Data assimilation and optimization for non-linear regression problems in tokamak plasma equilibrium

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Outline

I do not pretend to be complete. My aim is to supply some information and potential useful links to other fields (Mathematics, Meteorology, Engineering, Numerical Analysis and Optimization) where similar problems are analysed.

Outline

- Problem and notation
- Some useful Theorems
- Data assimilation
  - Hindcast vs Forcast (meteo problems)
  - Stochastic nature of the problem (nonlinear regression)
  - Discrete problem
    - Constrained regularised Least-Squares
    - Iterative methods: Adjoint method, Interior Point methods, ...
    - SQD matrices
    - Energy norms of errors and Probabilistic stopping criteria (linear regression problem) for iterative methods
- Summary

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Semilinear elliptic equations

Let $\Omega \subset \mathrm{R}^n$ bounded and with smooth boundary Γ.

$$\begin{aligned} \mathscr{L} u &= f(u) \quad \text{in } \Omega \\ u &= 0 \quad \text{on } \Gamma \end{aligned}$$

where

$$\mathscr{L} u = -\mathbf{div}(\alpha(x)\mathbf{grad} u) + s(x)u \qquad s(x) \in L^\infty(\Omega),\ s(x) \geq 0.$$

$$(\star)\ \boxed{f : \mathrm{R} \to \mathrm{R},\ \ |f(t)| \leq a + b|t|^{2^*-1},\ \forall t \in \mathrm{R}\ a, b \geq 0, \quad 2^* = \frac{2n}{n-2}}$$

In weak form we have

$$\int_\Omega \alpha(x)\nabla u \nabla v + \int_\Omega s(x)uv \qquad \forall v \in H_0^1(\Omega)$$

is continuous and coercive in $H_0^1(\Omega)$.

Semilinear elliptic equations

Let

$$F(t) = \int_0^t f(s)\mathbf{d}s.$$

The critical points of

$$J(u) = \frac{1}{2}\int_\Omega |\nabla u|^2 \mathbf{d}x + \frac{1}{2}\int_\Omega s(x)u^2 \mathbf{d}x - \int_\Omega F(u)\mathbf{d}x$$

are the solutions of

$$\int_\Omega \nabla u \nabla v \mathbf{d}x + \int_\Omega s(x)uv\mathbf{d}x - \int_\Omega f(u)v\mathbf{d}x = 0$$

Mountain pass Theorem

MP-1 $J \in C^1(H_0^1(\Omega), \mathbb{R})$, $J(0) = 0$ and $\exists r, \rho > 0$ such that $J(u) \geq \rho \ \forall u \in S_r = \{u \in H_0^1(\Omega) \ : \ \|u\| = r\}$

MP-2 $\exists e \in H_0^1(\Omega)\ \|e\| > r$ s.t. $J(e) \leq 0$

Palais-Smale conditions

$(\bigstar) \quad \Rightarrow$

for all $\quad \|u_k\|_{H_0^1(\Omega)} \leq C\ \forall k$ then $\exists u_{k_i}(x) \to u(x)$

a.e. in Ω (Palais-Smale)

Mountain pass Theorem

$H_0^1(\Omega) \hookrightarrow L^q(\Omega) \;\; \forall q \in \left[1, \frac{2n}{n-2}\right)$ compact.

We have existence also for $\frac{2n}{n-2}$ P.L. Lions 1981. Very difficult numerically Budd,Humphries, Wathen 1999.

$|f(t)| \leq a + b|t|^p \;\; p > \frac{2n}{n-2} - 1$ NO SOLUTION Pohozaev1965

Mountain pass Theorem

Theorem mountain pass Ambrosetti-Malchiodi 2003

Let J satisfy MP-1 and MP-2 and PS condition. Let

$$\boxed{\Upsilon = \left\{\gamma \in C\big([0,1], H_0^1(\Omega)\big) : \gamma(0) = 0, \;\; \gamma(1) = e\right\}}.$$

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$\Upsilon \neq \emptyset \quad \gamma(t) = te \in \Upsilon$

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$$c = \inf_{\gamma\in\Upsilon} \max_{t\in[0,1]} J\big(\gamma(t)\big)$$

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From MP-1 and since any γ crosses S_r we have

$$c \geq \min_{u\in S_r} J(u) \geq \rho > 0$$

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$$c = \inf_{\gamma \in \Upsilon} \max_{t \in [0,1]} J\big(\gamma(t)\big)$$

Then c is a positive critical level for J, and exists $z \in H_0^1(\Omega)$ s.t. $J(z) = c$ and $J'(z) = 0$, with $z \neq 0$ a.e.

Problem and notation

Let $\Omega \subset \mathrm{R}^n$ bounded and with smooth boundary Γ.

$$f(x,s) : \Omega \times \mathrm{R} \longrightarrow \mathrm{R} \ \text{ s.t.}$$

$$\begin{array}{ll} f(x,s) = 0 & \forall s \leq 0, \quad x \in \Omega \\ f(x,s) > 0 & \forall s > 0, \quad x \in \Omega \end{array}$$

$$\lim_{s \to +\infty} \frac{f(x,s)}{s^p} = 0 \qquad \text{uniformly in } \Omega$$

$$p = \frac{n}{n-2}, \quad n > 2, \quad \text{or for some } p \text{ if } \ n = 2.$$

Problem and notation

Problem: Given Ω, f as above and $\lambda, I \in \mathrm{R}^+$ find $u \in H^1(\Omega)$ and $k \in \mathrm{R}$ s.t.

$$\begin{aligned}
\mathscr{L} u &= \lambda f(x,u) && \textit{in } \Omega \\
u &= -k && \textit{on } \Gamma \\
-\int_\Gamma \frac{\partial u}{\partial \nu} \mathbf{d}\Gamma &= I && \nu \text{ outer normal at } \Gamma.
\end{aligned}$$

Some useful Theorems

$$f_+ = f_+(x) = \liminf_{s \to +\infty} f(x,s) \qquad f_+ = +\infty \text{ is allowed.}$$

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Theorem 1

(i)

$$\int_\Omega f_+ = +\infty$$

Problem has solution $\forall\ I$

(ii)

$$\int_\Omega f_+ < +\infty$$

$\exists b \geq \lambda \int f_+$ s.t.
Problem has solution $\forall\ 0 < I < b$

Teman 1979, Ambrosetti Mancini 1980, Berestycki Brezis 1980

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Some useful Theorems

Theorem 2

Let λ_1 the first eigenvalue of $\mathscr{L} u = \lambda_1 u, \;\; u_{|\Gamma} = 0.$

(i) Let assume $\exists \beta > 0$ s.t. $f(x, s) \leq \beta s, \; \forall \, x \in \Omega.$ Then $\exists \underline{\lambda} \geq \lambda_1 \beta^{-1}$ s.t. $\forall \lambda \leq \underline{\lambda}$ any solution of **Problem** satisfies $\boxed{u_{|\Gamma} \geq 0}$.

NO FREE BOUNDARY

(ii) Let assume $\exists \alpha > 0$ s.t. $f(x, s) \geq \alpha s, \; \forall \, x \in \Omega.$ Then $\exists \overline{\lambda} \leq \lambda_1 \alpha^{-1}$ s.t. $\forall \lambda \geq \overline{\lambda}$ any solution of **Problem** satisfies $\boxed{u_{|\Gamma} < 0}$.

THERE IS FREE BOUNDARY

Teman 1979, Ambrosetti Mancini 1980, Berestycki Brezis 1980

Inverse Problem

We do not know the explicit form of $f(x, u)$

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We do not know the explicit form of $f(x, u)$ Based on Theorem 2, we assume that

$$f(x, u) = \sum_{i=1}^{m} \pi_i \max(u(x)^i, 0) = \boldsymbol{\pi}^T \mathscr{D}(u).$$

where we denote by

$$\boldsymbol{\pi} = (\pi_1, \ldots, \pi_m) \geq 0$$

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What value for m ?

Inverse Problem

We have an Inverse Problem to solve.
Using the experimental data (y) and after Tikhonov regularization (J_ϵ), we want to solve in $\Omega \subset \mathbb{R}^2$

$$(\star\star) \quad \begin{array}{c} \text{Find } u \in H^1(\Omega) \cap H^2(\Omega) \text{ and } k > 0 \text{ s.t.} \\ \min_{\boldsymbol{\pi}} \left(\|\vec{\mathbf{g}}(u, \boldsymbol{\pi}) - \mathcal{Y}\|_W^2 + J_\epsilon(f'') \right) \\ \text{such that} \\ \mathscr{L} u(\boldsymbol{\pi}) = \lambda \boldsymbol{\pi}^T \mathscr{D}(u(\boldsymbol{\pi})) + g \\ -\int_\Gamma \frac{\partial u}{\partial \nu} \mathbf{d}\Gamma = I, \\ u_{|\Gamma} = -k \\ \boldsymbol{\pi} \geq 0. \end{array}$$

OR

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Inverse Problem

$u = v - k$

$$(\star\star)\quad \boxed{\begin{array}{c}\text{Find } v \in H_0^1(\Omega) \cap H^2(\Omega) \;\text{ and }\; k > 0 \;\text{ s.t.}\\ \min_{\boldsymbol{\pi}}\left(\|\vec{\mathbf{g}}(v-k,\boldsymbol{\pi}) - \mathcal{Y}\|_W^2 + J_\epsilon(f'')\right)\\ \text{such that}\\ \mathscr{L}v(\boldsymbol{\pi}) = \lambda\boldsymbol{\pi}^T\mathscr{D}(v(\boldsymbol{\pi}) - k) + g\\ -\int_\Gamma \frac{\partial v}{\partial \nu}\mathbf{d}\Gamma = I,\\ \boldsymbol{\pi} \geq 0.\end{array}}$$

Stochastic nature of the problem

The experimental data $\mathcal{Y}$ in ($\bigstar\bigstar$) are Stochastic Variables that we can assume to be $\mathcal{N}(0, \sigma^2 \mathbf{I})$. We denote the realizations of $\mathcal{Y}$ by $\mathbf{y}_k, \; k = 1, \ldots, \ell$.

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Problem ($\bigstar\bigstar$) is a nonlinear regression with constraints.

Data Assimilation

The inverse problem (★★) is recurrent in other fields of research

- Meteorology
- Oceanography and Hearth studies
- Engineering

Data Assimilation

The name for these problems is DATA ASSIMILATION where two approaches are used

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HINDCAST vs FORECAST

- FORECAST = Equinox ! We use this for real time applications.

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Data Assimilation

The name for these problems is DATA ASSIMILATION where two approaches are used

HINDCAST vs FORECAST

- FORECAST = Equinox ! We use this for real time applications.
- HINDCAST (backtesting in BE) = testing a mathematical model. Inputs for past events are entered into the model to see how well the output matches the known results.

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Discrete problem

Let $X_h = (V_h, \|\cdot\|_X)$ be the finite-dimensional subspaces of $X = H_0^1(\Omega)$ with the indicated induced norm topology. and let $\{\psi_i\}_{1\le i\le n}$ denote a basis of X_h and let $\mathbf{H}$ denote the Grammian (or Riesz) matrix corresponding to the inner product $(\cdot,\cdot)_X$:

$$(\mathbf{H})_{ij} = (\psi_i, \psi_j)_X \qquad 1 \le i,j \le n$$

so that

$$\|u_h\|_X = \|\mathbf{u}\|_H$$

where $\mathbf{u} \in \mathrm{R}^n$ denotes the vector of the coefficients of u_h expanded in the basis $\{\psi_i\}$.

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Discrete problem

Therefore, we have a nonlinear problem in finite dimension as

$$\mathbf{Lu} = \tilde{\lambda}_h \mathbf{D}(\mathbf{u})\boldsymbol{\pi} + \mathbf{g},$$

where $\mathbf{L}_{ij} = \mathbf{a}(\psi_i, \psi_j)$ with $i, j = 1, \ldots, n$, $\mathbf{g}$ is the vector corresponding to the Dirichlet boundary conditions, $\tilde{\lambda}_h$ the computed value of λ, and $\mathbf{D}(\mathbf{u}) \in \mathrm{R}^{n \times m}$ with

$$\mathbf{D}_{i,j}(\mathbf{u}) = \int_\Omega \max(u_h^j, 0)\psi_i \, \mathbf{d}x \quad (j = 1, \ldots, m) \ .$$

finally, the objective function of (★★) can be approximated by

$$\|\mathbf{G}(u_h)\boldsymbol{\pi} - \mathbf{y}\|_2^2 + \frac{\varepsilon}{2}\boldsymbol{\pi}^T \mathbf{M}\boldsymbol{\pi},$$

where $\mathbf{G} \in \mathrm{R}^{\ell \times m}$, $\mathbf{M} \in \mathrm{R}^{m \times m}$ and the norm is the standard euclidean norm.

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Discrete problem

$$(\star\star)_h \quad \boxed{\begin{array}{c} \min_{\boldsymbol{\pi}} \left(\|\mathbf{G}(\mathbf{u}, k)\boldsymbol{\pi} - \mathbf{y}\|_2^2 + \frac{\varepsilon}{2}\boldsymbol{\pi}^T \mathbf{M}\boldsymbol{\pi} \right) \\ \text{such that} \\ \mathbf{L}\mathbf{u} = \tilde{\lambda}_h \mathbf{D}(\mathbf{u})\boldsymbol{\pi} + \mathbf{g}, \\ -\int_\Gamma \frac{\partial u_h}{\partial \nu} \mathbf{d}\Gamma = I_h, \\ \boldsymbol{\pi} \geq 0. \end{array}}$$

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Discrete problem

Standard Problem

$$\min_{\mathbf{x}} \tilde{f}(\mathbf{x})$$

$$\boxed{\begin{array}{c} \mathbf{b}(\mathbf{x}) \geq 0 \\ \mathbf{c}(\mathbf{x}) = 0 \end{array}}$$

where $\mathbf{x} = \begin{bmatrix} \mathbf{u} \\ \boldsymbol{\pi} \\ \lambda \\ k \end{bmatrix}$

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Iterative methods

Equinox solves the problem $(\bigstar\bigstar)_h$ using a forward approach.

- Estimate a solution of the constraint equations
- Estimate the solution of the normal equations

Alternatives?

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Iterative methods

$$\mathfrak{L}(\mathbf{x}, \boldsymbol{\mu}, \boldsymbol{\sigma}) = \tilde{f}(\mathbf{x}) - \boldsymbol{\mu}^T \mathbf{b}(\mathbf{x}) - \boldsymbol{\sigma}^T \mathbf{c}(\mathbf{x})$$

Lagrangian of the Standard problem.

Iterative methods

$$\mathfrak{L}(\mathbf{x}, \boldsymbol{\mu}, \boldsymbol{\sigma}) = \tilde{f}(\mathbf{x}) - \boldsymbol{\mu}^T \mathbf{b}(\mathbf{x}) - \boldsymbol{\sigma}^T \mathbf{c}(\mathbf{x})$$

Lagrangian of the Standard problem. We can use

- Sequential Quadratic Programming: at each point $\mathbf{x}_j$, we seek a decreasing direction $\mathbf{d}$ s.t.

$$\min_{\mathbf{d}} \mathfrak{L}(\mathbf{x}_j, \boldsymbol{\mu}_j, \boldsymbol{\sigma}_j) + \nabla \mathfrak{L}(\mathbf{x}_j, \boldsymbol{\mu}_j, \boldsymbol{\sigma}_j)^T \mathbf{d} + \frac{1}{2} \mathbf{d}^T \nabla^2_{\mathbf{xx}} \mathfrak{L}(\mathbf{x}_j, \boldsymbol{\mu}_j, \boldsymbol{\sigma}_j) \mathbf{d}$$

$$\text{s.t. } \mathbf{b}(\mathbf{x}_j) + \nabla \mathbf{b}(\mathbf{x}_j)^T \mathbf{d} \geq 0, \quad \mathbf{c}(\mathbf{x}_j) + \nabla \mathbf{c}(\mathbf{x}_j)^T \mathbf{d} = 0, \quad \boldsymbol{\mu}_j \geq 0.$$

- Adjoint methods (see http://dolfin-adjoint.org/about/index.html , Farrell et al. at Imperial College London)

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$$\text{s.t. } \mathbf{b}(\mathbf{x}_j) + \nabla \mathbf{b}(\mathbf{x}_j)^T \mathbf{d} \geq 0, \quad \mathbf{c}(\mathbf{x}_j) + \nabla \mathbf{c}(\mathbf{x}_j)^T \mathbf{d} = 0, \quad \boldsymbol{\mu}_j \geq 0.$$

- Adjoint methods (see http://dolfin-adjoint.org/about/index.html , Farrell et al. at Imperial College London)

Both methods require the evaluation in a point of derivative of nonlinear functions. This can be achieved using Automatic Differentiation (AD) Griewank, Walther, (2008). Evaluating Derivatives: Principles and Techniques of Algorithmic Differentiation, SIAM.

Constrained Optimization with regularization

An other notation simplification and a standard problem

Constrained Optimization with regularization

$\mathbf{Q} = \nabla^2_{\mathbf{xx}} \mathfrak{L}(\mathbf{x}_j, \boldsymbol{\mu}_j, \boldsymbol{\sigma}_j)$ Semidefinite Positive

$$\min_{\mathbf{x}} \mathbf{q}^T \mathbf{x} + \frac{1}{2} \mathbf{x}^T \mathbf{Q} \mathbf{x}$$

$$\text{s.t. } \mathbf{A}^T \mathbf{x} = \mathbf{e}, \quad \mathbf{x} \geq 0.$$

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Constrained Optimization with regularization

$\mathbf{Q} = \nabla^2_{\mathbf{xx}}\mathfrak{L}(\mathbf{x}_j, \boldsymbol{\mu}_j, \boldsymbol{\sigma}_j)$ Semidefinite Positive

$$\min_{\mathbf{x}} \mathbf{q}^T\mathbf{x} + \frac{1}{2}\mathbf{x}^T\mathbf{Q}\mathbf{x}$$

$$\text{s.t. } \mathbf{A}^T\mathbf{x} = \mathbf{e}, \quad \mathbf{x} \geq 0.$$

Primal-Dual Regularisation

$$\min_{\mathbf{x},\mathbf{r}} \mathbf{q}^T\mathbf{x} + \frac{1}{2}\mathbf{x}^T\mathbf{Q}\mathbf{x} + \frac{1}{2}\rho||\mathbf{x} - \mathbf{x}_k||^2_{\mathbf{H}} + \frac{1}{2}\nu||\mathbf{r} + \mathbf{y}_k||^2_{\mathbf{N}}$$

$$\text{s.t. } \mathbf{A}^T\mathbf{x} + \nu\mathbf{N}\mathbf{r} = \mathbf{e}, \quad \mathbf{x} \geq 0 \quad \rho > 0 \quad \nu > 0.$$

$(\mathbf{H},\ \mathbf{N},\ \mathbf{Q}\ \text{SPD})$ can be solved by INTERIOR-POINT METHODS

Friedlander Orban 2012 Math. Prog. Comp. and Wright 1997 SIAM

SQD matrices

The choice of the regularization matrices **H**, **N** is crucial for good performance The optimality conditions produce linear systems

$$\begin{bmatrix} \tilde{\mathbf{Q}} & \mathbf{A} \\ \mathbf{A}^T & -\mathbf{N} \end{bmatrix} \begin{bmatrix} \mathbf{x} \\ \mathbf{y} \end{bmatrix} = \begin{bmatrix} \mathbf{g}_1 \\ \mathbf{g}_2 \end{bmatrix}$$

where

$$\tilde{\mathbf{Q}} = \mathbf{Q} + \rho\mathbf{H} + \mathbf{D}, \ \text{SPD} \qquad \mathbf{D} \geq 0 \text{ diagonal.}$$

SQD matrices

The choice of the regularization matrices **H**, **N** is crucial for good performance The matrices

$$\begin{bmatrix} \tilde{\mathbf{Q}} & \mathbf{A} \\ \mathbf{A}^T & -\mathbf{N} \end{bmatrix}$$

are called SQD (symmetric quasi-definite) and they have several important properties Arioli Orban, Venderbei 1995 Siam, ...

- We can compute the $L^T DL$ Gaussian decomposition without pivoting (It will be backward stable)
- The spectrum of the SQD matrices is real and symmetric around the origin.
- The Krylov methods can be efficiently implemented!

Energy norms and probabilistic stopping criteria

- We need stopping criteria for the Iterative Solvers that respect the norm we introduced

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Energy norms and probabilistic stopping criteria

- We need stopping criteria for the Iterative Solvers that respect the norm we introduced
- The $\mathbf{H}$ norm correspond to the $H_0^1(\Omega)$ norm computed on the finite-element test functions: we must use this to measure the error $\mathbf{e} = \mathbf{u} - \mathbf{u}_k$.

Energy norms and probabilistic stopping criteria

- We need stopping criteria for the Iterative Solvers that respect the norm we introduced
- The **H** norm correspond to the $H^1_0(\Omega)$ norm computed on the finite-element test functions: we must use this to measure the error $\mathbf{e} = \mathbf{u} - \mathbf{u}_k$.
- Using specialized Krylov space methods this can be estimated cheaply and accurately.

Energy norms and probabilistic stopping criteria

- We need stopping criteria for the Iterative Solvers that respect the norm we introduced
- The **H** norm correspond to the $H_0^1(\Omega)$ norm computed on the finite-element test functions: we must use this to measure the error $\mathbf{e} = \mathbf{u} - \mathbf{u}_k$.
- Using specialized Krylov space methods this can be estimated cheaply and accurately.
- For the LINEAR regression, probabilistic stopping criteria have been introduced Arioli Gratton CPC 2012. With probability 10^{-8} of being wrong, they stop the iterative process with a solution of a linear regression problem having standard deviation close to the standard deviation of the original problem.

Summary

- We left out several important topics

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- Mesh generation and ADAPTIVITY

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The HINDCAST approach can help to identify which $f(u(x))$ is the best, i.e. which polynomial in $u(x)$ is appropriate.

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$$f(u) = \pi_1 u + \pi_p u^p \qquad ??$$

Summary

$$f(u) = \pi_1 u + \pi_p \cancel{u^p} \;\; u^s \qquad s \in \mathrm{R}_+, \;\; s > 1 \;\; ??$$

Summary

Supercomputers and collaborations between JET and RAL
(Improving GS2 scalability using mixed-mode
programming:Gyrokinetic Plasma Turbulence)

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Summary

THANK YOU !!