Implicit regularization

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Implicit regularization/bias

- why do very expressive models generalize?
- overparametrized/underdermined models
- with many global solutions
- no capacity control specified in the objective

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Arora et al. (2019); Woodworth et al. (2020)). Different optimization choices, such as using different optimization methods (Gunasekar et al., 2018b), or different optimization parameters can significantly change the algorithmic bias, and thus completely change the effective inductive bias of learning and the ability to generalize in specific scenarios. In

Setting

only gradient descent (GD)

- least squares
- logistic regression
- (simple) nonlinear models

Examples of implicit biases

- algorithm used
- ▶ large batch sizes → sharp solutions [Keskar et al., 2017]

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- ▶ large **step sizes** → flatter minima
- initialization
- early stopping

Underdetermined least squares

$$\min_{w} \|Xw - y\|^2$$

- We assume $\exists \bar{w} : X\bar{w} = y$
- Q: Which solution does GD converge to?¹
- A: minimal distance to the starting point.

¹irresspective of the step size

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Also extends to momentum methods.

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$$\min_{w} \sum_{i=1}^{n} \exp(-y_i x_i^{\mathsf{T}} w)$$

- no solution exists (iterates diverge to infinity)
- GD converges to the maximum-margin classifier^a
- ► the solution to hard-margin SVM $\min_{w} ||w||^2 \text{ s.t. } y_i(w^{\mathsf{T}}x_i) \ge 1$



^anormalized iterates

The convergence is **extremely slow** $O(1/\log t)$.

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least squares for non-Euclidian geometries

Mirror descent:

$$w_{t+1} = \operatorname*{arg\,min}_{w} \left\{ \eta_t \langle w,
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angle + D_{\psi}(w, w_t)
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- negative entropy $\psi(w) = \sum_i w_i \log w_i$
- Kullback-Leibler divergence D_{ψ}
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In general: Iterates converge to $\underset{w:Xw=y}{\operatorname{arg\,min}} D_{\psi}(w, w_0)$

For KL divergence we get the maximum entropy solution.

Convex vs. Nonconvex

- previous models where convex
- observed bias *irresspective* of the step size
- non-convex case is more delicate then in convex GD
 - manifold spanned by the gradients is no longer flat
 - step size or momentum make you fall off

diagonal linear network, [Woodworth et al., 2020] Consider the following nonconvex parametrization: $\min \sum_{n=1}^{n} \|(u \otimes u, u) - u\|^2$

$$\min_{u} \sum_{i=1}^{n} \|\langle u \odot u, x_i \rangle - y_i \|^2.$$

- GD wrt to u can be seen as *mirror descent* in predictor space $w = u \odot u$
- **b** the Bregman distance depends on initialization $\alpha \mathbf{e}$
- small initialization gives minimal L1 norm the "rich" regime
- large initialization gives known L2 regularization the "kernel" or "lazy" regime

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Caveat: holds for gradient flow.

ity. In particular, we show how using large step size for non-centered data can change the implicit bias from a "kernel" type behavior to a "rich" (sparsity-inducing) regime — even when gradient flow, studied in previous works, would not escape the "kernel" regime. We do so by using

Matrix factorization

$$\min_{U,V} \sum_{i=1}^n \|\langle UV^{\mathsf{T}}, X_i \rangle - y_i \|^2$$

Similar results for infinitesimal step sizes

- implicit bias depends on initialization
- nuclear norm instead of L1 [Gunasekar et al., 2017]
- requires restricted isometry (RIP) [Li et al., 2018]

Thank You!

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