Deep Linear Networks

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Session 2 : Implicit Acceleration

References

- **On the Optimization of Deep Networks: Implicit Acceleration by Overparameterization**, Sanjeev Arora, Nadav Cohen, Elad Hazan (2018)
- **The geometry of the deep linear network**, Govind Menon (2024)

Recap: Key Questions for Gradient Flow

For the gradient flow dynamics on a loss surface $\mathcal{L}(\mathbf{W})$:

$$\frac{d}{dt}\mathbf{W}(t) = -\nabla_{\mathbf{W}}\mathcal{L}(\mathbf{W}(t))$$

We want to understand:

- Convergence guarantees? (*Yes, for balanced cases*)
- **Convergence rate?**
- Characterization of the minimizer reached?
- Effect of noise and discretization?

Today, we address the second question: can overparameterization improve the **rate of convergence**?

The Counter-Intuitive Message

The conventional wisdom is that increasing depth improves expressiveness but complicates optimization. Today's message, based on Arora, Cohen, & Hazan (2018), is that sometimes:

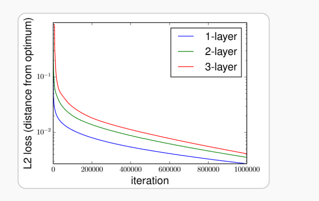
Increasing depth can *accelerate* optimization.

We will see that overparameterization via depth can act as an implicit preconditioner, combining the effects of momentum and adaptive learning rates.

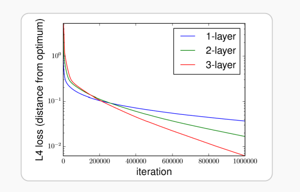
Empirical Evidence: Acceleration with Depth

Comparison of gradient descent on a linear regression task with ℓ_p loss. (Fig 3 from Arora et al. 2018)

L2 Loss Convergence



L4 Loss Convergence



- **Left (ℓ_2 loss):** Increasing depth slightly *slows down* convergence, consistent with prior work.
- **Right (ℓ_4 loss):** Increasing depth provides a **massive acceleration**, outperforming the shallow model significantly.

The End-to-End Update Rule

Let $W_e = W_N W_{N-1} \cdots W_1$ be the end-to-end matrix. The paper shows that its gradient flow dynamics can be written purely in terms of W_e itself.

Theorem 1 (Arora et al. 2018). Under the balanced initialization assumption, $W_{j+1}(t_0)^T W_{j+1}(t_0) = W_j(t_0) W_j(t_0)^T$, the gradient flow for W_e is:

$$\dot{W}_e(t) = -\eta \sum_{j=1}^{N} \left[W_e(t) W_e(t)^T\right]^{\frac{N-j}{N}} \cdot \nabla\mathcal{L}(W_e(t)) \cdot \left[W_e(t)^T W_e(t)\right]^{\frac{j-1}{N}}$$

The standard gradient $\nabla\mathcal{L}(W_e)$ is pre-multiplied and post-multiplied by fractional matrix powers of $W_e W_e^T$ and $W_e^T W_e$.

A Geometric Interpretation

The complex update rule from Theorem 1 seems arbitrary. But it has a beautiful geometric meaning. Let's define the linear preconditioning operator from Theorem 1 as A_{N,W_e}:

$$A_{N,W_e}(Z) = \sum_{k=1}^{N} (W_e W_e^T)^{\frac{N-k}{N}} Z (W_e^T W_e)^{\frac{k-1}{N}}$$

So the dynamics are $\dot{W}_e = -A_{N,W_e}(E'(W_e))$, where $E'(W_e) = \nabla\mathcal{L}(W_e)$ is the standard Euclidean gradient.

Following Menon (Sec 4.3), we define a position-dependent Riemannian metric g^N on the tangent space at W_e via the inner product:

Definition: A New Metric.

$$g^N(W_e)(Z_1, Z_2) := \mathrm{Tr}\left(Z_1^T (A_{N,W_e})^{-1} Z_2\right)$$

(Assuming W_e has full rank, A_{N,W_e} is invertible.)

Under this specific metric, the complicated dynamics of Theorem 1 become a simple and natural **Riemannian gradient flow**:

$$\dot{W}_e(t) = -\mathbf{grad}_{g^N} E(W_e(t))$$

Interpreting the Dynamics (Single Output Case)

For the special case of a single output ($k = 1$), the preconditioning scheme simplifies to a more intuitive form.

Claim 2 (Arora et al. 2018). For a single output network, the end-to-end dynamics are equivalent to:

$$\dot{W}_e = -\eta \underbrace{\|W_e\|^{2-\frac{2}{N}}}_{\text{Adaptive LR}} \left(\nabla\mathcal{L}(W_e) + \underbrace{(N-1)\,\mathrm{Pr}_{W_e}(\nabla\mathcal{L}(W_e))}_{\text{Momentum-like term}} \right)$$

where $\mathrm{Pr}_{W_e}(V)$ is the orthogonal projection of vector V onto the direction of vector W_e.

- **Adaptive Learning Rate:** As the weight vector $\|W_e\|$ grows (moves away from zero init), the effective learning rate increases.
- **Momentum:** The gradient is amplified along the direction of the current weight vector W_e. Since W_e is the integral of past updates, this promotes movement along the historical trajectory.

Detailed Derivations

Proof of Theorem 1 (N=2 case)

Let's derive the end-to-end dynamics for $W_e = W_2 W_1$. The time derivative is $\dot{W}_e = \dot{W}_2 W_1 + W_2 \dot{W}_1$.

1. Substitute the gradient flow dynamics for each layer:

$$\dot{W}_1 = -\eta W_2^T \nabla\mathcal{L}(W_e) \quad , \quad \dot{W}_2 = -\eta \nabla\mathcal{L}(W_e) W_1^T$$

2. Plug these into the expression for $\dot{W}_e$:

$$\dot{W}_e = (-\eta\nabla\mathcal{L}(W_e) W_1^T) W_1 + W_2(-\eta W_2^T \nabla\mathcal{L}(W_e))$$

3. Rearrange the terms:

$$\dot{W}_e = -\eta\left((W_2 W_2^T)\nabla\mathcal{L}(W_e) + \nabla\mathcal{L}(W_e)(W_1^T W_1)\right)$$

4. Using the identities for the N=2 case, $W_2 W_2^T = (W_e W_e^T)^{1/2}$ and $W_1^T W_1 = (W_e^T W_e)^{1/2}$:

$$\dot{W}_e = -\eta\left((W_e W_e^T)^{1/2}\nabla\mathcal{L}(W_e) + \nabla\mathcal{L}(W_e)(W_e^T W_e)^{1/2}\right)$$

This matches the general formula from Theorem 1 for $N = 2$.

Deriving the Preconditioner

SVD Setup (N=3 case)

Let's analyze $N = 3$. Let the SVD of each layer be $W_j = U_j \Sigma_j V_j^T$.

- **Balance Invariants:** $W_2^T W_2 = W_1 W_1^T$. Hence, their spectra are equal as well $\implies W_1$ and W_2 have the same set of singular values.
- In terms of Polar decomposition, the balance equation implies $P_2 = W_2^T W_2 = W_1 W_1^T = R_1$. Hence, V_2 and U_1 can be chosen to be equal. Therefore, we get the SVD decompositions: $W_2 = U_2 \Sigma V_2^T$ and $W_1 = V_2 \Sigma V_1^T$.
- Similarly using the balance equation for W_2 and W_3, we get the SVDs: $W_3 = U_3 \Sigma V_3^T$, $W_2 = V_3 \Sigma V_2^T$ and $W_1 = V_2 \Sigma V_1^T$.

Simplifying the Product

Let's express the end-to-end matrix $W_e = W_3 W_2 W_1$ using the SVDs and the relationships we found. The expression simplifies because the intermediate orthogonal matrices cancel out:

$$W_e = U_3 \Sigma^3 V_1^T$$

This looks like an SVD for W_e, with singular value matrix Σ^3 and orthogonal matrices U_3 and V_1^T.

Final Identities

From $W_e = U_3 \Sigma^3 V_1^T$, we can identify the SVD components of $W_e = U_e \Sigma_e V_e^T$ as $U_e = U_3$, $\Sigma_e = \Sigma^3$, $V_e = V_1$.

Now we can express the individual layer terms using the end-to-end SVD components.

- For the last layer, $W_3 W_3^T = U_3 \Sigma^2 U_3^T$. Since $U_3 = U_e$ and $\Sigma = \Sigma_e^{1/3}$:

$$W_3 W_3^T = U_e (\Sigma_e^{1/3})^2 U_e^T = (U_e \Sigma_e U_e^T)^{2/3} = (W_e W_e^T)^{2/3}$$

- For the first layer, $W_1^T W_1 = V_1 \Sigma^2 V_1^T$. Using $\Sigma = \Sigma_e^{1/3}$ and $V_1 = V_e$:

$$W_1^T W_1 = V_1 (\Sigma_e^{1/3})^2 V_1^T = (V_e^T \Sigma_e V_e)^{2/3} = (W_e^T W_e)^{2/3}$$

How This Leads to Acceleration

Setup

We analyze a simple, ill-conditioned linear regression problem with ℓ_4 loss and $N = 2$ overparameterization.

- **Data:** Two points, $([1, 0], y_1)$ and $([0, 1], y_2)$.
- **Loss:** $L(w_1, w_2) = \frac{1}{4}(w_1 - y_1)^4 + \frac{1}{4}(w_2 - y_2)^4$.
- **Ill-Conditioning:** Assume $|y_1| \gg |y_2| \approx 1$.
- **Initialization:** Near-zero weights, $w_1^{(0)} = \epsilon_1, w_2^{(0)} = \epsilon_2$, with $\epsilon_2/\epsilon_1 \approx y_2/y_1$.

Standard GD

The standard gradient descent update for each coordinate is decoupled:

$$w_i^{(t+1)} \leftarrow w_i^{(t)} - \eta(w_i^{(t)} - y_i)^3$$

- To avoid divergence, the learning rate η is limited by the coordinate with the largest gradient, which is w_1. The stability condition requires: $\eta < \frac{2}{(w_1 - y_1)^2} \approx \frac{2}{y_1^2}$.
- This very small learning rate, dictated by y_1, is then applied to the update for w_2.
- The convergence for w_2 is extremely slow. The error $\Delta_2 = w_2 - y_2$ shrinks by a factor of approximately $(1 - \eta y_2^2)$ at each step, which is very close to 1.

Overparameterized GD

For $N = 2$, the discrete update rule for a single output network is:

$$\mathbf{w}^{(t+1)} \leftarrow \mathbf{w}^{(t)} - \eta\left(\|\mathbf{w}^{(t)}\|\nabla\mathcal{L}(\mathbf{w}^{(t)}) + \mathrm{Pr}_{\mathbf{w}^{(t)}}(\nabla\mathcal{L}(\mathbf{w}^{(t)}))\right)$$

Using the condition $\epsilon_2/\epsilon_1 \approx y_2/y_1 \ll 1$, we have $\|\mathbf{w}^{(0)}\| \approx \epsilon_1$. The updates simplify to:

$$w_1^{(1)} \approx \epsilon_1 + \eta(2\epsilon_1 y_1^3) \quad , \quad w_2^{(1)} \approx \epsilon_2 + \eta(\epsilon_1 y_2^3 + \epsilon_2 y_1^3)$$

The Punchline

1. **Choose η:** We can now choose a large learning rate for w_1 to make it converge in one step. Let $\eta = \frac{1}{2\epsilon_1 y_1^2}$. This gives $w_1^{(1)} \approx y_1$.
2. **Analyze w_2 update:** With this η, the update for w_2 becomes approximately $\frac{y_2}{2}$.
3. **Compare Rates:** In one step, w_2 has moved halfway to its target y_2. The effective learning rate for w_2 after w_1 converges is $\eta_{OP} \approx \frac{1}{2\epsilon_1 y_1}$. The speedup is:

$$\frac{\eta_{OP}}{\eta_{GD}} > \frac{1/(2\epsilon_1 y_1)}{2/y_1^2} = \frac{y_1}{4\epsilon_1} \gg 1$$

Overparameterization allows the large coordinate to "lend" its scale to accelerate the small coordinate.

Next Time...

Characterizing the Minimizer

Thank You!

Any Questions?