Deep Learning - Parameters and Functions Implicit Biases

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• "Implicit Bias of Gradient Descent for Mean Squared Error Regression with Two-Layer Wide Neural Networks"

Intuition



Figure 1: In an overparametrized model, there may be many different parameters and model functions that perfectly fit the training data

1 Implicit Bias and Algorithmic Regularization

2 Implicit Bias in Wide Shallow ReLU Networks

Motivation

- Neural networks in practice are often overparameterized
 - Number of model parameters \gg Number of training samples
 - Can fit random labels
- Many global minima fit the training data perfectly
 - Most of them generalize horribly
- Nevertheless, deep models often generalize well, even without any explicit regularization
- The capacity of the hypothesis class alone does not explain this¹

Motivation

- One possible explanation is that optimization algorithms are implicitly biased towards selecting simple solutions
- Question: What kinds of minima does an optimization algorithm converge to?
 - Examples: maximum margin classifier, smooth interpolation, sparse function, ...
 - Depends on loss function, optimization algorithm, learning model, ...

Factors

- Loss: ℓ_2 loss (for regression); logistic loss (for classification).
- **Optimization algorithm:** gradient descent; stochastic gradient descent; mirror descent; steepest descent.
- Learning model: linear models; linear neural networks; neural networks; parametrization
- Hyperparameters: learning rate; initialization; mini-batch size;

Gradient Descent

Consider the following linear model with loss function $\ell(y_1, y_2)$:

$$L(w) = \sum_{i=1}^{n} \ell(\langle x_i, w \rangle, y_i),$$

and the gradient descent iterations

$$w_{t+1} = w_t - \eta \nabla L(w_t) = w_t - \eta \sum_{i=1}^n \nabla_1 \ell(\langle x_i, w_t \rangle, y_i) \cdot x_i.$$

Gradient Descent

Theorem 1 (Gunasekar et al. 2018a)

Consider a convex loss function ℓ with a unique finite minimizer $(\ell(y_1, y_2) = 0 \text{ iff } y_1 = y_2)$. Assume that the gradient descent iteration converges to the global minimum of L(w) with zero loss, i.e., $L(w_t) \rightarrow 0$. Then the algorithm returns the unique solution of following constrained optimization problem:

$$\min_{w} \|w - w_0\|_2 \quad s.t. \ \langle x_i, w \rangle = y_i, \quad i = 1, \dots, n.$$
 (1)

The key idea is that the gradients are restricted to a *n*-dimensional subspace that is spanned by $\{x_i\}_{i=1}^n$ and is independent of *w*.

Proof

Gradient Descent.

• Let $w_{\infty} = \lim_{t \to \infty} w_t$. By assumption, $\langle x_i, w \rangle = y_i, i = 1, ..., n$. The gradient descent iteration gives

$$w_{\infty} = w_0 - \sum_{t=0}^{\infty} \eta \sum_{i=1}^{n} \nabla_1 \ell(\langle x_i, w_t \rangle, y_i) \cdot x_i$$
$$= w_0 - \eta \sum_{i=1}^{n} x_i \sum_{t=0}^{\infty} \nabla_1 \ell(\langle x_i, w_t \rangle, y_i).$$

• The constrained optimization problem (1) is strongly convex. The first order optimality condition is

$$\begin{cases} w - w_0 + \sum_{i=1}^n \lambda_i x_i = 0, \\ \langle x_i, w \rangle = y_i, \quad i = 1, \dots, n. \end{cases}$$
(2)

Setting λ_i = ∑_{t=0}[∞] ∇₁ℓ(⟨x_i, w_t⟩, y_i), one has that w_∞ satisfies
 (2). So w_∞ is the solution of problem (1).

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Mirror Descent

Given a strongly convex and differentiable potential ϕ , the mirror descent updates are:

$$w_{t+1} = \arg\min_{w} \eta \langle w, \nabla L(w_t) \rangle + D_{\phi}(w, w_t),$$

where $D_{\phi}(w, w') = \phi(w) - \phi(w') - \langle \nabla \phi(w'), w - w' \rangle$ is the Bregman divergence with respect to ϕ .

The first order optimality condition for the parameter update gives

$$abla \phi(w_{t+1}) =
abla \phi(w_t) - \eta
abla L(w_t).$$

Examples of ϕ :

- ℓ_2 norm: $\phi(w) = \frac{1}{2} ||w||_2^2$, which leads to gradient descent;
- unnormalized negative entropy: $\phi(w) = \sum_{i} w_i \log w_i w_i$.

Mirror Descent

Theorem 2 (Gunasekar et al. 2018a)

For any strongly convex potential ϕ . Assume that the mirror descent iteration converges to the global minimum of L(w) with zero loss, i.e., $L(w_t) \rightarrow 0$. Then the algorithm returns the solution of following constrained optimization problem:

$$\min_{w} D_{\phi}(w, w_0) \quad s.t. \ \langle x_i, w \rangle = y_i, \quad i = 1, \dots, n.$$
(3)

The key idea is that $\nabla \phi(w_{t+1})$ (called dual iterates) are restricted to a *n*-dimensional manifold $\nabla \phi(w_0) + \operatorname{span}(\{x_i\})$.

Proof

Mirror Descent.

The constrained optimization problem (3) is strongly convex. The first order optimality condition of the problem is

$$\begin{cases} \nabla \phi(w) - \nabla \phi(w_0) + \sum_{i=1}^n \lambda_i x_i = 0, \\ \langle x_i, w \rangle = y_i, \quad i = 1, \dots, n. \end{cases}$$
(4)

Since

$$egin{aligned}
abla \phi(w_{t+1}) &=
abla \phi(w_t) - \eta
abla \mathcal{L}(w_t) \
abla \phi(w_\infty) &=
abla \phi(w_0) - \eta \sum_{i=1}^n x_i \sum_{t=0}^\infty
abla_1 \ell(\langle x_i, w_t
angle, y_i). \end{aligned}$$

One sees that w_{∞} satisfies (4). So w_{∞} is the solution of (3).

Reparametrization and change of geometry

• D_{ϕ} can be approximated locally by a quadratic function

$$D_{\phi}(w,w') = (w-w')^{T} \nabla^{2} \phi(w'')(w-w').$$

If we use D_{\(\phi\)}(w, w') = (w - w')^TK(w - w'), the mirror descent iterations become:

$$w_{t+1} = w_t - \eta K^{-1} \nabla L(w_t).$$

For mirror descent we have the update rule:

$$w_{t+1} = w_t - \eta(\nabla^2 \phi(w''))^{-1} \nabla L(w_t).$$

• If step size goes to 0, we have the following gradient flow:

$$\dot{w}_t = -(\nabla^2 \phi(w_t))^{-1} \nabla L(w_t).$$

Reparametrization and change of geometry

• Consider the least squares problem and reparametrization:

$$L(w) = \frac{1}{2} \sum_{i=1}^{n} (\langle x_i, u \rangle - y_i)^2 = \frac{1}{2} ||Xu - y||_2^2$$

where $X = [x_1, ..., x_n]$ and $u = (w_1^2, ..., w_d^2)$ is the entry-wise square of w.

• The gradient flow over w is

$$\dot{w}(t) = -\nabla_w L(w(t)).$$

• If we consider the space of *u*, the above iteration becomes

$$\begin{split} \dot{u}(t) &= D_w \cdot \dot{w}(t) = -D_w \cdot \nabla_w L(w(t)) \\ &= -2D_w \cdot D_w \cdot X^T (Xu - y) \\ &= -2D_u \cdot X^T (Xu - y) \\ &= -2D_u \cdot \nabla_u L(u(t)), \end{split}$$

where $D_u = \text{diag}(u)$ and $D_w = \text{diag}(w).$

Montúfar 2024 Example taken from 18.408 Lecture 4: https://people.csail.mit.edu/moitra/408b.html

Reparametrization and change of geometry

If we let
$$\phi(u) = \sum_{i=1}^d (u_i \log u_i - u_i)$$
, then we have $(
abla^2 \phi(u(t)))^{-1} = D_u.$

Then we can show that the following two iterations are equivalent:

- 1. Gradient descent under square parametrization;
- 2. Mirror descent under $\phi(u)$.

According to the implicit bias of mirror descent, u(t) converges to the solution of the following optimization problem:

$$\min_{u} D_{\phi}(u, u_0) \quad \text{s.t.} \ \langle x_i, u \rangle = y_i, \quad i = 1, \dots, n.$$

If $u_0 = \alpha \mathbf{1}$: as $\alpha \to 0$, we have $D_{\phi}(u, u_0) \to C_{\alpha} \|u\|_1$.

Classification

In classification problems, gradient descent on linear models converges to the ℓ_2 maximum margin solution if training data is linearly separable^2



Figure 2: Implicit bias of gradient descent for classification problems.

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Classification: Linear Classifier

- Consider binary classification problem $y_i \in \{-1, +1\}$
- Linear decision boundaries $f(x) = \langle x_i, w \rangle$
- Decision rule $\hat{y}(x) = \operatorname{sign}(f(x))$
- Consider the exponential loss function $\ell(y_1, y_2) = \exp(-y_1y_2)$,

$$L(w) = \sum_{i=1}^{n} \ell(\langle x_i, w \rangle, y_i)$$

Gradient descent iteration

$$w_{t+1} = w_t - \eta \nabla L(w_t) = w_t - \eta \sum_{i=1}^n \ell(\langle x_i, w_t \rangle, y_i)(-x_i y_i)$$

- If the dataset is linearly separable, $L(w) \rightarrow 0$ only as $||w|| \rightarrow \infty$.
- Study the limit direction $\bar{w}_{\infty} = \lim_{t \to \infty} \frac{w_t}{\|w_t\|}$.

Classification: Linear Classifier

Theorem 3 (Soudry et al. 2018)

For any dataset which is linearly separable, suitable learning rate η , and any starting point w_0 , $\frac{w_t}{\|w_t\|}$ converges to the unique solution of the SVM problem:

$$\max_{w} \min_{i} y_i \langle x_i, w \rangle \quad s.t. \ \|w\|_2 \leq 1.$$

Classification: Linear Classifier

Proof idea.

Suppose ^{w_t}/_{||w_t||} converges to some limit w_∞, so w_t = g(t)w_∞ + ρ(t) with g(t) → ∞ and lim_{t→∞} ^{ρ(t)}/_{g(t)} = 0.
 The undiant star is given by

• The gradient at *w_t* is given by:

$$\nabla L(w_t) = \sum_{i=1}^{n} \exp(-w_t^T x_i) x_i$$
$$= \sum_{i=1}^{n} \exp(-g(t) \bar{w}_{\infty}^T x_i) \exp(-\rho(t)^T x_i) x_i$$

As g(t) → ∞, only those samples with the largest exponents will contribute to the gradient. So w_t are asymptotically dominated by a non-negative linear combination of support vectors. These are precisely the KKT conditions for the SVM problem.

Classification: Steepest Descent

Steepest descent with respect to a generic norm is given by:

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

For classification problem we consider the exponential loss.

Theorem 4 (Gunasekar et al. 2018a)

For any dataset which is linearly separable, any norm $\|\cdot\|$, suitable learning rate η and any starting point w_0 , $\frac{w_t}{\|w_t\|}$ converges to the solution of the optimization problem:

$$\max_{w} \min_{i} y_i \langle x_i, w \rangle \quad s.t. \|w\| \leq 1.$$

Implicit Bias for Linear Networks

- Deep linear networks can be regarded as parameterizations of linear models.
- Gunasekar et al. 2018b showed that gradient descent on full-width linear convolutional networks of depth *L* converges to a linear predictor related to the $\ell_{2/L}$ penalty in frequency domain.
- And gradient descent on fully-connected linear networks converges to ℓ_2 maximum margin solution regardless of depth.
- This elucidates the impact of the network architectures.
- The approximation ability may be the same, but the implicit bias of gradient descent is different.

1 Implicit Bias and Algorithmic Regularization

2 Implicit Bias in Wide Shallow ReLU Networks

Implicit bias of gradient descent

Consider a shallow ReLU network with n hidden units,

$$f(x, \theta) = \sum_{i=1}^{n} W_i^{(2)}[\langle W_i^{(1)}, x \rangle + b_i^{(1)}]_+ + b^{(2)}.$$

- Initialize the parameters by independent samples of $(\mathcal{W}, \mathcal{B})$.
- For data $\{(x_j, y_j)\}_{j=1}^M$, select a function by gradient descent minimization of the squared error $L(\theta) = \sum_{j=1}^M \|f(x_j, \theta) y_j\|^2$.

Montúfar 2024 We discuss results for shallow ReLU networks from Jin and Montufar 2023.

- Consider first the univariate setting, $x \in \mathbb{R}$.
- A rectified linear unit $[w_i x + b_i]_+$ has breakpoint at $c_i = -b_i/w_i$.
- A density $p_{W,B}$ induces a breakpoint density p_C .



Implicit bias of GD in wide ReLU networks

Theorem 5 (Univariate regression)

- Consider a feedforward network with a single input unit, a hidden layer of n rectified linear units, skip connections, and a single linear output unit.
- Assume standard parametrization and that for each hidden unit the input weight and bias are initialized from a sub-Gaussian (W, B) with joint density p_{W,B}.
- Then, for any finite data set $\{(x_j, y_j)\}_{j=1}^M$ and sufficiently large n optimization of the MSE by full-batch gradient descent with sufficiently small step size converges to a parameter θ^* for which the output function $f(x, \theta^*)$ attains zero training error.

• Moreover,

Implicit bias of GD in wide ReLU networks

Theorem 5 (Univariate regression) *letting*

$$\zeta(x) = \int_{\mathbb{R}} |W|^3 p_{\mathcal{W},\mathcal{B}}(W, -Wx) \, \mathrm{d}W$$

and $S = \text{supp}(\zeta) \cap [\min_i x_j, \max_i x_j]$, we have

$$\|f(x, \theta^*) - g^*(x)\|_2 = O(n^{-\frac{1}{2}}), \quad x \in S$$

with high probability over the random initialization θ_0 , where g^* solves following variational problem:

$$\min_{g \in C^2(S)} \int_S \frac{1}{\zeta(x)} (g''(x) - f''(x,\theta_0))^2 \, \mathrm{d}x$$

subject to $g(x_j) = y_j, \quad j = 1, \dots, M.$ (5)

Numerical illustration



The curvature penalty function



- The reciprocal curvature penalty is $\begin{aligned} \zeta(x) &= \\ \int_{\mathbb{R}} |W|^3 p_{\mathcal{W},\mathcal{B}}(W, -Wx) \, \mathrm{d}W. \end{aligned}$
 - We obtain the explicit form of ζ for various initialization procedures.
- We obtain parameter initialization procedures leading to any desired ζ.

Explicit form of the curvature penalty

Theorem 6 (Curvature penalty for various initializations)

- 1. Gaussian initialization. Assume that W and \mathcal{B} are independent, $W \sim \mathcal{N}(0, \sigma_w^2)$ and $\mathcal{B} \sim \mathcal{N}(0, \sigma_b^2)$. Then ζ is given by $\zeta(x) = \frac{2\sigma_w^3 \sigma_b^3}{\pi(\sigma_b^2 + x^2 \sigma_w^2)^2}$.
- Binary-uniform initialization. Assume that W and B are independent, W ∈ {−1,1} and B ~ U(−a_b, a_b) with a_b ≥ L. Then ζ is constant on [−L, L].
- Uniform initialization. Assume that W and B are independent, W ~ U(-a_w, a_w) and B ~ U(-a_b, a_b) with ^{a_b}/_{a_w} ≥ L. Then ζ is constant on [-L, L].

Gaussian initialization



Figure 3: Initialization $W \sim N(0,1)$ and $B \sim N(0,1)$.

Sharp Gaussian initialization



Figure 4: Initialization $W \sim N(0, 1)$ and $B \sim N(0, 0.1)$. In this case ζ that is more peaked at x = 0. Solutions more curvy around x = 0.

Exploiting the initialization

- With the presented bias description we can formulate heuristics for parameter initialization either to ease optimization or also to induce specific smoothness priors on the solutions.
- In particular, any curvature penalty $1/\zeta$ can be implemented by an appropriate choice of the initialization distribution.

Proposition 7 (Constructing any curvature penalty)

Given any function $\varrho \colon \mathbb{R} \to \mathbb{R}_{>0}$, satisfying $Z = \int_{\mathbb{R}} \frac{1}{\varrho} < \infty$, if we set the density of C as $p_{\mathcal{C}}(x) = \frac{1}{Z} \frac{1}{\varrho(x)}$ and make \mathcal{W} independent of C with non-vanishing second moment, then

$$(\mathbb{E}(W^2|\mathcal{C}=x)p_{\mathcal{C}}(x))^{-1}=(\mathbb{E}(W^2)p_{\mathcal{C}}(x))^{-1}\propto \varrho(x), \quad x\in\mathbb{R}.$$

Optimization trajectory in function space

• Optimization trajectory described by smoothing splines

$$\min_{g \in C^2(S)} \quad \sum_{j=1}^M \left[g(x_j) - y_j\right]^2 + \frac{1}{\bar{\eta}t} \int_S \frac{1}{\zeta(x)} (g''(x) - f''(x,\theta_0))^2 \, \mathrm{d}x.$$

Trajectories of functions

2D PCA of the trajectories



Early stopping and spectral bias

- The result can be interpreted in combination with early stopping.
- The training trajectory is approximated by a smoothing spline, meaning that the network will filter out high frequencies which are usually associated to noise in the training data.
- This behavior is sometimes referred to as a spectral bias³.

Generalization to multivariate regression

Theorem 8 (Multivariate regression)

- Use the same network setting as in Theorem 5 except that the number of input units changes to d.
- Assume that for each hidden unit the input weight and bias are initialized from a sub-Gaussian (W, B) where W is a d-dimensional random vector and B is a random variable.
- Let U = ||W||₂, V = W/||W||₂, C = -B/||W||₂, and let p_{V,C} be the joint density of (V,C).
- Then, for any finite data set $\{(\mathbf{x}_j, y_j)\}_{i=1}^M$ and sufficiently large n optimization of the MSE by full-batch gradient descent with sufficiently small step size converges to a parameter θ^* for which $f(\cdot, \theta^*)$ attains zero training error.
- Moreover,

Generalization to multivariate regression

Theorem 8 (Multivariate regression) letting $\zeta(\mathbf{V}, c) = p_{\mathbf{V}, \mathcal{C}}(\mathbf{V}, c) \mathbb{E}(\mathcal{U}^2 | \mathbf{V} = \mathbf{V}, \mathcal{C} = c)$, we have $\|f(\mathbf{x}, \theta^*) - g^*(\mathbf{x})\|_2 = O(n^{-\frac{1}{2}}), \quad \mathbf{x} \in \mathbb{R}^d$

(the 2-norm over $\mathbb{R}^d)$ whp over $\theta_0,$ where g^* solves

$$\min_{g \in C(\mathbb{R}^d)} \quad \int_{\operatorname{supp}(\zeta)} \frac{1}{\zeta(\mathbf{V},c)} \left(\mathcal{R}\{(-\Delta)^{(d+1)/2}(g-f(\cdot,\theta_0))\}(\mathbf{V},c) \right)^2 \, \mathrm{d}\mathbf{V} \mathrm{d}c$$
s.t. $g(\mathbf{x}_j) = y_j, \quad j = 1, \dots, M,$
 $\mathcal{R}\{(-\Delta)^{(d+1)/2}(g-f(\cdot,\theta_0))\}(\mathbf{V},c) = 0, \quad (\mathbf{V},c) \notin \operatorname{supp}(\zeta).$

Here \mathcal{R} is the Radon transform, $\mathcal{R}{f}(\omega, b) \coloneqq \int_{\langle \omega, \mathbf{x} \rangle = b} f(\mathbf{x}) ds(\mathbf{x})$, and the power of the negative Laplacian $(-\Delta)^{(d+1)/2}$ is the operator defined in Fourier domain by $(-\Delta)^{(d+1)/2} f(\boldsymbol{\xi}) = \|\boldsymbol{\xi}\|^{d+1} \widehat{f}(\boldsymbol{\xi})$.

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Generalization to other activation functions

Theorem 9 (Different activation functions)

- Use the same setting as in Theorem 5 except that we use the activation function ϕ instead of ReLU.
- Suppose that ϕ is a Green's function of a linear operator L, i.e. $L\phi = \delta$, where δ denotes the Dirac delta function.
- Assume that the activation function φ is homogeneous of degree k, i.e. φ(ax) = a^kφ(x) for all a > 0.
- Then we can find a function p satisfying $Lp \equiv 0$ and adjust training data $\{(x_j, y_j)\}_{j=1}^M$ to $\{(x_j, y_j p(x_j)\}_{j=1}^M$.

Generalization to other activation functions

Theorem 9 (Different activation functions)

After that, the statement in Theorem 5 holds with

$$\min_{g \in C^2(S)} \quad \int_S \frac{1}{\zeta(x)} [\mathrm{L}(g(x) - f(x, \theta_0))]^2 \, \mathrm{d}x$$

s.t. $g(x_j) = y_j - p(x_j), \quad j = 1, \dots, M,$

where

$$\zeta(x) = p_{\mathcal{C}}(x) \mathbb{E}(\mathcal{W}^{2k} | \mathcal{C} = x)$$

and $S = \operatorname{supp}(\zeta) \cap [\min_i x_i, \max_i x_i].$

Generalization

From Theorem 5 we can extract generalization results such as

 In the univariate noisless model for a target g₀ on [a, b], if ζ uniform, then

$$\|g^* - g_0\|_{\infty} \le C \|g_0^{(4)}\|_{\infty} h^4$$

where $g^{(4)}$ is the fourth derivative of g_0 and $h = \max_i x_{i+1} - x_i$.

For univariate noisy models with y_j = g₀(x_j) + ε_j, ε_j independent zero mean with variance σ², if x_i uniform partition and ζ uniform, using early stopping with t = Θ(M^{4/5}), then

$$\mathbb{E}\|g^* - g_0\|_2^2 = O(M^{-4/5})$$

• Similar observations can be obtained in more general settings such as non-uniform training inputs, non-constant ζ

Related works

- Zhang et al. 2019 described the implicit bias of gradient descent in the kernel regime as minimizing a kernel norm from initialization, subject to fitting the training data.
- Savarese et al. 2019 showed infinite-width networks with 2-norm weight regularization represent functions with smallest 1-norm of the second derivative, an example of which are linear splines.
- Williams et al. 2019 showed a similar result for univariate shallow ReLU nets training only the output layer from zero initialization.



- Gradient descent training of overparametrized ReLU networks is biased towards functions with low curvature.
- The parameter initialization procedure determines the curvature penalty function $1/\zeta$.
- Generalizations to multivariate ReLU networks, different activation functions, and optimization trajectories.

Further topics

- Spectral bias
- Implicit bias in mildly overparametrized nets
- Other optimizers and stability
- Role of the data

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