Source identification from image-type measurement data for atmospheric chemistry models

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Motivation

- Image type measurement data in air quality applications (large volume of data with unknown value w.r.t. the considered inverse modelling task):
  - Time-series (air quality sensors produce concentration time-series data up to 1 minute discretization).
  - Vertical concentration profiles (aircraft sensing, lidar profiles, etc).
  - Satellite images.

- Current technological context (HPC):
  - The number of sequential iterations should be reduced.
  - An iteration should be computationally intensive (in the sense of parallel computations).

- Existing algorithms
  - Variational algorithms [V. Penenko et al. {1976,1981,…}], [Elbern et al. {1997, 2000, 2007,…},…] et al. (in Atm. Chem.)
  - Representer methods for nonlinear models [Iglesias, Dawson, 2009]

Problem statement

Production-destruction type model for transformation processes

$$\frac{\partial \varphi_l}{\partial t}(t) + P_l(t,\varphi(t))\varphi_l(t) = \Pi_l(t,\varphi(t)) + r_l(t), \quad t \in [0,T], \quad l = 1,\dots,N_c,$$

$$\varphi_l(0) = \varphi_l^0, \quad l = 1,\dots,N_c,$$

Let $\varphi[\varphi^0, r]$ denote the solution of the direct problem

Measurement data

For $l \in L_{mes}$ $\varphi_l[\varphi^0, r^{(*)}] = I_l + \delta I_l$

Time series with noise

Inverse problem

$$A: \begin{cases} \mathbb{R}^{N_c} \times F \to U_{mes} \\ \{\varphi^0, r\} \mapsto \left\{ \begin{cases} \varphi_l[\varphi^0, r], l \in L_{mes} \\ 0, l \notin L_{mes} \end{cases} \right\}_{l=1}^{N_c}, \end{cases}$$

$$I = A\left(\varphi^0, r^{(*)}\right) + \delta I,$$

$$U_{mes} = \left\{ \left\{ \begin{cases} h_l, l \in L_{mes} \\ 0, l \notin L_{mes} \end{cases} \right\}_{l=1}^{N_c} \middle| h_l \in L_2(0,T) \right\},$$

$\varphi^0 \in \mathbb{R}^{N_c}, I \in U_{mes}$ are known

$\delta I \in U_{mes}$ is partially known (e.g. its norm or distribution)

Applications

• Chemical kinetics

• **Augmented [Stockwell,2002] (22 substances, 20 reactions)**

$$
\begin{array}{cc}
hv + NO_2 \rightarrow NO + O_3P & hv + O_3 \rightarrow O^1D + O_2 \\
HCHO + hv \rightarrow CO + 2HO_2 & HCHO + hv \rightarrow CO + H_2 \\
O_2 + O_3P \rightarrow O_3 & N_2 + O^1D \rightarrow N2 + O_3P \\
O^1D + O_2 \rightarrow O_2 + O_3P & H_2O + O^1D \rightarrow 2OH \\
HO_2 + NO \rightarrow NO_2 + OH & NO + O_3 \rightarrow NO_2 + O_2 \\
NO + RO_2 \rightarrow HCHO + HO_2 + NO_2 & CO + OH \rightarrow CO_2 + HO_2 \\
HC + OH \rightarrow H_2O + RO_2 & HCHO + OH \rightarrow CO + H_2O + HO_2 \\
NO_2 + OH \rightarrow HNO_3 & 2HO_2 \rightarrow H_2O_2 + O_2 \\
H_2O + 2HO_2 \rightarrow H_2O + H_2O_2 + O_2 & HO_2 + RO_2 \rightarrow O_2 + ROOH \\
2RO_2 \rightarrow HCHO + HO_2 & OH + SO_2 \rightarrow HO_2 + SULF.
\end{array}
$$

Chemical reaction rates depend on time: incoming solar radiation (photochemistry), temperature, pressure, moisture etc.

$$P_{NO}(t,\varphi) = \left(k_9[HO_2](t) + k_{10}[O_3](t) + k_{11}[RO](t)\right),$$

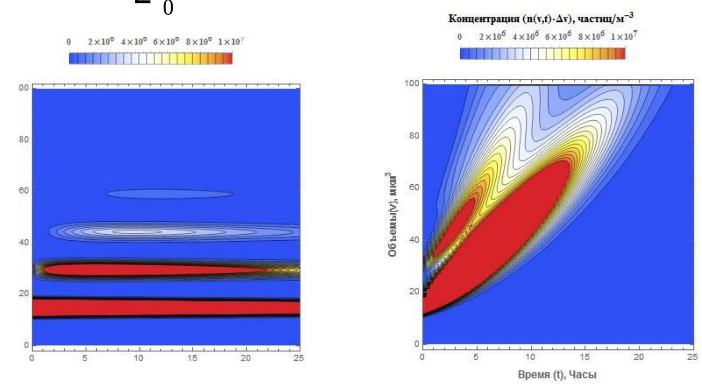
$$\Pi_{NO}(t,\varphi) = k_1(t)[NO_2](t),$$

• **RADM2 Model [Stockwell et al, 1990]**

•Aerosol population dynamics

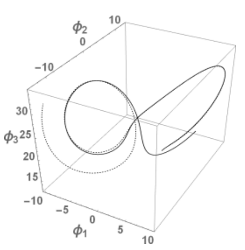
$$P(c;t,r) = \alpha_D(r) + \alpha_S(r) + \int_0^{r_{max}} K(r,r')c(r',t)dr'$$

$$\Pi(c;t,r) = \frac{1}{2}\int_0^r K(q(r,r'),r')c(q(r,r'),t)c(r',t)w(r,r')dr'$$



•Climatology (Lorenz 63 model)

$$P(t,\varphi) = \begin{bmatrix} a \\ 1 \\ c \end{bmatrix}, \quad \Pi(t,\varphi) = \begin{bmatrix} a\varphi_2 \\ b\varphi_1 - \varphi_1\varphi_3 \\ \varphi_1\varphi_2 \end{bmatrix},$$



Adjoint problem

Lagrange type identity (sensitivity relation)

$$\langle h, \delta\varphi \rangle_{L_2^{N_c}(0,T)} = \delta\varphi^0 \cdot \Psi(0) + \langle \delta r, \Psi \rangle_{L_2^{N_c}(0,T)},$$

$$\cdot\,\cdot : \begin{cases} \mathbb{R}^{N_c} \times \mathbb{R}^{N_c} \to \mathbb{R} \\ \{a,b\} \mapsto a^T diag(\rho) b = \sum_{l=1}^{N_c} a_l b_l \rho_l \end{cases}, \quad \langle .,. \rangle_{L_2^{N_c}(0,T)} : \begin{cases} L_2^{N_c}(0,T) \times L_2^{N_c}(0,T) \to \mathbb{R} \\ \{h, \varphi\} \mapsto \int_0^T h(t) \cdot \varphi(t)\, dt \end{cases},$$

Adjoint problem

$$-\frac{\partial \Psi}{\partial t} + \left(diag\left(P(t, \varphi + \delta\varphi) \right) + \bar{\nabla} P(t, \varphi + \delta\varphi, \varphi)^* diag(\varphi) - \bar{\nabla} \Pi(t, \varphi + \delta\varphi, \varphi)^* \right) \Psi = h,$$

$$\Psi(T) = 0,$$

Let $\Psi[\varphi^0, r, \delta\varphi^0, \delta r, h]$ denote the solution of the adjoint problem where the divided difference operators

$$S(t, \varphi + \delta\varphi) - S(t, \varphi) = \bar{\nabla} S(t, \varphi + \delta\varphi, \varphi) \delta\varphi.$$

Gradient algorithms

Given the cost functional

$$J(r)=\sum_{l\in L_{mes}}\left\|\varphi_l[\varphi^0,r]-I_l\right\|^2_{L_2(0,T)}\rho_l.$$

if the parameters are smooth enough, then

$$\nabla J(r)=\Psi[\varphi^0,r,0,0,h],\qquad h=\left\{\begin{cases}2\left(\varphi_l[\varphi^0,r]-I_l\right), l\in L_{mes}\\ 0, l\notin L_{mes}\end{cases}\right\}_{l=1}^{N_c}.$$

E.g. Polak-Ribiere conjugate gradient algorithm implemented in GSL

$$r^{(k+1)}:=r^{(k)}-\alpha^{(k)}s^{(k)},\quad \alpha^{(k)}=\arg\min_{\alpha>0}\bar{J}\left(r^{(k)}-\alpha s^{(k)}\right),$$

$$s^{(k)}=\begin{cases}g^{(k)}+\beta^{(k)}s^{(k-1)}, & k>1\\ g^{(k)}, & k=1\end{cases},\quad \beta^{(k)}=\frac{\left\langle g^{(k)},g^{(k)}-g^{(k-1)}\right\rangle}{\left\langle g^{(k-1)},g^{(k-1)}\right\rangle},\quad g^{(k)}=-\nabla_r\bar{J}(\phi^0,r^{(k)}).$$

Sensitivity operator

Given a system of (orthogonal) functions $U = \{u_\xi\}_{\xi \in \Xi} \subset L_2^{N_c}(0,T)$

Image to structure operator [Dimet et al,2015]

$$H_U\left(A(r_2) - A(r_1)\right) = \sum_{\xi \in \Xi} \left\langle A(r_2) - A(r_1), u_\xi \right\rangle_{L_2^{N_c}(0,T)} e_\xi, \quad \text{where} \quad A(r) := A[\varphi^0, r]$$

Sensitivity relation (Lagrange type identity)

$$\left\langle A(r_2) - A(r_1), u_\xi \right\rangle_{L_2^{N_c}(0,T)} = \left\langle M[r_2, r_1; u_\xi], r_2 - r_1 \right\rangle_{L_2^{N_c}(0,T)}.$$

Sensitivity operator

$$M_U[r_2, r_1]: \begin{cases} F \to \mathbb{R}^\Xi \\ z \mapsto \sum_{\xi \in \Xi} \left\langle M[r_2, r_1; u_\xi], z \right\rangle_{L_2^{N_c}(0,T)} e_\xi, \end{cases}$$

$$H_U\left(A(r_2) - A(r_1)\right) = M_U[k_2, k_1](r_2 - r_1),$$

The inverse problem solution $r^{(*)}$ for any r and U satisfy

$$H_U\left(\mathbf{I} - A(r)\right) = M_U[r^{(*)}, r]\left(r^{(*)} - r\right),$$

$$H_U A(r^{(*)})' = M_U[r^{(*)}, r^{(*)}].$$

Theoretical foundations

- Transformation of the inverse problem with the perturbation theory. An adjoint problem is stated for the element of measurement data.
  - G. I. Marchuk, On the formulation of certain inverse problems, Dokl. Akad. Nauk SSSR, 156:3 (1964), 503–506 (In Russian).
  - Marchuk, G. I. Adjoint Equations and Analysis of Complex Systems Springer Netherlands, 1995

- Practical application to the linear inverse source problem by the sparse *in situ* measurements.
  - Issartel, J.-P. Rebuilding sources of linear tracers after atmospheric concentration measurements // Atmospheric Chemistry and Physics, Copernicus GmbH, 2003 , 3 , 2111-2125

- Dealing with linear and quasi linear ill-posed operator equations:
  - **r-pseudoinverse operators (inverse problem analysis with SVD):** Cheverda V.A., Kostin V.I. r-pseudoinverse for compact operators in Hilbert space: existence and stability. J. Inverse and Ill-Posed Problems. 1995. V.3. № 2. P. 131–148. doi: 10.1515/jiip.1995.3.2.131.
  - **Iterative algorithms based on the truncated SVD:** Kaltenbacher B. Some Newton-type methods for the regularization of nonlinear ill-posed problems. Inverse Problems. 1997. V.13. № 3. P. 729–753. doi: 10.1088/0266-5611/13/3/012.
  - **Iterative regularization in the case of inexact measurements:** Vainikko, G. M.,Veretennikov, A. Yu. Iterative procedures in ill-posed problems Moskow, Nauka, 1986 (In Russian).

Operator equations family

$$H_U A(r+\delta r,\varphi^0+\delta\varphi^0)-H_U A(r,\varphi^0)=M_U^0[\varphi^0,r,\delta\varphi^0,\delta r]\delta\varphi^0+M_U[\varphi^0,r,\delta\varphi^0,\delta r]\delta r,$$

$$M_U[\varphi^0,r,\delta\varphi^0,\delta r]:\begin{cases} F\to\mathbb{R}^{\Xi} \\ z\mapsto\int_0^T\left\{\Psi_l\left[u_\xi\right](t)\right\}_{\xi=1,\,l=1}^{\Xi,\,N_c} diag(\rho)\,z(t)\,dt \end{cases},$$

$$M_U^0[\varphi^0,r,\delta\varphi^0,\delta r]:\begin{cases} \mathbb{R}^{N_c}\to\mathbb{R}^{\Xi} \\ z\mapsto\left\{\Psi_l\left[u_\xi\right](0)\right\}_{\xi=1,\,l=1}^{\Xi,\,N_c} diag(\rho)\,z \end{cases},$$

$$\Psi\left[u_\xi\right]=\Psi\left[\varphi^0,r,\delta\varphi^0,\delta r,u_\xi\right]$$

Family of operator equations depending on U,r

$$H_U\left(I-A(\varphi^0,r)\right)=M_U[\varphi^0,r,0,0]\left(r^{(*)}-r\right)+w,$$

$$w=\left(M_U[\varphi^0,r,0,r^{(*)}-r]-M_U[\varphi^0,r,0,0]\right)\left(r^{(*)}-r\right)+H_U\delta I.$$

Direct problem solution

- With the locally adjoint-problems [Penenko, Tsvetova, 2013]

$$\varphi_l(t^{j+1}) = \varphi_l(t^j)\varphi_l^*(t^j) + \int_{t_j}^{t_{j+1}} \Pi_l(\xi,\varphi(\xi))\varphi_l^*(\xi)\,d\xi, \quad l = 1,\dots,N_c,$$

$$-\frac{\partial \varphi_l^*}{\partial t} + P_l(t,\varphi)\varphi_l^* = 0, \;\; t \in \left[t^j, t^{j+1}\right], \quad \varphi_l^*(t^{j+1}) = 1.$$

- In the first order scheme the local adjoint-problem solution can be approximated with the solution for the constant coefficient

$$\phi_l^{j+1} = \phi_l^j e^{-P_l(t^j,\phi^j)\Delta t} + \int_0^{\Delta t} e^{-P_l(t^j,\phi^j)(\Delta t-\xi)}d\xi\left(\Pi_l(t^j,\phi^j) + r_l^j\right).$$

Positive solution

- Species can be grouped with respect to the life time (destruction rate P) (QSSA method [Hesstvedt, Hov, Isaksen, 1978])

$$\phi_l^{j+1} = \phi_l^j L(P_l(t^j,\phi^j)) + G(P_l(t^j,\phi^j))(\Pi_l(t^j,\phi^j) + r_l^j),$$

$$L(P) = \begin{cases} 0 & P\Delta t > \varepsilon_{\max} \\ e^{-P\Delta t} & P\Delta t \in \left[\varepsilon_{\min}, \varepsilon_{\max}\right] \\ 1 - P\Delta t & 0 < P\Delta t < \varepsilon_{\min} < 1 \end{cases}, \qquad G(P) = \begin{cases} 1/P & P\Delta t > \varepsilon_{\max} \\ \dfrac{1-e^{-P\Delta t}}{P\Delta t}\Delta t & P\Delta t \in \left[\varepsilon_{\min}, \varepsilon_{\max}\right] \\ \Delta t & 0 < P\Delta t < \varepsilon_{\min} < 1 \end{cases}.$$

Consistent numerical schemes

Lagrange type identity: $\langle \delta\phi, h \rangle_{\overline{L_2^{N_c}(0,T)}} = \delta\phi^0 \cdot \psi^0 \delta t^0 + \sum_{j=1}^{N_t-1} \delta r^j \cdot R(t^j, \phi^j) \psi^j \delta t^j,$

Adjoint problem: $\begin{cases} \psi^{j-1} \dfrac{\delta t^{j-1}}{\delta t^j} = \left(w^j(t^j, \phi^j, r^j, \delta\phi^j, \delta r^j) \right)^* \psi^j + h^j, \quad j = 1, \ldots, N_t, \\ \psi^{N_t} = 0, \end{cases}$

Let $\psi[\phi^0, r, \delta\phi^0, \delta r, h]$ denote the solution of the adjoint problem

$$w^j(t^j, \phi^j, r^j, \delta\phi^j, \delta r^j) = \underset{l=1,\ldots,N_c}{diag}\ L^j\left(p_l^2\right) + \left\{ S_l^j\left(t^j, \phi^j, r^j, \delta\phi^j, \delta r^j\right) \right\}_{l=1}^{N_c}, \quad R^j(t^j, \phi^j) = \underset{l=1,\ldots,N_c}{diag}\ G^j\left(p_l^1\right)$$

$$p_l^2 = P_l(t^j, \phi^j + \delta\phi^j), \qquad p_l^1 = P_l(t^j, \phi^j).$$

If $p_l^2 = p_l^1$

$$S_l^j\left(t^j, \phi^j, r^j, \delta\phi^j, \delta r^j\right) = G^j\left(p_l^1\right) \bar{\nabla} \Pi_l\left(t, \phi^j + \delta\phi^j, \phi^j\right),$$

Else

$$S_l^j\left(t^j, \phi^j, r^j, \delta\phi^j, \delta r^j\right) = G^j\left(p_l^1\right) \bar{\nabla} \Pi_l\left(t, \phi^j + \delta\phi^j, \phi^j\right) +$$

$$\left(\phi_l^j \frac{L^j(p_l^2) - L^j(p_l^1)}{p_l^2 - p_l^1} + \frac{G^j\left(p_l^2\right) - G^j\left(p_l^1\right)}{p_l^2 - p_l^1} (\Pi_l(t, \phi^j + \delta\phi^j) + r_l^j + \delta r_l^j) \right) \bar{\nabla} P_l\left(t, \phi^j + \delta\phi^j, \phi^j\right).$$

Consistent numerical schemes

For gradient-type methods:

$$\bar{J}(\phi^0,r)=\sum_{l\in L_{mes}}\sum_{j=1}^{N_t}\left(\phi_l^{\,j}[\phi^0,r]-\bar{I}_l^{\,j}\right)^2\delta t^j\rho_l,\qquad h_l^j=\begin{cases}2\left(\phi_l^{\,j}[\phi^0,r]-\bar{I}_l^{\,j}\right), l\in L_{mes}\\ 0, l\notin L_{mes}\end{cases},$$

$$\left(\nabla_r\bar{J}(\phi^0,r)\right)^j=diag(\rho)R(t^j,\phi^j)\psi^j[\phi^0,r,0,0,h]\delta t^j,\ j=1,\dots,N_t-1.$$

For sensitivity operator computation:

$$\bar{H}_{\bar{U}}\left(\bar{A}(r+\delta r,\phi^0+\delta\phi^0)-\bar{A}(r,\phi^0)\right)=m_{\bar{U}}^0[\phi^0,r,\delta\phi^0,\delta r]\delta\phi^0+m_{\bar{U}}[\phi^0,r,\delta\phi^0,\delta r]\delta r,$$

$$m_{\bar{U}}[\phi^0,r,\delta\phi^0,\delta r]:\begin{cases}\mathbb{R}^{N_c\times N_t-1}\to\mathbb{R}^{\Xi}\\ z\mapsto\sum_{j=1}^{N_t-1}\left\{R_l(t^j,\phi^j)\psi_l^{\,j}\left[\bar{u}_\xi\right]\right\}_{\xi=1,\,l=1}^{\Xi,\,N_c}diag(\rho)\,z^j\delta t^j\end{cases},$$

Parallel WRT ξ

$$m_{\bar{U}}^0[\phi^0,r,\delta\phi^0,\delta r]:\begin{cases}\mathbb{R}^{N_c}\to\mathbb{R}^{\Xi}\\ z\mapsto\left\{\psi_l^0\left[\bar{u}_\xi\right]\delta t^0\right\}_{\xi=1,\,l=1}^{\Xi,\,N_c}diag(\rho)\,z\end{cases},\qquad \psi\left[\bar{u}_\xi\right]=\psi\left[\phi^0,r,\delta\phi^0,\delta r,\bar{u}_\xi\right]$$

The Choice of Basis

«*a priori*» approach – the basis for the class of problems

- Fourier cos-basis

$$U_\Theta = \left\{ e_{\eta\theta} \,|\, 1 \le \theta \le \Theta, \eta \in L_{mes} \right\}, \quad e^{j}_{\eta\theta} = \left\{ \left\{ \begin{cases} \begin{cases} \sqrt{2} / \sqrt{T\,\rho_\eta} \cos\left(\dfrac{\pi\theta t^j}{T} \right), \theta > 0 \\ 1 / \sqrt{T\,\rho_\eta}, \qquad \theta = 0 \end{cases}, & l = \eta \\ 0, & l \ne \eta \end{cases} \right\}_{l=1}^{N_c} \right\}, \quad j = 1, \ldots, N_t.$$

- Wavelets, curvlets, etc. [Dimet et al.,2015]

«*a posteriori*» approach – the basis for the considered problem

- Singular vectors of the operator $m_{\bar{U}}[r^{(0)}, 0] m_{\bar{U}}[r^{(0)}, 0]^T$.

Penenko, A. V.; Nikolaev, S. V.; Golushko, S. K.; Romashenko, A. V. & Kirilova, I. A. Numerical Algorithms for Diffusion Coefficient Identification in Problems of Tissue Engineering // Math. Biol. Bioinf., 2016 , 11 , 426-444 (In Russian)

Inversion algorithm

$$\bar{H}_{\bar{U}}\left(\bar{I}-\bar{A}\left(\phi^0,r\right)\right)=m_{\bar{U}}[r,0]\left(\bar{r}^{(*)}-r\right)+w,$$

$$w=\left(m_{\bar{U}}[r,\bar{r}^{(*)}-r]-m_{\bar{U}}[r,0]\right)\left(\bar{r}^{(*)}-r\right)+\bar{H}_{\bar{U}}\delta\bar{I}.$$

$$\begin{cases} m_{\bar{U}}[r,\delta r]:=m_{\bar{U}}[\phi^0,r,\delta\phi^0,\delta r], \\ m_{\bar{U}}[r,\delta r]:\mathbb{R}^{N_c\times N_t-1}\to\mathbb{R}^{\Xi} \end{cases}$$

$$CC^T z=\sum_{l=1}^{\Xi}\sigma_l^2 U_l\left\langle z,U_l\right\rangle_{\mathbb{R}^{\Xi}}, \qquad \text{SVD}\ \left(\Xi\times\Xi\right)\quad \sigma_l\geq 0,\ \left\langle U_m,U_l\right\rangle_{\mathbb{R}^{\Xi}}=\delta_{ml}$$

(Right) r-pseudoinverse

$$\left[CC^T\right]^{-p}=\sum_{l=1}^{\min\{p,rank(C)\}}\frac{U_l}{\sigma_l^2}\left\langle \cdot,U_l\right\rangle_{\mathbb{R}^{\Xi}},$$

Parallel wrt l

$$C^T\left[CC^T\right]^{-p}\left(=\sum_{l=1}^{\min\{p,rank(C)\}}\frac{V_l}{\sigma_l}\left\langle \cdot,U_l\right\rangle_{\mathbb{R}^{\Xi}}\right)=\sum_{l=1}^{\min\{p,rank(C)\}}\frac{C^TU_l}{\sigma_l}\left\langle \cdot,U_l\right\rangle_{\mathbb{R}^{\Xi}},$$

Newton-Kantorovich type iteration with right r-pseudoinverse

$$\delta r=m_{\bar{U}}[r,0]^T\left[m_{\bar{U}}[r,0]m_{\bar{U}}[r,0]^T\right]^{-p}\bar{H}_{\bar{U}}\left(\bar{I}-\bar{A}(\phi^0,r)\right).$$

How to choose p?

The Iterative Algorithm

Initial setup: $U = U_{\Theta}, r^{(0)}$

Divide operator spectra on N_p intervals $\Delta p = \left[\frac{\Theta |L_{mes}|}{N_p}\right], \quad p = \Delta p,$

Outer iteration with respect to considered spectra intervals $p := p + \Delta p,$

Inner iterations up to the stabilization

$$\delta r^{(k)} = \Pr_{src} m_{\bar{U}}[r^{(k)}, 0]^T \left[m_{\bar{U}}[r^{(k)}, 0] m_{\bar{U}}[r^{(k)}, 0]^T \right]^{-p} \bar{H}_{\bar{U}} \left(\bar{I} - \bar{A}(\phi^0, r^{(k)}) \right),$$

$$r^{(k+1)} = r^{(k)} + \gamma^{(k)} \delta r^{(k)}.$$

Considered source regularization

$$\Pr_{src} z : \begin{cases} \mathbb{R}^{N_c \times N_t} \to \mathbb{R}^{N_c \times N_t} \\ z \mapsto \left\{ \begin{cases} z_l, l \in L_{src} \\ 0, l \notin L_{src} \end{cases} \right\}_{l=1}^{N_c} \end{cases}.$$

Step parameter according to the discrepancy principle and monotone decrease of the discrepancy

$$\left\| \bar{H}_{\bar{U}} \delta \bar{I} \right\|_{\mathbb{R}^{\Xi}} \le \left\| \bar{H}_{\bar{U}} \left(\bar{I} - \bar{A}(\phi^0, r^{(k)} + \gamma \delta r^{(k)}) \right) \right\|_{\mathbb{R}^{\Xi}} < \left\| \bar{H}_{\bar{U}} \left(\bar{I} - \bar{A}(\phi^0, r^{(k)}) \right) \right\|_{\mathbb{R}^{\Xi}},$$

Numerical experiment setup

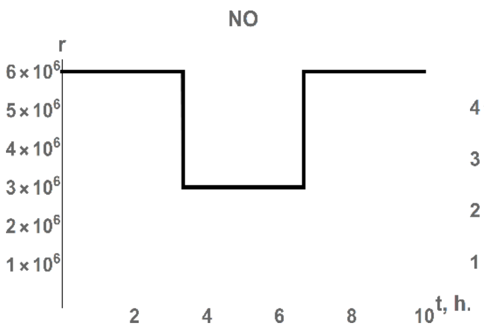
$$\mathrm{hv + NO_2 \to NO + O_3P}$$
$$\mathrm{HCHO + hv \to CO + 2HO_2}$$
$$\mathrm{O_2 + O_3P \to O_3}$$
$$\mathrm{O^1D + O_2 \to O_2 + O_3P}$$
$$\mathrm{HO_2 + NO \to NO_2 + OH}$$
$$\mathrm{NO + RO_2 \to HCHO + HO_2 + NO_2}$$
$$\mathrm{HC + OH \to H_2O + RO_2}$$
$$\mathrm{NO_2 + OH \to HNO_3}$$
$$\mathrm{H_2O + 2HO_2 \to H_2O + H_2O_2 + O_2}$$
$$\mathrm{2RO_2 \to HCHO + HO_2}$$
$$\mathrm{hv + O_3 \to O^1D + O_2}$$
$$\mathrm{HCHO + hv \to CO + H_2}$$
$$\mathrm{N_2 + O^1D \to N2 + O_3P}$$
$$\mathrm{H_2O + O^1D \to 2OH}$$
$$\mathrm{NO + O_3 \to NO_2 + O_2}$$
$$\mathrm{CO + OH \to CO_2 + HO_2}$$
$$\mathrm{HCHO + OH \to CO + H_2O + HO_2}$$
$$\mathrm{2HO_2 \to H_2O_2 + O_2}$$
$$\mathrm{HO_2 + RO_2 \to O_2 + ROOH}$$
$$\mathrm{OH + SO_2 \to HO_2 + SULF.}$$

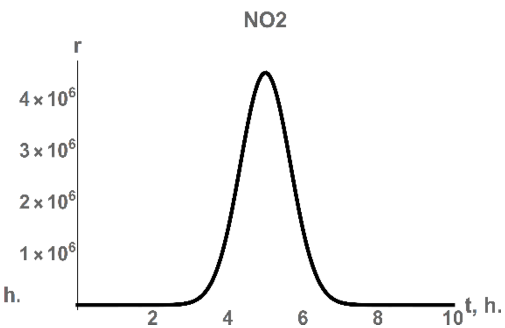
Photochemical reactions rates depend on time (of day)

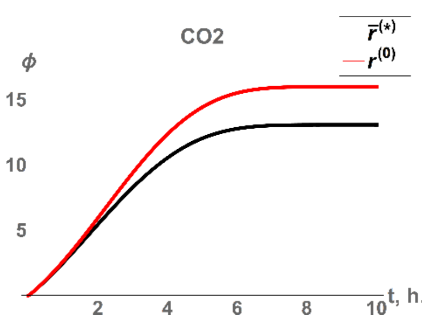
$$L_{mes} = \{CO_2, O_3\}$$
$$L_{src} = \{NO, NO_2\}$$
$$r^{(0)} = 0$$

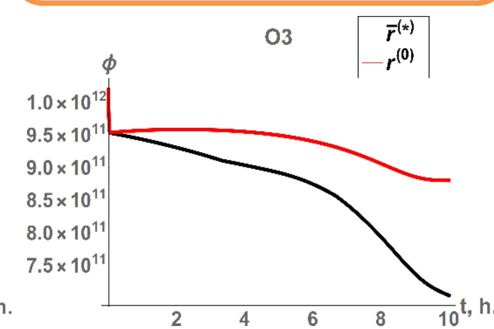
$$T = 10 \times 3600$$
$$N_t = 3000$$
$$N_c = 22$$
$$N_p = 25$$

$$\rho_{CO_2} = 10^{12}$$
$$\rho_{O_3} = 1$$

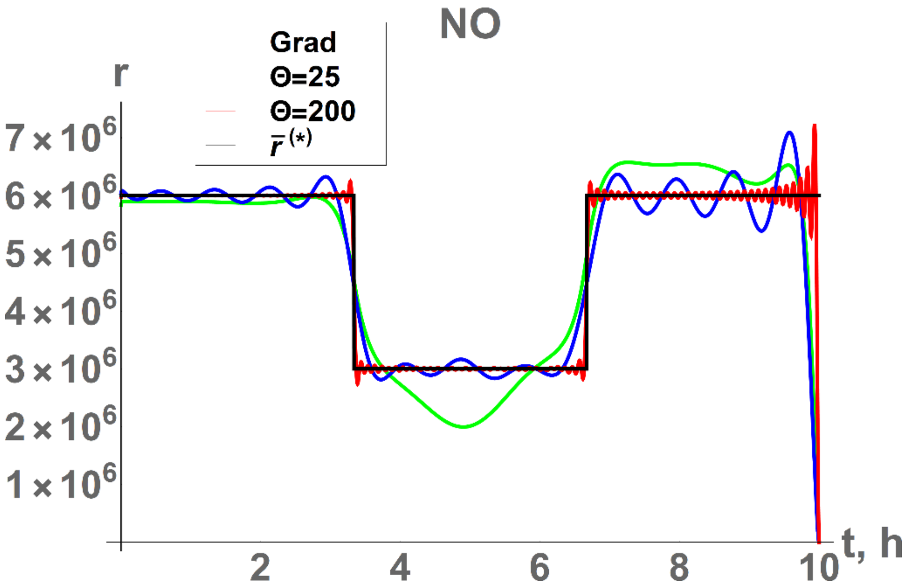


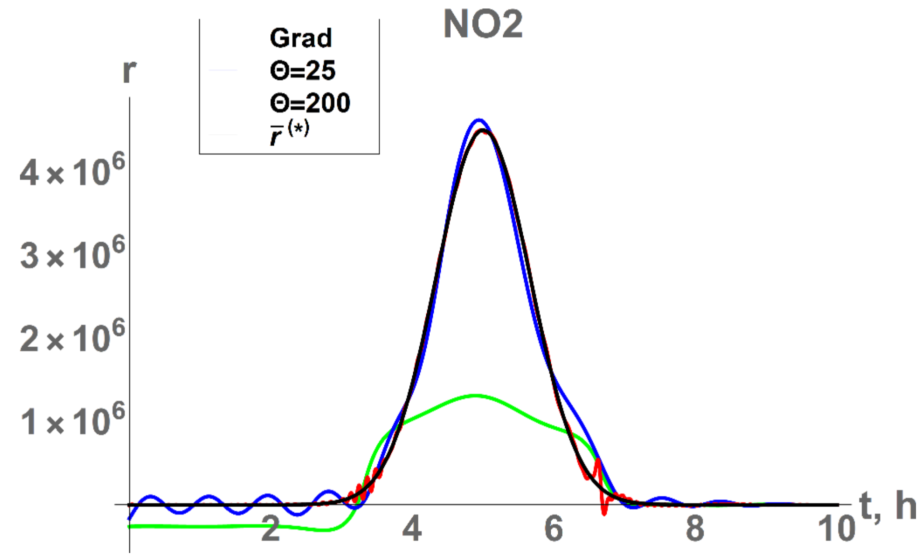


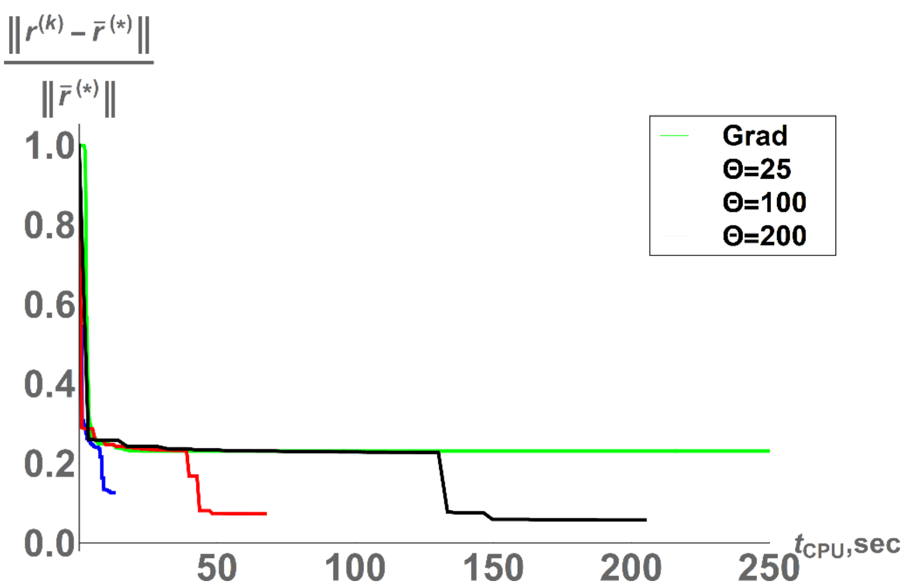


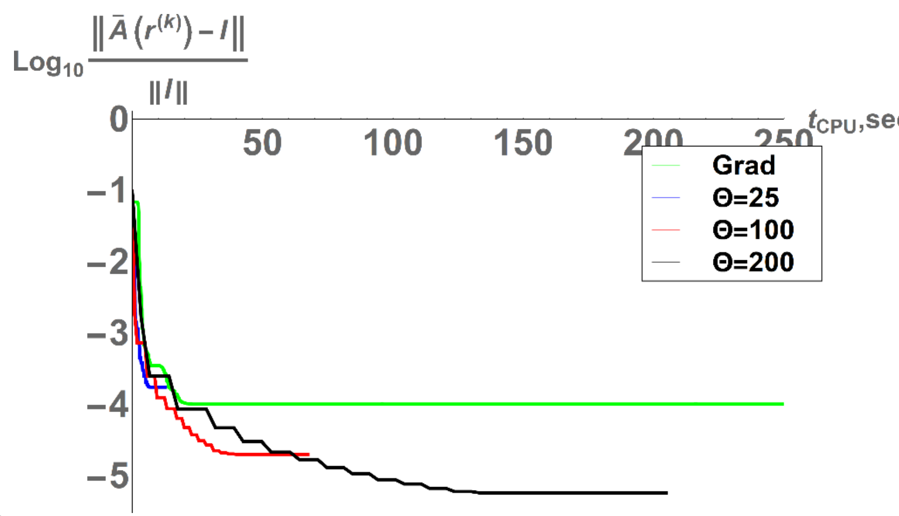


Exact measurements

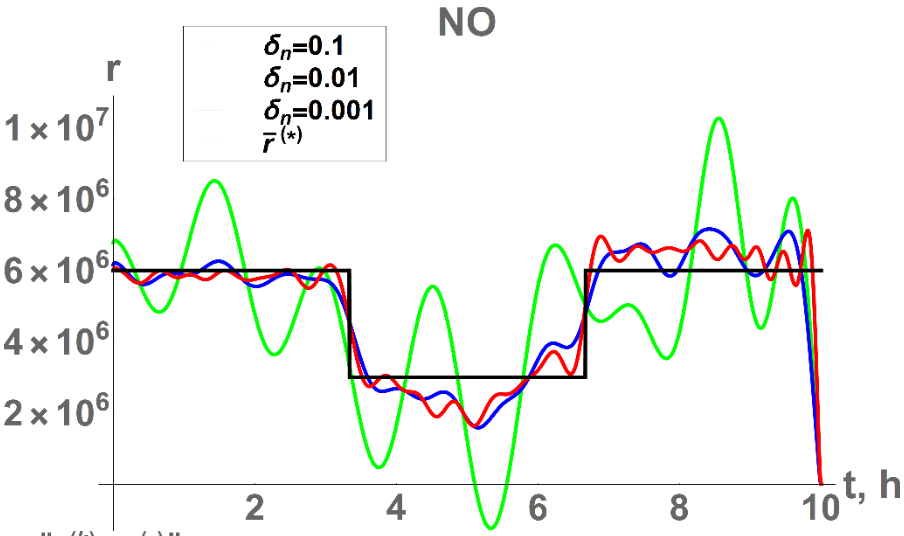


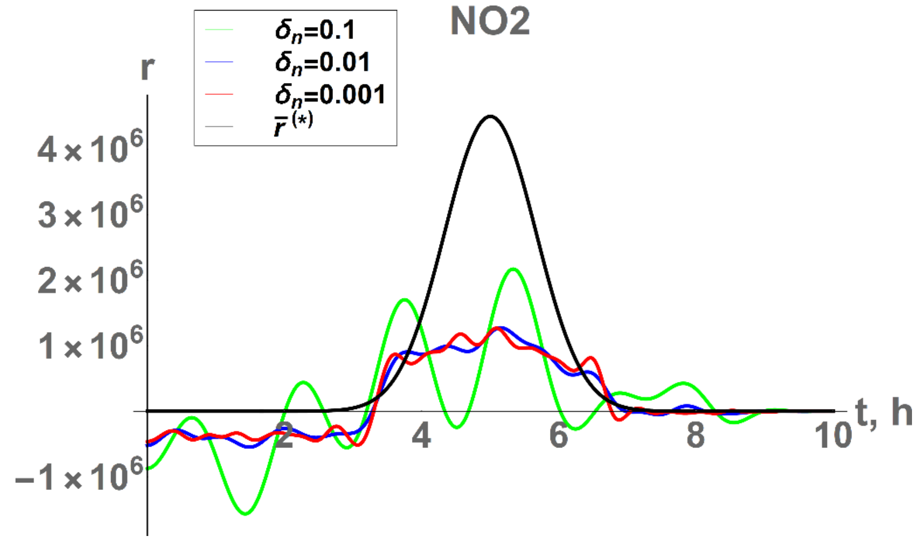


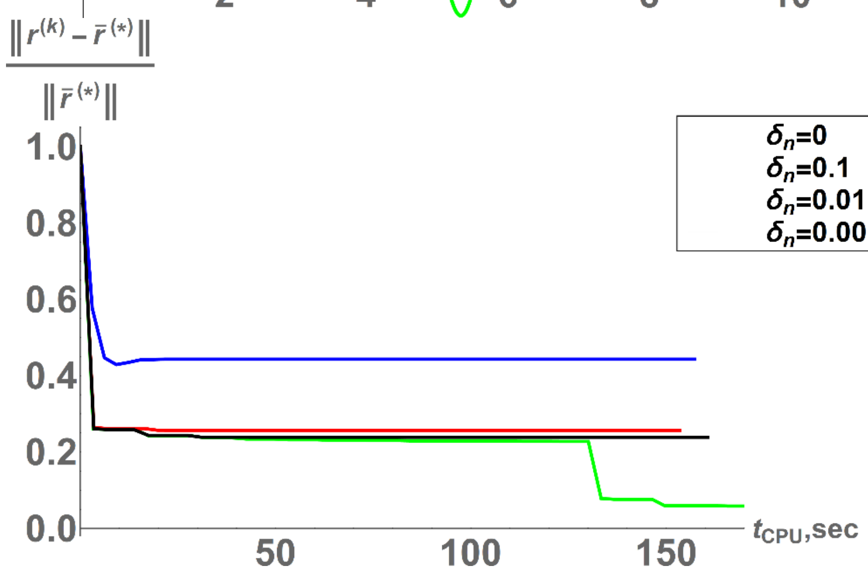


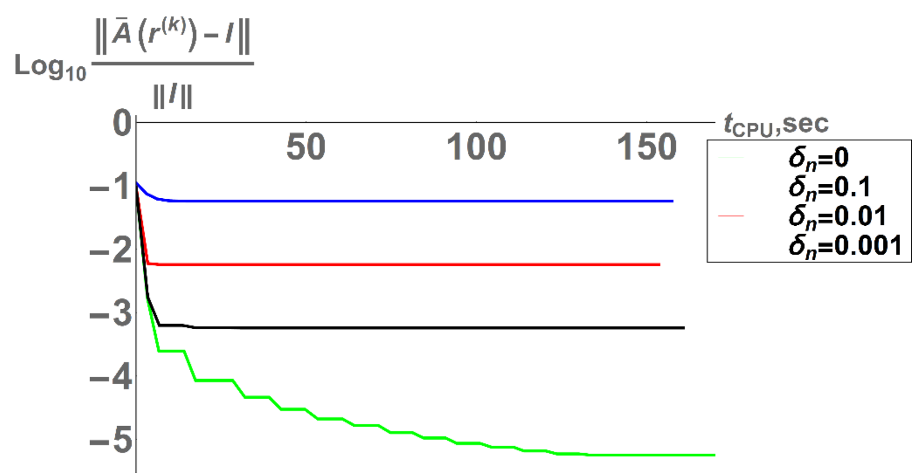


Inexact measurements



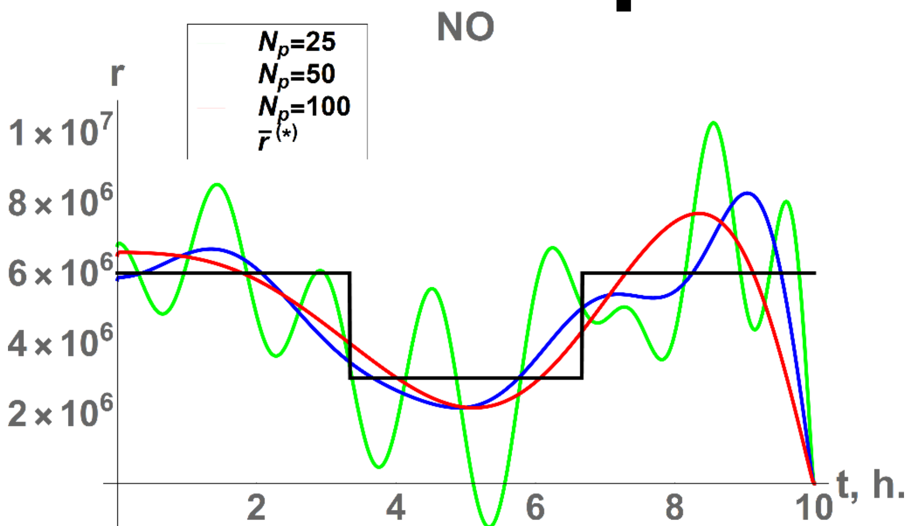


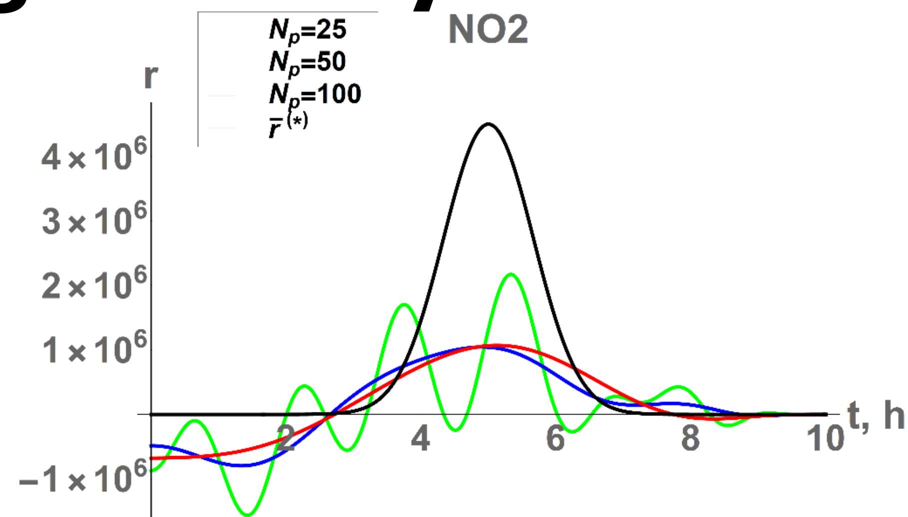


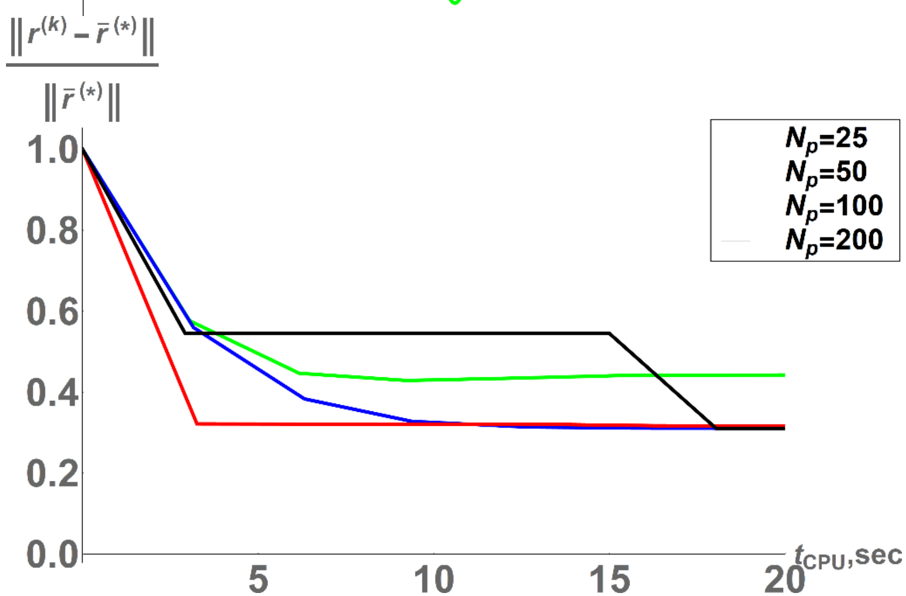


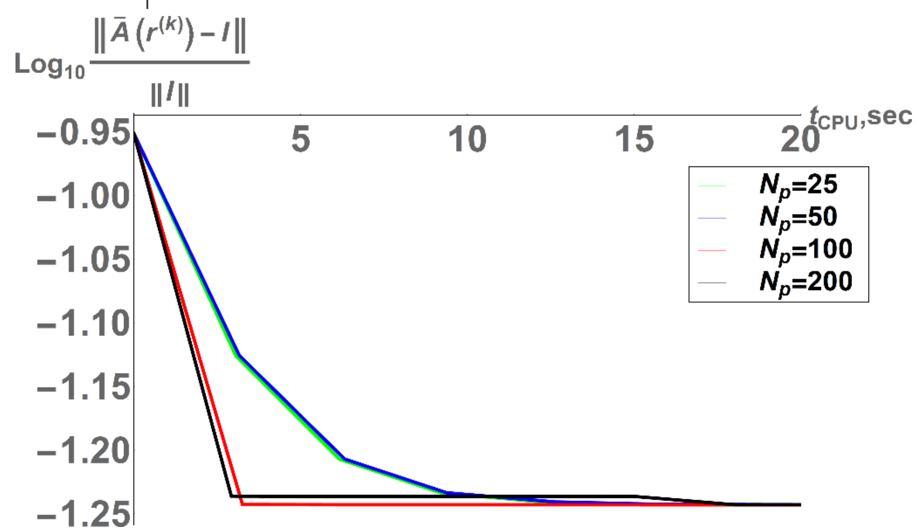
$$\bar{I}_l^{\,j} = (1+\delta_n n)\left(\bar{A}(\phi^0, \bar{r}^{(*)})\right)_l^j, l = 1,\ldots,N_c,\ j = 1,\ldots,N_t,$$

Improving Stability









$$\delta_n = 0.1$$

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Summary

- The inverse source identification problem for a production destruction model has been considered.

- Ajoint problems can be used for both cost functional gradient and sensitivity operator construction

- The sensitivity operator allow to reformulate the problem as a family of quasilinear operator equations

- To solve the equations, the inversion algorithm has been proposed using
  - Sequential increase of the considered spectrum
  - Right r-pseudoinverse matrices
  - Discrepancy principle and the iterative regularization

- The algorithm was tested in a scenario for an atmospheric chemistry model

Thank you for your attention!

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