Stochastic Runge-Kutta methods and adaptive SGD-G2 stochastic gradient descent ICPR 2020 paper # 2258

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Adaptive Stochastic Gradient Descent

• training neural networks (NN) e.g., for classification to simplify, often relies on the minimization of a loss function : $f(X) := \frac{1}{N} \sum_{i=1}^{N} f(\omega_i, X)$, where the sum is over all available samples. Equivalent writing: $f(X) = \mathbb{E}_{\omega} f(\omega, X)$. $X \in \mathbb{R}^d$ = parameters of the NN.

• classical gradient descent procedure : $X_{n+1} = X_n - h\nabla f(X_n)$, h > 0 is the learning rate (="step size").

• BUT computing $\nabla f(X_n)$ is too costly because of the average (many samples).

• it is replaced by a crude approximation $X_{n+1} = X_n - h\nabla f(\omega_{\gamma_n}, X_n)$ where $(\gamma_n)_{n\geq 1}$ are i.i.d uniform random variables in $\{1, 2, ..., N\}$. This is the Stochastic Gradient Descent (SGD)

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Adaptive Stochastic Gradient Descent

• Stochastic Gradient Descent $X_{n+1} = X_n - h\nabla f(\omega_{\gamma_n}, X_n)$ $(\gamma_n)_{n\geq 1}$ are i.i.d uniform in $\{1, 2, ..., N\}$. Problem: small *h* converge slowly, large *h* unstable.

- MAIN QUESTION: how to (optimally) choose the learning rate (I.r.) h?
- Flow interpretation : in the limit $h \to 0$ the minimization of f(X) is some approximation of the 'continuous time' evolution equation $X'(t) = \nabla_X f(X(t))$. SGD: $X_n \simeq X(t_n)$, $t_n = n \cdot h$.
- MAIN IDEA:
- 1/ construct a better approximation Y_{n+1} of $X(t_{n+1})$ such that $Y_{n+1} X_{n+1}$ is an estimation of the error $X_{n+1} X(t_{n+1})$.
- 2/ Using Y_{n+1} compute the largest l.r. *h* such that stability still holds
- Question 1: find a high order scheme consistent for the flow dynamics
- Question 2: is the procedure performing well in practice..

The second order Stochastic Runge Kutta "SRK" scheme

Stochastic Runge Kutta (SRK)

$$\tilde{Y}_{n+1} = Y_n - h\nabla f_{\gamma_n}(Y_n), \ Y_{n+1} = Y_n - \frac{h}{2} \left[\nabla f_{\gamma_n}(Y_n) + \nabla f_{\gamma_n}(\tilde{Y}_{n+1}) \right].$$
(1)

Theorem (Convergence of SGD and SRK schemes, I.A., G.T. 2019)

Suppose $\forall k, \nabla f_k$ is a Lipschitz function, ∇f_k and its partial derivatives up to order 6 have at most polynomial increase at ∞ and ∇f_k increases at most linearly at infinity. Then the SGD scheme converges at (weak) order 1 (in h) while the SRK scheme (1) converges at (weak) order 2.

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Adaptive step SGD: the SGD-G2 algorithm

Algorithm 1 SGD-G2

Set hyper-parameter: β , mini-batch size *M*, choose stopping criterion **Input:** initial learning rate h_0 , initial guess X_0 Initialize iteration counter: n = 0while stopping criterion not met do select next mini-batch γ_n^m , m = 1, ..., MCompute $g_n = \frac{1}{M} \sum_{m=1}^{M} \nabla f_{\gamma_n^m}(X_n)$ Compute $\tilde{g}_n = \frac{1}{M} \sum_{m=1}^{M} \nabla f_{\gamma_n^m}(X_n - h_n g_n)$ Compute $h_n^{opt} = \begin{cases} \frac{3}{2} \frac{h_n \langle g_n - \tilde{g}_n, g_n \rangle}{\|g_n - \tilde{g}_n\|^2} & \text{if } \langle g_n - \tilde{g}_n, g_n \rangle > 0 \\ h_n & \text{otherwise.} \end{cases}$ if $h_n^{opt} > h_n$ then $h_{n+1} = \beta h_n + (1-\beta) h_n^{opt}$ else $h_{n+1} = h_n^{opt}$ end if Update $X_{n+1} = X_n - h_{n+1}g_n$ Update $n \rightarrow n+1$ end while

Empirical validation (MNIST / FMNIST / CIFAR10)

Results on standard datasets are very convincing, start with h small then let it adapt itself.



Figure: Left: SGD vs. SGD-G2 on FMNIST . Right: SGD vs. SGD-G2 on CIFAR10 (10 epochs).

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Adaptive SGD: SGD-G2 algor

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Empirical validation on CIFAR100



Figure: SGD , SGD-G2 and Adam (100 epochs) on CIFAR100.

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Conclusion

• We presented a new adaptive learning rate procedure that performs well on standard datasets (MNIST, FMNIST, CIFAR10, CIFAR100)

• in the process we came up with a proof for the convergence of the Stochastic Runge-Kutta second order scheme

Want to know more:

• the paper: https://arxiv.org/abs/2002.09304 (Arxiv ID= arXiv:2002.09304)

• these slides: https://doi.org/10.5281/zenodo.4314299 (DOI=10.5281/zenodo.4314299)

• this video: https://youtu.be/z_V2OIM0UmI

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