Algorithmic Regularization: Bias Us Toward “Simple” Models

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Deep learning achieves big successes

- The rise of deep learning in various applications
  - Image classification, semantic segmentation
  - Natural language processing
  - AlphaGo
  - AlphaFold
  - ...

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- The rise of deep learning in various applications
  - Image classification, semantic segmentation
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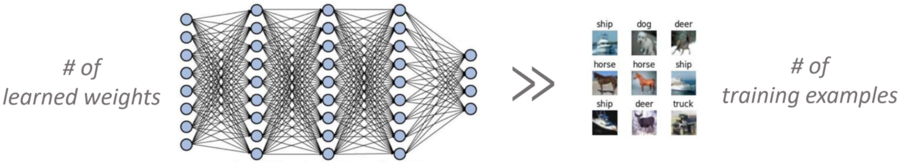
- Deep models often generalize well even without explicit regularization

- Algorithmic regularization: the optimization algorithm biases us toward a "simple" model that generalize well

Generalaization in deep learning

Deep neural networks are typically over-parameterized



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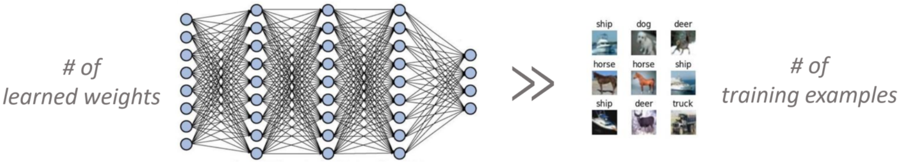
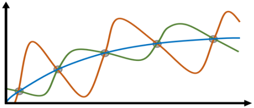


Many possible solutions fit training data



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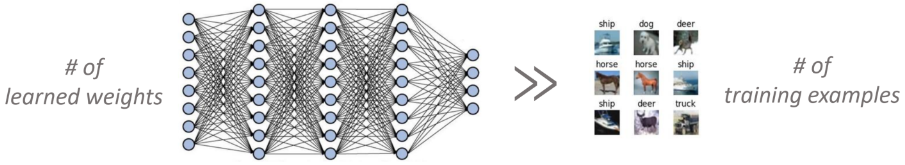

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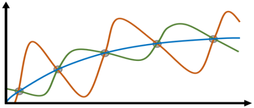

Variants of gradient descent (GD) usually find solutions that generalize well

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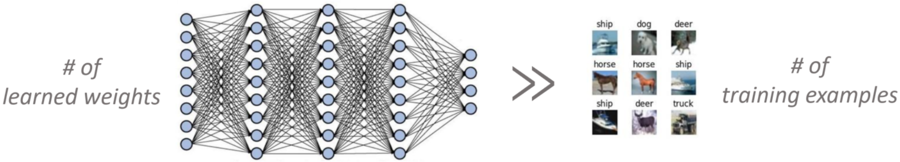

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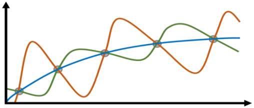


Variants of gradient descent (GD) usually find solutions that generalize well

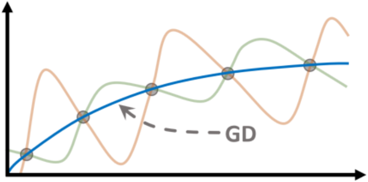
↑

Even without explicit regularization!

Implicit regularization

Imiplict regularization prefers “simpler” models

- GD fits trainning data with predictors of lowest possible complexity



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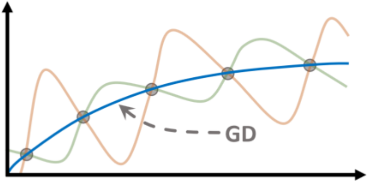
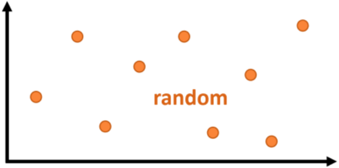


- Natural data can be fit with low complexity, other data cannot



Challenge: how to formalize the implicit regularization?

Goal

Mathematically formalize implicit regularization in deep learning

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Mathematically formalize implicit regularization in deep learning

Approach

- Start with simple models and standard GD algorithms
- Investigate the implicit bias for variants of GD on general models

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Let's start with a simple model

Consider linear regression with the squared loss function

Empirical risk minimization

$$L(w) = \sum_{i=1}^{n} (w^T x^{(i)} - y^{(i)})^2$$

- $n < d$ and the objective function is realizable, i.e., $\min_w L(w) = 0$

Let's start with a simple model

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- $n < d$ and the objective function is realizable, i.e., $\min_w L(w) = 0$
- The objective function has multiple global minima

$$\mathcal{G} = \{w : \forall i, w^T x^{(i)} = y^{(i)}\}$$

GD induces a unique minimum

Proposition 1 ([GLSS18])

Consider GD updates w_t starting with w_0. For any step-size schedule that minimizes $L(w)$, the algorithm returns a special global minimizer that implicitly also minimizes the Euclidean distance to w_0:

$$w_t \to \arg\min_{w \in \mathcal{G}} \|w - w_0\|_2^2 \tag{1}$$

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- GD implicitly induces a unique minimum that also minimizes the Euclidean distance to w_0

Proof sketch

Proof.

Note that $\forall w$, $\nabla L(w) = \sum_i (w^T x^{(i)} - y^{(i)}) x^{(i)} \in \text{span}(x^{(i)})$.
The gradients are restricted to a n dimensional subspace that is independent of w. The GD updates from initialization w_0, thus $w_t - w_0 = \sum_{t'<t} \eta \nabla L(w_{t'})$ are also constrained to the n dimensional subspace.

Proof sketch

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The gradients are restricted to a *n* dimensional subspace that is independent of w. The GD updates from initialization w_0, thus $w_t - w_0 = \sum_{t'<t} \eta \nabla L(w_{t'})$ are also constrained to the n dimensional subspace.
There exists a unique global minimizer that both fits the data ($w \in \mathcal{G}$) and is reachable by GD $w \in w_0 + \text{span}(x^{(i)})$. It is exactly the KKT condition of

$$\min_{w \in \mathcal{G}} ||w - w_0||_2^2 \tag{2}$$

which completes the proof $\square$

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Geometry induced by updates of local search algorithm

GD iterations can be alternatively specified as a local approximation while constraining the step length

$$w_{t+1} = \arg\min_{w} \langle w, \nabla L(w_t) \rangle + \frac{1}{2\eta} \|w - w_t\|_2^2 \tag{3}$$

Motivated by this connection, we can study other families of algorithms that work under different geometries

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Motivated by this connection, we can study other families of algorithms that work under different geometries

- Mirror descent w.r.t. Bregman divergence with potential ψ
- Steepest descent w.r.t. general norms

Mirror descent

Mirror descent w.r.t. Bregman divergence with potential ψ

Mirror descent updates are defined for any strongly convex and differentiable potential ψ as

$$\begin{aligned} w_{t+1} &= \arg\min_{w} \eta\langle w, \nabla L(w_t)\rangle + D_{\psi}(w, w_t) \\ &\Rightarrow \nabla\psi(w_{t+1}) = \nabla\psi(w_t) - \eta\nabla L(w_t) \end{aligned} \tag{4}$$

where $D_{\psi}(w, w') = \psi(w) - \psi(w') - \langle\nabla\psi(w'), w - w'\rangle$ is the Bregman divergence.

- $\psi(w) = \frac{1}{2}||w||_2^2$ leads to gradient descent
- Entropy potential $\psi(w) = \sum_i w[i]\log w[i] - w[i]$

Mirror update induced minima

Theorem 1 ([BT03])

For any realizable dataset $\{x^{(i)}, y^{(i)}\}_{i=1}^{n}$, and any strongly convex potential ψ, consider the mirror descent iterates w_t that minimizes $L(w)$. For w_0, if the step-size schedule minimizes $L(w)$, then then the asymptotic solution of the algorithm is given by

$$w_t \to \arg\min_{w \in \mathcal{G}} D_{\psi}(w, w_0) \tag{5}$$

Steepest descent

GD is also a special case of steepest descent (SD) w.r.t. a generic norm $||\cdot||$

Steepest descent w.r.t. general norms

$$w_{t+1} = w_t + \eta_t \Delta w_t, \text{ where } \Delta w_t = \arg\min_v \langle \nabla L(w_t), v \rangle + \frac{1}{2}||v||^2 \quad (6)$$

- ℓ_2 norm leads to gradient descent
- ℓ_1 norm leads to coordinate descent

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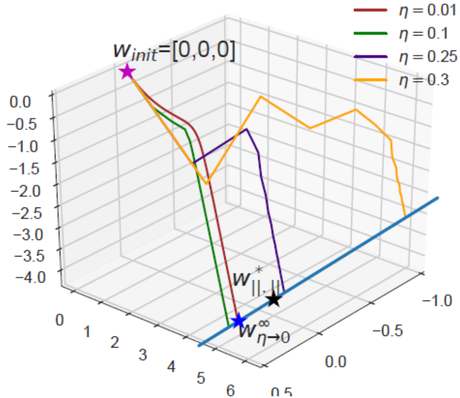
- ℓ_2 norm leads to gradient descent
- ℓ_1 norm leads to coordinate descent

- We may expect the steepest descent iterates to converge to the solution closest to w_0 in the corresponding norm
- It is only true for quadratic norms $||v||_D = \sqrt{v^T D v}$
- Unfortunately, it does not hold for general norms

Example: the global minimum depends on the step size

Consider the dataset
$\{(x^{(1)} = [1, 1, 1], y^{(1)} = 1), (x^{(2)} = [1, 2, 0], y^{(2)} = 10)\}$ using steepest descent updates w.r.t. $\ell_{4/3}$ norm



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Matrix factorization as a prediction problem

Matrix completion: recover an unknown matrix given its subset of entries

Bob	4	?	?	4
Alice	?	5	4	?
Joe	?	5	?	?

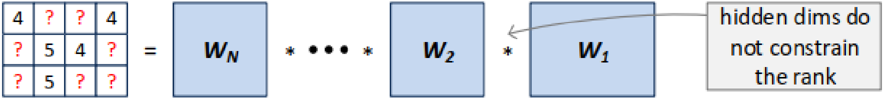
observations $\{y_{ij}\}_{(i,j)\in\Omega}$

$n \times p$ matrix completion $\Longleftrightarrow$ prediction from $\{1, \cdots, n\} \times \{1, \cdots, p\}$ to $\mathbb{R}$

Matrix Factorization $\longleftrightarrow$ Linear Neural Network

Matrix Factorization (MF)

Parameterize solution as product of matrices and fit observations via GD



$$\min_{W_1,\ldots,W_N} \sum_{(i,j)\in\Omega} \left([W_N W_{N-1} \cdots W_1]_{ij} - y_{ij} \right)^2$$

MF $\longleftrightarrow$ matrix completion via linear NN (with no explicit regularization)

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Matrix Factorization (MF)

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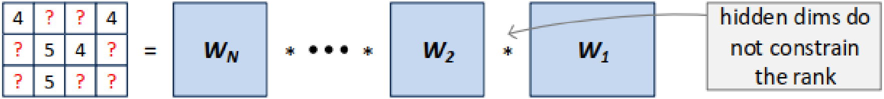


$$\min_{W_1,\dots,W_N} \sum_{(i,j)\in\Omega} \left([W_N W_{N-1} \cdots W_1]_{ij} - y_{ij}\right)^2$$

MF $\longleftrightarrow$ matrix completion via linear NN (with no explicit regularization)

Empirical phenomenon [GWB$^+$18]

MF (with small init and step size) accurately recovers low rank matrices

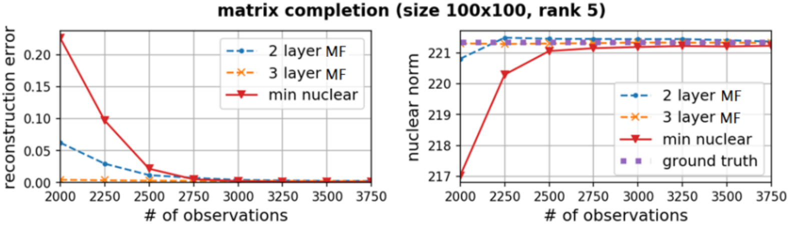
Implicit regularization of GD for MF

Classic results [CR09]

If (i) unknown matrix has low rank; (ii) observations are sufficiently many, then minimizing nuclear norm yields accurate recovery

Conjecture [GWB$^+$18]

MF of depth 2 (with small init and step size) fits observations while minimizing nuclear norm



Dynamical analysis of implicit regularization

Denote: $W_e := W_d \cdots W_1$ – end matrix of MF, $\{\sigma_r\}_r$ – singular vals of W_e

Theorem 2 ([ACHL19])

In training MF of depth d (with small init and step size): $\frac{d}{dt}\sigma_r \propto \sigma_r^{2-2/d}$

Depth speeds up (slows down) large (small) singular vals!

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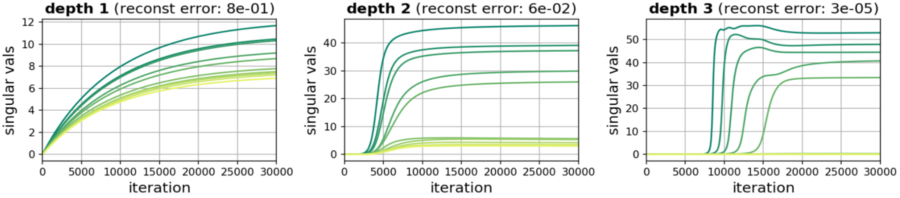
Completion of low rank matrix via MF



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

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Linear models in classification

- Consider linear classification with exponential loss
  $\ell(u, y) = \exp(-uy)$

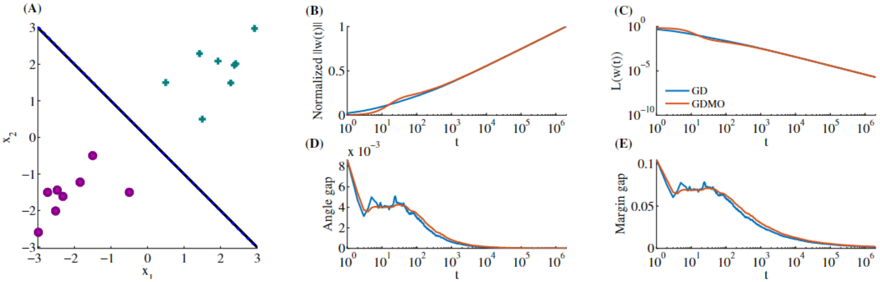
Empirical risk minimization

$$L(w) = \sum_{i=1}^{n} \exp\left(-y^{(i)} w^T x^{(i)}\right)$$

where $y^{(i)} \in \{-1, 1\}$

- Similarly, we consider the gradient descent and steepest descent

Empirical phenomena of GD



- (A) The asymptotic solution of GD coincides with the Max-Margin separator
- (B) $\|w(t)\|$ increases logarithmically
- (C) The loss decrease as t^{-1}
- GD with momentum (GDMO) behaviors similarly

Gradient descent induces ℓ_2 max-margin vector

Theorem 3 ([SHN$^+$18])

For any dataset which is linearly separable, any β-smooth decreasing loss function with an exponential tail, any stepsize $\eta < 2\beta^{-1}\sigma_{\max}^{-2}(X)$, where X is the data matrix and any starting point $w(0)$, the GD iterates will behave as:

$$w(t) = \hat{w}\log t + \rho(t),$$

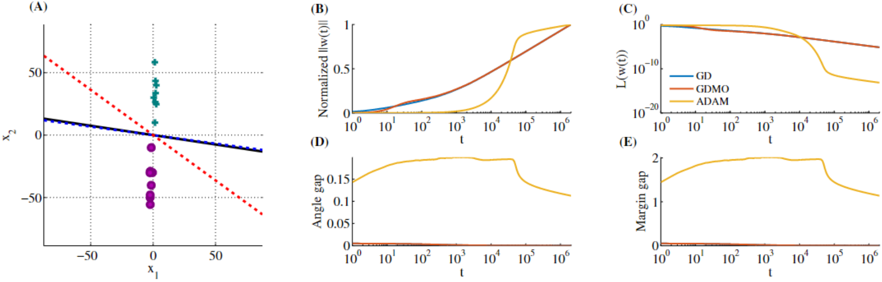
where $\hat{w}$ is the L_2 max margin vector (the solution to hard margin SVM):

$$\hat{w} = \arg\max_{w\in\mathbb{R}^d} \|w\|^2 \ s.t.\ w^T x_n \geqslant 1$$

and the residual grows at most as $\|\rho\| = O(\log\log(t))$, and so

$$\lim_{t\to\infty} \frac{w(t)}{\|w(t)\|} = \frac{\hat{w}}{\|\hat{w}\|}$$

Different algorithms behaves differently



- (A) ADAM [KB15] does not converges to the Max-Margin solution
- GD and GDMO converges to the Max-Margin solution

Implicit bias of steepest descent

Theorem 4 ([GLSS18])

For any separable dataset and any norm $||\cdot||$, consider the steepest descent updates for minimizing $L(w)$ with the exponential loss $\ell(u,y) = exp(-uy)$. For all initialization w_0, and all bounded step-sizes satisfying $\eta_t \leqslant \min\{\eta_+, \frac{1}{B^2 L(w_t)}\}$ where $B := \max_n ||x_n||_*$, $||x||_* := \sup_{||y||\leqslant 1} ||x^T y||$ and $\eta_+ < \infty$. The iterates w_t satisfy

$$\lim_{t\to\infty} \min_n \frac{y_i\langle w_t, y_i\rangle}{||w_t||} = \max_{w:||w||\leqslant 1} \min_n y_i\langle w, x_i\rangle =: \gamma.$$

If the maximum-$||\cdot||$ margin solution $w^* = \arg\max_{||w||\leqslant 1} \min_i y_i\langle w_t, y_i\rangle$ exist, then the direction satisfy $\lim_{t\to\infty} \frac{w_t}{||w_t||_2} = w^*$

- It is a generalization of Theorem 3

The implicit bias of GD for importance weighting

- Assigning importance weights to instances is common practice

$$L(\theta; w) = \frac{1}{N}\sum_{i=1}^{N} w_i \ell(y_i f(\theta, x_i)),$$

  where θ is the parameter of the network and $w_i \in [1/M, M]$ is the bounded importance weight

- [BL19] observes that the effect of importance weights diminishes as the training proceeds

- Question: What is the implicit bias of GD in the presence of importance weights?

The effect of importance weights diminishes

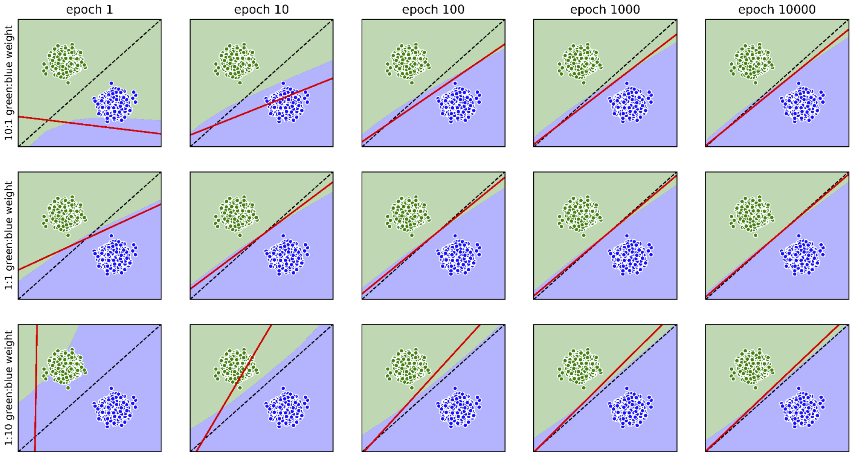


Figure: The decision boundaries are single-layered MLP with 64 hidden units [BL19]. **Black dashed line** shows the max-margin separator and the red dashed line shows the boundary of MLP

Implicit bias of GD for importance weighting

Theorem 5 (informal [XYR21])

For a separable data, with a sufficiently small constant rate η_t, for any $w \in [1/M, M]^n$, we have

$$\left| \frac{\theta^{(t)}}{\|\theta^{(t)}\|} - \theta^* \right| \precsim \frac{\log N + D_{KL}(p^* \| w) + M}{\gamma^* \log t},$$

where $p^* = [p_1^*, \ldots, p_N^*] \geqslant 0$ and $\sum_{i=1}^N p_i^*$ is the dual optimal for the hard margin SVM where $\theta^* = \sum_{i=1}^N y_i x_i p_i^*$, and D_{KL} is the Kullback-Leibler divergence.

- Importance weights does not change the convergence result as well as the convergence rate
- GD still induces the Max-Margin separator

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Homogeneous models with exponential tailed loss

Consider the asymptotic behavior of GD when the prediction is a homogeneous function

Definition 6 (α-homogeous)

$$L(w) = \sum_{i=1}^{n} \exp(-y_i f_i(w)),$$

where $f_i(cw) = c^\alpha f_i(w)$ is α-homogeous. $f_i(w)$ is the output of the prediction.

The associated non-linear margin maximization

$$\min \|w\|^2 \text{ s.t. } y_i f_i(w) \geqslant \gamma$$

First-order stationary point

- The max-margin problem itself is a constrained non-convex problem
- Instead, we show that GD iterates converge to the first-order stationary points of the max-margin problem

Definition 7 (First-order stationary point)

The first-order optimality conditions of Max-Margin are:

- $\forall i, y_i f_i(w) \geqslant \gamma$
- There exists Lagrange multipliers $\lambda \in R_+^N$ such that $w = \sum_n \lambda_n \nabla f_n(w)$ and $\lambda_n = 0$ for $n \notin S_m(w) := \{i : y_i f_i(w) = \gamma\}$, where $S_m(w)$ is the set of support vectors.

$\mathcal{W}^*$ indicates the set of firs-order stationary points

Implicit bias of GD for α-homogeneous function

Theorem 8

Define $\bar{w} = \lim_{t\to\infty} \frac{w_t}{||w_t||}$. *Suppose that* $f_i(w)$ *is a* C^2, $L(w_t) \to 0$, $\lim_{t\to\infty} \frac{w_t}{||w_t||}$ *and* $\lim_{t\to\infty} \frac{\ell_t}{||\ell_t||_1}$ *exist where* ℓ_t *is a vector whose* i*-th entry is* $\exp(-f_i(w_t))$, *and the linear independence constraint qualification (LICQ) holds, i.e.,* $\nabla\{f_i(w)\}_{i\in S_m(w)}$ *are linearly independent.* $\hat{w} \in \mathcal{W}$ *is a first-order stationary point of Max-Margin*

- Theorem 8 extends the result of linear models to α-homogeneous functions
- GD also converges to the Max-Margin solution in a sense

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Stability of GD on quadratic function

- Consider a convex quadratic function, gradient descent with step size η

$$f(x) = \frac{1}{2}x^T A x + b^T x + c$$

- **Sharpness**: the $\lambda_1 := A_{\max}$ is the largest eigenvalue of the Hessian of the objective function
  - If $\eta < 2/\lambda_1$, GD converges
  - If $\eta > 2/\lambda_1$, GD diverges
- In deep learning where the objective is nonconvex, similar analyses can show convergence towards stationary points and local minima
- However, recent empirical studies [CKL+21] showed compelling evidence to the contrary: Edge of Stability across various datasets and net structures

Dynamics of GD on neural networks training

Edge of Stability (EoS)

- Sharpness rises beyond $2/\eta$
- Sharpness stops rising but hovers noticeably above $2/\eta$ and even decreases a little
- Training loss behaves non-monotonically over individual iterations, yet consistently decreases over long timescales.

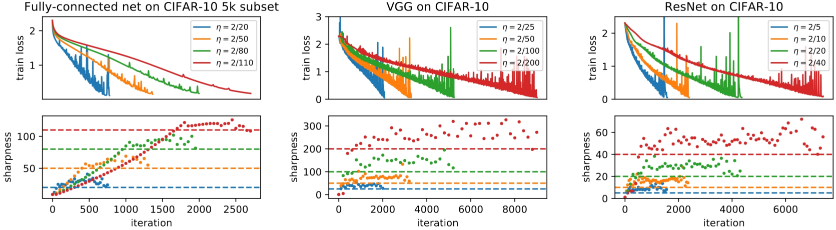


Figure: GD typically occurs at the Edge of Stability. [CKL+21] empirically observed this phenomenon.

GD enters EoS after sharpness reaches $2/\eta$

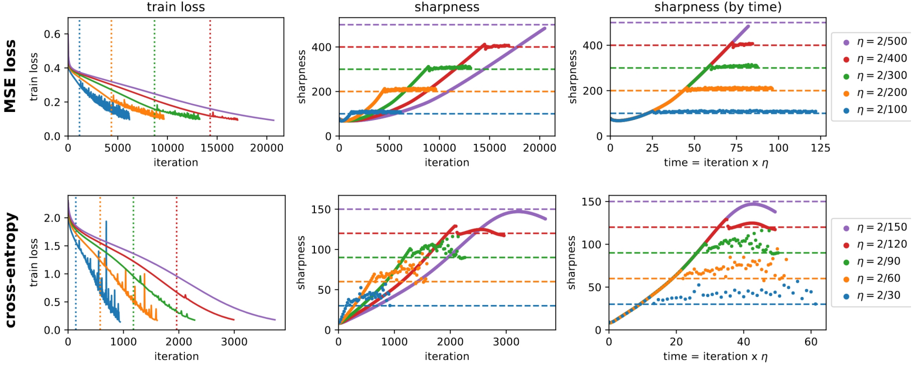
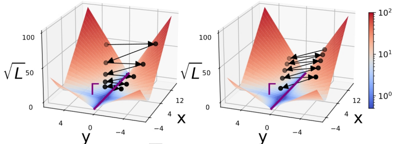


Figure: After progressive sharpening, GD enters the edge of stability

What happens after EoS?

Bias Towards Flattened Solutions

[ALP22] shows that normalized GD provably enters EoS, with associated flow on the manifold minimizing $\lambda_1(\nabla^2 L)$



(a) GD on $\sqrt{L}$ (b) Normalized GD on L

Explains SGD outperforms GD

[WS23] shows in a 2-layered neural network.

- SGD solution is linearly stable $\to Tr(\nabla^2 L) < 2/\eta$
- GD solution is linearly stable $\to \lambda_1(\nabla^2 L) < 2/\eta$

SGD often generalizes better than GD.

Summary

- Survey the recent advance on the implicit bias of gradient descent and other optimization algorithms
  - Linear regression model with squared loss
  - Matrix factorization
  - Linear classification model with exponential-tailed loss
  - Edge of stability
  - ...
- The implicit bias implies that those gradient descent prefers a "simpler" model
  - Bias towards max-margin solution
  - Bias towards "flatten" solution
- The implicit bias may partially explain why deep learning models trained with gradient descent generalize well

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