A definition of stiffness for initial value problems for ODEs

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Laurent O. Jay
Joint work with Manuel Calvo (University of Zaragoza, Spain)

Dedicated to the memory of Jan Verwer

Dept. of Mathematics, The University of Iowa, USA

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Initial value problems for ODEs and stiffness

$$\frac{d}{dt}x = f(t,x), \quad x(t_0) = x_0 \in \mathbb{R}^d. \quad \text{We suppose } f \in \mathcal{C}^1.$$

- What is the concept of *stiffness*?
- Our goal is to settle the problem of having a mathematical definition of stiffness for IVPs for ODEs. We want the definition to be rigorous, precise, simple, and general. We do not want to contradict many previous well-motivated and justified attempts, our definition should be unifying in this sense.

Citations on stiffness

- In Hairer and Wanner (1996):
  "The most pragmatical opinion is historically the first one (Curtiss and Hirschfelder 1952): *stiff equations are equations where certain implicit methods, in particular BDF, perform better, usually tremendously better, than explicit ones."*

- Curtiss and Hirschfelder (1952):
  "

$$\frac{dy}{dx} = [y - G(x)]/a(x, y)$$

If Δx is the desired resolution of x or the interval which will be used in the numerical integration, the equation is "stiff" if

$$\left| \frac{a(x, y)}{\Delta x} \right| \ll 1$$

and G is well behaved"

Citations on stiffness

- Dahlquist (1974):
  "Systems containing very fast components as well as very slow components."
- Shampine (1981):
  "A major difficulty is that stiffness is a complex of related phenomena, so that it is not easy to say what stiffness is."

Citations on stiffness

- Dekker and Verwer (1984):
  "The problems called stiff are diverse and it is rather cumbersome to give a mathematically rigorous definition of stiffness. [...] Stiff problems from practice are well recognized. [...] The essence of stiffness is that the solution to be computed is slowly varying but that perturbations exist which are rapidly damped."

- Higham and Trefethen (1993):
  "Instability and stiffness are transient phenomena, involving finite time intervals $[t_0, t_1]$*. [...] Not all complicated effects are due to nonlinearity or variable coefficients; some are due to non-normality. [...] A problem is stiff for* $t \approx t_0$ *if the pseudospectra of this linear approximation extend far into the left half-plane as compared with the time-scale of the solution for* $t \approx t_0$*."*

Citations on stiffness

- Hairer and Wanner (1996):
  "Stiff problems are problems for which explicit methods don't work."
  Remark: Should "explicit" exponential methods be considered as being explicit or implicit?

- K. Ekeland, Owren, and Øines (1998):
  "[...] a precise definition of stiffness is not crucial for practical purposes."

- Cash (2003):
  "One of the major difficulties associated with the study of stiff differential systems is that a good mathematical definition of the concept of stiffness does not exist."

Citations on stiffness

- Spiteri (2004):
  "Stiffness is about efficiency, so pragmatic definitions have more potential. [...] For a given IVP [...] on the sub-intervals where it is more efficient to use an implicit method than an explicit one, we say the problem is stiff.[...] Stiffness is an efficiency thing."

- Brugnano, Mazzia, and Trigiante (2009):
  "The needs of applications, especially those rising in the construction of robust and general purpose codes, require nowadays a formally precise definition."

Citations on stiffness

- Wikipedia (2011):
  "[...] a stiff equation is a differential equation for which certain numerical methods for solving the equation are numerically unstable, unless the step size is taken to be extremely small. It has proven difficult to formulate a precise definition of stiffness, but the main idea is that the equation includes some terms that can lead to rapid variation in the solution."

Our point of view on stifness

Stiffness is a concept local in time and state that is characterized by the strongest damping of infinitesimal perturbations to the solution during a time-scale of interest from a given time and state. We do not want to relate our definition of stiffness directly to numerical methods.

Ingredients for a definition of stiffness

Ingredients:

- the system of ODEs

$$\frac{d}{dt}x = f(t, x)$$

- a current value $t = a$
- a certain time-scale $h \geq 0$
- the solution $x(t)$ on $[a, a + h]$

One may think of the time-scale h as a potential stepsize to be used for a numerical method, but this is immaterial in our definition.

NOT in our definition of stiffness

Not in the list of ingredients:

- any class of numerical ODE methods
- any assumption about the existence of an invariant attractive manifold
- any assumption about the transient or nontransient behavior of the solution
- any assumption about various time-scales in the solution

Nevertheless, the last three assumptions can certainly be useful to prove that a solution is stiff is the sense of the definition that we propose.

Main tool used in our definition

We denote by $x(t, s, y)$ the solution of

$$\frac{d}{dt}x = f(t, x), \qquad x(s) = y \in \mathbb{R}^d.$$

Our main tool is the sensitivity matrix

$$R(t, s, y) := D_y x(t, s, y)$$

which is solution (resolvent) of the matrix variational equation

$$\frac{d}{dt}R = D_x f(t, x(t, s, y))R, \quad R(s, s, y) = I_d$$

Properties of the sensitivity matrix

The sensitivity matrix has the properties:

$$\det(R(t,s,y)) = e^{\int_s^t \mathrm{tr}(D_x f(r,x(r,s,y)))dr} > 0$$
$$R(t,s,y)^{-1} = R(s,t,x(t,s,y))$$

We have for $\delta y \to 0$

$$x(t,s,y+\delta y) = x(t,s,y) + R(t,s,y)\delta y + o\left(\|\delta y\|\right)$$

on $[\min(s,t), \max(s,t)]$. Hence, $R(t,s,y)$ characterizes infinitesimal perturbations of $x(s) = y$.

The stiffness factor and our definition of stiffness

Definition

The *stiffness factor* of the solution $x(t)$ of the system of ODEs $\frac{d}{dt}x = f(t,x)$ from a on the time-scale $h \geq 0$ is

$$S(x,a,h) := \min_{s \leq t \in [a,a+h]} \min_{j=1,\ldots,d} |\lambda_j(R(t,s,x(s)))| > 0.$$

If $S(x,a,h) \ll 1$, $x(t)$ is said to be *stiff from a on the time-scale h*.

A quantitative definition of stiffness

To be quantitative one can replace the relation $S(x, a, h) \ll 1$ for example by $\log(S(x, a, h)) \leq -10$ for *mildly stiff* and by $\log(S(x, a, h)) \leq -20$ for *stiff*. This is motivated from the fact that for the Dahlquist test equation $\frac{d}{dt}x = \lambda x$ for $\lambda < 0$ we have $S(x, a, h) = e^{h\lambda}$ and from considering the (linear) stability regions of typical explicit one-step and multistep methods applied to the Dahlquist test equation.

Remark on the time-scale h

Our definition of stiffness is not concerned about the time-scale h considered as being reasonable for certain numerical methods to be taken as an actual stepsize or not which is an accuracy and stability issue. We are also not concerned about the efficiency of any class of numerical integration methods. Those are different issues.

From $R(a, a, x(a)) = I$ we have

$$S(x, a, 0) = 1$$

Hence, for h sufficiently small the solution $x(t)$ is not stiff (even mildly) from a on the time-scale h. We also have that $0 < S(x, a, h) \leq 1$.

Stiffness is not a concept for time intervals

If the solution $x(t)$ is stiff from a on the time-scale h, this does NOT imply that for any b and k satisfying $[b, b+k] \subset [a, a+h]$ we have that $x(t)$ is stiff from b on the time-scale k. No definition of stiffness should have such a property since any solution $x(t)$ should not be considered as being stiff for sufficiently small time-scales k. The concept of stiffness should not be defined with respect to intervals and it should not be said that a solution is stiff on any particular interval.

Equivalent characterization of stiffness factor

Lemma

$$S(x,a,h) = \frac{1}{\max_{s \leq t \in [a,a+h]} \rho\left(R(s,t,x(t))\right)}$$

where ρ denotes the spectral radius

Equivalent characterization of stiffness factor (proof)

We have $\lambda_i(A^{-1}) = 1/\lambda_j(A)$ and $R(t,s,x(s))^{-1} = R(s,t,x(t))$.

$$\begin{aligned}
S(x,a,h) &= \min_{s\le t\in[a,a+h]} \min_{i=1,\dots,d} |\lambda_i\left(R(t,s,x(s))\right)| \\
&= \min_{s\le t\in[a,a+h]} \min_{i=1,\dots,d} \frac{1}{|\lambda_i\left(R(t,s,x(s))^{-1}\right)|} \\
&= \min_{s\le t\in[a,a+h]} \min_{i=1,\dots,d} \frac{1}{|\lambda_i\left(R(s,t,x(t))\right)|} \\
&= \min_{s\le t\in[a,a+h]} \frac{1}{\max_{i=1,\dots,d} |\lambda_i\left(R(s,t,x(t))\right)|} \\
&= \min_{s\le t\in[a,a+h]} \frac{1}{\rho\left(R(s,t,x(t))\right)} \\
&= \frac{1}{\max_{s\le t\in[a,a+h]} \rho\left(R(s,t,x(t))\right)}
\end{aligned}$$

Stiffness and numerical methods

A stepsize h to be used by a numerical method can be seen as the time-scale of interest. The fact that a numerical method is suited for a given problem using a certain stepsize h is an *accuracy and stability* issue.

C-stability

The main tool in proving convergence of one-step methods on a finite interval $[t_0, T]$ is provided by the concept of C-stability (convergence stability) introduced by Dekker and Verwer (1984):

Definition

A one-step method is *C-stable* $\iff \exists$ constants Λ of moderate size and $H > 0$ such that

$$\|x_{n+1} - y_{n+1}\| \leq (1 + \Lambda h_n)\|x_n - y_n\|$$

for all x_n, y_n sufficiently close to the exact solution $x(t_n)$ and for all $h_n \in]0, H]$.

This condition is implied by several stability concepts. For example B-stable Runge-Kutta methods for contractive ODEs are C-stable.

Conclusion

"In theory, there is no difference between theory and practice. But, in practice, there is." Jan L. A. van de Snepscheut, Yogi Berra.

Remarks, questions, and criticisms are welcome!