Experimenting Iterative Methods for Inverse Problems at Low Precision Levels

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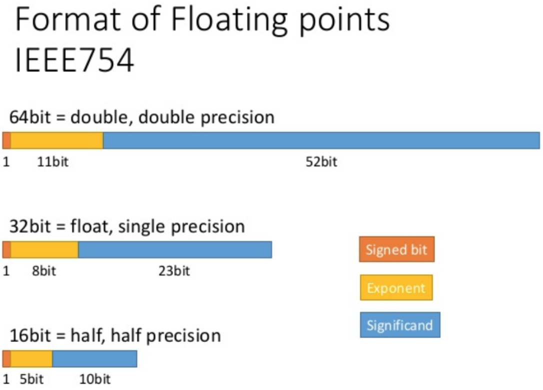
Outline

1. Chop
2. CGLS
3. Experiment

Chop: Overview

A closer look at double, single, fp16 precision:



[1]

[1] *Using tensor cores for mixed-precision scientific computing*. Oct-2021. URL: https://developer.nvidia.com/blog/tensor-cores-mixed-precision-scientific-computing/

Chop: Overview

- Simulate low-precision arithmetics
- Need to chop each operation

```
options.format = 'fp16';
chop([],options);

x = chop(x);
y = chop(y);
z = chop(z);
s = chop(x + chop(y * z));
```

```
options.format = 'c';
options.params = [11,23]
chop([],options);
```

Chop: Blocking

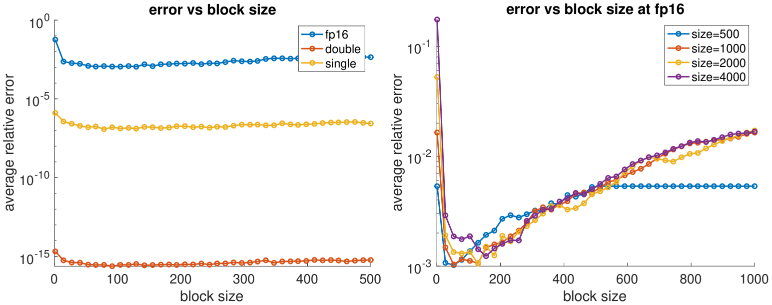
- Break an inner product into several smaller inner products
- Compute them independently and then sum

```
x = [x1, x2, x3, x4, x5, x6]
y = [y1, y2, y3, y4, y5, y6]

x_1 = [x1, x2, x3]
y_1 = [y1, y2, y3]

x_2 = [x4, x5, x6]
y_2 = [y4, y5, y6]
```

Chop: Blocking



Chop in Action

Matrix-vector multiplication:

```
function C = mv_blocked(X,y,block_size)
%
% compute the product of a matrix and a vector with chop
%

A = chop(chop(X).*chop(y'));

if nargin < 3
    block_size = 256; % default block size
end

[m, n] = size(X);

k = floor(n/block_size);
C = zeros(m,1);

for i = 1:k
    a=zeros(m,1);
    for j = (i-1)*block_size+1 : i*block_size
        a = chop(a+A(:,j));
    end
    C = chop(C + a);
end

if n-k*block_size ~= 0
    b=zeros(m,1);
    for i = k*block_size+1:n
        b = chop(b+ A(:,i));
    end
    C = chop(C + b);
end
```

```
Instead of:
a = chop(a+chop(chop(X(:,j))*chop(y(j))));
```

CGLS: Overview

- Conjugate Gradient Method: Solve $Ax = b$ for SPD matrices
- CGLS:
  - Generalize to all the matrices
  - A $\rightarrow$A^{T}A, b $\rightarrow$A^{T}b without explicitly calculating A^TA

CGLS: Our Modification

Chop each operation! :)

ALGORITHM 7.4.1. CGLS. Let $x^{(0)}$ be an initial approximation, set

$$r^{(0)} = b - Ax^{(0)}, \quad p^{(0)} = s^{(0)} = A^T r^{(0)}, \quad \gamma_0 = \|s^{(0)}\|_2^2,$$

and for $k = 0, 1, 2, \dots$ while $\gamma_k > tol$ compute

$$\begin{aligned} q^{(k)} &= Ap^{(k)}, \\ \alpha_k &= \gamma_k / \|q^{(k)}\|_2^2, \\ x^{(k+1)} &= x^{(k)} + \alpha_k p^{(k)}, \\ r^{(k+1)} &= r^{(k)} - \alpha_k q^{(k)}, \\ s^{(k+1)} &= A^T r^{(k+1)}, \\ \gamma_{k+1} &= \|s^{(k+1)}\|_2^2, \\ \beta_k &= \gamma_{k+1}/\gamma_k, \\ p^{(k+1)} &= s^{(k+1)} + \beta_k p^{(k)}. \end{aligned}$$

```
Ax = mv_blocked(A, x);normr2 = vv_blocked(d(:),d(:))
d = mv_blocked(A', b);
d = chop(d - mv_blocked(A', Ax));
normr2 = vv_blocked(d(:),d(:));

Ad = mv_blocked(A, d);
alpha = chop(normr2/normAd2);
x  = chop(x + chop(alpha*d));
r  = chop(r - chop(alpha*Ad));
s  = mv_blocked(A', r);
q = s; normr2_new = vv_blocked(q,q);
beta = chop(normr2_new/normr2);
d = chop(s + chop(beta*d));
```

[2]

[2] Åke Björck. *Numerical methods for least squares problems.* SIAM, 1996

Experiment: Image Deblurring (no noise)

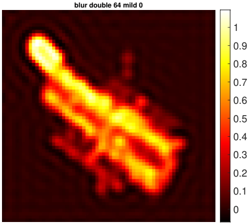


Figure: Double precision problem size 64 with mild blurring.

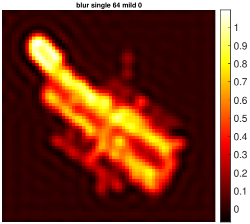


Figure: Single precision problem size 64 with mild blurring.

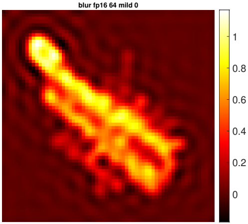


Figure: Half (fp16) precision problem size 64 with mild blurring.

Experiment: Image Deblurring (no noise)

-The error norm:

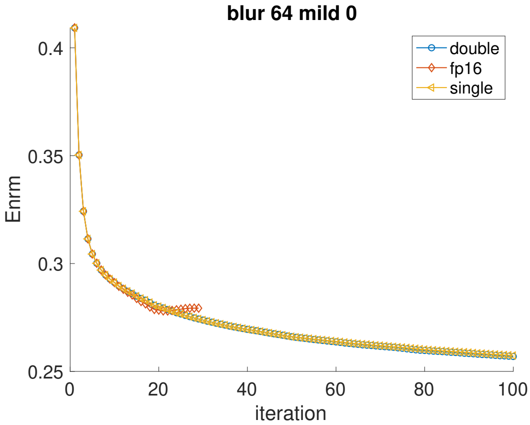


Figure: The error norm of a size 64 problem with mild blurring of different precisions.

Experiment: Image Deblurring (with noise)

-Single

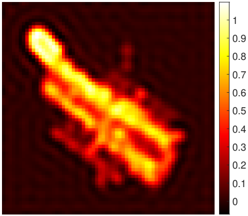


Figure: Single precision, problem size 64 with mild blurring and 0.1% noise.

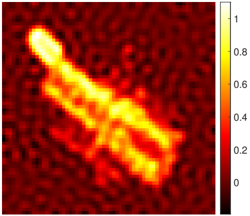


Figure: Single precision, problem size 64 with mild blurring and 1% noise.

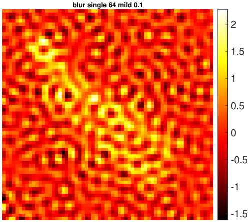


Figure: Single precision, problem size 64 with mild blurring and 10% noise.

Experiment: Image Deblurring (with noise)

-Half

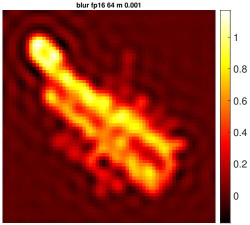


Figure: Half precision, problem size 64 with mild blurring and 0.1% noise.

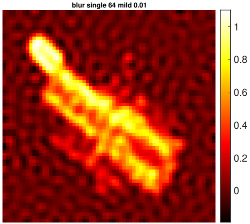


Figure: Half precision, problem size 64 with mild blurring and 1% noise.

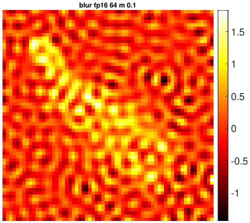


Figure: Half precision, problem size 64 with mild blurring and 10% noise.

Experiment: Image Deblurring (with noise)

- Error norm

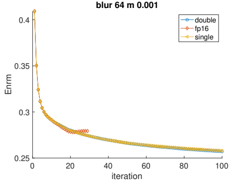


Figure: Error norm for problem size 64 with mild blurring and 0.1% noise.

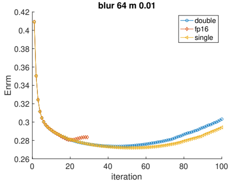


Figure: Error norm for problem size 64 with mild blurring and 1% noise.

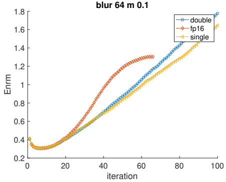


Figure: Error norm for problem size 64 with mild blurring and 10% noise.

Experiment: Tomography (no noise)

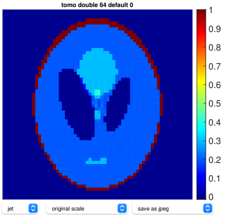


Figure: Double precision problem size 64 with default blurring.

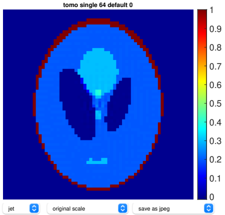


Figure: Single precision problem size 64 with default blurring.

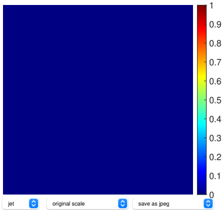


Figure: Half (fp16) precision problem size 64 with default blurring.

Experiment: Tomography (no noise)

- Why?

- NaNs!

ALGORITHM 7.4.1. CGLS. Let $x^{(0)}$ be an initial approximation, set

$$r^{(0)} = b - Ax^{(0)}, \quad p^{(0)} = s^{(0)} = A^T r^{(0)}, \quad \gamma_0 = \|s^{(0)}\|_2^2,$$

and for $k = 0, 1, 2, \ldots$ while $\gamma_k > tol$ compute

$$\begin{aligned}
q^{(k)} &= Ap^{(k)}, \\
\alpha_k &= \gamma_k / \|q^{(k)}\|_2^2, \\
x^{(k+1)} &= x^{(k)} + \alpha_k p^{(k)}, \\
r^{(k+1)} &= r^{(k)} - \alpha_k q^{(k)}, \\
s^{(k+1)} &= A^T r^{(k+1)}, \\
\gamma_{k+1} &= \|s^{(k+1)}\|_2^2, \\
\beta_k &= \gamma_{k+1} / \gamma_k, \\
p^{(k+1)} &= s^{(k+1)} + \beta_k p^{(k)}.
\end{aligned}$$

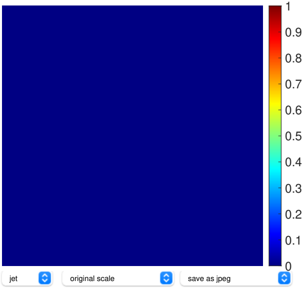
[3]

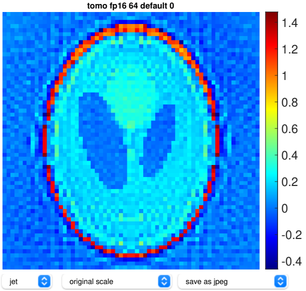
γ becomes Inf, there is an overflow.

[3] Björck, *Numerical methods for least squares problems*

Experiment: Tomography (no noise)

Our solution: A $\rightarrow A/100, b \rightarrow b/100$





Experiment: Tomography

- Error norm:

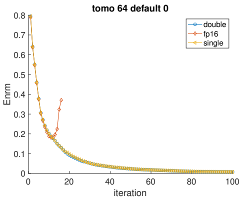


Figure: Error norm of size 64 problem with 0 noise at different precision level.

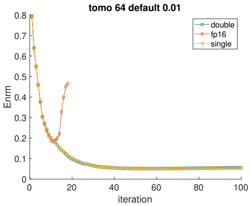


Figure: Error norm of size 64 problem with 1% noise at different precision level.

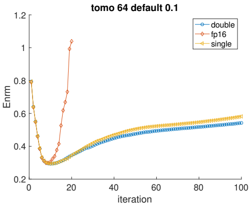


Figure: Error norm of size 64 problem with 10% noise at different precision level.

Experiment: Tomography (with noise)

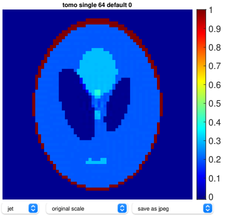


Figure: Single precision problem size 64 with zero noise.

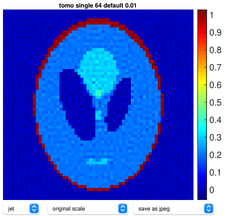


Figure: Single precision problem size 64 with 1% noise.

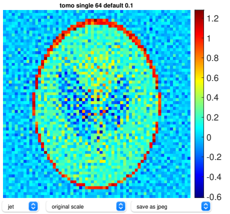


Figure: Single precision problem size 64 with 10% noise.

Experiment: Tomography (some interesting cases)

- γ becomes Inf in the original problem, the overflow results in NaNs from the first iteration
- After we divide both A and b by 10, $||q||_2^2$=Inf, $\alpha = x = 0$ in the first iteration. Later no underflow or overflow occurs, yet plot is always blur

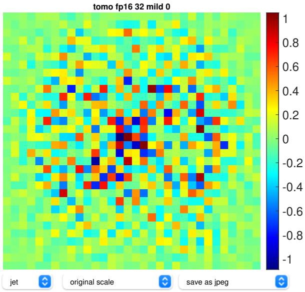


Figure: fp16 problem size 32 with zero noise

Experiment: Tomography (some interesting cases)

ALGORITHM 7.4.1. CGLS. Let $x^{(0)}$ be an initial approximation, set

$$r^{(0)} = b - Ax^{(0)}, \quad p^{(0)} = s^{(0)} = A^T r^{(0)}, \quad \gamma_0 = \|s^{(0)}\|_2^2,$$

and for $k = 0, 1, 2, \ldots$ while $\gamma_k > tol$ compute

$$\begin{aligned} q^{(k)} &= Ap^{(k)}, \\ \alpha_k &= \gamma_k / \|q^{(k)}\|_2^2, \\ x^{(k+1)} &= x^{(k)} + \alpha_k p^{(k)}, \\ r^{(k+1)} &= r^{(k)} - \alpha_k q^{(k)}, \\ s^{(k+1)} &= A^T r^{(k+1)}, \\ \gamma_{k+1} &= \|s^{(k+1)}\|_2^2, \\ \beta_k &= \gamma_{k+1}/\gamma_k, \\ p^{(k+1)} &= s^{(k+1)} + \beta_k p^{(k)}. \end{aligned}$$

[4]

$||q||_2^2$=Inf, $\alpha = x = 0$ in the first iteration.

[4] Björck, *Numerical methods for least squares problems*

Experiment: Tomography (some interesting cases)

- γ becomes Inf in the original problem, the overflow results in NaNs from the first iteration
- We set $A \to A/100$, and $b \to b/100$. This is the last iteration with all Inf and -Infs before NaN occurs.

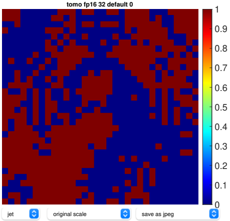


Figure: fp16 problem size 32 with default blur and zero noise, 14th iteration

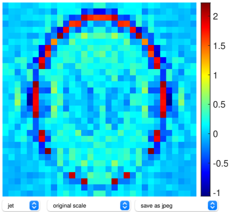


Figure: fp16 problem size 32 with default blur and zero noise, 13th iteration

Where We Will Go Next...

- Run experiments of larger sizes
- Implement other iterative methods that avoid inner products to eliminate NaNs

Bibliography

- Björck, Åke. *Numerical methods for least squares problems*. SIAM, 1996.
- *Using tensor cores for mixed-precision scientific computing*. Oct-2021. URL: https://developer.nvidia.com/blog/tensor-cores-mixed-precision-scientific-computing/.