Adjoint-based exact Hessian computation

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Today's talk is based on BIT Numerical Mathematics (2021)

Joint work with

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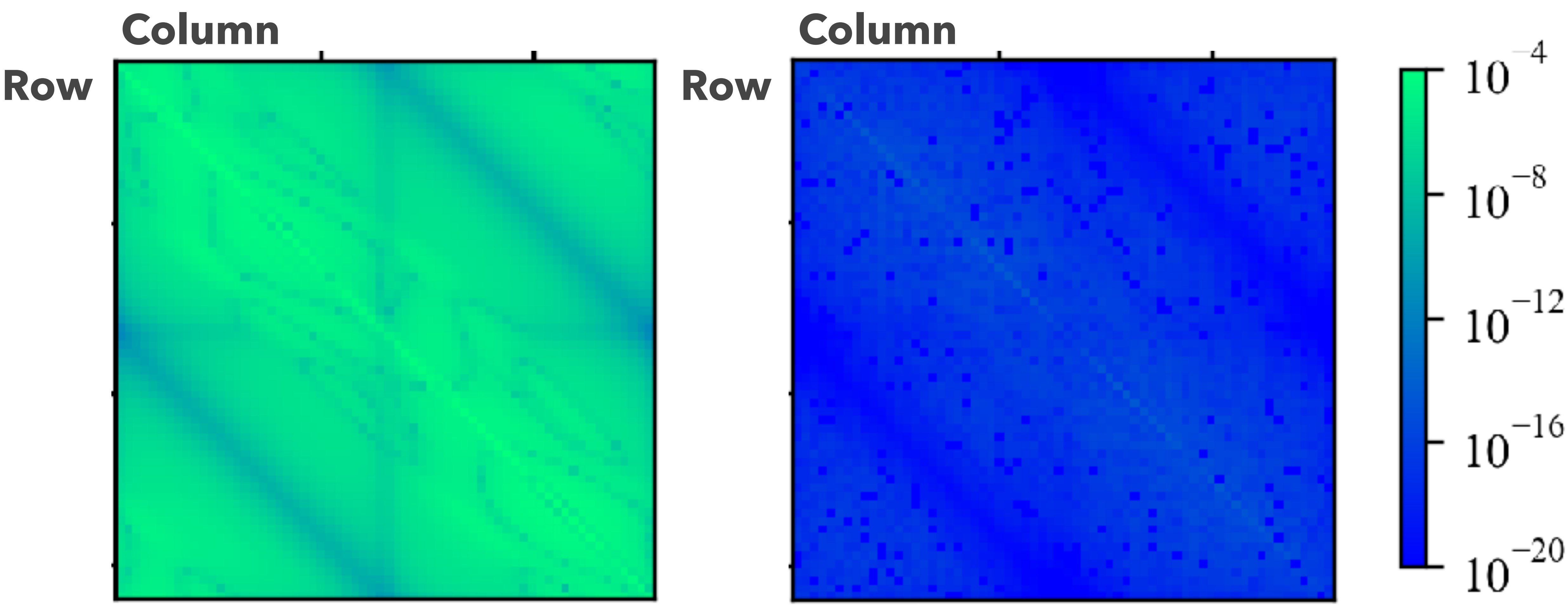
One-sentence summary

We developed an adjoint-based method that enables exact Hessian computations up to a given floating point limit.

Error in a Hessian matrix



Naive method

Our method

Outline

Introduction

Adjoint-based gradient and Hessian computations

Sanz-Serna’s idea

and exact Hessian computation

Numerical verifications

Introduction

Adjoint-based gradient and Hessian computations

Adjoint method

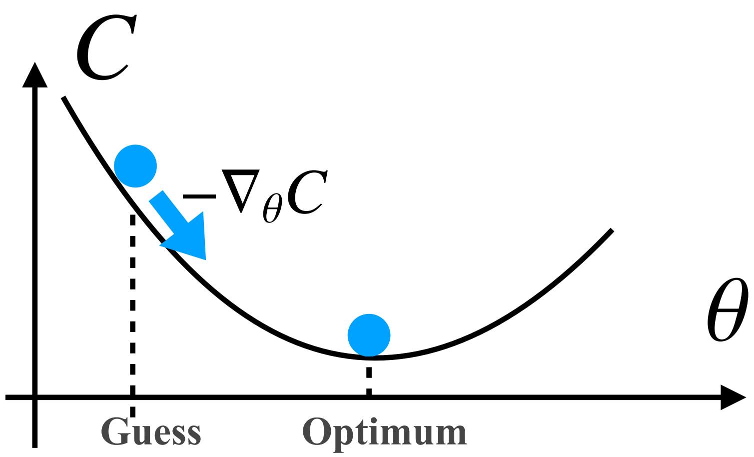
We consider an autonomous ordinary differential equation(ODE):

$$x_0 = \theta \rightarrow \boxed{\frac{d}{dt}x_t = f(x_t)} \rightarrow x_T(\theta)$$

Forward model

and a minimization problem of a cost function defined by the final state $t = T$

$$\min_{\theta} C\left(x_T(\theta)\right)$$



via an gradient method using a gradient $\nabla_\theta C$

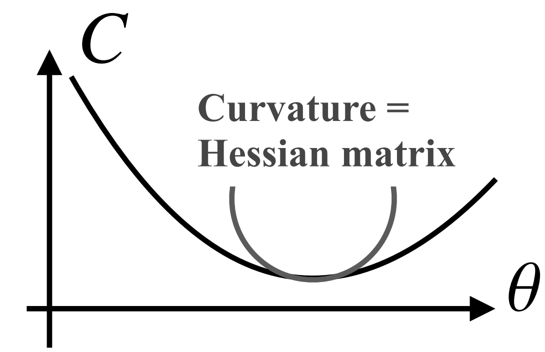
Adjoint method calculates $\nabla_\theta C$ exactly by solving

$$\boxed{\lambda_0 = \nabla_\theta C} \leftarrow \boxed{-\frac{d}{dt}\lambda_t = \left(\nabla_x f\right)^\top \lambda_t} \leftarrow \lambda_T = \nabla_{x_T} C$$

Adjoint model

Second-order adjoint method

Adjoint method is available for a first-order derivative computation, while second-order adjoint (SOA) method is available for a second-order derivative (Hessian matrix H_θ) computation.



$$\delta_0 = \gamma$$

$$\frac{d}{dt}\delta_t = (\nabla_x f)\,\delta_t$$

Tangent linear model

$$\delta_T$$

$$\xi_T = \mathsf{H}_{x_T}\delta_T$$

$$-\frac{d}{dt}\xi_t = (\nabla_x f)^\top \xi_t + \{(\nabla_x \nabla_x f)\,\delta_t\}^\top \lambda_t$$

SOA model

$$\xi_0 = \mathsf{H}_\theta \gamma$$

$$\mathsf{H}_\bullet = \nabla_\bullet \nabla_\bullet{}^\top C$$

*** These model are derived from the first-order perturbation of the forward and adjoint models.**

SOA provides an exact Hessian-vector product for arbitrary vectors.

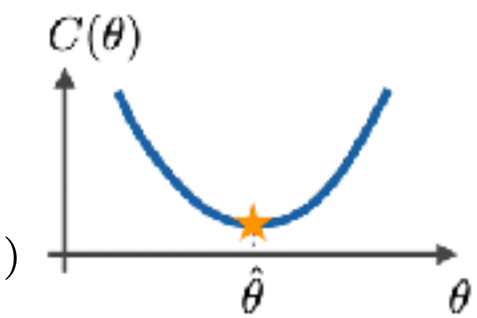
SOA is available for optimization methods, uncertainty quantification, ...

Application

- **Fast optimization**
  - **Newton method** $\theta \leftarrow \theta + y$ **where** $\mathrm{H}_\theta y = -\nabla_\theta C$ y **: Descent vector**
  - **Nonlinear conjugate gradient method**

$$
\begin{cases}
z \leftarrow \nabla_\theta C - \dfrac{z^\top \mathrm{H}_\theta \nabla_\theta C}{z^\top \mathrm{H}_\theta z} z \\
\theta \leftarrow \theta + \eta z
\end{cases}
$$

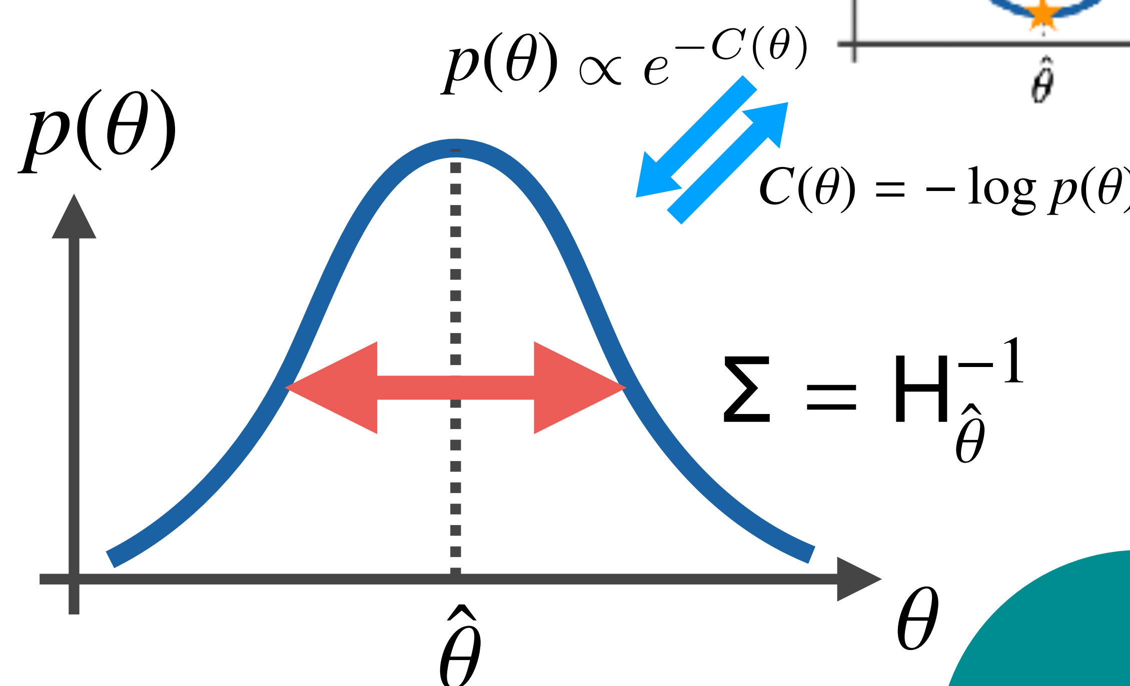
z **: Conjugate vector**
η **: Learning rate**



- **Uncertainty quantification (UQ)**

Solve $\mathrm{H}_{\hat{\theta}} \Sigma = \mathrm{I}$ **via Krylov subspace methods**

Ito et al., (2016)



Question

Adjoint and SOA methods give exact gradient $\nabla_\theta C$ and Hessian-vec. prod. $\mathrm{H}_\theta \gamma$

if all of the models are solved analytically.

In practice, all of the models are solved numerically,

using time integral schemes, e.g., Runge–Kutta methods.

→ inexact due to discretization errors, machine errors

Forward model

$$\frac{d}{dt}x_t = f(x_t)$$

Tangent linear (TL) model

$$\frac{d}{dt}\delta_t = (\nabla_x f)\,\delta_t$$

?

Adjoint model

$$-\frac{d}{dt}\lambda_t = (\nabla_x f)^\top \lambda_t$$

?

SOA model

$$-\frac{d}{dt}\xi_t = (\nabla_x f)^\top \xi_t + \{(\nabla_x \nabla_x f)\,\delta_t\}^\top \lambda_t$$

?

For a given forward scheme, are there "optimal schemes" for other models?

Question

Adjoint and SOA methods give **exact** gradient $\nabla_\theta C$ and Hessian-vec. prod. $\mathsf{H}_\theta \gamma$ if all of the models are solved **analytically**.

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→ **inexact** due to discretization errors, machine errors

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Sanz-Serna (2016)

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?

For a given forward scheme, are there "optimal schemes" for other models?

→ Yes. There exists **an optimal scheme for the adjoint model** that can avoid any discretization errors.

Question

Adjoint and SOA methods give exact gradient $\nabla_\theta C$ and Hessian-vec. prod. $\mathrm{H}_\theta \gamma$ if all of the models are solved analytically.

In practice, all of the models are solved numerically, using time integral schemes, e.g., Runge–Kutta methods.

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SOA model

$$-\frac{d}{dt} \xi_t = (\nabla_x f)^\top \xi_t + \{(\nabla_x \nabla_x f)\, \delta_t\}^\top \lambda_t$$

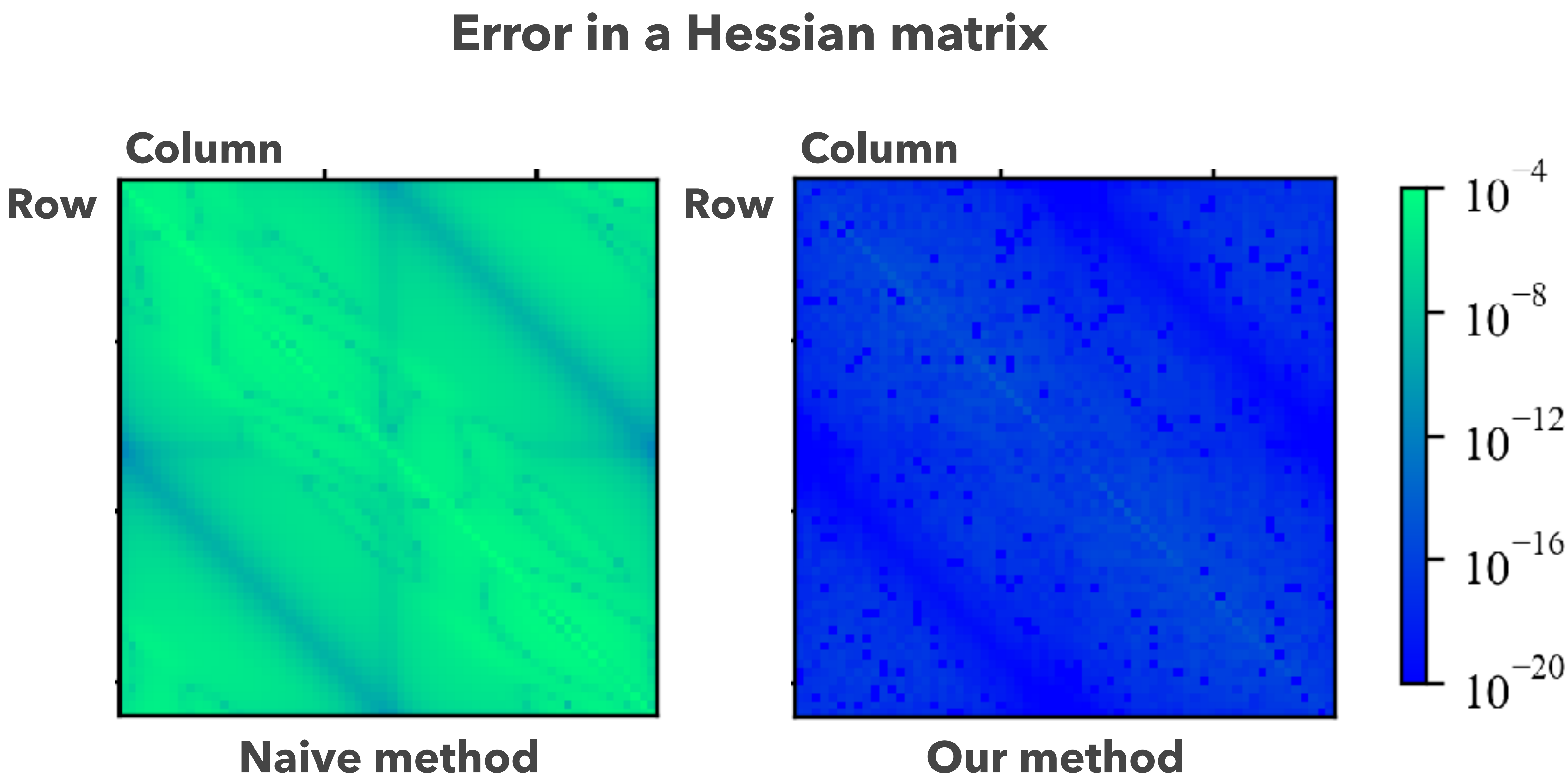
Ours

For a given forward scheme, are there "optimal schemes" for other models?

→ Yes. There exists a set of optimal schemes for all of these models that can avoid any discretization errors.

Importance of exact Hessian computation

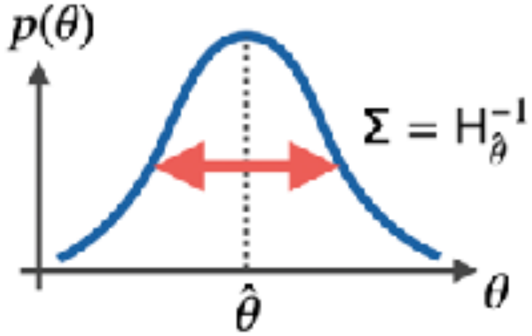
＊ Numerical details will be explained later.

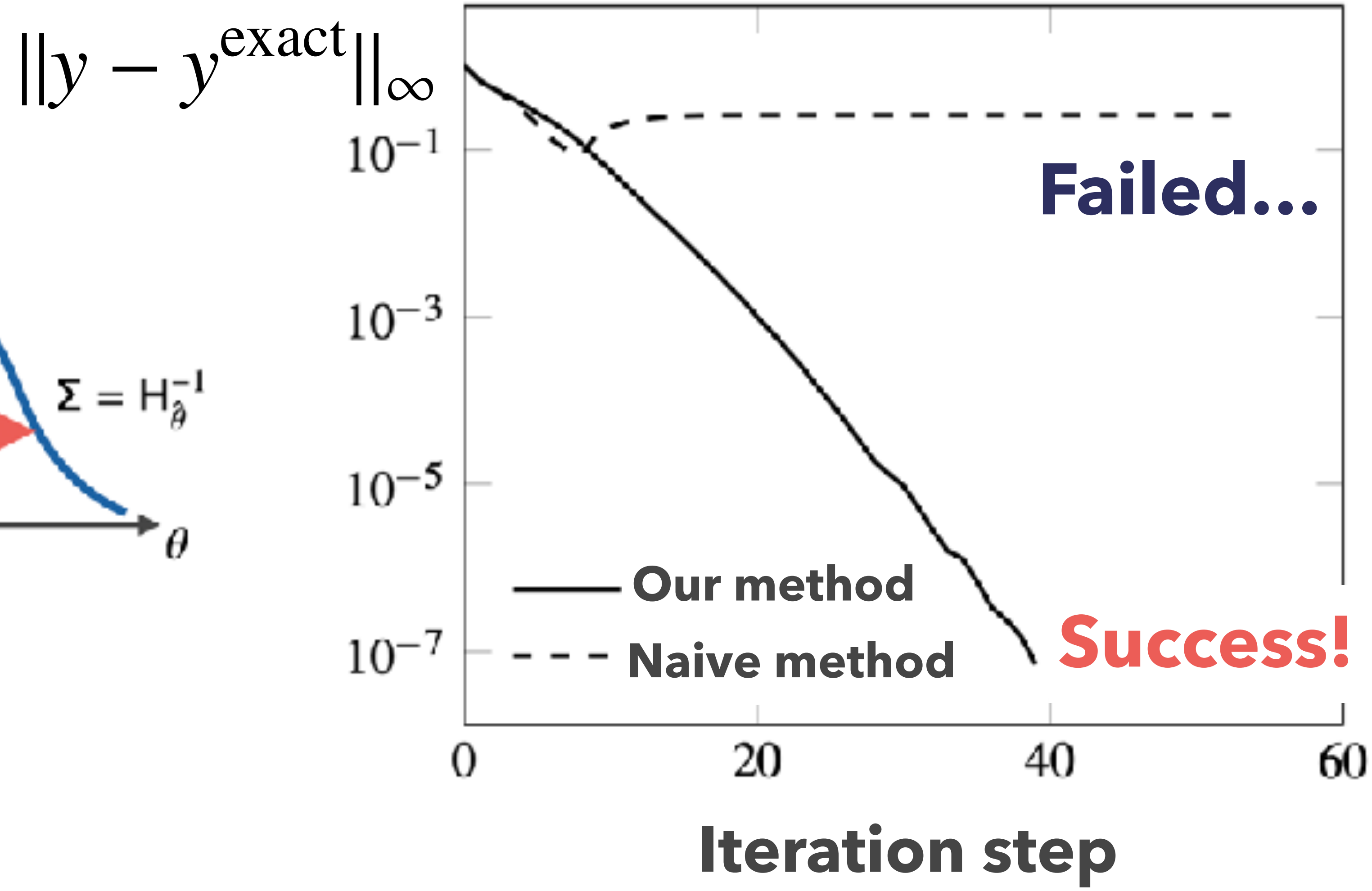


Our method allows exact Hessian computation up to a given floating point limit.

Importance of exact Hessian computation

Convergence behavior when solving $\mathrm{H}y = b$





When using an incorrect scheme,

- Optimization may not converge to correct solution.
- Uncertainty quantification may fail.

Sanz-Serna's idea

and exact Hessian computation

Invariant

Why can the analytical solution of the adjoint model provide the exact gradient ?

A product of TL and adjoint variables is time-invariant

$$\frac{d}{dt}\left(\delta_t^\top \lambda_t\right) = \left(\frac{d}{dt}\delta_t\right)^\top \lambda_t + \delta_t^\top \frac{d}{dt}\lambda_t = 0$$

$$\boxed{\delta_t^\top \lambda_t = \delta_0^\top \lambda_0}$$

TL model

$$\frac{d}{dt}\delta_t = (\nabla_x f)\,\delta_t$$

Adjoint model

$$-\frac{d}{dt}\lambda_t = (\nabla_x f)^\top \lambda_t$$

If we choose $\lambda_t = \nabla_{x_t} C(x_t(\theta))$ **, we obtain**

$$\delta_t^\top \nabla_{x_t} C(x_t) = ((\nabla_\theta x_t)\,\delta_0)^\top \nabla_{x_t} C(x_t)$$

$$= \delta_0^\top \left[(\nabla_\theta x_t)^\top \nabla_{x_t} C(x_t)\right] = \delta_0^\top \nabla_\theta C(x_t)$$

$$\because\ x_t(\theta + \epsilon\delta_0) = x_t(\theta) + \epsilon\delta_t + O(\epsilon^2)$$

$$\Rightarrow\ \delta_t = (\nabla_\theta x_t)\,\delta_0$$

$$\Rightarrow\ \lambda_0 = \nabla_\theta C(x_t(\theta))$$

Runge–Kutta family

Forward model

$$\frac{d}{dt}x_t = f(x_t)$$

Discretize

$$x_n := x_{t_n}$$
$$x_{n+1} := x_{t_n+h}$$

s-stage Runge–Kutta (RK) method

$$x_{n+1} = x_n + h\sum_{i=1}^{s} b_i k_{n,i},$$
$$k_{n,i} = f(X_{n,i}) \quad (i = 1,\dots,s),$$
$$X_{n,i} = x_n + h\sum_{j=1}^{s} a_{ij} k_{n,j} \quad (i = 1,\dots,s).$$

h **: stepsize**
a_{ij}, b_i **: weights**

* (…) : order

- **Classical 4-stage RK (4)**

$$x_{n+1} = x_n + \frac{h}{6}(k_{n,1} + 2k_{n,2} + 2k_{n,3} + k_{n,4}),$$
$$k_{n,i} = f(X_{n,i}) \quad (i = 1,\dots,4),$$
$$X_{n,1} = x_n \qquad X_{n,3} = x_n + \frac{h}{2}k_{n,2}$$
$$X_{n,2} = x_n + \frac{h}{2}k_{n,1} \qquad X_{n,4} = x_n + hk_{n,3}$$

- **Explicit Euler (1)**

$$x_{n+1} = x_n + hk_{n,1},$$
$$k_{n,1} = f(X_{n,1}),$$
$$X_{n,1} = x_n$$

- **Heun (2)**

$$x_{n+1} = x_n + \frac{h}{2}(k_{n,1} + k_{n,2}),$$
$$k_{n,i} = f(X_{n,i}) \quad (i = 1,\dots,2),$$
$$X_{n,1} = x_n$$
$$X_{n,2} = x_n + hk_{n,1}$$

- **Adaptive stepsize RK: Bogacki–Shampine(2-3), Runge-Kutta-Fehlberg(4-5), Dormand-Prince(4-5), …**

Sanz-Serna's idea

Solve forward models via a s-stage Runge–Kutta (RK) method

$$\frac{d}{dt}x_t = f(x_t) \quad \Rightarrow \quad \begin{aligned} x_{n+1} &= x_n + h\sum_{i=1}^{s} b_i k_{n,i}, \\ k_{n,i} &= f(X_{n,i}) \quad (i = 1, \ldots, s), \\ X_{n,i} &= x_n + h\sum_{j=1}^{s} a_{ij} k_{n,j} \quad (i = 1, \ldots, s). \end{aligned}$$

$$\frac{d}{dt}\delta_t = (\nabla_x f)\,\delta_t \quad \Rightarrow \quad \begin{aligned} \delta_{n+1} &= \delta_n + h\sum_{i=1}^{s} b_i d_{n,i}, \\ d_{n,i} &= \nabla_x f(X_{n,i}) D_{n,i} \quad (i = 1, \ldots, s), \\ D_{n,i} &= \delta_n + h\sum_{j=1}^{s} a_{ij} d_{n,j} \quad (i = 1, \ldots, s). \end{aligned}$$

and solve adjoint model via another s-stage RK method

$$-\frac{d}{dt}\lambda_t = (\nabla_x f)^\top \lambda_t \quad \Rightarrow \quad \begin{aligned} \lambda_{n+1} &= \lambda_n + h\sum_{i=1}^{s} B_i l_{n,i}, \\ l_{n,i} &= -\nabla_x f(X_{n,i})^\top \Lambda_{n,i} \quad (i = 1, \ldots, s), \\ \Lambda_{n,i} &= \lambda_n + h\sum_{j=1}^{s} A_{ij} l_{n,j} \quad (i = 1, \ldots, s). \end{aligned}$$

Sanz-Serna (2016) provided a relation between (a, b) and (A, B)

so that $\boxed{\delta_{n+1}^\top \lambda_{n+1} = \delta_n^\top \lambda_n}$ **exactly.**

Sanz-Serna's idea

$$\boxed{\delta_{n+1}^\top \lambda_{n+1} = \delta_n^\top \lambda_n} \quad \Longleftrightarrow \quad \boxed{\begin{aligned} & b_i = B_i \quad (i = 1, \ldots, s)\,, \\ & b_i A_{ij} + B_j a_{ji} = B_i b_j \quad (i, j = 1, \ldots, s)\,. \end{aligned}}$$

$$\delta_{n+1} = \delta_n + h \sum_{i=1}^{s} b_i d_{n,i},$$

$$d_{n,i} = \nabla_x f(X_{n,i}) D_{n,i} \quad (i = 1, \ldots, s)\,,$$

$$D_{n,i} = \delta_n + h \sum_{j=1}^{s} a_{ij} d_{n,j} \quad (i = 1, \ldots, s)\,.$$

$$\lambda_{n+1} = \lambda_n + h \sum_{i=1}^{s} B_i l_{n,i},$$

$$l_{n,i} = -\nabla_x f(X_{n,i})^\top \Lambda_{n,i} \quad (i = 1, \ldots, s)\,,$$

$$\Lambda_{n,i} = \lambda_n + h \sum_{j=1}^{s} A_{ij} l_{n,j} \quad (i = 1, \ldots, s)\,.$$

Proof

$$S(\delta_t, \lambda_t) = \delta_t^\top \lambda_t$$

$$\begin{aligned}
& S(\delta_{n+1}, \lambda_{n+1}) - S(\delta_n, \lambda_n) \\
&\quad = h \sum_{i=1}^{s} B_i S(\delta_n, l_{n,i}) + h \sum_{i=1}^{s} b_i S(d_{n,i}, \lambda_n) + h^2 \sum_{i,j=1}^{s} B_i b_j S(d_{n,i}, l_{n,j}) \\
&\quad = h \sum_{i=1}^{s} B_i S(D_{n,i}, l_{n,i}) - h^2 \sum_{i,j=1}^{s} B_i a_{ij} S(d_{n,j}, l_{n,i}) \\
&\qquad + h \sum_{i=1}^{s} b_i S(d_{n,i}, \Lambda_{n,i}) - h^2 \sum_{i,j=1}^{s} b_i A_{ij} S(d_{n,i}, l_{n,j}) + h^2 \sum_{i,j=1}^{s} B_i b_j S(d_{n,i}, l_{n,j}) \\
&\quad = h \sum_{i=1}^{s} \underbrace{(b_i - B_i)}_{=0} S\left(D_{n,i}, \nabla_x f(X_{n,i})^\top \Lambda_{n,i}\right) + h^2 \sum_{i,j=1}^{s} \underbrace{\left(B_i b_j - b_i A_{ij} - B_j a_{ji}\right)}_{=0} S(d_{n,i}, l_{n,j})
\end{aligned}$$

Exact gradient computation

Forward models solved by a s-stage Runge–Kutta (RK) method

$$\frac{d}{dt}x_t = f(x_t) \quad \Rightarrow \quad \begin{aligned} x_{n+1} &= x_n + h\sum_{i=1}^{s} b_i k_{n,i}, \\ k_{n,i} &= f(X_{n,i}) \quad (i = 1, \ldots, s), \\ X_{n,i} &= x_n + h\sum_{j=1}^{s} a_{ij} k_{n,j} \quad (i = 1, \ldots, s). \end{aligned}$$

$$\frac{d}{dt}\delta_t = (\nabla_x f)\,\delta_t \quad \Rightarrow \quad \begin{aligned} \delta_{n+1} &= \delta_n + h\sum_{i=1}^{s} b_i d_{n,i}, \\ d_{n,i} &= \nabla_x f(X_{n,i}) D_{n,i} \quad (i = 1, \ldots, s), \\ D_{n,i} &= \delta_n + h\sum_{j=1}^{s} a_{ij} d_{n,j} \quad (i = 1, \ldots, s). \end{aligned}$$

and adjoint model solved by another s-stage RK method

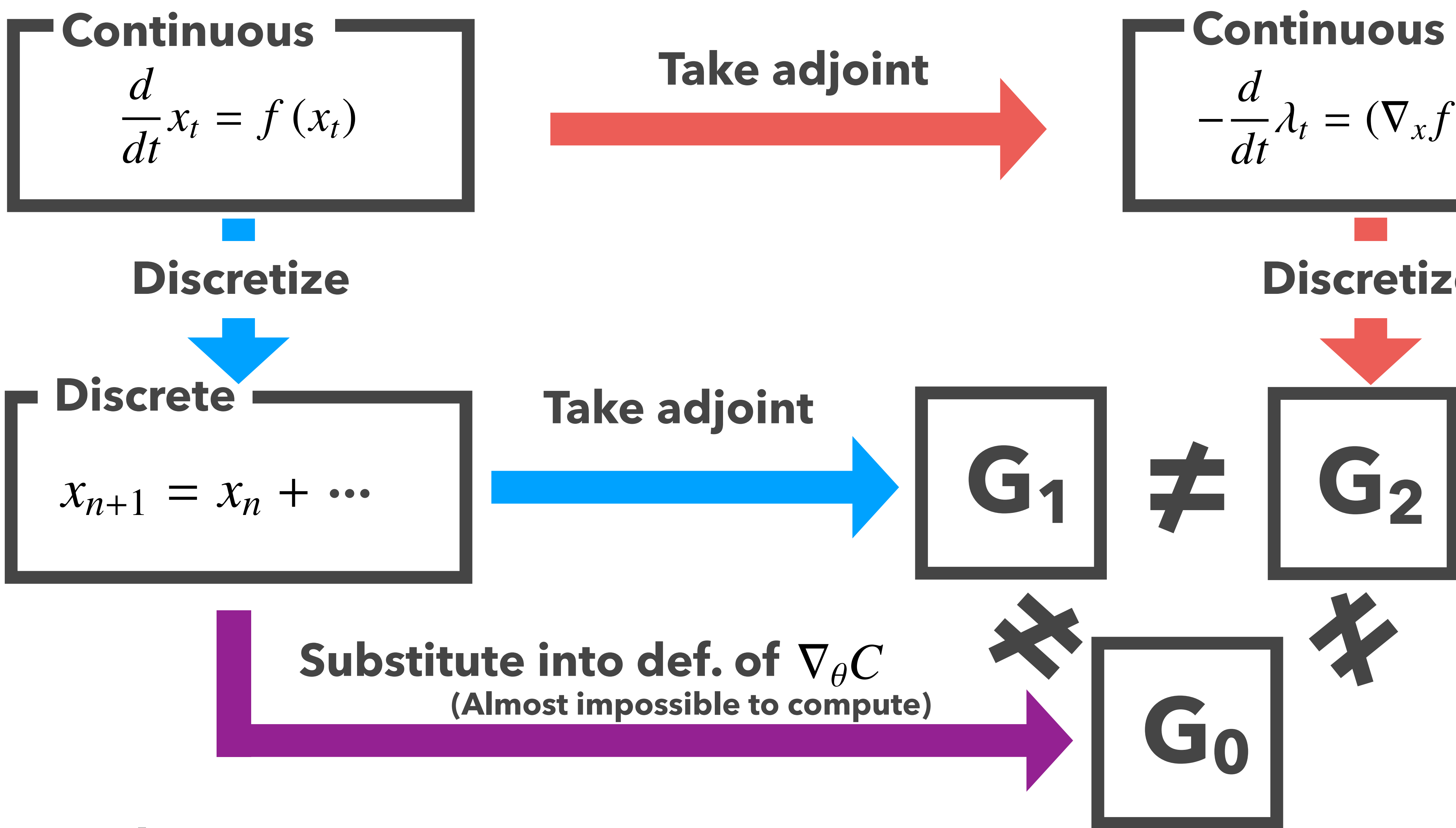
$$-\frac{d}{dt}\lambda_t = (\nabla_x f)^\top \lambda_t \quad \Rightarrow \quad \begin{aligned} \lambda_{n+1} &= \lambda_n + h\sum_{i=1}^{s} B_i l_{n,i}, \\ l_{n,i} &= -\nabla_x f(X_{n,i})^\top \Lambda_{n,i} \quad (i = 1, \ldots, s), \\ \Lambda_{n,i} &= \lambda_n + h\sum_{j=1}^{s} A_{ij} l_{n,j} \quad (i = 1, \ldots, s). \end{aligned}$$

where

$$\boxed{\begin{aligned} b_i &= B_i \quad (i = 1, \ldots, s), \\ b_i A_{ij} + B_j a_{ji} &= B_i b_j \quad (i, j = 1, \ldots, s). \end{aligned}}$$

provide exact gradient as $\lambda_0 = \nabla_\theta C$

Adjoint consistency in time



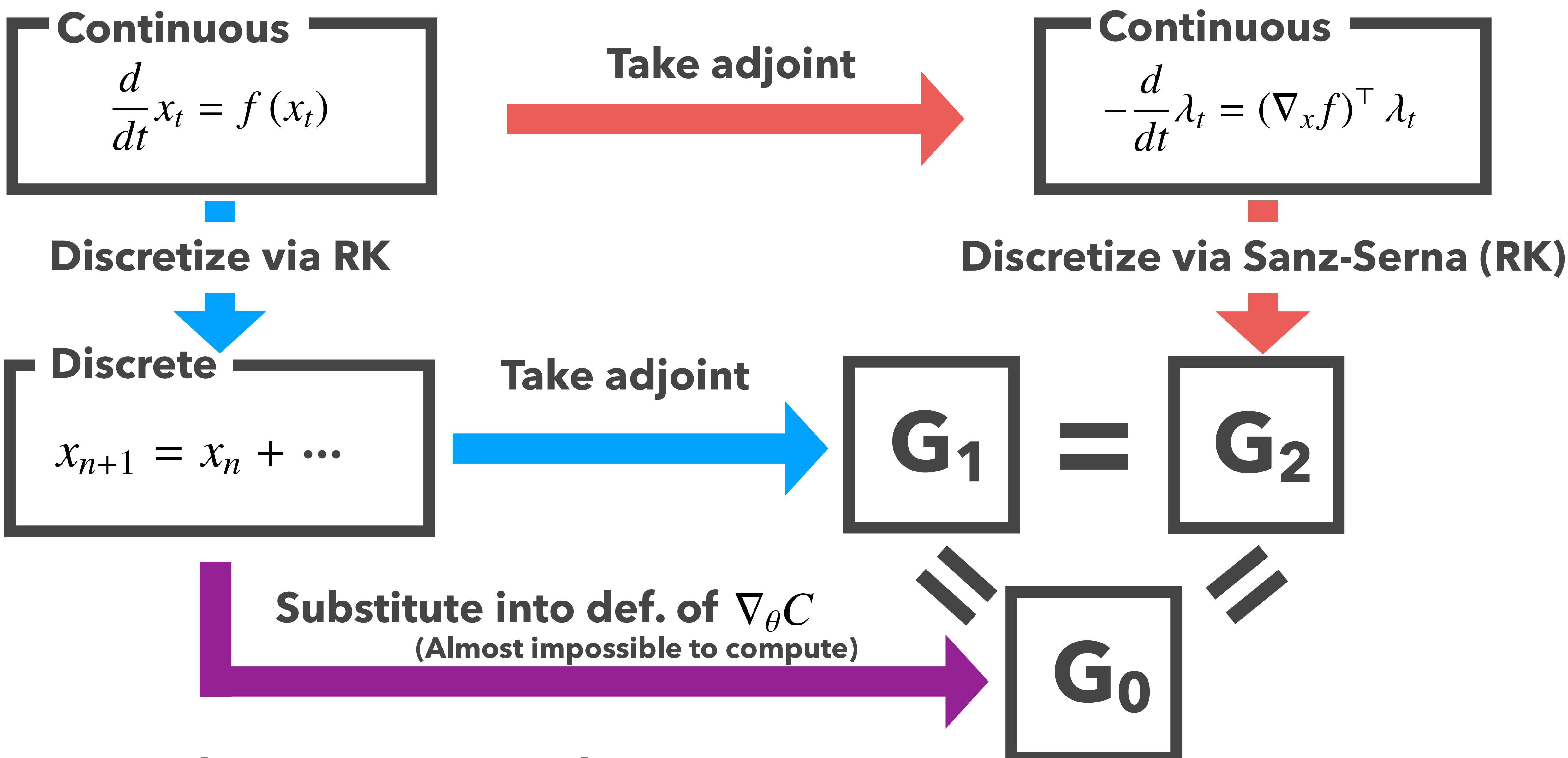
In general,

G_1 and G_2 are different.

Neither G_1 nor G_2 gives an exact gradient (G_0)

because $\delta_{n+1}^\top \lambda_{n+1} \neq \delta_n^\top \lambda_n$ in both cases.

Adjoint consistency in time



Sanz-Serna's scheme guarantees that

G_1 and G_2 are identical

They give an exact gradient (G_0)

since $\delta_{n+1}^\top \lambda_{n+1} = \delta_n^\top \lambda_n$

Open problems(?)

Other types of schemes

Consistency in space, i.e., PDEs

(e.g., advection eq.)

Towards exact Hessian computation

Exact gradient can be computed by using Sanz-Serna's scheme.

Exact Hessian ???

Forward model

$$\frac{d}{dt}x_t = f(x_t)$$

Adjoint model

$$-\frac{d}{dt}\lambda_t = (\nabla_x f)^\top \lambda_t$$

Sanz-Serna (2016)

Tangent linear (TL) model

$$\frac{d}{dt}\delta_t = (\nabla_x f)\,\delta_t$$

SOA model

$$-\frac{d}{dt}\xi_t = (\nabla_x f)^\top \xi_t + \{(\nabla_x \nabla_x f)\,\delta_t\}^\top \lambda_t$$

?

Towards exact Hessian computation

Our idea: Equivalence between SOA model and adjoint model

$$\frac{d}{dt}x_t = f(x_t) \qquad \frac{d}{dt}\delta_t = (\nabla_x f)\,\delta_t$$

$$-\frac{d}{dt}\lambda_t = (\nabla_x f)^\top \lambda_t \qquad -\frac{d}{dt}\xi_t = (\nabla_x f)^\top \xi_t + \{(\nabla_x \nabla_x f)\,\delta_t\}^\top \lambda_t$$

Define augmented vectors: $q_t = \begin{bmatrix} x_t \\ \delta_t \end{bmatrix}$ **and** $p_t = \begin{bmatrix} \lambda_t \\ \xi_t \end{bmatrix}$

$$\boxed{\begin{aligned} \frac{d}{dt}q_t &= \begin{bmatrix} f(x_t) \\ (\nabla_x f)\,\delta_t \end{bmatrix} = G(q_t) \\ -\frac{d}{dt}p_t &= \begin{bmatrix} (\nabla_x f)^\top \lambda_t \\ (\nabla_x f)^\top \xi_t + \{(\nabla_x \nabla_x f)\,\delta_t\}^\top \lambda_t \end{bmatrix} = \left(\nabla_q G\right)^\top p_t \end{aligned}}$$

Set of adjoint and SOA models constitutes a large adjoint system

→ **Many techniques for adjoint method can be used for SOA method.**
e.g., Sanz-Serna’s idea, adjoint code generator

Exact gradient and Hessian computations

The augmented models solved by Sanz-Serna (2016), i.e.,

the augmented forward model solved by a s-stage RK method

$$\frac{d}{dt}q_t = G(q_t) \quad \Rightarrow \quad \begin{aligned} q_{n+1} &= q_n + h\sum_{i=1}^{s} b_i k_{n,i}, \\ k_{n,i} &= G(Q_{n,i}) \quad (i = 1, \ldots, s), \\ Q_{n,i} &= q_n + h\sum_{j=1}^{s} a_{ij} k_{n,j} \quad (i = 1, \ldots, s). \end{aligned}$$

and the augmented adjoint model solved by another s-stage RK method

$$-\frac{d}{dt}p_t = \left(\nabla_q G\right)^\top p_t \quad \Rightarrow \quad \begin{aligned} p_{n+1} &= p_n + h\sum_{i=1}^{s} B_i l_{n,i}, \\ l_{n,i} &= -\nabla_q G(Q_{n,i})^\top P_{n,i} \quad (i = 1, \ldots, s), \\ P_{n,i} &= p_n + h\sum_{j=1}^{s} A_{ij} l_{n,j} \quad (i = 1, \ldots, s). \end{aligned}$$

where

$$\boxed{\begin{aligned} &b_i = B_i \quad (i = 1, \ldots, s), \\ &b_i A_{ij} + B_j a_{ji} = B_i b_j \quad (i, j = 1, \ldots, s). \end{aligned}}$$

provide exact gradient and Hessian computations.

Note that our method itself is not limited to RK.

Numerical verifications

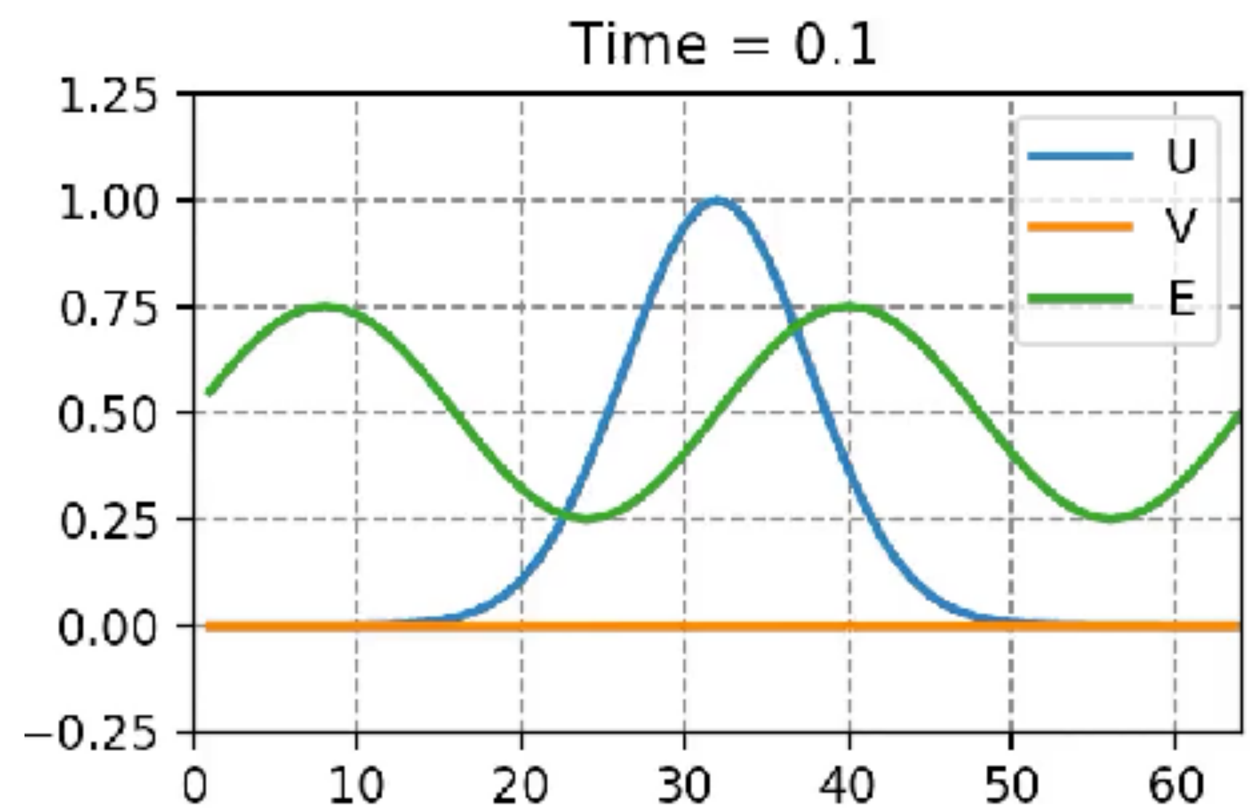
- Inhomogeneous wave equation

Inhomogeneous wave equation

Validate our method through numerical test of data assimilation based on a one-dimensional inhomogeneous wave equation

$$\frac{\partial^2 U(z,t)}{\partial t^2} = \frac{\partial}{\partial z}\left[E(z)\frac{\partial}{\partial z}U(z,t)\right]$$

(discretized in space by finite volume method)



Time integral scheme:

Heun method (2-stage RK)

Assume initial states of U and $\dot{U}$ are known but E is not.

Cost function:

$$C(E) = \sum_{t_n \in T^{\mathrm{obs}}} \|U_n(E) - U_n^{\mathrm{obs}}\|_2^2,$$

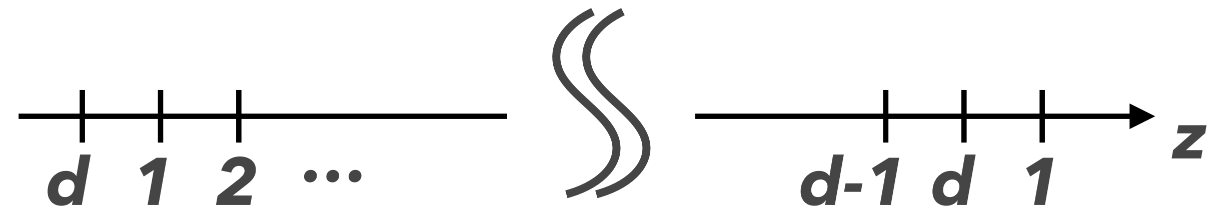
where

$T^{\mathrm{obs}} = \{0, 0.2, 0.4, \ldots, 1.8, 2.0\}$

U^{obs} : U **in the above movie**

Discretization in space

$$\frac{\partial^2 U(z,t)}{\partial t^2} = \frac{\partial}{\partial z}\left[E(z)\frac{\partial}{\partial z}U(z,t)\right]$$



Discretization via finite volume method (staggered lattice)

$$\frac{\mathrm{d}}{\mathrm{d}t}U_i = V_i \quad (i = 1, \ldots, d)$$

$$\frac{\mathrm{d}}{\mathrm{d}t}V_i = \frac{1}{\Delta z^2}\begin{cases} E_{\frac{3}{2}}\left(U_2 - U_1\right) - E_{d+\frac{1}{2}}\left(U_1 - U_d\right) & (i = 1) \\ E_{i+\frac{1}{2}}\left(U_{i+1} - U_i\right) - E_{i-\frac{1}{2}}\left(U_i - U_{i-1}\right) & (i = 2, \ldots, d-1) \\ E_{d+\frac{1}{2}}\left(U_1 - U_d\right) - E_{d-\frac{1}{2}}\left(U_d - U_{d-1}\right) & (i = d) \end{cases}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}E_{i+\frac{1}{2}} = 0 \quad (i = 1, \ldots, d),$$

Time integral schemes

Augmented forward model

$$\frac{d}{dt}q_t = G(q_t)$$

Heun method

$$q_{n+1} = q_n + \frac{h}{2}\left(k_{n,1} + k_{n,2}\right),$$
$$k_{n,1} = G(Q_{n,1}),$$
$$k_{n,2} = G(Q_{n,2}),$$
$$Q_{n,1} = q_n,$$
$$Q_{n,2} = q_n + hk_{n,1}.$$

Augmented adjoint model

$$-\frac{d}{dt}p_t = \left(\nabla_q G\right)^\top p_t$$

Naively

Our method

$$p_n = p_{n+1} + \frac{h}{2}\left(\bar{l}_{n,1} + \bar{l}_{n,2}\right),$$
$$\bar{l}_{n,2} = \nabla_q G(Q_{n,2})^\top P_{n,2},$$
$$\bar{l}_{n,1} = \nabla_q G(q_n)^\top P_{n,1},$$
$$P_{n,2} = p_{n+1},$$
$$P_{n,1} = p_{n+1} + h\bar{l}_{n,2}.$$

Heun method

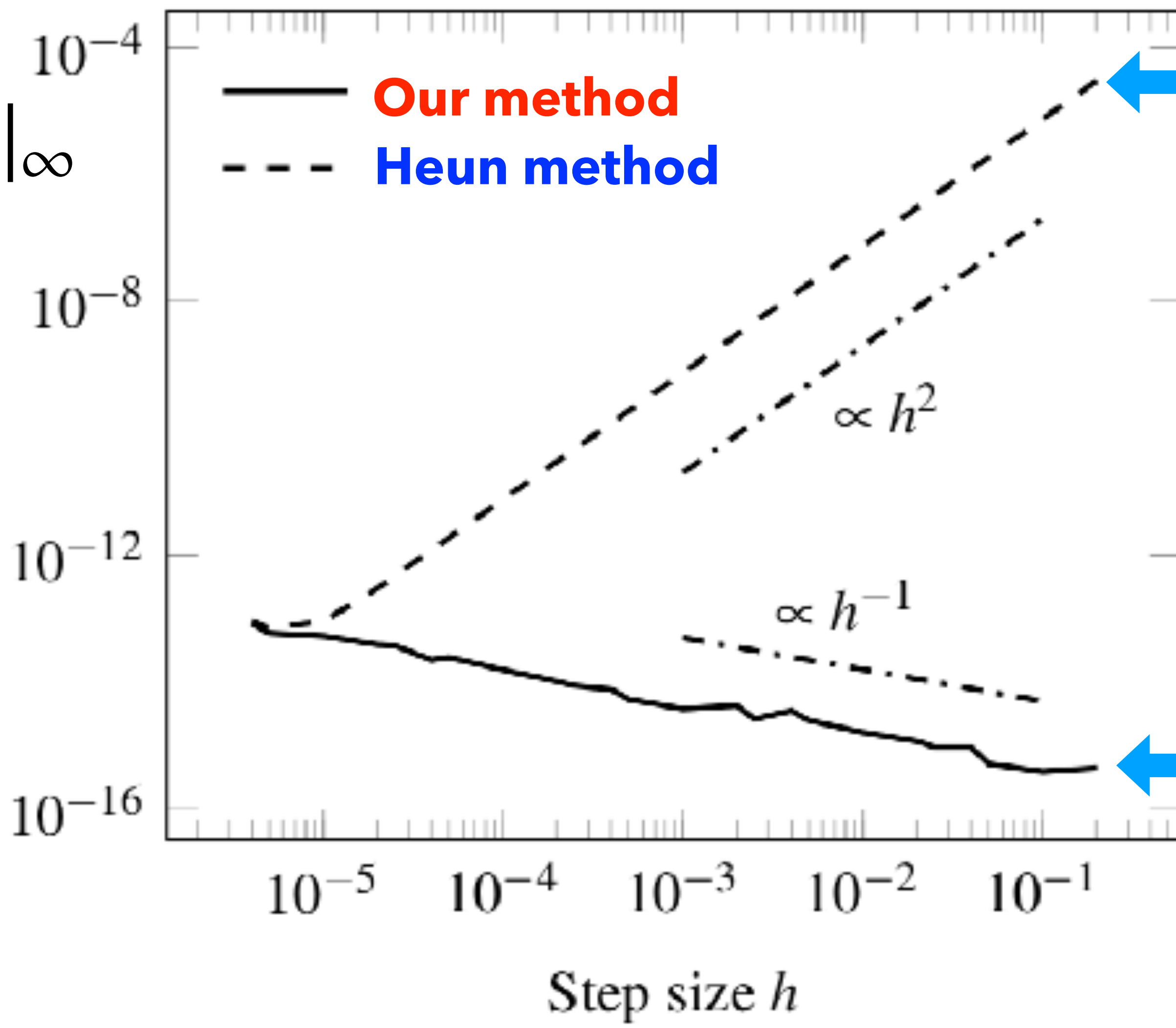
$$p_n = p_{n+1} + \frac{h}{2}\left(\bar{l}_{n,1} + \bar{l}_{n,2}\right),$$
$$\bar{l}_{n,2} = \nabla_q G(q_{n+1})^\top P_{n,2},$$
$$\bar{l}_{n,1} = \nabla_q G(q_n)^\top P_{n,1},$$
$$P_{n,2} = p_{n+1},$$
$$P_{n,1} = p_{n+1} + h\bar{l}_{n,2}.$$

Symmetry of Hessian matrix

$\|\mathrm{H}_\theta - \mathrm{H}_\theta{}^\top\|_\infty$: **Degree of asymmetry, which is zero if H_θ is symmetric.**

$\|\mathrm{H}_{\hat\theta} - \mathrm{H}_{\hat\theta}{}^\top\|_\infty$

$\hat\theta$: **Optimum sol.**



Discretization errors resulting from Heun method

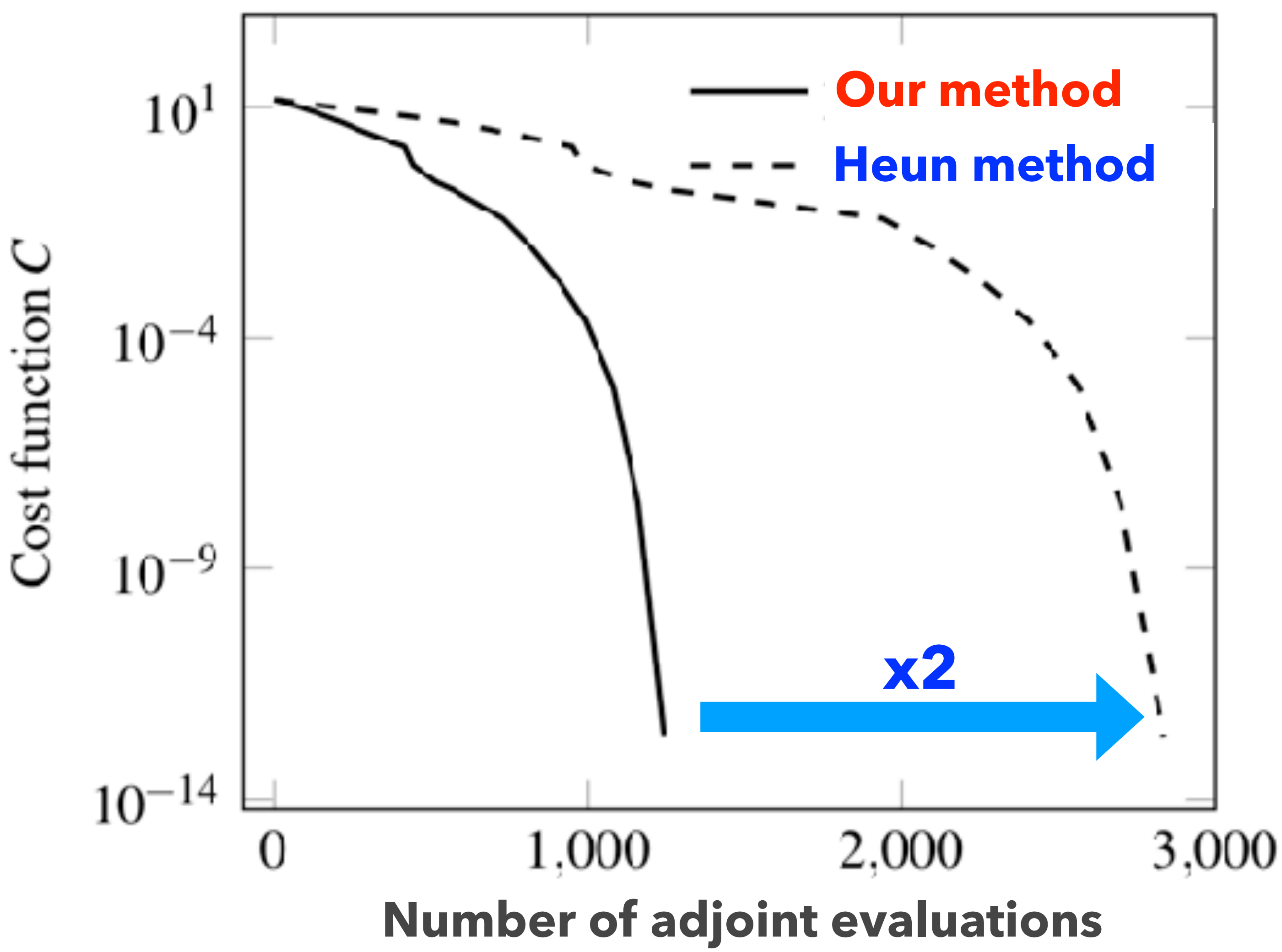
Only accumulation of machine errors (e.g., round-off error)

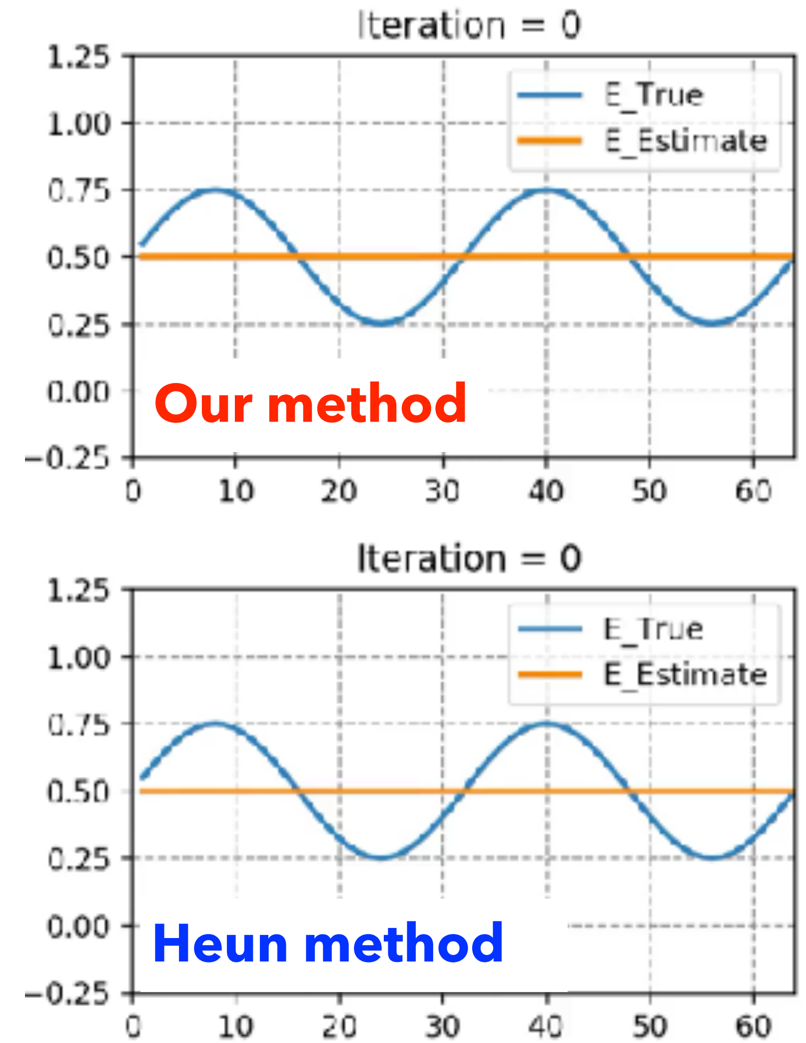
Our method reproduces the symmetry of Hessian without any discretization errors even when using a large step size.

Convergence to optimum solution

Optimizer : Regularized Newton method

$$\theta \leftarrow \theta + y \quad \text{where} \quad (\mathsf{H}_\theta + \sigma \mathsf{I})\, y = -\nabla_\theta C$$

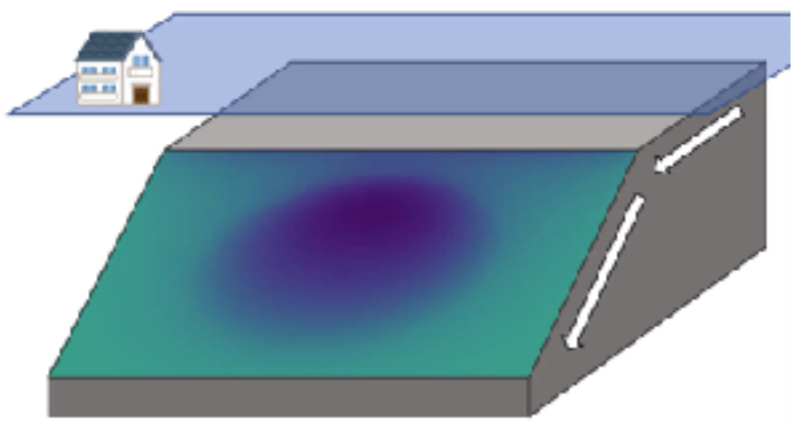




Our method contributes to rapid convergence.

Large-scale uncertainty quantification

Slow-slip motion model



* Damped EOM [Hirahara *et al.*(2019)]

$$\frac{d\tau}{dt} = \mathscr{G} \bullet (V_{plate} - V) + \mathrm{K}(V_{plate} - V_{lock}) - \frac{G}{2c}\frac{dV}{dt}$$

* Rate-and-state dependent friction law

$$\tau = \tau_0 + A \log V + B \log \theta$$

* Aging law

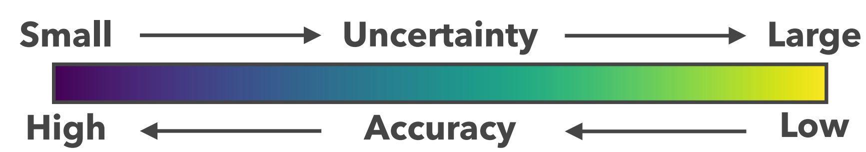
$$\frac{d\theta}{dt} = 1 - \frac{V\theta}{L}$$

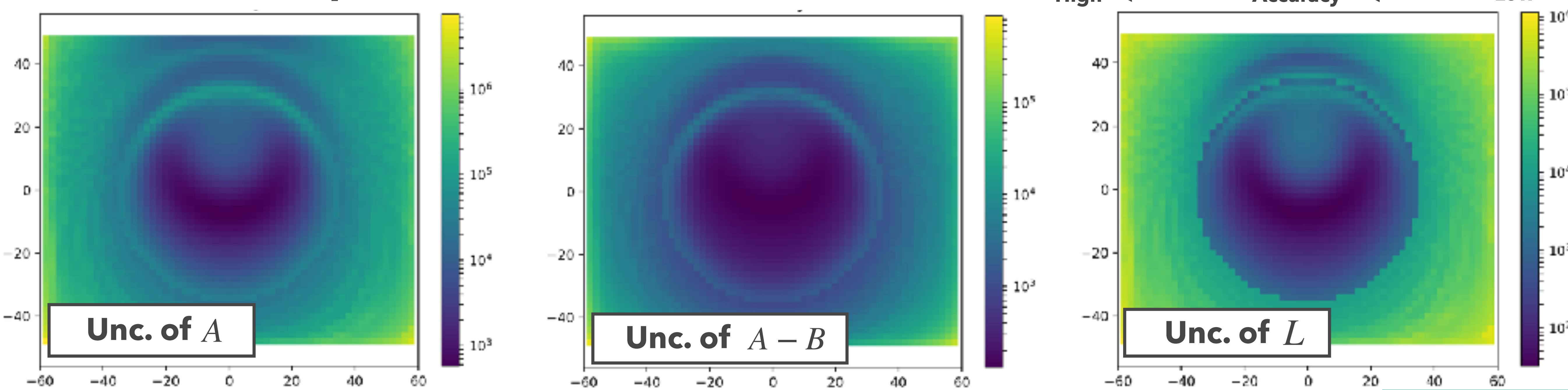
A, B, and L are spatially dependent

Ito et al., in prep.

Time integrator: Runge-Kutta-Fehlberg method

UQ for frictional parameter fields





Conclusions

* We proposed a method to compute an exact Hessian-vector product.

* The fact that the second-order adjoint system can be reformulated to a part of a large adjoint system is the key point to obtain the exact Hessian-vector product based on the Sanz-Serna scheme.

* Our method is capable of being applied to various types of ODEs.
    * Seismic imaging, aerodynamic design, structural materials, ...
    * Neural ODE

* Thank you for your attention

End