MACHINE LEARNING FOR LATTICE FIELD THEORY AND BEYOND — TRENTO 30/06/2023

STATISTICAL MECHANICS OF DEEP LEARNING BEYOND THE INFINITE-WIDTH LIMIT

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DI PARMA

[arXiv:2209.04882 (2022)]

OUTLINE OF THE TALK

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- Overparametrised DNNs / generalisation / Stat. phys. approaches

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  - ② Statistical mechanics of deep linear networks

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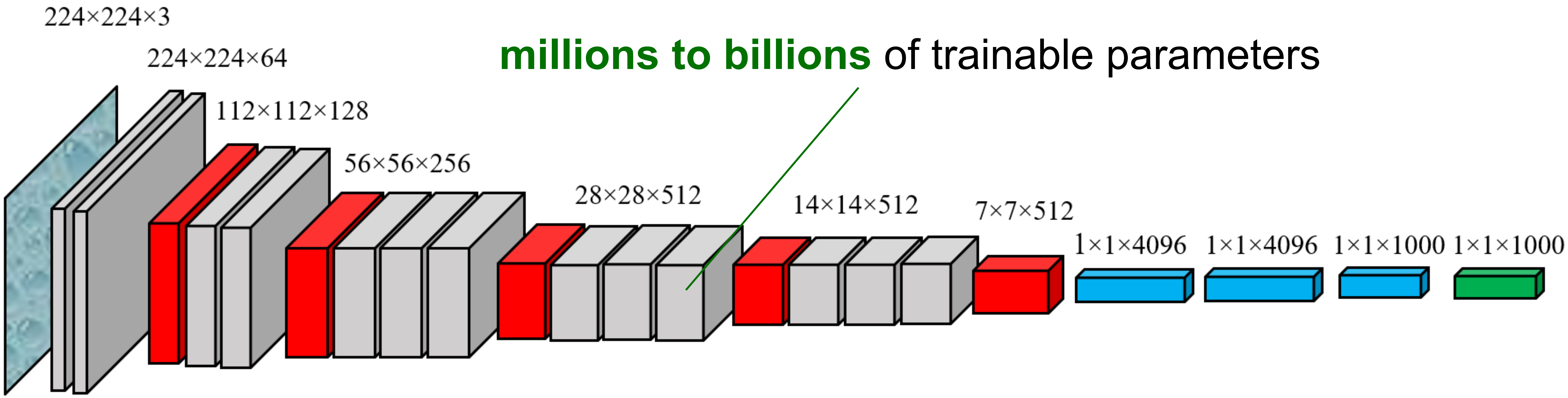
- Two important ideas for this work:

    ① Infinite-width limit

    ② Statistical mechanics of deep linear networks

- Results: an analytical framework to investigate the partition function of DNNs at “finite width”

OVERPARAMETRISATION IN DEEP NETS: A BLESS FOR PRACTITIONERS, A PROBLEM FOR THEORISTS



millions to billions of trainable parameters

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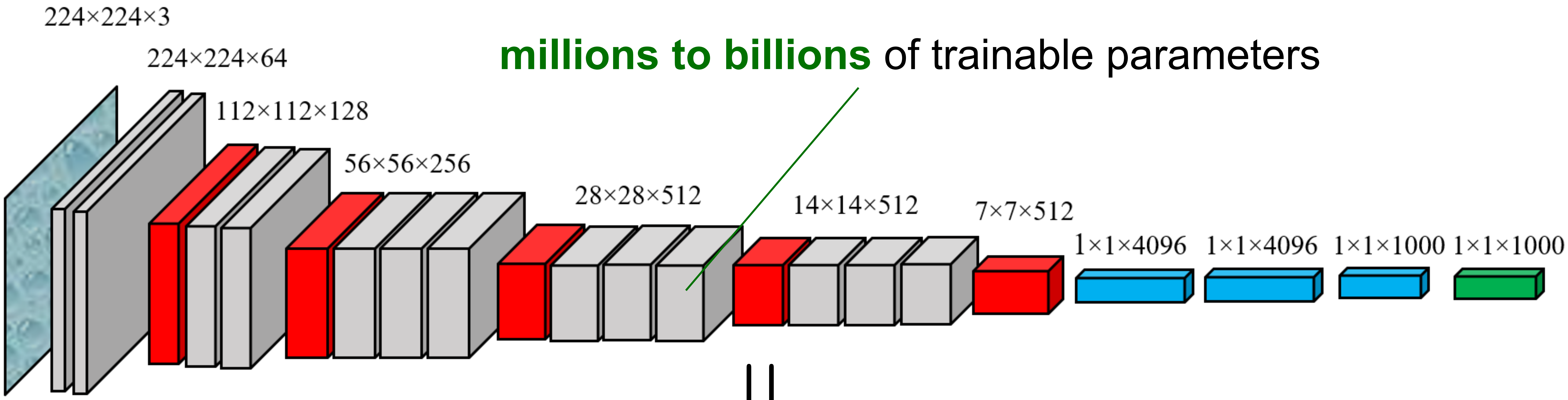

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$$f_{\mathrm{DNN}}(\mathbf{x}) = v \circ \sigma \circ W^{(L)} \circ \sigma \circ W^{(L-1)} \circ \cdots \circ \sigma \circ W^{(1)}(\mathbf{x})$$

non-linear activation function

affine transformation

$$f : \mathbb{R}^N \to \mathbb{R}$$

N is typically large

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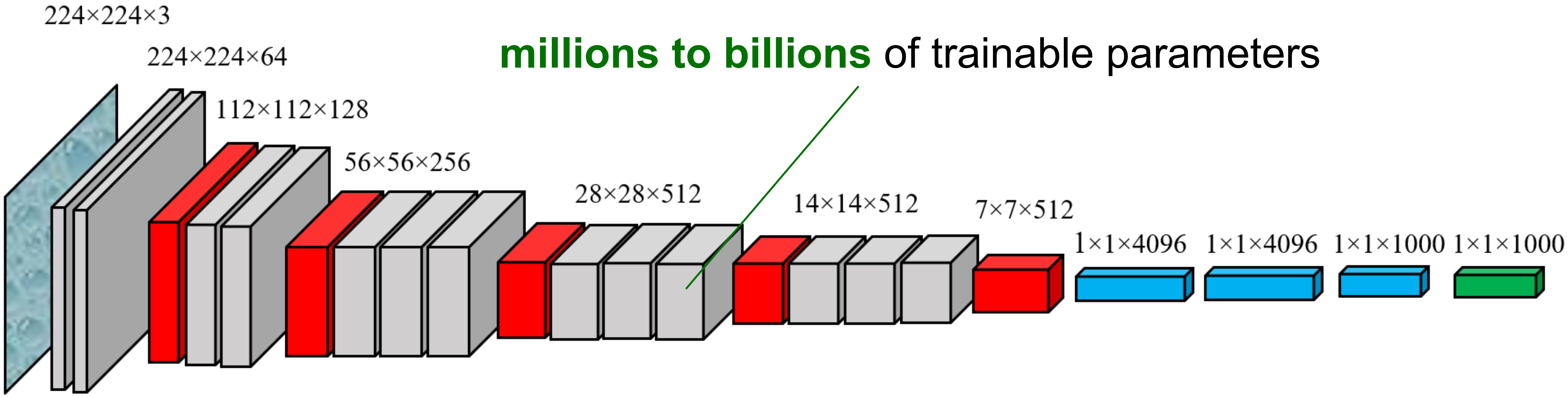


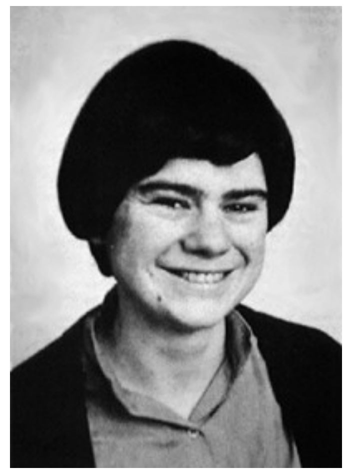
millions to billions of trainable parameters

overparametrised regime

number of trainable parameters $\gg$ **size of the training set**

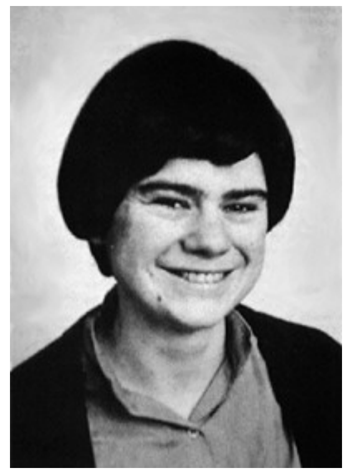
$L \times N^2$ P

STATISTICAL MECHANICS APPROACHES ARE LIMITED TO VERY SIMPLE ARCHITECTURES (FOR THE MOMENT)



E. Gardner

H. Sompolinsky



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what we would like to investigate

Deep neural networks
(fully-connected and/or convolutional)

vs

what we know how to investigate

Linear model (perceptron)
Random feature model
Kernel learning (SVMs)
Committee machine

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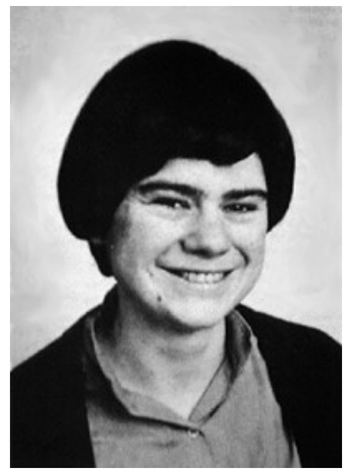

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$$\mathcal{T} = \{(\mathbf{x}^\mu, y^\mu)\}_{\mu=1}^P \text{———} P(\mathbf{x}, y)$$

input-output probability distribution

training set

$$Z = \int \mathcal{D}\theta \, e^{-\beta \sum_{\mu=1}^P \ell(y^\mu, f_\theta(\mathbf{x}^\mu))}$$

partition function

$$\langle \log Z \rangle = \lim_{n \to 0} \frac{\langle Z^n \rangle - 1}{n}$$

replica trick

WHAT DO WE KNOW? (1) THE INFINITE-WIDTH LIMIT OF DEEP NEURAL NETWORKS

[R. M. Neal, “Bayesian Learning for Neural Networks”, Springer (1996)]
[J. Lee et al., ICLR (2018)] [A. Jacot, F. Gabriel, C. Hongler, NeurIPS (2018)]

$$\boxed{N_\ell \gg P \quad \forall\, \ell = 1, \ldots, L}$$

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- Infinite-width deep neural networks are equivalent to Gaussian processes

$$K_\ell(\mathbf{x}_1, \mathbf{x}_2) = \int dz_1 dz_2\, \mathcal{N}\left(\begin{bmatrix} z_1 \\ z_2 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} K_{\ell-1}(\mathbf{x}_1, \mathbf{x}_1) & K_{\ell-1}(\mathbf{x}_1, \mathbf{x}_2) \\ K_{\ell-1}(\mathbf{x}_2, \mathbf{x}_1) & K_{\ell-1}(\mathbf{x}_2, \mathbf{x}_2) \end{bmatrix} \right) \sigma(z_1)\sigma(z_2) \qquad K_0(\mathbf{x}_1, \mathbf{x}_2) = \frac{\mathbf{x}_1 \cdot \mathbf{x}_2}{N_0}$$

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Bayesian vs Gradient Descent:
NNGP vs NTK!!

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- Data-averaged partition functions can be studied in this limit

[A. Canatar, B. Bordelon, C. Pehlevan, Nat. Comm. (2020)]
[R. Dietrich, M. Opper, H. Sompolinsky, PRL (1999)]

WHAT DO WE KNOW? (2) STATISTICAL MECHANICS OF DEEP LINEAR NETWORKS

[Q. Li & H. Sompolinsky, PRX (2021)] [A. Saxe, J. McClelland, S. Ganguli, ICLR (2014)]

$$f_{\mathrm{DLN}}(\mathbf{x}) = v \circ \xcancel{\sigma} \circ W^{(L)} \circ \xcancel{\sigma} \circ W^{(L-1)} \circ \cdots \circ \xcancel{\sigma} \circ W^{(1)}(\mathbf{x})$$

$$Z = \int \mathcal{D}\theta \, e^{-\beta \sum_{\mu=1}^{P} \ell(y^\mu, f_\theta(\mathbf{x}^\mu))}$$

$$\ell(y^\mu, f_\theta(\mathbf{x}^\mu)) = (y^\mu - f_\theta(\mathbf{x}^\mu))^2$$

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- **IDEA: integrate the weights backwards, starting from the output layer!**

(Backpropagating kernel renormalisation)

$$u_\ell \qquad \ell = 1, \ldots, L \qquad\qquad P\,, N_\ell \to \infty \qquad \alpha_\ell = \frac{P}{N_\ell}$$

determined self-consistently

Thermodynamic limit

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average generalisation error over a new unseen example

isotropic limit

$$\alpha_\ell = \alpha = \frac{P}{N}$$

linear kernel

$$(K_0)_{\mu\nu} = \frac{\mathbf{x}^\mu \cdot \mathbf{x}^\nu}{N_0}$$

$$\langle \epsilon_{\mathrm{g}}(\mathbf{x}^0, y^0) \rangle = \left[y^0 - \sum_{\mu\nu} \kappa_\mu(\mathbf{x}^0)(K_0^{-1})_{\mu\nu}\, y_\nu, \right]^2 + u_0^L \left[\kappa_0(\mathbf{x}^0) - \sum_{\mu\nu} \kappa_\mu(\mathbf{x}^0)(K_0^{-1})_{\mu\nu}\, \kappa_\nu(\mathbf{x}^0) \right]$$

$$r_0 = \frac{\sigma^{2L}}{P} y^T K_0^{-1} y$$

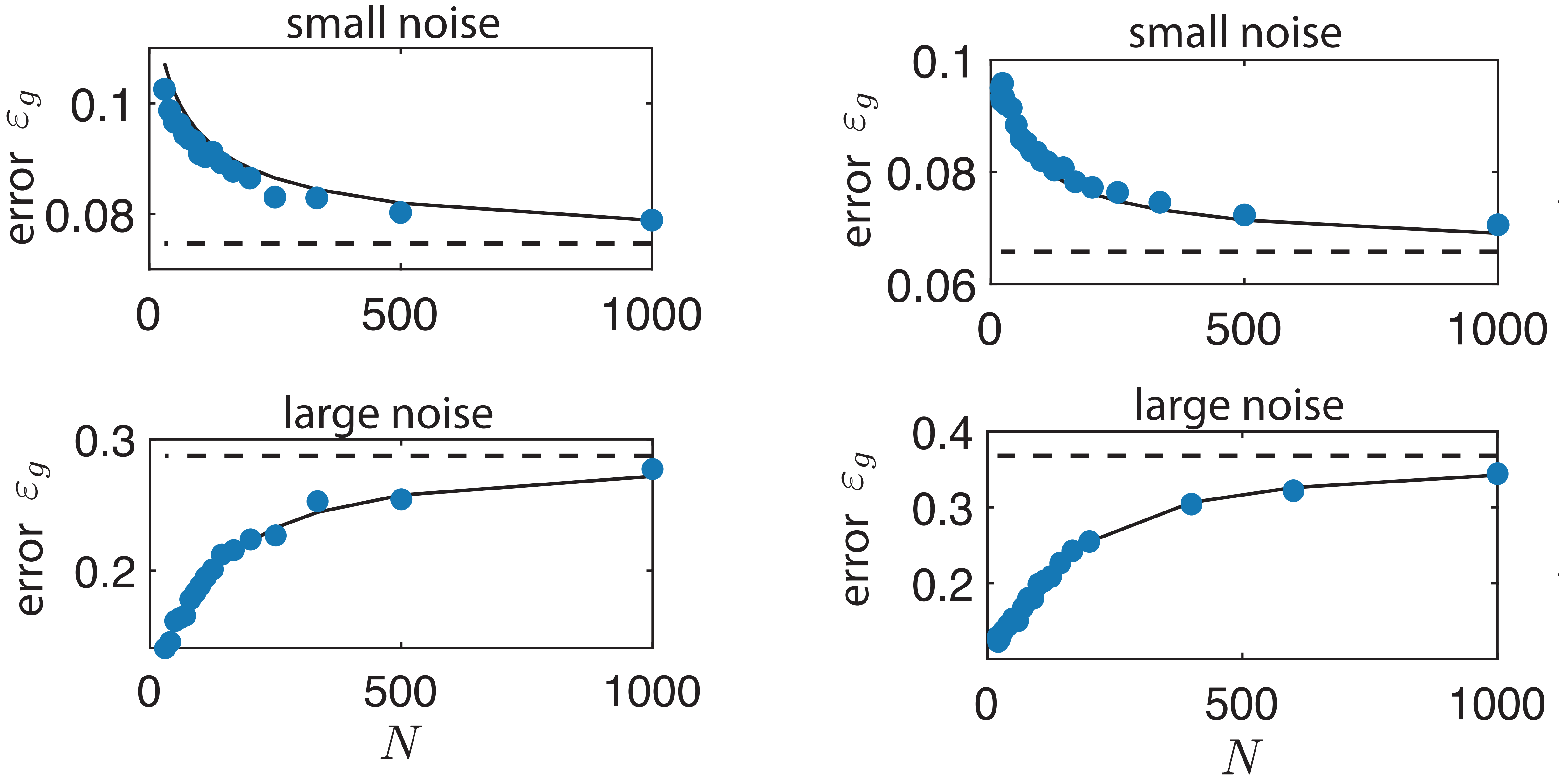
$$1 - \frac{u_0}{\sigma^2} = \alpha \left(1 - \frac{r_0}{u_0^L} \right)$$

WHAT DO WE KNOW? (3) AN HEURISTIC THEORY FOR RELU ACTIVATION

[Q. Li & H. Sompolinsky, PRX (2021)]

- **IDEA! Replace the linear kernel with the nonlinear kernel for ReLU activation**

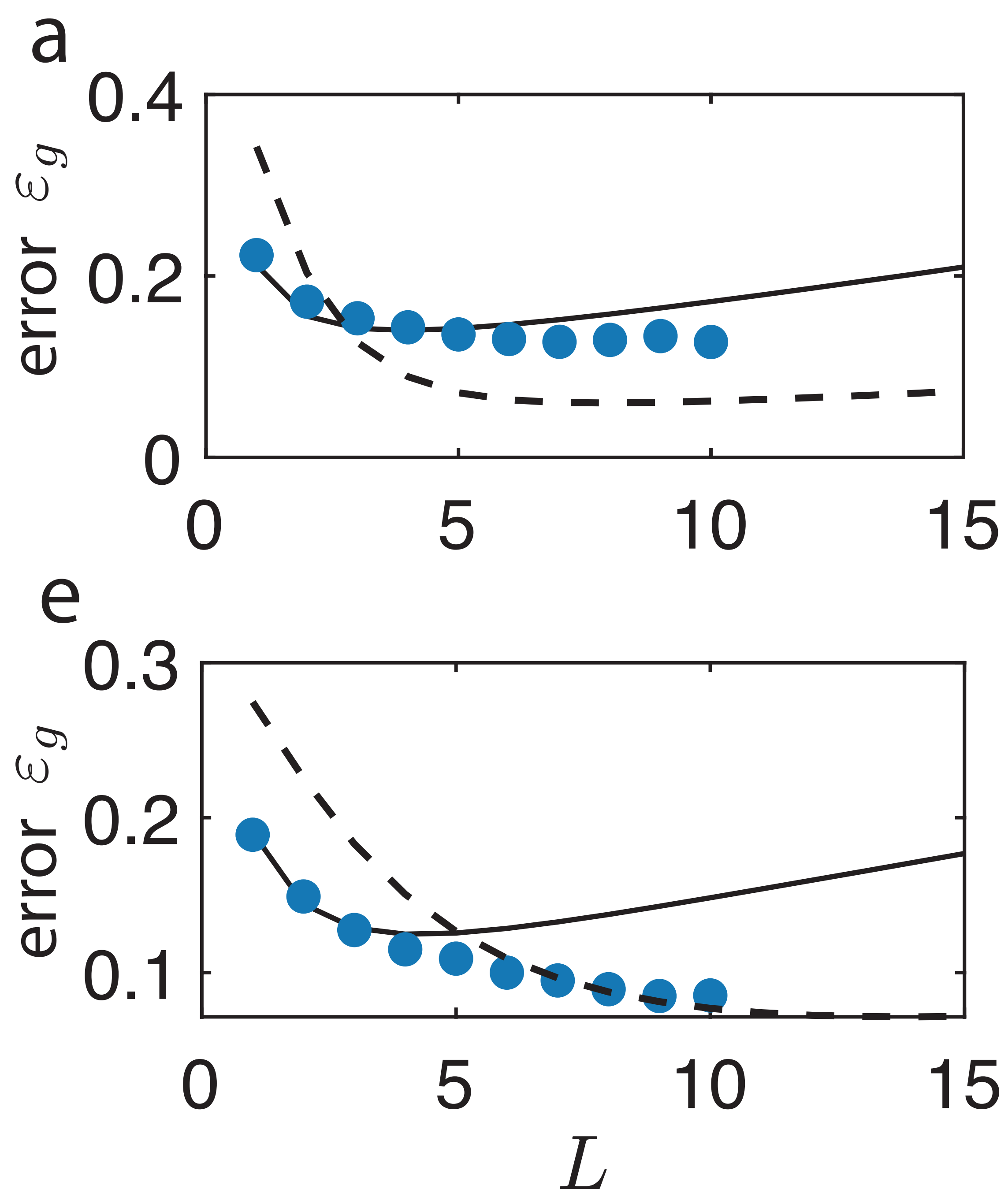
1-hidden layer (ReLU)



binary classification MNIST

noisy linear teacher

L-hidden layer (ReLU)



MAIN GOAL: developing an analytical framework based on statistical mechanics to describe deep learning beyond the infinite-width limit

① $P\,, N_\ell \to \infty \qquad \alpha_\ell = \dfrac{P}{N_\ell} \qquad \ell = 1, \dots, L$ (Thermodynamic limit)

② Fixed instance of the training set $\mathcal{T} = \{(\mathbf{x}^\mu, y^\mu)\}_{\mu=1}^{P}$

SETTING OF THE LEARNING PROBLEM

- $$h^{(\ell)}_{i_\ell} = \frac{1}{\sqrt{N_{\ell-1}}} \sum_{i_{\ell-1}=1}^{N_{\ell-1}} W^{(\ell)}_{i_\ell i_{\ell-1}} \, \sigma\left(h^{(\ell-1)}_{i_{\ell-1}}\right) + b^{(\ell)}_{i_\ell} \,,$$

  pre-activations at each layer

  $$h^{(1)}_{i_1} = \frac{1}{\sqrt{N_0}} \sum_{i_0=1}^{N_0} W^{(1)}_{i_1 i_0} x_{i_0} + b^{(1)}_{i_1}$$

  $$f_{\mathrm{DNN}}(\mathbf{x}) = \frac{1}{\sqrt{N_L}} \sum_{i_L=1}^{N_L} v_{i_L} \sigma\left[h^{(L)}_{i_L}(\mathbf{x})\right]$$

  readout layer

- $$\mathcal{L} = \frac{1}{2} \sum_{\mu=1}^{P} \left[y^\mu - f_{\mathrm{DNN}}(\mathbf{x}^\mu)\right]^2 + \mathcal{L}_{\mathrm{reg}} \,,$$

  $$\mathcal{L}_{\mathrm{reg}} = \frac{\lambda_L}{2\beta} \sum_{i_L=1}^{N_L} v_{i_L}^2 + \frac{1}{2\beta} \sum_{\ell=0}^{L-1} \lambda^{(\ell)} \|W^{(\ell)}\|^2$$

regression problem
quadratic loss function

$$\mathcal{T} = \{(\mathbf{x}^\mu, y^\mu)\}_{\mu=1}^{P}$$

A BAYESIAN DESCRIPTION OF LEARNING (AKA EQUILIBRIUM STATISTICAL MECHANICS)

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$$\boxed{Z} = \int \mathcal{D}\theta \, e^{-\beta \mathcal{L}(\theta)}$$

linked to the posterior distribution of the weights after training

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Regularisation should be interpreted as a Gaussian prior over the weights

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Regularisation should be interpreted as a Gaussian prior over the weights

$$\langle O(\theta) \rangle = \frac{1}{Z} \int \mathcal{D}\theta \; O(\theta) e^{-\beta \mathcal{L}(\theta)}$$

average of a generic observable of the weights

$$\epsilon_{\mathrm{g}}(\mathbf{x}^0, y^0; \theta) = \left(y^0 - f_\theta(\mathbf{x}^0) \right)^2$$

generalisation error

PARTITION FUNCTION FOR ONE HIDDEN LAYER NN IN THE ASYMPTOTIC LIMIT (1)

$$Z = \int \prod_{i_1}^{N_1} dv_{i_1} \prod_{i_1, i_0}^{N_1, N_0} dw_{i_1 i_0} \, \exp\left\{ -\frac{\lambda_1}{2} \sum_{i_1}^{N_1} v_{i_1}^2 - \frac{\lambda_0}{2} \|w\|^2 - \frac{\beta}{2} \sum_{\mu}^{P} \left[y^\mu - \frac{1}{\sqrt{N_1}} \sum_{i_1}^{N_1} v_{i_1} \sigma \left(\sum_{i_0}^{N_0} \frac{w_{i_1, i_0} x_{i_0}^\mu}{\sqrt{N_0}} \right) \right]^2 \right\}$$

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- I want to integrate over the weights of the network (I cannot do it for free)

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- I want to integrate over the weights of the network (I cannot do it for free)
- I introduce all possible deltas over the pre-activations

$$1 = \int \prod_{\mu}^{P} \prod_{i_1}^{N_1} dh_{i_1}^\mu \, \delta\left(h_{i_1}^\mu - \frac{1}{\sqrt{N_0}} \sum_{i_0}^{N_0} w_{i_1 i_0} x_{i_0}^\mu \right)$$

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$$1 = \int \prod_{\mu}^{P} ds^\mu \,\delta\left[s^\mu - \frac{1}{\sqrt{N_1}}\sum_{i}^{N_1} v_{i_1}\sigma(h_{i_1}^\mu)\right]$$

Once I employ an integral representation of the deltas I realise all the integrals over the weights are Gaussian

PARTITION FUNCTION FOR ONE HIDDEN LAYER NN IN THE ASYMPTOTIC LIMIT (2): THE CRITICAL STEP

$$Z = \int \prod_{\mu}^{P} \frac{ds^\mu d\bar{s}^\mu}{2\pi} e^{-\frac{\beta}{2}\sum_\mu (y^\mu - s^\mu)^2 + i\sum_\mu^P s^\mu \bar{s}^\mu} \left\{ \int \frac{dq}{\sqrt{2\pi}} e^{-\frac{q^2}{2}} \int d^P h \, P_1(\{h^\mu\}) \delta\left[q - \frac{1}{\sqrt{\lambda_1 N_1}} \sum_\mu \bar{s}^\mu \sigma(h^\mu)\right] \right\}^{N_1}$$

$$P_1(\{h^\mu\}) = \mathcal{N}(0, C) \qquad C_{\mu\nu} = \frac{1}{\lambda_0 N_0} \sum_{i_0}^{N_0} x^\mu_{i_0} x^\nu_{i_0}$$

$$P(q) = \int d^P h \, P_1(\{h^\mu\}) \delta\left[q - \frac{1}{\sqrt{\lambda_1 N_1}} \sum_\mu \bar{s}^\mu \sigma(h^\mu)\right]$$

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This probability is Gaussian for the Breuer-Major Theorem (1983)!!

$$Q = \frac{1}{\lambda_1 N_1} \sum_{\mu\nu}^{P} \bar{s}^\mu K_{\mu\nu} \bar{s}^\nu$$

$$K_{\mu\nu}(C) = \int \frac{dt_1 dt_2}{\sqrt{(2\pi)^2 \det \tilde{C}}} e^{-\frac{1}{2}\mathbf{t}^T \tilde{C}^{-1} \mathbf{t}} \sigma(t_1)\sigma(t_2) \qquad \tilde{C} = \begin{pmatrix} C_{\mu\mu} & C_{\mu\nu} \\ C_{\mu\nu} & C_{\nu\nu} \end{pmatrix}$$

This is just the NNGP kernel that describes the infinite-width limit

PARTITION FUNCTION FOR ONE HIDDEN LAYER NN IN THE ASYMPTOTIC LIMIT (3): SADDLE-POINT ACTION

$$Z = \int dQ d\bar{Q} \, \exp\left[-\frac{N_1}{2} S(Q, \bar{Q}) \right]$$

The model is “solved”, in the sense that the partition function is now in a form suitable to saddle-point integration

$$S = -Q\bar{Q} + \log(1+Q) + \frac{\alpha_1}{P} \mathrm{Tr} \log \beta \left[\frac{\mathbb{I}_P}{\beta} + \frac{\bar{Q}K}{\lambda_1} \right] + \frac{\alpha_1}{P} y^\top \left[\frac{\mathbb{I}_P}{\beta} + \frac{\bar{Q}K}{\lambda_1} \right]^{-1} y$$

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explicit formula for the generalisation error

$$\left\langle \epsilon_{\mathrm{g}}(\mathbf{x}^0, y^0) \right\rangle = \left\langle \left(y^0 - f(\mathbf{x}^0)\right)^2 \right\rangle$$

$$= \left[y^0 - \frac{\bar{Q}}{\lambda_1}\sum_{\mu\nu}\kappa_\mu(\mathbf{x}^0)\left(\frac{\mathbb{I}_P}{\beta} + \frac{\bar{Q}K}{\lambda_1}\right)^{-1}_{\mu\nu} y_\nu\right]^2 + \frac{\bar{Q}}{\lambda_1}\left[\kappa_0(\mathbf{x}^0) - \frac{\bar{Q}}{\lambda_1}\sum_{\mu\nu}\kappa_\mu(\mathbf{x}^0)\left(\frac{\mathbb{I}_P}{\beta} + \frac{\bar{Q}K}{\lambda_1}\right)^{-1}_{\mu\nu}\kappa_\nu(\mathbf{x}^0)\right]$$

A CORRESPONDENCE BETWEEN FINITE-WIDTH ONE HIDDEN LAYER ARCHITECTURES AND STUDENT-T PROCESSES

$$p(\{\bar{s}^\mu\}) \sim \left(1 + \frac{1}{\lambda N_1} \sum_{\mu,\nu}^{P} \bar{s}^\mu K_{\mu\nu}(C) \bar{s}^\nu \right)^{-\frac{N_1}{2}} \sim e^{-\frac{1}{2\lambda} \sum_{\mu,\nu}^{P} \bar{s}^\mu K_{\mu\nu}(C) \bar{s}^\nu}$$

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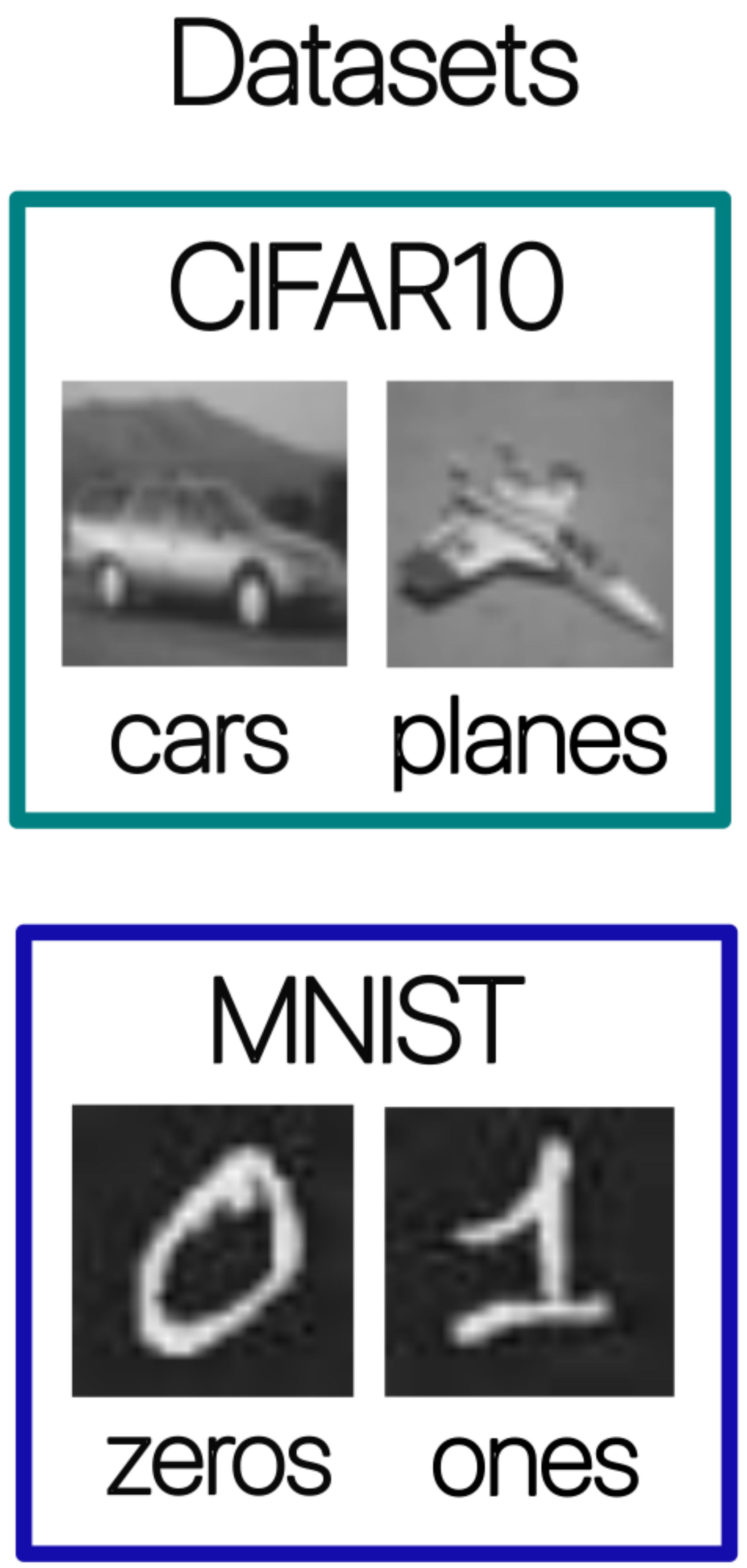
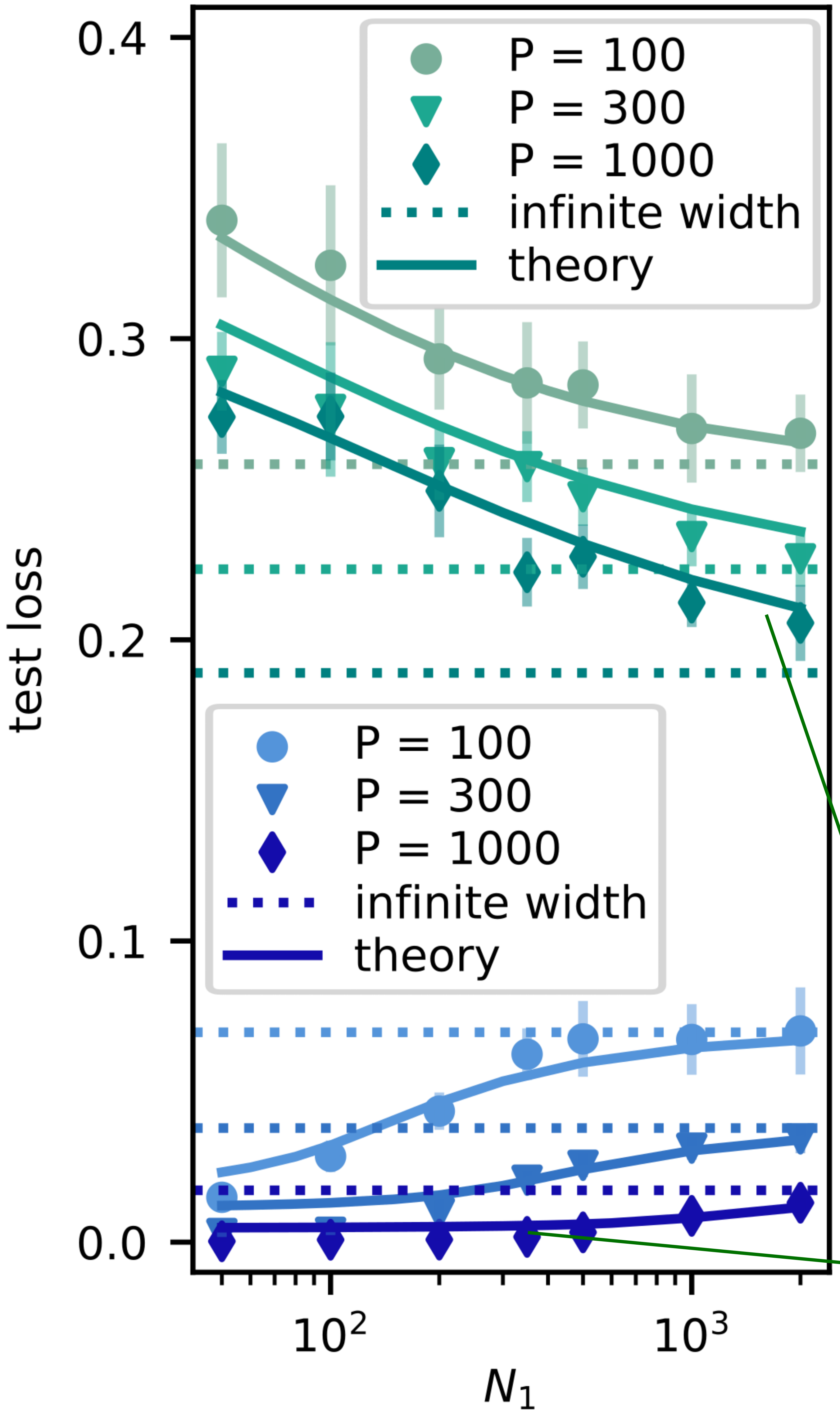
- **Finite-width one hidden layer neural networks are related to Student-t stochastic processes**
- **Finite-width deep linear networks are also related to Student-t processes!**

VERIFYING THE PREDICTIONS OF THE THEORY AT 1HL USING A DISCRETE LANGEVIN DYNAMICS (1)





Best test accuracy on the binary classification problem achieved: 86% (CIFAR), 99.9% (MNIST)

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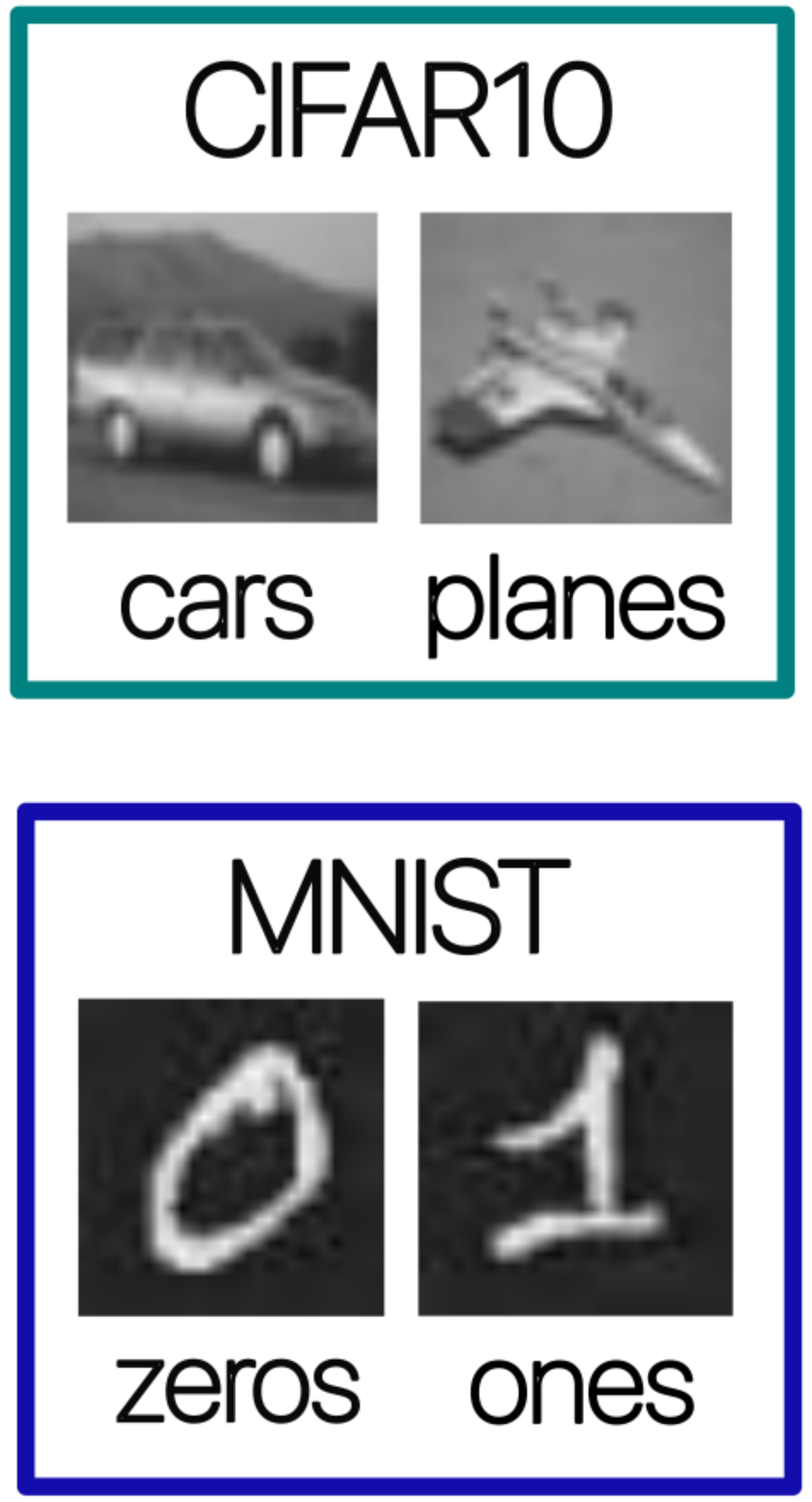
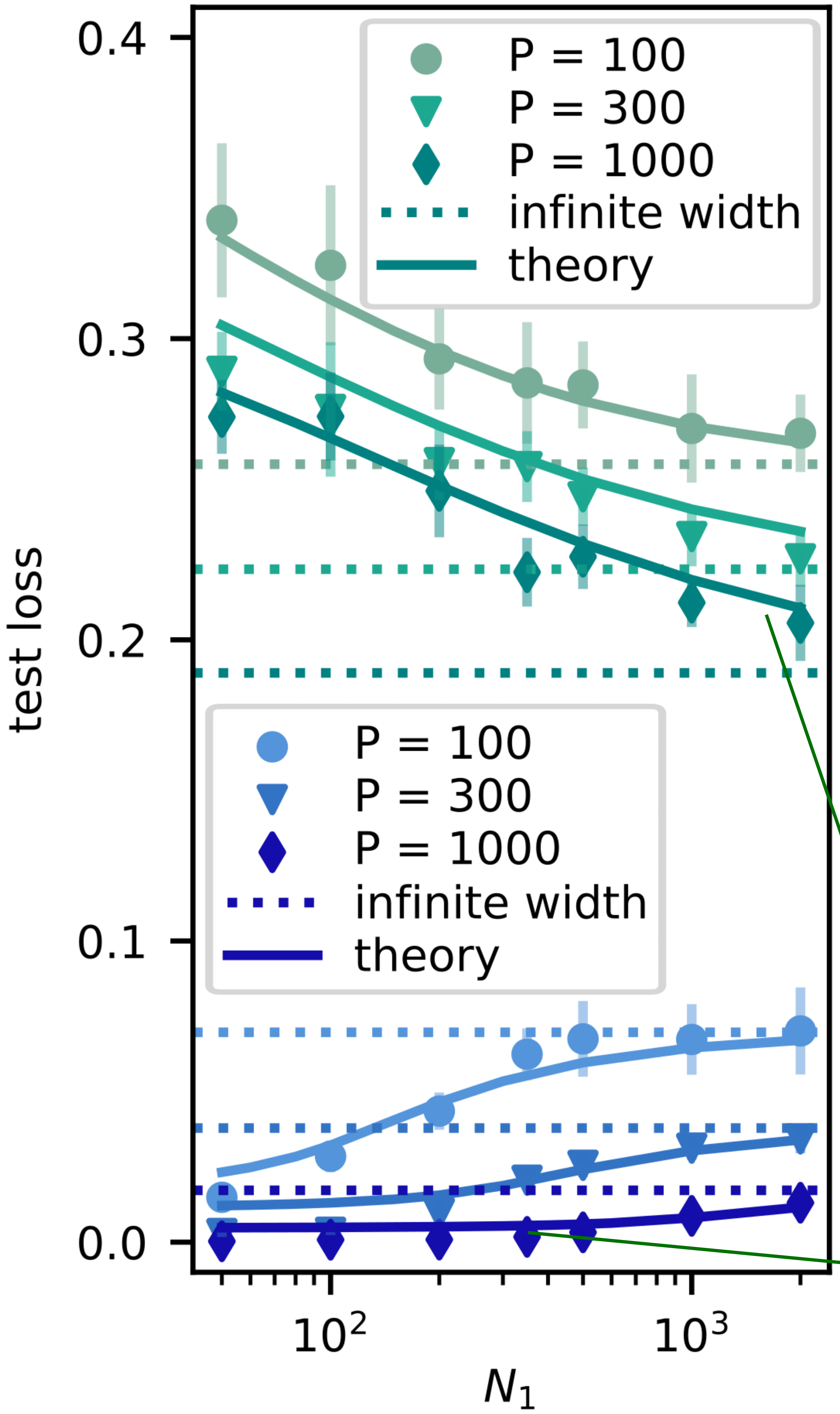
Datasets





Learning curves are **monotonically increasing/decreasing** in the range explored (smallest N = 50)

WHY?

analytical criterion

$$y^T K^{-1} y > P$$

ANOTHER CONNECTION WITH STUDENT-T! [Tracey & Wolpert (2018)]

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VERIFYING THE PREDICTIONS OF THE THEORY AT 1HL USING A DISCRETE LANGEVIN DYNAMICS (2)

Datasets

CIFAR10

cars planes

MNIST

zeros ones

General observations

(i) At T = 0 the bias in constant as a function of N_1 and of the Gaussian prior of the last layer λ_1

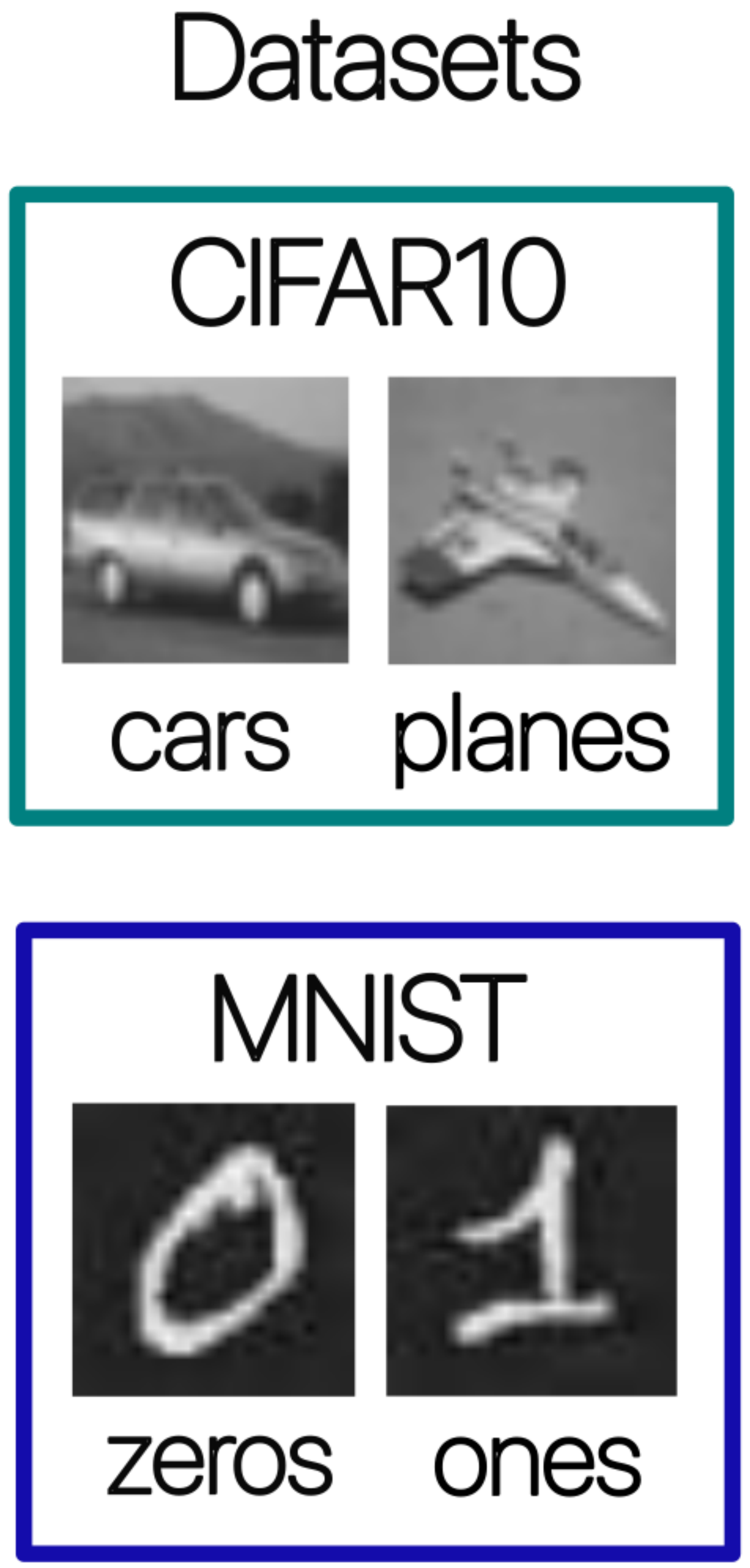
(ii) At T = 0 the variance depends on N_1 and goes to zero as $1/\sqrt{\lambda_1}$

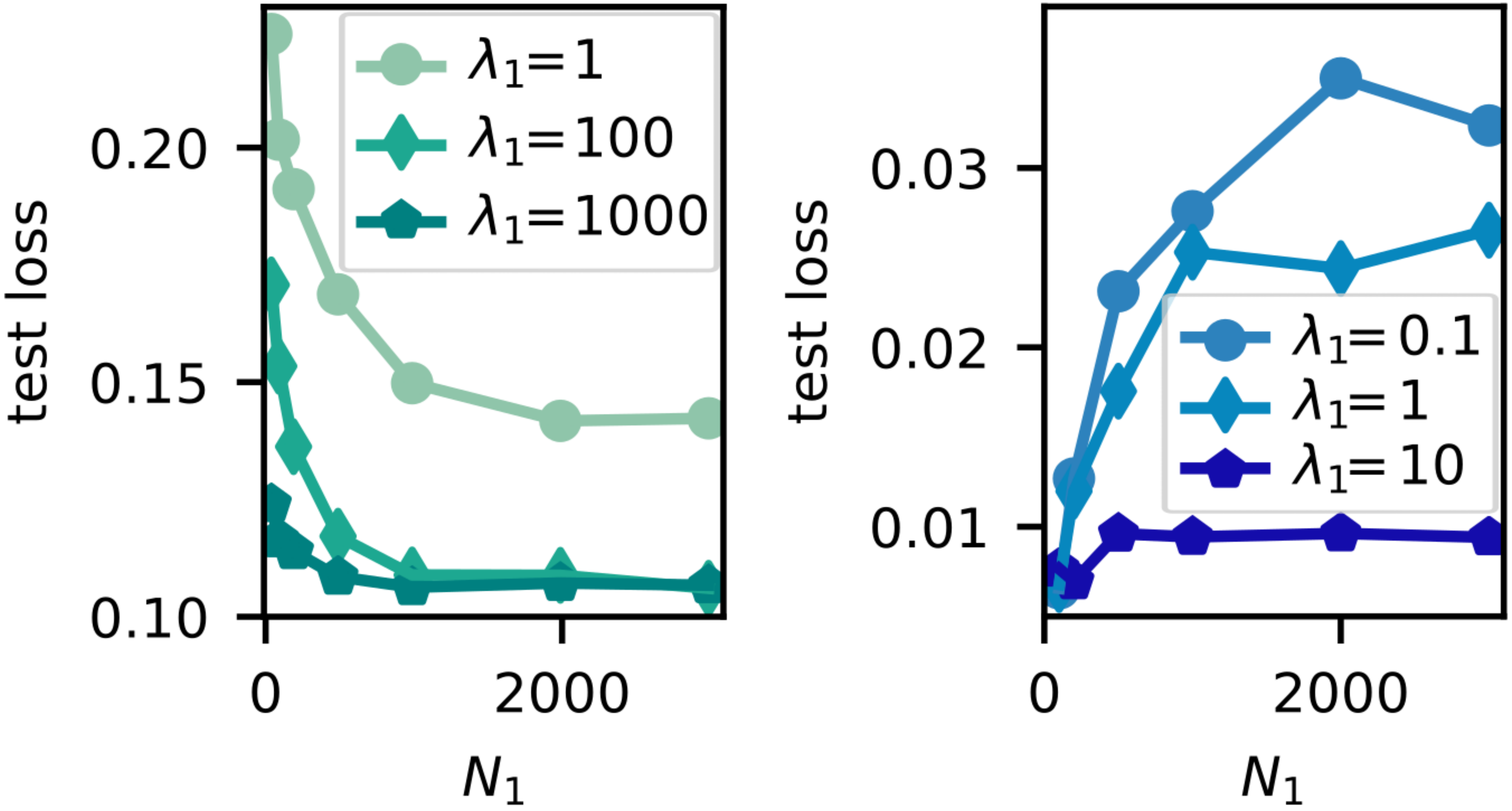
Physical consequences

(i) increasing the magnitude of the last layer Gaussian prior should lead to better generalisation at **ANY** N_1

(ii) For large values of λ_1 the dependence on the size of the hidden layer in the learning curve should disappear

VERIFYING THE PREDICTIONS OF THE THEORY AT 1HL USING A DISCRETE LANGEVIN DYNAMICS (2)





APPROXIMATE PARTITION FUNCTION FOR DNNS WITH ODD ACTIVATION FUNCTION: A RECURRENCE BASED ON STUDENT-T

$$P_{\ell-1}(\{\mathbf{h}^{\mu}_{\ell-1}\}) \longrightarrow P_{\ell}(\{\mathbf{h}^{\mu}_{\ell}\})$$

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$$Z_{\mathrm{DNN}} = \int \prod_{\ell=1}^{L} dQ_\ell d\bar{Q}_\ell e^{-\frac{N_L}{2} S_{\mathrm{DNN}}(\{Q_\ell, \bar{Q}_\ell\})}$$

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Effective action for finite-width fully-connected architectures with L hidden layers

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APPROXIMATE PARTITION FUNCTION FOR DEEP NEURAL NETWORKS: A RECURRENCE BASED ON STUDENT-T

IMPORTANT!

From this effective theory I am able to recover the Li-Sompolinsky heuristic theory valid for ReLU activation found in the isotropic limit

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GENERALISING THE APPROACH TO NON-ODD ACTIVATION FUNCTION: BEYOND LI-SOMPOLINSKY HEURISTIC THEORY

Let us go back to the derivation of the one hidden layer effective action…

$$P(q) = \int d^P h \, P_1(\{h^\mu\}) \delta\left[q - \frac{1}{\sqrt{\lambda N_1}} \sum_\mu \bar{s}^\mu \sigma\left(h^\mu\right) \right] \to \mathcal{N}(0, Q)$$

This random variable has zero mean **ONLY** if the activation function is odd

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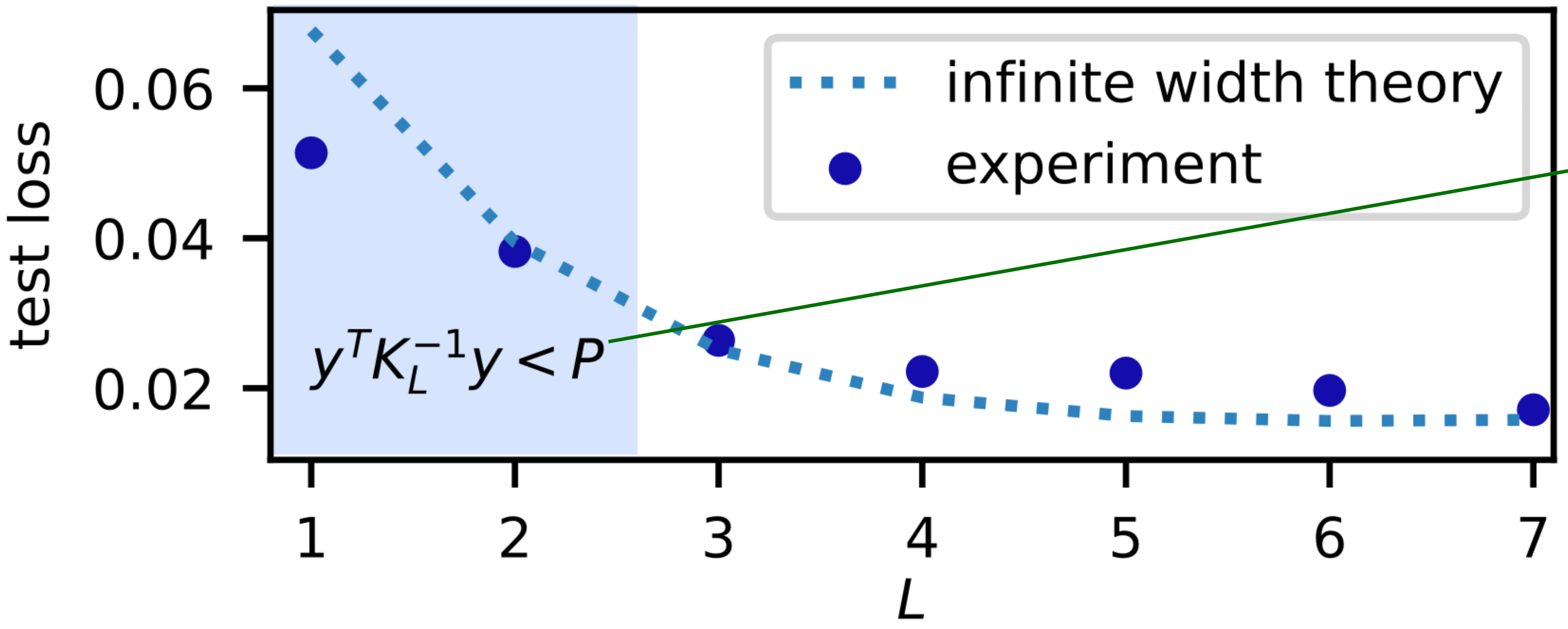
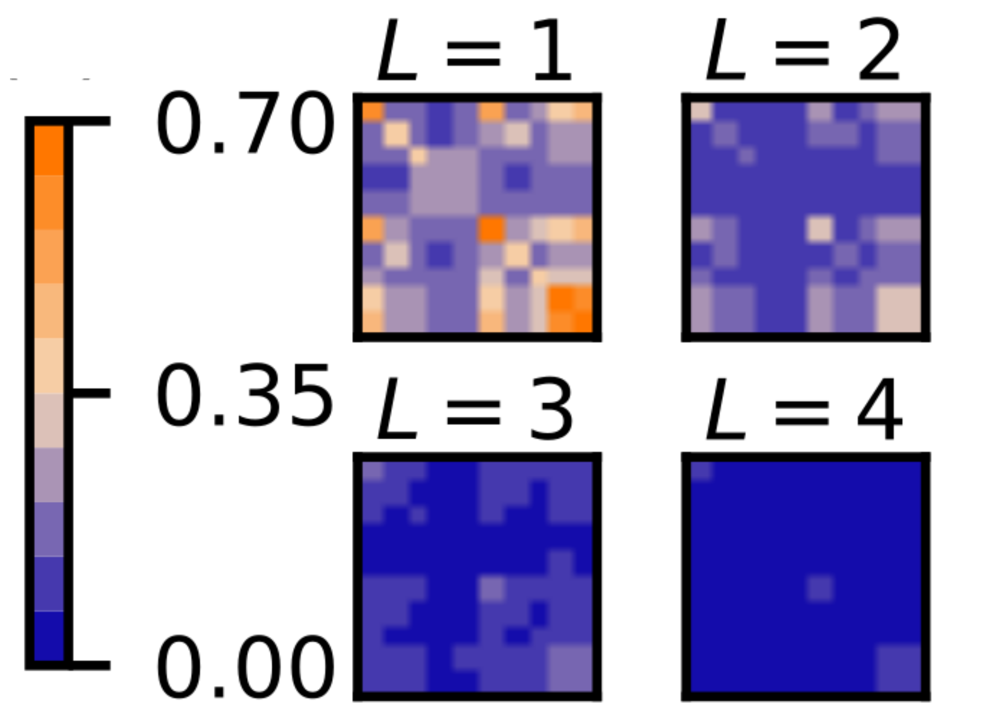
$$\boxed{\bar{Q}K \to \bar{Q}K - \left(\bar{Q} + \frac{1}{1+Q}\right)K^{(1)} \qquad K^{(1)}_{\mu\nu} = m^\mu m^\nu}$$

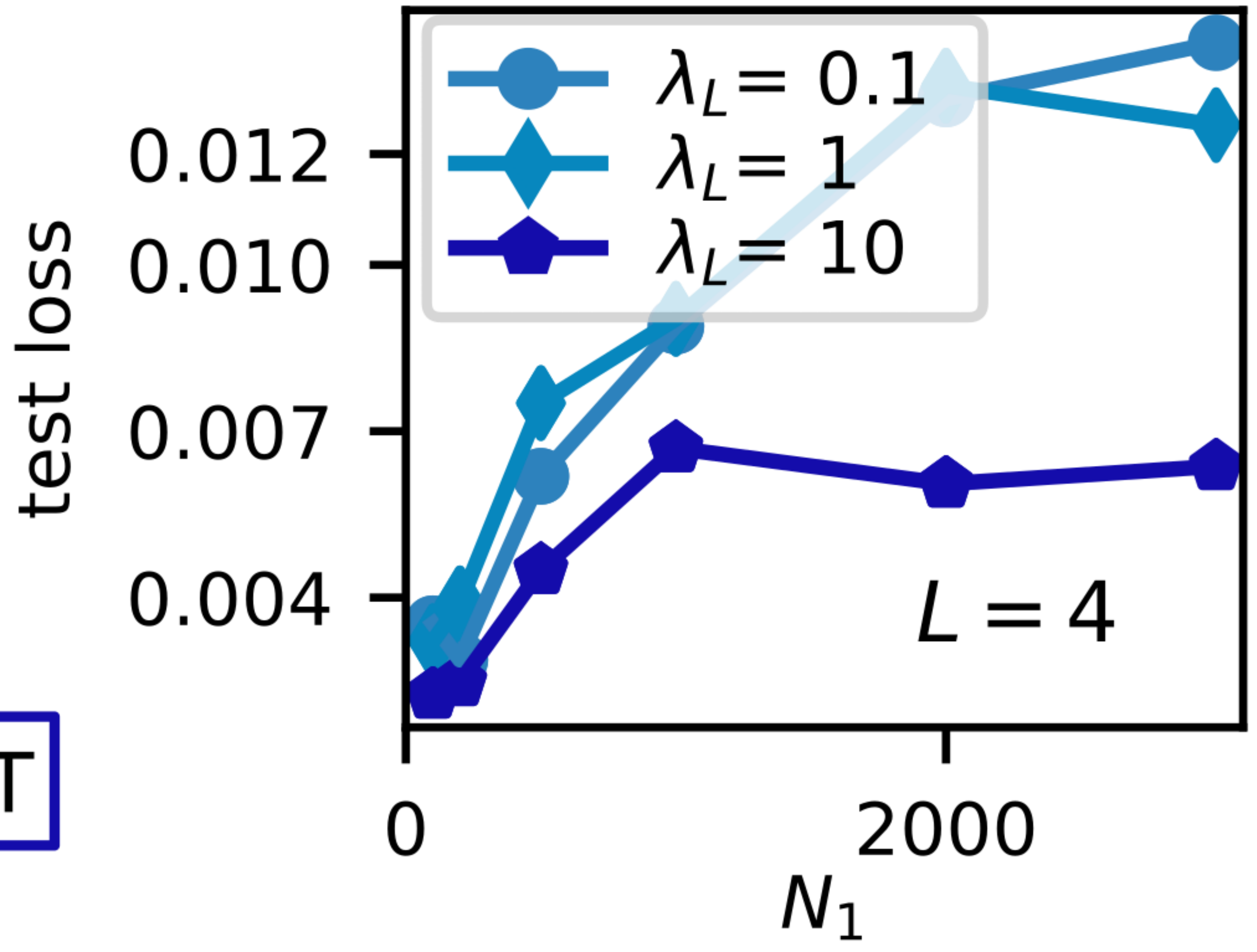
PRELIMINARY VERIFICATION OF THE THEORY AT L LAYERS



a criterion to establish if finite-width networks will outperform their infinite-width counterpart holds for ReLU



MNIST



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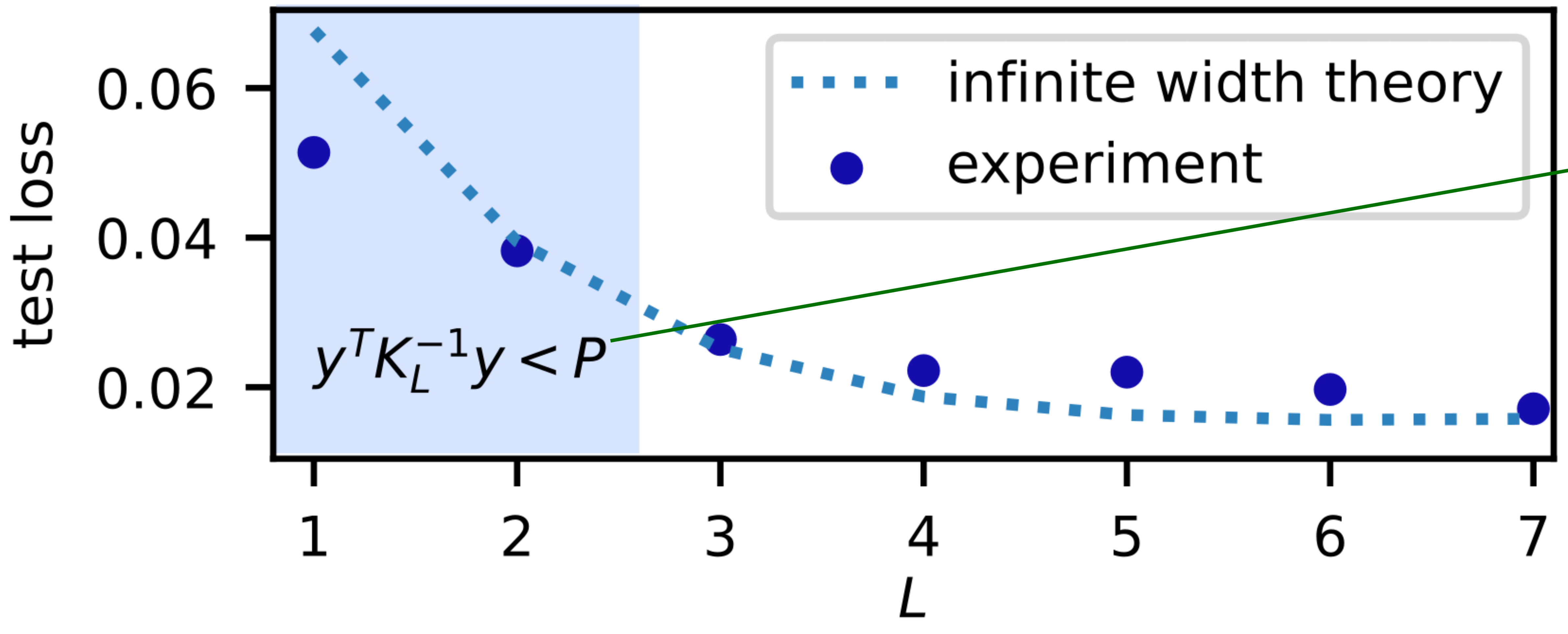

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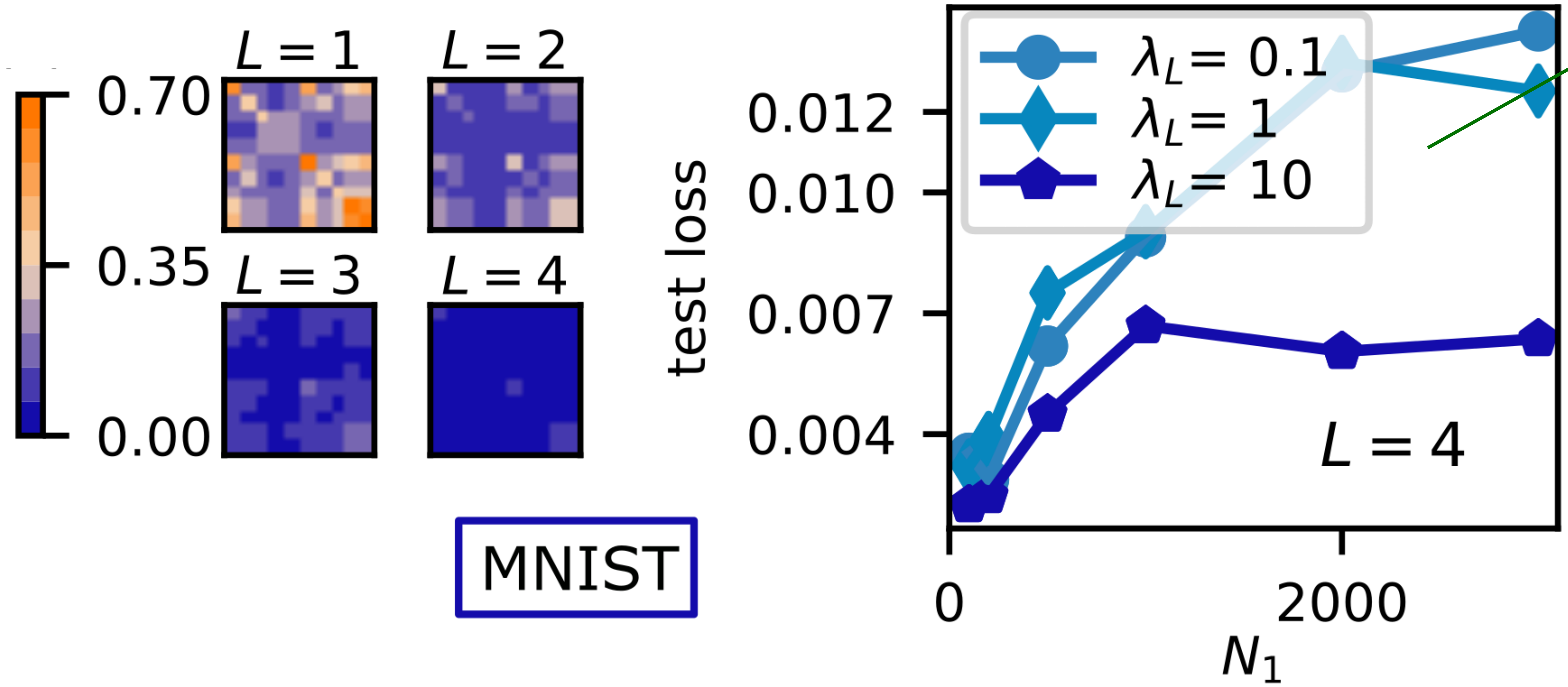

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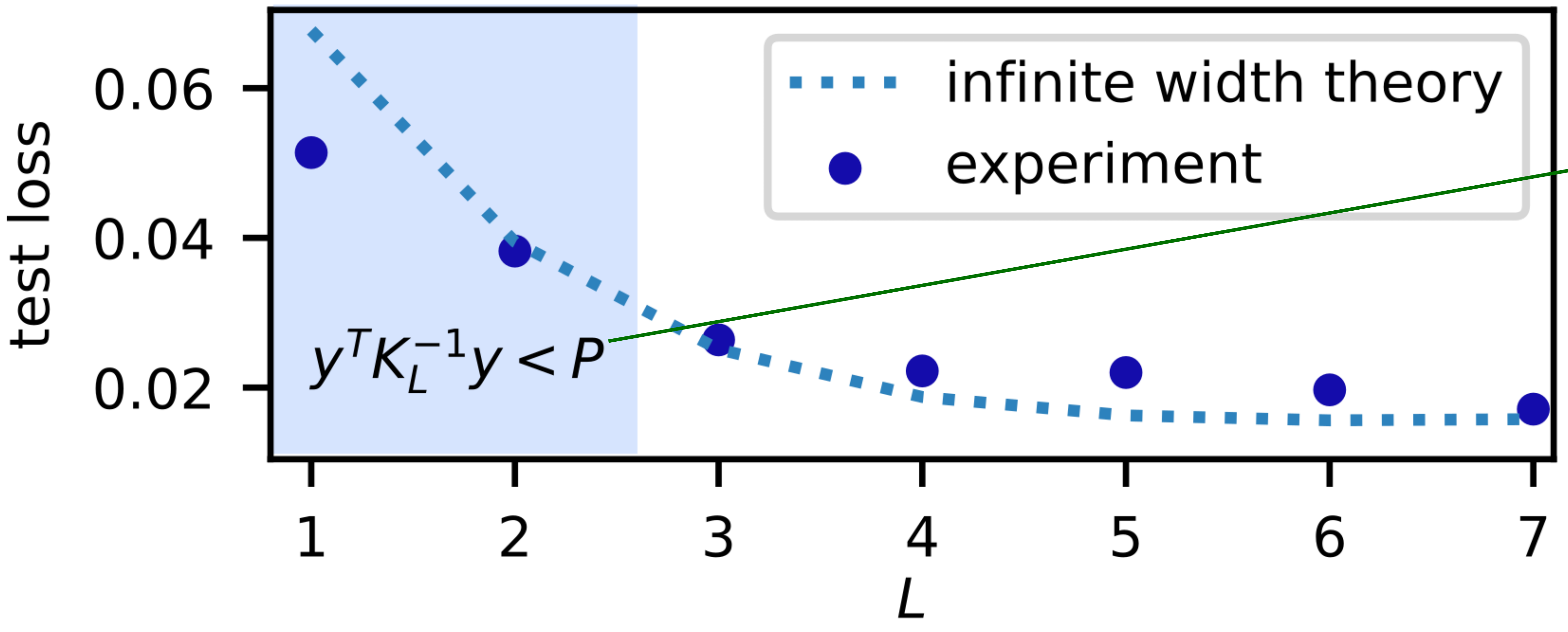

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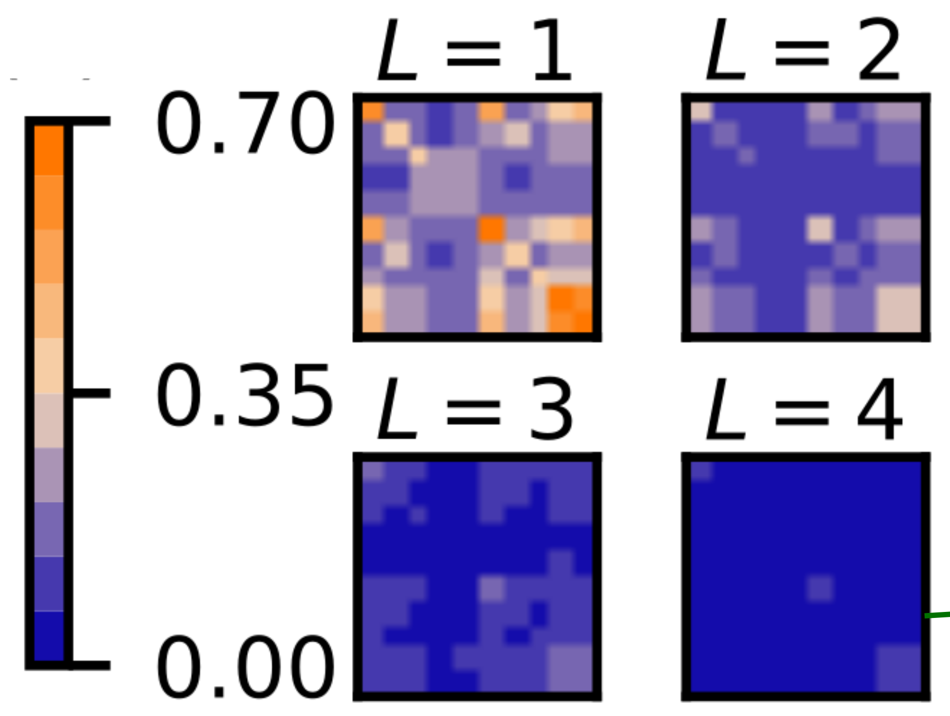

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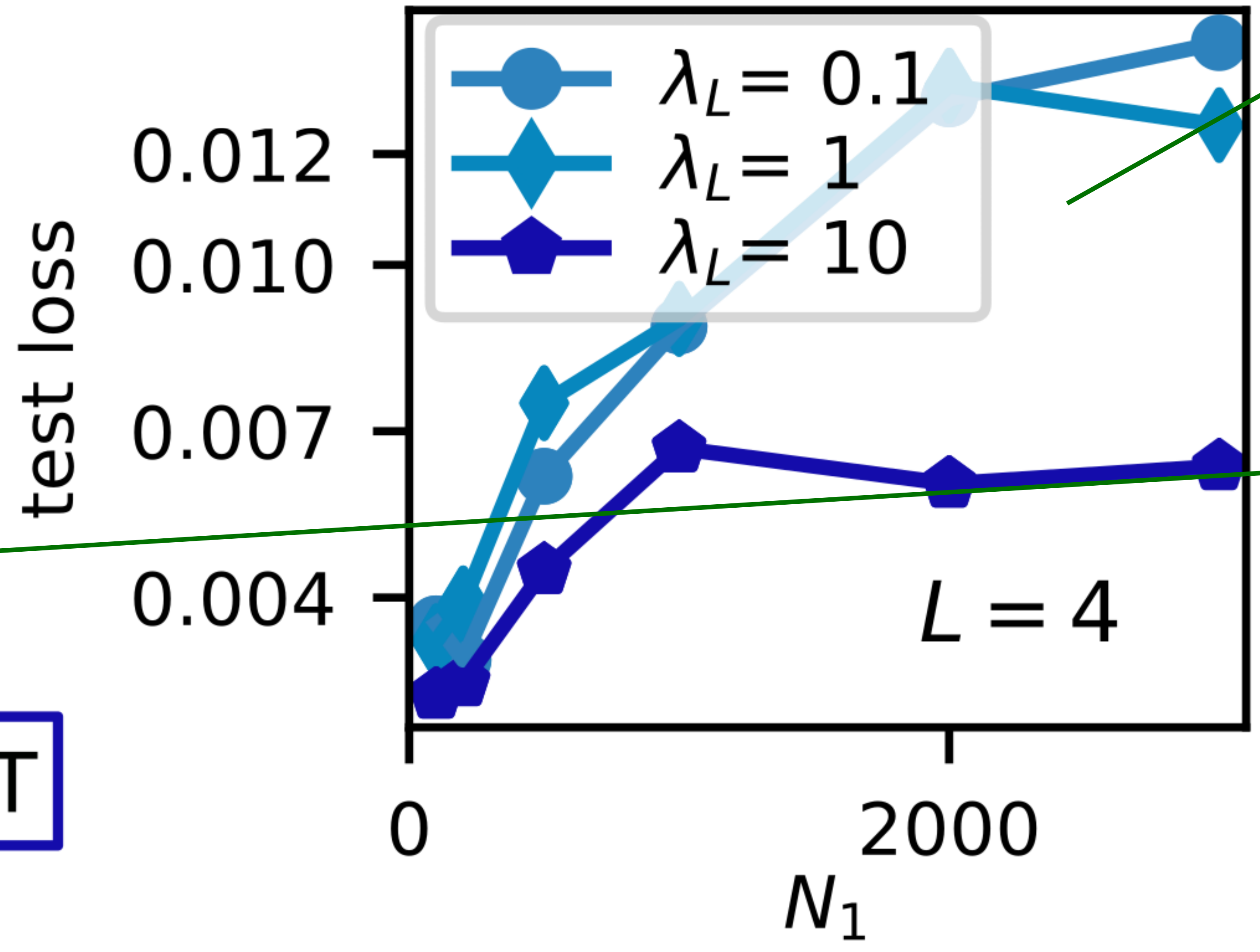

The same reasoning on the Gaussian prior of the last layer holds, but **for L layer the bias is not constant as a function of N!**

For ReLU, after a certain critical L, infinite-width outperforms finite width, since the NNGP kernel develops at least one almost singular eigenvalue

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- Effective theory for gradient descent dynamics? Convolutions? Feature learning? Generalisation performance at finite-width and edge of chaos? Role of skip connections (residual networks)?

THANKS!

Sebastiano Ariosto

Mauro Pastore

Francesco Ginelli

Marco Gherardi

Rosalba Pacelli

[arXiv:2209.04882 (2022)]