Levenberg-Marquardt method for nonlinear least-squares problems with noisy function and gradient

Elisa Riccietti

Institut de Recherche en Informatique de Toulouse (IRIT)

Joint work with: Stefania Bellavia (Università di Firenze), Serge Gratton (INPT-ENSEEIHT, Toulouse)

Institut de Recherche en Informatique de Toulouse
CNRS
INPT
UPS
UT1

Manchester, 23 January 2018

Large scale problems with noisy function and noisy gradient

Let us consider the following nonlinear least squares problem:

$$\min_{x \in \mathbb{R}^n} f(x) = \frac{1}{2}\|F(x)\|^2$$

where $F : \mathbb{R}^n \to \mathbb{R}^N$ with $N \geq n$, continuously differentiable.

Noisy function and noisy gradients

We are interested in **large scale** problems for which either:

- exact values for the function and the gradient are not available,
- computing exact values is computationally demanding.

Function approximations

- We want to rely on cheap approximations f_δ to f of known accuracy.
- We consider an iterative process that employs a sequence of approximations $\{f_{\delta_k}\}$ and at each iteration k considers an approximated problem:

$$\min_{x\in\mathbb{R}^n} f_{\delta_k}(x) = \frac{1}{2}\|F_{\delta_k}(x)\|^2, \quad F_{\delta_k} \sim F$$

- δ_k is the accuracy level of the approximations:

$$|f_{\delta_k}(x_k) - f(x_k)| \leq \delta_k.$$

- We assume that the accuracy level can be improved along the optimization process: $\delta_k \searrow 0$.

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Notations

- J_{δ_k} approximation to the Jacobian matrix J of F,
- g_{δ_k} approximation to the gradient g of f.

Typical applications

Subsampling techniques

- Machine learning, Data assimilation.
- Large set of data at disposal: $\{1, \dots, N\}$.
  Subsampling: $X_k \subseteq \{1, \dots, N\}$ such that $|X_k| = K_k \leq N$ is selected.
- $F_{\delta_k} : \mathbb{R}^n \to \mathbb{R}^{K_k}$ such that $(F_{\delta_k})_i = F_j$, $j \in X_k$ is built.
- $f_{\delta_k}(x) = \frac{1}{2}\|F_{\delta_k}(x)\|^2$
- approximation can be improved by considering more observations.

Iterative methods

- f is the result of an iterative process (solution of a nonlinear equation or an inversion process) that can be stopped when a certain accuracy level is reached.
- By varying the stopping criterion we vary the accuracy of the approximation.

We propose a **Levenberg-Marquardt method**.

Algorithm : k-th iteration

1. Step computation: define the LM model

$$\min_{p\in\mathbb{R}^n} m_k(x_k+p) = \frac{1}{2}\|F_{\delta_k}(x_k)+J_{\delta_k}(x_k)p\|^2 + \frac{1}{2}\lambda_k\|p\|^2,$$

   and compute the step p_k^{LM}.
2. Check the noise level. If noise is too high reduce it.
3. Step acceptance is based on $\rho_k^{\delta_k}(p_k^{LM}) = \frac{f_{\delta_{k-1}}(x_k)-f_{\delta_k}(x_k+p_k^{LM})}{m_k(x_k)-m_k(x_k+p_k^{LM})}$.
4. Regularization parameter update.

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1) The step

- The step is the solution of the linearized least squares subproblem:

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  where $\lambda_k > 0$ is an appropriately chosen regularization parameter.
- This is equivalent to:

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- Large scale problems: an inexact step is computed.
- For a residual, $\|r_k\|\leq \epsilon_k\|g_{\delta_k}\|$ with ϵ_k small enough, the step achieves the Cauchy decrease:

$$m_k(x_k)-m_k(x_k+p)\geq \frac{\theta}{2}\frac{\|g_{\delta_k}(x_k)\|^2}{\|J_{\delta_k}(x_k)\|^2+\lambda_k}, \qquad \theta>0.$$

  which is sufficient to get global convergence.

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2) Noise control

Assumption

1. It exists $\bar{K} > 0$ and $\delta_k \geq 0$, such that:

$$|f_{\delta_k}(x_k) - f(x_k)| = \left| \frac{1}{2}\|F_{\delta_k}(x_k)\|^2 - \frac{1}{2}\|F(x_k)\|^2 \right| \leq \delta_k,$$

$$\|g(x_k) - g_{\delta_k}(x_k)\| \leq \bar{K}\delta_k.$$

2. It is possible to drive δ_k to zero.

- The optimization process starts with a given initial noise level $\delta = \delta_0$.
- **Noise control**: our method relies on a mechanism to control the noise: at each iteration the noise is measured and reduced if it is judged to be too large.

2) Noise control

- Given the noise level δ_k, in [Trust region methods, Conn, Gould, Toint] this condition is used:

$$\delta_k \leq \eta_0[m_k(x_k) - m_k(x_k + p_k^{LM})],$$

with η_0 appropriately chosen, to ensure a true reduction in the noise-free objective function f.

- $m_k(x_k) - m_k(x_k + p_k^{LM}) = O(\lambda_k \|p_k^{LM}\|^2)$.
- Noise control:

$$\delta_k \leq \kappa_d \lambda_k^{\alpha} \|p_k^{LM}\|^2,$$

for suitable constants $\kappa_d > 0$ and $\alpha \in \left[\frac{1}{2}, 1\right)$.

- The noise tends to zero:

$$\lim_{k \to \infty} \lambda_k \|p_k^{LM}\|^2 = 0.$$

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4. Regularization parameter update.

3) Step acceptance

Step acceptance based on ratio between actual and predicted reduction:

$$\rho_k^{\delta_k}(p_k^{LM}) = \frac{f_{\delta_{k-1}}(x_k) - f_{\delta_k}(x_k + p_k^{LM})}{m_k(x_k) - m_k(x_k + p_k^{LM})}.$$

Given $0 < \eta_1 < 1$.

1. If $\rho_k^{\delta_k}(p_k^{LM}) \geq \eta_1$, accept the step: $x_{k+1} = x_k + p_k^{LM}$,
2. Otherwise reject the step: $x_{k+1} = x_k$.

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4) Parameter update

The parameter update is inspired by [Bergou, Gratton, Vicente, 2016] and [Bandeira, Scheinberg, Vicente, 2014].

Given $\gamma > 1$

- Successful step:

$$\lambda_{k+1} = \begin{cases} \min\{\gamma\lambda_k, \lambda_{\max}\} & \text{if } \|g_{\delta_k}(x_k)\| < \eta_2/\lambda_k, \\ \lambda_k & \text{if } \|g_{\delta_k}(x_k)\| \geq \eta_2/\lambda_k. \end{cases}$$

- Unsuccessful step:

$$\lambda_{k+1} = \gamma\lambda_k.$$

We increase the parameter even in case of successful iterations.

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We increase the parameter even in case of successful iterations.

$$\frac{\|g(x_k)\|}{(1+c_k)} \leq \|g_{\delta_k}(x_k)\| \leq \frac{\|g(x_k)\|}{(1-c_k)}, \text{ with } c_k = O\left(\frac{1}{\lambda_k^{1-\alpha/2}}\right).$$

Theoretical results

Assumptions

- Assumption 1:
  Function f is continuously differentiable, and it exists $\kappa_J > 0$ such that for all $k \geq 0$ and all $x \in [x_k, x_k + p_k^{LM}]$, $\|J_{\delta_k}(x)\| \leq \kappa_J$.
- Assumption 2: f has Lipschitz continuous gradient:
  $\|g(x) - g(y)\| \leq L\|x - y\|$ for all $x, y \in \mathbb{R}^n$.

Global Convergence

Let the residual be small enough, i.e. r_k satisfies $\|r_k\| \leq \epsilon_k \|g_{\delta_k}\|$, with

$$\epsilon_k \leq \min\left\{\frac{\theta_1}{\lambda_k^{\alpha}}, \sqrt{\theta_2 \frac{\lambda_k}{\|J_{\delta_k}(x_k)\|^2 + \lambda_k}}\right\}$$

where $\theta_1 > 0$, $\theta_2 \in \left(0, \frac{1}{2}\right]$ and $\alpha \in \left[\frac{1}{2}, 1\right)$.

Lemma

The sequences $\{\delta_k\}$ and $\{x_k\}$ generated by the Algorithm are such that

$$\lim_{k\to\infty} \delta_k = 0, \qquad \lim_{k\to\infty} \|g(x_k)\| = 0.$$

Local convergence

Asymptotic step behaviour

The LM step asymptotically tends to the direction of the negative perturbed gradient:

$$\lim_{k\to\infty}(p_k^{LM})_i + \frac{\theta}{\kappa_J^2+\lambda_k}(g_{\delta_k}(x_k))_i = 0 \quad \text{for} \quad i = 1,\dots,n,$$

where $(\cdot)_i$ denotes the i-th vector component.

Lemma

Let $p_k^{SD} = -\frac{\theta}{\kappa_J^2+\lambda_k} g_{\delta_k}(x_k)$ *and* $x_{k+1} = x_k + p_k^{SD}$. *If* $x_{\bar{k}} \in B_r(x^*)$ *and* $\lambda_{\bar{k}}$ *big enough,*

- $\|x_{k+1} - x^*\| < \|x_k - x^*\|$, *for all* $k \geq \bar{k}$.
- $\|x_k - x^*\|$ *tends to zero.*

Complexity analysis

Assumption

Let assume that the procedure is stopped when $\|g_{\delta_k}(x_k)\| \leq \epsilon$.

- The number of successful iterations N_1 is bounded above by:

$$N_1 \leq f_{\delta_{k_s-1}}(x_{k_s}) \frac{2}{\eta_1} \frac{\kappa_J^2 + \lambda_{\max}}{\theta \epsilon^2} = O(\epsilon^{-2}).$$

- The number of unsuccessful iterations N_3 is bounded above by a constant independent of ϵ:

$$N_3 \leq \frac{\log \frac{\lambda_{\max}}{\lambda_0}}{\log \gamma}.$$

Complexity

Standard Levenberg-Marquardt methods complexity is preserved:

$$N_T = O(\epsilon^{-2}),$$

Numerical Results

Test problems

We consider two problems of the form

$$\min_{x\in\mathbb{R}^n} f(x) = \frac{1}{2}\|F(x)\|^2 + \frac{1}{2}\|x\|^2 = \sum_{j=1}^{N} F_j(x)^2 + \frac{1}{2}\|x\|^2,$$

with $F_j : \mathbb{R}^n \to \mathbb{R}$, for $j = 1, \dots, N$, N total number of samples.

- P1: Data assimilation problem
- P2: Machine learning problem

Approximations

- Function approximations are built by means of a random subsampling.
- $J_{\delta_k}(x) \in \mathbb{R}^{K_k \times n}$ is the Jacobian matrix of $F_{\delta_k}(x)$.
- $g_{\delta_k} \in \mathbb{R}^n$ the gradient of f_{δ_k}.

Linear algebra phase

- CGLS method.
- $\|r_k\| \leq \epsilon_k \|g_{\delta_k}(x_k)\|$, $\epsilon_k \sim 10^{-1}$.

Performance evaluation criteria

We compare subsampled Levenberg-Marquardt method **(SSLM)** and full Levenberg-Marquardt method **(FLM)** ($K_k = N, \forall k$).

Cost counters

We evaluate savings arising from the employment of the noise control strategy.

- $cost_f$ weighted counter of function evaluations costs (if $|X_k| = N$ cost=1, if $|X_k| = K_k$ cost=K_k/N.) $\rightarrow$ $save_f$ savings in function evaluations.
- $cost_p$ weighted counter of products costs (if $|X_k| = N$ cost=1, if $|X_k| = K_k$ cost=K_k/N.) $\rightarrow$ $save_p$ savings in products.

Given the current sample set X_k, s.t. $|X_k| = K_k$.

Noise update

Given the step, check the noise: $\delta_k \leq \kappa_d \lambda_k^{\alpha} \|p_k^{LM}\|^2$?
If not, repeat:

1. Increase the samples set size: $|X_{k+1}| = K_* |X_k|$.
2. Recompute function, Jacobian and gradient.
3. Need to check condition again $\rightarrow$ Need to recompute the step: $(J_{\delta_k}(x_k)^T J_{\delta_k}(x_k) + \lambda_k I) p_k = -g_{\delta_k}(x_k) + r_k$.

$\rightarrow$ Resulting samples set size: $|X_{k+1}| = K_*^{n_k} |X_k|$.

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Parameters affecting the cost

- $\delta_k \leq \kappa_d \lambda_k^\alpha \|p_k^{LM}\|^2$.
- $|X_{k+1}| = K_*^{n_k} |X_k|$.

Nonlinear wave equation:

$$\begin{aligned}
&\frac{\partial^2 u(z,t)}{\partial t^2} - \frac{\partial^2 u(z,t)}{\partial z^2} + \mu e^{\nu u} = 0,\\
&u(0,t) = u(1,t) = 0,\\
&u(z,0) = u_0(z),\ \frac{\partial u(z,0)}{\partial t} = 0,\\
&0 \le t \le T,\ 0 \le z \le 1.
\end{aligned}$$

- We look for the initial state $u_0(z)$, from the knowledge of observations $u(z_i, t_j)$, $t_j > 0$.
- We consider a mesh involving $n = 360$ grid points for the spatial discretization and $N_t = 64$ for the temporal one.
- We assume to have an observation at each grid point: $N = n \times N_t = 23040$.

P1: Data assimilation problem

It is possible to recover $u_0(z)$ solving the following data assimilation problem:

$$\min_{x\in\mathbb{R}^n} \frac{1}{2}\|x - x_b\|^2_{B^{-1}} + \frac{1}{2}\sum_{j=0}^{N_t} \|H_j(x(t_j)) - y_j\|^2_{R_j^{-1}}$$

- $\|x\|^2_M = x^T M x$ for a symmetric positive definite matrix M,
- $x_b \in \mathbb{R}^n$ is the background vector (a priori estimate)
- $y_j \in \mathbb{R}^{m_j}$ is the vector of observations at time t_j, $m_j \leq n$.
- H_j is the operator modelling the observation process at t_j
- $x(t_j)$ the state vector, solution of the nonlinear model at time t_j.

P1: Data assimilation problem

- Background vector and observations from a chosen initial true state by adding noise $N(0, \sigma_b^2)$ and $N(0, \sigma_o^2)$ with $\sigma_b = 0.2$, $\sigma_o = 0.05$.
- Covariances matrices are diagonal: $B = \sigma_b^2 I_n$ and $R_j = \sigma_o^2 I_{m_j}$ $\forall j$.
- Least-squares problem reformulation:

$$F(x) = \begin{bmatrix} \frac{1}{\sigma_o}(H_0(x(t_0)) - y_0) \\ \vdots \\ \frac{1}{\sigma_o}(H_{N_t}(x(t_{N_t})) - y_{N_t}) \end{bmatrix}$$

where $(H_j(x(t_j)) - y_j) \in \mathbb{R}^{m_j}$ for $j = 1, \dots, N_t$.

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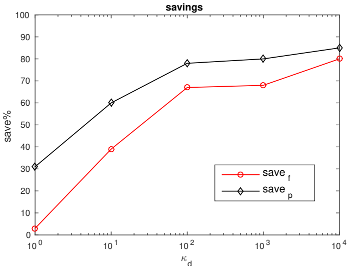
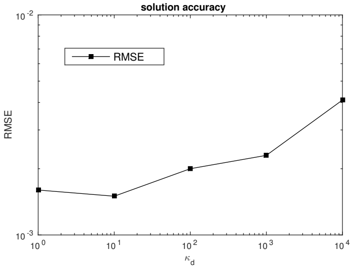
where $(H_j(x(t_j)) - y_j) \in \mathbb{R}^{m_j}$ for $j = 1, \dots, N_t$.

- Kept $K_* = 1.5$ fixed, we study the effect of κ_d.

P1: effect of κ_d

$K_0 = 2000$ $K_* = 1.5$	FLM	SSLM $\kappa_d = 1$	$\kappa_d = 10$	$\kappa_d = 100$	$\kappa_d = 1000$	$\kappa_d = 10000$
it	9	11	12	12	12	11
$\mathbf{CG_{it}}$	2.4	5.4	4.9	4.2	4.2	3.9
$\mathbf{cost_f}$	10	9.7	6.1	3.3	3.2	2.0
$\mathbf{cost_p}$	67	46.1	26.8	14.9	13.5	10.3
$\lvert\mathbf{X_{it}}\rvert$	23040	15188	6750	3000	3000	2000
RMSE	1.2e-2	3.0e-2	2.8e-2	3.8e-2	4.4e-2	7.8e-2
$\mathbf{save_f}$		3%	39%	67%	68%	80%
$\mathbf{save_p}$		31%	60%	78%	80%	85%





P2: Machine learning problem

Binary classification problem: $\{(z^i, y^i)\}$ with $z^i \in \mathbb{R}^n$, $y^i \in \{-1, +1\}$ and $i = 1, \ldots, N$.
Training objective function: logistic loss with l_2 regularization

$$f(x) = \frac{1}{2N} \sum_{i=1}^{N} \log(1 + \exp(-y^i x^T z^i)) + \frac{1}{2N} \|x\|^2.$$

Least-squares form:

$$F(x) = \frac{1}{N} \begin{bmatrix} \sqrt{\log(1 + \exp(-y^1 x^T z^1))} \\ \vdots \\ \sqrt{\log(1 + \exp(-y^N x^T z^N))} \end{bmatrix}.$$

Approximations to f are built as:

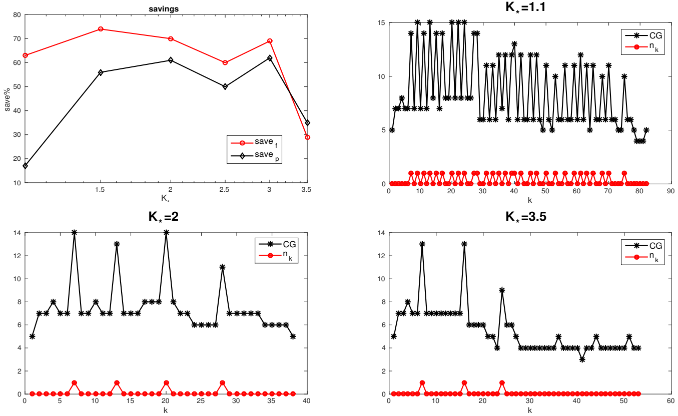
$$f_{\delta_k}(x) = \frac{1}{2K_k} \sum_{i \in X_k} \log(1 + \exp(-y^i x^T z^i)) + \frac{1}{2K_k} \|x\|^2.$$

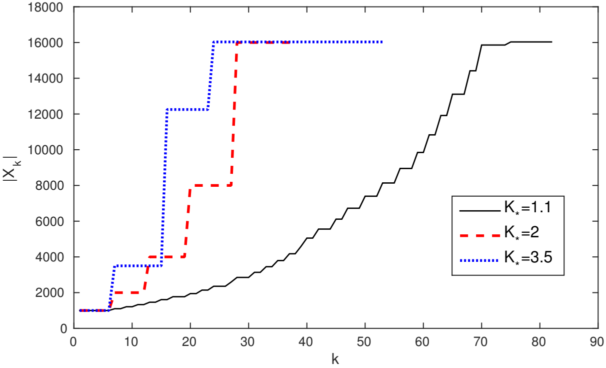
We consider the **CINA dataset** [http://www.causality.inf.ethz.ch/data/CINA.html], for which $n = 132$, $N = 16033$ for the training set, $\tilde{N} = 10000$ for the testing set.

Noise control condition parameters

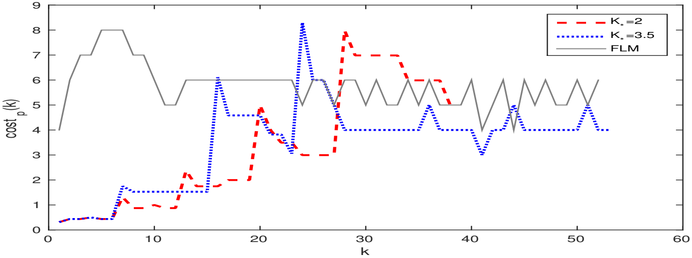
- $K_0 = 132$.
- $\kappa_d = 10$.
- We study the effect of K_*.

	FLM	SSLM					
		$K_* = 1.1$	$K_* = 1.5$	$K_* = 2$	$K_* = 2.5$	$K_* = 3$	$K_* = 3.5$
it	52	82	43	38	39	34	53
$\mathbf{CG_{it}}$	5.7	8.5	8.0	7.5	7.3	7.2	5.5
$\mathbf{cost_f}$	53	19.8	14.1	15.9	21.2	16.5	37.7
$\mathbf{cost_p}$	808	671.2	351.3	316.7	400.7	310.4	521.1
RMSE	6.0e-2	1.0e-1	6.6e-2	5.4e-2	4.7e-2	4.1e-2	3.9e-2
$\mathbf{save_f}$		63%	74%	70%	60%	69%	29%
$\mathbf{save_p}$		17%	56%	61%	50%	62%	35%





18000
16000
14000
12000
10000
8000
6000
4000
2000
0
0 10 20 30 40 50 60 70 80 90
k
|X_k|
K_*=1.1
K_*=2
K_*=3.5



9
8
7
6
5
4
3
2
1
0
0 10 20 30 40 50 60
k
cost_p(k)
K_*=2
K_*=3.5
FLM

For more details:

A Levenberg-Marquardt method for large nonlinear least-squares problems with dynamic accuracy in functions and gradients, Stefania Bellavia, Serge Gratton, Elisa Riccietti, under review in Numerische Mathematik

THANK YOU FOR YOUR ATTENTION!