Random Matrix Theory in Deep Learning: An Introduction

Log-gases in Caeli Australi - Recent Developments in and around Random MATRIX Theory

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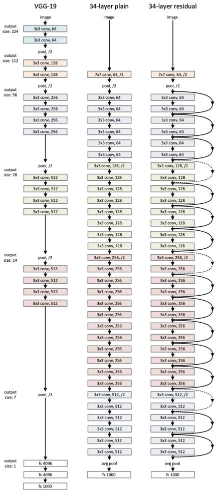
Outline

1. An Introduction Deep Learning for Mathematicians
2. Important Theoretical Questions for DL
3. Random (and Not-so Random) Matrix Theory in DL
   - Shallow and deep NN with random weights
   - NN with nonrandom weights
4. Conclusion

Outline

Question: what are deep neural networks?



Deep Learning (DL) ≈ **multilayered neural network** (NN) is becoming the most popular machine learning (ML) model, but

- what is machine learning?
- what is a deep neural network (DNN)?
- how is such as network trained (i.e., the learning procedure)?
- is there any theory for DL, and if yes, how far is the theory from practice?

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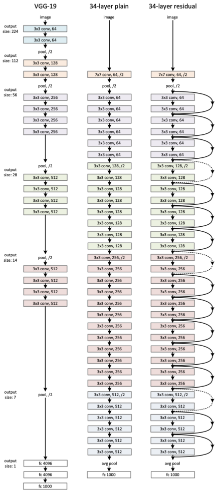

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Credit: most materials in this part are borrowed from [HH19].

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Example: binary classification of points in $\mathbb{R}^2$

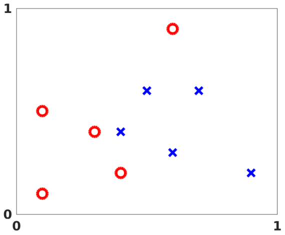

Figure: Labeled data points $\mathbf{x} \in \mathbb{R}^2$. Circles denote points in class $\mathcal{C}_1$. Crosses denote points in class $\mathcal{C}_2$.

- build a model/**function** f (from above historical data) that takes any points $\mathbf{x} \in \mathbb{R}^2$ and returns $\mathcal{C}_1$ or $\mathcal{C}_2$
- **logistic regression**: $\boxed{f(\mathbf{x}) = \sigma(\mathbf{w}^\top \mathbf{x} + b)}$ for $\mathbf{w} \in \mathbb{R}^2$ and $b \in \mathbb{R}$ to be determined, and sigmoid function $\sigma(t) = \frac{1}{1+e^{-t}}$

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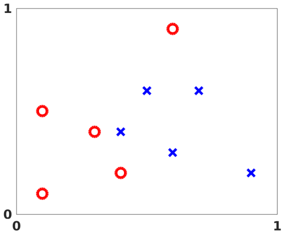

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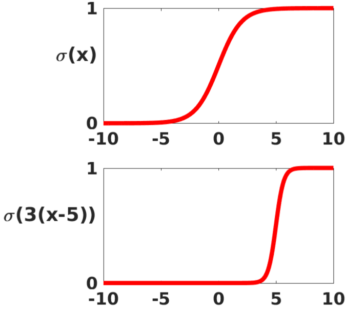

Figure: Sigmoid function.

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- "learn" or estimate parameters $\mathbf{w}, b$ from data/samples, by minimizing some cost function (e.g., negative likelihood, MSE)
- predict $\mathbf{x} \in \mathcal{C}_1$ if $f(\mathbf{x}) < 1/2$ and $\mathbf{x} \in \mathcal{C}_2$ otherwise.

Neural networks are nothing but "cascaded" logistic regressors

- logistic regression $f(\mathbf{x}) = \sigma(\mathbf{w}^\top \mathbf{x} + b) \in \mathbb{R}$ for $\mathbf{w} \in \mathbb{R}^2$, $b \in \mathbb{R}$ extends to

$$\boxed{f(\mathbf{x}) = \sigma(\mathbf{W}\mathbf{x} + \mathbf{b}) \in \mathbb{R}^N} \quad \mathbf{W} \in \mathbb{R}^{N\times 2}, \mathbf{b} \in \mathbb{R}^N \tag{1}$$

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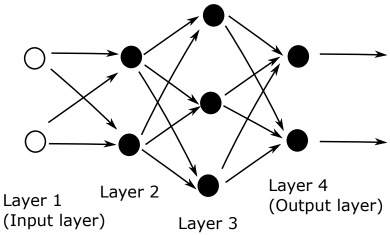

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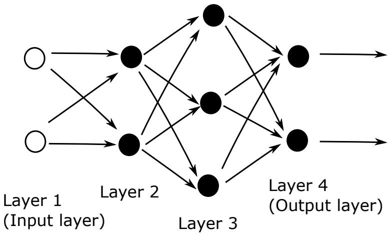

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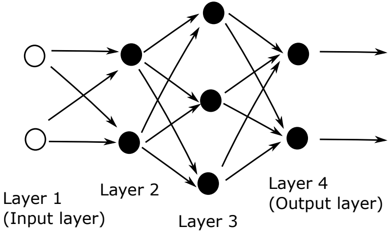

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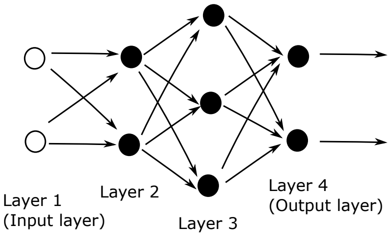

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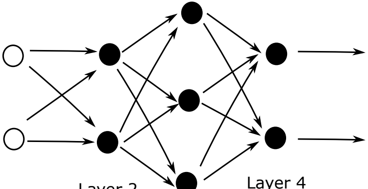

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Define the label/target output as

$$\mathbf{y}(\mathbf{x}_i) = \begin{cases} \begin{bmatrix} 1 \\ 0 \end{bmatrix} & \mathbf{x}_i \in \mathcal{C}_1, \\ \begin{bmatrix} 0 \\ 1 \end{bmatrix} & \mathbf{x}_i \in \mathcal{C}_2. \end{cases} \tag{2}$$

the MSE cost function writes $\mathrm{Cost}\left(\mathbf{W}_2, \mathbf{W}_3, \mathbf{W}_4, \mathbf{b}_2, \mathbf{b}_3, \mathbf{b}_4\right) = \frac{1}{10} \sum_{i=1}^{10} \|\mathbf{y}(\mathbf{x}_i) - f_{4L-NN}(\mathbf{x}_i)\|^2$

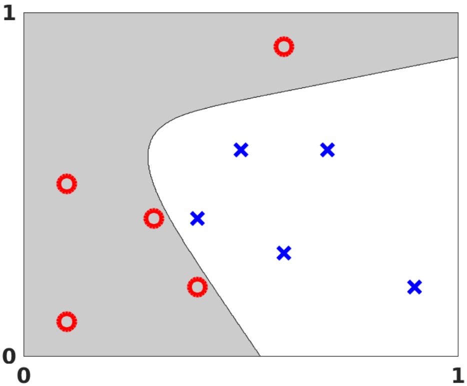

Figure: Visualization of output from a multilayered neural network applied to the data.

- from training to test!

General formulation and gradient decent training of DNN

We can define the network in a **layer-by-layer** fashion:

$$\mathbf{a}_0 = \mathbf{x} \in \mathbb{R}^{N_0}, \quad \boxed{\mathbf{a}_\ell = \sigma\left(\mathbf{W}_\ell \mathbf{a}_{\ell-1} + \mathbf{b}_\ell\right)} \in \mathbb{R}^{N_\ell}, \quad \ell = 1, \ldots, L,$$

with weights $\mathbf{W}_\ell \in \mathbb{R}^{N_\ell \times N_{\ell-1}}$ and bias $\mathbf{b} \in \mathbb{R}^{N_\ell}$ at layer ℓ.

- $\mathbf{W}_\ell$s and $\mathbf{b}_\ell$s obtained by minimizing cost function on a given training set $\{(\mathbf{x}_i, \mathbf{y}_i)\}_{i=1}^n$ of size n:

$$\text{Cost} = \frac{1}{n} \sum_{i=1}^n \frac{1}{2} \|\mathbf{y}_i - \mathbf{a}_L(\mathbf{x}_i)\|^2. \tag{3}$$

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- update using (stochastic) gradient descent, for parameter P,

$$P(t+1) = P(t) - \eta \nabla_P \text{Cost}(P(t)). \tag{4}$$

Matlab code to train a simple NN

```
%%%%%% DATA %%%%%%%%%%%
x1 = [0.1,0.3,0.1,0.6,0.4,0.6,0.5,0.9,0.4,0.7]; x2 = [0.1,0.4,0.5,0.9,0.2,0.3,0.6,0.2,0.4,0.6]; y = [ones(1,5) zeros(1,5); zeros(1,5) ones(1,5)];

% Initialize weights and biases
W2 = 0.5*randn(2,2); W3 = 0.5*randn(3,2); W4 = 0.5*randn(2,3); b2 = 0.5*randn(2,1); b3 = 0.5*randn(3,1); b4 = 0.5*randn(2,1);

% Forward and Back propagate
eta = 0.05;                % learning rate
Niter = 1e6;               % number of SG iterations
savecost = zeros(Niter,1); % value of cost function at each iteration
for counter = 1:Niter
    k = randi(10);         % choose a training point at random
    x = [x1(k); x2(k)];
    % Forward pass
    a2 = activate(x,W2,b2); a3 = activate(a2,W3,b3); a4 = activate(a3,W4,b4);
    % Backward pass
    delta4 = a4.*(1-a4).*(a4-y(:,k)); delta3 = a3.*(1-a3).*(W4'*delta4); delta2 = a2.*(1-a2).*(W3'*delta3);
    % Gradient step
    W2 = W2 - eta*delta2*x'; W3 = W3 - eta*delta3*a2'; W4 = W4 - eta*delta4*a3'; b2 = b2 - eta*delta2; b3 = b3 - eta*delta3; b4 = b4 - eta*delta4;
    % Monitor progress
    newcost = cost(W2,W3,W4,b2,b3,b4)   % display cost to screen
    savecost(counter) = newcost;
end

% Show decay of cost function
semilogy([1:1e4:Niter],savecost(1:1e4:Niter))

  function costval = cost(W2,W3,W4,b2,b3,b4)
     costvec = zeros(10,1);
     for i = 1:10
         x =[x1(i);x2(i)];
         a2 = activate(x,W2,b2); a3 = activate(a2,W3,b3); a4 = activate(a3,W4,b4);
         costvec(i) = norm(y(:,i) - a4,2);
     end
     costval = norm(costvec,2)^2;
  end % of nested function
```

Matlab code to train a simple NN

```
function y = activate(x,W,b)
%ACTIVATE  Evaluates sigmoid function.
%
%  x is the input vector,  y is the output vector
%  W contains the weights, b contains the shifts
%
%  The ith component of y is activate((Wx+b)_i)
%  where activate(z) = 1/(1+exp(-z))

y = 1./(1+exp(-(W*x+b)));
```

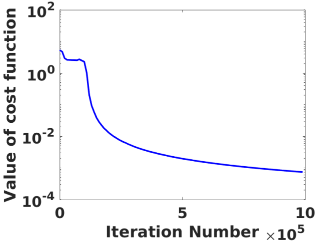

Figure: Vertical axis shows a scaled value of the cost function. Horizontal axis shows the iteration number. Here we used the stochastic gradient descent to train the aforementioned simple network.

Some commonly used tricks in DNN

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\begin{bmatrix} 1 & -1 & & & & \\ & 1 & -1 & & & \\ & & 1 & -1 & & \\ & & & 1 & -1 & \\ & & & & 1 & -1 \end{bmatrix} \in \mathbb{R}^{5\times 6}. \tag{5}
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- use of **tensors** instead of vectors or matrices for input data or intermediate representations

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- **too many** "tuning" hyperparameters in DNN design: number of layers, operator, width, and activation in each layer, different tricks, etc.
- for safety-related applications (e.g., self driving, healthcare), we need theory-supported DL

A (too) brief review of DL theory

From an approximation theoretical perspective:

- **universal approximation theorem**: for any (somewhat regular, e.g., Lebesgue p-integrable) function of interest $f \colon \mathbb{R}^{p \times K}$ and given $\varepsilon > 0$, there exists a fully-connected ReLU network F with width at least m such that $\int_{\mathbb{R}^p} \|f(\mathbf{x}) - F(\mathbf{x})\|^p d\mathbf{x} < \varepsilon$.
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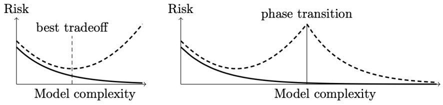
From an optimization perspective:

- DNN training involves non-convex (and possibly non-smooth) optimization: challenging!
- **empirically** simple (stochastic) gradient descent seems to work well, WHY?
- GUESS: DL landscape has nice properties?
- e.g., how to converge better and faster?
- **IMPORTANT**: pure optimization deals only with training, and **NOT** test/**generalization**

From a statistical perspective:

- **generalization theory**: for which type of **data**, and by using which **ML model** (trained with which **algorithm**), can we get a high probability error bound of which **metric**



(a) Classical U-shaped curve (b) Modern double descent "UL"-shaped test curve

A Good DL theory should cover **both** optimization **and** generalization!

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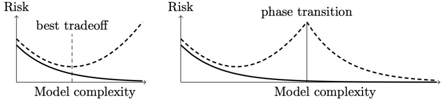

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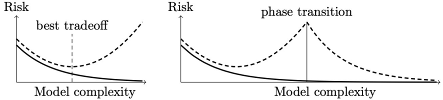

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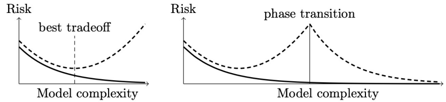

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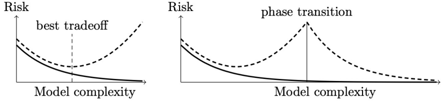

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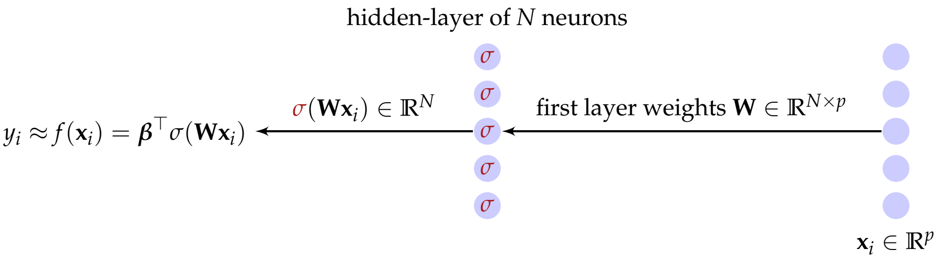
- PS: kernels are widely studied in the ML literature, we know quite a lot (reproducing kernel Hilbert space, RKHS, etc.)

Example of a two-layer NN model



- Given training set $\{(\mathbf{x}_i, y_i)\}_{i=1}^n$ with $\mathbf{x}_i \in \mathbb{R}^p$ and $y_i \in \mathbb{R}$

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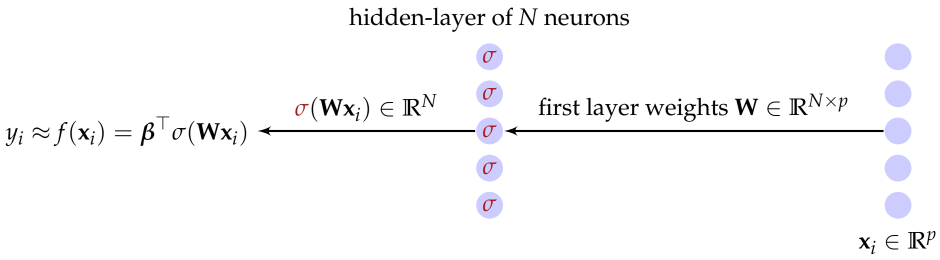

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- linearization of the network at initialization, by Taylor expansion

$$f(\mathbf{x}; \boldsymbol{\theta}) \approx f_{\text{lin}}(\mathbf{x}; \boldsymbol{\theta}) = f(\mathbf{x}; \boldsymbol{\theta}_0) + (\boldsymbol{\theta} - \boldsymbol{\theta}_0)^\top \boxed{\nabla_\theta f(\mathbf{x}; \boldsymbol{\theta}_0)}. \tag{8}$$

and

$$f_{\text{lin}}(\mathbf{x}; \boldsymbol{\theta}_0 + \delta) = f(\mathbf{x}; \boldsymbol{\theta}_0) + \boldsymbol{\delta}^\top \phi_{\text{NTK}}(\mathbf{x}), \quad K_{e-NTK}(\mathbf{x}, \mathbf{y}) = \phi_{\text{NTK}}(\mathbf{x})^\top \phi_{\text{NTK}}(\mathbf{y}). \tag{9}$$

The big picture of NTK

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Now, if there exists a neighborhood $B(\boldsymbol{\theta}_0)$ of $\boldsymbol{\theta}_0$ such that

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2. it suffices to optimize in $B(\boldsymbol{\theta}_0)$ to reach an approx. global min, i.e., $f(\mathbf{x};\boldsymbol{\theta}_0) \approx f_{\rm lin}(\mathbf{x};\boldsymbol{\theta}_0) \approx 0$
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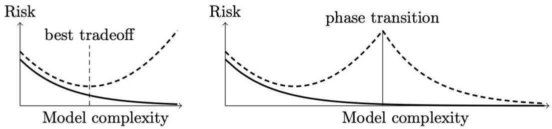
To reach the above is **over-parameterization** and/or **proper random initialization**, with small stochasticity (e.g., small learning rate or full batch GD)

- cost function (e.g., MSE) $\text{Cost}(f_{\boldsymbol{\theta}}(\mathbf{x}), \mathbf{y}) \approx \text{Cost}(f_{\text{lin}}(\mathbf{x}), \mathbf{y})$ linear (in the parameter $\boldsymbol{\theta}$) and convex!
- for MSE, $\text{Cost}(f_{\text{lin}}(\mathbf{X}), \mathbf{y}) = \frac{1}{n} \sum_{i=1}^n (f_{\text{lin}}(\mathbf{x}_i) - y_i)^2$, nothing but linear regression of type $\text{Cost} = \|\mathbf{y}' - \boldsymbol{\Phi}_{NTK}(\mathbf{X})^\top \delta\|^2$ with $y_i' = f(\mathbf{x}_i; \boldsymbol{\theta}_0) - y$



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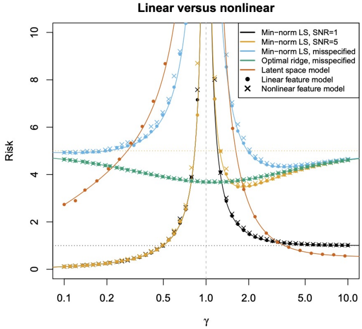

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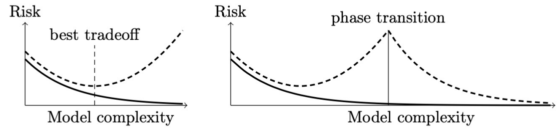

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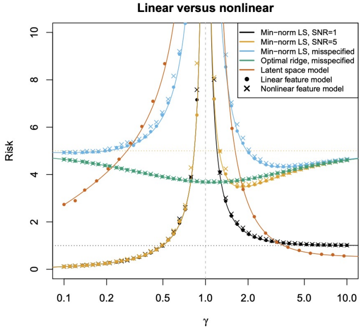

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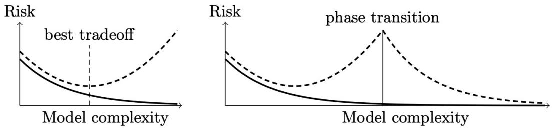

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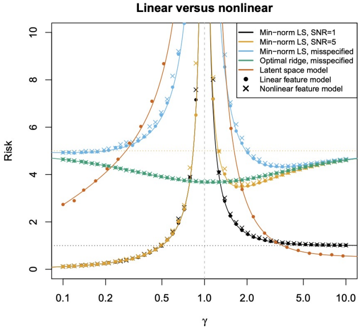

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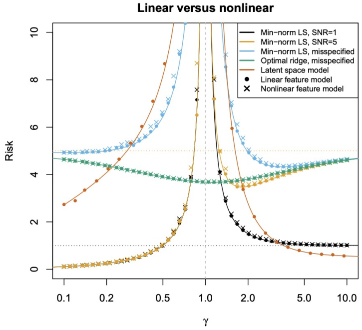

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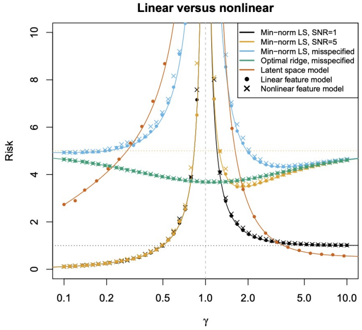

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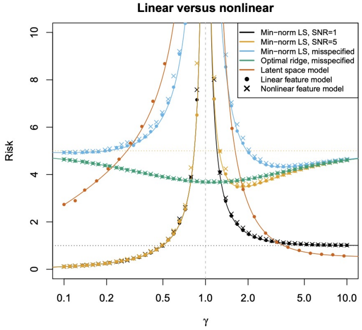

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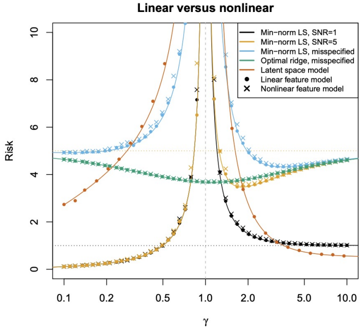

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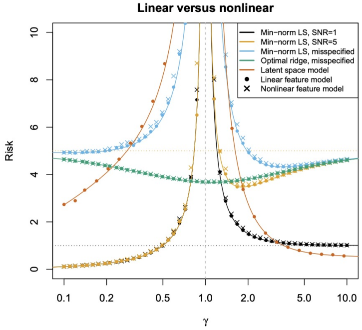
- tons of extensions: relaxing assumption, (slightly) more involved models, etc., less progress in the sense of deep though



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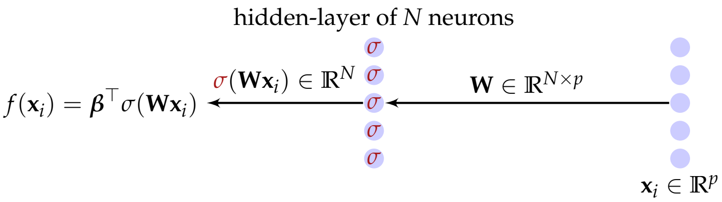
Two-layer network with random first layer



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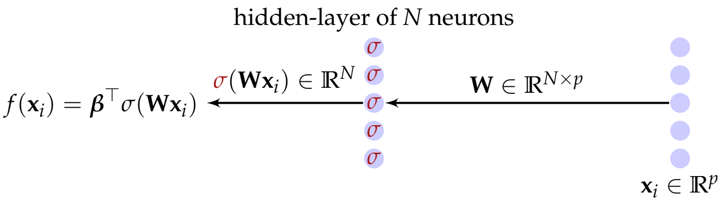

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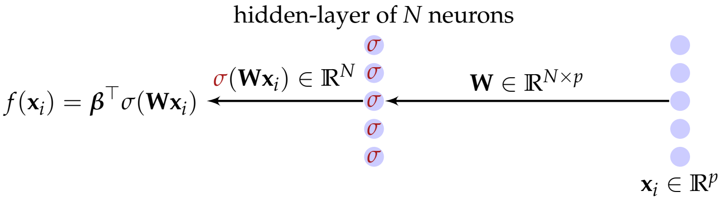

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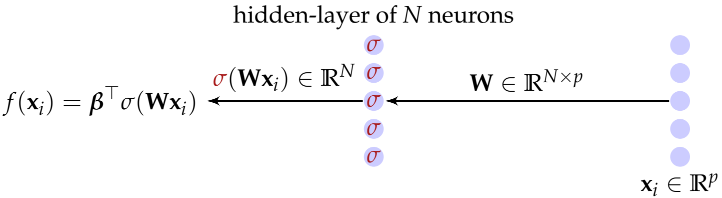

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- Similarly, the test MSE on a test set $(\hat{\mathbf{X}}, \hat{\mathbf{y}}) \in \mathbb{R}^{p \times \hat{n}} \times \mathbb{R}^{d \times \hat{n}}$ of size $\hat{n}$: $E_{\rm test} = \frac{1}{\hat{n}}\|\hat{\mathbf{y}} - \hat{\boldsymbol{\Sigma}}^\top \boldsymbol{\beta}\|_F^2, \quad \hat{\boldsymbol{\Sigma}} = \sigma(\mathbf{W}\hat{\mathbf{X}})$.

Nonlinear resolvent

$$\mathbf{Q}(\gamma) = \left(\frac{1}{n} \sigma(\mathbf{W}\mathbf{X})^\top \sigma(\mathbf{W}\mathbf{X}) + \gamma \mathbf{I}_n \right)^{-1} \tag{13}$$

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Lemma (Concentration of nonlinear quadratic form, [LLC18, Lemma 1])

For $\mathbf{w} \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_p)$, 1-*Lipschitz* $\sigma(\cdot)$, *and* $\mathbf{A} \in \mathbb{R}^{n \times n}, \mathbf{X} \in \mathbb{R}^{p \times n}$ *such that* $\|\mathbf{A}\|, \|\mathbf{X}\|$ *bounded, then*

$$\mathbb{P}\left(\left| \frac{1}{n} \sigma(\mathbf{w}^\top \mathbf{X}) \mathbf{A} \sigma(\mathbf{X}^\top \mathbf{w}) - \frac{1}{n} \operatorname{tr} \mathbf{A}\mathbf{K} \right| > t \right) \leq C e^{-cn \min(t, t^2)}$$

for some $C, c > 0$, $p/n \in (0, \infty)$ *with* $\mathbf{K} \equiv \mathbf{K}_{\mathbf{X}\mathbf{X}} \equiv \mathbb{E}_{\mathbf{w} \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_p)}[\sigma(\mathbf{X}^\top \mathbf{w}) \sigma(\mathbf{w}^\top \mathbf{X})] \in \mathbb{R}^{n \times n}$.

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- $\mathbf{K}$ is in fact the **conjugate kernel** (**CK**) matrix
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- get deterministic equivalent for $\mathbf{Q}$, establish (limiting) eigenvalue distribution of $\frac{1}{n}\sigma(\mathbf{W}\mathbf{X})^\top \sigma(\mathbf{W}\mathbf{X})$, etc.

Theorem (Resolvent for nonlinear Gram matrix, [LLC18])

Let $\mathbf{W} \in \mathbb{R}^{N \times p}$ *be a random matrix with i.i.d. standard Gaussian entries,* $\sigma(\cdot)$ *be* 1*-Lipschitz, and* $\mathbf{X} \in \mathbb{R}^{p \times n}$ *be of bounded operator norm. Then, as* $n, p, N \to \infty$ *at the same pace, for* $\mathbf{Q} = (\sigma(\mathbf{X}^\top \mathbf{W}^\mathsf{T})\sigma(\mathbf{W}\mathbf{X})/n + \gamma \mathbf{I}_n)^{-1}$ *with* $\gamma > 0$,

$$\|\mathbb{E}[\mathbf{Q}] - \bar{\mathbf{Q}}\| \to 0, \quad \bar{\mathbf{Q}} \equiv \left(\frac{N}{n} \frac{\mathbf{K}}{1+\delta} + \gamma \mathbf{I}_n \right)^{-1}$$

for δ *the unique positive solution to* $\delta = \frac{1}{n} \operatorname{tr} \bar{\mathbf{Q}}\mathbf{K}$ *and* $\mathbf{K} = \mathbb{E}_{\mathbf{w} \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_p)}[\sigma(\mathbf{X}^\top \mathbf{w})\sigma(\mathbf{w}^\top \mathbf{X})] \in \mathbb{R}^{n \times n}$.

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Corollary (Asymptotic training and test MSEs)

Under the setting and notations of Theorem 2, for bounded $\mathbf{X}, \hat{\mathbf{X}}, \mathbf{y}, \hat{\mathbf{y}}$*, then the training and test MSES, satisfy, as* $n, p, N \to \infty$*, we have* $E_{\text{train}} - \bar{E}_{\text{train}} \to 0$ *and* $E_{\text{test}} - \bar{E}_{\text{test}} \to 0$ *with*

$$\bar{E}_{\text{train}} = \frac{\gamma^2}{n} \mathbf{y}^\top \bar{\mathbf{Q}} \left(\frac{\frac{1}{N} \operatorname{tr} \bar{\mathbf{Q}} \bar{\mathbf{K}} \bar{\mathbf{Q}}}{1 - \frac{1}{N} \operatorname{tr} \bar{\mathbf{K}} \bar{\mathbf{Q}} \bar{\mathbf{K}} \bar{\mathbf{Q}}} \bar{\mathbf{K}} + \mathbf{I}_n \right) \bar{\mathbf{Q}} \mathbf{y}$$

$$\bar{E}_{\text{test}} = \frac{1}{\hat{n}} \|\hat{\mathbf{y}} - \bar{\mathbf{K}}_{\mathbf{X}\hat{\mathbf{X}}}^\top \bar{\mathbf{Q}} \mathbf{y}\|_F^2 + \frac{\frac{1}{N} \mathbf{y}^\top \bar{\mathbf{Q}} \bar{\mathbf{K}} \bar{\mathbf{Q}} \mathbf{y}}{1 - \frac{1}{N} \operatorname{tr} \bar{\mathbf{K}} \bar{\mathbf{Q}} \bar{\mathbf{K}} \bar{\mathbf{Q}}} \left(\frac{1}{\hat{n}} \operatorname{tr} \bar{\mathbf{K}}_{\hat{\mathbf{X}}\hat{\mathbf{X}}} - \frac{1}{\hat{n}} \operatorname{tr} (\mathbf{I}_n + \gamma \bar{\mathbf{Q}})(\bar{\mathbf{K}}_{\mathbf{X}\hat{\mathbf{X}}} \bar{\mathbf{K}}_{\mathbf{X}\hat{\mathbf{X}}}^\top \bar{\mathbf{Q}}) \right)$$

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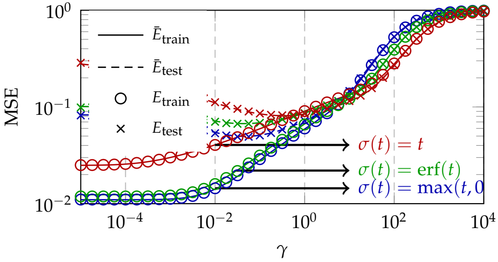
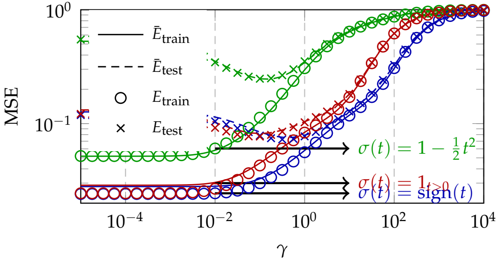
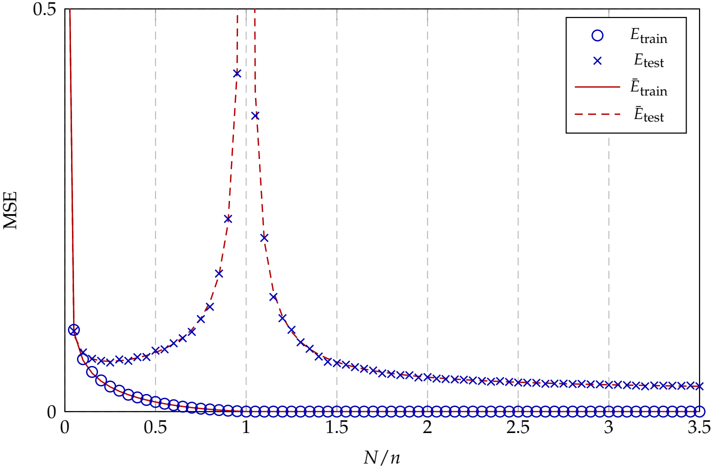
Numerical results





Numerical results: double descent



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Eigenspectra of $\frac{1}{n}\sigma(\mathbf{WX})^\top\sigma(\mathbf{WX})$:

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Question: what happen if either $\mathbf{W}$ or $\mathbf{X}$ has some structure? Any different phase transition behavior?

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Some further RMT investigations on random DNNs

- design of DNN to achieve dynamical isometry, **accelerate** training at the **beginning** stage of training

- Jeffrey Pennington, Samuel Schoenholz, and Surya Ganguli. "Resurrecting the Sigmoid in Deep Learning through Dynamical Isometry: Theory and Practice". In: *Advances in Neural Information Processing Systems*. Vol. 30. NIPS'17. Curran Associates, Inc., 2017, pp. 4785–4795
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- understand how weight distribution **interact** with activation in DNNs
  - Leonid Pastur. "On Random Matrices Arising in Deep Neural Networks. Gaussian Case". In: *arXiv* (2020). eprint: `2001.06188`
  - Leonid Pastur and Victor Slavin. "On Random Matrices Arising in Deep Neural Networks: General I.I.D. Case". In: *Random Matrices: Theory and Applications* 12.01 (Jan. 2023), p. 2250046
  - Leonid Pastur. "Eigenvalue Distribution of Large Random Matrices Arising in Deep Neural Networks: Orthogonal Case". In: *Journal of Mathematical Physics* 63.6 (2022), p. 063505
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Outline

Gradient descent dynamics on linear regression model

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$$L(\mathbf{w}) = \frac{1}{2n} \|\mathbf{y} - \mathbf{X}^\top \mathbf{w}\|^2 + \frac{\gamma}{2} \|\mathbf{w}\|^2 \tag{14}$$

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  for some regularization penalty $\gamma \geq 0$.
- gradient given by $\nabla L(\mathbf{w}) = -\frac{1}{n}\mathbf{X}(\mathbf{y} - \mathbf{X}^\top \mathbf{w}) + \gamma \mathbf{w}$ so that, for small gradient descent steps (or learning rate) α, continuous-time approximation (in fact, **gradient flow**) of the time evolution $\mathbf{w}(t)$ of $\mathbf{w}$:

$$\frac{\partial \mathbf{w}(t)}{\partial t} = -\alpha \nabla L(\mathbf{w}) = \frac{\alpha}{n}\mathbf{X}\mathbf{y} - \alpha \left(\frac{1}{n}\mathbf{X}\mathbf{X}^\top + \gamma \mathbf{I}_p \right) \mathbf{w}$$

  solution explicitly given by

$$\boxed{\mathbf{w}(t) = e^{-\alpha t \left(\frac{1}{n}\mathbf{X}\mathbf{X}^\top + \gamma \mathbf{I}_p \right)} \mathbf{w}_0 + \left(\mathbf{I}_p - e^{-\alpha t \left(\frac{1}{n}\mathbf{X}\mathbf{X}^\top + \gamma \mathbf{I}_p \right)} \right) \mathbf{w}_\infty} \tag{15}$$

  with $\mathbf{w}_0 = \mathbf{w}(t=0)$ (the initialization of gradient descent) and

$$\mathbf{w}_\infty = \left(\frac{1}{n}\mathbf{X}\mathbf{X}^\top + \gamma \mathbf{I}_p \right)^{-1} \frac{1}{n}\mathbf{X}\mathbf{y} \tag{16}$$

  the ridge regression solution with regularization parameter γ.

Some RMT results on GDD in classification

- to study statistical evolution of $\mathbf{w}(t)$, consider binary Gaussian mixture model for input data

$$\mathcal{C}_1 : \mathbf{x}_i \sim \mathcal{N}(-\boldsymbol{\mu}, \mathbf{I}_p) \quad \mathcal{C}_2 : \mathbf{x}_i \sim \mathcal{N}(\boldsymbol{\mu}, \mathbf{I}_p)$$

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- study training and test **misclassification error rates** as

$$\mathbb{P}(\mathbf{x}_i^\top \mathbf{w}(t) > 0 \mid y_i = -1), \quad \text{and} \quad \mathbb{P}(\hat{\mathbf{x}}^\top \mathbf{w}(t) > 0 \mid \hat{y} = -1),$$

  for $\hat{\mathbf{x}} \sim \mathcal{N}(-\boldsymbol{\mu}, \mathbf{I}_p)$ a new test datum (independent of the training set $(\mathbf{X}, \mathbf{y})$) of genuine label $\hat{y} = -1$.

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- we can of course consider different statistical **model** and/or different **task** (e.g., regression)

Theorem (Training and test performance of GDD, [LC18])

For a random initialization $\mathbf{w}_0 \sim \mathcal{N}(\mathbf{0}, \sigma^2 \mathbf{I}_p/p)$ *independent of* $\mathbf{X}$, $\mathbf{x}$ *a column of* $\mathbf{X}$ *of mean* $\boldsymbol{\mu}$ *and* $\hat{\mathbf{x}}$ *an independent copy of* $\mathbf{x}$, *as* $n, p \to \infty$ *with* $p/n \to c \in (0, \infty)$, *we have*

$$\mathbb{P}(\hat{\mathbf{x}}^\top \mathbf{w}(t) > 0 \mid \hat{y} = -1) - Q\left(\frac{E_{\rm test}}{\sqrt{V_{\rm test}}}\right) \to 0, \quad \mathbb{P}(\mathbf{x}^\top \mathbf{w}(t) > 0 \mid y = -1) - Q\left(\frac{E_{\rm train}}{\sqrt{V_{\rm train}}}\right) \to 0,$$

almost surely, where

$$E_{\rm test} = -\frac{1}{2\pi\imath} \oint_\Gamma \frac{1 - f_t(z)}{z} \frac{\rho m(z)\, dz}{(\rho + c)\, m(z) + 1}, \quad V_{\rm test} = \frac{1}{2\pi\imath} \oint_\Gamma \left[\frac{\frac{1}{z^2} (1 - f_t(z))^2}{(\rho + c)\, m(z) + 1} - \sigma^2 f_t^2(z) m(z) \right] dz$$

$$E_{\rm train} = -\frac{1}{2\pi\imath} \oint_\Gamma \frac{1 - f_t(z)}{z} \frac{dz}{(\rho + c)\, m(z) + 1}, \quad V_{\rm train} = \frac{1}{2\pi\imath} \oint_\Gamma \left[\frac{\frac{1}{z} (1 - f_t(z))^2}{(\rho + c)\, m(z) + 1} - \sigma^2 f_t^2(z) z m(z) \right] dz - E_{\rm train}^2$$

with $\rho = \lim_{p\to\infty} \|\boldsymbol{\mu}\|^2$, Γ *a positive contour surrounding the support of the Marčenko–Pastur law (shifted by* $\gamma \geq 0$*) and the points* $(\gamma, 0)$ *and* $(\gamma + \lambda_s, 0)$ *with* $\lambda_s = c + 1 + \rho + c/\rho$, $f_t(z) \equiv \exp(-\alpha t z)$ *and* $m(z)$ *unique ST solution to* $c(z-\gamma)m^2(z) - (1 - c - z + \gamma)m(z) + 1 = 0$.

Some further simplifications

- choose the contour Γ as, e.g., rectangle circling around both **main bulk** and **isolated eigenvalue** (if any)

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This leads to

$$E_{\rm test} = \int \frac{1-f_t(x+\gamma)}{x+\gamma}\omega(dx) \quad V_{\rm test} = \frac{\rho+c}{\rho}\int \frac{(1-f_t(x+\gamma))^2\omega(dx)}{(x+\gamma)^2} + \sigma^2 \int f_t^2(x+\gamma)\mu(dx)$$

$$E_{\rm train} = \frac{\rho+c}{\rho}\int \frac{1-f_t(x+\gamma)}{x+\gamma}\omega(dx), \quad V_{\rm train} = \frac{\rho+c}{\rho}\int \frac{x(1-f_t(x+\gamma))^2\omega(dx)}{(x+\gamma)^2} + \sigma^2 \int x f_t^2(x+\gamma)\mu(dx) - E_{\rm train}^2$$

where we recall $\rho = \lim \|\boldsymbol{\mu}\|^2$, $f_t(x) = \exp(-\alpha t x)$, $\mu(x)$ the MP law

$$\mu(dx) = \frac{\sqrt{(x-\lambda_-)^+(\lambda_+-x)^+}}{2\pi c x}dx + (1-c^{-1})^+\delta(x), \tag{17}$$

and

$$\omega(dx) \equiv \frac{\sqrt{(x-\lambda_-)^+(\lambda_+-x)^+}}{2\pi(\lambda_s - x)}dx + \frac{(\rho^2-c)^+}{\rho}\delta_{\lambda_s}(x) \tag{18}$$

for $\lambda_s = c + 1 + \rho + c/\rho$ the (possible) spike location.

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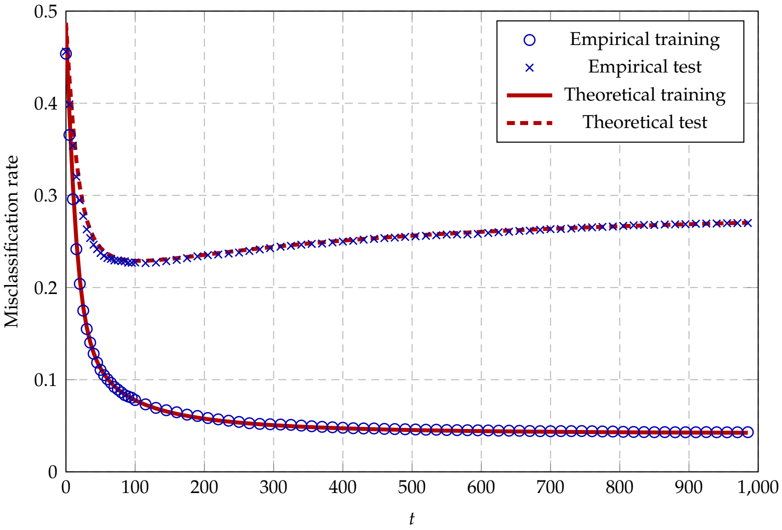
Numerical results



Some further RMT efforts on high-dimensional dynamics

From the statistical physics community: reduces to low-dimensional ODE or SDE

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And from the RMT community as well

- Gerard Ben Arous, Reza Gheissari, and Aukosh Jagannath. "Online Stochastic Gradient Descent on Non-Convex Losses from High-Dimensional Inference". In: *Journal of Machine Learning Research* 22.106 (2021), pp. 1–51
- Gerard Ben Arous, Reza Gheissari, and Aukosh Jagannath. "High-Dimensional Limit Theorems for SGD: Effective Dynamics and Critical Scaling". In: *Advances in Neural Information Processing Systems* 35 (Dec. 2022), pp. 25349–25362
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One step gradient beyond random network

- extends to wide DNN model via NTK, see, e.g., Y. Du, Z. Ling, R. C. Qiu, Z. Liao, "High-dimensional Learning Dynamics of Deep Neural Nets in the Neural Tangent Regime", High-dimensional Learning Dynamics Workshop, The Fortieth International Conference on Machine Learning (ICML'2023), 2023

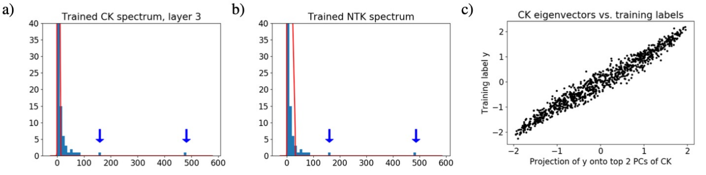

Figure 3: Eigenvalues of (a) K^{CK} and (b) K^{NTK} in a *trained* network, for training labels $y_\alpha = \sigma(\mathbf{x}_\alpha^\top \mathbf{v})$. The limit spectra at random initialization of weights are shown in red. Large outlier eigenvalues, indicated by blue arrows, emerge over training. (c) The projection of training labels onto the first 2 eigenvectors of the trained matrix K^{CK} accounts for 96% of the training label variance.

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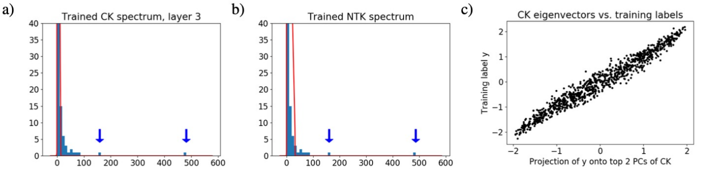

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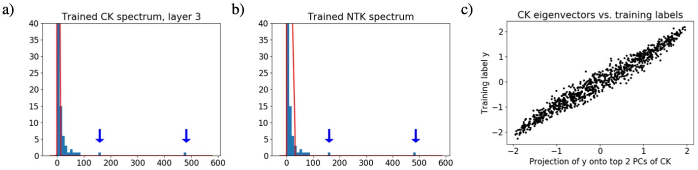

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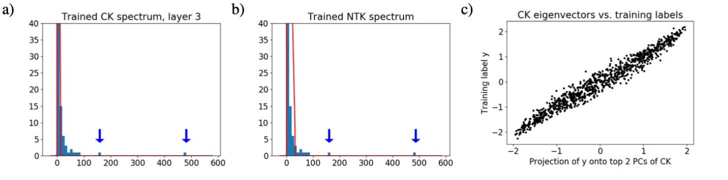
- **empirical observation**: spikes appear in the NTK spectra during gradient descent training [FW20]



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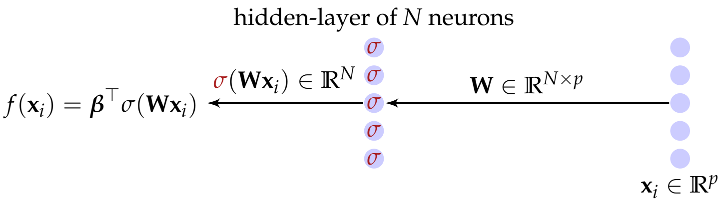
Two-layer random network after one step training



- two-layer NN having N neurons, with output $f(\mathbf{x}) = \frac{1}{\sqrt{N}} \boldsymbol{\beta}^\top \sigma(\mathbf{W}\mathbf{x})$, for input $\mathbf{x} \in \mathbb{R}^p$, first-layer weight $\mathbf{W} \in \mathbb{R}^{N \times p}$, second-layer weight $\boldsymbol{\beta} \in \mathbb{R}^N$, and nonlinear σ

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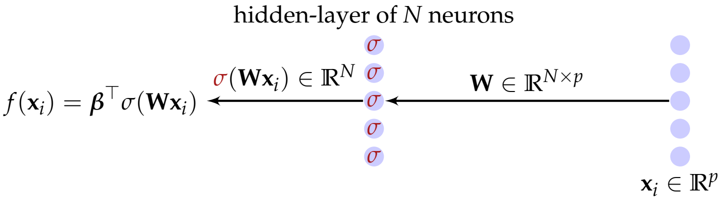

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- model trained on $\{(\mathbf{x}_i, y_i)\}_{i=1}^n$ of size n, by minimizing

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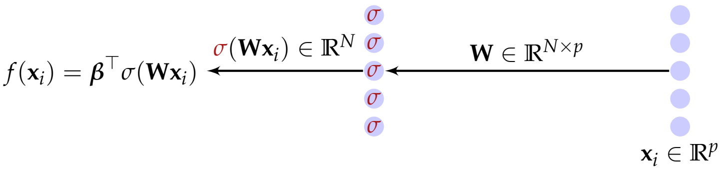

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- first-layer gradient explicitly given by

$$\frac{\partial \text{Cost}}{\partial \mathbf{W}} = -\frac{1}{n}\left(\left(\frac{1}{\sqrt{N}}\boldsymbol{\beta}\left(\mathbf{y}^\top - \frac{1}{\sqrt{N}}\boldsymbol{\beta}^\top\sigma(\mathbf{W}\mathbf{X})\right)\right)\odot\sigma'(\mathbf{W}\mathbf{X})\right)\mathbf{X}^\top \in \mathbb{R}^{N\times p}, \tag{20}$$

with $\mathbf{X} = [\mathbf{x}_1, \ldots, \mathbf{x}_n] \in \mathbb{R}^{p\times n}$, and $\mathbf{y} = [y_1, \ldots, y_n]^\top \in \mathbb{R}^n$.

Two-layer random network after one step GD training

- consider first step gradient update on $\mathbf{W}$ as $\mathbf{W}_1 = \mathbf{W}_0 + \sqrt{N}\eta_0 \mathbf{G}_0$, with $\mathbf{G}_0 = \frac{1}{n}\left(\left(\frac{1}{\sqrt{N}}\boldsymbol{\beta}_0\left(\mathbf{y}^\top - \frac{1}{\sqrt{N}}\boldsymbol{\beta}_0^\top \sigma(\mathbf{W}_0\mathbf{X})\right)\right) \odot \sigma'(\mathbf{W}_0\mathbf{X})\right)\mathbf{X}^\top$

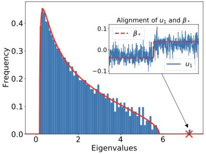

Figure 3: Main: empirical singular values of $\boldsymbol{W}_1$ (blue) vs. analytic prediction (red). Subfigure: overlap between $\boldsymbol{u}_1$ and the teacher vector $\boldsymbol{\beta}_* \propto [-\mathbf{1}_{d/2}; \mathbf{1}_{d/2}] \in \mathbb{R}^d$. We set $\sigma = \tanh$, $f^*(\boldsymbol{x}) = \mathrm{ReLU}(\langle \boldsymbol{x}, \boldsymbol{\beta}_* \rangle)$, $\eta = 2$, $\psi_1 = 4, \psi_2 = 2$, and $\sigma_\varepsilon = 0.2$.

[11] Jimmy Ba et al. "High-Dimensional Asymptotics of Feature Learning: How One Gradient Step Improves the Representation". In: *Advances in Neural Information Processing Systems*. May 2022

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- **key observation** made in [Ba+22]: under standard assumption and for Gaussian $\mathbf{W}_0, \boldsymbol{\beta}_0$ and $\mathbf{X}$, the first step gradient $\mathbf{G}_0$ is approximately of **rank one**!

$$\left\| \mathbf{G}_0 - \frac{\mathbb{E}[\sigma'(\xi)]}{n\sqrt{N}} \boldsymbol{\beta}_0 \mathbf{y}^\top \mathbf{X}^\top \right\| \to 0. \tag{21}$$

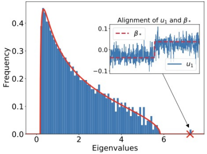

Figure 3: Main: empirical singular values of $\boldsymbol{W}_1$ (blue) vs. analytic prediction (red). Subfigure: overlap between $\boldsymbol{u}_1$ and the teacher vector $\boldsymbol{\beta}_* \propto [-\mathbf{1}_{d/2}; \mathbf{1}_{d/2}] \in \mathbb{R}^d$. We set $\sigma = \tanh$, $f^*(\boldsymbol{x}) = \mathrm{ReLU}(\langle \boldsymbol{x}, \boldsymbol{\beta}_* \rangle)$, $\eta = 2, \psi_1 = 4, \psi_2 = 2$, and $\sigma_\varepsilon = 0.2$.

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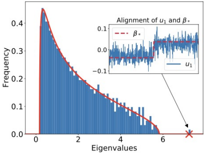

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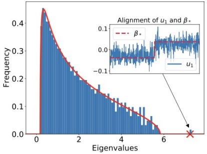
- built upon this, results on **generalization** can be obtained, etc.



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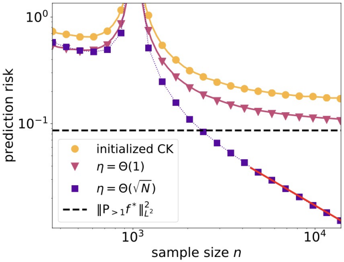
Discussion on the step size and its impact

- since $\|\mathbf{W}_0\| = O(1)$, $\|\mathbf{W}_0\|_F = \sqrt{N}$, and $\sqrt{N}\|\mathbf{G}_0\| = O(1)$, $\sqrt{N}\|\mathbf{G}_0\|_F = O(1)$, may consider:

1. small step $\eta = O(1)$ (same order in spectral norm): improve over initial CK, but not as good as optimal linear model
2. large step $\eta = O(\sqrt{N})$ (same order in Frobenius norm): improve over a class of **nonlinear** model, match **neural scaling law** in some cases



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Outline

Conclusion and take-away message

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- A recent (short) review focusing on RMT4DL: Zhenyu Liao and Michael W. Mahoney. *Random Matrix Theory for Deep Learning: Beyond Eigenvalues of Linear Models*. 2025. arXiv: 2201.04753 [cs, math]

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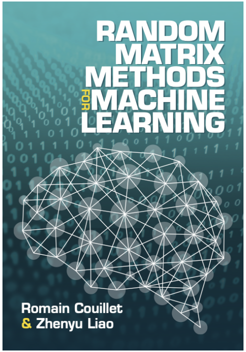

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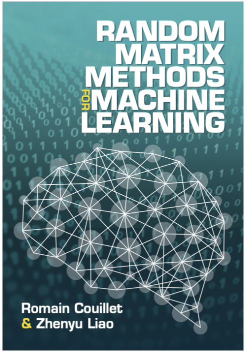

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Thank you! Q & A?