Applying CTSE within an ODE solver

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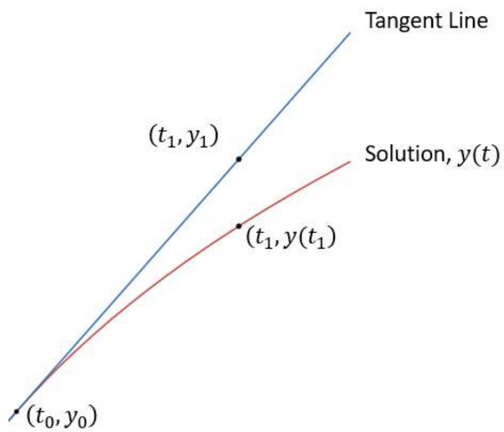
Ordinary Differential Equation (ODE) Solver

- CTSE can be employed within an ODE algorithm in order to obtain sensitivities of the dependent variable $y(x)$ with respect to model constants, i.e., $dy(x)/d\theta$, where θ is any constant in the ODE including initial conditions. This can be done for any ODE solver that supports complex variables including built-in solvers in C, Fortran, Mathematica, Matlab, Python, etc. The accuracy of the solver and its convergence rate are unaltered by CTSE.

Consider the simple case of Euler's method to solve equations of the form $y'(x) = f(x, y)$. Euler's method uses the slope $f(x_i, y_i)$ at y_i to project the solution to y_{i+1} that is,

$$y_{i+1} = y_i + f(x_i, y_i)h_{ode}.$$



Where h_{ode} is a step size to solve the ODE **NOT** the step size for CTSE.

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ODE solver – Euler's method

- Consider the following ODE with parameters: a, b, g. The sensitivities $dy(x)/da$, $dy(x)/db$, and $dy(x)/dg$ can be obtained by perturbing each parameter by ih and executing the traditional ODE solver method but now with complex variables. This will work with any ODE solver, e.g., RK45, as long as the solver supports complex variables.

$$y'(x) = ay(x) + bx - x^2 \qquad y(0) = g$$
$$a = 1, b = 2, g = 1$$

<u>Exact solutions:</u>

$y(x) = x^2 + e^x$ $\frac{dy(x)}{da} = -2 - 2x - x^2 + (2 + x)e^x$	$\frac{dy(x)}{db} = -1 - x + e^x$ $\frac{dy(x)}{dg} = e^x$

ODE solver – Euler's method

- The numerical results using Euler's method are shown below using a step size of $h_{ode} = 0.1$.

$$y'(x) = f(x, y) = ay(x) + bx - x^2$$

$$y(0) = g$$

$$a = 1, b = 2, g = 1$$

<u>Euler's method:</u>

$$y_{i+1}(x) = y_i + y'(x)h_{ode}$$

$$y'(x) = 1y(x) + 2x - x^2$$
$$y_0(0) = 1$$
$$h_{ode} = 0.1$$

h_{ode} is the step size used for Euler's method – this is independent from the h used by CTSE.

<u>Numerical solution:</u>

x	$\boldsymbol{y_i}$	$\boldsymbol{y'(x)}$	$\boldsymbol{y_{i+1}}$	$\boldsymbol{y_{exact}}$	Relative Error
0.0	1.0	1.0	1.1	1.0	---
0.1	1.1	1.129	1.290	1.1152	$9.80 * 10^{-2}$
0.2	1.229	1.589	1.388	1.2614	$1.09 * 10^{-1}$
0.3	1.388	1.898	1.578	1.4399	$1.20 * 10^{-1}$
0.4	1.578	2.218	1.799	1.6518	$1.29 * 10^{-1}$

ODE solver – $dy(x)/da$ result

- The sensitivity $dy(x)/da$ can be obtained using the standard Euler's method but now with complex variable parameters. As shown below, parameter a is replaced by $a + ih$ (with $a = 1$) and the derivative with respect to a is obtained as $\frac{dy(x)}{da} \approx \frac{1}{h} Im(y(x))$.

$$y'(x) = (1 + ih)y(x) + 2x - x^2 \text{ with } y(0) = 1$$

x	$y(x)$	dy/da	dy/da_{exact}	Relative Error
0.0	---	1.0	0	---
0.1	$1.1 + 1 * 10^{-1}\ i$	0.1	0.1108	$9.80 * 10^{-2}$
0.2	$1.229 + 2.2 * 10^{-11} i$	0.22	0.2471	$1.09 * 10^{-1}$
0.3	$1.388 + 3.649 * 10^{-1}\ i$	0.3649	0.4147	$1.20 * 10^{-1}$
0.4	$1.578 + 5.402 * 10^{-11} i$	0.5402	0.6204	$1.29 * 10^{-1}$

CTSE results ($h = 10^{-10}$ was used).

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ODE solver – $dy(x)/db$ result

- The sensitivity $dy(x)/db$ can be obtained using the standard Euler's method but now with complex variable parameters. As shown below, parameter b is replaced by $b + ih$ (with $b = 2$) and the derivative with respect to b is obtained as $dy(x)/db \approx \frac{1}{h} Im(y(x))$.

$$y'(x) = 1y(x) + (2 + ih)x - x^2 \text{ with } y(0) = 1$$

x	$y(x)$	dy/db	dy/db_{exact}	Relative Error
0.0	---	---	0	---
0.1	$1.1 + 0i$	0.0	0.0052	1
0.2	$1.229 + 1.0 * 10^{-12}i$	0.01	0.0214	0.532
0.3	$1.388 + 3.1 * 10^{-12}i$	0.031	0.0499	0.378
0.4	$1.578 + 6.41 * 10^{-12}i$	0.0641	0.0918	0.301

CTSE results ($h = 10^{-1}$ was used).

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ODE solver – $dy(x)/dg$ result

- The sensitivity $dy(x)/dg$ can be obtained using the standard Euler's method but now with complex variable parameters. As shown below, parameter g is replaced by $g + ih$ (with $\mathrm{g} = 1$) and the derivative with respect to g is obtained as $dy(x)/dg \approx \frac{1}{h} Im(y(x))$.

$y'(x) = 1y(x) + 2x - x^2$ with $y(0) = (1 + ih)$

x	$\boldsymbol{y(x)}$	$\boldsymbol{dy/dg}$	$\boldsymbol{dy/dg_{exact}}$	Relative Error
0.0	---	---	1.000	---
0.1	$1.1 + 1.1 * 10^{-10}i$	1.1	1.105	$4.68 * 10^{-3}$
0.2	$1.229 + 1.21 * 10^{-10}i$	1.21	1.221	$9.33 * 10^{-3}$
0.3	$1.388 + 1.331 * 10^{-10}i$	1.33	1.350	$1.40 * 10^{-2}$
0.4	$1.578 + 1.464 * 10^{-10}i$	1.46	1.492	$1.86 * 10^{-2}$

CTSE results ($h = 10^{-10}$ was used).

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