Benign Overfitting of Constant-Stepsize SGD for Linear Regression

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Abstract

There is an increasing realization that algorithmic inductive biases are central in preventing overfitting; empirically, we often see a benign overfitting phenomenon in overparameterized settings for natural learning algorithms, such as stochastic gradient descent (SGD), where little to no explicit regularization has been employed. However, such algorithmic aspects of generalization are far less well understood, where we lack a sharp characterization of it and when benign overfitting occurs.

In addition to the existing works that mostly focus on the classical underparameterized regime, the focus of this work is on the overparameterization regime. In particular, we study the generalization ability of SGD in arguably the most basic setting: constant-stepsize SGD, with iterate averaging or tail averaging, for overparameterized linear regression. Our main result provides a sharp excess risk bound, stated in terms of the full eigenspectrum of the data covariance matrix, that reveals a bias-variance decomposition characterizing when generalization is possible: (i) the variance bound is characterized in terms of an effective dimension (specific for SGD) and (ii) the bias bound provides a sharp geometric characterization in terms of the location of the initial iterate (and how it aligns with the data covariance matrix). In addition, for SGD with iterate averaging (output the average of all iterates), we demonstrate the sharpness of the established excess risk bound by proving a matching lower bound (up to constant factors). For SGD with tail averaging (output the average of tail iterates), we demonstrate its improvements over SGD with iterate averaging by proving a better excess risk bound together with a nearly matching lower bound. Moreover, we reflect on a number of notable differences between the algorithmic regularization afforded by (unregularized) SGD in comparison to ordinary least squares (minimum-norm interpolation) and ridge regression. Experimental results well corroborate our theoretical findings\(^1\).

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