

A FAST ALGORITHM FOR LEAST SQUARES PROBLEMS

Inner-Outer Iteration Method for Least Squares Problems

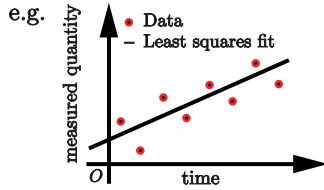
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WHAT FOR ?

- Survey
- Control
- Signal processing
- Statistical processing
- Image processing
- Optimization
- etc.



HOW ?

- Development of solvers for solving least squares problems
- Theoretical analysis of the property of the solvers
- Verification through numerical experiments

WHAT DO WE UNDERSTAND ?

Property of the solutions of least squares problems

$$\min_{\mathbf{x} \in \mathbb{R}^n} \|\mathbf{b} - A\mathbf{x}\|_2$$

where $A \in \mathbb{R}^{m \times n}$ is "large", i.e., find \mathbf{x} which minimizes $\|\mathbf{b} - A\mathbf{x}\|_2$

$$\min \left\| \begin{bmatrix} \mathbf{b} \\ -A \end{bmatrix} \begin{bmatrix} \mathbf{x} \end{bmatrix} \right\|_2 \quad \text{or} \quad \min \left\| \begin{bmatrix} \mathbf{b} \\ -A \end{bmatrix} \begin{bmatrix} \mathbf{x} \end{bmatrix} \right\|_2 \quad \text{nonzero element}$$

HOW IS IT RELATED TO US ?

For example...

- To determine the 3-D structure of protein molecules
- To determine the inner constitution of the earth from the analysis of seismic waves

WHY DO WE STUDY ?

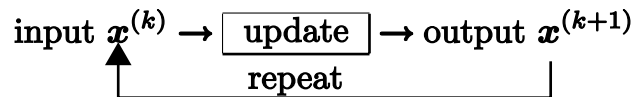
- To develop faster, more accurate, and more efficient methods for solving least squares problems
- To solve larger and larger, more and more ill-conditioned problems
- Theoretical understanding of the properties of the solvers

ITERATIVE METHOD

Iterative methods have advantages for large, sparse problems

The process is described as

1. Choose the initial solution \mathbf{x}_0
2. For $j = 1, 2, \dots$, Do
3. Update \mathbf{x}_j with an algorithm
4. EndDo



We should choose or have to develop **better algorithms** to achieve **faster**, more **robust**, and more **accurate** convergence

Krylov subspace iterative methods for linear systems use

$\mathcal{K}_m(A, \mathbf{r}_0) = \text{span} \{ \mathbf{r}_0, A\mathbf{r}_0, \dots, A^{m-1}\mathbf{r}_0 \}$ for $A \in \mathbb{R}^{n \times n}$ and initial residual $\mathbf{r}_0 = \mathbf{b} - A\mathbf{x}_0$

- The **generalized minimal residual** (GMRES) method minimizes $\|\mathbf{b} - A\mathbf{x}\|_2$ over the subspace $\text{span} \{ \mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_k \} = \mathcal{K}_m(A, \mathbf{r}_0)$, where $(\mathbf{v}_{j+1}, \mathbf{v}_i) = 0$ for $i = 1, 2, \dots, j$ and $(\mathbf{v}_{j+1}, \mathbf{v}_{j+1}) = 1$
- The **conjugate gradient** method for least squares problems (CGLS) applies the CG method to $A^T A \mathbf{x} = A^T \mathbf{b}$

NUMERICAL EXPERIMENTS

Table 1: Information of the matrices

| Problem | m | n | nnz | dens. [%] | rank | $\kappa(A)$ |
|-----------|---------|---------|-------------|-----------|--------|--------------------|
| Maragal-6 | 21, 251 | 10, 144 | 537, 694 | 0.25 | 8, 331 | 2.91×10^6 |
| Maragal-8 | 60, 845 | 33, 093 | 1, 308, 415 | 0.06 | - | - |

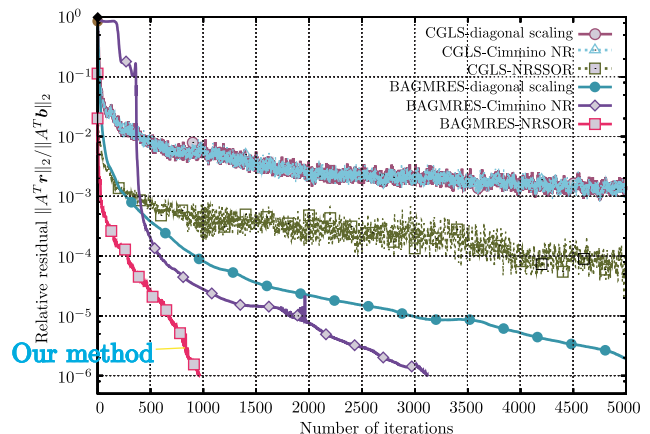
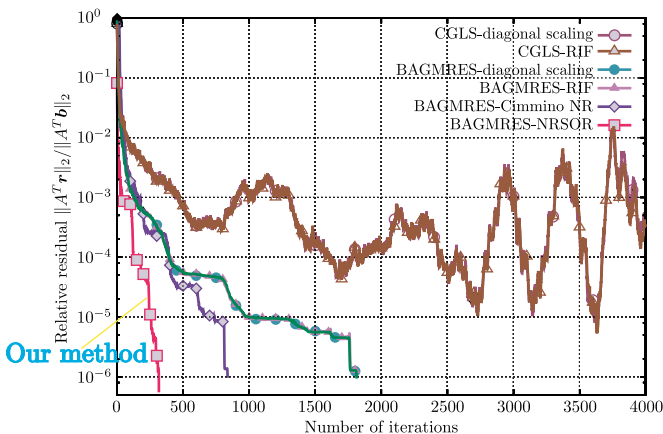


Figure 1: Convergence history of the relative residuals for Maragal-6 and -8

