

TTIC 31230, Fundamentals of Deep Learning

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Implicit Regularization

Implicit Regularization

Any stochastic learning algorithm, such as SGD, determines a stochastic mapping from training data to models.

The algorithm, especially with early stopping, can implicitly incorporate a preference or bias for models.

Implicit Regularization in Linear Regression

Linear regression with many more parameters than data points has many solutions.

But SGD converges to the minimum norm solution.

Implicit Regularization in Linear Regression

For linear regression SGD maintains the invariant that Φ is a linear combination of the (small number of) training vectors.

Any zero-loss (squared loss) solution can be projected on the span of training vectors to give a smaller (or no larger) norm solution.

It can be shown that when the training vectors are linearly independent any zero loss solution in the span of the training vectors is a least-norm solution.

Implicit Regularization of SGD

In a labeling problem a model with parameters Φ defines a model probability $P_{\Phi}(y|x)$.

This defines a log loss $-\ln P_{\Phi}(y|x)$ on which we do gradient descent.

Let $\text{SGD}[P_{\Phi}, \Phi_{\text{Init}}, \text{Train}]$ be the vector that results from running SGD on model P_{Φ} with initial parameters Φ_{Init} using training data Train (and a fixed set of hyperparameters, learning rate schedule, and fixed order in which training instances are considered, and fixed number of iterations).

Implicit Regularization of SGD

To get a generalization bound when learning a continuous parameter vector we add Gaussian noise to simulate limited precision of the real numbers.

$$\Phi' = \text{SGD}[P_\Phi, \Phi_{\text{Init}}, \text{Train}] + \epsilon$$

The algorithm defines an **implicit prior**:

$$p(\Phi' \mid P_\Phi, \Phi_{\text{Init}}, \text{Pop}) = E_{\left(\text{Train} \sim \text{Pop}^N\right)} p(\Phi' \mid P_\Phi, \Phi_{\text{Init}}, \text{Train})$$

The implicit prior $p(\Phi' \mid P_\Phi, \Phi_{\text{Init}}, \text{Pop})$ is a valid prior! It does not depend on training data!

Implicit Priors: the General Case

Let A be any algorithm mapping a training set to a probability density over model parameters.

Let $p(\Phi|A, \text{Train})$ be the probability density on parameter vectors defined by the stochasticity of the algorithm A run on the given training set.

The implicit prior defined by algorithm A and the given population distribution is

$$p(\Phi|A, \text{Pop}) = E_{\left(\text{Train} \sim \text{Pop}^N\right)} p(\Phi|A, \text{Train})$$

A PAC-Bayes Analysis of Implicit Regularization

$$\mathcal{L}(\Phi, \text{Pop}) = E_{\langle x, y \rangle \sim \text{Pop}} \mathcal{L}(\Phi, x, y)$$

$$\mathcal{L}(\Phi, \text{Train}) = E_{\langle x, y \rangle \sim \text{Train}} \mathcal{L}(\Phi, x, y)$$

$$\mathcal{L}(A) = E_{\left(\text{Train} \sim \text{Pop}^{N_{\text{Train}}}\right)} E_{\Phi \sim p(\Phi | A, \text{Train})} \mathcal{L}(\Phi, \text{Pop})$$

$$\hat{\mathcal{L}}(A) = E_{\left(\text{Train} \sim \text{Pop}^{N_{\text{Train}}}\right)} E_{\Phi \sim p(\Phi | A, \text{Train})} \mathcal{L}(\Phi, \text{Train})$$

A PAC-Bayes Analysis of Implicit Regularization

$$\mathcal{L}(A) \leq \frac{10}{9} \left(\hat{\mathcal{L}}(A) + \frac{5L_{\max}}{N_{\text{Train}}} \left(E_{\text{Train} \sim \text{Pop}}^{N_{\text{Train}}} KL(p(\Phi|A, \text{Train}), p(\Phi|A, \text{Pop})) + \ln \frac{1}{\delta} \right) \right)$$

There is no obvious way to calculate this guarantee.

However, it can be shown that $p(\Phi|A, \text{Pop})$ is the optimal PAC-Bayesian prior for algorithm A when run on the given population.

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