Optimization and Generalization for Deep Linear Neural Networks via Trajectories of Gradient Descent

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Tel Aviv University

Princeton University, Computer Science Department

Theoretical Deep Learning Course (COS 597B)

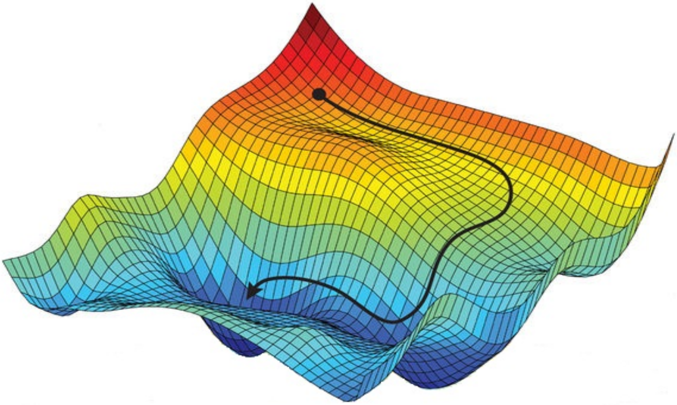
6 December 2019

Outline

1. Optimization and Generalization in Deep Learning via Trajectories
2. Case Study: Linear Neural Networks
   - Trajectory Analysis
   - Optimization
   - Generalization
3. Conclusion

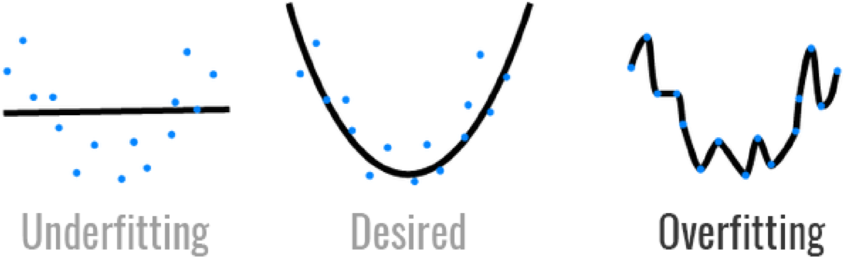
Optimization

Fitting training data by minimizing an objective (loss) function

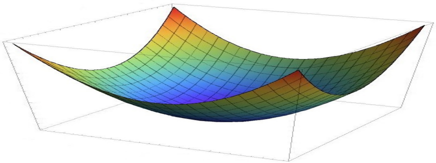


Generalization

Controlling gap between train and test errors, e.g. by adding regularization term/constraint to objective



Classical Machine Learning



Theme: make sure objective is convex!

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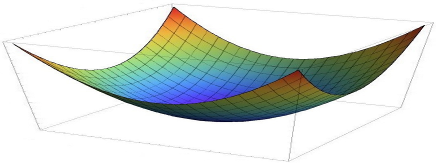

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- Choice of algorithm affects only speed of convergence

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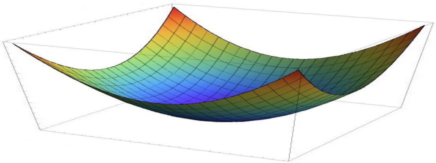

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Bias-variance trade-off:

regularization	*train/test gap*	*train err*
more	↘	↗
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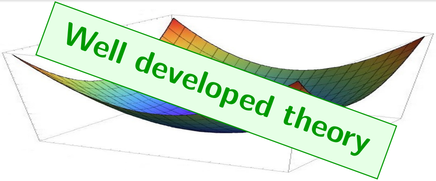

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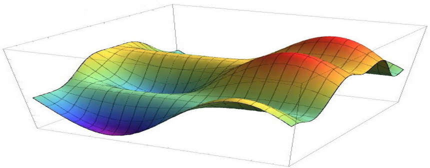

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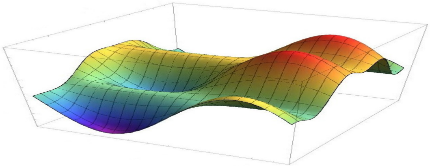

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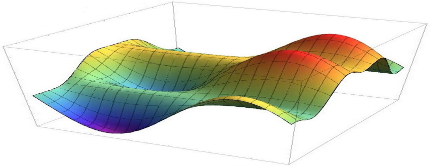

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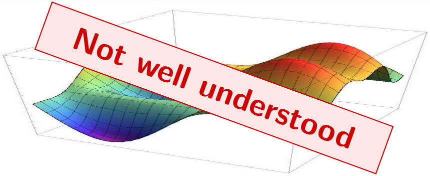

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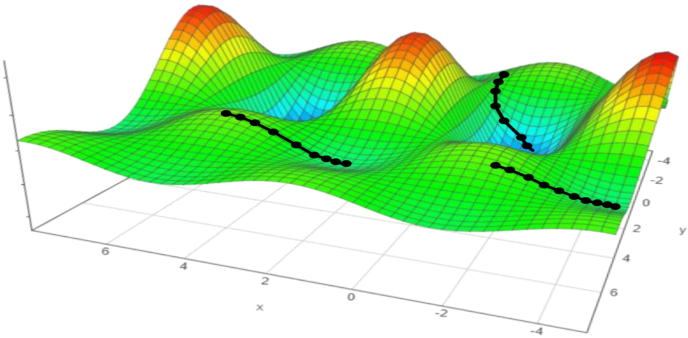

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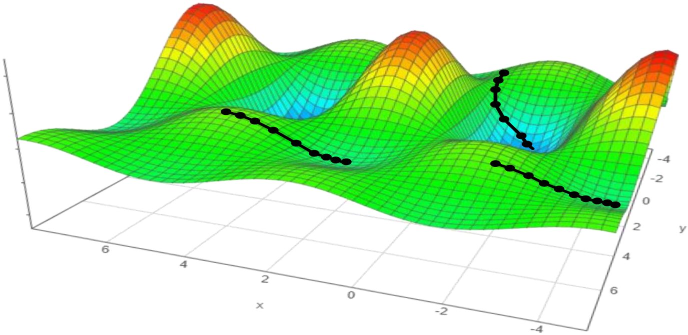


We will demonstrate this for deep linear neural networks

Outline

Sources

On the Optimization of Deep Networks:
Implicit Acceleration by Overparameterization

Arora + ***C*** + Hazan

International Conference on Machine Learning (ICML) 2018

A Convergence Analysis of Gradient Descent for Deep Linear Neural Networks

Arora + ***C*** + Golowich + Hu

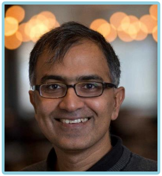
International Conference on Learning Representations (ICLR) 2019

Implicit Regularization in Deep Matrix Factorization

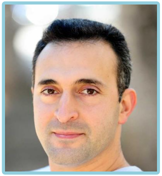
Arora + ***C*** + Hu + Luo

Conference on Neural Information Processing Systems (NeurIPS) 2019

Collaborators



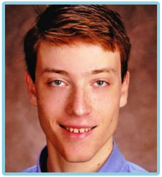
Sanjeev Arora



Elad Hazan

Yuping Luo

Wei Hu



Noah Golowich

Linear Neural Networks

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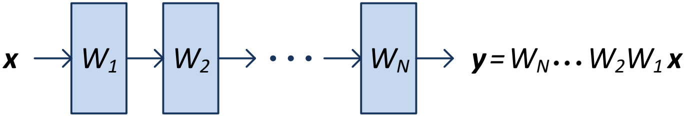

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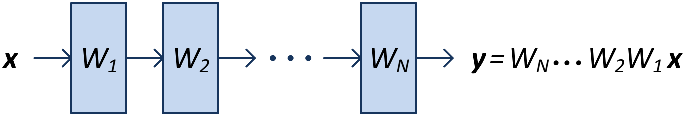

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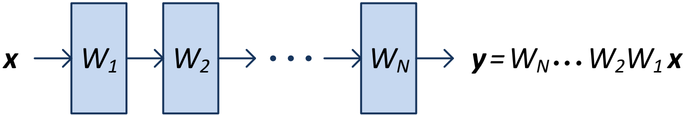

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Studied extensively as surrogate for non-linear neural networks:

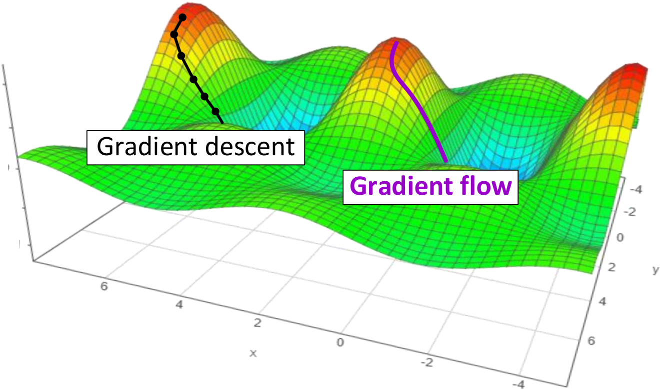
- Saxe et al. 2014
- Kawaguchi 2016
- Advani & Saxe 2017
- Hardt & Ma 2017
- Laurent & Brecht 2018
- Gunasekar et al. 2018
- Ji & Telgarsky 2019
- Lampinen & Ganguli 2019

Outline

Gradient Flow

Gradient flow (GF) is a continuous version of GD (step size $\rightarrow 0$):

$$\frac{d}{dt}\boldsymbol{\alpha}(t) = -\nabla f(\boldsymbol{\alpha}(t)) \quad , \; t \in \mathbb{R}_{>0}$$



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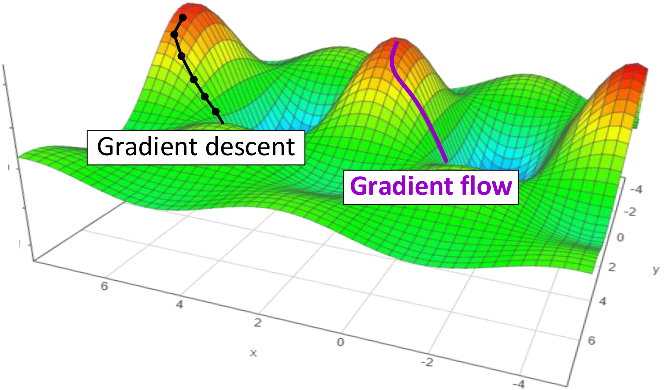
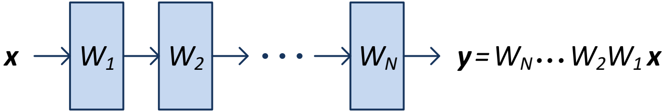


Admits use of theoretical tools from differential geometry/equations

Balanced Trajectories



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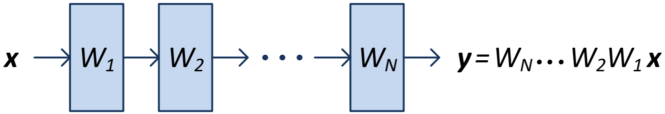

Loss $\ell(\cdot)$ for linear model induces **overparameterized objective** for LNN:

$$\phi(W_1, \ldots, W_N) := \ell(W_N \cdots W_2 W_1)$$

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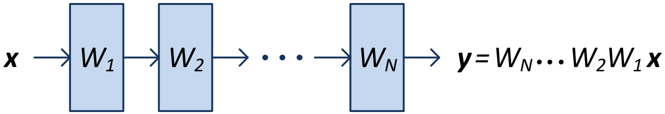

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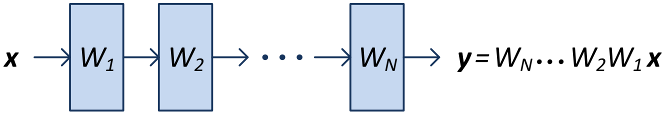

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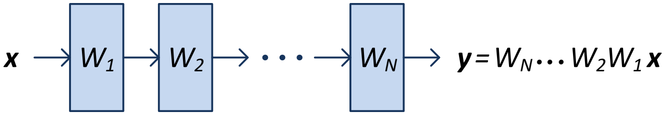

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Trajectories of GF over LNN preserve balancedness: if $W_1 \ldots W_N$ are balanced at init, they remain that way throughout GF optimization

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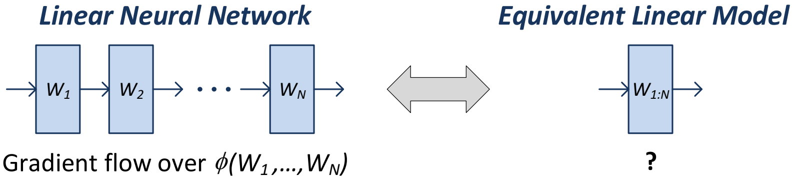
Balance at init $\implies$ $const = 0$ □

Implicit Preconditioning

Question

How does **end-to-end matrix** $W_{1:N} := W_N \cdots W_1$ move on GF trajectories?



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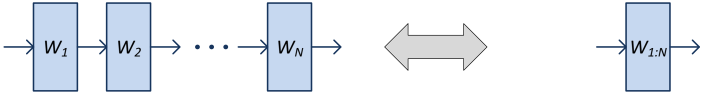

Gradient flow over $\phi(W_1,\ldots,W_N)$

Preconditioned gradient flow over $\ell(W_{1:N})$

Theorem

*If $W_1 \ldots W_N$ are balanced at init, $W_{1:N}$ follows **end-to-end dynamics**:*

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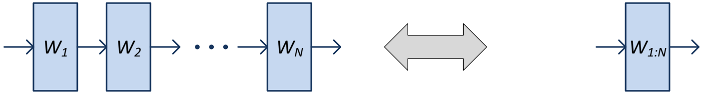

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$$vec\left[\sum_{j=1}^{N} \left[W_{1:N}(t) W_{1:N}(t)^\top\right]^{\frac{N-j}{N}} \cdot \nabla \ell(W_{1:N}(t)) \cdot \left[W_{1:N}(t)^\top W_{1:N}(t)\right]^{\frac{j-1}{N}}\right]$$

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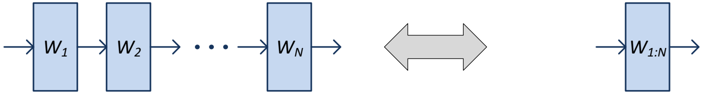

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Adding (redundant) linear layers to classic linear model induces preconditioner promoting movement in directions already taken!

Implicit Preconditioning — Proof Sketch

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$$\sum_{j=1}^{N} \prod_{j+1}^{i=N} W_i(t) \cdot \left(- \tfrac{\partial}{\partial W_j} \phi(W_1(t), \dots, W_N(t)) \right) \cdot \prod_{1}^{i=j-1} W_i(t)$$

Implicit Preconditioning — Proof Sketch

Theorem

If $W_1 \ldots W_N$ are balanced at init, $W_{1:N}$ follows ***end-to-end dynamics****:*

$$\tfrac{d}{dt} vec\left[W_{1:N}(t)\right] = -P_{W_{1:N}(t)} \cdot vec\left[\nabla \ell(W_{1:N}(t))\right]$$

where $P_{W_{1:N}(t)}$ is a preconditioner (PSD matrix) that "reinforces" $W_{1:N}(t)$

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SVD: $W_j(t) = U_j(t) S_j(t) V_j(t)^\top$

Balance $(W_j(t) W_j(t)^\top \equiv W_{j+1}(t)^\top W_{j+1}(t)) \implies S_j(t) \equiv S_{j+1}(t) \wedge U_j(t) \equiv V_{j+1}(t)$

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Vectorizing gives end-to-end dynamics (with closed-form expression for $P_{W_{1:N}(t)}$)

Trajectories Cannot Be Emulated via Regularization

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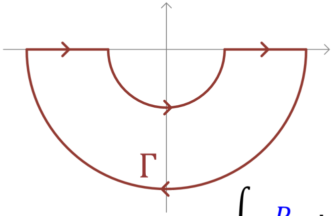


contradicts gradient theorem!

$$\int_{\Gamma} P_W \cdot vec\left[\nabla \ell(W)\right] \neq 0$$

Outline

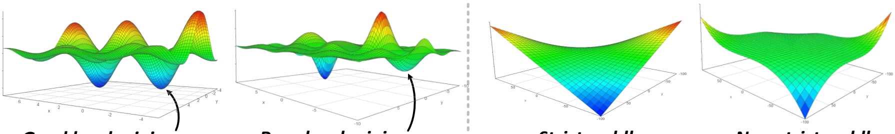
1. Optimization and Generalization in Deep Learning via Trajectories

2. Case Study: Linear Neural Networks
   - Trajectory Analysis
   - Optimization
   - Generalization

3. Conclusion

Classic Approach: Characterization of Critical Points

Prominent approach for analyzing optimization in DL (in spirit of classical learning theory) is via critical points in the objective



Good local minimum* (≈ *global minimum*)** | ***Poor local minimum | ***Strict saddle*** | ***Non-strict saddle***

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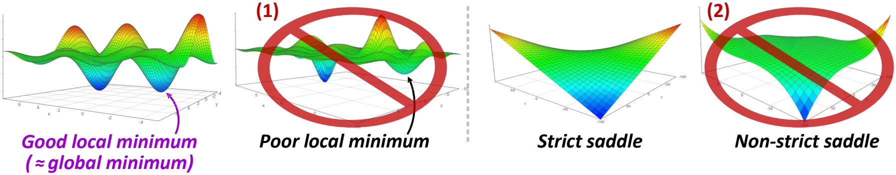

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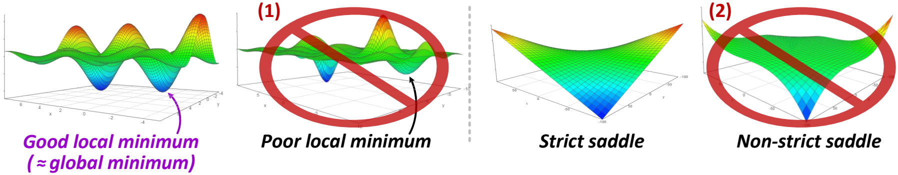

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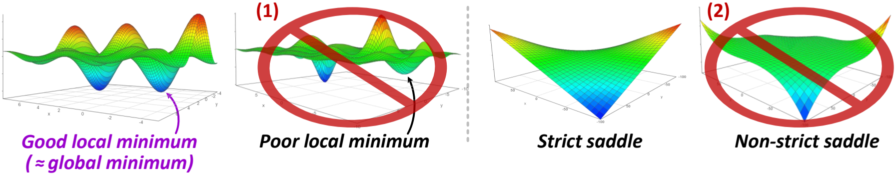

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Limitation: deep (≥ 3 layer) models violate **(2)** (consider all weights $= 0$)!

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Trajectory analysis revealed implicit preconditioning on end-to-end matrix:

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Assume $\ell(\cdot)$ is convex and LNN is init such that:

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Guarantee of efficient (linear rate) convergence to global min!
Most general guarantee to date for GD efficiently training deep net.

Effect of Depth on Optimization

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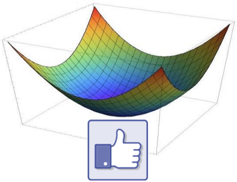
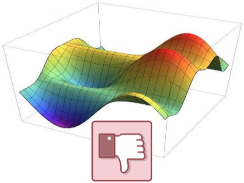
Viewpoint of classical learning theory:

- Convex optimization is easier than non-convex





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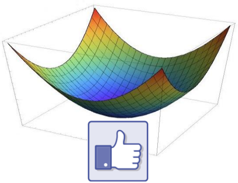
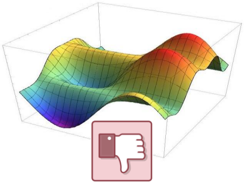
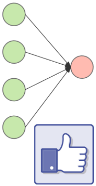
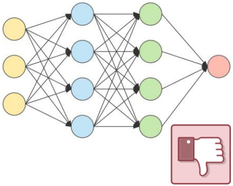




- Hence depth complicates optimization





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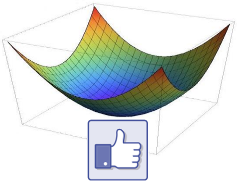

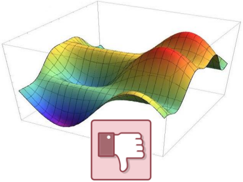

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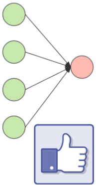

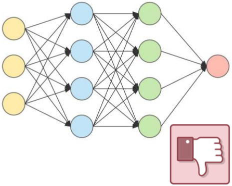

Our trajectory analysis reveals: not always true...

Acceleration by Depth

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Discrete version of end-to-end dynamics for LNN:

$$vec\left[W_{1:N}(t+1)\right] \leftarrow vec\left[W_{1:N}(t)\right] - \eta \cdot P_{W_{1:N}(t)} \cdot vec\left[\nabla\ell(W_{1:N}(t))\right]$$

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$\forall p > 2$, $\exists$ settings where $\ell(\cdot) = \ell_p$ loss (i.e. $\ell(W) = \frac{1}{m}\sum_{i=1}^{m} \|W\mathbf{x}_i - \mathbf{y}_i\|_p^p$) and disc end-to-end dynamics reach global min arbitrarily faster than GD

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$\forall p > 2$, $\exists$ settings where $\ell(\cdot) = \ell_p$ loss (i.e. $\ell(W) = \frac{1}{m}\sum_{i=1}^{m} \|W\mathbf{x}_i - \mathbf{y}_i\|_p^p$) and disc end-to-end dynamics reach global min arbitrarily faster than GD

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Discrete version of end-to-end dynamics for LNN:

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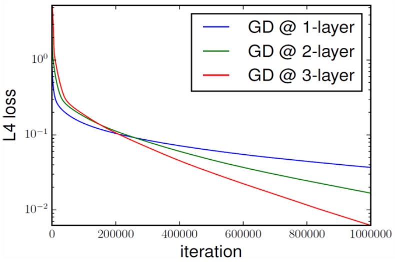

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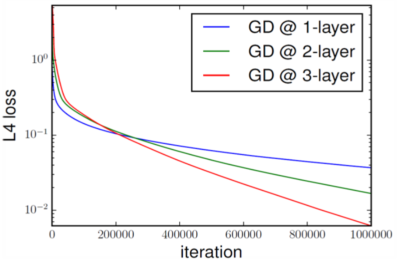
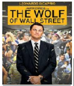


Depth can speed-up GD, even without any gain in expressiveness, and despite introducing non-convexity!

Outline

Setting: Matrix Completion

Matrix completion: recover matrix given subset of entries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				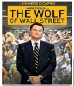
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Classical Result *(cf. Candes & Recht 2008)*

Nuclear norm minimization (convex program) perfectly recovers ("almost any") low rank matrix if observations are sufficiently many

Two-Layer Network $\longleftrightarrow$ Matrix Factorization

Matrix completion via two-layer LNN:

- Parameterize ground truth as $W_2 W_1$

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$$\begin{bmatrix} 4 & ? & ? & 4 \\ ? & 5 & 4 & ? \\ ? & 5 & ? & ? \end{bmatrix} = \boldsymbol{W_2} * \boldsymbol{W_1}$$

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Gunasekar et al. proved conjecture for certain restricted setting

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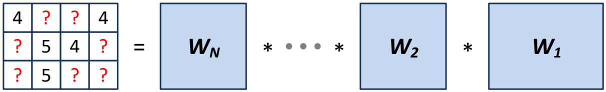

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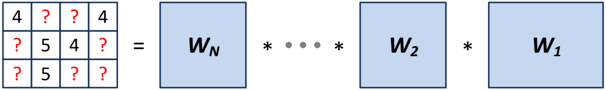

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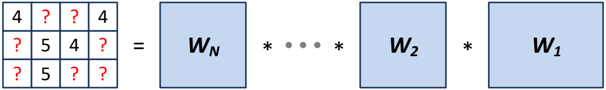

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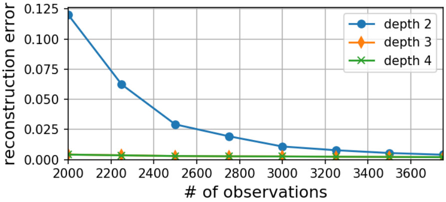

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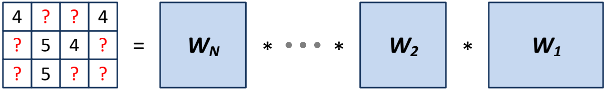

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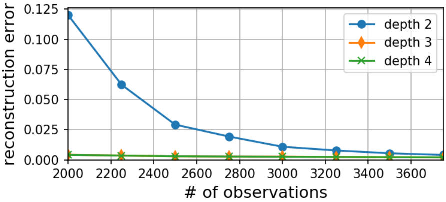

Depth enhanced implicit regularization towards low rank!

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- $0 < p < 1$: closer to rank, may correspond to higher depths

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But our experiment shows depth changes implicit regularization!

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Experiments Testing Nuclear Norm Conjecture (cont')

Few (2K) Observations:

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Hypothesis

Single norm (or quasi-norm) not enough to capture implicit regularization, detailed account for trajectories is needed

Trajectory Analysis $\longrightarrow$ Dynamics of Singular Values

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Trajectory analysis gave dynamics for end-to-end matrix of N-layer LNN:

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- $N = 1$ (classic linear model): factors reduce to 1
- $N \geq 2$: factors speed up (slow down) large (small) singular vals, more so for larger N (higher depth)

Dynamics of Singular Values — Proof Sketch

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Proof Sketch

SVD: $W_{1:N}(t) = U(t)S(t)V(t)^\top \quad \big(S = diag(\sigma_1, \sigma_2, ...) \quad U = [\mathbf{u}_1, \mathbf{u}_2, ...] \quad V = [\mathbf{v}_1, \mathbf{v}_2, ...]\big)$

$$\implies \tfrac{d}{dt}W_{1:N}(t) = \tfrac{d}{dt}U(t) \cdot S(t) \cdot V(t)^\top + U(t) \cdot \tfrac{d}{dt}S(t) \cdot V(t)^\top + U(t) \cdot S(t) \cdot \tfrac{d}{dt}V(t)^\top$$

$$\implies U(t)^\top \cdot \tfrac{d}{dt}W_{1:N}(t) \cdot V(t) = U(t)^\top \cdot \tfrac{d}{dt}U(t) \cdot S(t) + \tfrac{d}{dt}S(t) + S(t) \cdot \tfrac{d}{dt}V(t)^\top \cdot V(t)$$

End-to-end dynamics:

$$\tfrac{d}{dt}W_{1:N}(t) = -\textstyle\sum_{j=1}^{N} \Big[W_{1:N}(t)W_{1:N}(t)^\top\Big]^{\frac{N-j}{N}} \cdot \nabla\ell(W_{1:N}(t)) \cdot \Big[W_{1:N}(t)^\top W_{1:N}(t)\Big]^{\frac{j-1}{N}}$$

Dynamics of Singular Values — Proof Sketch

Theorem

$$\frac{d}{dt}\sigma_r(t) = -N \cdot \sigma_r^{2-\frac{2}{N}}(t) \cdot \langle \nabla \ell(W_{1:N}(t)), \mathbf{u}_r(t)\mathbf{v}_r^\top(t) \rangle$$

Proof Sketch

SVD: $W_{1:N}(t) = U(t)S(t)V(t)^\top$ $\quad \big(S = diag(\sigma_1, \sigma_2, \ldots) \quad U = [\mathbf{u}_1, \mathbf{u}_2, \ldots] \quad V = [\mathbf{v}_1, \mathbf{v}_2, \ldots]\big)$

$$\implies \frac{d}{dt}W_{1:N}(t) = \frac{d}{dt}U(t) \cdot S(t) \cdot V(t)^\top + U(t) \cdot \frac{d}{dt}S(t) \cdot V(t)^\top + U(t) \cdot S(t) \cdot \frac{d}{dt}V(t)^\top$$

$$\implies U(t)^\top \cdot \frac{d}{dt}W_{1:N}(t) \cdot V(t) = U(t)^\top \cdot \frac{d}{dt}U(t) \cdot S(t) + \frac{d}{dt}S(t) + S(t) \cdot \frac{d}{dt}V(t)^\top \cdot V(t)$$

End-to-end dynamics:

$$\frac{d}{dt}W_{1:N}(t) = -\sum_{j=1}^{N} \left[W_{1:N}(t)W_{1:N}(t)^\top\right]^{\frac{N-j}{N}} \cdot \nabla \ell(W_{1:N}(t)) \cdot \left[W_{1:N}(t)^\top W_{1:N}(t)\right]^{\frac{j-1}{N}}$$

Dynamics of Singular Values — Proof Sketch

Theorem

$$\frac{d}{dt}\sigma_r(t) = -N \cdot \sigma_r^{2-\frac{2}{N}}(t) \cdot \langle \nabla \ell(W_{1:N}(t)), \mathbf{u}_r(t)\mathbf{v}_r^\top(t) \rangle$$

Proof Sketch

SVD: $W_{1:N}(t) = U(t)S(t)V(t)^\top$ $\quad \big(S = diag(\sigma_1, \sigma_2, \ldots) \quad U = [\mathbf{u}_1, \mathbf{u}_2, \ldots] \quad V = [\mathbf{v}_1, \mathbf{v}_2, \ldots]\big)$

$$\implies \frac{d}{dt}W_{1:N}(t) = \frac{d}{dt}U(t) \cdot S(t) \cdot V(t)^\top + U(t) \cdot \frac{d}{dt}S(t) \cdot V(t)^\top + U(t) \cdot S(t) \cdot \frac{d}{dt}V(t)^\top$$

$$\implies U(t)^\top \cdot \frac{d}{dt}W_{1:N}(t) \cdot V(t) = U(t)^\top \cdot \frac{d}{dt}U(t) \cdot S(t) + \frac{d}{dt}S(t) + S(t) \cdot \frac{d}{dt}V(t)^\top \cdot V(t)$$

End-to-end dynamics:

$$\frac{d}{dt}W_{1:N}(t) = -\sum_{j=1}^{N} U(t)\Big[S(t)S(t)^\top\Big]^{\frac{N-j}{N}} U(t)^\top \cdot \nabla \ell(W_{1:N}(t)) \cdot V(t)\Big[S(t)^\top S(t)\Big]^{\frac{j-1}{N}} V(t)^\top$$

Dynamics of Singular Values — Proof Sketch

Theorem

$$\frac{d}{dt}\sigma_r(t) = -N \cdot \sigma_r^{2-\frac{2}{N}}(t) \cdot \langle \nabla \ell(W_{1:N}(t)), \mathbf{u}_r(t)\mathbf{v}_r^\top(t) \rangle$$

Proof Sketch

SVD: $W_{1:N}(t) = U(t)S(t)V(t)^\top \quad \big(S = diag(\sigma_1, \sigma_2, \ldots) \quad U = [\mathbf{u}_1, \mathbf{u}_2, \ldots] \quad V = [\mathbf{v}_1, \mathbf{v}_2, \ldots]\big)$

$$\implies \frac{d}{dt}W_{1:N}(t) = \frac{d}{dt}U(t) \cdot S(t) \cdot V(t)^\top + U(t) \cdot \frac{d}{dt}S(t) \cdot V(t)^\top + U(t) \cdot S(t) \cdot \frac{d}{dt}V(t)^\top$$

$$\implies U(t)^\top \cdot \frac{d}{dt}W_{1:N}(t) \cdot V(t) = U(t)^\top \cdot \frac{d}{dt}U(t) \cdot S(t) + \frac{d}{dt}S(t) + S(t) \cdot \frac{d}{dt}V(t)^\top \cdot V(t)$$

End-to-end dynamics:

$$\frac{d}{dt}W_{1:N}(t) = -\sum_{j=1}^{N} U(t)\left[S(t)S(t)^\top\right]^{\frac{N-j}{N}} U(t)^\top \cdot \nabla \ell(W_{1:N}(t)) \cdot V(t)\left[S(t)^\top S(t)\right]^{\frac{j-1}{N}} V(t)^\top$$

$$\implies U(t)^\top \cdot \frac{d}{dt}W_{1:N}(t) \cdot V(t)$$
$$= -\sum_{j=1}^{N} \left[S(t)S(t)^\top\right]^{\frac{N-j}{N}} U(t)^\top \cdot \nabla \ell(W_{1:N}(t)) \cdot V(t)\left[S(t)^\top S(t)\right]^{\frac{j-1}{N}}$$

Dynamics of Singular Values — Proof Sketch

Theorem

$$\frac{d}{dt}\sigma_r(t) = -N \cdot \sigma_r^{2-\frac{2}{N}}(t) \cdot \langle \nabla \ell(W_{1:N}(t)), \mathbf{u}_r(t)\mathbf{v}_r^\top(t) \rangle$$

Proof Sketch

SVD: $W_{1:N}(t) = U(t)S(t)V(t)^\top$ $\quad \big(S = diag(\sigma_1, \sigma_2, \ldots) \quad U = [\mathbf{u}_1, \mathbf{u}_2, \ldots] \quad V = [\mathbf{v}_1, \mathbf{v}_2, \ldots]\big)$

$$\Longrightarrow \frac{d}{dt}W_{1:N}(t) = \frac{d}{dt}U(t) \cdot S(t) \cdot V(t)^\top + U(t) \cdot \frac{d}{dt}S(t) \cdot V(t)^\top + U(t) \cdot S(t) \cdot \frac{d}{dt}V(t)^\top$$

$$\Longrightarrow U(t)^\top \cdot \frac{d}{dt}W_{1:N}(t) \cdot V(t) = U(t)^\top \cdot \frac{d}{dt}U(t) \cdot S(t) + \frac{d}{dt}S(t) + S(t) \cdot \frac{d}{dt}V(t)^\top \cdot V(t)$$

End-to-end dynamics:

$$\frac{d}{dt}W_{1:N}(t) = -\sum_{j=1}^{N} U(t)\left[S(t)S(t)^\top\right]^{\frac{N-j}{N}} U(t)^\top \cdot \nabla\ell(W_{1:N}(t)) \cdot V(t)\left[S(t)^\top S(t)\right]^{\frac{j-1}{N}} V(t)^\top$$

$$\Longrightarrow U(t)^\top \cdot \frac{d}{dt}W_{1:N}(t) \cdot V(t)$$

$$= -\sum_{j=1}^{N} \left[S(t)S(t)^\top\right]^{\frac{N-j}{N}} U(t)^\top \cdot \nabla\ell(W_{1:N}(t)) \cdot V(t)\left[S(t)^\top S(t)\right]^{\frac{j-1}{N}}$$

Dynamics of Singular Values — Proof Sketch

Theorem

$$\frac{d}{dt}\sigma_r(t) = -N \cdot \sigma_r^{2-\frac{2}{N}}(t) \cdot \langle \nabla \ell(W_{1:N}(t)), \mathbf{u}_r(t)\mathbf{v}_r^\top(t) \rangle$$

Proof Sketch

SVD: $W_{1:N}(t) = U(t)S(t)V(t)^\top$ $\big(S = diag(\sigma_1, \sigma_2, \ldots) \quad U = [\mathbf{u}_1, \mathbf{u}_2, \ldots] \quad V = [\mathbf{v}_1, \mathbf{v}_2, \ldots]\big)$

$$\implies \frac{d}{dt}W_{1:N}(t) = \frac{d}{dt}U(t) \cdot S(t) \cdot V(t)^\top + U(t) \cdot \frac{d}{dt}S(t) \cdot V(t)^\top + U(t) \cdot S(t) \cdot \frac{d}{dt}V(t)^\top$$

$$\implies U(t)^\top \cdot \frac{d}{dt}W_{1:N}(t) \cdot V(t) = U(t)^\top \cdot \frac{d}{dt}U(t) \cdot S(t) + \frac{d}{dt}S(t) + S(t) \cdot \frac{d}{dt}V(t)^\top \cdot V(t)$$

End-to-end dynamics:

$$\frac{d}{dt}W_{1:N}(t) = -\sum\nolimits_{j=1}^{N} U(t)\left[S(t)S(t)^\top\right]^{\frac{N-j}{N}} U(t)^\top \cdot \nabla\ell(W_{1:N}(t)) \cdot V(t)\left[S(t)^\top S(t)\right]^{\frac{j-1}{N}} V(t)^\top$$

$$\implies \quad U(t)^\top \cdot \frac{d}{dt}U(t) \cdot S(t) + \frac{d}{dt}S(t) + S(t) \cdot \frac{d}{dt}V(t)^\top \cdot V(t)$$

$$= -\sum\nolimits_{j=1}^{N} \left[S(t)S(t)^\top\right]^{\frac{N-j}{N}} U(t)^\top \cdot \nabla\ell(W_{1:N}(t)) \cdot V(t)\left[S(t)^\top S(t)\right]^{\frac{j-1}{N}}$$

Dynamics of Singular Values — Proof Sketch

Theorem

$$\tfrac{d}{dt}\sigma_r(t) = -N \cdot \sigma_r^{2-\frac{2}{N}}(t) \cdot \langle \nabla\ell(W_{1:N}(t)), \mathbf{u}_r(t)\mathbf{v}_r^\top(t) \rangle$$

Proof Sketch

SVD: $W_{1:N}(t) = U(t)S(t)V(t)^\top \quad \big(S = diag(\sigma_1, \sigma_2, \ldots) \quad U = [\mathbf{u}_1, \mathbf{u}_2, \ldots] \quad V = [\mathbf{v}_1, \mathbf{v}_2, \ldots] \big)$

$$\implies \tfrac{d}{dt}W_{1:N}(t) = \tfrac{d}{dt}U(t) \cdot S(t) \cdot V(t)^\top + U(t) \cdot \tfrac{d}{dt}S(t) \cdot V(t)^\top + U(t) \cdot S(t) \cdot \tfrac{d}{dt}V(t)^\top$$

$$\implies U(t)^\top \cdot \tfrac{d}{dt}W_{1:N}(t) \cdot V(t) = U(t)^\top \cdot \tfrac{d}{dt}U(t) \cdot S(t) + \tfrac{d}{dt}S(t) + S(t) \cdot \tfrac{d}{dt}V(t)^\top \cdot V(t)$$

End-to-end dynamics:

$$\tfrac{d}{dt}W_{1:N}(t) = -\textstyle\sum_{j=1}^{N} U(t)\Big[S(t)S(t)^\top\Big]^{\frac{N-j}{N}} U(t)^\top \cdot \nabla\ell(W_{1:N}(t)) \cdot V(t)\Big[S(t)^\top S(t)\Big]^{\frac{j-1}{N}} V(t)^\top$$

$$\implies \quad U(t)^\top \cdot \tfrac{d}{dt}U(t) \cdot S(t) + \tfrac{d}{dt}S(t) + S(t) \cdot \tfrac{d}{dt}V(t)^\top \cdot V(t)$$

$$= -\textstyle\sum_{j=1}^{N} \Big[S(t)S(t)^\top\Big]^{\frac{N-j}{N}} U(t)^\top \cdot \nabla\ell(W_{1:N}(t)) \cdot V(t)\Big[S(t)^\top S(t)\Big]^{\frac{j-1}{N}}$$

Restrict attention to r'th diagonal element:

Dynamics of Singular Values — Proof Sketch

Theorem

$$\frac{d}{dt}\sigma_r(t) = -N \cdot \sigma_r^{2-\frac{2}{N}}(t) \cdot \langle \nabla \ell(W_{1:N}(t)), \mathbf{u}_r(t)\mathbf{v}_r^\top(t) \rangle$$

Proof Sketch

SVD: $W_{1:N}(t) = U(t)S(t)V(t)^\top \quad \big(S = diag(\sigma_1, \sigma_2, ...) \quad U = [\mathbf{u}_1, \mathbf{u}_2, ...] \quad V = [\mathbf{v}_1, \mathbf{v}_2, ...]\big)$

$$\implies \tfrac{d}{dt}W_{1:N}(t) = \tfrac{d}{dt}U(t) \cdot S(t) \cdot V(t)^\top + U(t) \cdot \tfrac{d}{dt}S(t) \cdot V(t)^\top + U(t) \cdot S(t) \cdot \tfrac{d}{dt}V(t)^\top$$

$$\implies U(t)^\top \cdot \tfrac{d}{dt}W_{1:N}(t) \cdot V(t) = U(t)^\top \cdot \tfrac{d}{dt}U(t) \cdot S(t) + \tfrac{d}{dt}S(t) + S(t) \cdot \tfrac{d}{dt}V(t)^\top \cdot V(t)$$

End-to-end dynamics:

$$\tfrac{d}{dt}W_{1:N}(t) = -\textstyle\sum_{j=1}^N U(t)\Big[S(t)S(t)^\top\Big]^{\frac{N-j}{N}} U(t)^\top \cdot \nabla\ell(W_{1:N}(t)) \cdot V(t)\Big[S(t)^\top S(t)\Big]^{\frac{j-1}{N}} V(t)^\top$$

$$\implies \quad U(t)^\top \cdot \tfrac{d}{dt}U(t) \cdot S(t) + \tfrac{d}{dt}S(t) + S(t) \cdot \tfrac{d}{dt}V(t)^\top \cdot V(t)$$

$$= -\textstyle\sum_{j=1}^N \Big[S(t)S(t)^\top\Big]^{\frac{N-j}{N}} U(t)^\top \cdot \nabla\ell(W_{1:N}(t)) \cdot V(t)\Big[S(t)^\top S(t)\Big]^{\frac{j-1}{N}}$$

Restrict attention to r'th diagonal element:

$$\mathbf{u}_r(t)^\top \cdot \tfrac{d}{dt}\mathbf{u}_r(t) \cdot \sigma_r(t) + \tfrac{d}{dt}\sigma_r(t) + \sigma_r(t) \cdot \tfrac{d}{dt}\mathbf{v}_r(t)^\top \cdot \mathbf{v}_r(t) =$$

$$-\textstyle\sum_{j=1}^N \sigma_r^{2\frac{N-j}{N}}(t) \cdot \mathbf{u}_r(t)^\top \cdot \nabla\ell(W_{1:N}(t)) \cdot \mathbf{v}_r(t) \cdot \sigma_r^{2\frac{j-1}{N}}(t)$$

Dynamics of Singular Values — Proof Sketch

Theorem

$$\frac{d}{dt}\sigma_r(t) = -N \cdot \sigma_r^{2-\frac{2}{N}}(t) \cdot \langle \nabla \ell(W_{1:N}(t)), \mathbf{u}_r(t)\mathbf{v}_r^\top(t) \rangle$$

Proof Sketch

SVD: $W_{1:N}(t) = U(t)S(t)V(t)^\top \quad \left(S = diag(\sigma_1, \sigma_2, ...) \quad U = [\mathbf{u}_1, \mathbf{u}_2, ...] \quad V = [\mathbf{v}_1, \mathbf{v}_2, ...] \right)$

$$\implies \frac{d}{dt}W_{1:N}(t) = \frac{d}{dt}U(t) \cdot S(t) \cdot V(t)^\top + U(t) \cdot \frac{d}{dt}S(t) \cdot V(t)^\top + U(t) \cdot S(t) \cdot \frac{d}{dt}V(t)^\top$$

$$\implies U(t)^\top \cdot \frac{d}{dt}W_{1:N}(t) \cdot V(t) = U(t)^\top \cdot \frac{d}{dt}U(t) \cdot S(t) + \frac{d}{dt}S(t) + S(t) \cdot \frac{d}{dt}V(t)^\top \cdot V(t)$$

End-to-end dynamics:

$$\frac{d}{dt}W_{1:N}(t) = -\sum_{j=1}^{N} U(t)\left[S(t)S(t)^\top\right]^{\frac{N-j}{N}} U(t)^\top \cdot \nabla\ell(W_{1:N}(t)) \cdot V(t)\left[S(t)^\top S(t)\right]^{\frac{j-1}{N}} V(t)^\top$$

$$\implies \quad U(t)^\top \cdot \frac{d}{dt}U(t) \cdot S(t) + \frac{d}{dt}S(t) + S(t) \cdot \frac{d}{dt}V(t)^\top \cdot V(t)$$

$$= -\sum_{j=1}^{N} \left[S(t)S(t)^\top\right]^{\frac{N-j}{N}} U(t)^\top \cdot \nabla\ell(W_{1:N}(t)) \cdot V(t)\left[S(t)^\top S(t)\right]^{\frac{j-1}{N}}$$

Restrict attention to r'th diagonal element:

$$\mathbf{u}_r(t)^\top \cdot \frac{d}{dt}\mathbf{u}_r(t) \cdot \sigma_r(t) + \frac{d}{dt}\sigma_r(t) + \sigma_r(t) \cdot \frac{d}{dt}\mathbf{v}_r(t)^\top \cdot \mathbf{v}_r(t) =$$

$$-\sum_{j=1}^{N} \sigma_r^{2\frac{N-1}{N}}(t) \cdot \mathbf{u}_r(t)^\top \cdot \nabla\ell(W_{1:N}(t)) \cdot \mathbf{v}_r(t)$$

Dynamics of Singular Values — Proof Sketch

Theorem

$$\frac{d}{dt}\sigma_r(t) = -N \cdot \sigma_r^{2-\frac{2}{N}}(t) \cdot \langle \nabla\ell(W_{1:N}(t)), \mathbf{u}_r(t)\mathbf{v}_r^\top(t)\rangle$$

Proof Sketch

SVD: $W_{1:N}(t) = U(t)S(t)V(t)^\top \quad \left(S = diag(\sigma_1, \sigma_2, ...) \quad U = [\mathbf{u}_1, \mathbf{u}_2, ...] \quad V = [\mathbf{v}_1, \mathbf{v}_2, ...]\right)$

$$\implies \frac{d}{dt}W_{1:N}(t) = \frac{d}{dt}U(t) \cdot S(t) \cdot V(t)^\top + U(t) \cdot \frac{d}{dt}S(t) \cdot V(t)^\top + U(t) \cdot S(t) \cdot \frac{d}{dt}V(t)^\top$$

$$\implies U(t)^\top \cdot \frac{d}{dt}W_{1:N}(t) \cdot V(t) = U(t)^\top \cdot \frac{d}{dt}U(t) \cdot S(t) + \frac{d}{dt}S(t) + S(t) \cdot \frac{d}{dt}V(t)^\top \cdot V(t)$$

End-to-end dynamics:

$$\frac{d}{dt}W_{1:N}(t) = -\sum_{j=1}^{N} U(t)\left[S(t)S(t)^\top\right]^{\frac{N-j}{N}} U(t)^\top \cdot \nabla\ell(W_{1:N}(t)) \cdot V(t)\left[S(t)^\top S(t)\right]^{\frac{j-1}{N}} V(t)^\top$$

$$\implies \quad U(t)^\top \cdot \frac{d}{dt}U(t) \cdot S(t) + \frac{d}{dt}S(t) + S(t) \cdot \frac{d}{dt}V(t)^\top \cdot V(t)$$
$$= -\sum_{j=1}^{N} \left[S(t)S(t)^\top\right]^{\frac{N-j}{N}} U(t)^\top \cdot \nabla\ell(W_{1:N}(t)) \cdot V(t)\left[S(t)^\top S(t)\right]^{\frac{j-1}{N}}$$

Restrict attention to r'th diagonal element:

$$\mathbf{u}_r(t)^\top \cdot \frac{d}{dt}\mathbf{u}_r(t) \cdot \sigma_r(t) + \frac{d}{dt}\sigma_r(t) + \sigma_r(t) \cdot \frac{d}{dt}\mathbf{v}_r(t)^\top \cdot \mathbf{v}_r(t) =$$
$$-N \cdot \sigma_r^{2\frac{N-1}{N}}(t) \cdot \mathbf{u}_r(t)^\top \cdot \nabla\ell(W_{1:N}(t)) \cdot \mathbf{v}_r(t)$$

Dynamics of Singular Values — Proof Sketch

Theorem

$$\frac{d}{dt}\sigma_r(t) = -N \cdot \sigma_r^{2-\frac{2}{N}}(t) \cdot \langle \nabla \ell(W_{1:N}(t)), \mathbf{u}_r(t)\mathbf{v}_r^\top(t) \rangle$$

Proof Sketch

SVD: $W_{1:N}(t) = U(t)S(t)V(t)^\top \quad \big(S = diag(\sigma_1, \sigma_2, ...) \quad U = [\mathbf{u}_1, \mathbf{u}_2, ...] \quad V = [\mathbf{v}_1, \mathbf{v}_2, ...]\big)$

$$\implies \frac{d}{dt}W_{1:N}(t) = \frac{d}{dt}U(t) \cdot S(t) \cdot V(t)^\top + U(t) \cdot \frac{d}{dt}S(t) \cdot V(t)^\top + U(t) \cdot S(t) \cdot \frac{d}{dt}V(t)^\top$$

$$\implies U(t)^\top \cdot \frac{d}{dt}W_{1:N}(t) \cdot V(t) = U(t)^\top \cdot \frac{d}{dt}U(t) \cdot S(t) + \frac{d}{dt}S(t) + S(t) \cdot \frac{d}{dt}V(t)^\top \cdot V(t)$$

End-to-end dynamics:

$$\frac{d}{dt}W_{1:N}(t) = -\sum_{j=1}^{N} U(t)\left[S(t)S(t)^\top\right]^{\frac{N-j}{N}} U(t)^\top \cdot \nabla \ell(W_{1:N}(t)) \cdot V(t)\left[S(t)^\top S(t)\right]^{\frac{j-1}{N}} V(t)^\top$$

$$\implies \quad U(t)^\top \cdot \frac{d}{dt}U(t) \cdot S(t) + \frac{d}{dt}S(t) + S(t) \cdot \frac{d}{dt}V(t)^\top \cdot V(t)$$
$$= -\sum_{j=1}^{N} \left[S(t)S(t)^\top\right]^{\frac{N-j}{N}} U(t)^\top \cdot \nabla \ell(W_{1:N}(t)) \cdot V(t)\left[S(t)^\top S(t)\right]^{\frac{j-1}{N}}$$

Restrict attention to r'th diagonal element:

$$\mathbf{u}_r(t)^\top \cdot \frac{d}{dt}\mathbf{u}_r(t) \cdot \sigma_r(t) + \frac{d}{dt}\sigma_r(t) + \sigma_r(t) \cdot \frac{d}{dt}\mathbf{v}_r(t)^\top \cdot \mathbf{v}_r(t) =$$
$$-N \cdot \sigma_r^{2\frac{N-1}{N}}(t) \cdot \left\langle \nabla \ell(W_{1:N}(t)), \mathbf{u}_r(t)\mathbf{v}_r^\top(t) \right\rangle$$

Dynamics of Singular Values — Proof Sketch

Theorem

$$\frac{d}{dt}\sigma_r(t) = -N \cdot \sigma_r^{2-\frac{2}{N}}(t) \cdot \langle \nabla \ell(W_{1:N}(t)), \mathbf{u}_r(t)\mathbf{v}_r^\top(t) \rangle$$

Proof Sketch

SVD: $W_{1:N}(t) = U(t)S(t)V(t)^\top$ $\quad \big(S = diag(\sigma_1, \sigma_2, ...) \quad U = [\mathbf{u}_1, \mathbf{u}_2, ...] \quad V = [\mathbf{v}_1, \mathbf{v}_2, ...]\big)$

$$\implies \frac{d}{dt}W_{1:N}(t) = \frac{d}{dt}U(t) \cdot S(t) \cdot V(t)^\top + U(t) \cdot \frac{d}{dt}S(t) \cdot V(t)^\top + U(t) \cdot S(t) \cdot \frac{d}{dt}V(t)^\top$$

$$\implies U(t)^\top \cdot \frac{d}{dt}W_{1:N}(t) \cdot V(t) = U(t)^\top \cdot \frac{d}{dt}U(t) \cdot S(t) + \frac{d}{dt}S(t) + S(t) \cdot \frac{d}{dt}V(t)^\top \cdot V(t)$$

End-to-end dynamics:

$$\frac{d}{dt}W_{1:N}(t) = -\sum_{j=1}^{N} U(t)\left[S(t)S(t)^\top\right]^{\frac{N-j}{N}} U(t)^\top \cdot \nabla \ell(W_{1:N}(t)) \cdot V(t)\left[S(t)^\top S(t)\right]^{\frac{j-1}{N}} V(t)^\top$$

$$\implies \quad U(t)^\top \cdot \frac{d}{dt}U(t) \cdot S(t) + \frac{d}{dt}S(t) + S(t) \cdot \frac{d}{dt}V(t)^\top \cdot V(t)$$
$$= -\sum_{j=1}^{N} \left[S(t)S(t)^\top\right]^{\frac{N-j}{N}} U(t)^\top \cdot \nabla \ell(W_{1:N}(t)) \cdot V(t)\left[S(t)^\top S(t)\right]^{\frac{j-1}{N}}$$

Restrict attention to r'th diagonal element:

$$\mathbf{u}_r(t)^\top \cdot \frac{d}{dt}\mathbf{u}_r(t) \cdot \sigma_r(t) + \frac{d}{dt}\sigma_r(t) + \sigma_r(t) \cdot \frac{d}{dt}\mathbf{v}_r(t)^\top \cdot \mathbf{v}_r(t) =$$
$$-N \cdot \sigma_r^{2\frac{N-1}{N}}(t) \cdot \left\langle \nabla \ell(W_{1:N}(t)), \mathbf{u}_r(t)\mathbf{v}_r^\top(t) \right\rangle$$

Dynamics of Singular Values — Proof Sketch

Theorem

$$\frac{d}{dt}\sigma_r(t) = -N \cdot \sigma_r^{2-\frac{2}{N}}(t) \cdot \langle \nabla\ell(W_{1:N}(t)), \mathbf{u}_r(t)\mathbf{v}_r^\top(t) \rangle$$

Proof Sketch

SVD: $W_{1:N}(t) = U(t)S(t)V(t)^\top \quad \big(S = diag(\sigma_1, \sigma_2, \ldots) \quad U = [\mathbf{u}_1, \mathbf{u}_2, \ldots] \quad V = [\mathbf{v}_1, \mathbf{v}_2, \ldots]\big)$

$$\implies \frac{d}{dt}W_{1:N}(t) = \frac{d}{dt}U(t) \cdot S(t) \cdot V(t)^\top + U(t) \cdot \frac{d}{dt}S(t) \cdot V(t)^\top + U(t) \cdot S(t) \cdot \frac{d}{dt}V(t)^\top$$

$$\implies U(t)^\top \cdot \frac{d}{dt}W_{1:N}(t) \cdot V(t) = U(t)^\top \cdot \frac{d}{dt}U(t) \cdot S(t) + \frac{d}{dt}S(t) + S(t) \cdot \frac{d}{dt}V(t)^\top \cdot V(t)$$

End-to-end dynamics:

$$\frac{d}{dt}W_{1:N}(t) = -\sum\nolimits_{j=1}^{N} U(t)\Big[S(t)S(t)^\top\Big]^{\frac{N-j}{N}} U(t)^\top \cdot \nabla\ell(W_{1:N}(t)) \cdot V(t)\Big[S(t)^\top S(t)\Big]^{\frac{j-1}{N}} V(t)^\top$$

$$\implies \quad U(t)^\top \cdot \frac{d}{dt}U(t) \cdot S(t) + \frac{d}{dt}S(t) + S(t) \cdot \frac{d}{dt}V(t)^\top \cdot V(t)$$

$$= -\sum\nolimits_{j=1}^{N} \Big[S(t)S(t)^\top\Big]^{\frac{N-j}{N}} U(t)^\top \cdot \nabla\ell(W_{1:N}(t)) \cdot V(t)\Big[S(t)^\top S(t)\Big]^{\frac{j-1}{N}}$$

Restrict attention to r'th diagonal element:

$$\frac{1}{2}\frac{d}{dt}\|\mathbf{u}_r(t)\|_2^2 \cdot \sigma_r(t) + \frac{d}{dt}\sigma_r(t) + \sigma_r(t) \cdot \frac{1}{2}\frac{d}{dt}\|\mathbf{v}_r(t)\|_2^2 = -N \cdot \sigma_r^{2\frac{N-1}{N}}(t) \cdot \Big\langle \nabla\ell(W_{1:N}(t)), \mathbf{u}_r(t)\mathbf{v}_r^\top(t) \Big\rangle$$

Dynamics of Singular Values — Proof Sketch

Theorem

$$\frac{d}{dt}\sigma_r(t) = -N \cdot \sigma_r^{2-\frac{2}{N}}(t) \cdot \langle \nabla \ell(W_{1:N}(t)), \mathbf{u}_r(t)\mathbf{v}_r^\top(t) \rangle$$

Proof Sketch

SVD: $W_{1:N}(t) = U(t)S(t)V(t)^\top \quad \big(S = diag(\sigma_1, \sigma_2, ...) \quad U = [\mathbf{u}_1, \mathbf{u}_2, ...] \quad V = [\mathbf{v}_1, \mathbf{v}_2, ...]\big)$

$$\implies \frac{d}{dt}W_{1:N}(t) = \frac{d}{dt}U(t) \cdot S(t) \cdot V(t)^\top + U(t) \cdot \frac{d}{dt}S(t) \cdot V(t)^\top + U(t) \cdot S(t) \cdot \frac{d}{dt}V(t)^\top$$

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$$\implies U(t)^\top \cdot \frac{d}{dt}U(t) \cdot S(t) + \frac{d}{dt}S(t) + S(t) \cdot \frac{d}{dt}V(t)^\top \cdot V(t)$$

$$= -\sum_{j=1}^{N} \left[S(t)S(t)^\top\right]^{\frac{N-j}{N}} U(t)^\top \cdot \nabla\ell(W_{1:N}(t)) \cdot V(t)\left[S(t)^\top S(t)\right]^{\frac{j-1}{N}}$$

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$$\frac{d}{dt}\sigma_r(t) = -N \cdot \sigma_r^{2-\frac{2}{N}}(t) \cdot \langle \nabla \ell(W_{1:N}(t)), \mathbf{u}_r(t)\mathbf{v}_r^\top(t) \rangle$$

Proof Sketch

SVD: $W_{1:N}(t) = U(t)S(t)V(t)^\top \quad \left(S = diag(\sigma_1, \sigma_2, \ldots) \quad U = [\mathbf{u}_1, \mathbf{u}_2, \ldots] \quad V = [\mathbf{v}_1, \mathbf{v}_2, \ldots] \right)$

$$\Longrightarrow \frac{d}{dt}W_{1:N}(t) = \frac{d}{dt}U(t) \cdot S(t) \cdot V(t)^\top + U(t) \cdot \frac{d}{dt}S(t) \cdot V(t)^\top + U(t) \cdot S(t) \cdot \frac{d}{dt}V(t)^\top$$

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$$\Longrightarrow \quad U(t)^\top \cdot \frac{d}{dt}U(t) \cdot S(t) + \frac{d}{dt}S(t) + S(t) \cdot \frac{d}{dt}V(t)^\top \cdot V(t)$$

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Restrict attention to r'th diagonal element:

$$0 \cdot \sigma_r(t) + \frac{d}{dt}\sigma_r(t) + \sigma_r(t) \cdot 0 = -N \cdot \sigma_r^{2\frac{N-1}{N}}(t) \cdot \left\langle \nabla \ell(W_{1:N}(t)), \mathbf{u}_r(t)\mathbf{v}_r^\top(t) \right\rangle$$

Dynamics of Singular Values — Proof Sketch

Theorem

$$\tfrac{d}{dt}\sigma_r(t) = -N \cdot \sigma_r^{2-\frac{2}{N}}(t) \cdot \langle \nabla\ell(W_{1:N}(t)), \mathbf{u}_r(t)\mathbf{v}_r^\top(t) \rangle$$

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$$= -\sum_{j=1}^N \left[S(t)S(t)^\top\right]^{\frac{N-j}{N}} U(t)^\top \cdot \nabla\ell(W_{1:N}(t)) \cdot V(t)\left[S(t)^\top S(t)\right]^{\frac{j-1}{N}}$$

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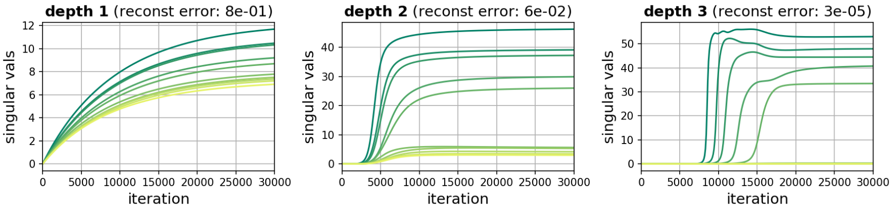
□

Implicit Bias Towards Low Rank

Implicit Bias Towards Low Rank

Experiment

Completion of low rank matrix via GD over LNN



Implicit Bias Towards Low Rank

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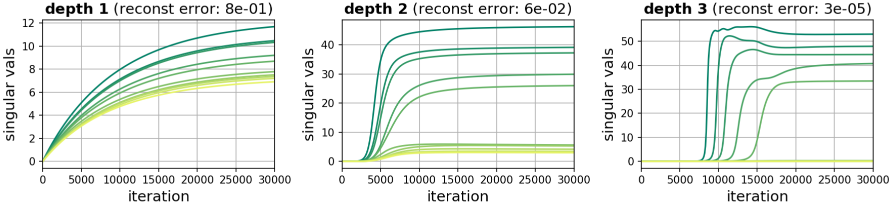
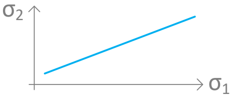


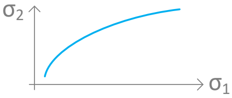
Theoretical Example

For one observed entry and ℓ_2 loss, relationship between singular vals is:

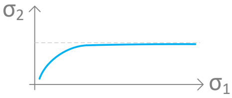
depth 1: linear



depth 2: polynomial



depth ≥ 3: asymptotic



Implicit Bias Towards Low Rank

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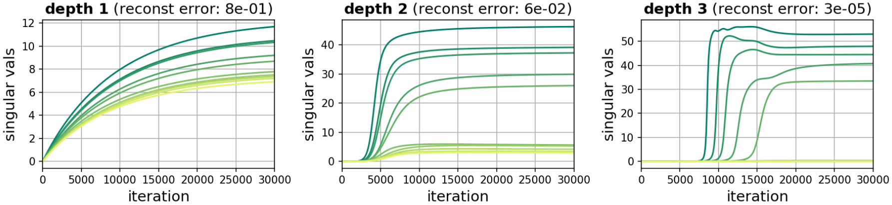
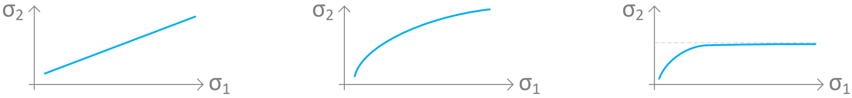


Theoretical Example

For one observed entry and ℓ_2 loss, relationship between singular vals is:

depth 1: linear | *depth 2: polynomial* | *depth* ≥ 3*: asymptotic*



Depth leads to larger gaps between singular vals (lower rank)!

Outline

Recap

Recap

Perspective

To understand optimization and generalization in deep learning:

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- Language of classical learning theory may be insufficient

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Case Study — Deep Linear Neural Networks

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Trajectory analysis:

Recap

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Trajectory analysis:

- **Depth induces preconditioner** promoting movement in directions taken

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Optimization:

Recap

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Optimization:

- **Guarantee of efficient convergence to global min** (most general yet)
- **Depth can accelerate convergence** (w/o any gain in expressiveness)!

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Generalization:

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Optimization:

- **Guarantee of efficient convergence to global min** (most general yet)
- **Depth can accelerate convergence** (w/o any gain in expressiveness)!

Generalization:

- **Depth enhances implicit regularization towards low rank**, yielding generalization for problems such as matrix completion

Outline

Thank You