Collection of Useful Problem Features

Science Challenge Project TZZT2019-B1.1

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Solving large-scale linear algebraic systems is a fundamental component of computer simulation of many science and engineering problems. Performance of linear solvers are largely affected by stage of evolution of physics, physical parameters, characteristics of discretization methods, requirement of accuracy, closeness to solution, limitation in computing resources, and so on. In this document, we discuss a few problem features (most of them are algebraic) which have been shown to be influential to the performance of linear solution methods [5, 2, 3, 7, 6, 4]. There is a paper discussing the issues about how to design meta data structures for storing this kind of features [1].

1 Simple properties

This is a set of parameters which can be obtained easily. They are related on problem size, number of nonzero entries, nonzero pattern of diagonal entries.

1.1 nrows : number of rows in the matrix.

1.2 block-size : integer size of blocks that comprise matrix block structure.

1.3 **nnz** : total number of structural nonzeros (could be zero) in the matrix [4].

1.4 **nnzeros** : number of nonzero elements in the matrix [4]?

1.5 nnzup : number of nonzeros in upper triangle.

1.6 nnzlow : number of nonzeros in lower triangle.

1.7 avg-nnzeros-per-row : average number of nonzero elements per row.

1.8 max-nnzeros-per-row : maximum number of nonzero elements per row.

1.9 **min-nnzeros-per-row** : minimum number of nonzero elements per row [4].

1.10 **nnzdia** : number of nonzero diagonal elements [4].

1.11 n-zero-diags : number of zero diagonals?

1.12 diag-zerostart : position of first zero element on the diagonal?

1.13 diag-definite : whether all diagonal elements are positive.

2 Structural properties

These parameters are matrix-structure related, including isolated rows, diagonal distribution, symmetry, bandwidth, etc.

2.1 n-dummy-rows : number of rows with only one element.

2.2 dummy-rows-kind : type of dummy rows (one, not-one, or not-on-diagonal).

2.3 ntdiags-ratio : the ratio of "true" to all diagonals? (Tan group)

2.4 avg-distfromdiag : average distance of nonzeros to the diagonal?

2.5 **avg-diag-dist** : average distance of nonzero diagonal to main diagonal [4]?

2.6 sigma-diag-dist : standard deviation of diag-dist?

2.7 symmetry : 1 for symmetric matrix, 0 otherwise.

2.8 n-struct-unsymm : number of structurally unsymmetric elements.

2.9 ratio-struc-symm : ratio of structural symmetric elements to total number of off-diagonal nonzero elements.

2.10 avg-unsymm-strength : how unsymmetrical the matrix is

$$\phi_{as} = \sqrt{\frac{\sum_{j\neq i}(\frac{a_{ij}-a_{ji}}{|a_{ij}|+|a_{ji}|})^2}{\#|\{(i,j) : a_{ij} \neq a_{ji}\}|}},$$

where $\#$ is the cardinality of a finite set.

2.11 max-unsymm-strength :

$$\psi_{as} = \max_{j\neq i} \frac{|a_{ij} - a_{ji}|}{|a_{ij}| + |a_{ji}|}.$$

2.12 row-ratio-sign-diag : ratio of the off-diagonal elements with the same sign as the diagonal one in the row sense

$$\frac{\#|\{(i,j) : a_{ij} \cdot a_{ii} > 0, i \neq j\}|}{\#|\{(i,j) : a_{ij} \neq 0, i \neq j\}|}.$$

2.13 col-ratio-sign-diag : ratio of the off-diagonal elements with the same sign as the diagonal one in the column sense

$$\frac{\#|\{(i,j) : a_{ij} \cdot a_{jj} > 0, i \neq j\}|}{\#|\{(i,j) : a_{ij} \neq 0, i \neq j\}|}.$$

2.14 left-bandwidth : left bandwidth number.

2.15 right-bandwidth : right bandwidth number.

2.16 upband : bandwidth in the upper triangle?

2.17 loband : bandwidth in the lower triangle?

2.18 avg-row-dist : avergage number of nonzeros per row (Tan group)

2.19 max-row-dist : maximal number of nonzeros per row (Tan group)

2.20 var-row-dist : variance of number of nonzeros per row (Tan group)

2.21 power-law : the factor of power-law distribution $P(k) \sim k^{-R}$ (Tan group)

3 Norm-related properties

These parameters are norms of the coefficient matrix or its symmetric part.

3.1 trace : sum of diagonal elements.

3.2 trace-abs : sum of absolute values of diagonal elements.

3.3 **norm1** : 1-Norm, maximum column sum of absolute element [4].

3.4 normInf : Infinity-Norm, maximum row sum of absolute element.

3.5 normF : Frobenius-norm, square-root of sum of elements squared.

3.6 symmetry-snorm : infinity norm of symmetric part $\frac{1}{2}(A + A^T)$.

3.7 symmetry-anorm : infinity norm of anti-symmetric part $\frac{1}{2}(A - A^T)$.

3.8 symmetry-fsnorm : Frobenius norm of symmetric part $\frac{1}{2}(A + A^T)$.

3.9 symmetry-fanorm : Frobenius norm of anti-symmetric part $\frac{1}{2}(A - A^T)$.

4 Spectral properties $\star$

The asymptotic convergence rate of iterative methods can be estimated by spectral radius and spectrum of the coefficient matrices. For non-normal matrices, numerical radius and field of values can be used instead. This set of parameters can usually be used to estimate potential convergence speed directly.

4.1 **est-cond-num** : estimated condition number [4].

4.2 n-ritz-values : number of stored Ritz values[1].

[1]Eigenvalue approximations from a subspace are known as Ritz values. The set of all possible Ritz values of a matrix from a one dimensional subspace known as the field of values or numerical range.

4.3 ritz-values-r : real parts of stored Ritz values.

4.4 ritz-values-c : complex parts of stored Ritz values.

4.5 ellipse-ax : size of x-axis of the enclosing ellipse of numerical range.

4.6 ellipse-ay : size of y-axis of the enclosing ellipse of numerical range.

4.7 ellipse-cx : x-coordinate of the center of the enclosing ellipse of numerical range.

4.8 ellipse-cy : y-coordinate of the center of the enclosing ellipse of numerical range.

4.9 positive-fraction : fraction of computed eigenvalues that has positive real part.

4.10 sigma-max : maximum singular value.

4.11 sigma-min : minimum singular value.

4.12 lambda-max-by-magnitude-re : real part of maximum lambda by magnitude[2].

4.13 lambda-max-by-magnitude-im : imaginary part of maximum lambda by magnitude.

4.14 lambda-min-by-magnitude-re : real part of minimum lambda by magnitude.

4.15 lambda-min-by-magnitude-im : imaginary part of minimum lambda by magnitude.

4.16 lambda-max-by-real-part-re : real part of maximum lambda by real-part[3].

4.17 lambda-max-by-real-part-im : imaginary part of maximum lambda by real-part.

5 Variability properties

5.1 **row-variability** : $\max_i \log_{10} \frac{\max_j |a_{ij}|}{\min_{j, a_{ij} \neq 0} |a_{ij}|}$ [4].

5.2 **col-variability** : $\max_j \log_{10} \frac{\max_i |a_{ij}|}{\min_{i, a_{ij} \neq 0} |a_{ij}|}$ [4].

5.3 diagonal-average : average value of absolute diagonal elements.

5.4 diagonal-variance : standard deviation of diagonal average.

5.5 diagonal-sign : indicator of diagonal sign pattern.

5.6 diagonal-dominance-row $\star$: least positive or most negative value of diagonal element minus sum of absolute off-diagonal elements by row, $\min_i\{a_{ii} - \sum_{j \neq i} |a_{ij}|\}$.

[2] Order eigenvalues by magnitude and take the real part of the maximum lambda

[3] Order eigenvalues by real part and take the real part of the maximum lambda

5.7 diagonal-dominance-col $\star$: least positive or most negative value of diagonal element minus sum of absolute off-diagonal elements by column, $\min_j\{a_{jj} - \sum_{i\neq j} |a_{ij}|\}$.

5.8 n-diagonal-dominance-row $\star$: number of diagonal dominant rows.

5.9 n-diagonal-dominance-col $\star$: number of diagonal dominant columns.

6 Multiscale properties [7, 6]

6.1 theta-multi-scale $\star$: A matrix $A = (a_{ij})_{n\times n} \in \mathbb{R}^{n\times n}$ is a *multi-scale* matrix if there exists an index i that satisfies

$$\min_{j\neq i, a_{ij}\neq 0} |a_{ij}| < \theta_c \cdot \max_{j\neq i} |a_{ij}|,$$

where θ_c is a threshold of the strength of connection. In the following, we use the notations:

- $N_i = \{j : a_{ij} \neq 0, j \neq i\}$ denotes the set of neighbors;
- $S_i = \{j \in N_i : |a_{ij}| \geq \theta_c \cdot \max_{k\neq i} |a_{ik}|\}$ denotes the set of strong dependence;
- $S_i^T = \{j \in N_i : i \in S_j\}$ denotes the set of strong influence;
- $W_i = \{j \in N_i : j \notin S_i\}$ denotes the set of weak dependence;
- $W_i^T = \{j \in N_i : i \in W_j\}$ denotes the set of weak influence.

6.2 n-row-ms : $n_{\mathrm{ms}}(\theta_c) = \#|\Omega_{\mathrm{ms}}|$, where $\Omega_{\mathrm{ms}} = \{i \in \Omega : W_i \neq \emptyset\}$.

6.3 ratio-row-ms : $n_{\mathrm{ms}}(\theta_c)/n$.

6.4 n-row-ai : $n_{\mathrm{ai}}(\theta_c) = \#|\Omega_{\mathrm{ai}}|$, where $\Omega_{\mathrm{ai}} = \{i \in \Omega_{\mathrm{ms}} : W_i \cap S_i^T \neq \emptyset\}$.

6.5 ratio-row-ai : $n_{\mathrm{ai}}(\theta_c)/n$.

6.6 overall-row-variability : a measurement of multiscale strength of rows

$$\psi := \lfloor \log_{10}(\max_i v_i) \rfloor, \qquad \text{where } v_i = \frac{\max_{j\neq i} |a_{ij}|}{\min_{j\neq i, a_{ij}\neq 0} |a_{ij}|}.$$

6.7 n-row-magnitudes : ϱ is the number of magnitude intervals

$$\{v_i, i = 1, \cdots, n\} \subseteq \cup_{l=1}^{\varrho} [10^{k_l}, 10^{k_l+1}).$$

6.8 closeness-row-magnitudes : ϕ reflects how close these magnitude intervals are

$$\phi = \begin{cases} 0, & \text{if } \varrho = 1, \\ \sum_{i=2}^{\varrho} (k_i - k_{i-1} - 1), & \text{otherwise.} \end{cases}$$

6.9 max-dist-magn-interval

$$\max_{k_l} |\{i : v_i \in [10^{k_l}, 10^{k_l+1})\}|.$$

6.10 min-dist-magn-interval

$$\min_{k_l} |\{i : v_i \in [10^{k_l}, 10^{k_l+1})\}|.$$

6.11 max-gap-dist-magn

$$\max_{i=2,\cdots,\varrho} \{k_i - k_{i-1}\}.$$

Remark 1 In practice, we also draw a threshold $\theta_p > 0$ into the actual calculation of ϱ and ϕ, with the purpose to omit the disturbance of $[10^{k_l}, 10^{k_l+1})$ if $n_l/n < \theta_p$, where n_l is the number of elements in $\{v_i, i = 1, \cdots, n\}$ scattered in that magnitude interval.

7 Physics-related properties

7.1 diffusion-coeff : magnitude of diffusion coefficient.

7.2 Reynolds : Reynolds number, the ratio of inertial forces to viscous forces.

7.3 Peclet : Peclet number, relative importance of advection versus diffusion.

References

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