Stochastic Block BFGS: Squeezing More Curvature out of Data

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1. Problem

Find an approximate minima of

$$\min_{x\in\mathbb{R}^d} f(x) \overset{\text{def}}{=} \tfrac{1}{n}\sum_{i=1}^n f_i(x), \tag{1}$$

where $f_i : \mathbb{R}^d \to \mathbb{R}$ is convex and twice differentiable, d is large and **n is very large**.

2. Variable Metric Methods

Given $x_0 \in \mathbb{R}^d$, many successful methods for solving (1) fit the format

$$x_{t+1} = x_t - \eta H_t g_t,$$

where $\mathbf{E}[g_t] = \nabla f(x_t)$, $H_t \approx \nabla^2 f(x_t)^{-1}$, and $\eta > 0$ is a stepsize. To update g_t and H_t, effective methods use only the *subsampled gradient* and *subsampled Hessian*

$$\nabla f_S(x) \overset{\text{def}}{=} \frac{1}{|S|}\sum_{i\in S}\nabla f_i(x), \quad \nabla^2 f_T(x) \overset{\text{def}}{=} \frac{1}{|T|}\sum_{i\in T}\nabla^2 f_i(x)$$

where $S, T \subseteq [n] \overset{\text{def}}{=} \{1,2,\ldots,n\}$ selected uniformly at random.

Challenge: Update H_t using subsampled Hessians.

Novelty: We develop a new stochastic Block BFGS method for updating/maintaining H_t based on sketching. We also present a new limited memory variant.

3. Hessian Sketching

Fact: Evaluating Hessian-vector products is cheap

$$\nabla^2 f_T(x_t)v = \frac{d}{d\alpha}\nabla f_T(x_t+\alpha v)\Big|_{\alpha=0} \tag{2}$$

We would like H_t to satisfy the *inverse equation*

$$H_t\nabla^2 f_T(x_t) = I,$$

but calculating the inverse of $d\times d$ matrix is expensive.

Solution: finding H_t that satisfies a *sketched* version of inverse equation

$$H_t\nabla^2 f_T(x_t)D_t = D_t, \tag{3}$$

is cheap (2), where $D_t \in \mathbb{R}^{d\times q}$ and $q \ll \min\{d,n\}$.

We employ three different sketching strategies:

1) gauss. D_t has standard Gaussian entries sampled i.i.d at each iteration.

2) prev. Let $d_t = -H_t g_t$. Store search directions $D_t = [d_{t+1-q},\ldots,d_t]$ and update H_t once every q iterations.

3) fact. Sample $C_t \subseteq \{1,\ldots,d\}$ uniformly at random and set $D_t = L_{t-1}I_{:C_t}$,where $L_{t-1}L_{t-1}^T = H_{t-1}$ and $I_{:C_t}$ denotes the concatenation of the columns of the identity matrix indexed by a set $C_t \subset \{1,\ldots,d\}$.

4. Block BFGS Update

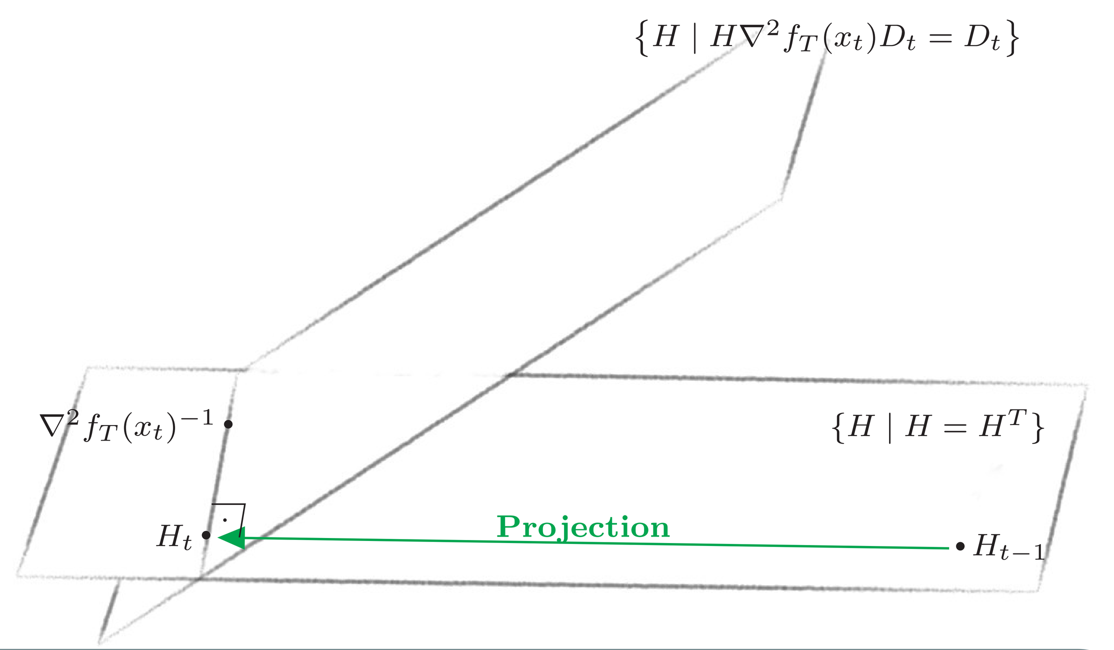
The sketched equation (3) is not enough to determine H_t uniquely. So we make use of the following projection

$$H_t = \arg\min_{H\in\mathbb{R}^{d\times d}} \|H - H_{t-1}\|_t^2$$
$$\text{subject to } H\nabla^2 f_T(x_t)D_t = D_t,\ H = H^T, \tag{4}$$

where $\|H\|_t^2 \overset{\text{def}}{=} \mathbf{Tr}\left(H\nabla^2 f_T(x_t)H^T\nabla^2 f_T(x_t)\right)$. The closed form solution of (4) is

$$H_t = D_t\Delta_t D_t^T + \left(I - D_t\Delta_t Y_t^T\right)H_{t-1}\left(I - Y_t\Delta_t D_t\right),$$

where $\Delta_t = (D_t^T Y_t)^{-1}$ and $Y_t = \nabla^2 f_T(x_t)D_t$.



5. Block L-BFGS update

Let $V_t = I - D_t\Delta_t Y_t^T$. Expanding M block BFGS updates applied to H_{t-M} gives

$$\begin{aligned} H_t &= V_t H_{t-1}V_t^T + D_t\Delta_t D_t^T \\ &= V_t\cdots V_{t+1-M}H_{t-M}V_{t+1-M}^T\cdots V_t^T \\ &+ \sum_{i=t}^{t+1-M} V_t\cdots V_{i+1}D_i\Delta_i D_i^T V_{i+1}^T\cdots V_t^T. \end{aligned}$$

Therefore H_t is a function of H_{t-M} and the triples

$$(D_{t+1-M}, Y_{t+1-M}, \Delta_{t+1-M}), \ldots, (D_t, Y_t, \Delta_t). \tag{5}$$

Set $H_{t-M} = I$ and **only store the triples in (5).**

Algorithm 1 Block L-BFGS Update (Two-loop Recursion)

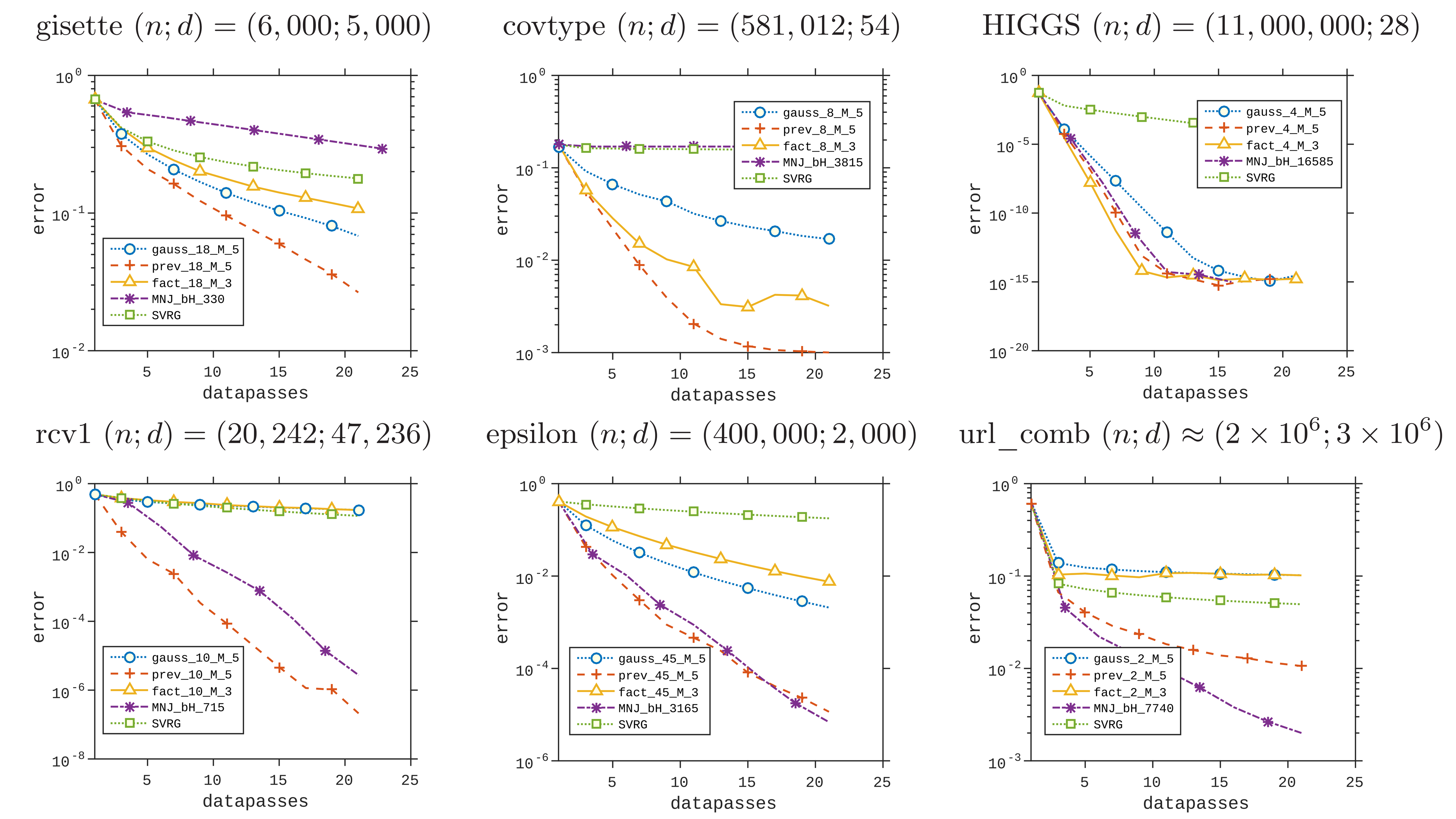
inputs: $g_t \in \mathbb{R}^d, D_i, Y_i \in \mathbb{R}^{d\times q}$ and $\Delta_i \in \mathbb{R}^{q\times q}$ for $i \in \{t+1-M,\ldots,t\}$.
initiate: $v \leftarrow g_t$
for $i = t,\ldots,t-M+1$ **do**
  $\alpha_i \leftarrow \Delta_i D_i^T v, \quad v \leftarrow v - Y_i\alpha_i$
end for
for $i = t-M+1,\ldots,t$ **do**
  $\beta_i \leftarrow \Delta_i Y_i^T v, \quad v \leftarrow v + D_i(\alpha_i - \beta_i)$
end for
output $H_t g_t \leftarrow v$

6. Algorithm

Algorithm 2 Stochastic Block BFGS Method

inputs: $w_0 \in \mathbb{R}^d$, stepsize $\eta > 0$, q = sample action size, and length of inner loop m.
initiate: $H_{-1} = I$
for $k = 0,1,2,\ldots$ **do**
  Compute the full gradient $\mu = \nabla f(w_k)$
  Set $x_0 = w_k$
  for $t = 0,\ldots,m-1$ **do**
    Sample $S_t, T_t \subseteq [n]$, independently
    Compute variance-reduced stochastic gradient
    $g_t = \nabla f_{S_t}(x_t) - \nabla f_{S_t}(w_k) + \mu$
    Form $D_t \in \mathbb{R}^{d\times q}$ so that $\text{rank}(D_t) = q$
    Compute sketch $Y_t = \nabla^2 f_{T_t}(x_t)D_t$
    Compute $d_t = -H_t g_t$ via Algorithm 1
    Set $x_{t+1} = x_t + \eta d_t$
  end for
  Option I: Set $w_{k+1} = x_m$
  Option II: Set $w_{k+1} = x_i$, where i is selected uniformly at random from $[m] = \{1,2,\ldots,m\}$
end for
output w_{k+1}

7. Tests on logistic loss with $L2$ regularizer



8. Convergence

Assumption 1. *There exist constants $0 < \lambda \le \Lambda$ such that*

$$\lambda I \preceq \nabla^2 f_T(x) \preceq \Lambda I \tag{6}$$

for all $x \in \mathbb{R}^d$ and all $T \subseteq [n]$.

Lemma 1. *There exists $\Gamma \ge \gamma > 0$ such that*

$$\gamma I \preceq H_t \preceq \Gamma I \qquad \forall t, \tag{7}$$

where

$$\frac{1}{1+M\Lambda} \le \gamma \le \Gamma \le (1+\sqrt{\kappa})^{2M}\left(1+\frac{1}{\lambda(2\sqrt{\kappa}+\kappa)}\right)$$

and $\kappa \overset{\text{def}}{=} \Lambda/\lambda$.

Theorem 1. *If we select parameters m, η such that*

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

then Algorithm 2 with Option II gives

$$\mathbf{E}\left[f(w_k) - f(w_*)\right] \le \rho^k\mathbf{E}\left[f(w_0) - f(w_*)\right], \quad k \ge 0$$

where the convergence rate is given by

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

9. Summary

We proposed a novel limited-memory stochastic block BFGS update for incorporating enriched curvature information in stochastic approximation methods. In our method, the estimate of the inverse Hessian matrix is updated at each iteration using a sketch of the Hessian. We presented three sketching strategies, a new quasi-Newton method that uses stochastic block BFGS updates combined with the variance reduction approach SVRG to compute batch stochastic gradients, and proved linear convergence of the resulting method.

References

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[4] R.M. Gower and Jacek Gondzio Action constrained quasi-Newton methods, *1412.8045* 2014.