Parameter Estimation Algorithms for kinetic modelling from noisy measurements.

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Overview

Comparative study of optimization algorithms for parameter estimation of kinetic terms in models of bio-chemical processes.

- Definition of a Test Problem to obtain synthetic data.
- Test of several optimization functions available in Matlab Optimization Toolbox and Tomlab library.
- Add Gaussian noise to synthetic data and apply Morozov's Discrepancy Principle.
- Corrupt synthetic data by impulsive noise and solve by L1 norm minimization.

Parameter Estimation Problem

- Estimation of the parameter q of a model (state equation) :

$$\min_q J(u,q) \quad s.t. \quad c(u,q) = 0 \qquad \text{ODE-PDE model}$$

  - $q \in Q$ parameter to be estimated.
  - $u \equiv u(q)$ (state variable) is the unique solution of state equation $c(u,q) = 0$.

- Reduced problem: $\boxed{\min_q \widehat{J}(q)}$ where $\widehat{J}(q) \equiv J(u(q), q)$
- Some measurements $y \in Y$ of the state variable $u(q)$ are available i.e. $y = \mathcal{C}(u(q))$ where $\mathcal{C}$ is the observation operator that maps the state $u \in U$ into the measurements space Y.
- The data-fidelity term $\widehat{J}(q)$ is: $\boxed{\widehat{J}(q) \equiv \|F(q) - y\|}$ where $F(q) \equiv \mathcal{C}(u(q))$

Discrete Optimization Problem

- $\mathbf{q} \in \mathbb{R}^P$ vector of the parameters to estimated.
- $\mathbf{y}^\delta \in \mathbb{R}^N$ Noisy data.
- Discrete minimization problem: $\min_{\mathbf{q}} \widehat{J}(\mathbf{q})$
  - Gaussian Noise: Nonlinear Least Squares Problem

$$\widehat{J}(\mathbf{q}) \equiv \frac{1}{2}\|F(\mathbf{q}) - \mathbf{y}^\delta\|_2^2$$

  - Impulsive noise: L1 norm minimization

$$\widehat{J}(\mathbf{q}) \equiv \|F(\mathbf{q}) - \mathbf{y}^\delta\|_1$$

- $F(\mathbf{q})$ is obtained by:
  1. Solve the discrete state equation (ODE-PDE) model:

$$\text{find} \quad \mathbf{u} \quad s.t. \quad c(\mathbf{u}, \mathbf{q}) = 0$$

  2. Compute the values corresponding to the measurements $\mathbf{y}^\delta$ by applying the observation operator $\mathcal{C}(\mathbf{u}, \mathbf{q})$.

The Differential Model

$$\begin{aligned} \frac{\partial u}{\partial t} &= -\nu \frac{\partial u}{\partial z} + D \frac{\partial^2 u}{\partial z^2} - R(u, v, \boldsymbol{\theta}) \\ \delta_v \frac{\partial v}{\partial t} &= R(u, v, \boldsymbol{\theta}) \end{aligned} \tag{1}$$

where

$$R(u, v, \boldsymbol{\theta}) = \theta_1 \left(u - \frac{\theta_2 v}{\theta_3 - v} \right)$$

- Spatial Domain: $z \in [z_a, z_b]$
- δ_v retardation factor
- Boundary Conditions: $u(t, z_a) = u_a$, $\frac{\partial u}{\partial z}(t, z_b) = 0$,
- Initial Condition: $u(0, z) = u_0(z)$, $v(0, z) = v_0(z)$

Ref. D. Frascari et al. *Olive mill wastewater valorisation through Phenolic compounds adsorption in a continuous flow column* Chemical Engineering Journal, submitted.

Test Problem

- Model state equation:

$$\begin{cases} \frac{\partial u}{\partial t} = -\nu \frac{\partial u}{\partial z} + D\frac{\partial^2 u}{\partial z^2} - R(u, v, \boldsymbol{\theta}) + f_u \\ \delta_v \frac{\partial v}{\partial t} = R(u, v, \boldsymbol{\theta}) + f_v \end{cases} \quad (2)$$

- Parameter vector $\mathbf{q}_{true} = [\theta_1, \theta_2, \theta_3] = [1, 2, 3]$
- f_u and f_v defined by the given solution:

$$u(t, z) = e^{(-\pi^2 t)}(\sin(\pi z^2)) \cos(0.5\pi z^2), \quad v(t, z) = e(-\pi^2 t)(\sin(\pi z))$$

- Initial and boundary conditions defined by the solution (u, v).
- Retardation factor $\delta_v = 2.2$
- Time interval $[0, 0.1]$.
- Solved by the method of lines using matlab `ode15s`.
- Data $\mathbf{y} = F(\mathbf{q}_{true})$ computed in a uniformly spaced grid of $N_t \times N_z$ points.

Nonlinear Least Squares Problem

Gauss Newton - Levemberg Marquardt Iteration step:

$$\mathbf{q}^{(k+1)} = \mathbf{q}^{(k)} + \alpha_k \mathbf{s}_k$$

where

$$\left((J_F^{(k)})^t J_F^{(k)} + \lambda_k I\right) \mathbf{s}_k = -(J_F^{(k)})^t (F(\mathbf{q}^{(k)}) - \mathbf{y}^\delta)$$

- $0 < \alpha_k \leq 1$ damping parameters.
- $\lambda_k = 0$ for the Gauss Newon method.
- $J_F^{(k)}$ is the Jacobian matrix $(J_F^{(k)})_{i,j} = \partial F_i(\mathbf{q}) / \partial \mathbf{q}_j$
- Main computation step: approximation of the Jacobian
  - Finite differences method (forward-central): solve P or $2P$ forward problems (state equation).
  - General: available in optimization libraries.
  - Time-consuming.

Nonlinear Least Squares Problem

Quasi Newton Iteration step:

$$\mathbf{q}^{(k+1)} = \mathbf{q}^{(k)} + \alpha_k \mathbf{s}_k$$

where

$$H^{(k)}\mathbf{s}_k = -\nabla_{\mathbf{q}} \widehat{J}(\mathbf{q}^{(k)})$$
$$\text{compute} \quad H^{(k+1)} = H^{(k)} + S(\mathbf{q}^{(k)})$$

- BFGS update: $$S(\mathbf{q}^{(k)}) = \frac{v_k v_k^t}{v_k^t \mathbf{s}_k} - \frac{H^{(k)}\mathbf{s}_k \mathbf{s}_k^t H^{(k)}}{\mathbf{s}_k^t H^{(k)} \mathbf{s}_k}$$

  where $v_k = \nabla_{\mathbf{q}}(\widehat{J}(\mathbf{q}^{(k+1)})) - \nabla_{\mathbf{q}}(\widehat{J}(\mathbf{q}^{(k)}))$
- Initial definition $H^{(0)} = \gamma I$, γ scaling of the variables.
- $0 < \alpha_k \leq 1$ damping parameters.

Ref.

Experiments without data noise

Methods used:

- Gauss Newton Method. Stopping criterion:

$$G_F \mathbf{s}^{(k)} < \tau_F \text{ and } \|G_F\|_\infty < 10(\tau_F + \tau_X), \quad \|s^{(k)}\|_\infty < \tau_X$$

  where $G_F = 2(J_F^{(k)})^t (F(\mathbf{q}^{(k)}) - \mathbf{y}^\delta)$

- Quasi Newton BFGS. Stopping criterion:

$$\|\nabla \widehat{J}(\mathbf{q}^{(k)})\|_\infty < \tau_F (1 + \|\nabla \widehat{J}(\mathbf{q}^{(0)})\|_\infty)$$

$$\max_i \left(\frac{|q_i^{(k+1)} - q_i^{(k)}|}{1 + |q_i|} \right) < \tau_X$$

$\tau_F = \tau_X = 10^{-6}$

Experiments without data noise

- Initial parameter guess $\mathbf{q}_0 = \mathbf{q}_{true}(1 + \delta_q)$

	N_t	N_z	$\delta_q(\%)$	PRE	ResN	fval (it)
Gauss Newton	5	5	25	3.7589e-13	1.9595e-29	24(5)
	20	10	25	2.3943e-13	1.7037e-27	24(5)
	20	20	25	3.2203e-13	3.9651e-26	24(5)
	5	5	40	8.6163e-14	8.4433e-29	32(8)
	20	10	40	3.5806e-12	5.9765e-26	32(7)
	20	20	40	3.3278e-12	1.6605e-24	32(8)

	N_t	N_z	$\delta_q(\%)$	*PRE*	*ResN*	fval (it)
Quasi Newton BFGS	5	5	25	1.2708e-02	2.8781e-09	80(18)
	20	10	25	1.3880e-02	3.0633e-08	80(18)
	20	20	25	1.2106e-04	5.4168e-12	116(28)
	5	5	40	5.1000e-02	3.9129e-08	104(24)
	20	10	40	4.0196e-04	3.0938e-11	132(28)
	20	20	40	6.9894e-04	1.9933e-10	120(26)

$PRE = \|\mathbf{q}_{true} - \mathbf{q}_{it}\| / \|\mathbf{q}_{true}\|$, $ResN = \|F(\mathbf{q}_{it}) - \mathbf{y}\|$

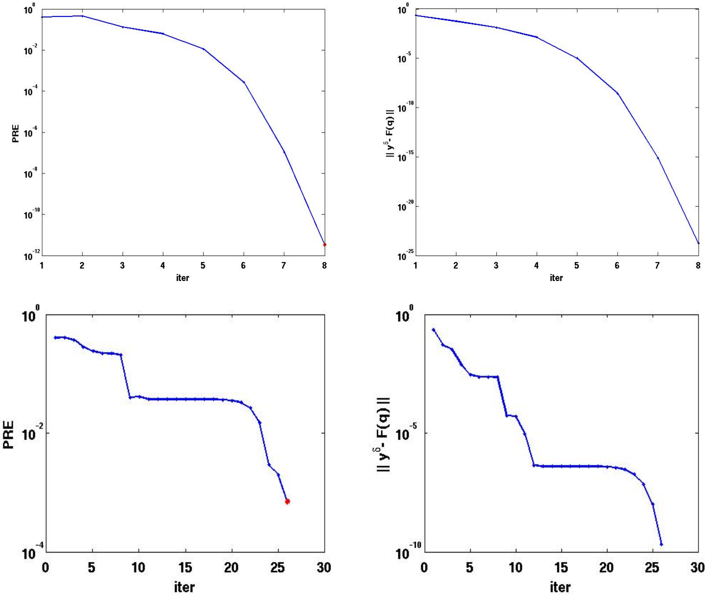
Convergence Plots: $\delta_q = 40\%$, $N_t = N_z = 20$

Gauss

Newton

Quasi

Newton



Case $N_t = 20$, $N_z = 10$, $\delta_q = 25\%$

Gaussian random noise of level δ:

$$\mathbf{y}^\delta = \mathbf{y} + \delta\|\mathbf{y}\|\boldsymbol{\eta}, \qquad \|\eta\| = 1$$

Gauss Newton

δ	PRE	$\|F(\mathbf{q}) - \mathbf{y}^\delta\|$	fval(it)
1e-6	8.6040e-5	9.5454e-11	24(6)
1e-4	8.6964e-3	9.5455e-07	24(6)
1e-3	**9.6303e-2**	9.5466e-05	24(6)
5e-3	9.1788e-1	2.3879e-03	28(7)

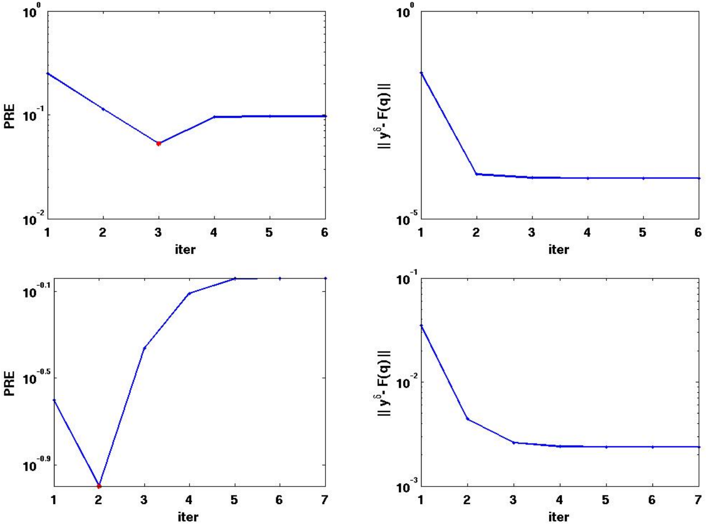
Quasi Newton

δ	PRE	$\|F(\mathbf{q}) - \mathbf{y}^\delta\|$	fval(it)
1e-6	1.3879e-02	3.1096e-8	80(18)
1e-04	1.3943e-02	9.8731e-7	80(18)
1e-3	**9.1184e-3**	9.7764e-5	124(28)
5e-03	2.0990e-01	2.4125e-3	132(31)
1e-02	2.9171e-01	9.7249e-3	136(32)

Convergence Plots: Gauss Newton

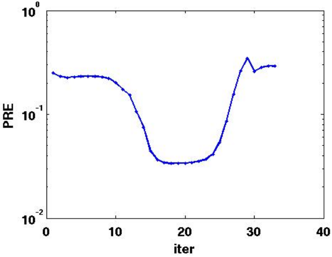
$\delta = 0.001$

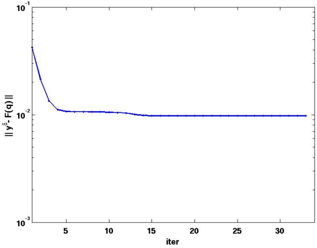
$\delta = 0.005$



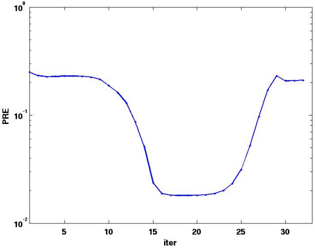
Convergence Plots: Quasi Newton BFGS

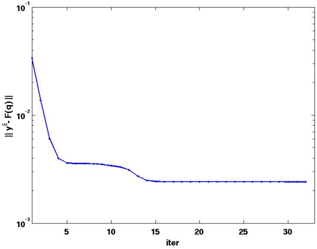
$\delta = 0.01$





$\delta = 0.005$





Regularization of semiconvergent iterations

- Semiconvergent error curve for BFGS.
- Improve the solution quality by suitable stopping rules.

Morozov's Discrepancy Principle (MDP).
When using MDP to compute a regularized solution of an iterative method, we stop the iterations at an index d s.t.

$$\|F(\mathbf{q}_d) - \mathbf{y}^\delta\| \leq \sigma(\delta), \quad \sigma(\delta) \simeq \delta \tag{3}$$

The success of this method is based on the correct estimation of the noise level δ.
Proposed stopping rule (SR_d):

$$\boxed{|J_k - J_{k-1}| < \tau|J_2 - J_1|, \quad \tau = 10^p, \quad p = \lceil \log_{10}(J_2^3) \rceil}$$

where $J_k = \widehat{J}(\mathbf{q}_k)$

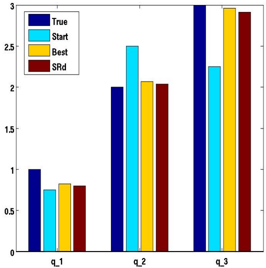
Quasi Newton BFGS with SR_d

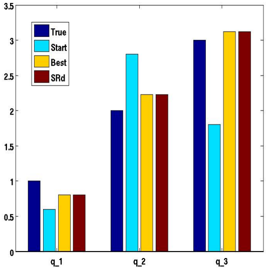
Results with $N_t = 20$, $N_z = 10$, $\delta_q = 25\%$

δ	PRE	fval(it)	PRE_{opt}	it	PRE_d	d
1e-6	1.3879e-2	80(18)	1.3853e-2	18	1.3963e-2	17
1e-4	1.3943e-2	80(18)	1.3912e-2	18	1.4037e-2	17
1e-3	1.5598e-1	132(30)	1.0628e-2	24	1.6370e-2	17
5e-3	2.0990e-01	132(31)	1.7999e-02	18	1.8132e-02	17
1e-2	2.9171e-01	136(32)	3.3698e-02	18	3.4146e-02	17

$\delta = 1e-2$

$\delta_q = 25\%$





$\delta = 1e-2$

$\delta_q = 40\%$

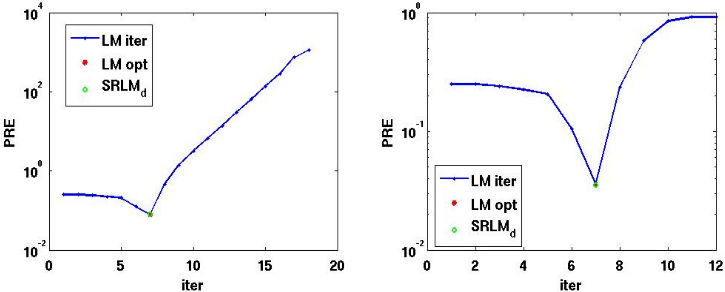
Regularization by Levemberg Marquardt

$$\left((J_F^{(k)})^t J_F^{(k)} + \lambda_k I\right) \mathbf{s}_k = -(J_F^{(k)})^t (F(\mathbf{q}^{(k)}) - \mathbf{y}^\delta)$$

- $\lambda_k = \lambda_0 10^{-k}$, $\lambda_0 > 0$ (Matlab)
- Proposed stopping rule ($SRLM_d$):

$$\boxed{|J_k - J_{k-1}| < \tau |J_2 - J_1|, \quad \tau = 10^p, \quad p = \lceil \log_{10}(J_2) \rceil}$$

$\delta = 0.01$ $\delta = 0.005$



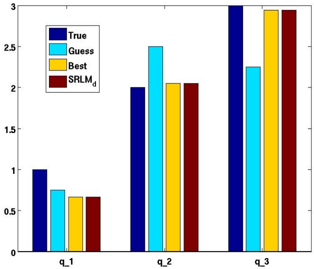
Regularization by Levemberg Marquardt

Levemberg Marquardt

δ	PRE	fval(it)	PRE_{opt}	it	PRE_d	d	λ_0
1e-4	9.5455e-07	32(7)	1.5835e-3	5	1.5835e-3	5	0.01
1e-3	9.6323e-2	32(7)	1.0942e-2	4	4.270019e-2	5	0.1
5e-3	9.1834e-1	48(11)	3.5532e-2	7	3.5532e-2	7	1
1e-2	1.1286e+3	72(17)	7.9780e-2	7	7.9780e-2	7	10

$\delta = 1e-2$

$\delta_q = 25\%$

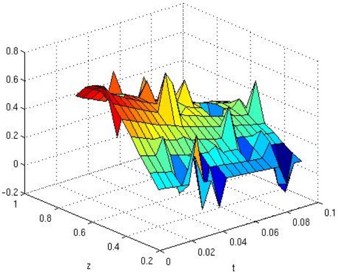


Data Corrupted by Impulsive Noise

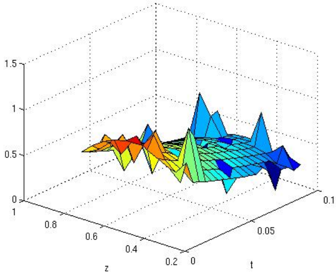
Given $\boldsymbol{\eta}$ vector with $\{0, \pm 1\}$ elements, define $\mathbf{y}^\delta$ corrupted by impulsive noise of level δ, as:

$$\mathbf{y}^\delta = \mathbf{y} + \delta \|\mathbf{y}\| \boldsymbol{\eta}, \quad \sum_i (|\eta_i|) = \lceil P \cdot N_t \cdot N_z \rceil, \quad P < 1$$

$\mathbf{y}_u^\delta$



$\mathbf{y}_v^\delta$



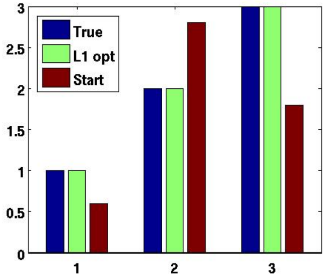
Case $N_t = 20,\ N_z = 10$

- Problem solved by `Tomlab` Solver `L1solve`:

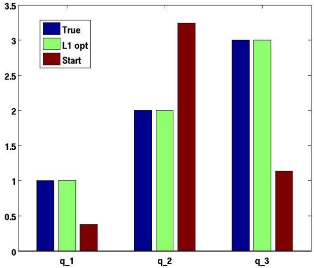
$$\min \|F(\mathbf{q}) - \mathbf{y}^\delta\|_1 \quad \Rightarrow \quad \min \sum_i w_i \ s.t. \ -\mathbf{w} \le F(\mathbf{q}) - \mathbf{y}^\delta \le \mathbf{w}$$

$P\%$	$\delta\%$	$\delta_p\%$	PRE	$\|F(\mathbf{q}) - \mathbf{y}\|_1$	fval(it)
80	50	40	1.4281e-12	8.3817e-12	15(13)
80	50	60	1.0567e-08	2.8787e-09	16(13)
80	50	62	1.9426e-06	7.5940e-07	39(27)

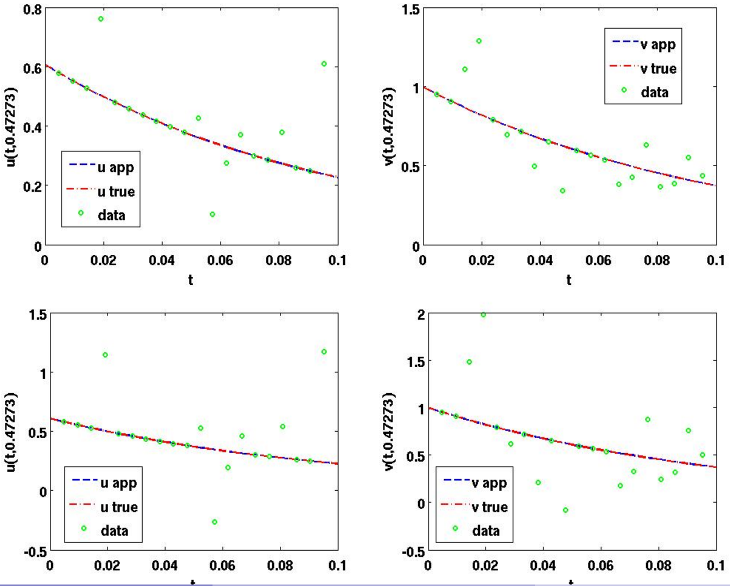
$\delta_p = 40\%$



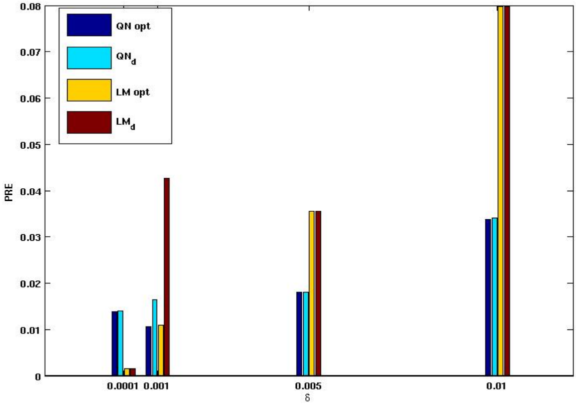
$\delta_p = 62\%$



Case $N_t = 20$, $N_z = 10$



Gaussian Random Noise



Low noise $\Rightarrow$ Levemberg Marquardt,

Medium-High noise $\Rightarrow$ Regularized BFGS

Final Remarks

- Computation Times ($\mathit{Intel}\ i5\ \mathit{CPU}, 1.60\mathit{GHz}\ x\ 4,\ 8\ \mathit{Gb}\ \mathit{RAM}$):
  - Gauss Noise $\delta = 0.01$:

$$QN\ BFGS + SR_d = 78\ sec. \quad LM + LMSR_d = 35\ sec.$$

  - Impulsive Noise $\delta_p = 40\%$:

$$\texttt{Tomlab}\ \ \texttt{L1Solve} = 63\ sec.$$

- Further steps:
  - Solve a regularized optimization problem:

$$\min_{\mathbf{q}} \widehat{J}(\mathbf{q}) + \alpha \mathcal{R}(\mathbf{q})$$

  - Application to Real Data.

Thanks for your attention