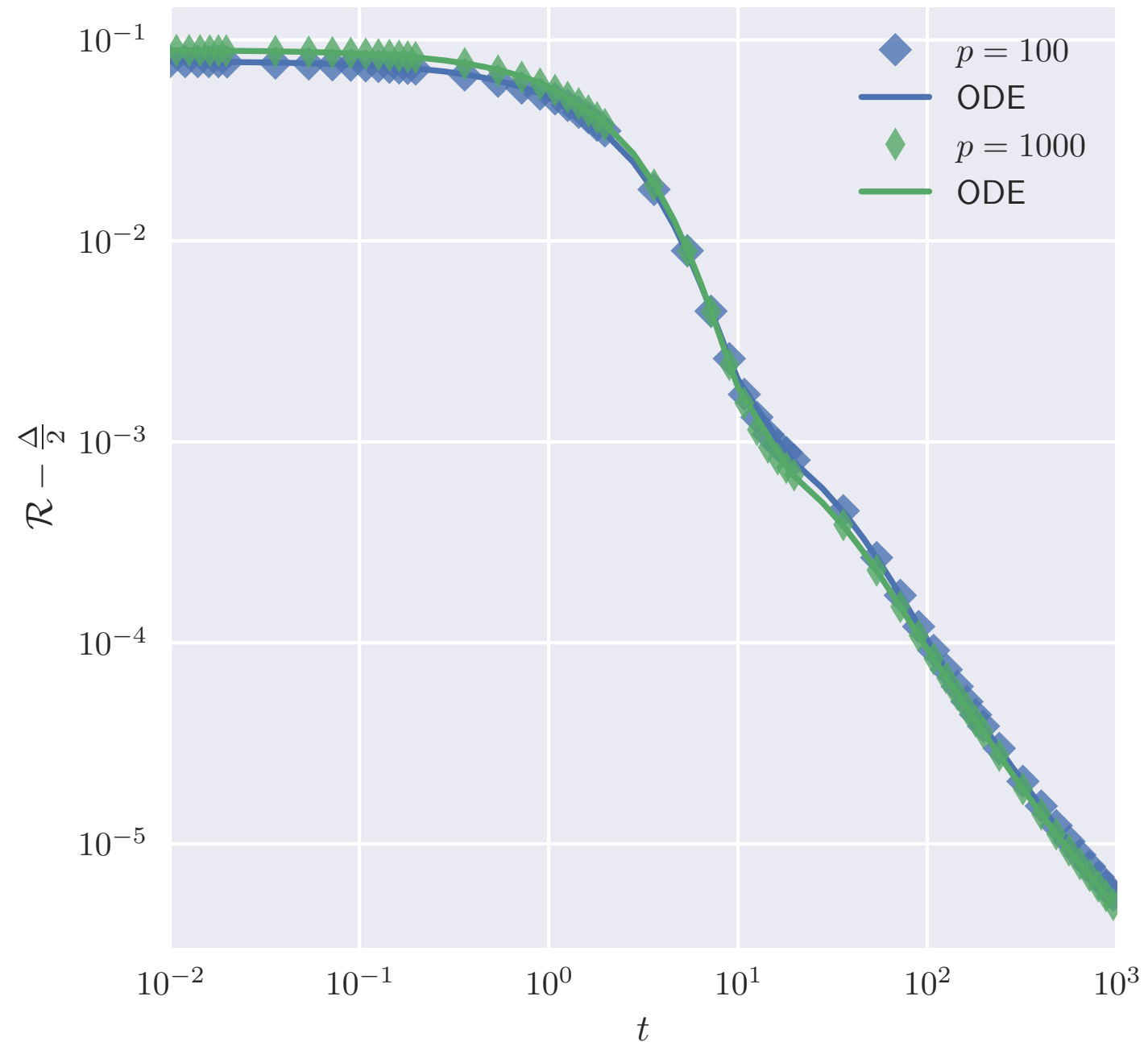


Mean-field regime



Mean field limit

$$p \rightarrow \infty$$
$$\gamma, d = O(1)$$



$$\dot{M}_{ri}(t) = \mathbb{E}[\Psi_M^{(\text{GF})}(\bar{M}, \bar{Q})] \quad \dot{Q}_{ji}(t) = \mathbb{E}[\Psi_Q^{(\text{GF})}(\bar{M}, \bar{Q})]$$

Mean-field limit

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

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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:

$$\rho_p^\nu(a, w) = \frac{1}{p} \sum_{i=1}^p \delta(a_i - a_i^\nu) \delta(w_i - w_i^\nu)$$

Mean-field limit



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

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

Mean-field limit



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

One-pass
SGD

$p \rightarrow \infty$
→

$$\partial_t \rho_t = \gamma \nabla_\theta \left(\rho_t \nabla_\theta \ell(\theta; \rho_t) \right)$$

“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](#):

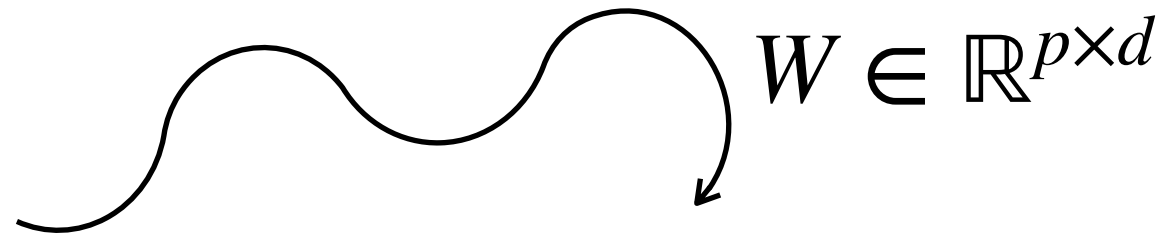
- This is only for $m = +\infty$, and we cannot provide an estimation of the number of particles needed to approximate the mean field regime that is not exponential in t (see such results e.g. in [\[28\]](#)).
- We cannot provide an estimation of the performance as the function of time, that would provide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

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

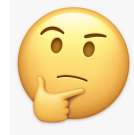
Mean-field regime



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



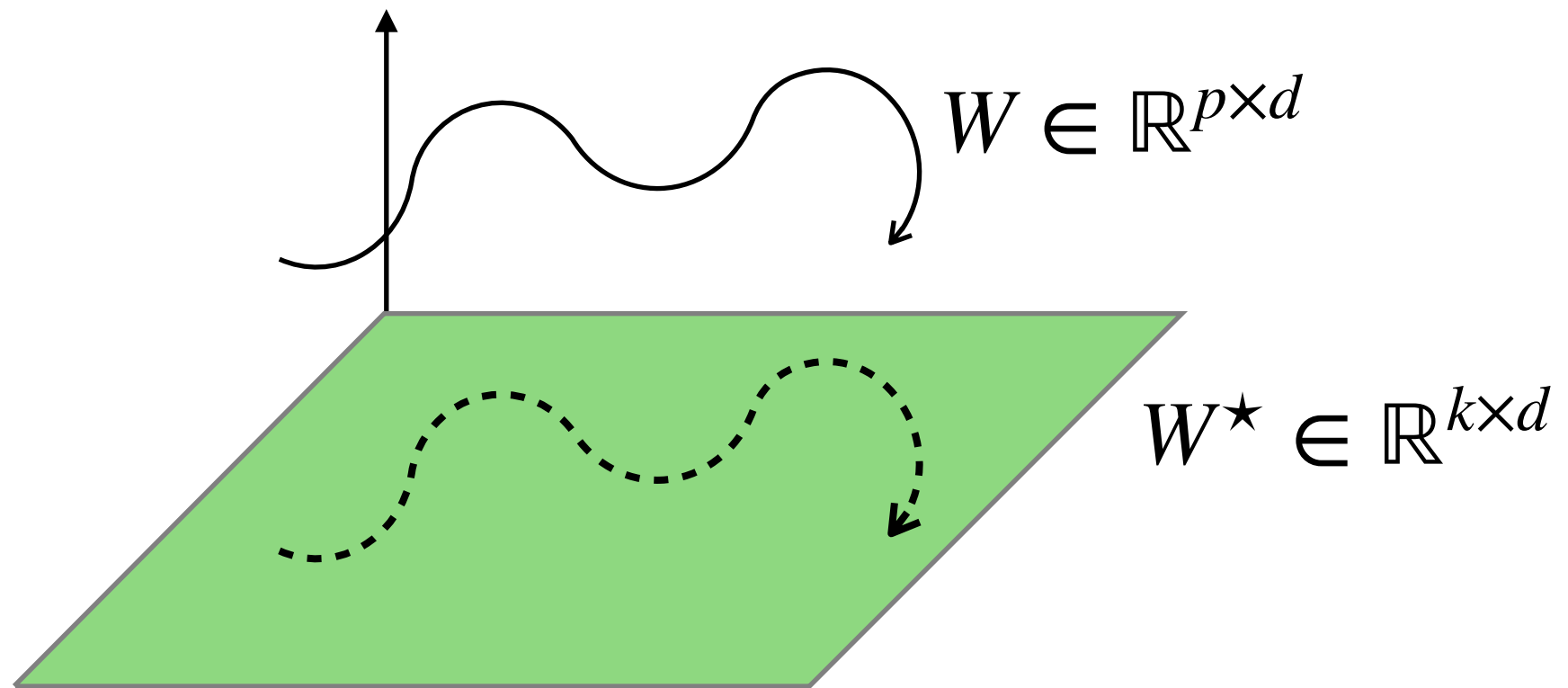
Mean-field regime



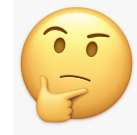
But $Q \in \mathbb{R}^{p \times p}$!!!

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

Teacher
subspace

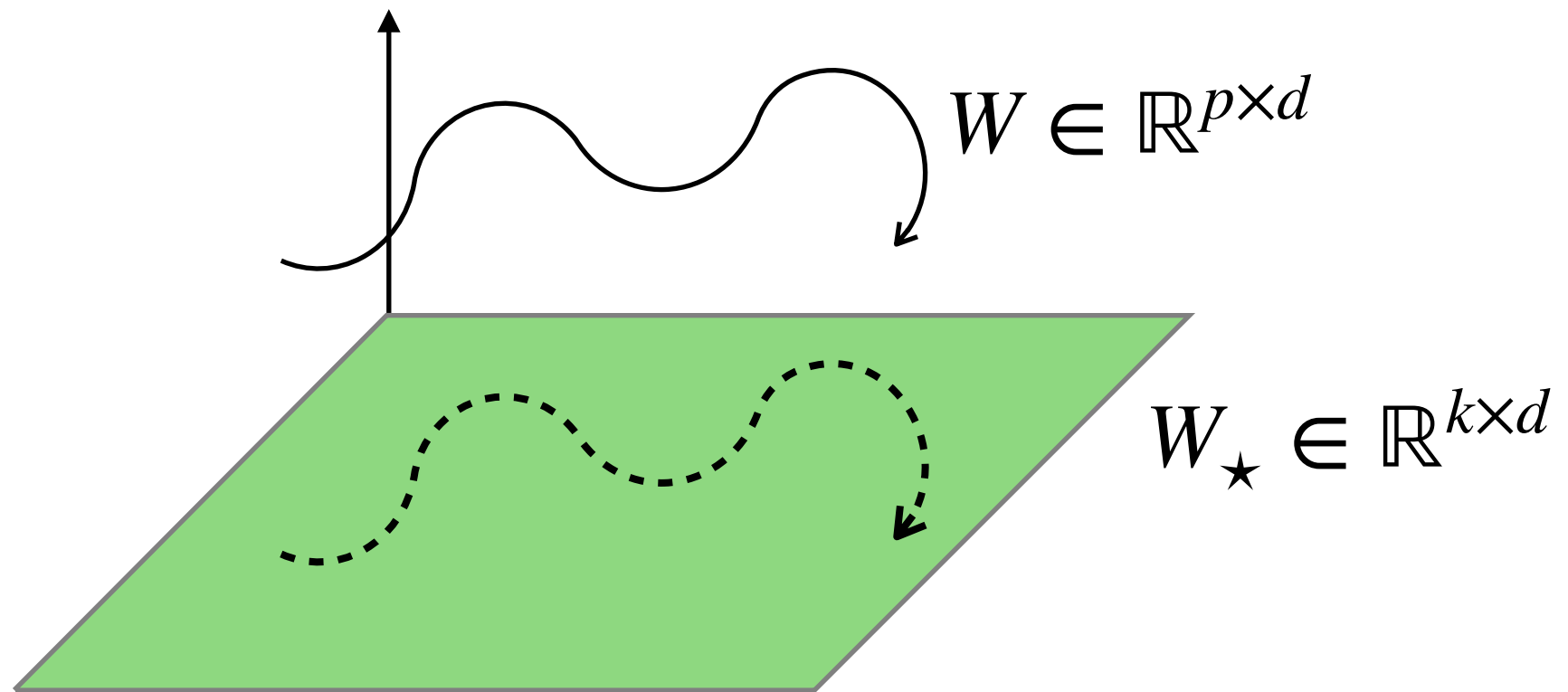


Mean-field regime



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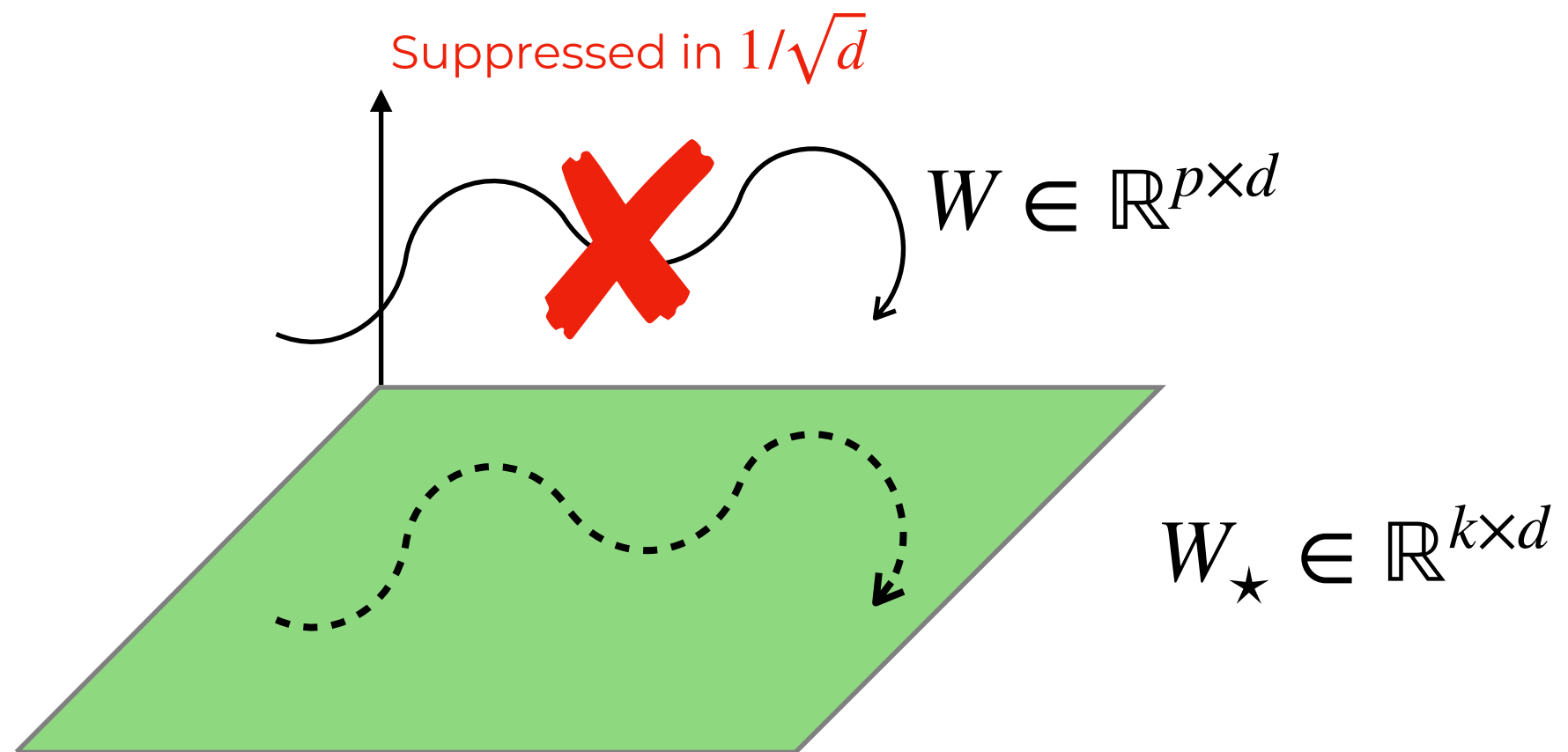
$$W = \underbrace{MP^{-1}W^\star}_{\text{Teacher subspace}} + W^\perp \longrightarrow Q \approx \underbrace{MPM^\top} + \underbrace{D_{\sqrt{q^\perp}} \Xi D_{\sqrt{q^\perp}}}_{\substack{\lambda \\ \mathbb{S}^{d-k-1}}}$$



Mean-field + high-d

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

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



Mean-field + high-d

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

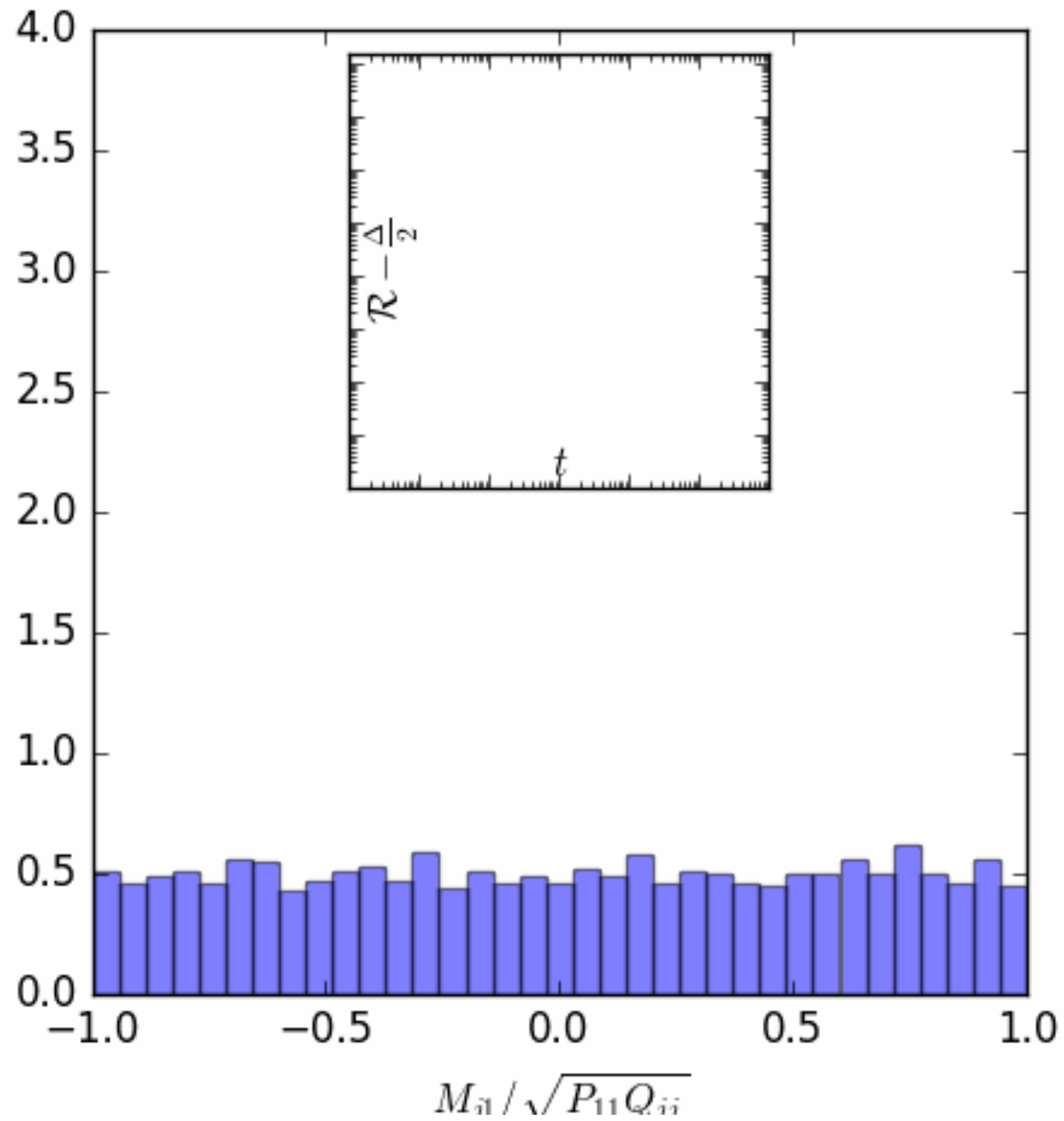
$$\mathbb{E} \left\| Q(t) - MP^{-1}M^\top + \text{diag}(Q^\perp) \right\|_\infty \leq e^{Ct} (p^{-1/2} + d^{-1/2})$$

This implies MF-like PDE for the sufficient statistics:

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

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

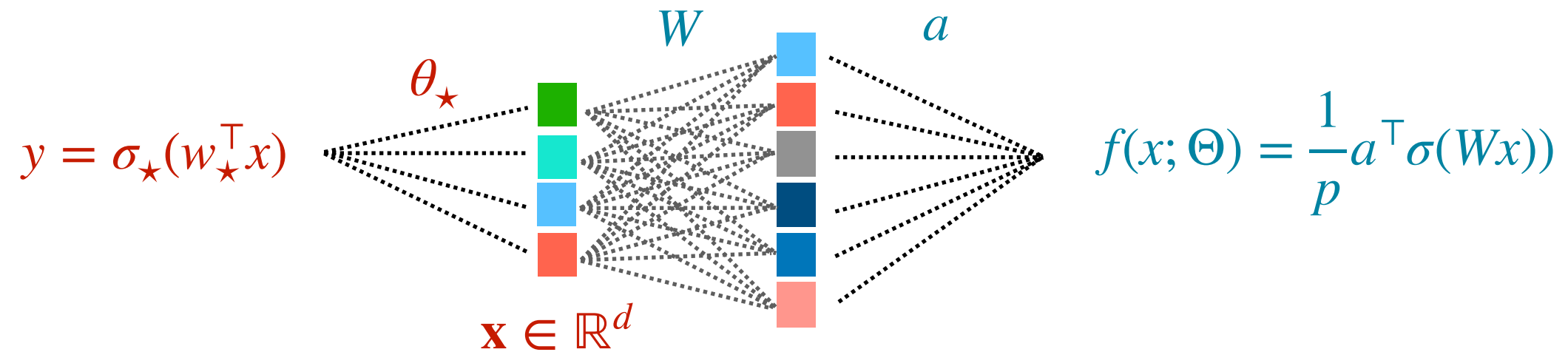
Mean-field and high-d



What can I do with that?

From [Berthier, Montanari & Zhou '23]

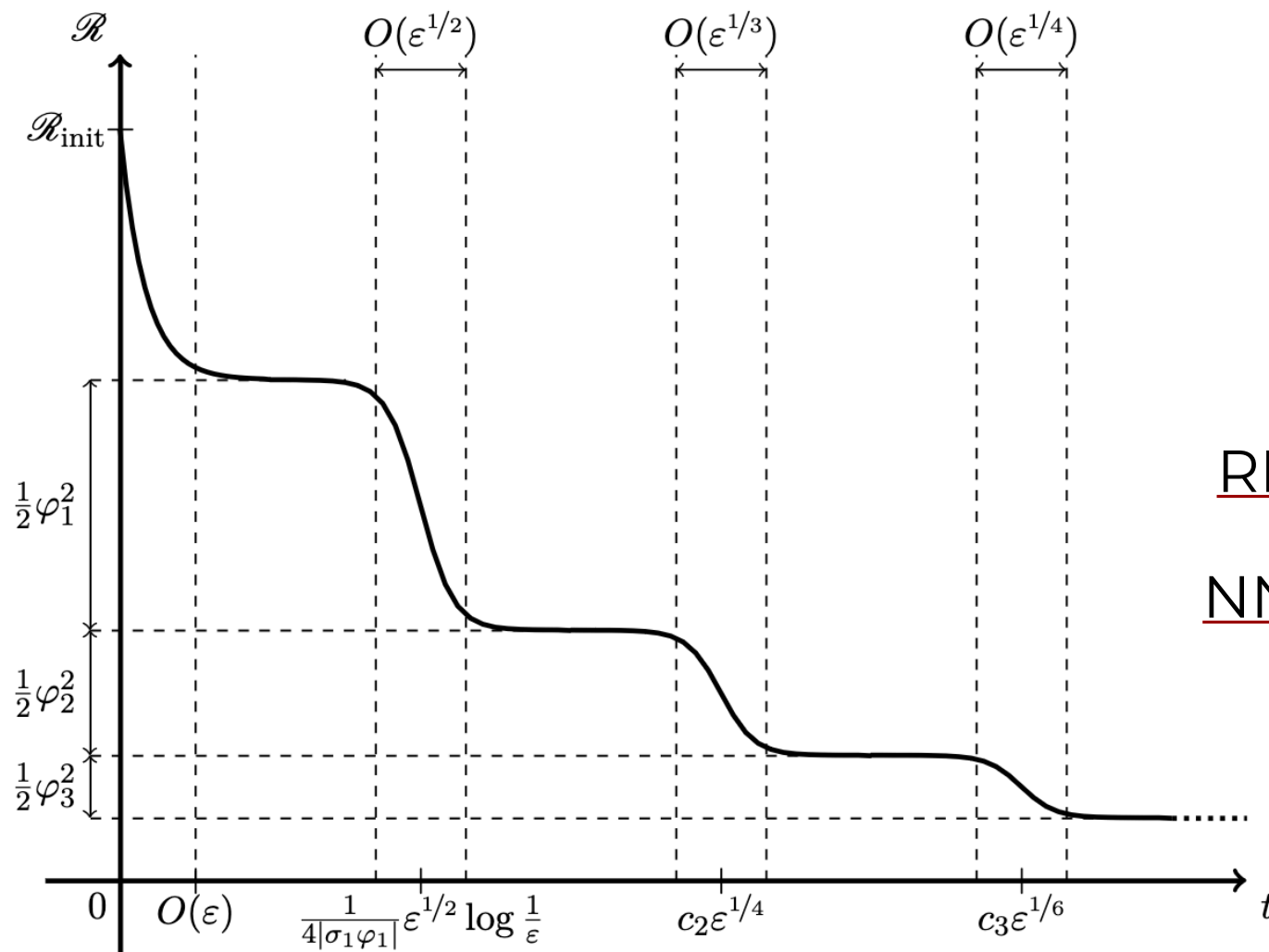
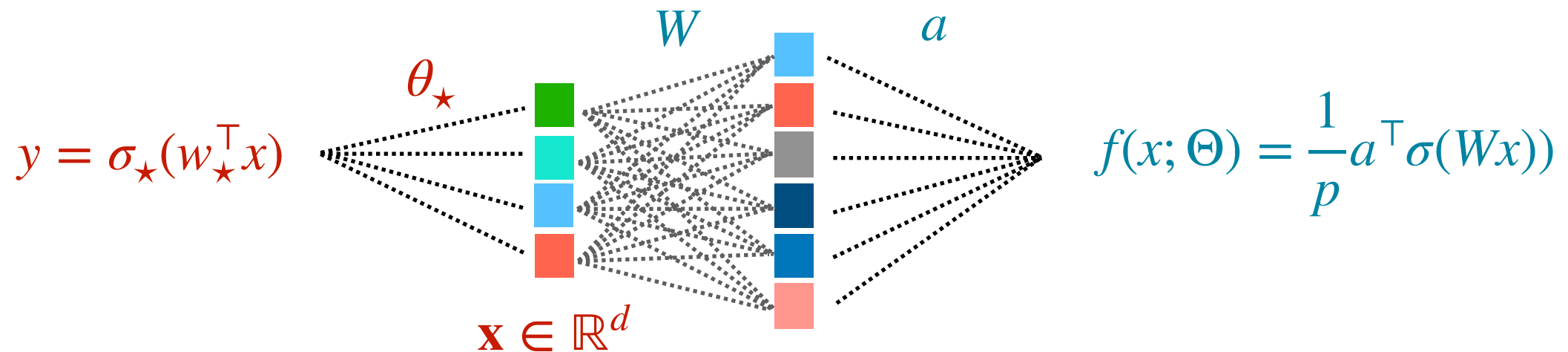
Consider simple case: $k = 1$ and $p \rightarrow \infty$



What can I do with that?

From [Berthier, Montanari & Zhou '23]

Consider simple case: $k = 1$ and $p \rightarrow \infty$



Recall: For $n \propto d$ and $x \sim \mathcal{N}(0, I_d)$

RF / Kernels: can only learn linear part

NNs: can learn non-linear components
if (σ_{\star}, σ) “standard”
(full Hermite expansion).

Follow-ups and challenges



Characterisation of the stochastic dynamics close to fixed points as a coloured diffusion

[Ben Arous, Gheissari, Jagannath NeurIPS '22]

Follow-ups and challenges



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Uniform control over the variance and convergence rates

Follow-ups and challenges



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Uniform control over the variance and convergence rates



Phenomenology of the dynamics:
Functions of increasing complexity?
Distributions of increasing complexity?

[Abbe, Adsera, Misiakiewicz, COLT '22; Berthier, Montanari '23]

[Refinetti, Ingrosso, Goldt, arXiv '22]

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Role of initialisation

Lecture III: Summary



Deterministic analysis of two-layer neural nets
in the “rich” regime

Lecture III: Summary



Deterministic analysis of two-layer neural nets
in the “rich” regime



Phenomenology in the classical
and high-dimensional regime

Lecture III: Summary

- ✓ Deterministic analysis of two-layer neural nets in the “rich” regime
- ✓ Phenomenology in the classical and high-dimensional regime
- ✓ Interplay between effective SGD noise and overparametrisation

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- ✓ Deterministic analysis of two-layer neural nets in the “rich” regime
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- ✓ Interplay between effective SGD noise and overparametrisation
- ✓ Dimension free limits in the mean-field regime

But this is only the tip of
an iceberg...



brloureiro@gmail.com