Independent Loops Search in Flow Networks Aiming for Well-Conditioned System of Equations

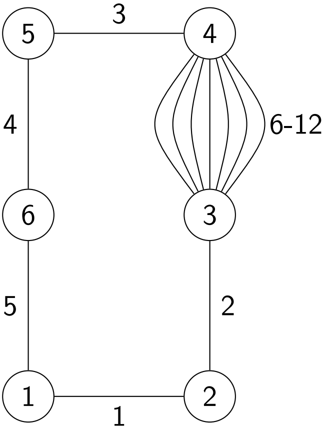
Jukka-Pekka Humaloja, Simo Ali-Löytty, Timo Hämäläinen and Seppo Pohjolainen

ECMI 2016

Outline

Introduction

- Consider a pipeflow network with m pipes and n nodes.
- In order to solve the flow rates in the pipes, we need to find a well-defined set of equations for them.
- The flow rates behave analogously to Kirchoff's circuit laws, i.e., flow into a node equals flow out, and the pressure loss over any closed loop equals zero.



Introduction

- We obtain n equations based on continuity of flow (flow in $=$ flow out), $n-1$ of which are linearly independent.
- Thus, we need to choose (at least) $m-n+1$ loops over which we compute the pressure losses.
- The pressure loss equations are nonlinear with respect to the flow rates, but they can be solved iteratively by solving a linearized version of them.
- Thus, we want to choose such $m-n+1$ loops that the resulting set of linear equations is well-conditioned.
- We will present ideas on how the loops should be chosen, and also, how can the condition of the equations be improved in general.

Concepts of Graph Theory

- In graph theory, a minimum set of edges that connect all the nodes is called a *spanning tree*.
- There are $n-1$ edges in the spanning tree, and the remaining $m-n+1$ edges are in the *cospanning tree*.
- When an edge from the cospanning tree is added to the spanning tree, a cycle (loop) is formed.
- By forming such cycle for every edge in the cospanning tree, we obtain a set of *fundamental cycles*.
- Since every fundamental cycle contains at least one unique edge, the set of fundamental cycles is linearly independent.
- Thus, the pressure loss loops have to be chosen to be a set of fundamental cycles to ensure linear independence.

How to Choose the Loops Optimally?

- Even though we know that the set of fundamental cycles gives a linearly independent set of loops, we do not know how well-conditioned the equations actually will be.
- Optimally we should find the set of fundamental cycles that is the most linearly independent.
- For PEEC problems, an algorithm that utilizes the topology of the circuit network has been presented by [Nguyen et al.] but such approach is problematic for pipeflow networks where the topology may differ significantly based on the application.
- Thus, we will resort to finding an excessive number of cycles in a network and aim to choose the ones that produce the best-conditioned equations.

Choosing the Best-Conditioned Submatrix

- The problem of choosing the loops optimally can be considered as choosing the best-conditioned submatrix, which is shown to be NP-hard in [Šrámek et al.].
- We will present the algorithm presented in [Šrámek et al.] and utilize it in our heuristics for choosing good loops.
- The main idea behind the heuristics is to choose such loops that the corresponding rows of A are as orthogonal as possible.
- Thus, the heuristics maximize $\mathrm{vol}(A) = \Pi_{i=1}^{m} \sigma_i$, whereas condition number is defined as $\mathrm{cond}(A) = \sigma_{\max}/\sigma_{\min}$.
- Maximal volume and minimal condition number are obtained when A is orthogonal, but in general these properties behave in a slightly different way.

SFVW Algorithm from [Šrámek et al.]

- Aim: find the best-conditioned $m \times m$ submatrix B of an $M \times m$ matrix A. ($M > m$)
- The heuristic repeats the following steps m times
  1. On the i:th step, find the row a_j of A that has the largest norm. Choose the row as the i:th row of B, i.e., $b_i = a_j$.
  2. For each row of A, Subtract its projection to b_i from itself, i.e., update the remaining rows a_k by $a_k = a_k - \langle a_k, b_i \rangle ||b_i||^{-2} b_i$.
- That is, on each step we choose the row of A most orthogonal to the previously chosen rows.
- Due to this criterion, the matrix B should be rather well-conditioned.
- The algorithm runs in $O(Mm^2)$.

Improving the Condition Number

- In addition to choosing the pressure loss loops such that the resulting linearized equations are well-conditioned, the condition number of the coefficient matrix can be improved by scaling.
- We will present three heuristics based on the SFVW algorithm for choosing the pressure loss loops.
- We will also consider scaling the rows of the coefficient matrix in order to improve its condition number.

Heuristic 1

- The SFVW algorithm can be used directly to find good loops.
- Firstly, generate a number of loops as the rows of A, e.g., by finding fundamental cycles with different spanning trees.
- Subtract the projection of A to B_0 from A, where B_0 contains the $n-1$ rows corresponding the continuity of flow equations, i.e, set $A = A - (B_0^T(B_0B_0^T)^{-1}B_0A^T)^T$.
- Use the SFVW algorithm to find a well-conditioned $m-n+1 \times m$ submatrix of A, which gives the choice of the required $m-n+1$ loops.

Heuristic 2

- Heuristic 2 can be described by the following steps:
  1. Generate a number of loops as the rows of A, and generate a random $m \times m$ matrix A_0.
  2. Find the row index j of A_0 that satisfies
  $$j = \max_{n \leq j \leq m} \sum_{k=1, k \neq j}^{m} |\langle a_{0j} ||a_{0j}||^{-1}, a_{0k} ||a_{0k}||^{-1} \rangle|$$
  and remove the row a_{0j} from A_0. Denote $\tilde{A}_0 = A_0 \setminus a_{0j}$.
  3. Compute the norm of the orthogonal component of a_{0j} to the rows of $\tilde{A}_0$, i.e., $r = ||a_{0j}^T - \tilde{A}_0^T (\tilde{A}_0 \tilde{A}_0^T)^{-1} \tilde{A}_0 a_{0j}^T||$.
  4. Find the row a_i of A that has norm-wise the largest orthogonal component to the rows of $\tilde{A}_0$.
  5. If $||a_i^T - \tilde{A}_0^T (\tilde{A}_0 \tilde{A}_0^T)^{-1} \tilde{A}_0 a_i^T|| > r$, swap a_{0j} and a_i and go to step 2, otherwise stop.

Heuristic 3

- Heuristic 3 combines the previous heuristics.
- Firstly, generate a number of loops as rows of A, and generate a random $m \times m$ matrix A_0.
- Compute $\sum_{k=1,k\neq j}^{m} |\langle a_{0j}||a_{0j}||^{-1}, a_{0k}||a_{0k}||^{-1}\rangle|$ for $n \leq j \leq m$. See for which rows the value is larger than the mean value and move them from A_0 to A. Denote $\tilde{A}_0 = A_0 \setminus A_{0,moved}$.
- Update A by $A = A - (\tilde{A}_0^T(\tilde{A}_0\tilde{A}_0^T)^{-1}\tilde{A}_0 A^T)^T$
- Use the SFVW algorithm to find a well-conditioned $N \times m$ submatrix of A that gives the choice of the N loops that replace the ones that were removed earlier.

Scaling the Equations

- Consider the linearized set of equations for the flow rates in the form $Ax = b$.
- Let the $n - 1$ first rows of A represent the continuity of flow equations, hence consisting of elements -1, 0 and 1.
- The rest of the rows represent the pressure loss loops, and the corresponding nonzero elements of A are of the scale $10^3 - 10^5$.
- Thus, the matrix A may be badly scaled and therefore badly conditioned.
- We will consider simple row scaling by a diagonal matrix S so that the equations become $SA = Sb$.

Scaling the Equations

- A heuristic given in [Golub & Van Loan, pp. 138–139] suggests that the scaling matrix S should be chosen such that every row of SA has approximately the same ∞-norm.
- Thus, if a_j denotes a row of A, a suitable choice for S would be, e.g., $S = \mathrm{diag}(||a_1||_\infty^{-1}, ||a_2||_\infty^{-1}, \ldots, ||a_m||_\infty^{-1})$ so that every row of SA has ∞-norm 1.
- We will also consider normalizing the rows of A with respect to the Euclidian (2-) norm.
- We will test the effect of scaling to the condition number of A in a few test cases.

Scaling the Equations

- The table below shows the average condition number of SA with different scalings S and the standard deviation for 100 different matrices A. The subindex of S refers to the norm and I is the identity matrix (no scaling).

S	Case 1 $m = 12, n = 6$	Case 2 $m = 618, n = 235$	Case 3 $m = 953, n = 78$
I	$(14.3 \pm 5.5) \cdot 10^3$	$(9.4 \pm 1.8) \cdot 10^5$	$(13.4 \pm 2.2) \cdot 10^5$
S_∞	17.6 ± 8.8	$(15.0 \pm 3.0) \cdot 10^3$	$(15.6 \pm 4.2) \cdot 10^3$
S_2	11.9 ± 4.2	$(12.2 \pm 2.7) \cdot 10^3$	$(7.7 \pm 2.4) \cdot 10^3$

- Scaling significantly reduces the condition number, and 2-norm seems to be more efficient than ∞-norm.

Choosing Loops for the Test Cases

- We consider choosing the pressure loss loops in the same test cases that we inspected the effect of scaling on.
- Since normalization with respect to 2-norm was found out to be effective, we will combine normalization with choosing the loops.
- We will perform the choosing of loops 100 times for each test case, and each time we generate a random initial matrix A_0 and approximately $10(m - n)$ additional loops.
- We will consider the mean values and standard deviations of numbers of iterations, computation times and obtained condition numbers for the heuristics over the 100 repetitions.

Case 1: 12 pipes, 6 nodes

	Heuristic 1	Heuristic 2	Heuristic 3
iterations	7	2.84 ± 1.58	3.18 ± 1.14
time (ms)	1.59 ± 0.26	0.76 ± 0.30	0.81 ± 0.31
cond(A)	7.11 ± 0.27	7.27 ± 0.21	7.26 ± 0.23
cond(A_0)	-	12.69 ± 4.16	12.69 ± 4.16

- All the heuristics produce virtually equal results and somewhat improve the condition number from the randomly chosen A_0.
- Computational times and the numbers of iterations are very low for all the heuristics due to the small size of the test case.

Case 2: 618 pipes, 235 nodes

	Heuristic 1	Heuristic 2	Heuristic 3
iterations	384	51.0 ± 31.8	216.7 ± 36.7
time (s)	30.6 ± 1.2	8.0 ± 4.8	19.0 ± 3.5
cond(A)	6905 ± 4228	7119 ± 3910	9332 ± 4437
cond(A_0)	-	12312 ± 3083	12312 ± 3083

- Heuristics 1 and 2 produce the best results and reduce the condition number of A_0 relatively as much as in Case 1, while Heuristic 2 is somewhat weaker
- Heuristic 2 performs almost as well as Heuristic 1 with much less computational effort.

Case 3: 953 pipes, 78 nodes

	Heuristic 1	Heuristic 2	Heuristic 3
iterations	876	???±???	???±???
time (s)	???±???	???±???	???±???
cond(A)	???±???	???±???	???±???
cond(A_0)	-	???±???	???±???

- Computation in progress...

Conclusions

- We considered improving the condition number of the coefficient matrix of a linearized set of equations.
- The inspected methods were choosing the pressure loss loops optimally and scaling the rows of the coefficient matrix.
- We found out that normalizing the rows with respect to 2-norm was more efficient than normalization with ∞-norm.
- Heuristic 1 appeared to produce best results when choosing the loops, but it was also required the most computation time.
- Heuristic 2 required much fewer iterations and less computation time than Heuristic 1 and still produced virtually the same results, so it can be considered the best option for choosing the pressure loss loops.

References

Golub, G. H. & Van Loan, C. F. Matrix Computations, 4th edition. The Johns Hopkins University Press, Baltimore, 2013. 756 p.

T.-S. Nguyen, J.-M. Guichon, O. Chadebec, G. Meunier, B. Vincent, An Independent Loops Search Algorithm for Solving Inductive PEEC Large Problems, *PIER M* **23**, 2013. pp. 53-63,

R. Šrámek, B. Fisher, E. Vicari, P. Widmayer, Optimal Transitions for Targeted Protein Quantification: Best Conditioned Submatrix Selection. Computing and Combinatorics, 15th Annual International Conference, COCOON 2009, Niagara Falls, NY, USA, July 13-15, 2009, Proceedings. pp. 287–296.

Thank you