Imperial College London

Non-linear inverse problems via sequential convex optimization

Filippo Pecci [1], Panos Parpas [2] and Ivan Stoianov [1]

[1]Department of Civil and Environmetal Engineering, Imperial College London

[2]Department of Computing, Imperial College London

Outline

- Inverse problem formulation
- Sequential Convex Optimization
- Application to fault estimation in water networks

System of non-linear equations

We consider a system governed by a set of non-linear equations:

$$F(x, \theta) = 0 \tag{1}$$

where $x \in \mathbb{R}^n$ represent system states and $\theta \in \Theta \subseteq \mathbb{R}^p$ the parameters.

- $F : \mathbb{R}^n \times \mathbb{R}^p \to \mathbb{R}^m$ continuously differentiable function
- For every $\theta \in \Theta$, there exist a unique $x(\theta)$ such that $F(x(\theta), \theta) = 0$, and we can compute it using simulation tools.
- Θ is a convex set.

Non-linear inverse problems

Objective: given some measurements of the system states, estimate parameters θ.

$$
\begin{aligned}
\underset{x,\theta}{\text{minimize}} \quad & l(x) + g(\theta) \\
\text{subject to} \quad & F(x,\theta) = 0 \\
& \theta \in \Theta
\end{aligned}
\tag{2}
$$

where $l : \mathbb{R}^n \to \mathbb{R}$ is a convex loss function, and $g : \mathbb{R}^p \to \mathbb{R}$ is a convex regularizer.

Some examples

- Examples of convex loss functions include:
  - $l(x) = \|Ax - b\|_2^2$ (least squares)
  - $l(x) = \|Ax - b\|_1$ (robust estimation)
  - $l(x) = \|Ax - b\|_\infty$ (Chebyshev approximation)
  - $l(x) = \sum_{i=1}^{m} \psi_{\text{hub}}((Ax - b)_i)$, with

$$\psi_{\text{hub}}(z) = \begin{cases} z^2 & |z| \leq M \\ M(2|z| - M) & |z| > M \end{cases}$$

    (Huber loss function)
  - others: deadzone linear, log barrier...
- Examples of convex regularization functions include:
  - $g(\theta) = \|\theta\|_2^2$ (Tikhonov)
  - $g(\theta) = \|\theta\|_1$ (Lasso)
  - ...

Problem reformulation

Let $\phi : \mathbb{R}^p \to \mathbb{R}^n$ be a continuously differentiable function such that

$$F(\phi(\theta), \theta) = 0.$$

We can reformulate the considered inverse problem as:

$$\begin{aligned} &\underset{\theta}{\text{minimize}} && l(\phi(\theta)) + g(\theta) \\ &\text{subject to} && \theta \in \Theta \end{aligned} \tag{3}$$

$$\begin{aligned} \underset{\theta}{\text{minimize}} \quad & l(\phi(\theta)) + g(\theta) \\ \text{subject to} \quad & \theta \in \Theta \end{aligned} \tag{4}$$

- $\phi(\cdot)$, is evaluated by a numerical iterative scheme.
- Functions $l(\cdot)$ and $g(\cdot)$ are convex and non-smooth.

Solution methods:

- Can be solved using regularization techniques, e.g. proximal methods [Lewis and Wright,2016].
- We consider a trust region method, which naturally handles box constraints on the parameters.

Sequential convex optimization

Iterative solution algorithm, at each step we:

- convexify the non-linear system model $\phi(\cdot)$;
- solve the resulting convex problem within a trust region.

Given an iterate θ_k, a new trial iterate θ^+ is obtained solving:

$$\begin{aligned} \underset{\theta}{\text{minimize}} \quad & l(\phi(\theta_k) + J_k(\theta - \theta_k)) + g(\theta) \\ \text{subject to} \quad & \|\theta - \theta_k\|_\infty \leq \Delta_k \\ & \theta \in \Theta \end{aligned} \tag{5}$$

where J_k is the Jacobian matrix of $\phi(\cdot)$ evaluated at θ_k.

- At each iteration, we need to solve the adjoint equation:

$$\frac{\partial F(\phi(\theta_k), \theta_k)}{\partial x} J_k + \frac{\partial F(\phi(\theta_k), \theta_k)}{\partial \theta} = 0 \tag{6}$$

- Computing the full Jacobian matrix J_k would require a significant computational effort when large systems are considered.

We introduce auxiliary variables $x \in \mathbb{R}^n$ and reformulate the convex sub-problem as

$$\begin{aligned} \underset{x,\theta}{\text{minimize}} \quad & l(x) + g(\theta) \\ \text{subject to} \quad & x = \phi(\theta_k) + J_k(\theta - \theta_k) \\ & \|\theta - \theta_k\|_\infty \leq \Delta_k \\ & \theta \in \Theta \end{aligned} \tag{7}$$

The convex sub-problem is equivalently reformulated as

$$\begin{aligned} \underset{x,\theta}{\text{minimize}} \quad & l(x) + g(\theta) \\ \text{subject to} \quad & \frac{\partial F_k}{\partial x}(x - x_k) + \frac{\partial F_k}{\partial \theta}(\theta - \theta_k) = 0 \\ & \|\theta - \theta_k\|_\infty \le \Delta_k \\ & \theta \in \Theta \end{aligned} \tag{8}$$

where $F_k := F(\phi(\theta_k), \theta_k)$ and $x_k := \phi(\theta_k)$.

The proposed reformulation is particularly convenient when matrices $\frac{\partial F_k}{\partial x}$ and $\frac{\partial F_k}{\partial \theta}$ are large and sparse.

Trust region based sequential convex optimization

Initialization: $\eta = 0.01$, $\gamma = 1.1$, $\alpha = 0.5$,

Select $\theta_{\mathbf{0}}$ and Δ_0 and set $x_0 = \phi(\theta_0)$;

repeat

  Trial iterate computation. Solve the convex sub-problem at (x_k, θ_k), let (x^+, θ^+) be the computed solution;

  Acceptance of trial iterate. Let

$$\rho_k = \frac{l(x_k) + g(\theta_k) - l(\phi(\theta^+)) - g(\theta^+)}{l(x_k) + g(\theta_k) - l(x^+) - g(\theta^+)}; \tag{9}$$

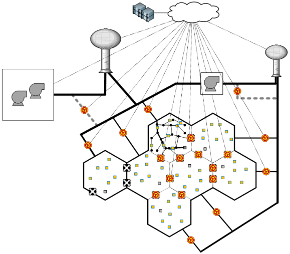
If $\rho_k \geq \eta$ then $\theta_{k+1} = \theta^+$, $x_{k+1} = \phi(\theta^+)$, $\Delta_{k+1} = \gamma\Delta_k$

else $\theta_{k+1} = \theta_k$, $x_{k+1} = x_k$, and $\Delta_{k+1} = \alpha\Delta_k$;

until Termination criteria are met

Head loss faults in water networks

- Water networks are equipped with an increasing level of instrumentation, like pressure control valves and isolation valves.
- Unreported changes to status or location of partially/fully closed valves results in discrepancies between hydraulic model predictions and real system states.



Previous literature

- Previously published approaches to identify head loss faults relied on genetic algorithms.
- These methods are not suitable for real-time implementation in fault diagnostic applications. As example, Do et al. (2018) reported an overall CPU time of more than 4 hours on a small benchmarking network.
- We propose an optimization-based estimation method for real-time fault detection and localization.

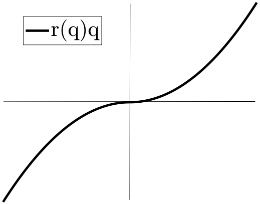
Do, N.C., Simpson, A.R., Deuerlein, J.W., and Piller, O. (2018) Locating Inadvertently Partially Closed Valves in Water Distribution Systems. Journal of Water Resources Planning and Management, 144 (8), 04018039. Available from: doi:10.1061/(asce)wr.1943-5452.0000958.

Faults modelling

Energy conservation laws:

$$h_{i_1} - h_{i_2} - r_j(q_j)q_j = f_j, \quad \forall i_1 \xrightarrow{j} i_2 \tag{10}$$

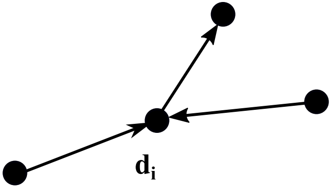
- Non-linear function $r_j(\cdot)$ depends on the frictional head loss formula used.
- The term f_j is used to model a fault on link j, e.g. pipe blockage or unknown valve status.



Mass conservation law

$$\sum_{j \in I^{\text{in}}(i)} q_j - \sum_{j \in I^{\text{out}}(i)} q_j = d_i \tag{11}$$

where d_i represents the demand at node i, which is estimated based on billing/historical data.



Network conservation laws

Energy and mass conservation laws are expressed in a more compact form as

$$A_{11}(q)q + A_{12}h + A_{10}h_0 + f = 0 \tag{12}$$

$$A_{12}^T q = d \tag{13}$$

where

- $q \in \mathbb{R}^{n_p}$ is the vector of unknown flows
- $h \in \mathbb{R}^{n_n}$ is the vector of unknown hydraulic heads
- $f \in \mathbb{R}^{n_p}$ is the vector of unknown faults
- $d \in \mathbb{R}^{n_n}$ is the vector of known demands
- $h_0 \in \mathbb{R}^{n_0}$ is the vector of known hydraulic heads

Sparsity-based fault estimation

We assume that most of the potential faults are not presented at the same time:

$$\|f\|_0 \leq \delta \tag{14}$$

However, the inclusion of a cardinally constraint would result in additional non-convexities.

We consider a convex relaxation based on the ℓ_1 norm.

Inverse problem formulation

We formulate the problem of head loss fault estimation as

$$\begin{aligned} \underset{q,h,f}{\text{minimize}} \quad & \frac{1}{2}\|Bh-\hat{h}\|_2^2 + \frac{1}{2}\|Cq-\hat{q}\|_2^2 + \lambda\|f\|_1 \\ \text{subject to} \quad & A_{11}(q)q + A_{12}h + A_{10}h_0 + f = 0 \\ & A_{12}^T q = d \end{aligned} \tag{15}$$

where

- $B \in \mathbb{R}^{n_t \times n_n}$ and $C \in \mathbb{R}^{n_s \times n_p}$ be sensor-node and sensor-link selection matrices, respectively.
- $\hat{h} \in \mathbb{R}^{n_t}$ is the vector of measured hydraulic heads
- $\hat{q} \in \mathbb{R}^{n_s}$ is the vector of measured flows

- Given a vector of faults $f \in \mathbb{R}^{n_p}$, there exists a unique pair $q(f)$ and $h(f)$ satisfying hydraulic conservation laws (Collins, 1978).
- The vector of hydraulic states that solves the network conservation laws is computed using tailored numerical schemes.

Collins, M. and Cooper, L. (1978) Solving the pipe network analysis problem using optimization techniques.

Management Science. 24 (7), 747–760

Non-linear least squares with ℓ_1 regularization:

$$\underset{f}{\text{minimize}} \quad \frac{1}{2}\|Bh(f)-\hat{h}\|_2^2+\frac{1}{2}\|Cq(f)-\hat{q}\|_2^2+\lambda\|f\|_1 \tag{16}$$

We apply the sequential convex optimization algorithm: at each step k, solve:

$$\begin{aligned} \underset{q,h,f}{\text{minimize}} \quad & \frac{1}{2}\|Bh-\hat{h}\|_2^2+\frac{1}{2}\|Cq-\hat{q}\|_2^2+\lambda\|f\|_1 \\ \text{subject to} \quad & A_{11}(q_k)q_k+G(q_k)(q-q_k)+A_{12}h+A_{10}h_0+f=0 \\ & A_{12}^T q = d \\ & \|f-f_k\|_\infty \leq \Delta_k \end{aligned} \tag{17}$$

Computational experience

- Trust region initial radius $\Delta_0 = 20$, and initial point $f_0 = 0$;
- the ℓ_1 penalty parameter is set to $\lambda = 0.01$;
- all experiments are conducted in MATLAB and the convex sub-problems within the sequential convex optimization algorithm are reformulated as quadratic programs and solved using GUROBI.

Case study - BWFLnet

The developed method is implemented to estimate head loss faults occurring in BWFLnet, the hydraulic model of a large operational water network from the UK operated by Bristol Water, Cla-Val, and Imperial College London.

- ~ 8000 customers
- 2606 pipes
- 545 valves
- 2546 nodes
- 27 pressure sensors

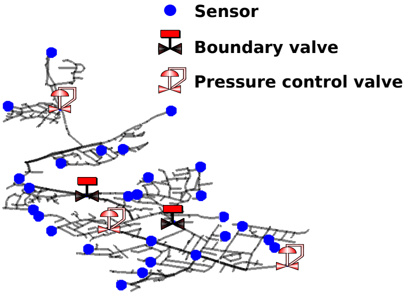
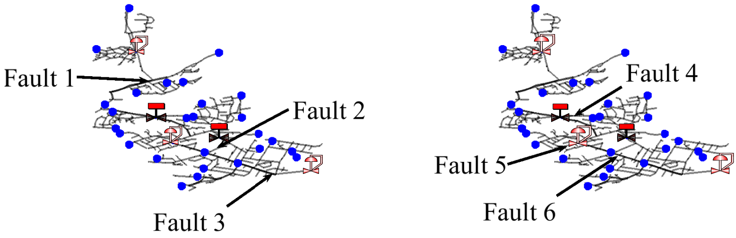


Figure: BWFLnet

Case study - Simulated data

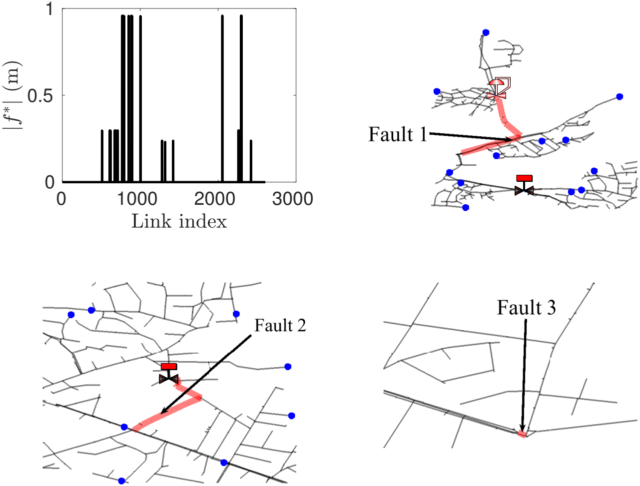
- We generate flow and hydraulic head measurements by simulating the water network model under different fault scenarios.
- Simulated faults correspond to partially/fully closed valves whose locations and status are unknown.



(a) Experiment 1. (b) Experiment 2.

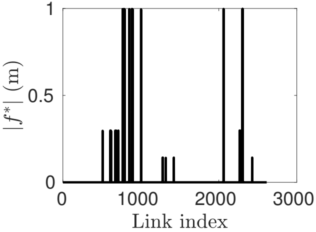
Multiple faults - Experiment 1

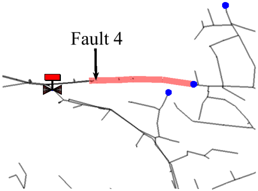
CPU time = 1.12 s

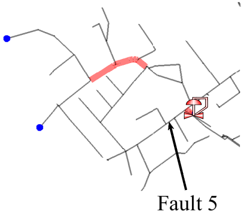


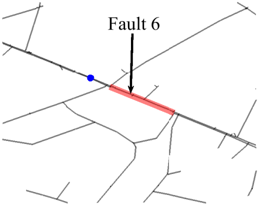
Multiple faults - Experiment 2

CPU time = 0.87 s



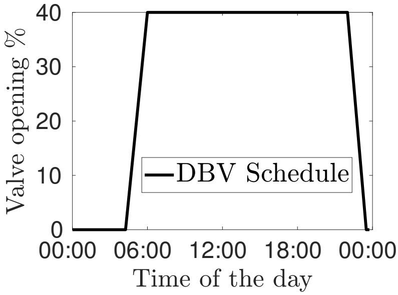




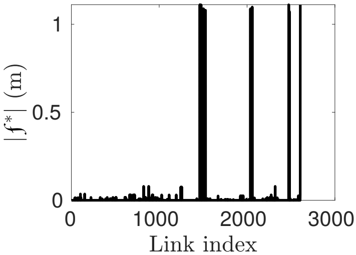


Case study - Experimental data

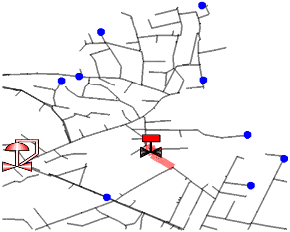
- The boundary valves are closed at 03:00 am.
- We assume that they are both open and attempt to recover their correct status.
- Measurements from the boundary valves are ignored.
- Measurements from the remaining locations are collected and the fault estimation problem is formulated and solved.



CPU time: 2.7 s



(k) Estimated fault state.



(l) Localization performance.

Conclusion

- We have presented a sequential convex optimization approach for solving inverse problems subject to non-linear equations.
- The developed algorithm has enabled the implementation of optimization-based fault estimation methods for water networks.
- The preliminary computational experience suggest that the proposed method is suitable for implementation in real time fault diagnosis applications.
- Further work should investigate ability of the algorithm to solve inverse problems where parameters and system states are coupled in time.

Thank you!

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For further information

f.pecci14@imperial.ac.uk