Stochastic Newton and quasi-Newton Methods for Large-Scale Convex Optimization

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Outline

- Newton-like and quasi-Newton methods for convex stochastic optimization problems using limited memory block BFGS updates.
- In the class of problems of interest, the objective functions can be expressed as the sum of a huge number of functions of an extremely large number of variables.
- We present preliminary numerical results on problems from machine learning.

Related work on L-BFGS for Stochastic Optimization

- P1 N.N. Schraudolph, J. Yu and S.Günter. A stochastic quasi-Newton method for online convex optim. Int'l. Conf. AI & Stat., 2007
- P2 A. Bordes, L. Bottou and P. Gallinari. SGD-QN: Careful quasi-Newton stochastic gradient descent. JMLR vol. 10, 2009
- P3 R.H. Byrd, S.L. Hansen, J. Nocedal, and Y. Singer. A stochastic quasi-Newton method for large-scale optim. arXiv1401.7020v2, 2014
- P4 A. Mokhtari and A. Ribeiro. RES: Regularized stochastic BFGS algorithm. IEEE Trans. Signal Process., no. 10, 2014.
- P5 A. Mokhtari and A. Ribeiro. Global convergence of online limited memory BFGS. to appear in J. Mach. Learn. Res., 2015.
- P6 P. Moritz, R. Nishihara, M.I. Jordan. A linearly-convergent stochastic L-BFGS Algorithm, 2015 arXiv:1508.02087v1
- P7 X. Wang, S. Ma, D. Goldfarb and W. Liu. Stochastic quasi-Newton methods for nonconvex stochastic optim. 2015, submitted.

(the first 6 papers are for strongly convex problems, the last one is for nonconvex problems)

Stochastic optimization

- Stochastic optimization

$$\min\ f(x) = \mathbb{E}[f(x,\xi)], \quad \xi \text{ is random variable}$$

- Or finite sum (with $f_i(x) \equiv f(x,\xi_i)$ for $i = 1,\ldots,n$ and very large n)

$$\min\ f(x) = \frac{1}{n}\sum_{i=1}^{n} f_i(x)$$

- f and ∇f are very expensive to evaluate; e.g., SGD methods randomly choose a random subset $\mathcal{S} \subset [n]$ and evaluate

$$f_{\mathcal{S}}(x) = \frac{1}{|\mathcal{S}|}\sum_{i\in\mathcal{S}} f_i(x) \quad \text{and} \quad \nabla f_{\mathcal{S}}(x) = \frac{1}{|\mathcal{S}|}\sum_{i\in\mathcal{S}} \nabla f_i(x)$$

- Essentially, only noisy info about f, ∇f and $\nabla^2 f$ is available
- Challenge: how to design a method that takes advantage of noisy 2nd-order information?

Using 2nd-order information

- Assumption: $f(x) = \frac{1}{n}\sum_{i=1}^{n} f_i(x)$ is strongly convex and twice continuously differentiable.
- Choose (compute) a sketching matrix S_k (the columns of S_k are a set of directions).
- Following Byrd, Hansen, Nocedal and Singer, we do not use differences in noisy gradients to estimate curvature, but rather compute the action of the sub-sampled Hessian on S_k. i.e.,
- compute $Y_k = \frac{1}{|\mathcal{T}|}\sum_{i\in\mathcal{T}} \nabla^2 f_i(x) S_k$, where $\mathcal{T} \subset [n]$.
- We choose $\mathcal{T} = \mathcal{S}$

block BFGS

Given $H_k = B_k^{-1}$, the block BFGS method computes a "least change" update to the current approximation H_k to the inverse Hessian matrix $\nabla^2 f(x)$ at the current point x, by solving

$$\begin{aligned} \text{min} \quad & \|H - H_k\| \\ \text{s.t.,} \quad & H = H^\top, \quad HY_k = S_k. \end{aligned}$$

This gives the updating formula (analgous to the updates derived by Broyden, Fletcher, Goldfarb and Shanno).

$$H_{k+1} = (I - S_k[S_k^\top Y_k]^{-1} Y_k^\top) H_k (I - Y_k[S_k^\top Y_k]^{-1} S_k^\top) + S_k[S_k^\top Y_k]^{-1} S_k^\top$$

or, by the Sherman-Morrison-Woodbury formula:

$$B_{k+1} = B_k - B_k S_k [S_k^\top B_k S_k]^{-1} S_k^\top B_k + Y_k [S_k^\top Y_k]^{-1} Y_k^\top$$

Limited Memory Block BFGS

After M block BFGS steps starting from H_{k+1-M}, one can express H_{k+1} as

$$\begin{aligned} H_{k+1} &= V_k H_k V_k^T + S_k \Lambda_k S_k^T \\ &= V_k V_{k-1} H_{k-1} V_{k-1}^T V_k + V_k S_{k-1} \Lambda_{k-1} S_{k-1}^T V_k^T + S_k \Lambda_k S_k^T \\ &\vdots \\ &= V_{k:k+1-M} H_{k+1-M} V_{k:k+1-M}^T + \sum_{i=k}^{k+1-M} V_{k:i+1} S_i \Lambda_i S_i^T V_{k:i+1}^T, \end{aligned}$$

where

$$V_k = (I - S_k \Lambda_k Y_k^T) \tag{1}$$

and $\Lambda_k = (S_k^T Y_k)^{-1}$ and $V_{k:i} = V_k \cdots V_i$.

Limited Memory Block BFGS

- Hence, when the number of variables d is large, instead of storing the $d \times d$ matrix H_k, we store the previous M block curvature pairs

$$\left(S_{k+1-M}, Y_{k+1-M}\right), \ldots, \left(S_k, Y_k\right),$$

  and the Cholesky factors of the matrices $(S_i^T Y_i) = \Lambda_i^{-1}$ for $i = k+1-M, \ldots, k$.
- Then, analogously to the standard L-BFGS method, for any vector $v \in \mathbb{R}^d$, $H_k v$ can be computed efficiently using a two-loop block recursion (in $Mp(4d + 2p) + O(p)$) operations), if all $S_i \in \mathbb{R}^{d \times p}$.

Intuition

- Limited memory - least change aspect of BFGS is important
- Each block update acts like a sketching procedure.

Choices for the Sketching Matrix S_k

We employ one of the following strategies

- Gaussian: $S_k \sim \mathcal{N}(0, I)$ has Gaussian entries sampled i.i.d at each iteration.
- Previous search directions s_i delayed: Store the previous L search directions $S_k = [s_{k+1-L}, \ldots, s_k]$ then update H_k only once every L iterations.
- Self-conditioning: Sample the columns of the Cholesky factors L_k of H_k (i.e., $L_k L_k^T = H_k$) uniformly at random. Fortunately we can maintain and update L_k efficiently with limited memory.

The matrix S is a sketching matrix, in the sense that we are sketching the, possibly very large equation $\nabla^2 f(x) H = I$ to which the solution is the inverse Hessian. Left multiplying by S^T compresses/sketches the equation yielding $S^T \nabla^2 f(x) H = S^T$.

Stochastic Variance Reduced Gradients

- Stochastic methods converge slowly near the optimum due to the variance of the gradient estimates $\nabla f_{\mathcal{S}}(x)$; hence requiring a decreasing step size.
- We use the control variates approach of Johnson and Zhang (2013) for a SGD method SVRG.
- It uses $\nabla f_{\mathcal{S}}(x_t) - \nabla f_{\mathcal{S}}(w_k) + \nabla f(w_k$, where w_k is a reference point, in place of $\nabla f_{\mathcal{S}}(x_t)$.
- w_k, and the full gradient, are computed after each full pass of the data, hence doubling the work of computing stochastic gradients.
- Other recently proposed SGD variance reduction techniques such as SAG, SAGA, SDCA, and S2GD, can be used in place of SVRG.

The Basic Algorithm

Algorithm 0.1: Stochastic Variable Metric Learning with SVRG

Input: $H_{-1} \in \mathbb{R}^{d \times d}$, $w_0 \in \mathbb{R}^d$, $\eta \in \mathbb{R}_+$, s = subsample size, q = sample action size and m

for $k = 0, \ldots, max\_iter$ **do**
- $\mu = \nabla f(w_k)$
- $x_0 = w_k$
- **for** $t = 0, \ldots, m-1$ **do**
  - Sample $\mathcal{S}_t, \mathcal{T}_t \subseteq [n]$ i.i.d from a distribution $\mathcal{S}$
  - Compute the sketching matrix $S_t \in \mathbb{R}^{d \times q}$
  - Compute $\nabla^2 f_{\mathcal{S}}(x_t) S_t$
  - $H_t =$update_metric$(H_{t-1}, S_t, \nabla^2 f_{\mathcal{T}}(x_t) S_t)$
  - $d_t = -H_t \left(\nabla f_{\mathcal{S}}(x_t) - \nabla f_{\mathcal{S}}(w_k) + \mu\right)$
  - $x_{t+1} = x_t + \eta d_t$
- **end**
- **Option I:** $w_{k+1} = x_m$
- **Option II:** $w_{k+1} = x_i$, i selected uniformly at random from $[m]$;

end

Convergence - Assumptions

There exist constants $\lambda, \Lambda \in \mathbb{R}_+$ such that

- f is λ–strongly convex

$$f(w) \geq f(x) + \nabla f(x)^T(w - x) + \frac{\lambda}{2} \|w - x\|_2^2, \qquad (2)$$

- f is Λ–smooth

$$f(w) \leq f(x) + \nabla f(x)^T(w - x) + \frac{\Lambda}{2} \|w - x\|_2^2, \qquad (3)$$

- These assumptions imply that

$$\lambda I \preceq \nabla^2 f_{\mathcal{S}}(w) \preceq \Lambda I, \quad \text{for all } x \in \mathbb{R}^d, \mathcal{S} \subseteq [n], \qquad (4)$$

- from which we can prove that there exist constants $\gamma, \Gamma \in \mathbb{R}_+$ such that for all k we have

$$\gamma I \preceq H_k \preceq \Gamma I. \qquad (5)$$

Linear Convergence

Theorem

Suppose that the Assumptions hold. Let w_* be the unique minimizer of $f(w)$. Then in our Algorithm, we have for all $k \geq 0$ that

$$\mathbb{E}f(w_k) - f(w_*) \leq \rho^k \mathbb{E}f(w_0) - f(w_*),$$

where the convergence rate is given by

$$\rho = \frac{1/2m\eta + \eta\Gamma^2\Lambda(\Lambda - \lambda)}{\gamma\lambda - \eta\Gamma^2\Lambda^2} < 1,$$

assuming we have chosen $\eta < \gamma\lambda/(2\Gamma^2\Lambda^2)$ and that we choose m large enough to satisfy

$$m \geq \frac{1}{2\eta\left(\gamma\lambda - \eta\Gamma^2\Lambda(2\Lambda - \lambda)\right)},$$

which is a positive lower bound given our restriction on η.

Upper and lower bounds on eigenvalues of H_k

- Under the assumption that

$$\lambda I \preceq \nabla^2 f_T(x) \preceq \Lambda I, \quad \forall x \in \mathbb{R}^d \tag{6}$$

there exist constants $\gamma, \Gamma \in \mathbb{R}_+$ such that for all k we have

$$\gamma I \preceq H_k \preceq \Gamma I. \tag{7}$$

where

$$\gamma \;\geq\; \frac{1}{1+M\Lambda}, \quad \Gamma \;\leq\; (1+\sqrt{\kappa})^{2M}(1+\frac{1}{\lambda(2\sqrt{\kappa}+\kappa)}), \quad \kappa \;\equiv\; \Lambda/\lambda. \tag{8}$$

- Previously derived bounds depend on the problem dimension d; e.g. $\Gamma \sim ((d+M)\kappa)^{d+M}$

gisette-scale $d = 5,000$, $n = 6,000$

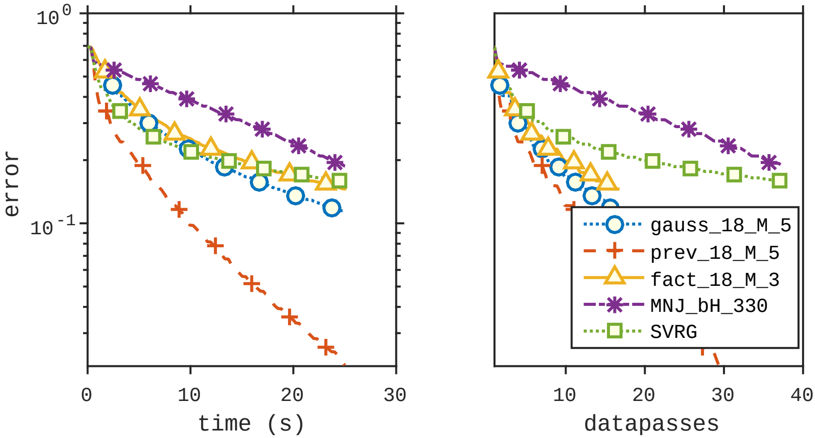

Figure: gisette

covtype-libsvm-binary $d = 54, n = 581,012$

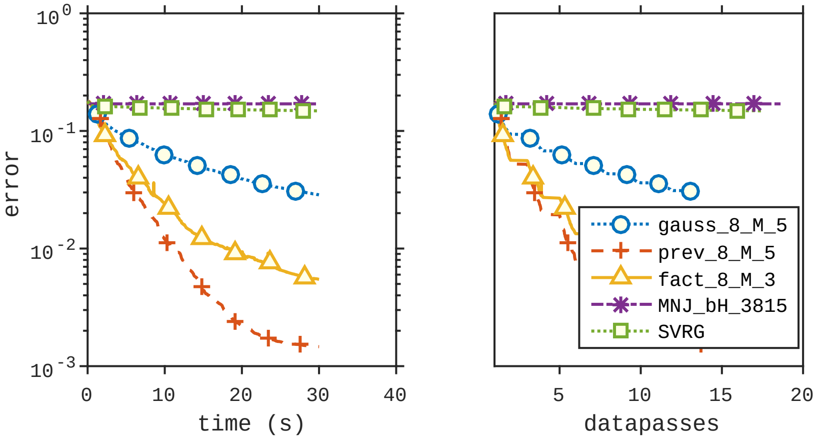

Figure: covtype.libsvm.binary

Higgs $d = 28, n = 11,000,000$

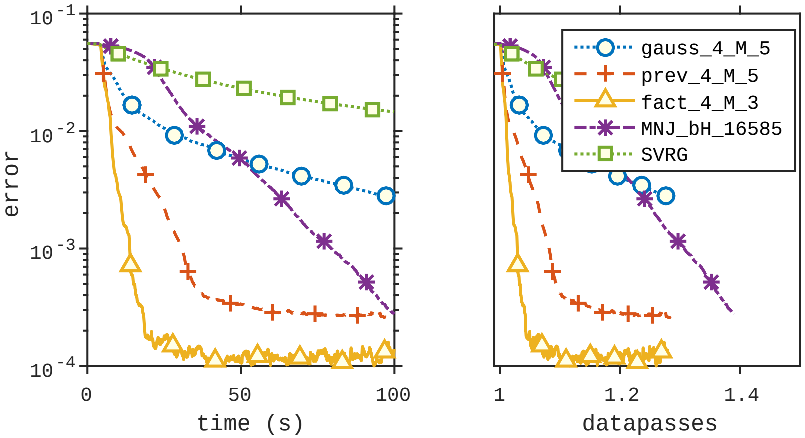

Figure: HIGGS

SUSY $d = 18, n = 3,548,466$

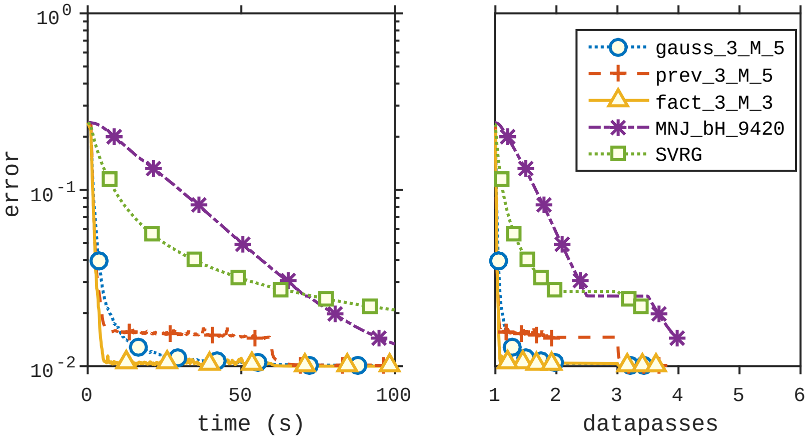

Figure: SUSY

epsilon-normalized $d = 2,000$, $n = 400,000$

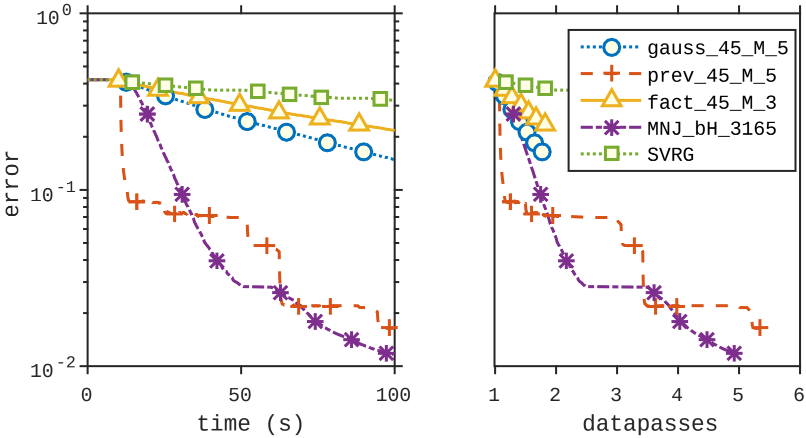

Figure: epsilon-normaliized

rcv1-training $d = 47,236$, $n = 20,242$

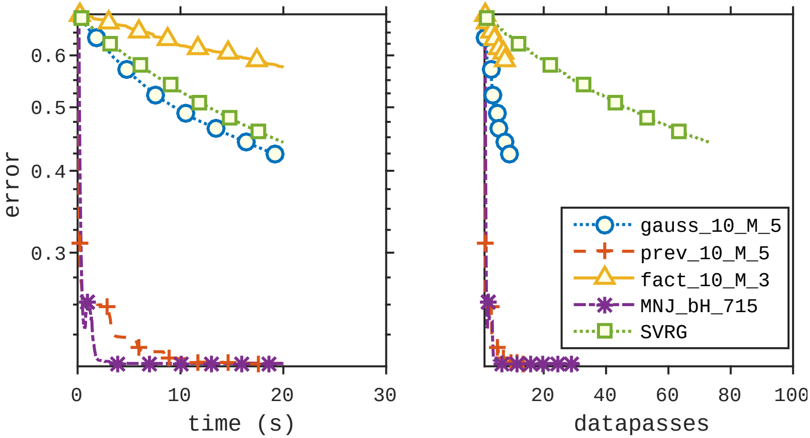

Figure: rcv1-train

url-combined $d = 3,231,961, n = 2,396,130$

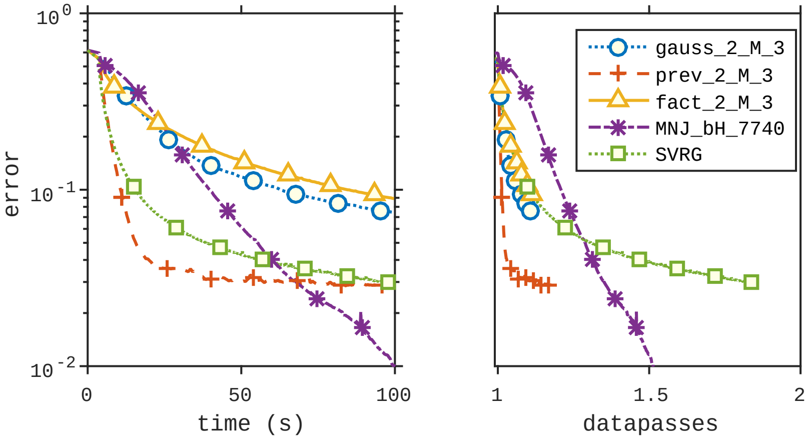

Figure: url-combined

Contributions

- *New metric learning framework.* A block BFGS framework for gradually learning the metric of the underlying function using a sketched form of the subsampled Hessian matrix
- *New limited-memory block BFGS method.* May also be of interest for non-stochastic optimization
- *New limited-memory factored form block BFGS method.*
- *Several sketching matrix possibilities.*
- *Linear convergence rate* proof for our methods.
- *Tighter upper and lower bounds* on the eigenvalues of the variable metric