Explicit expressions for state estimation sensitivity analysis in water systems

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ABSTRACT

The implementation of state estimation techniques to water systems enables the hydraulic state of a given network to be computed at any time. However, errors in both measurements and model parameters can severely affect the quality of the state estimate, thus sensitivity analysis is crucial to assess its performance. The aim of this paper is to provide general explicit expressions for the sensitivities of the objective function and the primal variables of the state estimation problem with respect to both measurements and roughness parameters based on the perturbation of the Karush-Kuhn-Tucker (KKT) conditions. Additionally, among all the possible applications of sensitivity analysis, we present two specific forms of such analysis for water systems: identifiability of roughness parameters and linear state estimate approximation. The merit of these applications is

illustrated by means of a case study, which highlights the usefulness of compact sensitivity formulae to further understanding of state estimation solutions.

Keywords: state estimation, sensitivity analysis, parameter identifiability, linear approximation

INTRODUCTION

As a result of the growing complexity of water networks, supervisory control and data acquisition (SCADA) systems are becoming essential tools in large urban areas. They are installed with the aim of collecting the available on-line information provided by the various sensors distributed throughout the network. In this context, state estimation techniques are a feasible approach to process the information provided by such platforms, as they have been implemented with the same purpose in the power supply field for many years (Schweppe and Wildes 1970). The state estimation problem is formulated as a weighted least-squares (WLS) problem that minimises the difference between the available measurements and the estimates themselves, thus allowing the computation of the most likely hydraulic state of the network at a given time (Díaz et al. 2016b). Note that typical hydraulic models use the measurement setting given by head levels at tanks and demand measurements to estimate the flow in the network. In contrast, state estimation is a more versatile tool that enables to take into account different measurement settings and their corresponding noise with the same purpose.

The state estimation problem has been tackled before in the context of water systems. Starting from the well-known WLS approach (Bargiela 1985; Powell et al. 1988; Brdys and Ulanicki 2002), several authors have proposed modified algorithms with different aims, such as dealing with gross errors (Sterling and Bargiela 1984), introducing graph-based theory (Carpentier and Cohen 1991; Kumar et al. 2008) or considering bounds for the state estimation problem (Bargiela and Hainsworth 1989; Andersen et al. 2001), among others. More recently, Díaz et al. (2016a) consider the state estimation problem with mathematical programming techniques, which enables the inclusion of high precision measurements and upper and lower bounds for the variables of the state estimation problem.

In any case, the state estimation problem can always be considered as an optimisation problem, whose performance depends on: (1) how accurate measurements are, and (2) how well model parameters have been calibrated. To begin with, each measurement is subjected to noise as a result of the inaccuracy associated with its metering device, and estimations of demand, which are traditionally used to counteract the scarcity of instrumentation in water systems (i.e., *pseudo-measurements* based on historical records), are subjected to even greater uncertainties (Bargiela and Hainsworth 1989). Additionally, great effort has been made in the last decades to better calibrate network parameters (e.g. Walski (1983), Lansey and Basnet (1991), Kumar et al. (2010)), with many of them considering pipe roughness coefficients as the calibration parameters (e.g. Lansey et al. (2001), Kapelan et al. (2007)). It is important to highlight that the state estimation problem has traditionally assumed a previously calibrated hydraulic model (Díaz et al. 2016). Thus, errors in both measurements and parameters can severely affect the quality of the state estimates. This is why analysing state estimation sensitivity to both sources of uncertainty is a matter of interest.

Sensitivity analysis is a technique that allows to understand how uncertain input sources can affect qualitatively or quantitatively the output of a given model (Saltelli et al. 2004). Four different approaches are normally distinguished to compute local sensitivity analysis in the context of water management: (1) finite differences, (2) automatic differentiation, (3) sensitivity equations, and (4) the adjoint method. A consistent literature review of these strategies in the water systems domain can be found in Piller et al. (2017), where the sensitivity equations approach is highlighted for its potential when explicit formulations can be derived. In this regard, Piller et al. (2017) present explicit formulas that improve the knowledge of the flow network solution and therefore enhance calibration and sampling design procedures. Vairavamoorthy and Ali (2005) and Fu et al. (2012) have enhanced optimal design of water systems by introducing sensitivity information to guide evolutionary algorithms. Concurrently, there is another approach in the literature to develop sensitivity analysis for optimisation problems based on the perturbation of the Karush-Kuhn-Tucker (KKT) conditions (Fiacco 1983; Conejo et al. 2006). The aim is to provide the sensitivities of the objective function and the primal and dual variable values with respect to model data (Castillo et al. 2006).

The objective of this paper is twofold: firstly, to adapt the general explicit expressions obtained by perturbation of the KKT conditions to water systems, and secondly, to present some related applications: (1) characterise the identifiability of roughness parameters, and (2) provide a linear state estimate approximation based on an average state estimation result. The rest of the paper is organised as follows: first, the state estimation formulation is presented together with the derived sensitivity expressions. Subsequently, the aforementioned applications are presented in the context of water systems. Then, the potential of such applications is presented by means of a case study. Finally, some conclusions are drawn.

STATE ESTIMATION SENSITIVITY ANALYSIS

In this section the state estimation problem is formulated as a constrained WLS problem and the expressions for sensitivity analysis are derived. Afterwards, these general expressions are formulated for water systems.

State Estimation Formulation

The state estimation problem can be written as a mathematical programming problem as follows:

$$\underset{\boldsymbol{x}}{\text{Minimize}}\ J(\boldsymbol{x}, \boldsymbol{z}, \boldsymbol{\theta}) = \frac{1}{2}\left[\boldsymbol{z} - \boldsymbol{h}(\boldsymbol{x}, \boldsymbol{\theta})\right]^T \boldsymbol{W} \left[\boldsymbol{z} - \boldsymbol{h}(\boldsymbol{x}, \boldsymbol{\theta})\right] \tag{1}$$

subject to

$$\boldsymbol{f}(\boldsymbol{x}, \boldsymbol{\theta}) = \boldsymbol{0} : \boldsymbol{\lambda} \tag{2}$$

where the objective function given by Eq. (1) is defined by the $\boldsymbol{x} \in \mathbb{R}^n$ state variable vector; the $\boldsymbol{z} \in \mathbb{R}^m$ measurement vector; the $\boldsymbol{\theta} \in \mathbb{R}^p$ parameter vector; the $\boldsymbol{h} : \mathbb{R}^n \times \mathbb{R}^p \rightarrow \mathbb{R}^m$ nonlinear relationship of the state variables with respect to measurements and parameters according to the model equations; and $\boldsymbol{W}$, which is the $m \times m$ diagonal matrix for the measurement weights. In this work, roughness coefficients are considered the only model parameters, as done before by other experts for calibration purposes (e.g. Kapelan et al. (2007), Kumar et al. (2010)). Also, the state variable vector needs to be defined. The state variables are the minimum set of variables that enable to compute the state of the system (Brdys and Ulanicki 2002). It is common in state estimation applications to consider nodal heads as the state variables of the system (Díaz et al. 2016). Note that, as mentioned before, the traditional state estimation approach assumes that the model has been previously calibrated, i.e. $\boldsymbol{\theta}$ values are known inputs and only $\boldsymbol{x}$ values are to be determined. This implies that all sources of error are captured in model parameters and every other property of the system (e.g. connectivity, diameters, pump and valve statuses, etc.) is exactly known. For this reason, state estimation sensitivity analysis is of utmost importance. Note that $\boldsymbol{h}(\boldsymbol{x}, \boldsymbol{\theta})$ is used instead of $\boldsymbol{h}(\boldsymbol{x})$ because this work intends to assess the sensitivity of the problem with respect to both measurements and parameters. More specifically, this non-linear relationship can be expanded as:

$$\boldsymbol{h}(\boldsymbol{x}, \boldsymbol{\theta}) \rightarrow \left\{ \begin{array}{ll} h_k = x_i; & i \in \mathcal{V}_k^{\mathrm{m}} \\ h_k = \frac{x_i - x_j}{\theta_{ij}^{\frac{1}{b}}} |x_i - x_j|^{\frac{1}{b}-1}; & ij \in \mathcal{L}_k^{\mathrm{m}} \\ h_k = -\sum_{\forall j \in \Omega_i^I} \frac{x_i - x_j}{\theta_{ij}^{\frac{1}{b}}} |x_i - x_j|^{\frac{1}{b}-1} + \sum_{\forall j \in \Omega_i^O} \frac{x_i - x_j}{\theta_{ij}^{\frac{1}{b}}} |x_i - x_j|^{\frac{1}{b}-1}; & i \in \mathcal{V}_{\mathrm{Q}_k}^{\mathrm{m}} \end{array} \right\}; \forall k = 1, \ldots, m, \tag{3}$$

where k is an index that represents the number of the measurement. Note that $\boldsymbol{h}(\boldsymbol{x}, \boldsymbol{\theta})$ considers three different types of measurements: head level ($x_i; \forall i \in \mathcal{V}_k^{\mathrm{m}}$), water flow through a pipe that goes from node i to node j ($\forall ij \in \mathcal{L}_k^{\mathrm{m}}$), and water consumption at a demand node ($\forall i \in \mathcal{V}_{\mathrm{Q}_k}^{\mathrm{m}}$), respectively. Note that $\mathcal{V}_k^{\mathrm{m}}$, $\mathcal{L}_k^{\mathrm{m}}$ and $\mathcal{V}_{\mathrm{Q}_k}^{\mathrm{m}}$ are sets of nodes that activate depending on the type of measurement of k. Additionally, θ_{ij} represents the flow resistance pipe coefficient and $b = 1.852$ is the exponential flow coefficient for the Hazen-Williams equation. In this work, it is assumed that water flows from the lower to the higher numbering node, i.e. $i < j$. Two subsets Ω_i^I and Ω_i^O are defined for each node i corresponding to water inflows to node i from the rest of nodes connected to i through a pipe, and water outflows from node i to the rest of nodes connected to i through a pipe, respectively. Note that Eq. (3) is a flexible way of formulating the problem, and it enables to take into account the required headloss and continuity equations depending on the available measurements. Additionally, Eq. (2) represents the problem's hydraulic constraints, with $\boldsymbol{\lambda}$ being the dual variable vector related to equality constraints. In this work, we consider demand at transit nodes ($\forall i \in \mathcal{V}_{\mathrm{T}}$) to be null, i.e. nodes known to have zero consumption, as the only equality constraints, so Eq. (4) can be specified as:

$$\boldsymbol{f}(\boldsymbol{x}, \boldsymbol{\theta}) \rightarrow f_i = -\sum_{\forall j \in \Omega_i^I} \frac{x_i - x_j}{\theta_{ij}^{\frac{1}{b}}} |x_i - x_j|^{\frac{1}{b}-1} + \sum_{\forall j \in \Omega_i^O} \frac{x_i - x_j}{\theta_{ij}^{\frac{1}{b}}} |x_i - x_j|^{\frac{1}{b}-1}; \quad \forall i \in \mathcal{V}_{\mathrm{T}}. \tag{4}$$

Thus, the number of equality constraints c is equal to the number of transit nodes of the network (the cardinality of $\mathcal{V}_{\mathrm{T}}$).

Additional equality constraints could be added if needed. Also, inequality constraints could be included in the formulation, as once the optimal solution of the state estimation problem $\hat{\boldsymbol{x}}$ is computed, binding inequality constraints must be considered equality constraints and non-binding ones are disregarded. In such a case, specific derivative formulations for each type of equality constraint should be defined.

General Sensitivity Expressions

Once solution $\hat{\boldsymbol{x}}$ to problem (1)-(2) has been found, a sensitivity analysis is undertaken. For this purpose, the first order optimality conditions are differentiated in such a way that the KKT optimality conditions hold. By developing the associated equations (see Conejo et al. (2006) for detail), the following sensitivity matrices are obtained:

$$\begin{bmatrix} \frac{\partial \boldsymbol{x}}{\partial \boldsymbol{z}}_{(n\times m)} \\ \frac{\partial \boldsymbol{\lambda}}{\partial \boldsymbol{z}}_{(c\times m)} \end{bmatrix} = -\begin{bmatrix} \boldsymbol{J}_{\boldsymbol{xx}(n\times n)} & \boldsymbol{F}^T_{\boldsymbol{x}\,(n\times c)} \\ \boldsymbol{F}_{\boldsymbol{x}(c\times n)} & \boldsymbol{0}_{(c\times c)} \end{bmatrix}^{-1} \begin{bmatrix} \boldsymbol{J}_{\boldsymbol{xz}(n\times m)} \\ \boldsymbol{0}_{(c\times m)} \end{bmatrix}, \tag{5}$$

$$\begin{bmatrix} \frac{\partial \boldsymbol{x}}{\partial \boldsymbol{\theta}}_{(n\times p)} \\ \frac{\partial \boldsymbol{\lambda}}{\partial \boldsymbol{\theta}}_{(c\times p)} \end{bmatrix} = -\begin{bmatrix} \boldsymbol{J}_{\boldsymbol{xx}(n\times n)} & \boldsymbol{F}^T_{\boldsymbol{x}\,(n\times c)} \\ \boldsymbol{F}_{\boldsymbol{x}(c\times n)} & \boldsymbol{0}_{(c\times c)} \end{bmatrix}^{-1} \begin{bmatrix} \boldsymbol{J}_{\boldsymbol{x\theta}(n\times p)} \\ \boldsymbol{F}_{\boldsymbol{\theta}(c\times p)} \end{bmatrix}, \tag{6}$$

which provide the derivatives of the optimal state variables and dual variables of the equality constraints with respect to both measurements and parameters. Dimensions of each matrix are indicated in parenthesis. Note that in order for the sensitivities to be computed, the system of equations' coefficient matrix must be invertible, i.e. the system must be observable (Díaz et al.

2016). The derivatives of the objective function with respect to measurements and parameters can be written as:

$$\frac{\partial J}{\partial \boldsymbol{z}}_{(1\times m)} = \boldsymbol{J}_{\boldsymbol{z}\ (1\times m)}^{T} + \boldsymbol{J}_{\boldsymbol{x}\ (1\times n)}^{T} \frac{\partial \boldsymbol{x}}{\partial \boldsymbol{z}}_{(n\times m)}, \tag{7}$$

$$\frac{\partial J}{\partial \boldsymbol{\theta}}_{(1\times p)} = \boldsymbol{J}_{\boldsymbol{\theta}\ (1\times p)}^{T} + \boldsymbol{J}_{\boldsymbol{x}\ (1\times n)}^{T} \frac{\partial \boldsymbol{x}}{\partial \boldsymbol{\theta}}_{(n\times p)}. \tag{8}$$

Sensitivities provide information about how much the optimal estimated variables $\hat{\boldsymbol{x}}$ or the objective function $\hat{J}$ changes when parameters $\boldsymbol{\theta}$ or measurements $\boldsymbol{z}$ change one unit. Therefore, units of sensitivities correspond to the ratio between units of the variable whose sensitivity is being calculated, and the units of the parameter or measurement with respect to which sensitivities are being obtained. For instance, if units for head levels and flows within the state estimation problem are m and m^3/h, respectively, the sensitivities of estimated head levels with respect to flow measurements are $m/(m^3/h)$.

The main contribution of this work, which is to adapt these expressions to the reality of water networks, is now explained. Note that Eqs. (5)-(6) represent the derivatives of the state (i.e. the head levels) and dual variables with respect to measurements and parameters, but once these are obtained, the sensitivities of flows and demands can be inferred by applying the chain rule. Also, it is important to highlight that these expressions are a generalised version of those proposed by Piller et al. (2017), because they are suitable no matter the measurement setting as long as it is observable. Note that when only head levels at tanks and water demands are metered, problem (1)-(2) is equivalent to solving the flow network, and thus the sensitivities computed with Eqs. (5)-(6) are equivalent to those proposed by Piller et al. (2017) for demand driven models.

Specific Expressions for Water Distribution Systems

In order for these expressions to be specified for water systems, matrices $\boldsymbol{J_x}$, $\boldsymbol{J_{xx}}$ and $\boldsymbol{F_x}$ from (5)-(8) can be obtained as follows:

$$\boldsymbol{J}_{\boldsymbol{x}(n\times 1)} = \boldsymbol{\nabla_x} J(\hat{\boldsymbol{x}}, z, \boldsymbol{\theta}) = \left.\frac{\partial J}{\partial x_j}\right|_{\hat{\boldsymbol{x}}} = \sum_{i=1}^{m} \left[-\frac{\partial h_i(\hat{\boldsymbol{x}}, \boldsymbol{\theta})}{\partial x_j}\right]^T W_{ii}\left[z_i - h_i(\hat{\boldsymbol{x}}, \boldsymbol{\theta})\right] = -\boldsymbol{H}^T{}_{(n\times m)} \boldsymbol{W}_{(m\times m)} (\boldsymbol{z} - \hat{\boldsymbol{z}})_{(m\times 1)}, \tag{9}$$

$$\boldsymbol{J}_{\boldsymbol{xx}(n\times n)} = \boldsymbol{\nabla}_{\boldsymbol{xx}} J(\hat{\boldsymbol{x}}, z, \boldsymbol{\theta}) = \left.\frac{\partial^2 J}{\partial x_j \partial x_k}\right|_{\hat{\boldsymbol{x}}} =$$

$$\sum_{i=1}^{m} \left[\cancel{\left[-\frac{\partial^2 h_i(\hat{\boldsymbol{x}}, \boldsymbol{\theta})}{\partial x_j \partial x_k} \right]^T W_{ii} \left[z_i - h_i(\hat{\boldsymbol{x}}, \boldsymbol{\theta}) \right]} + \left[-\frac{\partial h_i(\hat{\boldsymbol{x}}, \boldsymbol{\theta})}{\partial x_j} \right]^T W_{ii} \left[-\frac{\partial h_i(\hat{\boldsymbol{x}}, \boldsymbol{\theta})}{\partial x_k} \right] \right] = \boldsymbol{H}^T{}_{(n\times m)} \boldsymbol{W}_{(m\times m)} \boldsymbol{H}_{(m\times n)}, \quad (10)$$

$$\boldsymbol{F}_{\boldsymbol{x}(c\times n)} = \boldsymbol{\nabla}_{\boldsymbol{x}} \boldsymbol{f}(\hat{\boldsymbol{x}}, z, \boldsymbol{\theta}) = \left.\frac{\partial f_i}{\partial x_j}\right|_{\hat{\boldsymbol{x}}}, \quad (11)$$

where $\boldsymbol{H}$ is the $m \times n$ available measurement Jacobian matrix, $\boldsymbol{F}_{\boldsymbol{x}}$ is the $c \times n$ equality constraint measurement Jacobian matrix and $\hat{\boldsymbol{z}} = \boldsymbol{h}(\hat{\boldsymbol{x}}, z, \boldsymbol{\theta})$ refers to the value of the estimated measured variable. Second order derivatives are here disregarded for the computation of matrix $\boldsymbol{J}_{\boldsymbol{xx}}$ because they have proven to have a negligible effect and sensitivity analysis is expected to be undertaken once the state estimation solution has been found. Note that this implies that outliers have been conveniently removed (Caro et al. 2011; Caro et al. 2013), hence there is no risk of assigning undeserved importance to those second order derivatives. Components of the measurement Jacobian matrix for the construction of $\boldsymbol{H}$ can be computed as shown below:

$$\boldsymbol{H} \rightarrow \left\{ \begin{array}{ll} \frac{\partial h_k}{\partial x_l} = \delta_{il}; & i \in \mathcal{V}_k^{\mathrm{m}} \\ \frac{\partial h_k}{\partial x_l} = \left\{ \begin{array}{ccc} \frac{1}{\theta_{ij} b |h_k|^{b-1}} & \text{if} & l = i \\ \frac{-1}{\theta_{ij} b |h_k|^{b-1}} & \text{if} & l = j \\ 0 & & \text{otherwise} \end{array} \right\}; & ij \in \mathcal{L}_k^{\mathrm{m}} \\ \frac{\partial h_k}{\partial x_l} = -\sum_{\forall j \in \Omega_i^I} \frac{\partial Q_{ij}}{\partial x_l} + \sum_{\forall j \in \Omega_i^O} \frac{\partial Q_{ij}}{\partial x_l}; & i \in \mathcal{V}_{\mathrm{Q}_k}^{\mathrm{m}} \end{array} \right\}; \forall l \in \mathcal{V}; \forall k = 1, \ldots, m, \quad (12)$$

where Q_{ij} is an auxiliary variable that refers to water flows and can be written as:

$$\frac{\partial Q_{ij}}{\partial x_l} = \left\{ \begin{array}{ccc} \frac{1}{\theta_{ij} b |\frac{x_i - x_j}{\theta_{ij}}|^{\frac{b-1}{b}}} & \text{if} & l = i \\ \frac{-1}{\theta_{ij} b |\frac{x_i - x_j}{\theta_{ij}}|^{\frac{b-1}{b}}} & \text{if} & l = j \end{array} \right\} \forall ij \in \mathcal{L}; \forall l \in \mathcal{V} \quad (13)$$

with $\mathcal{V}$ and $\mathcal{L}$ representing the whole set of nodes and link elements in the system, respectively. On the other hand, the components of $\boldsymbol{F_x}$ can be obtained as:

$$\boldsymbol{F_x} \rightarrow \frac{\partial f_i}{\partial x_l} = -\sum_{\forall j \in \Omega_i^I} \frac{\partial Q_{ij}}{\partial x_l} + \sum_{\forall j \in \Omega_i^O} \frac{\partial Q_{ij}}{\partial x_l}; \quad \forall i \in \mathcal{V}_\mathrm{T}; \quad \forall l \in \mathcal{V} \tag{14}$$

Similarly, matrices $\boldsymbol{J_\theta}$, $\boldsymbol{J_{x\theta}}$ and $\boldsymbol{F_\theta}$ can be obtained as:

$$\boldsymbol{J}_{\boldsymbol{\theta}(p\times1)} = \boldsymbol{\nabla_\theta} J(\hat{\boldsymbol{x}}, z, \boldsymbol{\theta}) = \left.\frac{\partial J}{\partial \theta_{lr}}\right|_{\hat{\boldsymbol{x}}} = \sum_{i=1}^{m} \left[-\frac{\partial h_i(\hat{\boldsymbol{x}}, \boldsymbol{\theta})}{\partial \theta_{lr}}\right]^T W_{ii} \left[z_i - h_i(\hat{\boldsymbol{x}}, \boldsymbol{\theta})\right] = -\boldsymbol{P}^T{}_{(p\times m)} \boldsymbol{W}_{(m\times m)} (\boldsymbol{z} - \hat{\boldsymbol{z}})_{(m\times1)}, \tag{15}$$

$$\boldsymbol{J}_{\boldsymbol{x\theta}(n\times p)} = \boldsymbol{\nabla_{x\theta}} J(\hat{\boldsymbol{x}}, z, \boldsymbol{\theta}) = \left.\frac{\partial^2 J}{\partial x_j \partial \theta_{lr}}\right|_{\hat{\boldsymbol{x}}} = \sum_{i=1}^{m} \left[\cancel{\left[-\frac{\partial^2 h_i(\hat{\boldsymbol{x}}, \boldsymbol{\theta})}{\partial x_j \partial \theta_{lr}}\right]^T W_{ii} \left[z_i - h_i(\hat{\boldsymbol{x}}, \boldsymbol{\theta})\right]} + \left[-\frac{\partial h_i(\hat{\boldsymbol{x}}, \boldsymbol{\theta})}{\partial x_j}\right]^T W_{ii} \left[-\frac{\partial h_i(\hat{\boldsymbol{x}}, \boldsymbol{\theta})}{\partial \theta_{lr}}\right]\right] = \boldsymbol{H}^T{}_{(n\times m)} \boldsymbol{W}_{(m\times m)} \boldsymbol{P}_{(m\times p)}, \tag{16}$$

$$\boldsymbol{F}_{\boldsymbol{\theta}(c\times p)} = \boldsymbol{\nabla_\theta} \boldsymbol{f}(\hat{\boldsymbol{x}}, z, \boldsymbol{\theta}) = \left.\frac{\partial f_i}{\partial \theta_{lr}}\right|_{\hat{\boldsymbol{x}}}, \tag{17}$$

where $\boldsymbol{P}$ is the $m \times p$ roughness Jacobian matrix. As before, second order derivatives have been neglected for the computation of $\boldsymbol{J_{x\theta}}$, and $\boldsymbol{F_\theta}$ is the $c \times p$ equality constraint roughness Jacobian matrix. Also, note that θ_{lr} is here used in order to refer to the fact that roughness is a property of a pipe that goes from node l to node r, but $\boldsymbol{\theta}$ represents a vector (i.e. not a matrix). Components of the roughness Jacobian matrix for the construction of $\boldsymbol{P}$ can be computed as shown below:

$$\boldsymbol{P} \rightarrow \left\{ \begin{array}{ll} \frac{\partial h_k}{\partial \theta_{lr}} = 0; & i \in \mathcal{V}_k^{\mathrm{m}} \\ \frac{\partial h_k}{\partial \theta_{lr}} = \left\{ \begin{array}{ll} \frac{-|h_k|^{b+1}}{b(x_i - x_j)} & \text{if} \quad l = i, r = j \\ 0 & \text{otherwise} \end{array} \right\}; & ij \in \mathcal{L}_k^{\mathrm{m}} \\ \frac{\partial h_k}{\partial \theta_{lr}} = \left\{ \begin{array}{ll} \frac{|Q_{lr}|^{b+1}}{b(x_l - x_r)} & \text{if} \quad r = i \\ \frac{-|Q_{lr}|^{b+1}}{b(x_l - x_r)} & \text{if} \quad l = i \\ 0 & \text{otherwise} \end{array} \right\}; & i \in \mathcal{V}_{\mathrm{Q}_k}^{\mathrm{m}} \end{array} \right\}; \forall lr \in \mathcal{L}; \forall k = 1, \ldots, m, \qquad (18)$$

where Q_{lr} can be obtained from Eq. (13). Also, $\boldsymbol{F}_{\boldsymbol{\theta}}$ components can be computed as:

$$\boldsymbol{F}_{\boldsymbol{\theta}} \rightarrow \frac{\partial f_i}{\partial \theta_{lr}} = \left\{ \begin{array}{ll} \frac{|Q_{lr}|^{b+1}}{b(x_l - x_r)} & \text{if} \quad r = i \\ \frac{-|Q_{lr}|^{b+1}}{b(x_l - x_r)} & \text{if} \quad l = i \\ 0 & \text{otherwise} \end{array} \right\}; \forall lr \in \mathcal{L}; \forall i \in \mathcal{V}_{\mathrm{T}} \qquad (19)$$

Finally, matrices $\boldsymbol{J}_{\boldsymbol{z}}$ and $\boldsymbol{J}_{\boldsymbol{xz}}$ can be computed as:

$$\boldsymbol{J}_{\boldsymbol{z}(m\times 1)} = \boldsymbol{\nabla}_{\boldsymbol{z}} J(\hat{\boldsymbol{x}}, \boldsymbol{z}, \boldsymbol{\theta}) = \left.\frac{\partial J}{\partial z_j}\right|_{\hat{\boldsymbol{x}}} = \sum_{i=1}^{m} W_{ii} \left[z_i - h_i(\hat{\boldsymbol{x}}, \boldsymbol{\theta}) \right] = \boldsymbol{W}_{(m\times m)} (\boldsymbol{z} - \hat{\boldsymbol{z}})_{(m\times 1)}, \qquad (20)$$

$$\boldsymbol{J}_{\boldsymbol{xz}(n\times m)} = \boldsymbol{\nabla}_{\boldsymbol{xz}} J(\hat{\boldsymbol{x}}, \boldsymbol{z}, \boldsymbol{\theta}) = \left.\frac{\partial^2 J}{\partial x_j \partial z_k}\right|_{\hat{\boldsymbol{x}}} = \sum_{i=1}^{m} \left[-\frac{\partial h_i(\hat{\boldsymbol{x}}, \boldsymbol{\theta})}{\partial x_j} \right]^T W_{ii} = -\boldsymbol{H}^T{}_{(n\times m)} \boldsymbol{W}_{(m\times m)}. \qquad (21)$$

APPLICATIONS

The general expressions derived for state estimation sensitivity analysis in water systems have interest on their own since they are explicit expressions that provide the value of the sensitivity of the primal variables, dual variables and objective function of the problem with respect to both measurements and model parameters. However, some other related applications can be derived from the computation of state estimation sensitivities in water systems. In this section, two applications are briefly presented: (1) identifiability of roughness parameters, and (2) linear state estimate approximation. Note that in this work only the potential of the sensitivities of the objective function and the state variables is explored, but additional studies could focus on dual variables. According to the formulation presented in this work, $\boldsymbol{\lambda}$ represents how the objective function changes as the water demand at transit nodes varies, hence $\frac{\partial \boldsymbol{\lambda}}{\partial \boldsymbol{z}}$ and $\frac{\partial \boldsymbol{\lambda}}{\partial \boldsymbol{\theta}}$ indicate how that marginal is affected by measurements and model parameters. This is a subject for further research.

Identifiability of roughness parameters

The concept of *identifiability analysis* refers to the assessment of how well model parameters (in this case, roughness parameters) can be estimated based on existing measurements. Such analysis is not just a matter of evaluating if sufficient measurements exist to calibrate them (i.e. observability analysis), but rather how well they could be estimated considering the uncertainty of the measurement setting. In this regard, the derivative of the objective function with respect to roughness parameters ($\frac{\partial J}{\partial \boldsymbol{\theta}}$) as given in Eq. (8) provides an insight of how susceptible the objective function is to changes in the roughness value, reflecting to what extent a given parameter could be adjusted in a calibration procedure. Therefore, this value can be used to rank the network pipes according to their importance for calibration, enabling to identify the pipes whose roughness value adjustment would better contribute to minimise the objective function. This information could be incorporated into calibration procedures, as it provides an additional criterion to, for example, guide evolutionary algorithms.

Note that sensitivities would provide a more intuitive value if they were computed with respect to the roughness value instead of the flow resistance pipe coefficient $\boldsymbol{\theta}$. Therefore, if for example the Hazen-Williams headloss equation is being considered, the derivative of the objective function with respect to the roughness value $\boldsymbol{C}$ could be computed by simply applying the chain rule as follows:

$$\frac{\partial J}{\partial \boldsymbol{C}} = \frac{\partial J}{\partial \boldsymbol{\theta}} \frac{\partial \boldsymbol{\theta}}{\partial \boldsymbol{C}} = -1.852 \frac{10.67L}{D^{4.871} C^{2.852}} \frac{\partial J}{\partial \boldsymbol{\theta}}, \tag{22}$$

when all terms expressed in SI units. Sensitivity expressions with respect to roughness value $\boldsymbol{C}$

have been recently used for the calibration of networks based on multi-period state estimation (Díaz et al. 2017). Note that as mentioned before, the state estimation approach enables to cover more possibilities in terms of measurement settings than traditional calibration procedures (Kumar et al. 2010).

Linear state estimate approximation

There are different methods to solve the state estimation problem. At present, the computational time associated with existing techniques is not extensive even for large systems. However, there may be situations in which a rough estimate may be sufficient, so it is not required to go through the expense of repeatedly evaluating the state estimation itself. For example, this may be the case of undertaking experiments (i.e. Monte Carlo method) to statistically evaluate how a particular aspect of the state estimation problem (output) varies with noisy measurements (input).

In such scenario, the previously presented sensitivity analysis formulae have potential to approximate the state estimate for different measured values as long as they are not subjected to gross errors and a linear approximation can be assumed. To begin with, the average hydraulic state can be estimated ($\hat{\boldsymbol{x}}_{\boldsymbol{m}}$) from the mean measured values ($\boldsymbol{z}_{\boldsymbol{m}}$), and the associated average sensitivities can be computed. Note that the mean measured values can be assumed to be equal to the solution of the flow network, around which noisy measurements are generated. Then, the value of the state variables could be estimated by corrupting the average sensitivities by the deviation between the mean measured value and the particular measurement $\boldsymbol{z}$ that is to be analysed:

$$\hat{\boldsymbol{x}} = \hat{\boldsymbol{x}}_{\boldsymbol{m}} + \left.\frac{\partial \boldsymbol{x}}{\partial \boldsymbol{z}}\right|_{\hat{\boldsymbol{x}}_{\boldsymbol{m}}} (\boldsymbol{z} - \boldsymbol{z}_{\boldsymbol{m}}). \tag{23}$$

Similarly, the chain rule could be applied to $\frac{\partial \boldsymbol{x}}{\partial \boldsymbol{z}}$ in order to obtain $\frac{\partial \boldsymbol{Q}}{\partial \boldsymbol{z}}$ and $\frac{\partial \boldsymbol{q}}{\partial \boldsymbol{z}}$, from which the updated values of flows ($\hat{\boldsymbol{Q}}$) and demands ($\hat{\boldsymbol{q}}$) can be computed analogously to Eq. (23). It must be highlighted that this simplification implies the assumption of a linear behaviour near the optimum. Its validity depends on the network response and uncertainty magnitude, which may be dubious at some locations that might be especially prone to non-linear behaviour. Nevertheless, it permits to significantly reduce the computational cost associated with simulation experiments without severely affecting the quality of results, as it will be shown in the case study.

CASE STUDY: HANOI NETWORK

The purpose of this case study is to demonstrate state estimation sensitivity analysis in water systems, as well as to show the potential of the aforementioned applications. With this aim, the well-known Hanoi network (Fujiwara and Khang 1990) is adopted for illustration in this work. The network originally consists of 1 tank, 31 demand nodes and 34 pipes, but as in Díaz et al. (2016a), nodes 3, 16, 23 and 25 are considered in this paper as nodes with null demand (i.e. transit nodes) to introduce some hydraulic constraints. Appendix S1 contains detailed characteristics of this example. Hanoi system is considered in this work as a water transport network. Water transport networks are pipeline systems that provide water to large communities, e.g. District Metered Areas (DMA), where incoming flows are normally monitored. Therefore, they constitute the "main arteries" that enable large urban areas to be supplied with water, and they are bettered metered than conventional water distribution systems. For this reason, they are the first areas where state estimation techniques are being applied at present (Vrachimis et al. 2016). Consequently, it is here assumed that water demand is metered in each of the demand nodes, as it is likely to be the case if each of them were actual DMAs. Also, the water level at the tank (x_1) and the pressure at node 30 (x_{30}) are metered, i.e. one degree of redundancy exists. This detail is important because redundancy helps to identify the most likely hydraulic state of the system despite measurement noise. As the uncertainty of flow meters is normally dependent on the circulating flow rate, a noise $\sigma_q = 2\text{‰}q$ is here assumed, where q corresponds to water demands in Appendix S1. On the other hand, we assume $\sigma_x = 0.01$ bar for pressure meters, and $\sigma_x = 0.01$ m for water level meters, which are usual values for such metering devices.

Identifiability of roughness parameters

As commented before, the derivative of the objective function with respect to the Hazen-Williams roughness value ($\frac{\partial J}{\partial C}$) provides an insight into how well each of the pipes can be calibrated: the greater the value of such derivative, the more sensitive the objective function is to the roughness value, i.e. the more crucial it is to adequately calibrate that particular roughness for a good adjustment of the model. Table 1 provides the network pipes sorted by $|\frac{\partial J}{\partial \boldsymbol{C}}|$ and the value of this derivative under three scenarios: (1) considering a roughness value of 90% of the real value $\boldsymbol{C} = 0.9\boldsymbol{C}_{real}$ for all pipes, (2) considering the exact roughness value $\boldsymbol{C} = \boldsymbol{C}_{real}$ for all pipes, and (3) considering a roughness value of 1.1 times the real value $\boldsymbol{C} = 1.1\boldsymbol{C}_{real}$ for all pipes.

These results show that when a roughness value below C_{real} is used to solve the state estimation problem, the associated derivatives are mainly negative, which indicates that their roughness should be increased to reduce the objective function, i.e. to achieve a better state estimation result. Note that some of the pipes may have the sign changed as a result of measurement noise or because of negative flows (flow is considered positive when it goes from the lower to the higher numbering node). Sensitivity is almost null for the last ones, which mainly correspond to the two branches that come out of node 10 and 20 according to Figure 1. Similarly, if the adopted roughness is above the real value, derivatives are positive, whereas they become almost zero when the real value of roughness is being used. Therefore, values of such sensitivities clearly different from zero are a trustworthy indicator of deviations with respect to the real roughness value. This would indicate a need for recalibrating the system.

Moreover, Table 1 shows that the relative importance of pipes is basically the same regardless of the roughness value being considered. This implies that even if the roughness assumed in the model is not correct, state estimation sensitivity analysis still provides information about the importance of each pipe, enabling identification of the most relevant pipes in terms of calibration. Figure 1 shows the relative importance of each pipe for the $\boldsymbol{C} = \boldsymbol{C}_{real}$ scenario. In this figure, the thickness of those pipes whose sensitivity is above the 50% percentile threshold varies according to the $\frac{\partial J}{\partial C}$ value, whereas the rest of pipes are only dotted. It can be seen that pipes with greater circulating flows (near the source tank) have a better identifiability. Also, length and diameter are important according to Eq. (22). Note that even though a higher flow circulates through pipe 1-2, identifiability in 2-3 is greater than in pipe 1-2 due to the pipe length.

Linear state estimate approximation

In this section, sensitivity analysis is used as an alternative to evaluate state estimation results under a Monte Carlo simulation of $1,000$ realizations. More specifically, state estimation results in terms of head levels are computed for this case study in two different ways: (1) solving the state estimation problem $1,000$ times via mathematical programming, and (2) solving the state estimation problem once (for the mean measurement configuration) and linearly approximating state estimation via sensitivity analysis using Eq. (23). Appendix S2 provides the mean and standard deviation of the estimated variables according to both methods, as well as the results of comparing such results by means of a two-sample Kolmogorov-Smirnov test with a confidence level of 95% for each head level in the network. This test shows that head level distributions are the same with both methods, thus proving that the linear approximation is valid to compute the state variables in the Hanoi network.

Table 2 provides the average computational time required to implement each of the steps of the aforementioned linear state estimate approximation in a MatLab 7.12.0 (R2011a) 64-bits version and a 23.3 GAMS 64-bits version when run in an Intel(R) Core(TM) i7-6700 CPU 3.40 GHz 16 GB RAM desktop computer. This table shows that the linear state estimate approximation is four orders of magnitude faster than solving state estimation via mathematical programming each time.

To finish with, it must be noted that the linear approximation proposed in Eq. (23) could also be used as initialisation strategy when state estimation is implemented on-line. If measurements are available at consecutive times, the linear approximation via sensitivity analysis could be used to initialise the following time step based on the previous one as long as the time step is small enough (i.e. measurements are relatively close), thus accelerating the state estimation process itself. Nevertheless, the computational time required for sensitivity analysis may be inadmissible for online processing. According to Table 2, sensitivity analysis computation needs about 30% of the time required to execute an average state estimation process via mathematical programming. Therefore, 30% extra time would be required to update the initialisation point for the subsequent time step at each time. Hence, if time steps are small, it may be worth just initialising each time step with the solution of the previous one. This avoids the sensitivity analysis burden, whose computational needs are doomed to increase with the size of the network, i.e. the size of the matrices. For this reason, the linear state estimate approximation presented in this paper is especially recommended for repetitive processes like the aforementioned Monte Carlo experiment, where sensitivity analysis only has to be computed once.

CONCLUSIONS

Sensitivity analysis is a useful strategy to extract information around the optimum of any optimisation problem, as it is the case of state estimation applied to water systems. With this aim, general expressions for local state estimation sensitivity analysis in water systems are derived in this paper by perturbing KKT conditions. Explicit expressions for the objective function and primal and dual variables of the state estimation problem with respect to both measurements and roughness parameters are given here. Additionally, two applications of the information provided by sensitivity analysis are presented and illustrated with a case study.

In this regard, sensitivity analysis enables to assess identifiability of the roughness value in the pipes of any water system and to rank them according to their relative importance for calibration purposes. In the case study presented in this work, the pipes near the source node are the most identifiable, hence they should be the target when calibrating the system. Moreover, sensitivity values clearly different from zero indicate that there is a deviation between the assumed roughness coefficient and the real one. These results would indicate that it is required to recalibrate the system. Secondly, sensitivity analysis is used here to provide a linear approximation of state estimation results in a Monte Carlo simulation, considerably accelerating the calculation process while providing similar results to ordinary state estimation via mathematical programming. Both applications present potential for gaining information and improving the understanding of the behaviour of the system when state estimation techniques are to be implemented.

SUPPLEMENTAL DATA

Appendixes S1-S2 are available online in the ASCE Library (www.ascelibrary.org).

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List of Tables

1 Identifiability of roughness parameters for Hanoi case study: Pipes sorted by $|\frac{\partial J}{\partial \boldsymbol{C}}|$ under different scenarios. Sensitivities are unitless. 21

2 Average computational time associated with linear state estimate approximation for Hanoi network case study 22

TABLE 1. Identifiability of roughness parameters for Hanoi case study: Pipes sorted by $|\frac{\partial J}{\partial \boldsymbol{C}}|$ under different scenarios. Sensitivities are unitless.

$\boldsymbol{C} = 0.9\boldsymbol{C}_{real}$		$\boldsymbol{C} = \boldsymbol{C}_{real}$		$\boldsymbol{C} = 1.1\boldsymbol{C}_{real}$	
Pipe	$\frac{\partial J}{\partial \boldsymbol{C}}$	Pipe	$\frac{\partial J}{\partial \boldsymbol{C}}$	Pipe	$\frac{\partial J}{\partial \boldsymbol{C}}$
2 - 3	-18.9520	2 - 3	-0.0078	2 - 3	17.7988
20 - 23	-2.9722	20 - 23	-0.0010	20 - 23	2.8642
3 - 20	-2.2070	3 - 20	-0.0008	3 - 20	2.0309
1 - 2	-1.5589	1 - 2	-0.0006	1 - 2	1.4415
23 - 24	-1.3453	17 - 18	-0.0006	23 - 24	1.3407
17 - 18	-1.1325	18 - 19	-0.0005	17 - 18	1.1870
18 - 19	-1.0161	16 - 17	-0.0005	18 - 19	1.0871
16 - 17	-0.9382	23 - 24	-0.0004	16 - 17	0.9889
28 - 29	-0.7692	25 - 32	-0.0004	25 - 32	0.9113
25 - 32	-0.7336	28 - 29	-0.0003	28 - 29	0.7454
31 - 32	-0.5537	3 - 19	-0.0003	3 - 19	0.5564
24 - 25	-0.5394	5 - 6	-0.0002	16 - 27	0.5124
3 - 19	-0.5224	4 - 5	-0.0002	24 - 25	0.5006
23 - 28	-0.4713	16 - 27	-0.0002	31 - 32	0.4974
5 - 6	-0.4462	31 - 32	-0.0002	5 - 6	0.4219
4 - 5	-0.4400	7 - 8	-0.0002	23 - 28	0.4193
7 - 8	-0.4263	3 - 4	-0.0002	4 - 5	0.4115
16 - 27	-0.3809	23 - 28	-0.0002	7 - 8	0.3929
3 - 4	-0.3577	24 - 25	-0.0002	3 - 4	0.3330
8 - 9	-0.3113	8 - 9	-0.0002	8 - 9	0.2920
29 - 30	-0.2248	9 - 10	-0.0001	29 - 30	0.2689
14 - 15	0.2241	29 - 30	-0.0001	9 - 10	0.1964
9 - 10	-0.2046	14 - 15	0.0001	14 - 15	-0.1445
15 - 16	0.1647	15 - 16	0.0001	26 - 27	0.1158
6 - 7	-0.0983	6 - 7	-0.0001	15 - 16	-0.1139
25 - 26	0.0901	26 - 27	-0.0000	6 - 7	0.0933
26 - 27	-0.0724	30 - 31	-0.0000	30 - 31	0.0425
30 - 31	-0.0443	10 - 14	-0.0000	25 - 26	0.0405
10 - 14	0.0052	25 - 26	0.0000	10 - 14	0.0236
10 - 11	-0.0000	10 - 11	0.0000	11 - 12	0.0000
11 - 12	0.0000	11 - 12	-0.0000	10 - 11	-0.0000
12 - 13	-0.0000	20 - 21	0.0000	12 - 13	-0.0000
20 - 21	0.0000	12 - 13	-0.0000	20 - 21	-0.0000
21 - 22	-0.0000	21 - 22	-0.0000	21 - 22	-0.0000

TABLE 2. Average computational time associated with linear state estimate approximation for Hanoi network case study

	Time (s)
State estimation via mathematical programming	0.7065
Sensitivity analysis computation	0.2345
Linear state estimate approximation from average state estimation	0.0001

List of Figures

1 Identifiability gradation for pipes with sensitivity above 50% percentile in Hanoi network case study 24

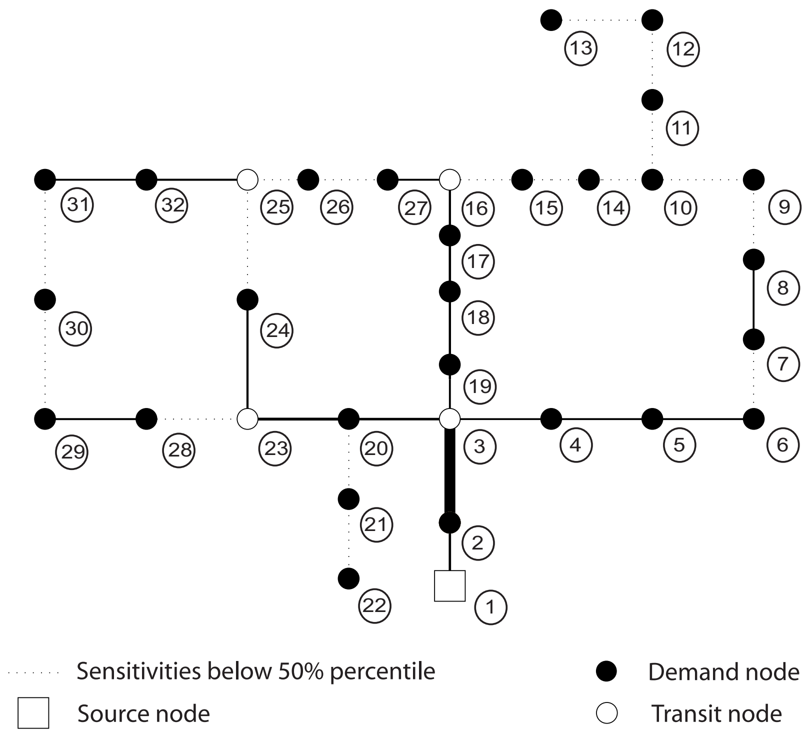

Fig. 1. Identifiability gradation for pipes with sensitivity above 50% percentile in Hanoi network case study