Sensitivity analysis for hyperbolic PDEs systems with discontinuous solution



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Outline of the talk

- Sensitivity analysis
- Sensitivity analysis for hyperbolic equations
- Riemann problem for the Euler equations and their sensitivity
- Classical numerical schemes
- Anti-diffusive numerical schemes
- Numerical results
- Uncertainty quantification

Sensitivity Analysis

Sensitivity Analysis

Sensitivity analysis: study of how changes in the **inputs** of a model affect the **outputs**



 $\begin{cases} \partial_t \mathbf{U} + \partial_x \mathbf{F}(\mathbf{U}) = 0 & \Omega \times (0, T), \\ \mathbf{U}(x, 0) = \mathbf{g}(x) & \Omega, \end{cases}$

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\begin{cases} \partial_a(\partial_t \mathbf{U}) + \partial_a(\partial_x \mathbf{F}(\mathbf{U})) = 0 & \Omega \times (0, T), \\ \partial_a \mathbf{U}(x, 0) = \partial_a \mathbf{g}(x) & \Omega, \end{cases}
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$$\begin{aligned} & \overbrace{\partial_a(\partial_t \mathbf{U}) + \partial_a(\partial_x \mathbf{F}(\mathbf{U})) = 0}^{\bullet} & \Omega \times (0, T), \\ & \overbrace{\partial_a \mathbf{U}(x, 0) = \partial_a \mathbf{g}(x)}^{\bullet} & \Omega, \end{aligned}$$

 $\begin{cases} \partial_t \mathbf{U}_a + \partial_x \mathbf{F}_a(\mathbf{U}, \mathbf{U}_a) = 0 & \Omega \times (0, T), \\ \mathbf{U}_a(x, 0) = \mathbf{g}_a(x) & \Omega, \end{cases}$

 $\begin{cases} \partial_t \mathbf{U}_a + \partial_x \mathbf{F}_a(\mathbf{U}, \mathbf{U}_a) = 0 & \Omega \times (0, T), \\ \mathbf{U}_a(x, 0) = \mathbf{g}_a(x) & \Omega, \end{cases}$

This can be done under hypotheses of regularity of the state U.

If these techniques are applied to hyperbolic equations, **Dirac delta functions** will appear in the sensitivity.

Sensitivity analysis for hyperbolic equations In order to have a sensitivity system which is valid also when the state is discontinuous, we add a correction term:

 $\begin{cases} \partial_t \mathbf{U}_a + \partial_x \mathbf{F}_a(\mathbf{U}, \mathbf{U}_a) = \mathbf{S} & \Omega \times (0, T), \\ \mathbf{U}_a(x, 0) = \mathbf{g}_a(x) & \Omega, \end{cases}$

 $\sum \rho_k \delta(x - x_{k,s}(t)),$

defined as follows:

 $\mathbf{S} = \mathbf{S}$

number of discontinuities

position of the k-th discontinuity

amplitude of the k-th correction (to be computed)

Remark: a shock detector is necessary to discretise such source term.

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Definition of the source term

To compute the amplitude of the correction, we consider an infinitesimal control volume containing a single discontinuity:

By integrating the sensitivity equations with the source term on the control volume, one has: $\boldsymbol{\rho}_k = (\mathbf{U}_a^- - \mathbf{U}_a^+)\boldsymbol{\sigma}_k + \mathbf{F}_a^+ - \mathbf{F}_a^-$

 $x_1 x_c$

 x_2

Rankine-Hugoniot conditions for the state: $(\mathbf{U}^+ - \mathbf{U}^-)\sigma_k = \mathbf{F}^+ - \mathbf{F}^-$

 t_2 -

 t_1

Differentiating them w.r.t. the parameter:

$$\mathbf{U}_{a}^{-} - \mathbf{U}_{a}^{+} \sigma_{k} + (\mathbf{U}^{-} - \mathbf{U}^{+}) \sigma_{k,a} + \sigma_{k} (\partial_{x} \mathbf{U}^{+} - \partial_{x} \mathbf{U}^{-}) \partial_{a} x_{k,s}(t) =$$
$$= \mathbf{F}_{a}^{-} - \mathbf{F}_{a}^{+} + \left(\frac{\partial \mathbf{F}(\mathbf{U}^{+})}{\partial \mathbf{U}} \partial_{x} \mathbf{U}^{+} - \frac{\partial \mathbf{F}(\mathbf{U}^{-})}{\partial \mathbf{U}} \partial_{x} \mathbf{U}^{-} \right) \partial_{a} x_{k,s}(t).$$

Finally, we obtain the following amplitude: $\rho_k = (\mathbf{U}^+ - \mathbf{U}^-)\sigma_{a,k}$

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Riemann problem for Euler equations and their sensitivity

The Riemann problem for Euler equations

The Euler equations write:

 $\begin{array}{l} \partial_t \rho + \partial_x (\rho u) = 0, \\ \partial_t (\rho u) + \partial_x (\rho u^2 + p) = 0, \\ \partial_t (\rho E) + \partial_x (u(\rho E + p)) = 0, \end{array} \end{array}$

Eigenvalues:	Eigenvectors:
$\lambda_1(\mathbf{U}) = u - c,$	$\mathbf{r}_1(\mathbf{U}) = (1, u - c, H - uc)^t,$
$\lambda_2(\mathbf{U}) = u,$	$\mathbf{r}_2(\mathbf{U}) = (1, u, \frac{u^2}{2})^t,$
$\lambda_3(\mathbf{U}) = u + c.$	$\mathbf{r}_3(\mathbf{U}) = (1, u + c, H + uc)^t.$

Genuinely nonlinear

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The Riemann problem for Euler equations

The Euler equations write:

 $\begin{array}{l} \partial_t \rho + \partial_x (\rho u) = 0, \\ \partial_t (\rho u) + \partial_x (\rho u^2 + p) = 0, \\ \partial_t (\rho E) + \partial_x (u(\rho E + p)) = 0, \end{array} \end{array}$

Eigenvalues:Eigenvectors:
$$\lambda_1(\mathbf{U}) = u - c,$$
 $\mathbf{r}_1(\mathbf{U}) = (1, u - c, H - uc)^t,$ $\lambda_2(\mathbf{U}) = u,$ $\mathbf{r}_2(\mathbf{U}) = (1, u, \frac{u^2}{2})^t,$ $\lambda_3(\mathbf{U}) = u + c.$ $\mathbf{r}_3(\mathbf{U}) = (1, u + c, H + uc)^t.$

Linearly degenerate

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The Riemann problem for Euler equations



The Riemann problem for the sensitivity equations

The sensitivity system writes:

$$\begin{aligned} \partial_t \rho_a &+ \partial_x (\rho u)_a = S_1, \\ \partial_t (\rho u)_a &+ \partial_x (\rho_a u^2 + 2\rho u u_a + p_a) = S_2, \\ \partial_t (\rho E)_a &+ \partial_x (u_a (\rho E + p) + u((\rho E)_a + p_a)) = S_3, \end{aligned}$$

Eigenvalues:

$$\lambda_1(\mathbf{U}) = u - c,$$

$$\lambda_2(\mathbf{U}) = u,$$

$$\lambda_3(\mathbf{U}) = u + c.$$



Classical Numerical Schemes



Remark: the state and the sensitivity systems are solved **separately**.

 $\begin{cases} \partial_t \mathbf{U} + \partial_x \mathbf{F}(\mathbf{U}) = 0\\ \partial_t \mathbf{U}_a + \partial_x \mathbf{F}_a(\mathbf{U}, \mathbf{U}_a) = \mathbf{S}(\mathbf{U}) \qquad \mathbf{S}(\mathbf{U}) = \sum_{k=1}^{N_s} \sigma_{a,k} (\mathbf{U}_k^+ - \mathbf{U}_k^-) \end{cases}$

Remark: HLL-type schemes cannot be used for the state, two intermediate star states are necessary to have a well-defined the source term for the sensitivity.

Approximate Riemann solver for the state

First order Roe-type scheme

$$\begin{split} \lambda_1^{ROE} &= \tilde{u} - \tilde{c}_3 \quad \lambda_2^{ROE} = \tilde{u} \quad \lambda_3^{ROE} = \tilde{u} + \tilde{c} \quad \text{Roe-averaged eigenvalues} \\ \mathbf{U}_R - \mathbf{U}_L &= \sum_{k=1}^{3} \alpha_i \tilde{\mathbf{r}}_i \quad \text{decomposition along Roe-averaged eigenvectors} \\ \mathbf{U}_L^* &= \mathbf{U}_L + \alpha_1 \tilde{\mathbf{r}}_1 \quad \mathbf{U}_R^* = \mathbf{U}_R - \alpha_3 \tilde{\mathbf{r}}_3 \end{split}$$

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Approximate Riemann solvers for the sensitivity

HLL-type scheme: simpler structure that the state solver.
 HLL consistency conditions yield:

 $\begin{aligned} \mathbf{U}_{a,j-1/2}^{*} &= \frac{1}{\lambda_{3}^{ROE} - \lambda_{1}^{ROE}} \left(\lambda_{3}^{ROE} \mathbf{U}_{a,j}^{n} - \lambda_{1}^{ROE} \mathbf{U}_{a,j-1}^{n} - \mathbf{F}_{a}(\mathbf{U}_{j}, \mathbf{U}_{a,j}) + \mathbf{F}_{a}(\mathbf{U}_{j-1}, \mathbf{U}_{a,j-1}) + \mathbf{S}_{j-1/2} \right) \\ &\qquad \mathbf{S}_{j-1/2} = \partial_{a} \lambda_{1,j-1/2}^{ROE} (\mathbf{U}_{L,j-1/2}^{*} - \mathbf{U}_{j-1}) d_{1,j-1/2} \\ &\qquad + \partial_{a} \lambda_{2,j-1/2}^{ROE} (\mathbf{U}_{R,j-1/2}^{*} - \mathbf{U}_{L,j-1/2}^{*}) \\ &\qquad + \partial_{a} \lambda_{3,j-1/2}^{ROE} (\mathbf{U}_{j} - \mathbf{U}_{R,j-1/2}^{*}) d_{3,j-1/2} \end{aligned}$

HLLC-type scheme: same structure as the state.

HLL consistency conditions + Rankine-Hugoniot conditions. Equivalent to:

$$\mathbf{U}_{a,L}^* = \mathbf{U}_{a,L} + \alpha_{1,a}\tilde{\mathbf{r}}_1 + \alpha_1\tilde{\mathbf{r}}_{1,a} \qquad \mathbf{U}_{a,R}^* = \mathbf{U}_{a,R} - \alpha_{3,a}\tilde{\mathbf{r}}_3 - \alpha_3\tilde{\mathbf{r}}_{3,a}$$

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Numerical Scheme without diffusion

Scheme without numerical diffusion

Step 0 : initial data discretisation

Step 1 : solution of the Riemann problems, one for each interface



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Scheme without numerical diffusion

Step 0 : initial data discretisation

- Step 1 : solution of the Riemann problems, one for each interface
- Step 2 : definition of a staggered mesh on which the average is performed



 $\overline{x}_{j-1/2} = x_{j-1/2} + \sigma_{j-1/2} \Delta t$

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Scheme without numerical diffusion

Step 0 : initial data discretisation

Step 1 : solution of the Riemann problems, one for each interface

Step 2 : definition of a staggered mesh on which the average is performed

Step 3 : projection on the initial mesh

$$\overline{\mathbf{U}_{j-1}} \qquad \overline{\mathbf{U}_{j}} \qquad \overline{\mathbf{U}_{j+1}}$$

$$\mathbf{U}_{j} = \begin{cases} \overline{\mathbf{U}}_{j-1} & \text{if } \alpha \in \left(0, \frac{\Delta t}{\Delta x} \max(\sigma_{j-1/2}, 0)\right), \\ \overline{\mathbf{U}}_{j} & \text{if } \alpha \in \left[\frac{\Delta t}{\Delta x} \max(\sigma_{j-1/2}, 0), 1 + \frac{\Delta t}{\Delta x} \min(\sigma_{j+1/2}, 0)\right), \\ \overline{\mathbf{U}}_{j+1} & \text{if } \alpha \in \left[1 + \frac{\Delta t}{\Delta x} \min(\sigma_{j+1/2}, 0), 1\right). \end{cases}$$

 $\alpha \sim \mathcal{U}([0,1])$

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Numerical results



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Numerical results



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Sensitivity Analysis for nonlinear hyperbolic PDEs

Convergence



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Sensitivity Analysis for nonlinear hyperbolic PDEs

Riemann problem with uncertain parameters: $\mathbf{a} = (\rho_L, \rho_R, u_L, u_R, p_L, p_R)^t$

Aim: determine a **confidence interval** $CI_X = [\mu_X - \kappa \sigma_X, \mu_X + \kappa \sigma_X]$

Monte Carlo approach: N samples X_k

$$\mu_X = \frac{1}{N} \sum_{k=1}^N X_k \qquad \sigma_X^2 = \frac{1}{N-1} \sum_{k=1}^N |\mu_X - X_k|^2$$

Sensitivity approach: state X, sensitivities X_{a_i}

$$\mu_X = X$$
 $\sigma_X^2 = \sum_{i=1}^{6} X_{a_i}^2 \sigma_{a_i}^2$

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Sensitivity Analysis for nonlinear hyperbolic PDEs



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Conclusion and future development

Conclusion:

- We defined a sensitivity system valid in case of discontinuous state
- The correction term is well defined
- The correction term is important in applications

Future development:

- Effects of the numerical diffusion for the applications
- Extension to 2D

Thank you for your attention!