Matrix Decomposition for Adaptive Optimization Regularization

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AdaGrad algorithm background

Suppose that we have a smooth loss function $f : \mathbb{R}^n \to \mathbb{R}$, and the following minimization problem:

$$f(x) \to \min_{x \in \mathcal{X}}$$

Denote $g_k \equiv \nabla f_x(x_k)$ and $\mathbf{G}_k = [g_k \; g_{k-1} \dots \; g_1]$, where $\mathbf{G}_k \in \mathbb{R}^{n \times k}$.
In this notation the k-th update step of full-matrix AdaGrad algorithm is:

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \frac{\eta}{\sqrt{\mathbf{G}_k \mathbf{G}_k^T + \varepsilon \mathbf{I}}} \nabla f(\mathbf{x}_k),$$

Problem formulation

GGT uses the preconditioner from full-matrix AdaGrad, with gradient history attenuated exponentially as in Adam, and truncated to a window parameter r.

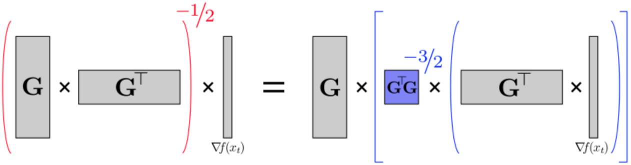
$$\mathbf{G}_k = [g_k g_{k-1} \dots g_{k-r+1}], \quad \text{where } g_{k-t} = \beta_2^t \widetilde{\nabla} f\left(x_{k-t}\right), \text{ or } 0 \text{ if } t \geq k$$

where $\beta_2 \leq 1$ and $\widetilde{\nabla} f\left(x_{k-t}\right)$ is stochastic gradient.
GGT iterative step is:

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \frac{\eta}{\sqrt{\mathbf{G}_k \mathbf{G}_k^T + \varepsilon \mathbf{I}}} \widetilde{\nabla} f(\mathbf{x}_k)$$

Key Idea

The inversion of the large low-rank matrix $\mathbf{GG}^T \in \mathbb{R}^{n\times n}$ can be performed by diagonalizing the small matrix $\mathbf{G}^T\mathbf{G} \in \mathbb{R}^{r\times r}$.



Key Idea

$$\left[\left(\mathbf{G}\mathbf{G}^\top\right)^{1/2} + \varepsilon\mathbf{I}\right]^{-1} v = \frac{1}{\varepsilon} v + \mathbf{U}_r \left[\left(\boldsymbol{\Sigma}_r + \varepsilon\mathbf{I}_r\right)^{-1} - \frac{1}{\varepsilon}\mathbf{I}_r\right] \mathbf{U}_r^\top v \qquad (*)$$

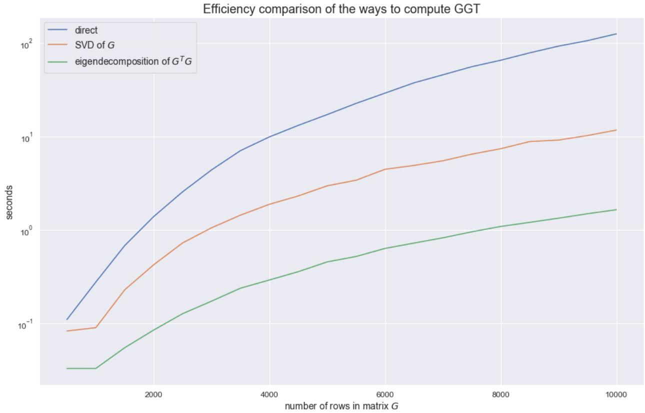
The first term is none other than an SGD update step. The rest can be computed by taking the eigendecomposition $\mathbf{G}^\top\mathbf{G} = \mathbf{V}\boldsymbol{\Sigma}_r^2\mathbf{V}^\top$, giving $\mathbf{U}_r = \mathbf{G}\mathbf{V}\Sigma_r^{-1}$

Iterative step matrix computation

So, there are several ways to compute matrix $\left[\left(\mathbf{G}\mathbf{G}^\top\right)^{1/2}+\varepsilon\mathbf{I}\right]^{-1}$ which is used at the iterative step:

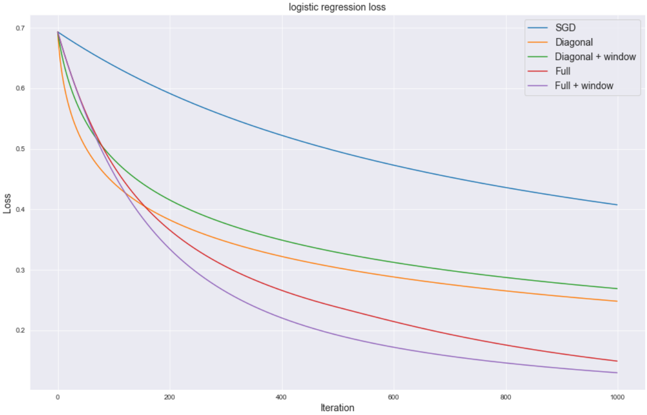
- direct: make eigendecomposition of symmetric matrix $\mathbf{G}\mathbf{G}^\top$ to compute its square root, and then compute the inverse
- use $(*)$, obtain $\mathbf{U}_r$ and $\mathbf{\Sigma}_r$ via SVD decomposition of matrix $\mathbf{G}$
- use $(*)$, obtain $\mathbf{U}_r$ and $\mathbf{\Sigma}_r$ via eigendecomposition of matrix $\mathbf{G}^T\mathbf{G}$ as was described on the previous slide

Iterative step matrix computation



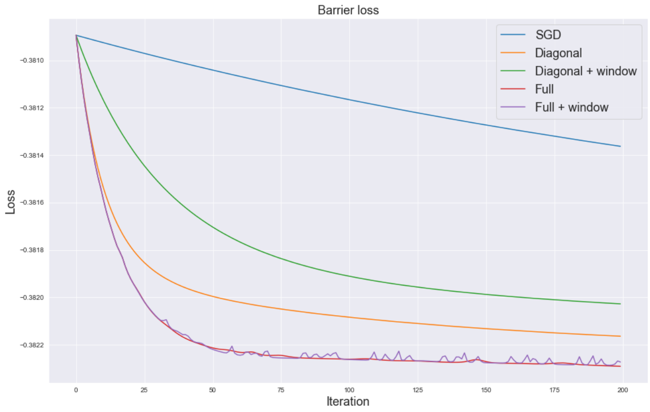
Results representation: syntetic data 1

We compared different full- and diagonal-matrix adaptive optimizers and SGD on the logistic regression problem on a set destibuted from an extremely anisotropic ($\sigma^2_{max}/\sigma^2_{min} \approx 10^4$) Gaussian distribution.



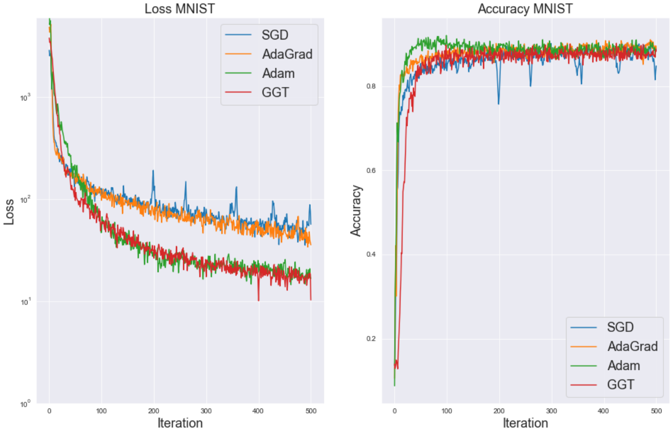
Results representation: syntetic data 2

We compared same optimizers on the the same set but now we minimized the barrier loss function: $f_i(w) = -\log\left(w^\top x_i + c_i\right)$ where c_i generated uniformly from $[0, 1]$.



Test on new data: MNIST

We compared modern state-of-the-art methods on a well known MNIST dataset. We used DNN with two hidden fully connected layers with 256 nodes.



Our modifications

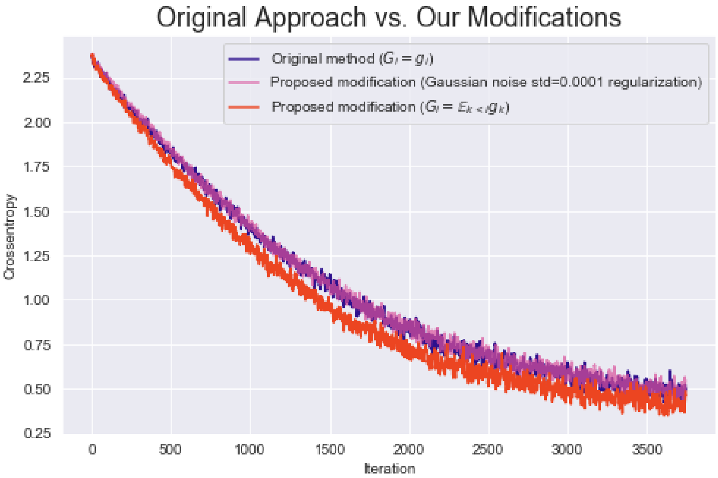
Original paper propose us to use the following matrix $\mathbf{G}_t$:

$$\mathbf{G}_t = \begin{pmatrix} g_t & g_{t-1} & \dots & g_{t-r+2} & g_{t-r+1} \end{pmatrix}$$

Where $g_{t-k} = \beta_2^k \nabla f(x_{t-k})$ (authors also suggest to use momentum with parameter $\beta_1 \approx 0.9$ and put $\beta_2 = 1$ on practice)
We considered several modifications of this method. The most important one is to replace matrix $\mathbf{G}_t$ by the following matrix:

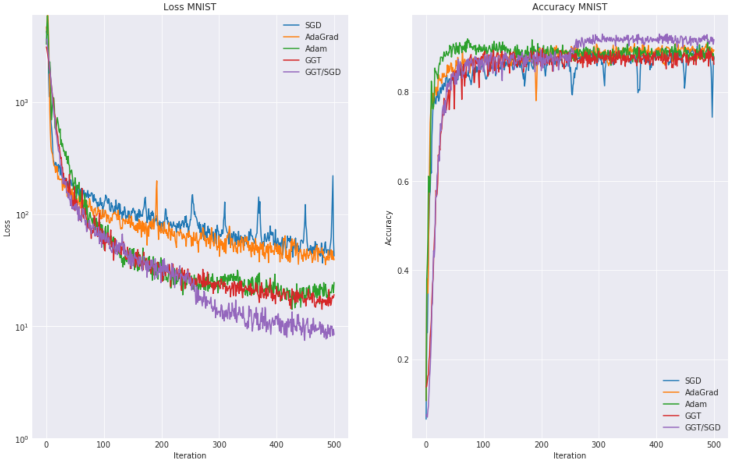
$$\mathbf{G}_t = \begin{pmatrix} \frac{1}{r}\sum_{j=t-r+1}^{t} g_j & \frac{1}{r-1}\sum_{j=t-r+1}^{t-1} g_j & \dots & \frac{1}{2}\sum_{j=t-r+1}^{t-r+2} g_j & \sum_{j=t-r+1}^{t-r+1} g_j \end{pmatrix}$$

Our modifications



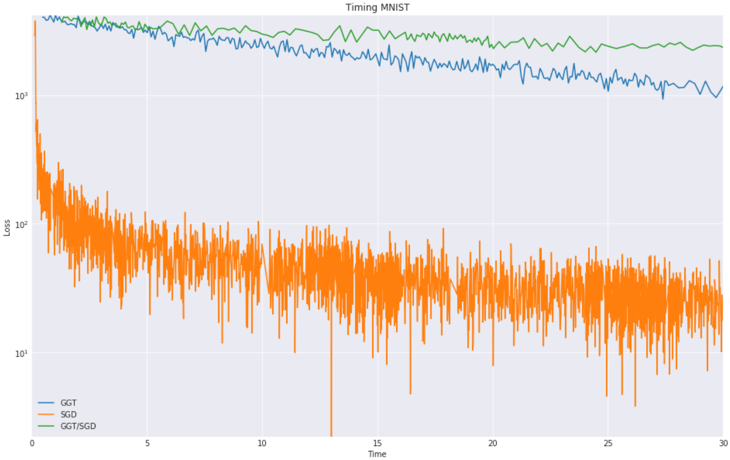
Combining GGT & SGD on MNIST

Combination of GGT and SGD converges faster *in terms of iteration*



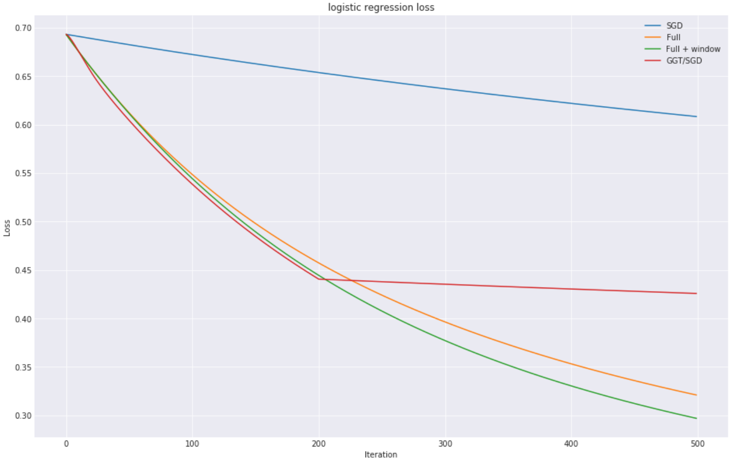
Timing GGT & SGD on MNIST

SGD converges faster *in terms of time* on image data



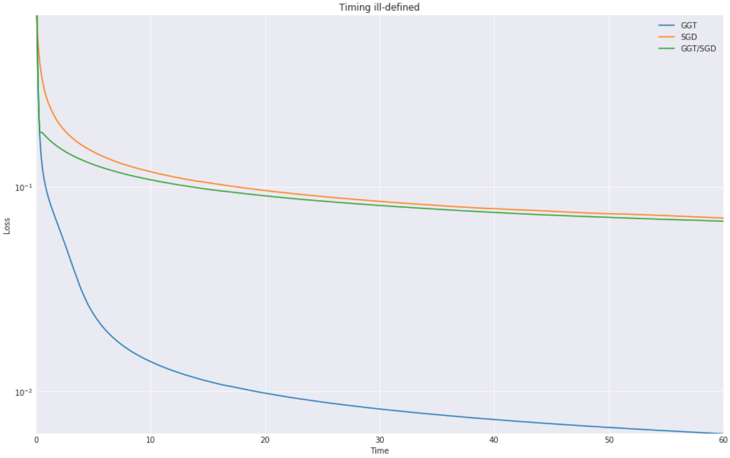
Combining GGT & SGD on ill-defined problem

Combination doesn't help for **ill-defined problems**. Pure GGT's still better



Timing GGT, SGD and GGT&SGD on ill-defined problem

Also *In terms of time*



Discussion

As we can see, the GGT method works on the same performance level as state-of-the-art optimizers such as Adam but it is better in case of ill-posed problem. In our work we succesfuly explored ways to improve this method. Further work could contain massive comparison of GGT with second order methods, study of GGT parameters influence and exploring new forms of matrix $\mathbf{G}_t$.

Contribution

Lusine Airapetyan	Combining GGT & SGD + Timing comparison
Daniil Chesakov	Data preprocessing and model validation
Vsevolod Glazov	Representation results on syntetic data and MNIST dataset
Evgeny Kovalev	Efficiency analysis of possible ways to compute matrix at the iterative step
Leonid Matyushin	Study of modifications of original method, Significant improvement