Lecture 8: Fast Linear Solvers (Part 5)

Conjugate Gradient (CG) Method

- Solve Ax = b with A being an $n \times n$ symmetric positive definite matrix.
 - proposed by Hestenes and Stiefel in 1951
- Define the quadratic function

$$\phi(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T A \mathbf{x} - \mathbf{x}^T \mathbf{b}$$

Suppose x minimizes $\phi(x)$, x is the solution to Ax = b.

- $\nabla \phi(\mathbf{x}) = \left(\frac{\partial \phi}{\partial x_1}, \dots, \frac{\partial \phi}{\partial x_n}\right) = A\mathbf{x} \mathbf{b}$
- The iteration takes form $\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \alpha_k \mathbf{v}^{(k)}$ where $\mathbf{v}^{(k)}$ is the search direction and α_k is the step size.
- Define $r^{(k)} = b Ax^{(k)}$ to be the residual vector.

• Let x and $v \neq 0$ $\phi(x + \alpha v)$ be fixed vectors and α a real number variable.

Define:

$$h(\alpha) = \phi(\mathbf{x} + \alpha \mathbf{v}) = \phi(\mathbf{x}) + \alpha < \mathbf{v}, A\mathbf{x} - \mathbf{b} > + \frac{1}{2}\alpha^2 < \mathbf{v}, A\mathbf{v} >$$

 $h(\alpha)$ has a minimum when $h'(\alpha) = 0$. This occurs when

$$\hat{\alpha} = \frac{\boldsymbol{v}^T(\boldsymbol{b} - A\boldsymbol{x})}{\boldsymbol{v}^T A \boldsymbol{v}}.$$

So
$$h(\hat{\alpha}) = \phi(\mathbf{x}) - \frac{1}{2} \frac{(\mathbf{v}^T (\mathbf{b} - A\mathbf{x}))^2}{\mathbf{v}^T A \mathbf{v}}$$
.

Suppose x^* is a vector that minimizes $\phi(x)$. So $\phi(x + \hat{\alpha}v) \ge \phi(x^*)$. This implies $v^T(b - Ax^*) = 0$. Therefore $b - Ax^* = 0$.

- For any $v \neq 0$, $\phi(x + \alpha v) > \phi(x)$ unless $v^T(b Ax) = 0$ with $\alpha = \frac{v^T(b Ax)}{v^T Av}$.
- How to choose the search direction v?
 - Method of steepest descent: $v = r = -\nabla \phi(x)$
 - Remark: Slow convergence for linear systems

Algorithm.

Let $x^{(0)}$ be initial guess.

for
$$k = 1, 2, ...$$

$$v^{(k)} = b - Ax^{(k-1)}$$

$$\alpha_k = \frac{\langle v^{(k)}, (b - Ax^{(k-1)}) \rangle}{\langle v^{(k)}, Av^{(k)} \rangle}$$

$$x^{(k)} = x^{(k-1)} + \alpha_k v^{(k)}$$

end

Steepest descent method when $\frac{\lambda_{max}}{\lambda_{min}}$ is large

• Consider to solve
$$Ax = b$$
 with $A = \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix}$,

$$\boldsymbol{b} = \begin{bmatrix} \lambda_1 \\ \lambda_2 \end{bmatrix}$$
 and the start vector $\boldsymbol{v} = \begin{bmatrix} -9 \\ -1 \end{bmatrix}$.

Reduction of $||Ax^{(k)} - b||_2 < 10^{-4}$.

- With $\lambda_1 = 1$, $\lambda_2 = 2$, it takes about 10 iterations
- With $\lambda_1 = 1$, $\lambda_2 = 10$, it takes about 40 iterations

- Second approach to choose the search direction \boldsymbol{v} ?
 - A-orthogonal approach: use a set of nonzero direction vectors $\{\boldsymbol{v}^{(1)},...,\boldsymbol{v}^{(n)}\}$ that satisfy $<\boldsymbol{v}^{(i)},A\boldsymbol{v}^{(j)}>=0$, if $i\neq j$. The set $\{\boldsymbol{v}^{(1)},...,\boldsymbol{v}^{(n)}\}$ is called A-orthogonal.
- Theorem. Let $\{v^{(1)}, \dots, v^{(n)}\}$ be an A-orthogonal set of nonzero vectors associated with the symmetric, positive definite matrix A, and let $\boldsymbol{x}^{(0)}$ be arbitrary. Define $\alpha_k = \frac{\langle v^{(k)}, (\boldsymbol{b} A\boldsymbol{x}^{(k-1)}) \rangle}{\langle v^{(k)}, A\boldsymbol{v}^{(k)} \rangle}$ and $\boldsymbol{x}^{(k)} = \boldsymbol{x}^{(k-1)} + \alpha_k \boldsymbol{v}^{(k)}$ for $k = 1, 2 \dots n$. Then $A\boldsymbol{x}^{(n)} = \boldsymbol{b}$ when arithmetic is exact.

Conjugate Gradient Method

- The conjugate gradient method of Hestenes and Stiefel.
- Main idea: Construct $\{ \pmb{v}^{(1)}, \pmb{v}^{(2)} \dots \}$ during iteration so that $\{ \pmb{v}^{(1)}, \pmb{v}^{(2)} \dots \}$ are A-orthogonal.
- Define:

$$K_k(A, \mathbf{r}^{(0)}) = span\{\mathbf{r}^{(0)}, A\mathbf{r}^{(0)}, A^2\mathbf{r}^{(0)}, \dots, A^{k-1}\mathbf{r}^{(0)}\}.$$

- Lemma (Kelly). Let A be spd and let $\{x^{(k)}\}$ be CG iterates, then $r_k^T r_l = 0$ for all $0 \le l < k$.
 - Remark: let $\{x^{(k)}\}$ be CG iterates. $r_l \in K_k$ for all l < k.
- **Lemma** (Kelly). Let A be spd and let $\{x^{(k)}\}$ be CG iterates. If $x^{(k)} \neq x^*$, then $x^{(k+1)} = x^{(k)} + \alpha_{k+1}v^{(k+1)}$ and $v^{(k+1)}$ is determined up to a scalar multiple by the conditions $v^{(k+1)} \in K_{k+1}$, $(v^{(k+1)})^T A \xi = 0$ for all $\xi \in K_k$.
 - Remark: This implies $\boldsymbol{v}^{(k+1)} = \boldsymbol{r}^{(k)} + \boldsymbol{w}^{(k)}$ with $\boldsymbol{w}^{(k)} \in K_k$

- Theorem (Kelly). Let A be spd and assume that $r^{(k)} \neq 0$. Define $v^{(0)} = 0$. Then $v^{(k+1)} = r^{(k)} + \beta_{k+1}v^{(k)}$ for some β_{k+1} and $k \geq 0$.
 - Remark (1): $v^{(k+1)} \cdot Ar^{(k-1)} = 0 = r^{(k)} \cdot Ar^{(k-1)} + \beta_{k+1}v^{(k)} \cdot Ar^{(k-1)}$
 - Remark (2): $\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \alpha_{k+1} \mathbf{v}^{(k+1)}$ implies $\mathbf{r}^{(k+1)} = \mathbf{r}^{(k)} \alpha_{k+1} A \mathbf{v}^{(k+1)}$, which leads to $\mathbf{r}^{(k)} \cdot A \mathbf{v}^{(k+1)} = \mathbf{r}^{(k)} \cdot \mathbf{r}^{(k)} / \alpha_{k+1} \neq 0$

• **Lemma** (Kelly). Let A be spd and assume that $r^{(k)} \neq 0$. Then

$$\alpha_k = \frac{\langle r^{(k-1)}, r^{(k-1)} \rangle}{\langle v^{(k)}, Av^{(k)} \rangle}$$

And

$$\beta_k = \frac{\langle r^{(k)}, r^{(k)} \rangle}{\langle r^{(k-1)}, r^{(k-1)} \rangle}$$

• Fact: Since $\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \alpha_{k+1} \mathbf{v}^{(k+1)}$, $\mathbf{r}^{(k+1)} = \mathbf{r}^{(k)} - \alpha_{k+1} A \mathbf{v}^{(k+1)}$.

Algorithm of CG Method

```
Let x^{(0)} be initial guess.
Set \mathbf{r}^{(0)} = \mathbf{b} - A\mathbf{x}^{(0)}: \mathbf{v}^{(1)} = \mathbf{r}^{(0)}.
for k = 1, 2, ...
       \alpha_k = \frac{\langle r^{(k-1)}, r^{(k-1)} \rangle}{\langle v^{(k)}, Av^{(k)} \rangle}
       \boldsymbol{x}^{(k)} = \boldsymbol{x}^{(k-1)} + \alpha_k \boldsymbol{v}^{(k)}
       \boldsymbol{r}^{(k)} = \boldsymbol{r}^{(k-1)} - \alpha_k A \boldsymbol{v}^{(k)} // construct residual
       \rho_k = \langle \boldsymbol{r}^{(k)}, \boldsymbol{r}^{(k)} \rangle
        if \sqrt{\rho_k} < \varepsilon exit. //convergence test
       S_k = \frac{\langle r^{(k)}, r^{(k)} \rangle}{\langle r^{(k-1)}, r^{(k-1)} \rangle}
       \boldsymbol{v}^{(k+1)} = \boldsymbol{r}^{(k)} + s_{\nu} \boldsymbol{v}^{(k)} // construct new search direction
end
```

Remarks

- Constructed $\{v^{(1)}, v^{(2)} \dots\}$ are pair-wise A-orthogonal.
- Each iteration, there are one matrix-vector multiplication, two dot products and three scalar multiplications.
- Due to round-off errors, in practice, we need more than n iterations to get the solution.
- If the matrix A is ill-conditioned, the CG method is sensitive to round-off errors (CG is not good as Gaussian elimination with pivoting).
- Main usage of CG is as iterative method applied to bettered conditioned system.

CG as Krylov Subspace Method

Theorem. $x^{(k)}$ of the CG method minimizes the function $\phi(x)$ with respect to the subspace

$$K_k(A, \boldsymbol{r}^{(0)}) =$$
 $span\{\boldsymbol{r}^{(0)}, A\boldsymbol{r}^{(0)}, A^2\boldsymbol{r}^{(0)}, \dots, A^{k-1}\boldsymbol{r}^{(0)}\}.$
I.e.

$$\phi(\mathbf{x}^{(k)}) = \min_{c_i} \phi(\mathbf{x}^{(0)} + \sum_{i=0}^{k-1} c_i A^i \mathbf{r}^{(0)})$$

The subspace $K_k(A, r^{(0)})$ is called Krylov subspace.

Error Estimate

- Define an energy norm $||\cdot||_A$ of vector \boldsymbol{u} with respect to matrix $A: ||\boldsymbol{u}||_A = (\boldsymbol{u}^T A \boldsymbol{u})^{1/2}$
- Define the (algebraic) error $e^{(k)} = x^{(k)} x^*$ where x^* is the exact solution.
- Theorem.

$$||\mathbf{x}^{(k)} - \mathbf{x}^*||_A \le 2(\frac{\sqrt{\kappa(A)} - 1}{\sqrt{\kappa(A)} + 1})^k ||\mathbf{x}^{(0)} - \mathbf{x}^*||_A \text{ with}$$

$$\kappa(A) = cond(A) = \frac{\lambda_{max}(A)}{\lambda_{min}(A)} \ge 1.$$

Remark: Convergence is fast if matrix A is well-conditioned.

Preconditioning

Let the symmetric positive definite matrix M be a preconditioner for A and $LL^T = M$ be its Cholesky factorization. $M^{-1}A$ is better conditioned than A (and not necessarily symmetric).

The preconditioned system of equations is

$$M^{-1}A\boldsymbol{x} = M^{-1}\boldsymbol{b}$$

or

$$L^{-T}L^{-1}Ax = L^{-T}L^{-1}b$$

where $L^{-T} = (L^T)^{-1}$.

Multiply with L^T to obtain

$$L^{-1}AL^{-T}L^T\boldsymbol{x} = L^{-1}\boldsymbol{b}$$

Define: $\widetilde{A} = L^{-1}AL^{-T}$; $\widetilde{\boldsymbol{x}} = L^T\boldsymbol{x}$; $\widetilde{\boldsymbol{b}} = L^{-1}\boldsymbol{b}$

Now apply CG to $\widetilde{A}\widetilde{x} = \widetilde{b}$.

Preconditioned CG for $M^{-1}Ax = M^{-1}b$

• Definition: Let A, M be spd. The M-inner product $<\cdot,\cdot>_M$ is said to be < x, $y>_M = < Mx$, $y> = x^T My$.

Fact:

- 1. $M^{-1}A$ is symmetric with respect to $<\cdot,\cdot>_M$, i.e., $< M^{-1}Ax$, $y>_M = < x$, $M^{-1}Ay>_M$
- 2. $M^{-1}A$ is positive definite with respect to $\langle \cdot, \cdot \rangle_M$, i.e., $\langle M^{-1}Ax, x \rangle_M > 0$ for all $x \neq 0$.
- We can apply the CG algorithm to $M^{-1}Ax = M^{-1}b$, replacing the standard inner product by the M-inner product.
 - Let r = b Ax. $z = M^{-1}r$. Then $\langle z, z \rangle_M = \langle r, z \rangle$ and $\langle M^{-1}Av, v \rangle_M = \langle Av, v \rangle$
 - Reference. Y. Saad. Iterative Methods for Sparse Linear Systems

Preconditioned CG Method

• Define $z^{(k)} = M^{-1}r^{(k)}$ to be the preconditioned residual. Let $x^{(0)}$ be initial guess. Set $\mathbf{r}^{(0)} = \mathbf{b} - A\mathbf{x}^{(0)}$: Solve $M\mathbf{z}^{(0)} = \mathbf{r}^{(0)}$ for $\mathbf{z}^{(0)}$ Set $v^{(1)} = z^{(0)}$ for k = 1.2... $\alpha_k = \frac{\langle z^{(k-1)}, r^{(k-1)} \rangle}{\langle v^{(k)}, av^{(k)} \rangle}$ $\boldsymbol{x}^{(k)} = \boldsymbol{x}^{(k-1)} + \alpha_{k} \boldsymbol{v}^{(k)}$ $\mathbf{r}^{(k)} = \mathbf{r}^{(k-1)} - \alpha_{\nu} A \mathbf{v}^{(k)}$ solve $M\mathbf{z}^{(k)} = \mathbf{r}^{(k)}$ for $\mathbf{z}^{(k)}$ $ho_k = <m{r}^{(k)},m{r}^{(k)}>$ if $\sqrt{\rho_k} < \varepsilon$ exit. //convergence test $S_k = \frac{\langle \mathbf{z}^{(k)}, \mathbf{r}^{(k)} \rangle}{\langle \mathbf{z}^{(k-1)}, \mathbf{r}^{(k-1)} \rangle}$

$$\boldsymbol{v}^{(k+1)} = \boldsymbol{z}^{(k)} + s_k \boldsymbol{v}^{(k)}$$

Split Preconditioner CG for $\widetilde{A}\widetilde{x} = \widetilde{b}$

- M is a Cholesky product.
- Define $\widehat{\boldsymbol{v}}^{(k)} = L^T \boldsymbol{v}^{(k)}$, $\widetilde{\boldsymbol{x}} = L^T \boldsymbol{x}$, $\widehat{\boldsymbol{r}}^{(k)} = L^T \boldsymbol{z}^{(k)} = L^T \boldsymbol{r}^{(k)}$, $\widetilde{A} = L^{-1} A L^{-T}$.
- Fact:
 - $< r^{(k)}, z^{(k)} > = < r^{(k)}, L^{-T}L^{-1}r^{(k)} > = < \hat{r}^{(k)}, \hat{r}^{(k)} >.$ $< Av^{(k)}, v^{(k)} > = < AL^{-T}\hat{v}^{(k)}, L^{-T}\hat{v}^{(k)} > = < \tilde{A}\hat{v}^{(k)}, \hat{v}^{(k)} >.$
 - With new variables, the preconditioned CG method solves $\widetilde{A}\widetilde{\boldsymbol{x}}=\widetilde{\boldsymbol{b}}$.

Split Preconditioner CG

Let $x^{(0)}$ be initial guess.

Set
$${m r}^{(0)}={m b}-A{m x}^{(0)}$$
; $\hat{m r}^{(0)}=L^{-1}{m r}^{(0)}$ and ${m v}^{(1)}=L^{-T}\hat{m r}^{(0)}$ for $k=1,2,...$

$$\begin{split} &\alpha_k = \frac{<\hat{r}^{(k-1)},\hat{r}^{(k-1)}>}{< v^{(k)},Av^{(k)}>} \\ &\boldsymbol{x}^{(k)} = \boldsymbol{x}^{(k-1)} + \alpha_k \boldsymbol{v}^{(k)} \\ &\hat{\boldsymbol{r}}^{(k)} = \hat{\boldsymbol{r}}^{(k-1)} - \alpha_k L^{-1} A \boldsymbol{v}^{(k)} \\ &\rho_k = <\boldsymbol{r}^{(k)},\boldsymbol{r}^{(k)}> \\ &\text{if } \sqrt{\rho_k} < \varepsilon \text{ exit.} \qquad //\text{convergence test} \\ &s_k = \frac{<\hat{r}^{(k)},\hat{r}^{(k)}>}{<\hat{r}^{(k-1)},\hat{r}^{(k-1)}>} \\ &\boldsymbol{v}^{(k+1)} = L^{-T}\hat{\boldsymbol{r}}^{(k)} + s_k \boldsymbol{v}^{(k)} \end{split}$$

end

Incomplete Cholesky Factorization

- Assume A is symmetric and positive definite. A is sparse.
- Factor $A = LL^T + R$, $R \neq \mathbf{0}$. L has similar sparse structure as A.

```
for k = 1, ..., n
   l_{kk} = \sqrt{a_{kk}}
   for i = k + 1, ..., n
      l_{ik} = \frac{a_{ik}}{l_{ik}}
       for j = k + 1, ..., n
         if a_{ij} = 0 then
             l_{ii} = 0
           else
              a_{ij} = a_{ij} - l_{ik}l_{kj}
           endif
        endfor
   endfor
endfor
```

Jacobi Preconditioning

In diagonal or Jacobi preconditioning

$$M = diag(A)$$

• Jacobi preconditioning is cheap if it works, i.e. solving $M\mathbf{z}^{(k)} = \mathbf{r}^{(k)}$ for $\mathbf{z}^{(k)}$ almost cost nothing.

References

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- M. J. Grote and T. Huckle, Parallel preconditioning with sparse approximate inverses, SIAM J. Sci. Comput. 18:838-853, 1997
- Y. Saad, Highly parallel preconditioners for general sparse matrices, G. Golub, A. Greenbaum, and M. Luskin, eds., *Recent Advances in Iterative Methods*, pp. 165-199, Springer-Verlag, 1994
- H. A. van der Vorst, High performance preconditioning, SIAM J. Sci. Stat. Comput. 10:1174-1185, 1989

Parallel CG Algorithm

 Assume a row-wise block-striped decomposition of matrix A and partition all vectors uniformly among tasks.

```
Let x^{(0)} be initial guess.
Set r^{(0)} = b - Ax^{(0)}; Solve Mz^{(0)} = r^{(0)} for z^{(0)}
Set v^{(1)} = z^{(0)}
for k = 1, 2, ...
    \boldsymbol{g} = A \boldsymbol{v}^{(k)}
                                           // parallel matrix-vector multiplication
    zr = <\mathbf{z}^{(k-1)} , \mathbf{r}^{(k-1)}> // parallel dot product by MPI_Allreduce
     \alpha_k = \frac{zr}{\langle v^{(k)}.q \rangle} // parallel dot product by MPI_Allreduce
    \boldsymbol{x}^{(k)} = \boldsymbol{x}^{(k-1)} + \alpha_k \boldsymbol{v}^{(k)}
    \mathbf{r}^{(k)} = \mathbf{r}^{(k-1)} - \alpha_k \mathbf{g}
                                         //
    solve M\mathbf{z}^{(k)} = \mathbf{r}^{(k)} for \mathbf{z}^{(k)} // Solve matrix system, can involve additional complexity
    \rho_k = < r^{(k)}, r^{(k)} >
                                  // MPI_Allreduce
    if \sqrt{\rho_k} < \varepsilon exit. //convergence test
    zr_n = \langle \mathbf{z}^{(k)}, \mathbf{r}^{(k)} \rangle // parallel dot product
    s_k = \frac{zr_n}{\pi}
    v^{(k+1)} = r^{(k)} + s_k v^{(k)}
```

end