A Genetic Algorithm for Matrix Bandwidth Reduction

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1 INTRODUCTION

A set of elementary reactions between time-dependent variables is randomly created. This set is also known as a kinetic mechanism. Due to its random nature, it can be seen that the associated Jacobian is generaly a sparse matrix lacking an ordered pattern. In this paper we report a genetic optimization procedure to find a variables ordering such that the Jacobian has minimum bandwidth. This problem is an NP-complete problem [1], therefore it is interesting in its own right, but its solution may have relevance to the problem of optimizing Gear's method in chemical kinetic problems.

2 GENETIC OPTIMIZATION

Genetic Algorithms (GA), as a global optimization procedure, has been increasingly used in a broad spectrum of areas in physics, chemistry and engineering. It searches efficiently and parallely in different regions of the space of solutions and seldom get trapped into local minima.

Next we describe the main implementation features of the GA used in the present work.

- **Chromosome Definition:** We used a vectors of natural numbers with a modification scheme to permit crossover and not have repetition (modified sequence representation).

- **Fitness Function:** In our problem the fitness function should give a measure of the sparsity matrix distribution. Since we focus on band-diagonalizing the system's Jacobian, the function should penalize nonzero elements far away the matrix diagonal and be a minimum when all nonzero matrix elements lie nearest to the main diagonal. A function satisfying such a requirement is:

$$f = \sum_{i,j} \mathcal{P}(|i - j|) \quad \text{where } \mathcal{P} \text{ is defined as:}$$

$$\mathcal{P}(k) = \begin{cases} 1 & \text{if } k = 0 \\ N + 1 & \text{if } k = 1 \\ (2N - 2k + 3)\mathcal{P}(k-1) & \text{if } k \geq 2 \end{cases}$$

- **Operators:** *Crossover* Given our chromosome definition we perform the crossover in the following way: generate a uniform random number that represents the crossing site and obtain two new chromosomes exchanging parts from the crossing site to the end. *Mutation.* We use four operators: exchange, inversion, left rotation and right rotation. These operators require that we define two random positions in the permutation. Both crossover and mutation satisfy GA operators requirements: Completeness and Soundness.

3 Results

In order to test the performance of our procedure we studied four random systems of increasing sizes ($N = 242$, $N = 347$, $N = 225$ and $N = 341$). Starting with a population of 50 strings and after 200 generations, the Jacobians transformed so in each case a narrow band is formed: respectively, 75, 145, 29 and 53 diagonals around the main diagonal (see *http://www.mor.itesm.mx/gecco/results.html).*

References

[1] D.S. Johnson M.R. Garey, R.L. Graham and D.E. Knuth, *Complexity results for bandwidth minimization*, SIAM Journal of Applied Mathematics 34 (1978), 477–495.