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:

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

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 step of optimization update:

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

Problem formulation

GGT uses the preconditioner from full-matrix AdaGrad.

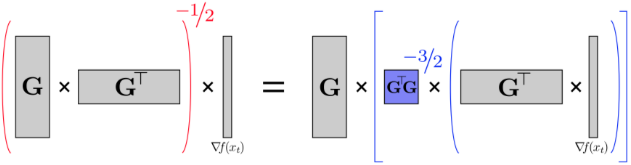
$$\mathbf{G}_k = [g_k g_{k-1} \ldots g_{k-r+1}], \quad \text{where } g_{k-t} = \beta_2^t \widetilde{\nabla} f\left(x_{k-t}\right), \text{ or } 0 \text{ if } t \geq k$$

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 $\mathbf{G}\mathbf{G}^T \in \mathbb{R}^{n\times n}$ can be performed by diagonalizing the small matrix $\mathbf{G}^T\mathbf{G} \in \mathbb{R}^{r\times r}$.



Key Idea

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

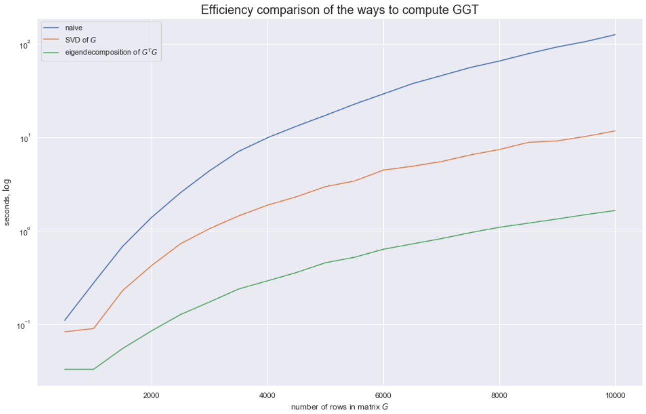
The first term is none other than an SGD update step. The rest can be computed by taking the eigendecomposition $\mathbf{G}^\top \mathbf{G} = \mathbf{V}\boldsymbol{\Sigma}_r^2 \mathbf{V}^\top$, giving $\mathbf{U}_r = \mathbf{G}\mathbf{V}\Sigma_r^{-1}$

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:

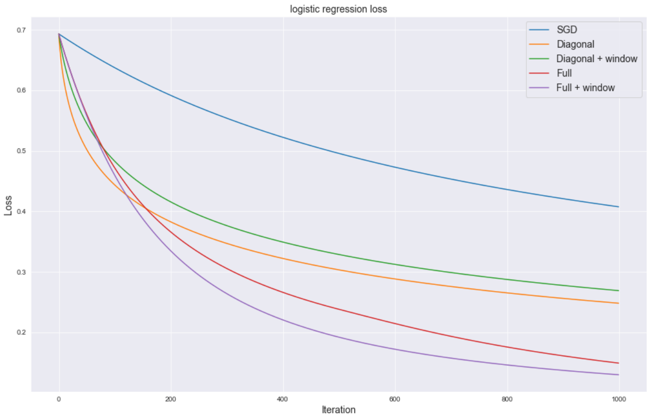
- naive way: use eigendecomposition of symmetric matrix $\mathbf{G}\mathbf{G}^\top$ to compute its square root, and then compute the inverse
- use $(*)$, obtain $\mathbf{U}_r$ and $\mathbf{\Sigma}_r$ via SVD decomposition of matrix $\mathbf{G}$
- use $(*)$, obtain $\mathbf{U}_r$ and $\mathbf{\Sigma}_r$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

Iterative step matrix computation



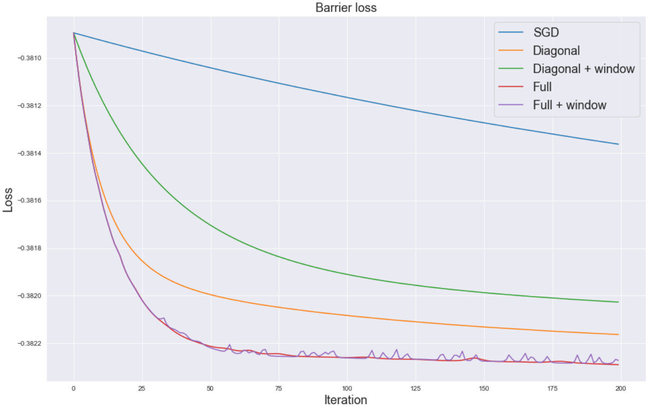
Results representation: syntetic data 1

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.



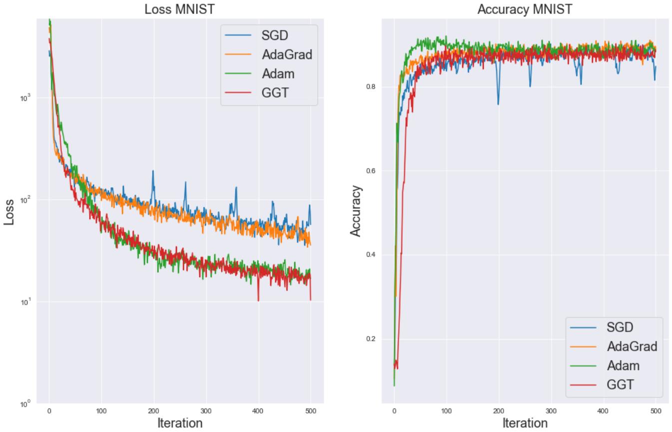
Results representation: syntetic data 2

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 DNN with two hidden fully connected layers with 256 nodes.



Our modifications

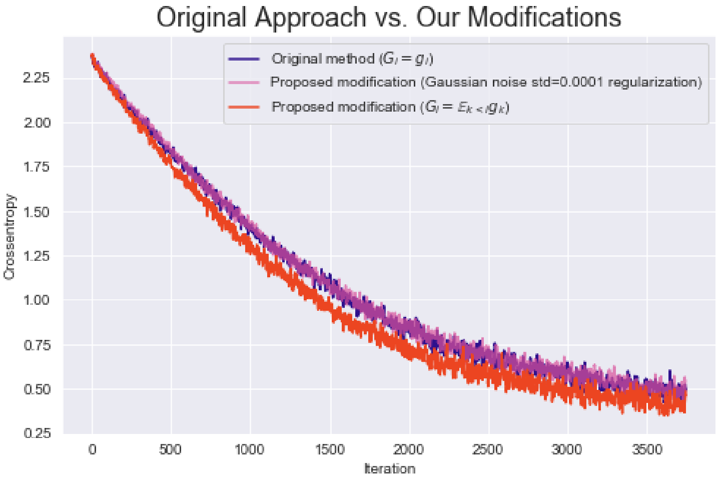
Original paper propose us to use the following matrix $\mathbf{G}_t$:

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

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



Low variance

High correlation (1.0)

Before

After

ROCs

Results

Model	Data	AUC-ROC
XGBoost	**tabular**	**0.9415**
Random Forest	tabular	0.9282
Logistic Regression	tabular	0.9003
KNN	tabular	0.8990
XGBoost	**TF – IDF**	**0.8622**
Random Forest	TF-IDF	0.8511
LSTM + Conv	**texts**	**0.8460**
KNN	TF-IDF	0.8350
Logistic Regression	TF-IDF	0.8316
LSTM	texts	0.8269

Feature importances

Conclusion

- Different approaches were compared
  - DL on texts
    - LSTM+Conv was better than LSTM
    - The worst results though
    - Probably model architecture should be more complex
  - ML on TF-IDF matrix
    - Best: XGBoost
  - ML on tabular data
    - Best: XGBoost
    - The best approach
- EDA was performed
  - Low variance, high correlation features were excluded
- Feature extraction from texts
  - Golden feature: stopwords share
- Model is applicable to a real-life scenario
  - It is interpretable, the quality is good
  - But better to train it on larger dataset