ISSN: 2278 – 1323
International Journal of Advanced Research in Computer Engineering & Technology (IJARCET)
Volume 1, Issue 8, October 2012

Global sensitivity and analysis of O.D.E by solving the P.D.E

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Abstract: ***In this work we discuss the global sensitivity analysis of O.D.E s by solving the P.D.E.***

$$\frac{\partial}{\partial t}u=-div\left(F.u\right)=Au,u\left(0,.\right)=u_0$$

Here we distinguish between methods that solve the O.D.E directly and method that solve the equivalent P.D.E formulation.We discuss general strategies for the solution of P.D.Es . This approaches is often referred to as stochastic sensitivity analysis .We give a brief overview of approaches to solving time dependent P.D.E

Key word: Global sensitivity, Linear sensitivity, sampled input values ,Density function semidiscretization in space.

Introduction: Depending on the problemunder study , the uncertainty and variability of an O.D.E model may effect initial values the parameters ,or both these will refer to as the model input.

In many cases , uncertainty can be regarded as small variations, or purterbation s around reference input values while variability generally refers to larger variations . Effect of small variations are often studied using a local approach . Local sensitivity analysis is basedlinearised solution s of the O.D.E around a reference input values .Llinearization facilities the analysis of the problem considerably, It involves the computation of partial derivative of the O.D.E with respect to the uncertain input variables so called sensibility indices which describes the varience of the out put uncertainty . The two terms ,Local and Linear sensitivity analysis , are often used interchangeably

The linear approach provide a good estimate of the true sensitivity only when variation are small, or when the modal dynamics are linear . In case of larger variations ,the sensitivity of a non linear model should there fore be studied globally .Global sensitivity analysis commonly considers the input values as a random variables with a given probability distribution . The problem can them =n be transformed to a system of O.D.Es with random initial values. By extending the state space to includes . The model parameters , this approach can account for variations in initial values and parameters within a single frame work . A straight forward approach is to solve this system for a set of sampled input values . An estimate of the sensitivity of the model can then be obtained from the out put produced with each of the sampled values . Sampling based approaches are called MONTE Carlo (MC) methods and are widely esed for sensitivity analysis of O.D.Es.

Based on the probability density function of the random initial values , The problem can be recast as a density propagation problem . The evolution of the density function is described by a first –order linear partial differential equation .CostanzaSeinfield , the numerical analysis of P.D.Es.is a broad field of ongoing research and extensive literature is dedicated to it . Therefore , The density propagation approach gives access to a rich theory and methodology that facilitate a lightly accurate estimation of the input uncertainty.

The analysis shown in this work reveals that , to guarantee convergence of the all numerical scheme , dependicies between the Spatial and temporal discretization have to be taken into account .These impose high accuracy constraints on the spatial descritization .

Acombination of the frame work presented here in with approximate approximizationson scattered grids may provide a powerful tool for the global sensitivity analysis of O.D.Es with moderate input dimensions.

Here we follow the presentation of linear sensitivity in

$$x^{\bullet}=F\left(x\right),\text{with } x\left(o\right)=x_0 \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(1)$$

Where $x_0=X_0$ is a random variable with probability density function u_o and consider a small change or perturbation δ_{x_0} around the initial value x_0 .The O.D.E with a perturbed initial value $x_0+\delta_{x_0}$ has the solution

$$x\left(t\right)=\phi_t\left(x_0+\delta_{x_0}\right) \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(2)$$

Using taylor expansion of ϕ_t atound x_0 , the linearized perturbation at time t

$$\delta_x(t) = \phi_t\left(x_0 + \delta_{x_0}\right) - \phi_t\left(x_0\right) \text{..........................(3)}$$

Can be written as

$$\delta_x(t) = W_t.\delta_{x_0} \text{ ....(4)}$$

Where W $W_t \in R^{d \times d}$ denotes the Jacobian of ϕ_t evaluated at $\phi_t x_0$

$$W_t = \frac{\partial}{\partial x}\phi_t(x) \ |_{x=\phi_t(x_0)} \text{ ....(5)}$$

Under the linearized dynamics , W_t propagates an initial perturbation along the trajectory $(\phi_t x_0, t)$ and is therefore called propagation matrix also wronski or sensitivity matrix .Since F and ϕ_t are assumed to be differentiable with respect to x we can establish O.D.E. for the evolution of the propagation matrix by

$$\frac{d}{dt}W_t = \frac{d}{dt}\left(\frac{\partial}{\partial x}\phi_t x\right) = \frac{\partial}{\partial x}\left(\frac{d}{dt}\phi_t x\right) = \frac{\partial}{\partial x}F\left(\phi_t x\right)W_t \text{.................................(6)}$$

Multiplication with δ_{x_0} and considering relation (4)yields the initial value problem

$$\frac{d}{dt}\delta_x(t) = \frac{\partial}{\partial x}F\left(\phi_t x\right)\delta_x(t),\ \delta_x(0) = \delta_{x_0}$$

....(7)

Which is called the variational equation in a parabolistic interpretation δ_{x_0} can denote the standard deviation of a normally distributed initial value $X_0 \sim N\left(\mu_0, \sum_0\right)$ with

$$\mu_0 = x_0 \text{ and } \sum_0 = \begin{pmatrix} \left(\delta_{x_0}\right)_1^2 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \left(\delta_{x_0}\right)_d^2 \end{pmatrix}$$

Where $\left(\delta_{x_0}\right)_i$ denotes the i-th component of δ_{x_0} since we assume that the uncertainty and or variability in the model input $x_0 = X_0$ is captured by the probability distribution of X_0, a straight forward approach is to sample points $\{\xi_1, \xi_2 .... \xi_n\}$ if the sample size M is sufficiently large , then by law of large numbers, the initial probabilitydistribution can be approximated by Global sensitivity analysis of O.D.Es can equivalently be studied by solving the P.D.E that describes the evolution of the probability density function associated with random state variable $x(t) = X_t$

Here we give a brief over view of approaches to solving time –dependent P.D.Es , The numerical solution of P.D.Es is a broad field of research and there is a such literature devoted to it . We confines ourselves to treating only those concept with more detail that are relevant to discuss the approach proposed in this work .

We focus on Trail ,a method by Horenko that was developed for a particular case of our problem .It was motivated by the attempt to transfer and apply Trail to the global sensitivity analysis of O.D.E.

Method of linear &Rothe method

A solution $u : R^d \times R^d \to R$ to a time dependent P.D.E is a function in time and space . Semi discretization in space corresponds to a computation of u at discrete space points or a representation in a finite dimensional function space . Semi discretization in time is the computation of u at discrete time .Depending on the order of semi- discretization we distinguish between methods of lines which first conduct a semi discretization in space and Rothe methods ,which first apply semi-discretization in time .Semi- discretization results in a reduced problem , a temporal problem in case of the method of lines and a spatial (stationary)problem in case of the Rothe method

Method of Lines Rothe method

$\frac{\partial}{\partial t}u$ = Au

Semi-discretization Semi discretization

In space in time

↓

System of O.D.E
Stationary P.D.E

The method of lines $\rightarrow$ For first order P.D.Es an initial semi –discretization in space results in a system of O.D.Es solving this system of O.D.Es yields a discrete solution along trajectories- or lines in time .We exemplify the derivation of such O.D.Es with a finite difference approximation of the spatial derivatives of the P.D.Es

Example : Semi –discretization in space by first order finite difference

Consider the one –dimensional case d=1 ,the P.D.E describing the evolution of an initial probability density function U_0 under deterministic dynamics F is given by

$$\frac{\partial}{\partial t}u = Au = -\frac{\partial}{\partial x}(F.u) \text{ with } u(0,\cdot) = u_0 \quad \text{............(8)}$$

A first order finite difference approximation of the spatial derivatives of $u(t,\cdot) = u_t$ yields

$$\frac{\partial}{\partial x}u_t(y) \approx \frac{u_t(y)-u_t(z)}{y-z},\ y,z \in R$$

…………………………..(9)

Given finite set of point $x_m \in R$ m=1……………..M

a substitution of $\frac{\partial}{\partial x}u$ for the above finite difference approximation transform to

$$\frac{\partial}{\partial t}u_t(x_m) = -F'(x_m).\ u_t(x_m) - F(x_m).\frac{u_t(x_m)-u_t(x_{m-1})}{x_m - x_{m-1}}$$

………………………(10)

With the remaining temporal derivative of u , the problem has been transformed in to a system of O.D.Es .It can be solved using the initial values

$u(o,x_m) = u_0(x_m)$,m=1,………………..M

Where $u(t,x_1),\ t \geq 0$ needs to specified by a boundary condition . Solution yields a fully discrete solution $u(t_j,x_m)$ at discrete time points $t_j \in R^+$, j =0,1,1,………, and space time m=1, ………………M

The above example shows how O.D.E.for the function values $u_t(x_m)$ can be derived by an approximation of the spatial derivatives . Alternatively ,u can be represented in a finite dimensional function space ie as a linear combination of a finite number of basis functions . Then , a system of O.D.Es for the coefficient of the linear combination can be derived in a similar way. Higher order P.D.E which require the inclusion of boundary condition , yield differential algebraic equation (DAE) INSTEAD OF o.d.Es . Due to the possibility of using standard numerical O.D.E (DAE) solvers , the method of lines is a popular tool for the solution of time dependent P.D.Es

The Rothe Method

The Rothe Method first conducts a semi –discretization in time , The basic idea is to consider the P.D.E as an O.D.E in a function space .We exemplify the derivation of the stationary problems using the implicit Euler method to approximate the temporal derivative .

Example: Semi discretization in timely the implicit euler

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International Journal of Advanced Research in Computer Engineering & Technology (IJARCET)
Volume 1, Issue 8, October 2012

Consider the same time –dependent P.D.E . Now we approximate the temporal derivative for a fixed time step τ

> 0 Applying an implicit Euler approximation of the temporal derivative yields the sequence of stationary or eliptic P.D.Es

$$\frac{u_{t_j} - u_{t_{j-1}}}{\tau} = Au_{t_j} \quad , \quad t_j = j.\tau \quad j=1,2,\ldots\ldots\ldots\ldots (11)$$

The stationary P.D.Es can be solved using spatial discretization techniques . Their solution yields a sequence of approximation to u at discrete time points t_j

In the above example we used a fixed time step τ .However ,time steps can also be chosen differently in each integration step $t_{j+1} = t_j + \tau_j$

Conclusion: The main advantage of the Rothemethod over the methods of lines relies on the repeated solution of the stationary spatial problems instead of choosing a semi-discretization in space on

at=0 , The solution of the spatial approximationcan be adapted according to the structure that a solution develops in the course of its temporal evolution Therefore ,the Rothe method allows for a fully adaptive integration of time dependent P.D.Es

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