

Benefits of Early Stopping in Gradient Descent for Overparameterized Logistic Regression

Hyojeong An Taesun Yeom

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Overview

1. Preliminaries, Backgrounds, and Setups
2. Part 1: Upper Bounds for Early-Stopped GD
3. Part 2: Early Stopping vs. Asymptotic Regime
4. Part 3: Early Stopping and ℓ_2 -Regularization
5. Conclusion

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Motivation

Q. Why do deep neural networks (or at least simplified models) generalize well, even when they are heavily overparameterized?



The need for an **easy-to-handle, tractable model and setup.**

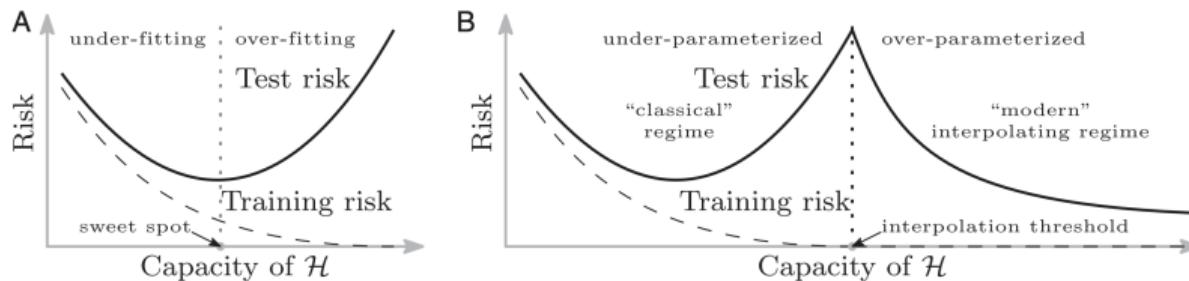


Figure: Deep Double Descent [1]

Back to Basic: Logistic Regression

- Given n data points $\{(\mathbf{x}_i, y_i)\}_{i=1}^n$

$$\mathbf{x}_i \in \mathbb{R}^d, \quad y_i \in \{+1, -1\}, \quad i \leq n. \quad (1)$$

- Trained with empirical logistic loss

$$\hat{\mathcal{L}}(\mathbf{w}) = \frac{1}{n} \sum_{i=1}^n \ell(y_i \mathbf{x}_i^\top \mathbf{w}) = \frac{1}{n} \sum_{i=1}^n \ln(1 + \exp(-y_i \mathbf{x}_i^\top \mathbf{w})). \quad (2)$$

- Update via a full-batch gradient descent

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \eta \nabla \hat{\mathcal{L}}(\mathbf{w}_t). \quad (3)$$

(Asymptotic) Implicit Bias

- Implicit bias is informally defined as a “characteristic” of the predictor at $t \rightarrow \infty$.
 - From regression (i.e., MSE loss) to classification (i.e., exp, logistic loss).
- From [3], if the training data distribution is **linearly separable**, the (normalized) predictor at limit $\tilde{\mathbf{w}}$ becomes ℓ_2 max-margin solution:

$$\tilde{\mathbf{w}} = \arg \max_{\|\mathbf{w}\|=1} \min_i y_i \mathbf{x}_i^\top \mathbf{w} > 0, \quad \frac{\mathbf{w}_t}{\|\mathbf{w}_t\|} \rightarrow \tilde{\mathbf{w}}. \quad (4)$$

Q. Does this formula always yield a favorable implicit bias?
Moreover, is it related to generalization?

Data model

$$\mathbf{x} \sim \mathcal{N}(0, \Sigma), \quad \Pr(y|\mathbf{x}) = \frac{1}{1 + \exp(-y\mathbf{x}^\top \mathbf{w}^*)}. \quad (5)$$

- Σ (covariance matrix): PSD + Bounded trace
- \mathbf{w}^* (true model): $\|\mathbf{w}^*\|_\Sigma := \mathbf{w}^{*\top} \Sigma \mathbf{w}^* < \infty \implies \text{Std}(\mathbf{x}^\top \mathbf{w}^*) < \infty$.
- Labels are generated by \mathbf{w}^* (Eq. 5), with **some inherent noise**.
- During the paper, we will consider the following setup.
 - *Noisy*, $\|\mathbf{w}^*\|_\Sigma \lesssim 1$: The true model generates “uncertain” labels (i.e., prediction near 0.5).
 - *Overparameterized*, $\text{rank}(\Sigma) \geq n$: Always exists a hyperplane that **perfectly separates the training set**, i.e., perfect train acc.

Theoretical Picture

Part 1. Early-stopped logistic regression achieves a vanishing risk upper bound.

Part 2. Which outperforms the model in the asymptotic regime.



Part 3. Indeed, there exists a strong connection
between early stopping time and ℓ_2 -regularization.

Metrics

Let $(\mathbf{x}, y) \in \mathbb{H} \times \{\pm 1\}$. \mathbb{H} is a finite or countably infinite-dimensional Hilbert space.

- **Logistic risk**

$$\mathcal{L}(\mathbf{w}) := \mathbb{E} \ell(y \mathbf{x}^\top \mathbf{w}), \quad \text{where } \ell(t) := \ln(1 + e^{-t}) \quad (6)$$

- Zero-one error

$$\mathcal{E}(\mathbf{w}) := \mathbb{E} \mathbf{1}[y \mathbf{x}^\top \mathbf{w} \leq 0] = \Pr(y \mathbf{x}^\top \mathbf{w} \leq 0) \quad (7)$$

- Calibration error

$$\mathcal{C}(\mathbf{w}) := \mathbb{E} |p(\mathbf{w}; \mathbf{x}) - \Pr(y = 1 | \mathbf{x})|^2 \quad (8)$$

In this presentation, we will mainly focus on the “logistic risk.”

Basic Properties

- **True model is the best model!**

- The true model \mathbf{w}^* (i.e., Bayes optimal classifier) satisfies

$$\mathbf{w}^* = \arg \min_{\mathbf{w}} \mathcal{L}(\mathbf{w}) \quad \text{and} \quad \mathbf{w}^* \in \arg \min_{\mathbf{w}} \mathcal{E}(\mathbf{w}). \quad (9)$$

- **Basic inequality.**

- The zero-one error is bounded by the calibration error, which is bounded by the logistic risk.

$$\underbrace{\mathcal{E}(\mathbf{w}) - \min \mathcal{E}}_{\text{Zero-one error}} \leq 2\sqrt{\mathcal{C}(\mathbf{w})} \leq \sqrt{2 \cdot \underbrace{(\mathcal{L}(\mathbf{w}) - \min \mathcal{L})}_{\text{Logistic risk}}} \quad (10)$$

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Definitions

Based on the Properties, minimizing logistic risk leads to the following properties:
An estimator $\hat{\mathbf{w}}$ is called

- **Calibrated** if $\mathcal{C}(\hat{\mathbf{w}}) \rightarrow 0$.
 ⇒ The model's predicts the true one.
- **Consistent** if $\mathcal{E}(\hat{\mathbf{w}}) - \min \mathcal{E} \rightarrow 0$.
 ⇒ The model achieves Bayes optimal zero-one error.

Theorem

Early-Stopped GD successfully minimizes the excess logistic risk, thereby achieving both calibration and consistency.

A bias-dominating risk bound

Theorem

Let k be an arbitrary index. Suppose that the stepsize η for GD satisfies $\eta \leq 1/(C_0(1 + \text{tr}(\boldsymbol{\Sigma}) + \lambda_1 \ln(1/\delta)/n))$ where $C_0 > 1$ is a universal constant. Then with probability at least $1 - \delta$, there exists a stopping time t such that

$$\hat{\mathcal{L}}(\mathbf{w}_t) \leq \hat{\mathcal{L}}(\mathbf{w}_{0:k}^*) \leq \hat{\mathcal{L}}(\mathbf{w}_{t-1}). \quad (11)$$

Moreover, for GD with this stopping time, we have

$$\mathcal{L}(\mathbf{w}_t) - \min \mathcal{L} \leq \sqrt{\max \{1, \text{tr}(\boldsymbol{\Sigma})\|\mathbf{w}_{0:k}^*\|^2\} \frac{\ln^2(n/\delta)}{n}} + \frac{1}{2} \|\mathbf{w}_{k:\infty}^*\|_{\boldsymbol{\Sigma}}^2, \quad (12)$$

where C is a constant.

Setup

Let $(\lambda_i, \mathbf{u}_i)$ be the eigenvalue, eigenvector pair of the covariance matrix Σ . Let $\pi(i)$ be resorted indexes such that $\lambda_{\pi(i)}(\mathbf{u}_{\pi(i)}^\top \mathbf{w}^*)^2$ is non-increasing function. Define

$$\begin{aligned}\mathbf{w}_{0:k}^* &:= \sum_{i=1}^k \mathbf{u}_{\pi(i)} \mathbf{u}_{\pi(i)}^\top \mathbf{w}^* \\ \mathbf{w}_{k:\infty}^* &:= \sum_{i=k+1}^{\infty} \mathbf{u}_{\pi(i)} \mathbf{u}_{\pi(i)}^\top \mathbf{w}^*\end{aligned}$$

- We pick k which satisfies $\|\mathbf{w}_{0:k}^*\| = o(\sqrt{n})$.
Then the **risk bound** implies that **logistic risk** vanishes:

$$\mathcal{L}(\mathbf{w}_t) - \min \mathcal{L} = o(1) \quad \text{as } n \text{ increases}$$

Proof Sketch (1)

To bound the risk $\mathcal{L}(\mathbf{w}_t) - \mathcal{L}(\mathbf{w}^*)$, we decompose it into four terms using the empirical risk $\widehat{\mathcal{L}}$ and the model $\mathbf{w}_{0:k}^*$.

$$\begin{aligned}\mathcal{L}(\mathbf{w}_t) - \mathcal{L}(\mathbf{w}^*) &= \underbrace{[\mathcal{L}(\mathbf{w}_t) - \widehat{\mathcal{L}}(\mathbf{w}_t)]}_{(1: \text{ Lemma B.3})} + \underbrace{[\widehat{\mathcal{L}}(\mathbf{w}_t) - \widehat{\mathcal{L}}(\mathbf{w}_{0:k}^*)]}_{(2)} \\ &\quad + \underbrace{[\widehat{\mathcal{L}}(\mathbf{w}_{0:k}^*) - \mathcal{L}(\mathbf{w}_{0:k}^*)]}_{(3: \text{ Lemma B.3})} + \underbrace{[\mathcal{L}(\mathbf{w}_{0:k}^*) - \mathcal{L}(\mathbf{w}^*)]}_{(4: \text{ Lemma B.2})}\end{aligned}$$

- We define the stopping time t such that $\widehat{\mathcal{L}}(\mathbf{w}_t) \leq \widehat{\mathcal{L}}(\mathbf{w}_{0:k}^*)$, then term (2) ≤ 0 .
- Before calculating generalization error, we must ensure the early-stopped parameter \mathbf{w}_t does not explode.

Boundedness

Lemma B.1

Let $\beta := C_0(1 + \text{tr}(\Sigma) + \lambda_1 \ln(1/\delta)/n)$, where $C_0 > 1$ is a sufficiently large constant. Assume that $\eta \leq 1/\beta$ and t is such that $\widehat{\mathcal{L}}(\mathbf{w}_{0:k}^*) \leq \widehat{\mathcal{L}}(\mathbf{w}_{t-1})$. Then with probability at least $1 - \delta$, we have $\|\mathbf{w}_t - \mathbf{w}_{0:k}^*\| \leq 1 + \|\mathbf{w}_{0:k}^*\|$.

Note that

$$\|\mathbf{w}_t - \mathbf{w}_{0:k}^*\| \leq \|\mathbf{w}_t - \mathbf{w}_{t-1}\| + \|\mathbf{w}_{t-1} - \mathbf{w}_{0:k}^*\|$$

- $\widehat{\mathcal{L}}$ is $\sqrt{\beta}$ -Lipschitz
- Let $\widehat{\mathcal{L}}(\cdot)$ be convex and β -smooth. Then for every \mathbf{u} , we have:

$$\frac{\|\mathbf{w}_t - \mathbf{u}\|^2}{2\eta t} + \widehat{\mathcal{L}}(\mathbf{w}_t) \leq \widehat{\mathcal{L}}(\mathbf{u}) + \frac{\|\mathbf{u}\|^2}{2\eta t} \quad (13)$$

Proof Sketch (2)

We need to show that $\widehat{\mathcal{L}}$ is β -smooth and $\sqrt{\beta}$ -Lipschitz for $\beta > 1$

Note that

$$\|\nabla \widehat{\mathcal{L}}(\mathbf{w})\| \leq \sqrt{\frac{1}{n} \sum_{i=1}^n \|\mathbf{x}_i\|^2}, \quad \|\nabla^2 \widehat{\mathcal{L}}(\mathbf{w})\| \leq \frac{1}{n} \sum_{i=1}^n \|\mathbf{x}_i\|^2.$$

By Bernstein's inequality, we have the following with probability at least $1 - \delta$:

$$\begin{aligned} \sum_{i=1}^n \|\mathbf{x}_i\|^2 &= \sum_{i=1}^n \sum_j \lambda_j z_{ij}^2 \leq n \text{tr}(\boldsymbol{\Sigma}) + C_1 \left(\sqrt{n \sum_j \lambda_j^2 \ln(1/\delta)} + \lambda_1 \ln(1/\delta) \right) \\ &\leq C_0(n \text{tr}(\boldsymbol{\Sigma}) + \lambda_1 \ln(1/\delta)) \leq \beta, \end{aligned}$$

where $C_0, C_1 > 1$ are constants.

Generalization Error

Lemma B.3

Let $C_1 > 1$ be a sufficiently large constant. Then with probability at least $1 - \delta$,

$$\sup_{\|\mathbf{w}\| \leq W} |\mathcal{L}(\mathbf{w}) - \hat{\mathcal{L}}(\mathbf{w})| \leq C_1 W \sqrt{\frac{(1 + \text{tr}(\boldsymbol{\Sigma})) \ln(n/\delta) \ln(1/\delta)}{n}}.$$

By applying Rademacher Complexity Bounds [2], we have

$$\begin{aligned} \sup_{\|\mathbf{w}\| \leq W} (L(\mathbf{w}) - \hat{\mathcal{L}}(\mathbf{w})) &\leq \frac{W}{n} + 2XW \sqrt{\frac{1}{n}} + XW \sqrt{\frac{\ln(1/(3\delta))}{2n}} \\ &\leq C_1 W \sqrt{\frac{(1 + \text{tr}(\boldsymbol{\Sigma})) \ln(n/\delta) \ln(1/\delta)}{n}}, \end{aligned}$$

where $C_1 > 1$ is a constant.

Approximation Error

Lemma B.2

Let $\mathbf{w}^* \in \arg \min \mathcal{L}(\mathbf{w})$, then for every \mathbf{w} , we have

$$\mathcal{L}(\mathbf{w}) \leq \mathcal{L}(\mathbf{w}^*) + \frac{1}{2} \|\mathbf{w} - \mathbf{w}^*\|_{\Sigma}^2. \quad (14)$$

Notice that

$$\nabla^2 \mathcal{L}(\mathbf{w}) = \mathbb{E} \ell''(y \mathbf{x}^\top \mathbf{w}) \mathbf{x} \mathbf{x}^\top = \mathbb{E} \frac{\mathbf{x} \mathbf{x}^\top}{(1 + \exp(\mathbf{x}^\top \mathbf{w}))(1 + \exp(-\mathbf{x}^\top \mathbf{w}))} \preceq \mathbb{E} \mathbf{x} \mathbf{x}^\top = \Sigma. \quad (15)$$

Moreover, we have $\nabla \mathcal{L}(\mathbf{w}^*) = 0$. Then by the midpoint theorem, there exists a \mathbf{v} such that

$$\mathcal{L}(\mathbf{w}) - \mathcal{L}(\mathbf{w}^*) = \langle \nabla \mathcal{L}(\mathbf{w}^*), \mathbf{w} - \mathbf{w}^* \rangle + \frac{1}{2} (\mathbf{w} - \mathbf{w}^*)^\top \nabla^2 \mathcal{L}(\mathbf{v}) (\mathbf{w} - \mathbf{w}^*) \leq \frac{1}{2} \|\mathbf{w} - \mathbf{w}^*\|_{\Sigma}^2. \quad (16)$$

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Asymptotic Behavior of the Logistic Risk

Theorem (Logistic risk at limit)

Suppose that Assumption 1 holds. Let $\tilde{\mathbf{w}}$ be a unit vector such that $\|\tilde{\mathbf{w}}\|_{\Sigma} > 0$ and let $(\mathbf{w}_t)_{t \geq 0}$ be a sequence of vectors such that

$$\|\mathbf{w}_t\| \rightarrow \infty, \quad \frac{\mathbf{w}_t}{\|\mathbf{w}_t\|} \rightarrow \tilde{\mathbf{w}}. \quad (17)$$

Then we have

$$\mathcal{L}(\mathbf{w}_t) = \infty. \quad (18)$$

If data are “noisy” ...

- Logistic risk (\mathcal{L}) at limit: Diverges!

Early stopping is better than asymptotic GD!

Proof Sketch (1)

Fix a small constant $\gamma > 0$. Define an *special* event

$$\mathcal{F} := \{\mathbf{x} : |\mathbf{x}^\top \mathbf{w}^*| \leq 10\|\mathbf{w}^*\|_{\Sigma}, \|\mathbf{x}\| \leq 10\sqrt{\text{tr}(\Sigma)}, |\mathbf{x}^\top \tilde{\mathbf{w}}| \geq \gamma\}. \quad (19)$$

Let t_0 be such that $\|\mathbf{w}_t/\|\mathbf{w}_t\| - \tilde{\mathbf{w}}\| \leq \gamma/(20\sqrt{\text{tr}(\Sigma)})$, for every $t \geq t_0$. Next, we have

$$\frac{|\mathbf{x}^\top \mathbf{w}_t|}{\|\mathbf{w}_t\|} \geq |\mathbf{x}^\top \tilde{\mathbf{w}}| - \left| \mathbf{x}^\top \left(\frac{\mathbf{w}_t}{\|\mathbf{w}_t\|} - \tilde{\mathbf{w}} \right) \right| \quad (20)$$

$$\geq |\mathbf{x}^\top \tilde{\mathbf{w}}| - \|\mathbf{x}\| \left\| \frac{\mathbf{w}_t}{\|\mathbf{w}_t\|} - \tilde{\mathbf{w}} \right\| \geq \frac{\gamma}{2}. \quad (21)$$

Proof Sketch (2)

Then for every $\mathbf{x} \in \mathcal{F}$ and $t \geq t_0$, we have the population risk

$$\mathcal{L}(\mathbf{w}_t) = \mathbb{E}_{\mathbf{x}} \mathbb{E}_y \ln(1 + \exp(-y \mathbf{x}^\top \mathbf{w}_t)) \quad (22)$$

$$\geq \mathbb{E} \sum_{y \in \{-1, +1\}} \frac{\ln(1 + \exp(-y \mathbf{x}^\top \mathbf{w}_t))}{1 + \exp(-y \mathbf{x}^\top \mathbf{w}^*)} \mathbf{1}[\mathbf{x} \in \mathcal{F}] \quad (23)$$

$$\geq \mathbb{E} \frac{\ln(1 + \exp(|\mathbf{x}^\top \mathbf{w}_t|))}{1 + \exp(|\mathbf{x}^\top \mathbf{w}^*|)} \mathbf{1}[\mathbf{x} \in \mathcal{F}] \quad (24)$$

$$\geq \mathbb{E} \frac{\|\mathbf{w}_t\| \gamma / 2}{1 + \exp(10 \|\mathbf{w}^*\|_\Sigma)} \Pr(\mathcal{F}) \rightarrow \infty. \quad (25)$$

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Early stopping vs. ℓ_2 -regularization

Theorem (Early stopping vs. ℓ_2 -reg.)

Let $\widehat{\mathcal{L}}(\cdot)$ be convex and β -smooth. Consider $(\mathbf{w}_t)_{t \geq 0}$ given by GD iteration with $\eta \leq 1/\beta$ and $(\mathbf{u}_\lambda)_{\lambda > 0} := \arg \min_{\mathbf{u}} \widehat{\mathcal{L}}(\mathbf{u}) + (\lambda/2)\|\mathbf{u}\|^2$. Set $\lambda = 1/(\eta t)$. Then we have ,

$$\|\mathbf{w}_t - \mathbf{u}_\lambda\| \leq \frac{1}{\sqrt{2}} \|\mathbf{w}_t\|. \quad (26)$$

As a direct consequence, we also have

$$\cos(\mathbf{w}_t, \mathbf{u}_\lambda) \geq \frac{1}{\sqrt{2}}, \quad \frac{\sqrt{2}}{\sqrt{2}+1} \|\mathbf{u}_\lambda\| \leq \|\mathbf{w}_t\| \leq \frac{\sqrt{2}}{\sqrt{2}-1} \|\mathbf{u}_\lambda\|. \quad (27)$$

- Under certain settings, the trajectories of ℓ_2 -reg. and early stopping do not differ significantly in terms of angle and norm.
- $\lambda = 1/(\eta t)$: **Short training (i.e., small t) \iff Strong reg. (i.e., large λ)**.

Proof Sketch (1)

For the first-order stationary point of the ℓ_2 -reg. ERM

$$\nabla \widehat{\mathcal{L}}(\mathbf{u}_\lambda) + \lambda \mathbf{u}_\lambda = \nabla \widehat{\mathcal{L}}(\mathbf{u}_\lambda) + \frac{1}{\eta t} \mathbf{u}_\lambda. \quad (28)$$

With the results of the early stopping + convexity, we have,

$$\frac{1}{2} \|\mathbf{w}_t - \mathbf{u}_t\|^2 - \frac{1}{2} \|\mathbf{u}_t\|^2 \leq \eta t (\widehat{\mathcal{L}}(\mathbf{u}_\lambda) - \widehat{\mathcal{L}}(\mathbf{w}_t)) \quad (29)$$

$$\leq \eta t \langle \nabla \mathcal{L}(\mathbf{u}_\lambda), \mathbf{u}_\lambda - \mathbf{w}_t \rangle = -\langle \mathbf{u}_\lambda, \mathbf{u}_\lambda - \mathbf{w}_t \rangle. \quad (30)$$

Rearranging the terms, we get

$$\frac{1}{2} \|\mathbf{w}_t - \mathbf{u}_\lambda\|^2 \leq \langle \mathbf{u}_\lambda, \mathbf{w}_t \rangle - \frac{1}{2} \|\mathbf{u}_\lambda\|^2 \iff \|\mathbf{w}_t - \mathbf{u}_\lambda\|^2 \leq \frac{1}{2} \|\mathbf{w}_t\|^2. \quad (31)$$

Proof Sketch (2)

1. Angle

From $2\langle \mathbf{u}_\lambda, \mathbf{w}_t \rangle \geq \frac{1}{2}\|\mathbf{w}_t\|^2 + \|\mathbf{u}_\lambda\|^2$, we obtain

$$\cos(\mathbf{u}_\lambda, \mathbf{w}_t) = \frac{\langle \mathbf{u}_\lambda, \mathbf{w}_t \rangle}{\|\mathbf{u}_\lambda\| \|\mathbf{w}_t\|} \geq \frac{\frac{1}{2}(\frac{1}{2}\|\mathbf{w}_t\|^2 + \|\mathbf{u}_\lambda\|^2)}{\|\mathbf{u}_\lambda\| \|\mathbf{w}_t\|} \geq \frac{1}{\sqrt{2}}. \quad (32)$$

2. Norm

We have

$$\frac{1}{\sqrt{2}}\|\mathbf{w}_t\| \geq \|\mathbf{w}_t - \mathbf{u}_\lambda\| \geq \begin{cases} \|\mathbf{w}_t\| - \|\mathbf{u}_\lambda\| \\ \|\mathbf{u}_\lambda\| - \|\mathbf{w}_t\|, \end{cases} \quad (33)$$

which implies

$$\frac{\sqrt{2}}{\sqrt{2}+1}\|\mathbf{u}_\lambda\| \leq \|\mathbf{w}_t\| \leq \frac{\sqrt{2}}{\sqrt{2}-1}\|\mathbf{u}_\lambda\|. \quad (34)$$

Blessing of Dimensionality?

Q. What if we care about the ℓ_2 distance between the predictors?

- In high dimension, the “support vector condition” typically holds, which is defined as

$$\text{rank}\{x_i : i \in \mathcal{S}_+\} = \text{rank}\{x_i : i \in [n]\}. \quad (35)$$

= the rank of the support vector should be same as the rank of the data matrix.

- Under this condition, we have,

$$\|\mathbf{w}_t - \mathbf{u}_{\lambda(t)}\| \rightarrow 0, \quad \text{while } \|\mathbf{w}_t\|, \|\mathbf{u}_{\lambda(t)}\| \rightarrow \infty, \quad \text{as } t \rightarrow \infty. \quad (36)$$

- But with low-dimensional vectors, there exists some exceptions, i.e., difference between the norm diverges.

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Conclusion & Discussion

So far, this work investigates:

- Early stopping in overparameterized logistic regression improves logistic risk, zero-one error, and calibration error,
 - Early stopping is better than asymptotic GD,
 - Strong connection between early stopping and ℓ_2 -regularization.
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However, several challenges remain to be addressed in future work:

- The results depends on the oracle-chosen stopping time.
- This work focuses on linear models, not deep nets.
 - Networks with more than two layers exhibit distinct and more complex phenomena (e.g., as the lazy-rich dynamic [4]).

Q & A

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