Investigating Quasi-Newton Compact Dense Representations on GPUs

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Outline

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The Good Old Days

Simulation-based Applications

- (Relatively) Small optimization problem
- (Relatively) Large simulation
- Computational cost dominated by governing equations (i.e.objective function and/or gradient evaluation)

CPU-based Architectures

- Homogeneous computing w/MPI
- Full instruction set
- Mature software stack

The Accelerator Takeover

- Top500 Rank: 2 (125 PFlop/s)
- CPU: IBM Power9 (2/node)
- GPU: NVIDIA Volta V100 (4/node)

- Top500 Rank: 1 (200 PFlop/s)
- CPU: IBM Power9 (2/node)
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- 1000+ Pflop/s
- CPU: Intel Xeon (2/node)
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Over 95% of flops from GPUs

Why does it matter?

Libraries and application codes are being ported to new architectures

- Necessity - CPUs amount to a small % compute power on the latest generation supercomputers
- SIAM PP20 Minisymposiums - FASTMath (MS3 & MS12) and PETSc (MS23 & MS34)

Emerging applications in data science, machine learning and artificial intelligence

- Perform a lot of tasks well suited to GPUs and/or heterogeneous systems
- Can generate (very) large optimization problems

Optimization (and other "outer loop" tools) must also run on GPUs

PETSc/TAO Overview

PETSc – Portable Extensible Toolkit for Scientific Computing

TAO – Toolkit for Advanced Optimization

- Parallelized with PETSc `Vec` and `Mat` data structures
- Provides gradient-based solvers for large-scale optimization
- Unconstrained and bound-constrained methods:
  - Nonlinear Conjugate Gradient (BNCG)
  - Quasi-Newton (BQNLS)
  - Truncated Newton (BNLS, BNTR)
- Constrained methods:
  - Alternating Directions Method of Multipliers (ADMM)
  - More to come in 2020

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Today: Investigating QN on GPUs

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Tomorrow: Profiling ADMM on GPUs, Todd Munson (MS23)

Outline

The Basics

$$\min_x f(x) \quad \Rightarrow$$

for k=0,1,2,...

$$\mathrm{p}_k = \arg\min_p \tfrac{1}{2} p_k^T \nabla_{xx}^2 f(x_k) p_k + p_k^T \nabla_x f(x_k)$$

$$\mathrm{x}_{k+1} = x_k + \alpha p_k$$

The Basics

$$\min_x f(x) \quad \Rightarrow \quad \begin{aligned} &\textbf{for } \mathrm{k=0,1,2,\ldots} \\ &\mathrm{p}_k = -\left[\nabla^2_{xx} f(x_{k+1})\right]^{-1} \nabla_x f(x_k) \\ &\mathrm{x}_{k+1} = x_k + \alpha p_k \end{aligned}$$

BFGS approximates the Hessian as

$$\left[\nabla^2_{xx} f(x_{k+1})\right]^{-1} \approx H_{k+1} = \left(I - \frac{s_k y_k^T}{y_k^T s_k}\right) H_k \left(I - \frac{y_k s_k^T}{y_k^T s_k}\right) + \frac{s_k s_k^T}{y_k^T s_k}$$

with $\quad s_k = x_k - x_{k-1} \quad$ and $\quad y_k = g_k - g_{k-1} \quad$ where $\quad g_k = \nabla_x f(x_k)$

Why quasi-Newton?

$$\left[\nabla^2_{xx} f(x_{k+1})\right]^{-1} \approx H_{k+1} = \left(I - \frac{s_k y_k^T}{y_k^T s_k}\right) H_k \left(I - \frac{y_k s_k^T}{y_k^T s_k}\right) + \frac{s_k s_k^T}{y_k^T s_k}$$

- First-order method – computing Hessians is prohibitively expensive for many applications
- L-BFGS is one of the most popular general-purpose gradient-based optimization algorithms
- Recent focus on developing stochastic variants for emerging ML/AI applications

A Practical Implementation

- Limited-memory implementation stores only $m \ll 100$ iterations of (s, y) pairs
- Matrix-free two-loop algorithm computes the action of the inverse Hessian on a vector
- Available as MATLMVMBFGS in PETSc/TAO

$q \leftarrow g_k$
for $i = k-1, k-2, \ldots, k-m$ **do**
  $\alpha_i \leftarrow \frac{s_i^T q}{y_i^T s_i}$
  $q \leftarrow q - \alpha_i y_i$
end for
$z \leftarrow H_0 q$
for i=k-m,k-m+1,...,k-1 **do**
  $\beta_i \leftarrow \frac{y_i^T z}{y_i^T s_i}$
  $z \leftarrow z + (\alpha_i - \beta_i) s_i$
end for

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Collective vector operations do not leverage GPU capabilities

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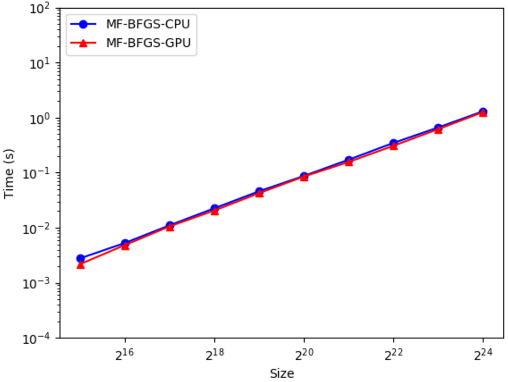
Collective vector operations do not leverage GPU capabilities

Can we trade-off storage for better performance?

Does it run on GPUs?



Computing $H_k z$ with two-loop algorithm

Disclaimer: Preliminary investigation, no general conclusions!

- Intel Core i5-9400F (262 GF)
- NVIDIA GTX 1080 (277 GF)
- CUDA 10.2
- $m = 5$
- `VECSEQ` vs. `VECSEQCUDA`

Outline

An Alternative View

BFGS can be reformulated as

$$\mathrm{H}_{k+1} = H_0 + \begin{bmatrix} H_0 Y_k & S_k \end{bmatrix} \begin{bmatrix} 0 & -\bar{R}_k^{-1} \\ -\bar{R}_k^{-T} & \bar{R}_k^{-T} \left(D_k + Y_k^T H_0 Y_k \right) \bar{R}_k^{-1} \end{bmatrix} \begin{bmatrix} Y_k^T H0 \\ S_k^T \end{bmatrix}$$

where $\mathrm{S}_k = \begin{bmatrix} s_1 & s_2 & \dots & s_k \end{bmatrix}, \; Y_k = \begin{bmatrix} y_1 & y_2 & \dots & y_k \end{bmatrix},$

$\mathrm{S}_k^T Y_k = L_k + D_k + R_k$ and $\bar{R}_k = D_k + R_k$

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$\mathrm{S}_k^T Y_k = L_k + D_k + R_k$ and $\bar{R}_k = D_k + R_k$

$$S_k^T Y_k,\ L_k,\ D_k,\ R_k, \bar{R}_k \ \in \ \mathbb{R}^{(m \times m)}$$

$$S_k,\ Y_k \ \in \mathbb{R}^{(n \times m)} \text{ where } x \ \in \ \mathbb{R}^n$$

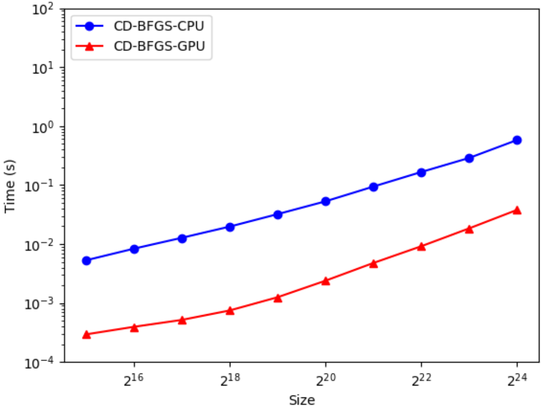
Implementation Notes

- $\begin{bmatrix} 0 & -\bar{R}_k^{-1} \\ -\bar{R}_k^{-T} & \bar{R}_k^{-T}\left(D_k + Y_k^T H_0 Y_k\right)\bar{R}_k^{-1} \end{bmatrix}$ can be assembled efficiently (see Alg. 1 from Erway and Marcia, 2016)
- Leverage fast mat-vec on GPUs – products with S_k and Y_k instead of looping over sequence of update vectors
- Theoretically requires only $(4m^3 + 4m^2)$ more storage but a practical implementation can approach a $2\times$ factor
- Approx. 40% savings on flop count compared to two-loop algorithm for $n \gg 100$

Method	**Flop Count**
Two-loop	4nm + 3m + n + 2m(2n - 1)
Compact dense	(2m + 1)(n + m + 1) + 2n + 13(40m^3 + 90m^2 + 122m) + (2n - 1)(m + 1)

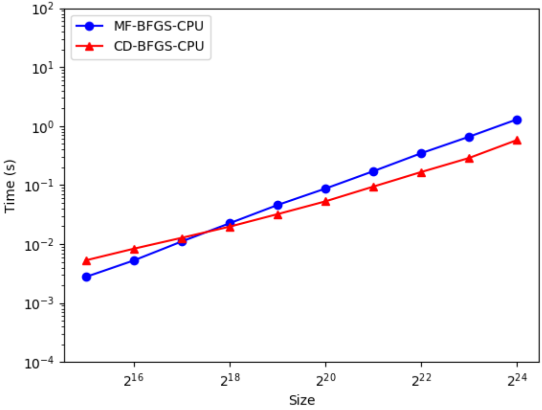
Outline

Compact Dense L-BFGS



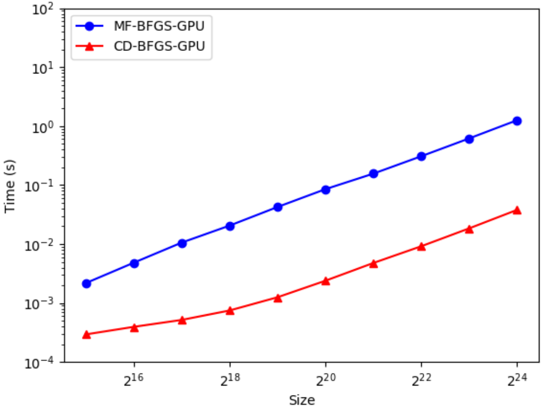
Computing $H_k z$ with the compact dense representation

Head-to-Head (CPU)



Compact dense vs. two-loop $H_k z$ calculation on the CPU

Head-to-Head (GPU)



Compact dense vs. two-loop $H_k z$ calculation on the GPU

What's the catch?

$H_k z$ calculation does not include the cost of updating S_k and Y_k matrices with new iterate information

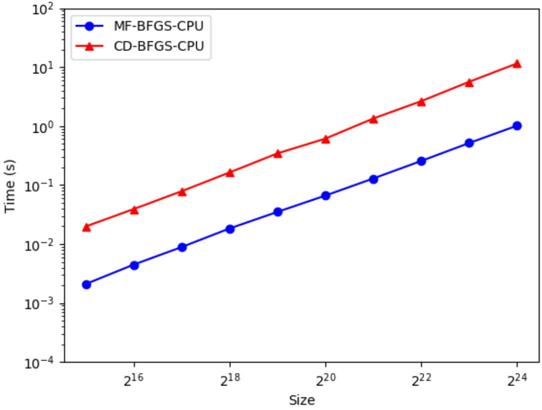
Matrix-free Two-loop BFGS:

- Store S_k and Y_k as array of vectors
- Vectors indexes for $i \geq k$ never used
- Reassign pointers to shift vectors when $k = m$

Compact Dense BFGS:

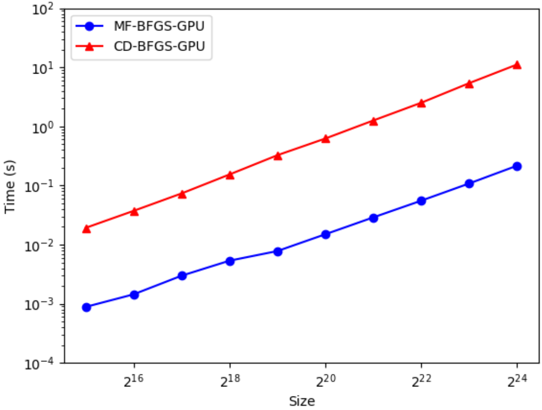
- Resize S_k and Y_k matrices when $k < m$
- Shift matrix columns when $k = m$
- Avoiding resizing/shifting requires custom mat-vec kernel

S_k and Y_k updates are not trivial!



Compact dense vs. two-loop updates on the CPU

S_k and Y_k updates are NOT trivial!



Compact dense vs. two-loop updates on the GPU

Outline

Observations

Compact dense BFGS might take better advantage of GPUs than the matrix-free two-loop algorithm when computing $H_k z$

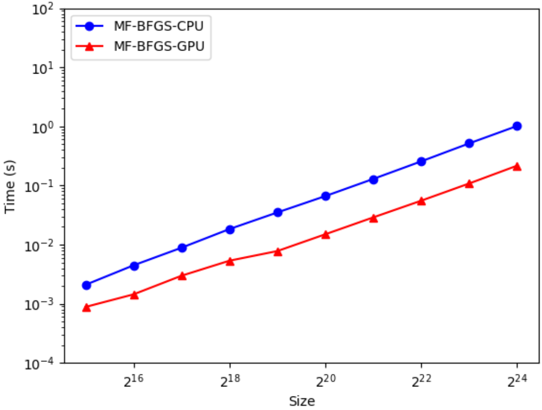
Future Work:

- Changing size of S_k and Y_k pose some implementation challenges – need to write dedicated kernel instead of using high-level interfaces
- Matrix algebra needs to be inspected carefully to avoid unnecessary CPU-GPU copy operations
- Lack of `MATMPIDENSECUDA` in PETSc means dense S_k and Y_k has to use `MATMPIAIJCUSPARSE` and incur overhead cost
- More profiling in HPC environments (ORNL Summit)

References:

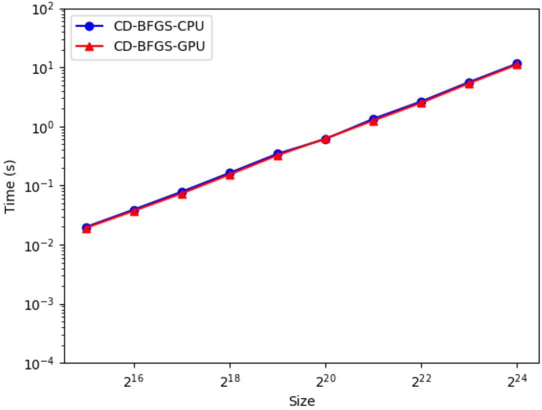
- Erway, Jennifer B., and Roummel F. Marcia. "On solving large-scale limited-memory quasi-Newton equations." Linear Algebra and its Applications 515 (2017): 196-225.
- Byrd, Richard H., Jorge Nocedal, and Robert B. Schnabel. "Representations of quasi-Newton matrices and their use in limited memory methods." Mathematical Programming 63.1-3 (1994): 129-156.

MF-BFGS Updates



Updating matrix-free BFGS with new s_k and y_k vectors

CD-BFGS Updates



Updating the S_k and Y_k matrices for compact dense BFGS