On the Explicit Role of Initialization on the Convergence and Implicit Bias of Overparametrized Linear Networks

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ABSTRACT

In this paper, we present a novel analysis of single-hidden-layer linear networks trained under gradient flow, which connects initialization, optimization, and overparametrization, specifically, we show

- The squared loss converges exponentially to its optimum at a rate that depends on the level of imbalance and the margin of the initialization.
- Proper initialization constrains the dynamics of the network parameters to lie within an invariant set. In turn, minimizing the loss over this set leads to the min-norm solution.
- Large hidden layer width, together with (properly scaled) random initialization, ensures proximity to such an invariant set during training, allowing us to derive a novel non-asymptotic upper-bound on the distance between the trained network and the min-norm solution.

PRELIMINARIES

We study the squared loss on a single-hidden-layer linear network

$$\mathcal{L}(U,V)=\frac{1}{2}\|Y-XUV^T\|_F^2$$

where $X\in\mathbb{R}^{P\times n}$, $Y\in\mathbb{R}^{P\times m}$, $U\in\mathbb{R}^{n\times k}$, $V\in\mathbb{R}^{m\times k}$ with $rank(X)=r$

n:	Input dimension	m:	Output dimension
k:	Hidden layer width	P:	# of data points
r:	rank of input data matrix		

and consider the gradient flow dynamics

$$\dot{U}=-\frac{\partial L}{\partial U},\dot{V}=-\frac{\partial L}{\partial V}$$

We decompose the weights of the first layer as

$$U=\Phi_1\overbrace{\Phi_1^TU}^{:=U_1}+\Phi_2\overbrace{\Phi_2^TU}^{:=U_2},\qquad X=W\begin{bmatrix}\Sigma_x^{1/2} & 0\end{bmatrix}\begin{bmatrix}\Phi_1^T\\ \Phi_2^T\end{bmatrix}$$

We also define the imbalance (invariant under gradient flow)

$$Q=U_1^TU_1-V^TV$$

MAIN RESULTS

Exponential convergence guarantees

$$Rate\geq\sqrt{(Imbalance)^2+4(Margin)^2}$$

Theorem 1. *(Exponential convergence) Let $\tilde{Y}=W^TY$, and*

$$\alpha=-\bar{\lambda}_++\underline{\lambda}_-+\sqrt{(\bar{\lambda}_++\underline{\lambda}_-)^2+4\left(max\left\{\sigma_m(\tilde{Y})-\left\|\tilde{Y}-\Sigma_x^{1/2}U_1V^T\right\|_F,0\right\}\right)^2/\lambda_1(\Sigma_x)}$$

$$-\bar{\lambda}_-+\underline{\lambda}_++\sqrt{(\bar{\lambda}_-+\underline{\lambda}_+)^2+4\left(max\left\{\sigma_r(\tilde{Y})-\left\|\tilde{Y}-\Sigma_x^{1/2}U_1V^T\right\|_F,0\right\}\right)^2/\lambda_1(\Sigma_x)},$$

where

$$\bar{\lambda}_+=max\{\lambda_1(Q),0\},\qquad \underline{\lambda}_-=max\{\lambda_m(-Q),0\}$$

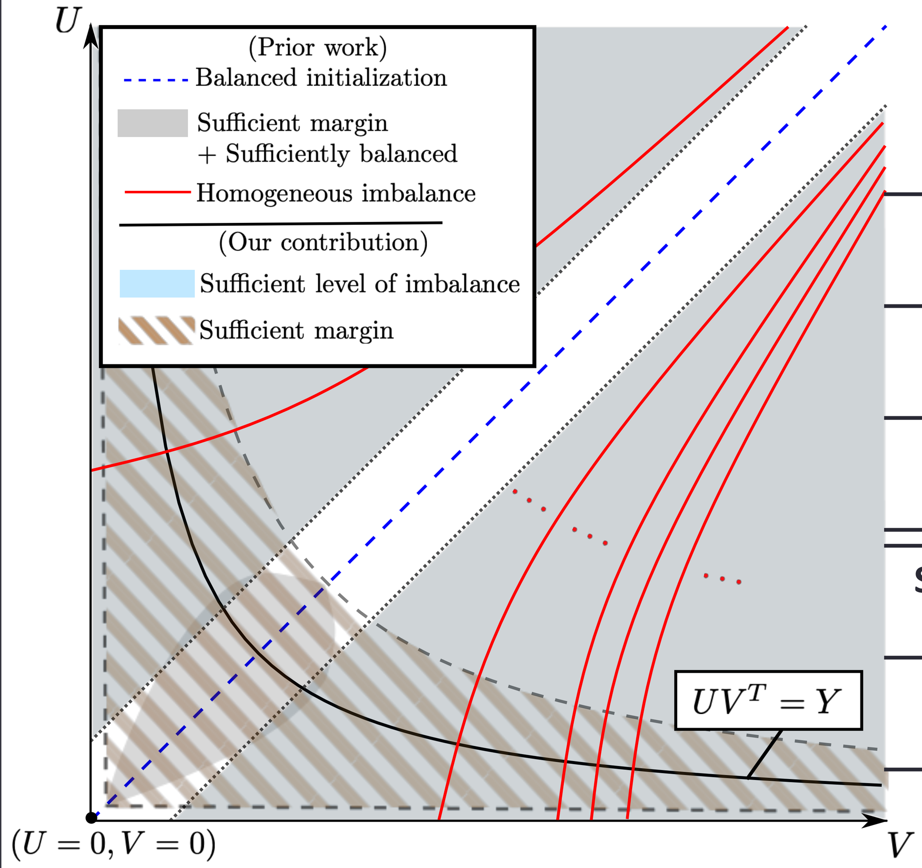
$$\bar{\lambda}_-=max\{\lambda_1(-Q),0\},\qquad \underline{\lambda}_+=max\{\lambda_n(Q),0\}$$

The gradient flow satisfies

$$L(t)-L^*\leq\exp(-\lambda_r(\Sigma_x)\alpha(0)t)(L(0)-L^*),t\geq 0$$

i.e., if $\alpha(0)>0$, $L(t)$ converges to its global minimum exponentially.

- Theorem 1 suggests that either **sufficient level of imbalance** or **sufficient margin** guarantees exponential convergence



Non-spectral initializations for the gradient flow on $\frac{1}{2}\|Y-UV^T\|_F^2$

Balanced initialization	$Q:=U^TU-V^TV=0$
Margin + approx. balanced [Arora'18]	$\sigma_{min}(Y)-\|Y-UV^T\|_F>\delta$ $\|Q\|_F\leq C\delta^2$
Homogeneous imbalance [Tarmoun'21]	$Q=\lambda_0I_h,\lvert\lambda_0\rvert>0$
Sufficient level of imbalance [Min'21]	$\underline{\lambda}_-+\underline{\lambda}_+>0$
Sufficient margin	$\sigma_{min}(Y)-\|Y-UV^T\|_F>0$

S Arora, N Cohen, and E Hazan. "On the optimization of deep networks: Implicit acceleration by overparameterization." ICML 2018
S Tarmoun, G França, B D Haeffele, and R Vidal. "Understanding the dynamics of gradient flow in overparameterized linear models." ICML 2021
H Min, S Tarmoun, R Vidal, and E Mallada. "On the explicit role of initialization on the convergence and implicit bias of overparametrized linear networks." ICML 2021.

MAIN RESULTS

Orthogonal Initialization Leads to Min-norm Solution

The min-norm solution is given by

$$\hat{\Theta}=argmin_\Theta\{\|\Theta\|_F:\|Y-X\Theta\|_F=min_\Theta\|Y-X\Theta\|_F\}$$

Proposition 1. (Informal) *If at initialization, we have*

$$V(0)U_2^T(0)=0,\qquad U_1(0)U_2^T(0)=0,$$

then the gradient flow, if converges, finds the min-norm solution.

- Extension of "initializing Θ within the span of the input data leads to min-norm solution" in standard linear regression problem
- For single-hidden-layer model, initialization within the span of the data $VU_2^T=0$ is not sufficient

Under **random initialization + large hidden layer width k**, w.h.p.:

- There is sufficiently positive level of imbalance
- Orthogonality conditions are approximately satisfied

Theorem 2. (Informal) *With random initialization (properly scaled) and large hidden layer width, the gradient flow finds a solution within $\mathcal{O}(k^{-1/2})$distance to the min-norm solution with high probability*

SUMMARY

We study the gradient flow on single-hidden-layer linear networks:

- **Sufficient Imbalance or Sufficient Margin** ⇒ exponential convergence
- **Orthogonal initialization** ⇒ exact min-norm solution
- **Random initialization + large network width** finds near min-norm solution efficiently

Future work:

- Deep Linear Networks and potentially nonlinear networks