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

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Problem Setup

- Training data $X = [x^{(1)} \quad \cdots \quad x^{(n)}]^T \in \mathbb{R}^{n\times D}, Y = [y^{(1)} \quad \cdots \quad y^{(n)}]^T \in \mathbb{R}^{n\times m}$
- Single-hidden layer linear network, squared loss

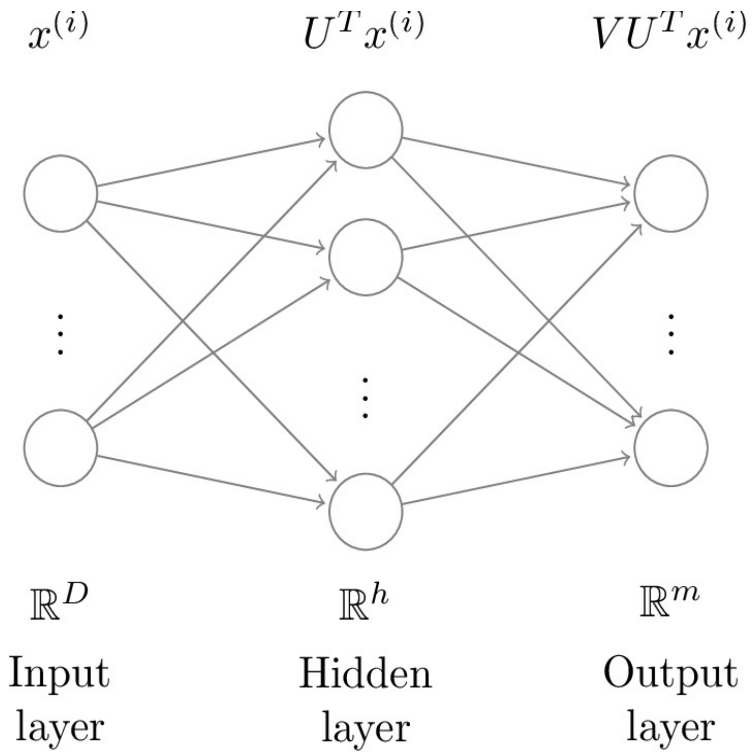
$$L(U,V) = \frac{1}{2}\|Y - XUV^T\|_F^2, \qquad U \in \mathbb{R}^{D\times h}, V \in \mathbb{R}^{m\times h}$$

  - Underdetermined linear regression: $D > n$
  - Overparametrized model: $h \geq min\{D, m\}$

- Gradient flow dynamics

$$\dot{U} = -\frac{\partial L}{\partial U} = (Y - XUV^T)V^T$$

$$\dot{V} = -\frac{\partial L}{\partial V} = (Y - XUV^T)^T U$$



Problem Setup

- Suppose $rank(X) = r$, we decompose the weight U using the SVD of X

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

- We have $U_1 \in \mathbb{R}^{r \times h}$, $U_2 \in \mathbb{R}^{m \times h}$, and

$$\dot{U}_1 = \Sigma_x^{1/2} \left(W^T Y - \Sigma_x^{1/2} U_1 V^T \right) V^T, \qquad \dot{U}_2 = 0,$$

$$\dot{V} = \left(W^T Y - \Sigma_x^{1/2} U_1 V^T \right)^T \Sigma_x^{1/2} U$$

- For **convergence**, it suffices to study the flow of U_1 and V, which is exactly the gradient flow dynamics on $\tilde{L}(U_1, V) = \frac{1}{2} \left\| W^T Y - \Sigma_x^{1/2} U_1 V^T \right\|_F^2$

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- We also study the **implicit bias towards the min-norm solution**

$$\widehat{\Theta} = \min_{\Theta} \left\{ \|\Theta\|_F : \ \|Y - X\Theta\|_F = \min_{\Theta} \|Y - X\Theta\|_F \right\}$$

Overview

- **Sufficient imbalance** or **sufficient margin** guarantees exponential convergence

- **Orthogonal initialization** leads to min-norm solution

- **Random initialization** + **large network width** approximately satisfies the two conditions above, allowing us to find near minimum norm solution efficiently

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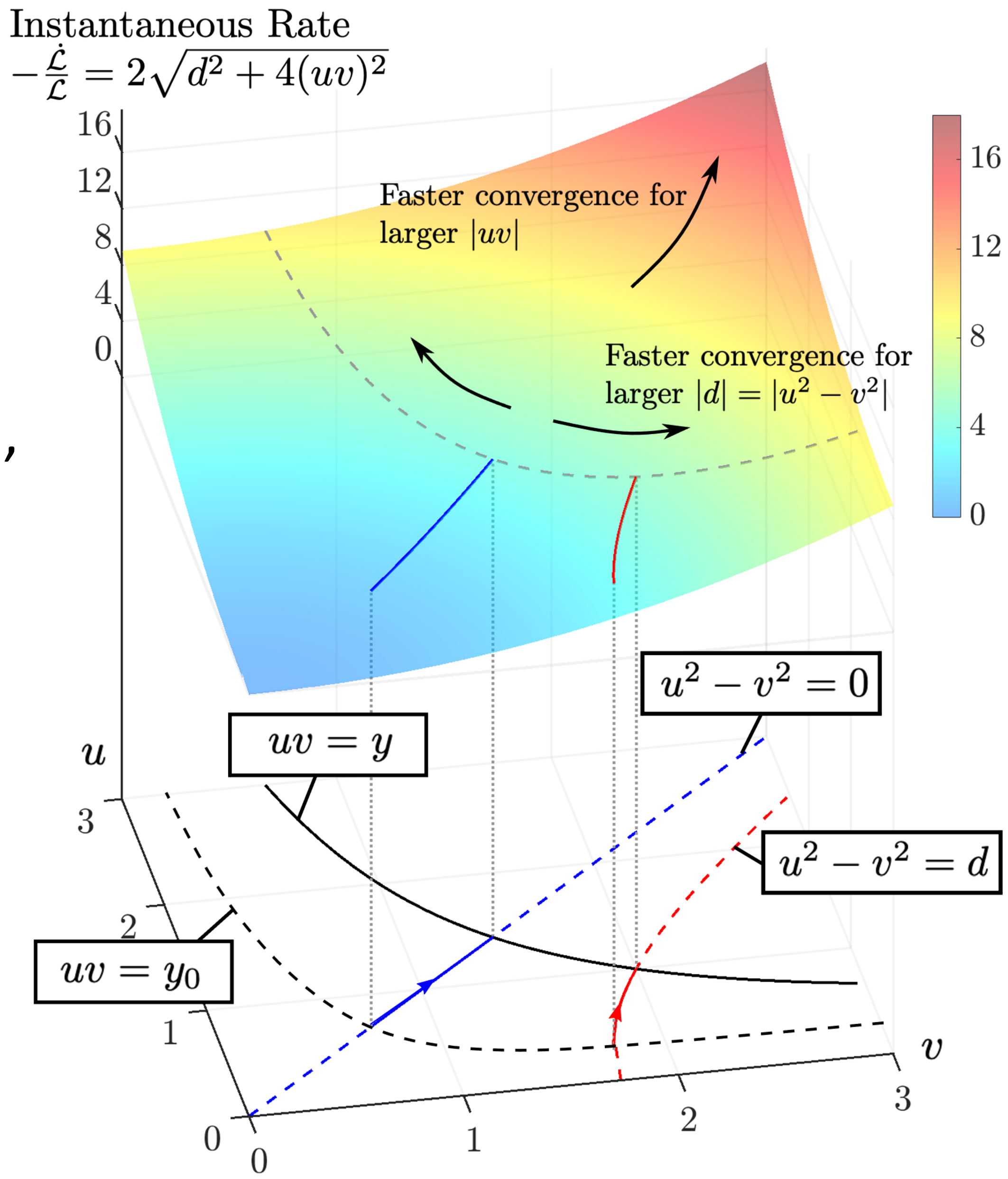
Convergence Analysis: Insights from Scalar Dynamics

Consider the gradient flow on

$$L(u, v) = |y - uv|^2/2$$

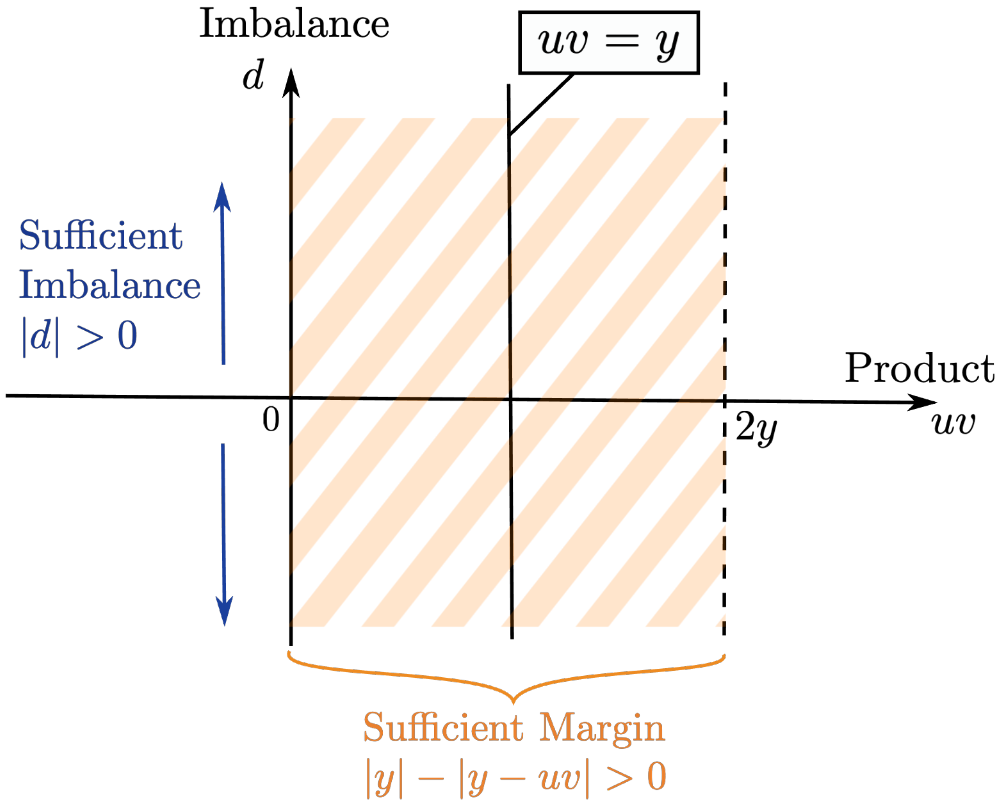
- The imbalance $d = u^2 - v^2$ is time invariant
- Start with same initial product $uv = y_0$, different imbalance leads to different trajectory (solid lines)

- The instantaneous rate $-\dot{L}/L$ is closely related to the exponential convergence
- Instantaneous rate depends on the **imbalance** d and the **product** uv



Convergence Analysis: Insights from Scalar Dynamics

Instantaneous rate depends on the **imbalance** $|d|$ and the **product** $|uv|$



Proper initialization controls d and uv for the entire trajectory:

- $|d|$ is time invariant
- Positive margin $|y| - |y - uv| > 0$ ensures $|uv|$ stays above margin

A lower bound on Instantaneous rate leads to exponential convergence

$$-\dot{L}(t)/L(t) \geq c \implies \int_0^t \dot{L}(t)/L(t)dt \leq -ct$$

$$\implies \log \frac{L(t)}{L(0)} \leq -ct \implies L(t) \leq \exp(-ct)\, L(0)$$

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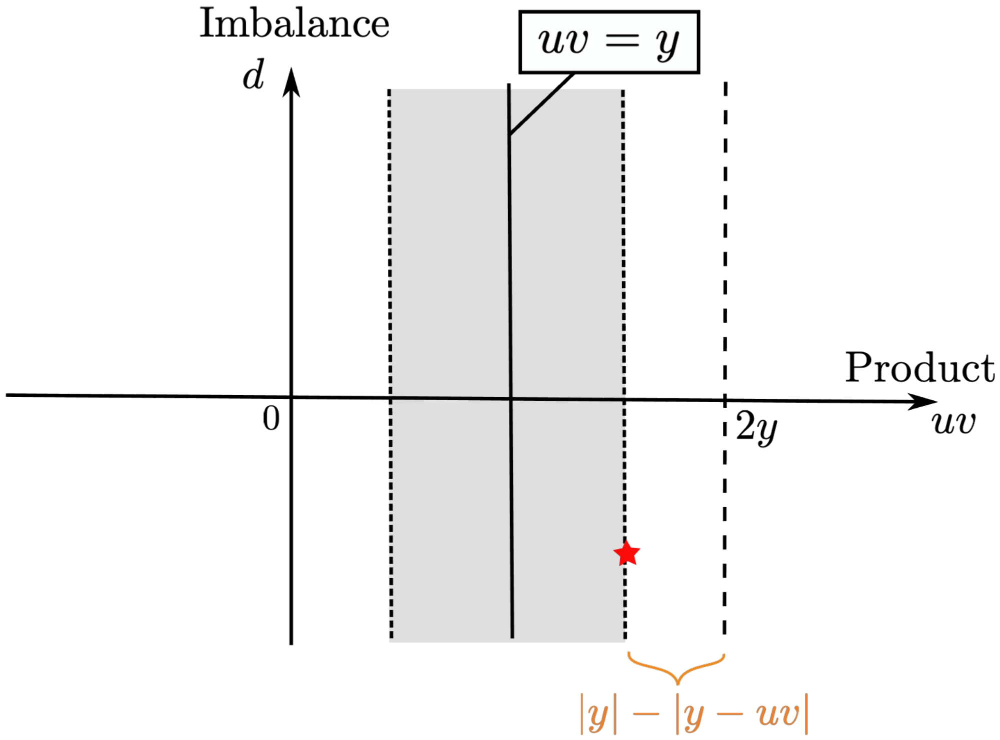

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Convergence Analysis: Our Contribution

In our problem setting, we study the gradient flow on $U_1 \in \mathbb{R}^{r\times h}, U_2 \in \mathbb{R}^{m\times h}$ with loss function

$$\tilde{L}(U_1, V) = \frac{1}{2}\left\|W^T Y - \Sigma_x^{1/2} U_1 V^T\right\|_F^2 = L(U,V) - L^*$$

We show

- A lower bound on the instantaneous rate $-\dot{\tilde{L}}/\tilde{L}$ that depends on the **imbalance** $D = U_1^T U_1 - V^T V$ and the **product** $U_1 V^T$
- Two types of initialization that guarantees initialization
  - Sufficient level of imbalance
  - Sufficient margin

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For simplicity, we present the results for the case $W = I_r, \Sigma_x = I_r$

Convergence Analysis: Instantaneous Rate

***Proposition** 1. (Lower bound on instantaneous rate, $\Sigma_x = I_r$) Define $D = U_1^T U_1 - V^T V$. Let $\dot{\tilde{L}}(U_1, V)$ be the time derivative of $\tilde{L}(U_1, V)$ under gradient flow. Then we have*

$$-\frac{\dot{\tilde{L}}(U_1,V)}{\tilde{L}(U_1,V)} \geq -\bar{\lambda}_+ + \underline{\lambda}_- + \sqrt{\left(\bar{\lambda}_+ + \underline{\lambda}_-\right)^2 + 4\sigma_m^2(U_1V^T)}$$
$$-\bar{\lambda}_- + \underline{\lambda}_+ + \sqrt{\left(\bar{\lambda}_- + \underline{\lambda}_+\right)^2 + 4\sigma_r^2(U_1V^T)},$$

where

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

- (Recall) insta. rate in scalar dynamics: $-\dot{L}/L = 2\sqrt{d^2 + 4(uv)^2}$
- Tightness: Fix imbalance D and product U_1V^T, there exists U_1, V that attains the exact lower bound for the insta. rate

Exponential Convergence Guarantee

***Theorem** 1. (Exponential convergence, $\Sigma_x = I_r$) Let*

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

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

then under gradient flow satisfies

$$\tilde{L}(t) \leq \exp(-c(0)t)\tilde{L}(0)\,, t \geq 0$$

i.e., if $c(0) > 0$, $\tilde{L}(t)$ converges to zero exponentially at a rate at least $c(0)$.

- Control the Imbalance and margin at initialization
- $\tilde{L}(U_1, V) = L(U, V) - L^*$, $L(t)$ converges to its global minimum exponentially
- First exponential convergence result for non-spectral initialization with general imbalance structure

Exponential Convergence Guarantee

***Corollary** 1. (Sufficient level of imbalance* [Min'21] *) If at initialization, we have*

$$c' = \underline{\lambda}_- + \underline{\lambda}_+ > 0,$$

then $\tilde{L}(t)$ converges to zero exponentially at a rate at least $2c'$.

- $-\bar{\lambda}_+ + \underline{\lambda}_- + \sqrt{\left(\bar{\lambda}_+ + \underline{\lambda}_-\right)^2 + 4(max\{\sigma_m(Y) - \|Y - U_1V^T\|_F, 0\})^2} \geq 2\underline{\lambda}_-$

***Corollary** 2. (Sufficient margin) If at initialization, we have*

$$\sigma_{min}(Y) - \|Y - U_1V^T\|_F > 0,$$

then $c(0) > 0$ and $\tilde{L}(t)$ converges to zero exponentially at a rate at least $c(0)$.

- Convergence with positive margin was studied for sufficiently balanced initialization [Arora'18]
- No requirement on imbalance here

Exponential Convergence Guarantee

***Corollary** 3. (Characterizing local convergence rate) If at some t_0, we have $t_0 > 0$, then*

$$\tilde{L}(t) \leq \exp(-c(t_0)t)\tilde{L}(t_0)\,, t \geq t_0.$$

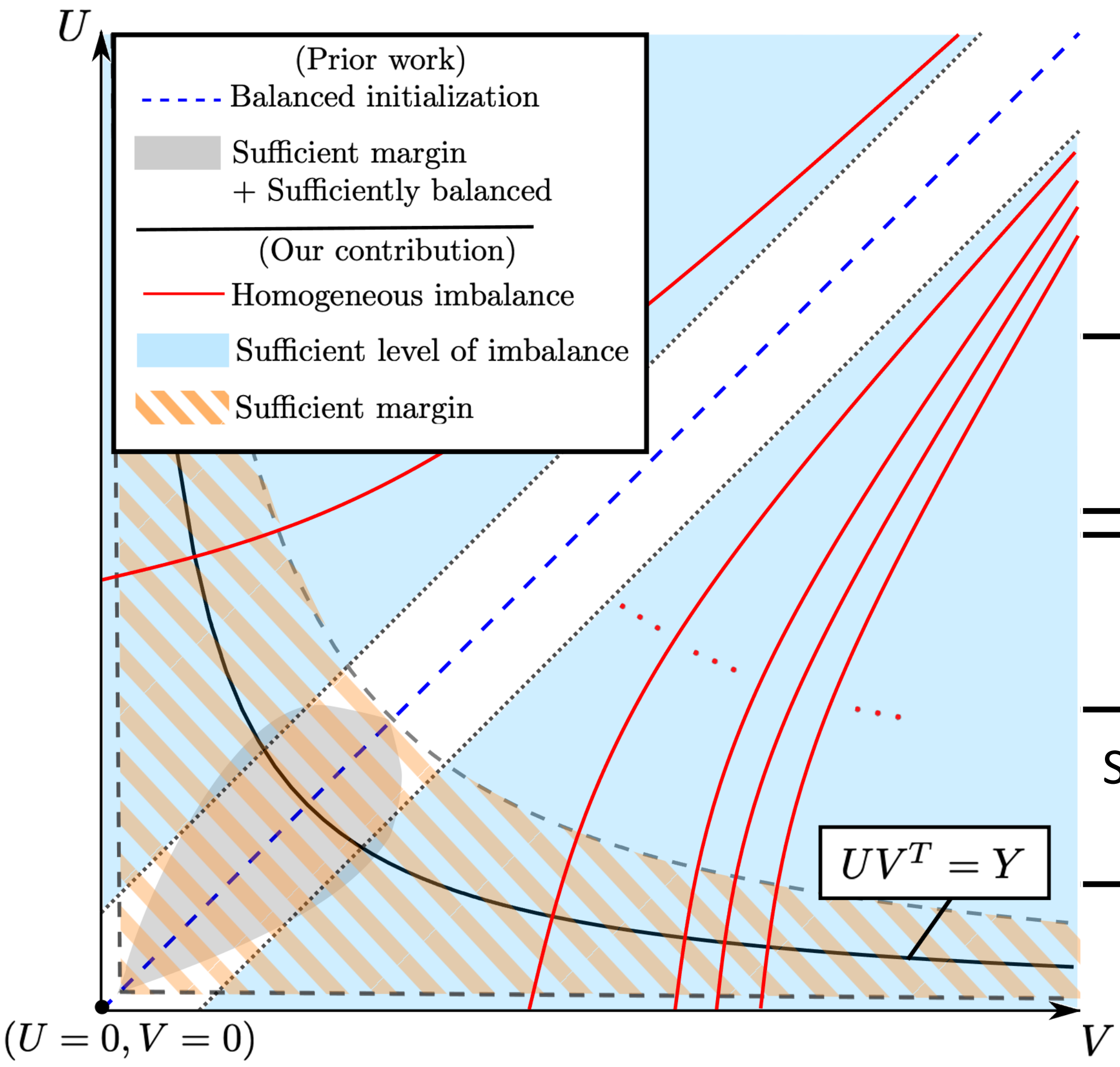
That is, after t_0, the loss converges to zero exponentially with a rate at least $c(t_0)$. Notably, for sufficiently large t_0, we have

$$c(t_0) \approx -\bar{\lambda}_+ + \underline{\lambda}_- + \sqrt{\left(\bar{\lambda}_+ + \underline{\lambda}_-\right)^2 + 4\sigma_m^2(Y)}$$

$$-\bar{\lambda}_- + \underline{\lambda}_+ + \sqrt{\left(\bar{\lambda}_- + \underline{\lambda}_+\right)^2 + 4\sigma_r^2(Y)}.$$

- Convergence rate around equilibrium: imbalance D and target Y
- [Salma'21] studies the local convergence rate when $D = \lambda_0 I_h, |\lambda_0| > 0$
- No assumption on the imbalance structure here

Exponential Convergence Guarantee: Summary



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

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

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Reference

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