Data-Dependent Stability of Stochastic Gradient Descent

A review

M. Zadem K. Abouda TH. Yen Vu

MAP670L - Generalisation properties of algorithms in ML

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Introduction

Algorithmic stability

Stability	
Uniform	On-average
- Restrictive - Not data-dependent	- Less restrictive - Data-dependent

- Pessimistic generalization bound.
- Insufficient to give deeper theoretical insights.

Outline

Notations

- $\mathcal{Z}$: Example space
- Training and testing examples are drawn iid from a probability distribution $\mathcal{D}$ over $\mathcal{Z}$.
- $S = \{z_i\}_{i=1}^m \sim \mathcal{D}^m$: A training set drawn according to $\mathcal{D}$.
- $A : \mathcal{Z}^m \mapsto \mathcal{H}$: A learning algorithm, $\mathcal{H}$ a parameter space
- $f(\boldsymbol{w}, z)$: Loss incurred by predicting with parameter $\boldsymbol{w} \in \mathcal{H}$

Outline

Uniform stability of a randomized algorithm

Definition

A randomized algorithm A is ϵ-uniformly stable if :
for all datasets $S, S^{(i)} \in \mathcal{Z}^m$ such that S and $S^{(i)}$ differ in the $i-th$ example we have

$$\sup_{z \in \mathcal{Z}, i \in [m]} \left\{ \mathbb{E}\left[f\left(A_S, z\right) - f\left(A_{S^{(i)}}, z\right) \right] \right\} \leqslant \epsilon$$

Outline

Uniform stability implies generalization in expectation

Theorem

Let A be ϵ-uniformly stable. Then,

$$\left| \underset{S,A}{\mathbb{E}} \left[\widehat{R}_S\left(A_S\right) - R\left(A_S\right) \right] \right| \leqslant \epsilon$$

Outline

On-average stability of a randomized algorithm

Here we introduce a data-dependent notion of stability. Therefore, we denote stability as a function of $\epsilon(\theta)$ where θ is a parameter of the algorithm that captures caracteristics of the given dataset.

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Outline

On-average stability implies generalization in expectation

Theorem

Let A be $\epsilon(\theta)$-uniformly stable. Then,

$$\left| \mathbb{E}_{S,A} \left[\widehat{R}_S(A_S) - R(A_S) \right] \right| \leqslant \epsilon(\theta)$$

Outline

SGD algorithm

- The studied SGD algorithm is the following: given a training set $S = \{z_i\}_{i=1}^{m} \sim^{iid} \mathcal{D}^m$, step sizes $\{\alpha_t\}_{t=1}^{T}$, random indices $I = \{j_t\}_{t=1}^{T}$, and an initialization point $\boldsymbol{w}_1$, perform updates

$$\boldsymbol{w}_{t+1} = \boldsymbol{w}_t - \alpha_t \nabla f\left(\boldsymbol{w}_t, z_{jt}\right)$$

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- The variance of the stochastic gradients verifies

$$\mathop{\mathbb{E}}_{S,z_z}\left[\left\|\nabla f\left(\boldsymbol{w}_{S,t}, z\right) - \nabla R\left(\boldsymbol{w}_{S,t}\right)\right\|^2\right] \leqslant \sigma^2 \quad \forall t \in [T]$$

Loss function

The loss function in the following theorems is assumed to be

- Non-negative
- Lipschitz: A loss function f is L-Lipschitz if $\|\nabla f(\boldsymbol{w}, z)\| \leqslant L, \forall \boldsymbol{w} \in \mathcal{H}$ and $\forall z \in \mathcal{Z}$
- β-Smooth: A loss function is β-smooth if $\forall \boldsymbol{w}, \boldsymbol{v} \in \mathcal{H}$ and $\forall z \in \mathcal{Z}, \|\nabla f(\boldsymbol{w}, z) - \nabla f(\boldsymbol{v}, z)\| \leqslant \beta \|\boldsymbol{w} - \boldsymbol{v}\|$

Outline

Generalisation bound for convex loss

Theorem

Assume that f is convex, and that the step for SGD are such that $\alpha_t = \frac{c}{\sqrt{t}} \leqslant \frac{1}{\beta}, \forall t \in [T]$. Then SGD is $\epsilon(\mathcal{D}, \boldsymbol{w}_1)$-on-average stable with

$$\epsilon(\mathcal{D}, w_1) = \mathcal{O}\left(\sqrt{c\left(R\left(w_1\right) - R^*\right)} \cdot \frac{\sqrt[4]{T}}{m} + c\sigma\frac{\sqrt{T}}{m}\right)$$

Generalisation bound for convex loss

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- The Data-dependant bound is tighter than the uniform bound given by [1] which corresponds to $\epsilon = \mathcal{O}(\sqrt{T/m})$ for the same step
- In the case that σ is not too large, the obtained bound depends on the initial point for the SGD which makes the choice of the starting point crucial to obtaining better stability
- On the other hand, for a large σ, the second term in the sum is dominant, and the bound is equivalent to the uniform bound.

Outline

Generalisation bound for non-convex loss

Theorem

Assume that $f(\cdot, z) \in [0,1]$ and has a ρ-Lipschitz Hessian, and that step sizes of a form $\alpha_t = \frac{c}{t}$ satisfy $c \leqslant \min\left\{\frac{1}{\beta}, \frac{1}{4(2\beta\ln(T))^2}\right\}$ Then SGD is $\epsilon(\mathcal{D}, \boldsymbol{w}_1)$-on-average stable with

$$\epsilon(\mathcal{D}, \boldsymbol{w}_1) \leqslant \frac{1 + \frac{1}{c\gamma}}{m}\left(2cL^2\right)^{\frac{1}{1+c\gamma}}\left(\mathop{\mathbb{E}}_{S,A}\left[R\left(A_S\right)\right] \cdot T\right)^{\frac{c\gamma}{1+c\gamma}}$$

where

$$\gamma := \mathcal{O}\left(\min\left\{\beta, \mathop{\mathbb{E}}_{z}\left[\left\|\nabla^2 f\left(\boldsymbol{w}_1, z\right)\right\|_2\right] + \Delta^*_{1,\sigma^2}\right\}\right)$$

$$\Delta^*_{1,\sigma^2} := \rho(c\sigma + \sqrt{c\left(R\left(\boldsymbol{w}_1\right) - R^*\right)})$$

Generalisation bound for non-convex loss

- The quantity γ expresses how the curvature of the loss function at the initial point affects the stability of the algorithm. Consequently, starting from a point that is less curved yields a better bound and thus smaller generalisation error. This statement corroborates the intuition.
- In [1], a similar bound was given, but instead of γ, the given bound included a Lipschitz constant relative to the gradient of f. This constant fails to represent the data dependency.

Generalisation bound for non-convex loss

Corollary

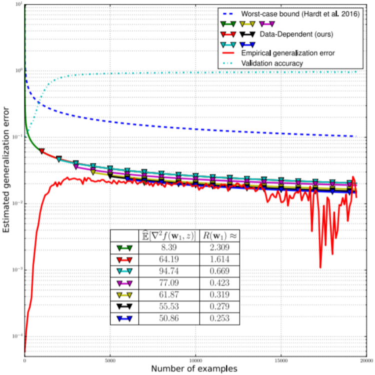
Under conditions of tthe previous theorem we have that SGD is $\epsilon\left(\mathcal{D}, \boldsymbol{w}_1\right)$-on-average stable with

$$\epsilon\left(\mathcal{D}, \boldsymbol{w}_1\right) = \mathcal{O}\left(\frac{1+\frac{1}{c\gamma}}{m}\left(R\left(\boldsymbol{w}_1\right)\cdot T\right)^{\frac{c\gamma}{1+c\gamma}}\right)$$

For $R\left(\boldsymbol{w}_1\right) \to 0$ we have that $\epsilon\left(\mathcal{D}, \boldsymbol{w}_1\right) \to 0$. As the initialisation point error diminishes, the generalisation error is close to zero. The uniform stability is incapable of showing these results seeing that it is distribution independent.

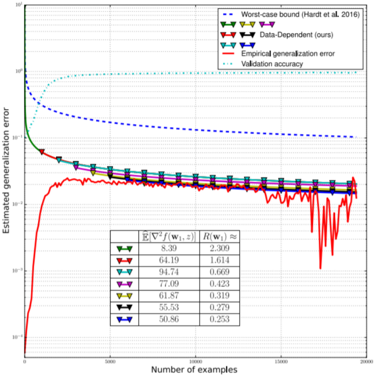
Remarks

- This article gives an average bound, while in [1] an uniform worst-case bound was given, which is more confident but far away from being optimal.



Remarks

- In non-convex case (the case for most Neural Nets), trade-off between curvature of the initial point $\widehat{\mathbb{E}}[\nabla^2 f(\mathbf{w}_1, z)]$ and the risk at the initial point $R(\mathbf{w}_1)$.



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- In non-convex case (the case for most Neural Nets), trade-off between curvature of the initial point $\widehat{\mathbb{E}}[\nabla^2 f(\mathbf{w}_1, z)]$ and the risk at the initial point $R(\mathbf{w}_1)$.
- A tighter bound can be obtained by taking the minimum of the two bounds.
- Require a knowledge on the prior distribution of the dataset for exact bound, otherwise only an estimation.

Conclusion

- Provide new data-dependent stability bounds for SGD on convex and non-convex loss functions.
- Better initial point (lower objective) makes the algorithm more stable and generalizes better.
- In non-convex case, starting from a point in a less-curved region yields a better generalisation error.

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