Stochastic gradient algorithms from ODE splitting perspective

ICLR 2020 DeepDiffEq workshop

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Finite sum problems

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We propose a new view on the continuous time SGD as a first-order splitting scheme.

Splitting scheme for ODE

Simplest example of initial value problem. We have $\boldsymbol{\theta}(0) = \boldsymbol{\theta}_0$ and $\boldsymbol{\theta}(h) = ?$:

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We split right-hand side into primitive summands and solve each problem separately with reinitialization.

$$\frac{d\boldsymbol{\theta_1}}{dt} = -\frac{1}{2} g_1(\boldsymbol{\theta_1}), \boldsymbol{\theta_1}(0) = \boldsymbol{\theta}_0 \;\rightarrow\; \boldsymbol{\theta}_1(h);$$

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First order splitting scheme: $\boldsymbol{\theta}^I(h) = \boldsymbol{\theta}_n(h) \circ \cdots \circ \boldsymbol{\theta}_1(h) \circ \boldsymbol{\theta}_0$

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Splitting step	Euler discretization	SGD Epoch	First-order splitting
$\frac{d\boldsymbol{\theta}}{dt} = -\frac{1}{2}\nabla f_1(\boldsymbol{\theta})$	$\tilde{\boldsymbol{\theta}}_I = \boldsymbol{\theta}_0 - \frac{h}{2}\nabla f_1(\boldsymbol{\theta}_0)$	$\tilde{\boldsymbol{\theta}}_{SGD} = \boldsymbol{\theta}_0 - h\nabla f_1(\boldsymbol{\theta}_0)$	$\tilde{\boldsymbol{\theta}}_I = \boldsymbol{\theta}_0 - \frac{h}{2}\nabla f_1(\boldsymbol{\theta}_0)$
$\frac{d\boldsymbol{\theta}}{dt} = -\frac{1}{2}\nabla f_2(\boldsymbol{\theta})$	$\boldsymbol{\theta}_I = \tilde{\boldsymbol{\theta}}_I - \frac{h}{2}\nabla f_2(\tilde{\boldsymbol{\theta}}_I)$	$\boldsymbol{\theta}_{SGD} = \tilde{\boldsymbol{\theta}}_{SGD} - h\nabla f_2(\tilde{\boldsymbol{\theta}}_{SGD})$	$\boldsymbol{\theta}_I = \tilde{\boldsymbol{\theta}}_I - \frac{h}{2}\nabla f_2(\tilde{\boldsymbol{\theta}}_I)$

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Thus, we can conclude, that one epoch of SGD is just the splitting scheme for the discretized Gradient Flow ODE with $2 \cdot h$ step size ($m \cdot h$ in case of m batches)

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Problem	Loss function	Batch gradient	Initial local ODE
Linear Least Squares	$f(\boldsymbol{\theta}) = \frac{1}{n}\sum\limits_{i=1}^{m} \lVert X_i\boldsymbol{\theta} - \mathbf{y_i}\rVert_2^2$	$\frac{1}{b}X_i^\top(X_i\boldsymbol{\theta} - \mathbf{y_i})$	$\frac{d\boldsymbol{\theta}}{dt} = -\frac{1}{n}X_i^\top(X_i\boldsymbol{\theta} - \mathbf{y_i})$
Binary logistic regression	$f(\boldsymbol{\theta}) = -\dfrac{1}{n}\sum\limits_{i=1}^{n}\Big(y_i \ln \sigma(\boldsymbol{\theta}^\top \mathbf{x_i}) + (1-y_i)\ln\big(1-\sigma(\boldsymbol{\theta}^\top\mathbf{x_i})\big)\Big)$	$\frac{1}{b}X_i^\top\left(\sigma\left(X_i\boldsymbol{\theta}\right) - \mathbf{y_i}\right)$	$\frac{d\boldsymbol{\theta}}{dt} = -\frac{1}{n}X_i^\top\left(\sigma\left(X_i\boldsymbol{\theta}\right) - \mathbf{y_i}\right)$
One FC Layer + softmax	$f(\Theta) = -\frac{1}{n}\sum\limits_{i=1}^{n}\log\left(\frac{\mathbf{y_i}^\top e^{\Theta^\top \mathbf{x_i}}}{\mathbf{1}^\top e^{\Theta^\top \mathbf{x_i}}}\right)$	$\frac{1}{b}X_i^\top\left(s(\Theta^\top X_i^\top) - Y_i\right)^\top$	$\frac{d\Theta}{dt} = -\frac{1}{n}X_i^\top\left(s(\Theta^\top X_i^\top) - Y_i\right)^\top$

Integration of local problems

It is important, that we can reduce dimensionality of the dynamic system via QR decomposition of each batch data matrix $X_i^\top = Q_i R_i$ and substitution $\boldsymbol{\eta}_i = Q_i^\top \boldsymbol{\theta}$.

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$$\frac{d\boldsymbol{\theta}}{dt} = -\frac{1}{n} X_i^\top (X_i \boldsymbol{\theta} - \mathbf{y_i}), \boldsymbol{\theta} \in \mathbb{R}^p$$

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$$\begin{cases} \frac{d\boldsymbol{\eta}_\mathbf{i}}{dt} = -\frac{1}{n} R_i \left(R_i^\top \boldsymbol{\eta}_\mathbf{i} - \mathbf{y_i} \right), \boldsymbol{\eta}_\mathbf{i} = Q_i^\top \boldsymbol{\theta}, \boldsymbol{\eta}_\mathbf{i} \in \mathbb{R}^b \\ \boldsymbol{\theta}(h) = Q_i \left(\boldsymbol{\eta}_\mathbf{i}(h) - \boldsymbol{\eta}_\mathbf{i}(0) \right) + \boldsymbol{\theta}_0 \end{cases}$$

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Initial local ODE	$\mathcal{P}_i^k$	**Integration**
$\frac{d\boldsymbol{\theta}}{dt} = -\frac{1}{n} X_i^\top (X_i \boldsymbol{\theta} - \mathbf{y_i})$	$\frac{d\boldsymbol{\eta}_\mathbf{i}}{dt} = -\frac{1}{n} R_i \left(R_i^\top \boldsymbol{\eta}_\mathbf{i} - \mathbf{y_i} \right), \boldsymbol{\eta}_\mathbf{i} = Q_i^\top \boldsymbol{\theta}$	analytical
$\frac{d\boldsymbol{\theta}}{dt} = -\frac{1}{n} X_i^\top \left(\sigma \left(X_i \boldsymbol{\theta} \right) - \mathbf{y_i} \right)$	$\frac{d\boldsymbol{\eta}_\mathbf{i}}{dt} = -\frac{1}{n} R_i \left(\sigma \left(R_i^\top \boldsymbol{\eta}_\mathbf{i} \right) - \mathbf{y_i} \right), \boldsymbol{\eta}_\mathbf{i} = Q_i^\top \boldsymbol{\theta}$	`odeint`
$\frac{d\Theta}{dt} = -\frac{1}{n} X_i^\top \left(s(\Theta^\top X_i^\top) - Y_i \right)^\top$	$\frac{dH_i}{dt} = -\frac{1}{n} R_i (s(H_i^\top R) - Y_i)^\top, H_i = Q_i^\top \Theta$	`odeint`

Algorithm

Algorithm 1: Splitting optimization

$\boldsymbol{\theta}_0$ - initial parameter; b - batch size; α - learning rate; m- total number of batches

$h := \alpha m$

$t := 0$

for $k = 0, 1, \ldots$ **do**

  for $i = 1, 2, \ldots, m$ **do**

    Formulate local ODE problem $\mathcal{P}_i^k$

    $\boldsymbol{\theta}_{t+1} =$ integrate $\mathcal{P}_i^k$ given an initial value $\boldsymbol{\theta}(0) = \boldsymbol{\theta}_t$ to the step h

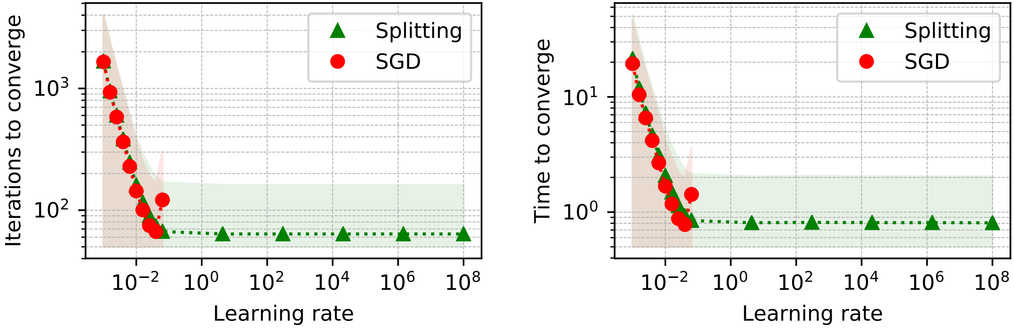
    $t := t + 1$

  end

end

Random linear system

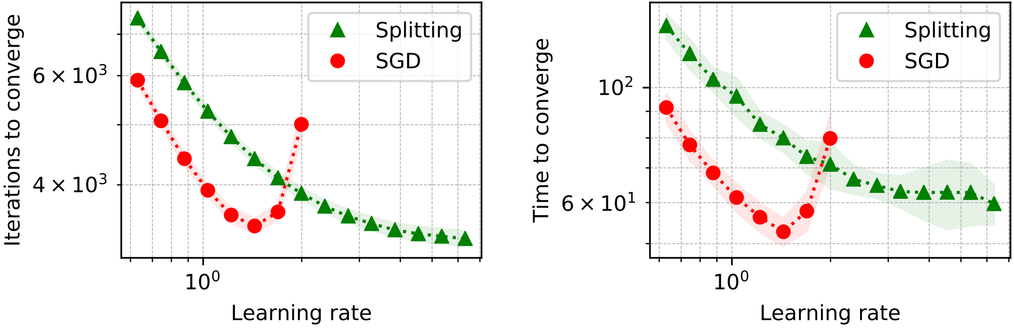
10000×500. $b = 20$. Relative error 10^{-3}



(a) Iterations (b) Time

Real linear system

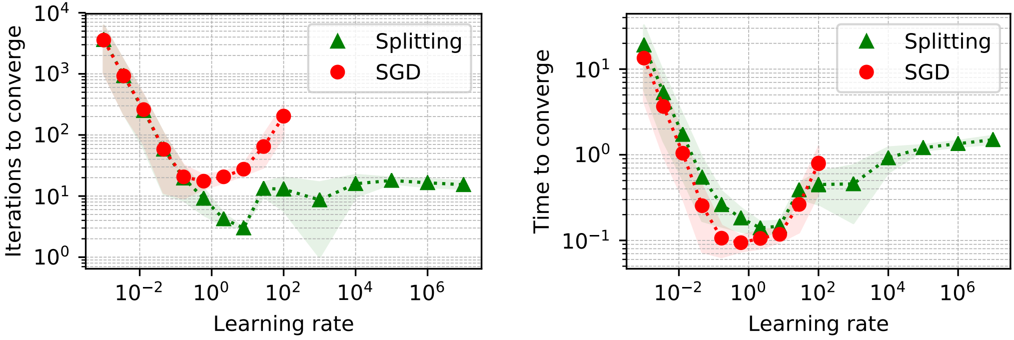
Tomogropy data from AIRTools II 12780×2500. $b = 60$. Relative error 10^{-3}



(a) `Iterations` (b) `Time`

Binary logistic regression

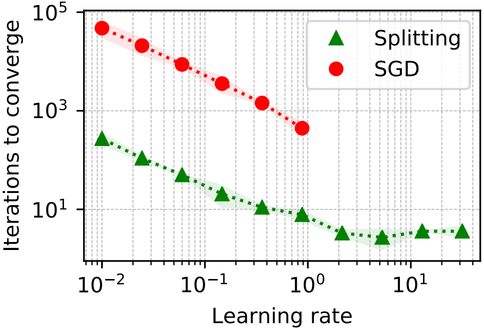
MNIST 0,1 dataset. $b = 50$. Test error 10^{-3}



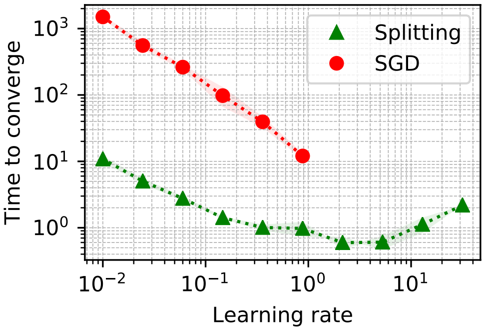
(a) Iterations (b) Time

Softmax regression

Fashion MNIST dataset. 10 classes. 28×28 images, $b = 64$. Test error 0.25

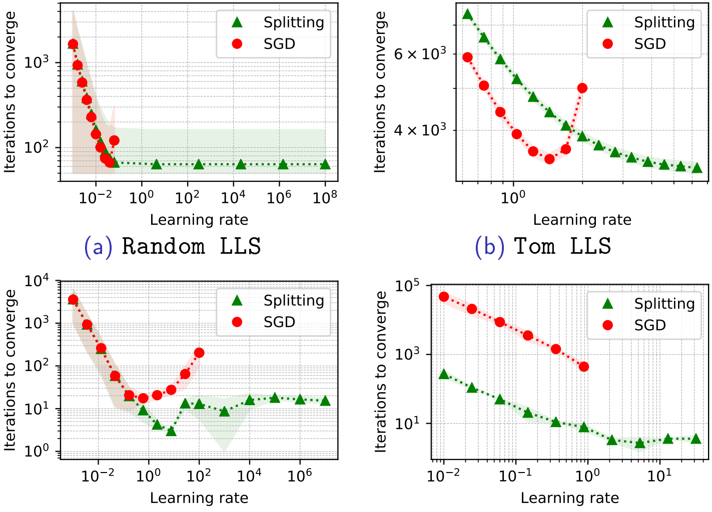


(a) Iterations



(b) Time

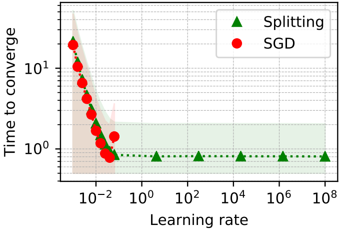
SGD vs Splitting. Iteration comparison



(a) Random LLS (b) Tom LLS

(c) LogReg (d) Softmax

SGD vs Splitting. Time comparison



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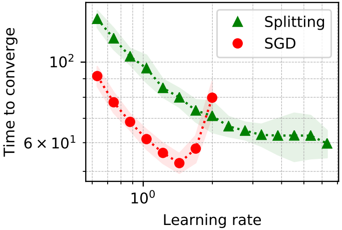
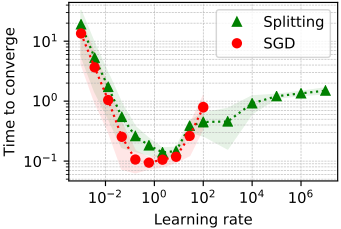
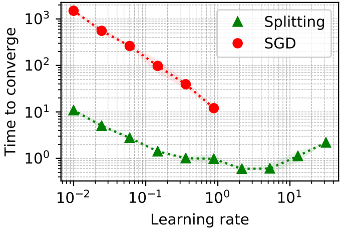


(b) Tom LLS



(c) LogReg



(d) Softmax

Thank you for your attention!

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Paper and code:

merkulov.top/sgd_splitting