On the spectral bias of two-layer linear networks

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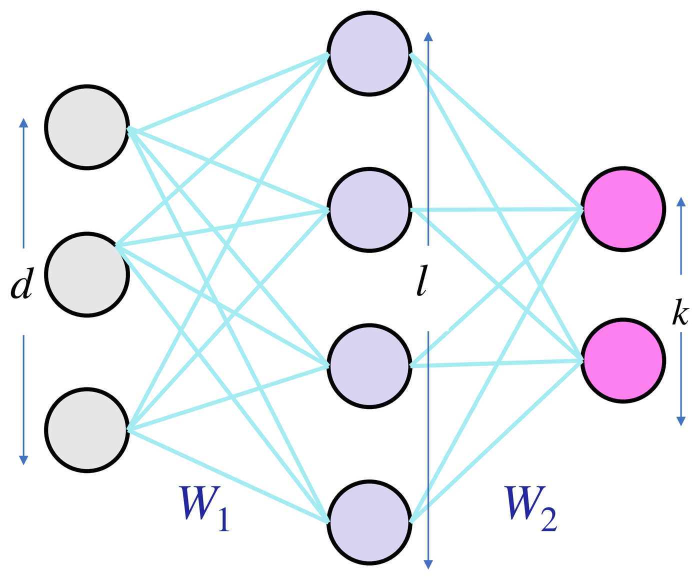
Regression with Linear Network

Setup: The $(x_i)_{i=1}^n$ from $\mathbb{R}^d$ and w.l.o.g assume the labels are generated by $y_i = \mathbf{U}_*^\top x_i \in \mathbb{R}^k$ and $\mathbf{U}_* \in \mathbb{R}^{d\times k}$.



A linear network representing function f

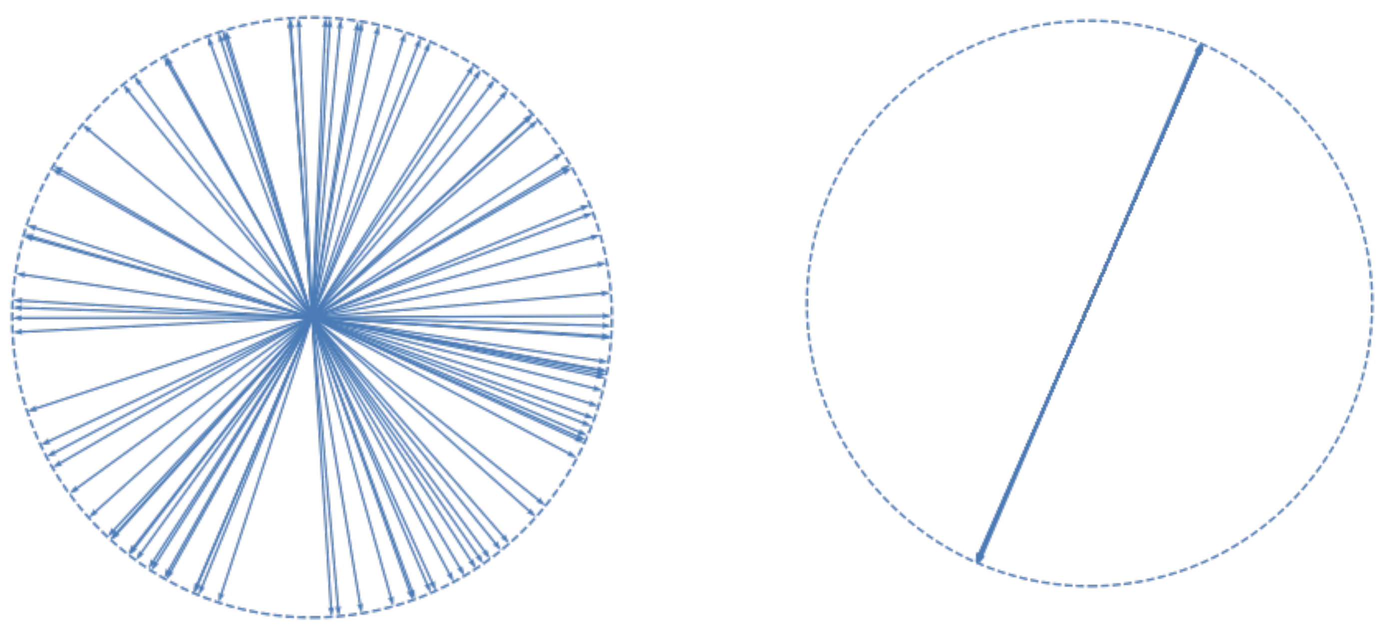
Linear Network: Let hidden layer be $W_1 \in \mathbb{R}^{d\times l}$ and weight layer $W_2 \in \mathbb{R}^{l\times k}$. The network represents the function

$$f(x) = W_2^\top W_1^\top x.$$

Square Loss: $L(W_1, W_2) = \frac{1}{2}\|Y - XW_1W_2\|^2$ which is **non-convex** in W_1, W_2 and X, Y denotes the data in a matrix form.

Dependence on initialization : Consider the problem of scalar regression, i.e., k = 1.

The direction of neurons of W_1 at the end of training.



W_1, W_2 initialized a **large** scale — W_1, W_2 initialized at a **small** scale

Different regimes: For higher scale of initialization, the neurons at convergence point in many directions (**lazy training**). For smaller scale of initialization, the neurons point towards a few feature directions (**feature learning**).

The aim of the paper: To rigorously study the impact of the initialization on the learning dynamics while training linear networks with gradient methods.

Implicit bias of the Parameters

Initialization (I) : $W = \sqrt{2\gamma}P$ where $P \in \mathbb{R}^{d\times l}$ and $PP^\top = I_d$ and $W_2 = 0$. Here γ refers to the **scale** of initialization.

Gradient Flow: We train with gradient flow (GF) on the loss L,

$$\dot{W}_1 = -\nabla_{W_1} L(W_1, W_2) = (X^\top(Y - XW_1W_2))W_2^\top,$$
$$\dot{W}_2 = -\nabla_{W_2} L(W_1, W_2) = W_1^\top(X^\top(Y - XW_1W_2)) .$$

Theorem : When trained with GF and initialized as (I), let $\beta = W_1W_2$,

a) Convergence to the solution: $\lim_{t\to\infty} L\left(W_1(t), W_2(t)\right) \to 0$

b) Implicit bias:

- ⋆ β : $\beta_\infty = \lim_{t\to\infty} \beta(t) = \operatorname{argmin}_{X\beta \in Y} \|\beta\|_2 = \beta_*$
- ⋆ W_1, W_2: $W_1^\infty, W_2^\infty = \operatorname{argmin}_{XW_1W_2 = Y} \|W_1\|_F^2 + \|W_2\|_F^2 - 2\gamma \log\det W_1^\top W_1$

Comments:

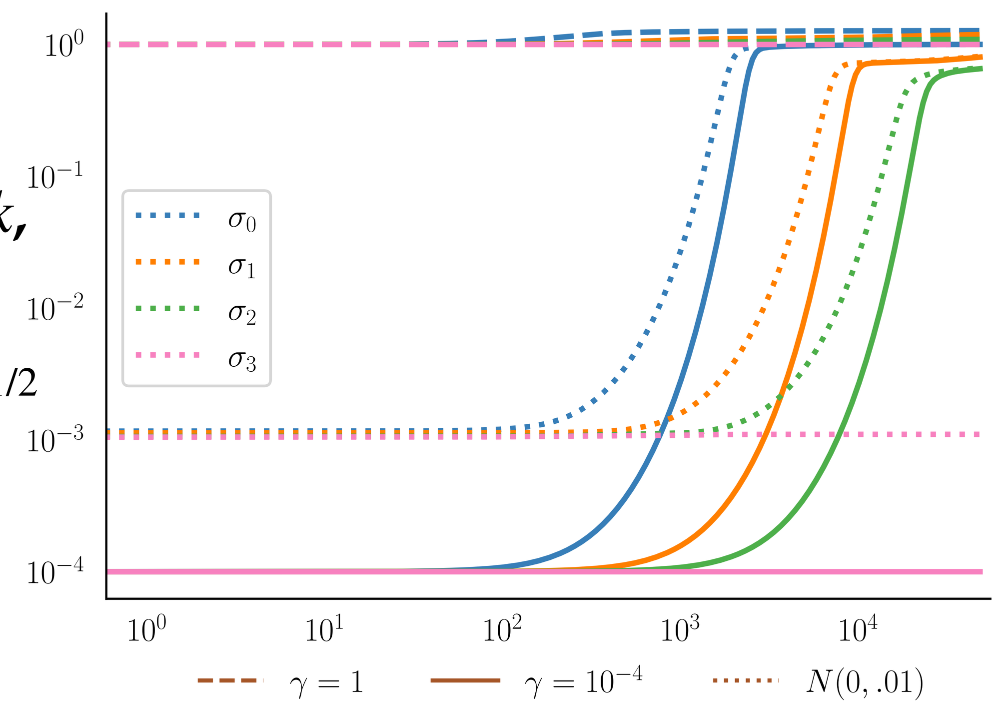
- when $\gamma \to 0$, GF converges to **min-norm interpolator** ensuring that $rank(W_1^\infty) = k$.
- $\log\det(\,.\,)$ is a smooth approximation of rank and intuitively larger γ pushes to large rank.

Corollary: We have the following expressions of final **singular values.** For $1 \le i \le k$,

$$\sigma_i\left(W_1^\infty\right) = \left(\sqrt{\sigma_i(\beta_*) + \gamma^2} + \gamma\right)^{1/2},$$

and for $k < i \le d$,

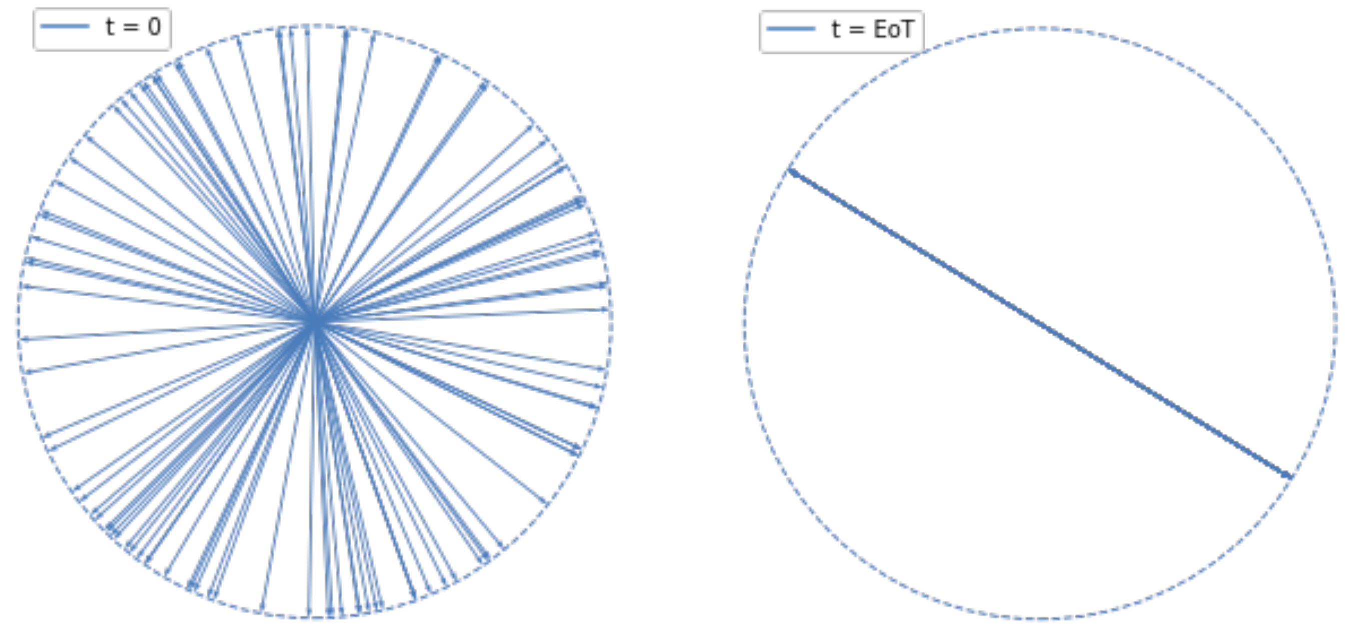
$$\sigma_i\left(W_1^\infty\right) = (2\gamma)^{1/2}$$



Evolution of singular values along the train when trained with different scales and init. shape.

GF converges to a **low-rank** W_1 at small γ (**rich** regime), whereas converges to a **high-rank** W_1 at large γ (**lazy** regime).

Going beyond small γ- noisy dynamics



Evolution of direction of neurons when trained with LNGD, shows **neuron alignment** at even **large** init. scale

LNGD: Let $\mathbf{B}_t$ denote a n-dimensional brownian motion,

$$dW = a(X^\top(Y - XW^\top a))^\top dt + a(X^\top(d\mathbf{B}_t))^\top,$$
$$da = W(X^\top(Y - XW^\top a))dt + W(X^\top d\mathbf{B}_t) .$$

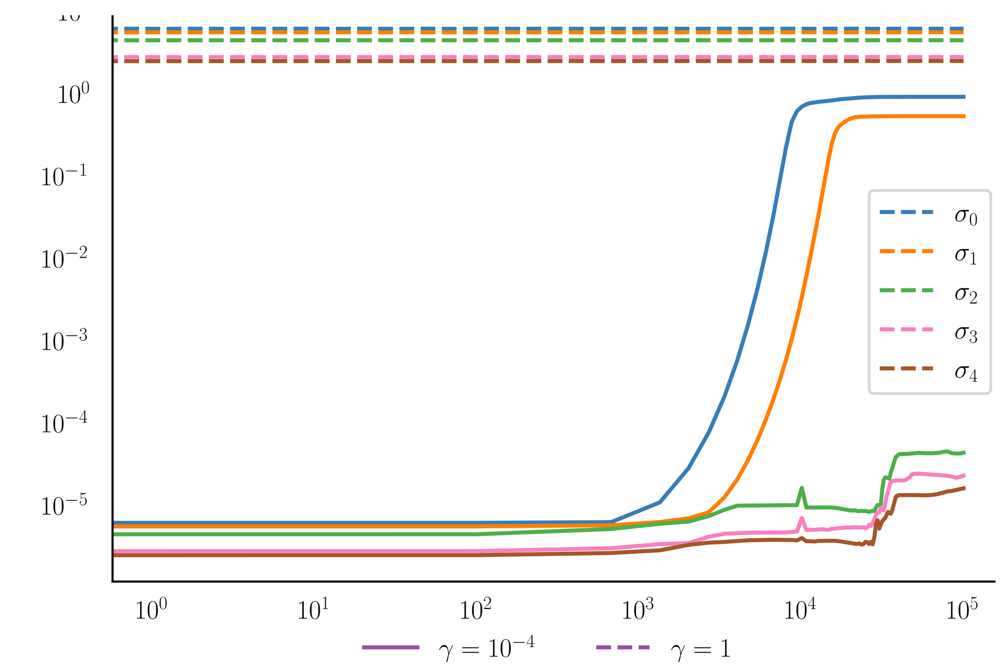
Non-linear ReLU activation

A simplified setup: Let u, v be any two orthogonal directions. We sample inputs $(x_i)_{i=1}^n$ from standard normal distribution, i.e., $x_i \sim \mathcal{N}(0, I)$ and we generate labels by a teacher network,

$$y_i = \sigma(u^\top x_i) + \sigma(v^\top x_i) .$$

We train a student network with 20 neurons on this data.

Small initialization is effective in recovering **features** even with ReLU activation.



Evolution of singular values along the train when trained with different scales for the ReLU network

References:

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