Closure to "Dealing With Zero Flows in Solving the Non-Linear Equations for Water Distribution Systems" by Sylvan Elhay and Angus R. Simpson October 2011,Vol 137, No. 10, pp. 1216-1224. **DOI:** 10.1061/(ASCE)HY.1943-7900.0000411

Sylvan Elhay* Angus R. Simpson†

The authors thank Profs. Kovalenko, Prokhorov, Gorev and Kodzhespirova for their interesting and insightful observations.

Extension of the regularization to cases where the full Jacobian is singular

All four correspondents make a useful (and nice) observation when they point out that the method can be extended to any case where the full Jacobian $\boldsymbol{J}$ is singular by virtue of the fact that there are more zero flows, n_z, than nodes, n_j, in the network. They might have argued as follows. The vector of required (correct) flows and heads $\boldsymbol{m}^* = \begin{pmatrix} \boldsymbol{q}^* \\ \boldsymbol{h}^* \end{pmatrix}$ is the solution to Eq (4) of the original paper. The Newton method finds $\boldsymbol{m}^*$ by solving Eq (10) using iteration. When the full Jacobian, on the left of Eq (10), is singular that system cannot be solved for the unique $\boldsymbol{m}^*$ that is sought even though that $\boldsymbol{m}^*$ may still exist. However, the matrix on the left of the regularized system in Eq (15) can always be made to be invertible (non-singular) by the appropriate choice of $\boldsymbol{T}$. Moreover, its solution is precisely the vector $\boldsymbol{m}^*$ which satisfies Eq (4).

The networks proposed by the four correspondents, all of which have $n_z > n_j$, are shown in Figs. 1–3. We did not investigate how well the regularization performs on those cases in Figs. 1–3 or any other cases where the full Jacobian is singular and we agree further investigation is warranted.

In order to apply the regularization to cases where $n_z > n_j$ the algorithm in the section of the original paper entitled "New Regularization Method for the Case of Zero Flows" should be changed by replacing its last paragraph by "Repeat steps 2 and 3 with $\sigma_{min}^{(m)}$ set in turn to $\sigma_{n_p-1}^{(m)}, \sigma_{n_p-2}^{(m)}, \ldots$ until exit occurs at step 3." i.e. where the last two sentences have been omitted.

Criteria for the applicability of the regularization

Profs. Kovalenko and Prokhorov, in discussing the applicability of the regularization technique, compare the performance of the regularization and that of EPANET and suggest that the performance of EPANET is better than that of regularization for some example networks. A key point here is that the Global Gardient Algorithm (GGA) of Todini & Pilati (1988), which is used in EPANET, cannot solve for the heads and flows of a network in which the head loss is modeled by the Hazen-Williams formula and there are zero flows. EPANET produces a solution for these cases by applying a strategy, described in the paper, that solves the wrong equations. This begs the question of what it means to compare the performance of the regularization technique and EPANET when there are zero flows. The regularization is applicable whenever the head loss is modeled by the Hazen-Williams formula and there are zero flows.

On the more general question of speed of convergence, the following can be said. The speed of convergence of a fixed point iteration (such as Netwon's method or the regularization of the GGA method of the original paper) is determined (Isaacson & Keller 1966, 111) by the behaviour of the partial derivatives of the iteration function in the vicinity of the fixed point which is sought and for each different network these differ. Estimates of the speed of convergence for a particular case can be found in terms of certain Lipschitz constants for that

*Visiting Research Fellow, School of Computer Science, University of Adelaide, South Australia, 5005.
†Professor, School of Civil, Environmental and Mining Engineering, University of Adelaide, South Australia, 5005.

case (see Isaacson & Keller (1966) for details) but finding these involves considerable effort.

Profs. Kovalenko and Prokhorov also mention the very real question of how one might distinguish (presumably a priori) between a network which will challenge the solver from one which will not. The regularization is intended to overcome a failure of the GGA and to optimize the bounds, given in Eq. (19) of the original paper, on the condition number of an important matrix in the process. The factor $cond_2(\boldsymbol{A}_1)$ in this bound is one indicator of how challenging the network will be to solve: if it is large then the results from the linear solver which determines the heads will be unreliable. But finding $cond_2(\boldsymbol{A}_1)$ requires computing the largest and smallest singular values of $\boldsymbol{A}_1$, a problem not without its own difficulties for large networks. To determine the condition of the problem (i.e. to find the sensitivity of the exact heads and flows solution to changes in the problem data) is a daunting problem that might be a good topic for future research.

Convergence error and error of the solution

Kovalenko and Prokhorov consider, in addition to the error measures used in the original paper, the quantities $\phi^\infty(\boldsymbol{q}^{(m)})$, ϕ^∞, $\|\rho\|_\infty$ and E_a. It is important to distinguish, as Kovalenko and Prokhorov do, between the quite different quantities that these measure: the first two measure the distance between successive iterates, the third measures the residual of a proposed solution and the fourth measures the difference between a proposed solution and the true solution. Unhappily, the difference between successive iterates is not necessarily a measure of the closeness of a proposed solution to the exact solution as the following example illustrates.

Example 1 Consider the solution of the non-linear equation $x = e^{x-\alpha}$. For $\alpha = 1$ the equation has exactly one solution at $x = 1$ which can be found, for example, by setting $x_0 = 0.9$ and applying the fixed point iteration $x_{j+1} = e^{x_j - \alpha}, \quad j = 0, 1, 2, \ldots$. Using the same iteration scheme with the same starting value but for the case $\alpha = 0.9999$ gives, after some early steps, the following iterates, rounded to five decimals, $x_{j-2} = 0.99977, x_{j-1} = 0.99987, x_j = 0.99997$. The difference between any two of these successive iterates is smaller in magnitude than 10^{-3} so a stopping test which terminated the iteration when $|x_j - x_{j-1}| \leq 10^{-3}$ might be thought to have found the solution to the equation. However, for $\alpha = 0.9999$, the equation has no solution, as can be easily verified. With a sufficient number of further iterations the process diverges. □

This example illustrates that, even when it is known that a solution exists, care should be exercised in interpreting the results for a problem which challenges the method. Although computable measures of the distance between a given iterate and the exact solution to a fixed point equation can sometimes be found they require bounds on certain derivatives which in this case may be too cumbersome, or perhaps even impossible, to find.

Using the residual measure, $\|\rho\|_\infty$, to decide when to terminate iteration also has its hazards. If one seeks only a solution with small residual then using the size of the residual makes sense. However, if one wants a solution which is close to the exact solution then using the residual can be misleading. The following example illustrates the problem.

Example 2 The 2-norm, defined for an n-vector by $\|\boldsymbol{z}\| = \sqrt{\sum_{k=1}^{n} |z_k|^2}$ (rather than the infinity norm used in the paper) will be used, with no loss of generality, in this example. Let

$$\boldsymbol{A} = \begin{pmatrix} 35223 & 42200 & 46527 \\ 5959 & 7140 & 7872 \\ 33406 & 40025 & 44129 \end{pmatrix}, \ \boldsymbol{b} = \begin{pmatrix} 123950 \\ 20971 \\ 117560 \end{pmatrix}, \ \boldsymbol{x}_1 = \begin{pmatrix} 1.3721 \\ -0.6604 \\ 0.6765 \end{pmatrix}, \text{ and } \boldsymbol{x}_2 = \begin{pmatrix} 1.6645 \\ -9.9706 \\ 10.4473 \end{pmatrix}.$$

Suppose the vectors $\boldsymbol{x}_1, \boldsymbol{x}_2$ are proposed as solutions to $\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}$. The exact solution to $\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}$ is easily seen to be $\boldsymbol{x}^* = (1, 1, 1)^T$ and so $\boldsymbol{x}_2$ is clearly further from the exact solution than $\boldsymbol{x}_1$ because $\|\boldsymbol{x}_2 - \boldsymbol{x}^*\| > \|\boldsymbol{x}_1 - \boldsymbol{x}^*\|$. However, the residuals of the two approximate solutions are, correctly rounded to four figures, $\|\boldsymbol{A}\boldsymbol{x}_1 - \boldsymbol{b}\| = 100,000$ and $\|\boldsymbol{A}\boldsymbol{x}_2 - \boldsymbol{b}\| = 1.732$: even though $\boldsymbol{x}_1$ is much closer to $\boldsymbol{x}^*$ than is $\boldsymbol{x}_2$, the residual of $\boldsymbol{x}_1$ is **five orders** of magnitude larger than that of $\boldsymbol{x}_2$. Thus, distance (or closeness) to the exact solution is not necessarily indicated by the size of the residual. However, a residual that is large is always an indication that the solution is not close to the exact solution. □

Thus, one cannot, in general, infer closeness to the exact solution from the size of the residual and so the recommendation in the original paper is that the residual test be used only to reject poor solutions. But the suggestion of Profs. Kovalenko and Prokhorov that both the flows and the heads should be used in deciding

when to stop an iteration has merit. It might be that the definition of ϕ^∞ should be extended so that iteration stops when both of the scale invariant versions of $\phi^\infty(\boldsymbol{q}^{(m)})$ and $\phi^\infty(\boldsymbol{h}^{(m)})$ are simultaneously smaller than preset tolerances:

$$\frac{\left\|\boldsymbol{q}^{(m+1)}-\boldsymbol{q}^{(m)}\right\|_\infty}{\left\|\boldsymbol{q}^{(m+1)}\right\|_\infty} \leq \epsilon_q, \text{ and } \frac{\left\|\boldsymbol{h}^{(m+1)}-\boldsymbol{h}^{(m)}\right\|_\infty}{\left\|\boldsymbol{h}^{(m+1)}\right\|_\infty} \leq \epsilon_h.$$

The different stopping tolerances are suggested in case the accuracies sought for the heads and flows are different.

A sufficient condition for the singularity of the Jacobian

The sufficient condition proposed by Profs. Gorev and Kodzhespirova gives a useful and more easily identified characterization of certain cases where the full Jacobian is singular. However, it cannot be, as Profs. Gorev and Kodzhespirova claim, more general than the condition given in the original paper which is both sufficient and necessary.

Profs. Gorev and Kodzhespirova also suggest that, for consistency, their changes to the matrix $\boldsymbol{G}$ should be applied. But, as was pointed out in the discussion by Profs. Kovalenko and Prokhorov, the regularization as it stands is applicable even when the full Jacobian is singular as a result of there being more zero flows than nodes in the network, $n_z > n_j$.

References

Isaacson, E. & Keller, H. (1966), *Analysis of numerical methods*, Wiley, New York.

Todini, E. & Pilati, S. (1988), *A gradient algorithm for the analysis of pipe networks.*, John Wiley and Sons, London, pp. 1–20. B. Coulbeck and O. Chun-Hou (eds).

LIST OF FIGURES

Fig. 1 . The first network in the discussion of Kovalenko and Prokhorov (non-zero demands at nodes 2 and 3 only; 9 pipes with zero flows).

Fig. 2. The second network in the discussion of Kovalenko and Prokhorov (non-zero demands at two nodes 6 and 7 only; 5 pipes with zero flows).

Fig. 3. The network in the discussion of Gorev and Kodzhespirova (non-zero demand at node 8 only; 9 pipes with zero flows)

Figure 1

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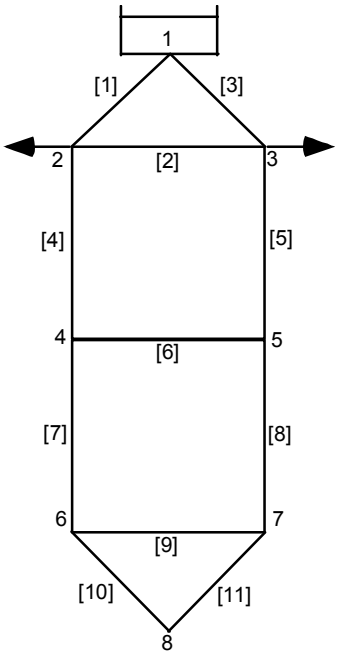

Figure 2

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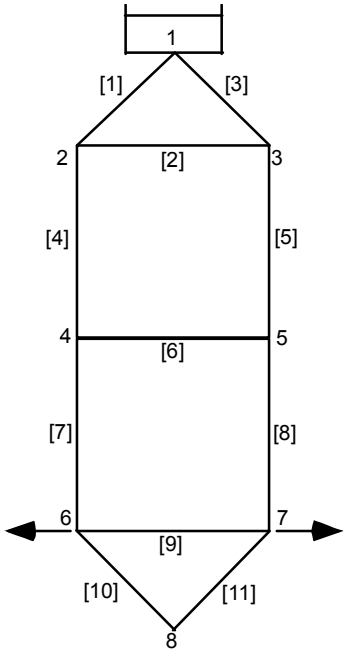

Figure 3

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