Gradient Descent for Deep Matrix Factorization

Dynamics and Implicit Bias towards Low Rank

Donata Buožytė

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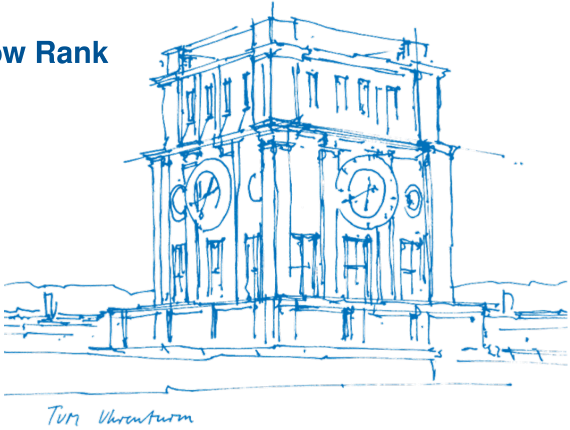

Gradient Descent for Deep Matrix Factorization: Dynamics and Implicit Bias towards Low Rank

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Outline

Motivation

theoretical studies	real situations
neural network trained with the (stochastic) gradient descent results in zero training error $\rightarrow$ model is overfitting	neural networks trained with the SDG lead to models that generalize pretty well

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observations:

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$\Rightarrow$ key task: understand nature of implicit bias

Feed Forward Neural Networks

General Case

- $h : \mathbb{R}^{n_0} \to \mathbb{R}^{n_N}$, $h(x) = g_N \circ \ldots \circ g_1(x)$, $N > 1$ with:
  - layers: $g_k : \mathbb{R}^{n_{k-1}} \to \mathbb{R}^{n_k}$, $h_k(x) = \sigma(W_k x + b_k)$
  - weight matrices: $W_k \in \mathbb{R}^{n_k \times n_{k-1}}$
  - bias terms: $b_k \in \mathbb{R}^{n_k}$
  - activation function: $\sigma : \mathbb{R} \to \mathbb{R}$, in general non-linear

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  - activation function: $\sigma : \mathbb{R} \to \mathbb{R}$, in general non-linear
- loss function: $\mathcal{L} : \mathbb{R}^{n_N} \times \mathbb{R}^{n_N} \to \mathbb{R}_+$
- approach in supervised learning:

$$\min_{W_1,\ldots,W_N} \frac{1}{M} \sum_{i=1}^{M} \mathcal{L}(h(x_i), y_i)$$

Feed Forward Neural Networks

Linear Case

- linear neural networks: $\sigma(x) = x$, $b_k = 0$, hence
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- approach with quadratic loss:
$$\min_{W_1,\dots,W_N} \frac{1}{M} \sum_{i=1}^{M} \|W_N \dots W_1 x_i - y_i\|_2^2 \tag{1}$$
- it can be shown: if $\operatorname{span}(\{x_i\}_{i=1}^{M}) = \mathbb{R}^{n_0}$, then the set of minimizers of (1) is equivalent to the set of minimizers of
$$\min_{W_1,\dots,W_N} \|W_N \dots W_1 - \hat{W}\|_F^2 \tag{2}$$

($\hat{W}$ = ground truth matrix)

Frobenius Norm

For $A \in \mathbb{R}^{m \times n}$:

$$
\begin{aligned}
\|A\|_F^2 &= \sum_{i=1}^{m} \sum_{j=1}^{n} (a_{ij})^2 \\
&= \operatorname{trace}(A^T A) \\
&= \operatorname{trace}((U \Sigma V^T)^T (U \Sigma V^T)) \\
&= \operatorname{trace}(\Sigma^T \Sigma) \\
&= \sum_{i=1}^{r} \sigma_i^2
\end{aligned}
$$

Gradient Descent

For the loss function:

$$\mathcal{L}(W) = \frac{1}{2}\|W - \hat{W}\|_F^2, \quad \nabla_W \mathcal{L}(W) = (W - \hat{W}) \tag{3}$$

$$\nabla_{W_j} \mathcal{L}(W) = (W_N \dots W_{j+1})^T \nabla_W \mathcal{L}(W)(W_{j-1} \dots W_1)^T \tag{4}$$

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the gradient descent is defined as:

$$W_j^{(0)} = \alpha W_0 \tag{5}$$

$$W_j^{(k+1)} = W_j^{(k)} - \eta \nabla_{W_j}\mathcal{L}(W^{(k)}) \tag{6}$$

Outline

Dynamics of Gradient Descent with Identical Initialization

Consider the (discrete) dynamics

$$W_j^{(0)} = \alpha W_0$$
$$W_j^{(k+1)} = W_j^{(k)} - \eta \nabla_{W_j} \mathcal{L}(W^{(k)})$$

with an identical initialization $W_0 = I$.

Dynamics of Gradient Descent with Identical Initialization

Now let $(W_j^{(k)})_{j=1}^N$ be solutions of the discrete dynamics with identical initialization and $\hat{W} = V\Lambda V^T$ the eigendecomposition of the symmetric ground truth matrix $\hat{W}$.

Dynamics of Gradient Descent with Identical Initialization

Now let $(W_j^{(k)})_{j=1}^N$ be solutions of the discrete dynamics with identical initialization and $\hat{W} = V\Lambda V^T$ the eigendecomposition of the symmetric ground truth matrix $\hat{W}$.Then:

1. $D^{(k)} = D_j^{(k)} := V^T W_j^{(k)} V \quad \forall j$ are real, diagonal, identical
2. $D^{(k)}$ follows the dynamics $D^{(k+1)} = D^{(k)} - \eta (D^{(k)})^{N-1}((D^{(k)})^N - \Lambda)$

Dynamics of Gradient Descent with Identical Initialization

Hence by definition:

- $W_j^{(k)} = VD^{(k)}V^T \quad \forall j, k$
- $W_N^{(k)} \dots W_1^{(k)} = (VD^{(k)}V^T)^N = V(D^{(k)})^N V^T \quad \forall k$

Dynamics of Gradient Descent with Identical Initialization

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- $W_N^{(k)} \dots W_1^{(k)} = (VD^{(k)}V^T)^N = V(D^{(k)})^N V^T \quad \forall k$

Additionally: as $D^{(k)}$ is diagonal, the dynamics can be reformulated as

$$d_{ii}^{(k+1)} = d_{ii}^{(k)} - \eta(d_{ii}^{(k)})^{N-1}((d_{ii}^{(k)})^N - \lambda_i) \tag{7}$$

where λ_i is the corresponding eigenvalue of $\hat{W}$.

Dynamics of Gradient Descent with Identical Initialization

Theorem 2.1 $N \geq 2$, $\lambda \in \mathbb{R}$, $\alpha > 0$, $\{d^{(k)}\}_k$ *the solution of* (7).
Let $M = \max(\alpha, |\lambda|^{\frac{1}{N}})$ *and* η *be s.t.*

$$0 < \eta < \begin{cases} \frac{1}{2NM^{2N-2}} & \textit{if } \lambda \geq 0 \\ \frac{1}{(3N-2)M^{2N-2}} & \textit{if } \lambda < 0. \end{cases}$$

Additionally let $\epsilon \in (0, |\alpha - \lambda_+^{\frac{1}{N}}|)$ *the desired error and* $T = \min\{k : |d^{(k)} - \lambda_+^{\frac{1}{N}}| \leq \epsilon\}$ *the minimal number of steps needed to achieve the desired error.*

Then: $T \leq T_N^{\mathrm{Id}}(\lambda, \epsilon, \alpha, \eta)$.
(Note: T_N^{Id} *is an estimation of the required number of steps with 5 different cases depending on the input values.)*

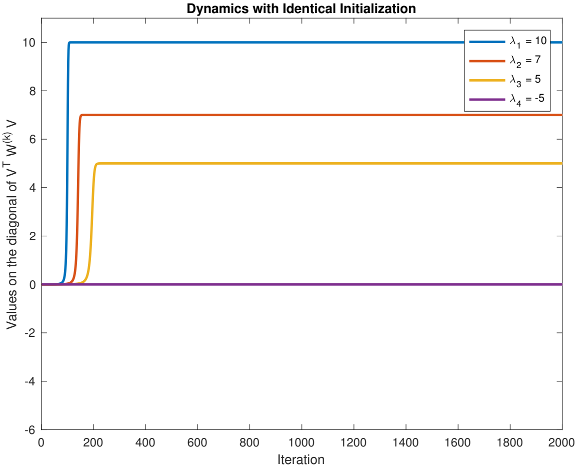
Recovery of positive eigenvalues

Theorem 2.2 *$N \geq 2$, $\hat{W} = V\Lambda V^T \in \mathbb{R}^{n\times n}$ an eigendecomposition the symmetric matrix $\hat{W}$.*
Let $W^{(k)} = W_N^{(k)} \dots W_1^{(k)}$ with $W_j^{(k)}$ defined by (5)-(6) *with loss function* (3)*, $W_0 = I$ and $\alpha > 0$.*
Let $M = \max(\alpha, \|\hat{W}\|_2^{\frac{1}{N}})$ and η be s.t.

$$0 < \eta < \frac{1}{(3N-2)M^{2N-2}}. \tag{8}$$

Then: $\lim_{k\to\infty} W^{(k)} = V\Lambda_+ V^T$ and the error is the diagonal matrix $E^{(k)} = V^T W^{(k)} V - \Lambda_+$.

Recovery of positive eigenvalues: Example



$$\hat{W} = \begin{pmatrix} 7/3 & 10/3 & -4 & 2/3 \\ 10/3 & 10/3 & 5 & 5/3 \\ -4 & 5 & 4 & 1 \\ 2/3 & 5/3 & 1 & -5 \end{pmatrix}$$

$$\Lambda = \begin{pmatrix} 10 & 0 & 0 & 0 \\ 0 & 7 & 0 & 0 \\ 0 & 0 & 5 & 0 \\ 0 & 0 & 0 & -5 \end{pmatrix}$$

$$N = 3, \ \alpha = 0.1$$

Recovery of positive eigenvalues

Conclusion of Theorem 2.2:
the dynamics

$$W_j^{(0)} = \alpha I$$
$$W_j^{(k+1)} = W_j^{(k)} - \eta \nabla_{W_j} \mathcal{L}(W^{(k)})$$

can recover the non-negative eigenvalues of $\hat{W}$ under certain conditions.

Outline

Dynamics of Gradient Descent with Perturbed Initialization

Idea:
instead of initializing all $W_j^{(0)}$ with only αI, perturb the initialization slightly by for example using

$$W_j^{(0)} = \begin{cases} (\alpha - \beta) I & \text{if } j = 1 \\ \alpha I & \text{otherwise} \end{cases} \tag{9}$$

with $0 < \beta < \alpha$.

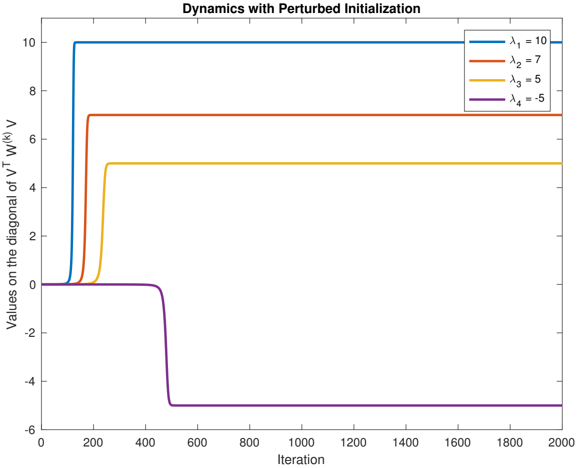
Recovery of arbitrary eigenvalues

Theorem 3.1 *$N \geq 2$, $\hat{W} = V\Lambda V^T \in \mathbb{R}^{n\times n}$ an eigendecomposition the symmetric matrix $\hat{W}$.*
Let $W^{(k)} = W_N^{(k)} \dots W_1^{(k)}$ with $W_j^{(k)}$ defined by (5) *and the perturbed initialization* (9) *with loss function* (3) *and $W_0 = I$.*
Let $M = \max(\alpha, \|\hat{W}\|_2^{\frac{1}{N}})$, $0 < \frac{\beta}{c-1} < \alpha$, $c \in (1,2)$ with c being the maximal real solution of $1 = (c-1)c^{N-1}$ and η be s.t.

$$0 < \eta < \frac{1}{9N(cM)^{2N-2}}. \tag{10}$$

Then: $\lim_{k\to\infty} W^{(k)} = V\Lambda V^T = \hat{W}$ and the error is the diagonal matrix $E^{(k)} = V^T W^{(k)} V - \Lambda$.

Recovery of arbitrary eigenvalues: Example



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$$N = 3,\ \alpha = 0.1,\ \beta = 0.05$$

Recovery of arbitrary eigenvalues

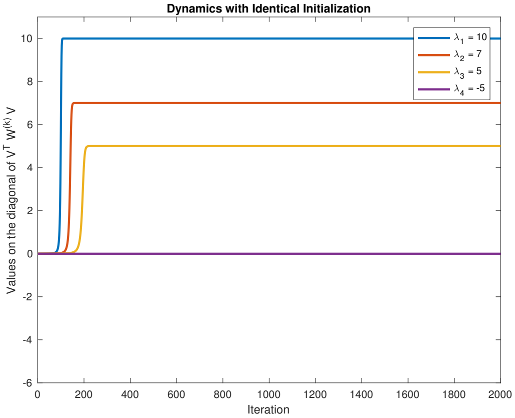
First conclusion of Theorem 3.1:
the dynamics

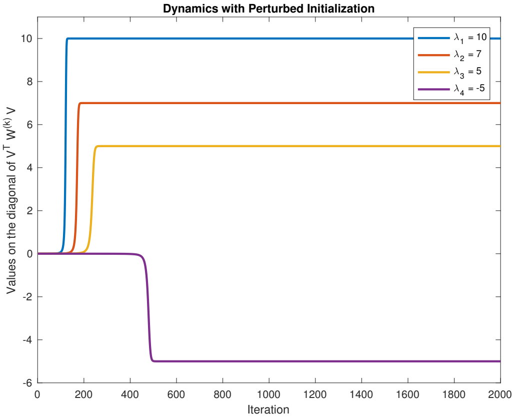
$$W_j^{(0)} = \begin{cases} (\alpha - \beta)I & \text{if } j = 1 \\ \alpha I & \text{otherwise} \end{cases}$$

$$W_j^{(k+1)} = W_j^{(k)} - \eta \nabla_{W_j} \mathcal{L}(W^{(k)})$$

can recover the all eigenvalues of $\hat{W}$ under certain conditions.

Recovery of arbitrary eigenvalues: Example





Recovery of arbitrary eigenvalues

Second conclusion of Theorem 3.1:
there are two different regimes of the dynamic:

1. if $\lambda_i > 0$: dynamics behave as in 2.2 ("only positive eigenvalues")

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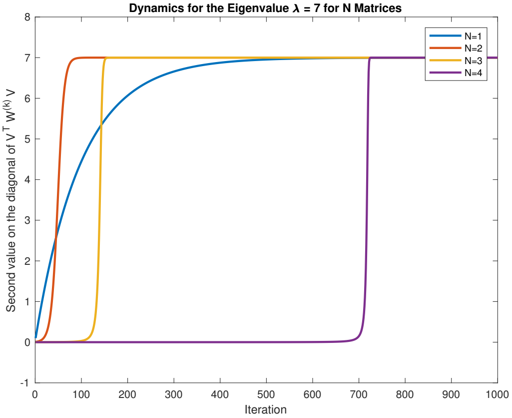
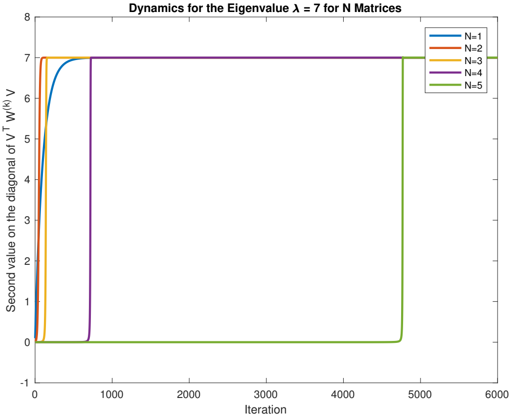
there are two different regimes of the dynamic:

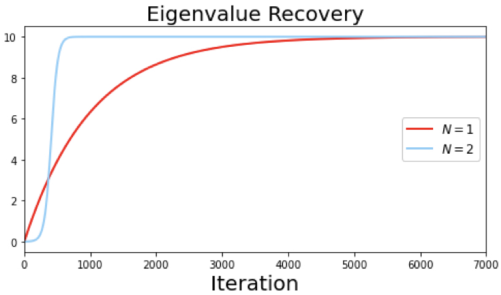
1. if $\lambda_i > 0$: dynamics behave as in 2.2 ("only positive eigenvalues")
2. if $\lambda_i < 0$: at first $(\lambda_i)_+$ is approximated up to β and only after reaching that level forced to take negative values

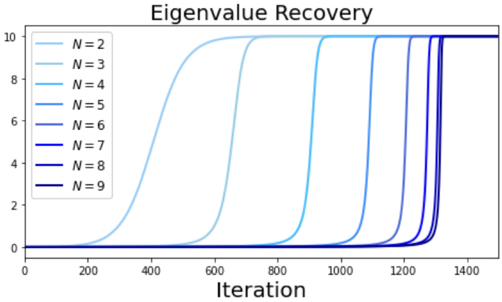
Eigenvalue Recovery for Different Depths: Example





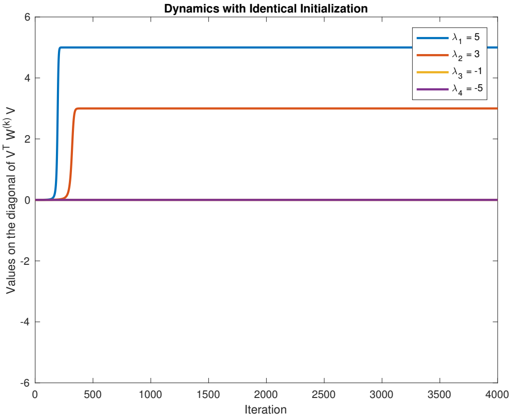
Eigenvalue Recovery for Different Depths

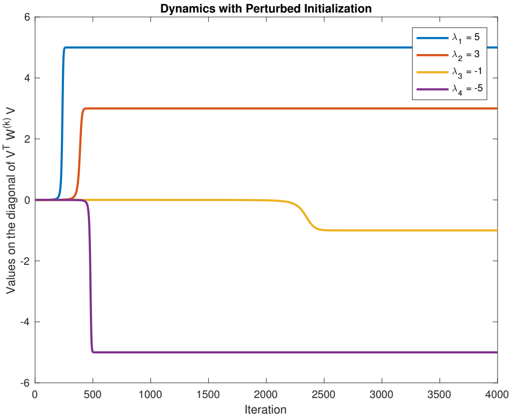




Outline

Implicit Bias Towards Low-Rank: Example





Implicit Bias Towards Low-Rank

The Theorems 2.2 and 3.1 suggest:

- as dominant eigenvalues will be approximated faster: stopping the gradient descent at a suitable finite k will result in a low rank matrix $W^{(k)}$

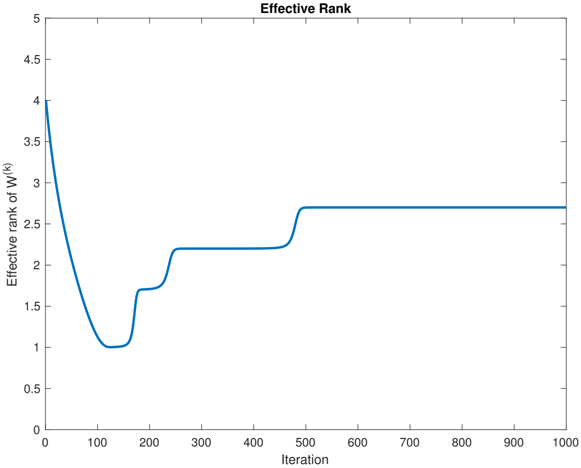
Implicit Bias Towards Low-Rank

The Theorems 2.2 and 3.1 suggest:

- as dominant eigenvalues will be approximated faster: stopping the gradient descent at a suitable finite k will result in a low rank matrix $W^{(k)}$
- it can be shown: effective rank of $W^{(k)}$ drops to one, then monotonically increases to plateau on effective ranks of various low-rank approximations of $\hat{W}$

Effective rank: $1 \leq r(W) = \frac{\|W\|_*}{\|W\|_2} = \frac{\sum_j \sigma(A)_j}{\|W\|_2} \leq \operatorname{rank}(W)$

Effective Rank: Example



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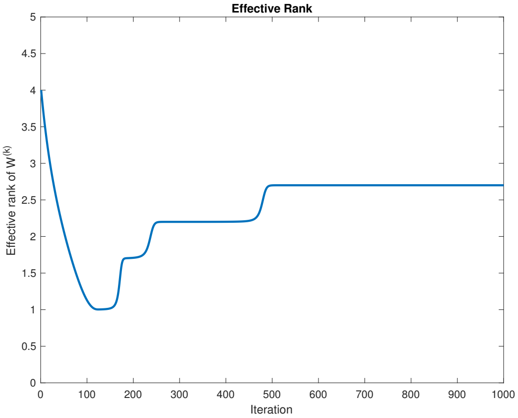

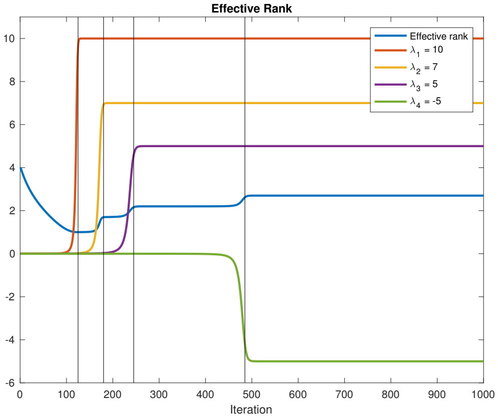

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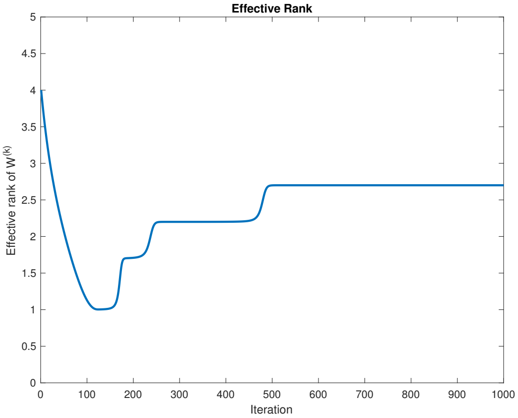

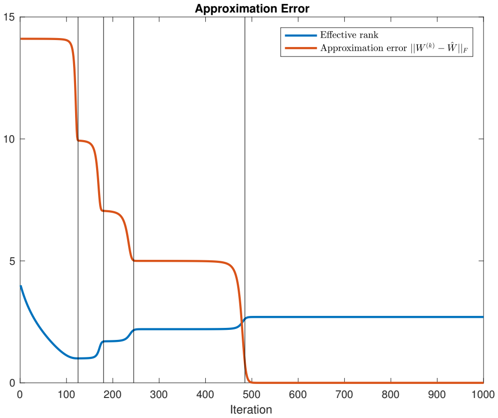

Outline

Central Observations

Three central observations:

1. recovery of positive eigenvalues
2. recovery of arbitrary eigenvalues
3. implicit bias towards low-rank

Thank you for your attention!