

# Chapter 1

## Fifty Years of Stiffness

Luigi Brugnano, Francesca Mazzia,  
and Donato Trigiante

**Abstract** The notion of *stiffness*, which originated in several applications of a different nature, has dominated the activities related to the numerical treatment of differential problems for the last fifty years. Contrary to what usually happens in Mathematics, its definition has been, for a long time, not formally precise (actually, there are too many of them). Again, the needs of applications, especially those arising in the construction of robust and general purpose codes, require nowadays a formally precise definition. In this paper, we review the evolution of such a notion and we also provide a precise definition which encompasses all the previous ones.

**Keywords** Stiffness · ODE problems · Discrete problems · Initial value problems · Boundary value problems · Boundary value methods

**Mathematics Subject Classification (2000)** [72J10](#)

*Frustra fit per plura quod potest per pauciora.  
Razor of W. of Ockham, doctor invincibilis.*

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L. Brugnano (✉)

Dipartimento di Matematica, Università di Firenze, Viale Morgagni 67/A, 50134 Firenze, Italy  
e-mail: [luigi.brugnano@unifi.it](mailto:luigi.brugnano@unifi.it)

F. Mazzia

Dipartimento di Matematica, Università di Bari, Via Orabona 4, 70125 Bari, Italy  
e-mail: [mazzia@dm.uniba.it](mailto:mazzia@dm.uniba.it)

D. Trigiante

Dipartimento di Energetica, Università di Firenze, Via Lombroso 6/17, 50134 Firenze, Italy  
e-mail: [trigiant@unifi.it](mailto:trigiant@unifi.it)

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## 1.1 Introduction

The struggle generated by the duality short times–long times is at the heart of human culture in almost all its aspects. Here are just a few examples to fix the idea:

- in historiography: Braudel's distinction among the geographic, social and individual times;<sup>1</sup>
- in the social sphere: Societies are organized according to three kinds of laws, i.e., codes (regulating short term relations), constitutions (regulating medium terms relations), and ethical laws (long term rules) often not explicitly stated but religiously accepted;
- in the economy sphere: the laws of this part of human activities are partially unknown at the moment. Some models (e.g., the Goodwin model [19]), permits us to say, by taking into account only a few variables, that the main evolution is periodic in time (and then predictable), although we are experiencing an excess of periodicity (chaotic behavior). Nevertheless, some experts claim (see, e.g., [18]) that the problems in the predictability of the economy are mainly due to a sort of gap in passing information from a generation to the next ones, i.e. to the conflict between short time and long time behaviors.<sup>2</sup>

Considering the importance of this concept, it would have been surprising if the duality “short times–long times” did not appear somewhere in Mathematics. As a matter of fact, this struggle not only appears in our field but it also has a name: *stiffness*.

Apart from a few early papers [10, 11], there is a general agreement in placing the date of the introduction of such problems in Mathematics to around 1960 [17]. They were the necessities of the applications to draw the attention of the mathematical community towards such problems, as the name itself testifies: “*they have been termed stiff since they correspond to tight coupling between the driver and the driven components in servo-mechanism*” ([12] quoting from [11]).

Both the number and the type of applications proposing difficult differential problems has increased exponentially in the last fifty years. In the early times, the problems proposed by applications were essentially initial value problems and, consequently, the definition of stiffness was clear enough and shared among the few experts, as the following three examples evidently show:

D1: *Systems containing very fast components as well as very slow components* (Dahlquist [12]).

D2: *They represent coupled physical systems having components varying with very different times scales: that is they are systems having some components varying much more rapidly than the others* (Liniger [31], translated from French).

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<sup>1</sup>Moreover, his concept of *structure*, i.e. events which are able to accelerate the normal flow of time, is also interesting from our point of view, because it somehow recalls the mathematical concept of large variation in small intervals of time (see later).

<sup>2</sup>Even Finance makes the distinction between short time and long time traders.

93 D3: *A stiff system is one for which  $\lambda_{max}$  is enormous so that either the stability*  
94 *or the error bound or both can only be assured by unreasonable restrictions*  
95 *on  $h$ . . . Enormous means enormous relative to the scale which here is  $\bar{t}$  (the*  
96 *integration interval) . . . (Miranker [34]).*

97 The above definitions are rather informal, certainly very far from the precise def-  
98 initions we are accustomed to in Mathematics, but, at least, they agree on a crucial  
99 point: the relation among stiffness and the appearance of different time-scales in the  
100 solutions (see also [24]).

101 Later on, the necessity to encompass new classes of difficult problems, such as  
102 Boundary Value Problems, Oscillating Problems, etc., has led either to weaken the  
103 definition or, more often, to define some consequence of the phenomenon instead  
104 of defining the phenomenon itself. In Lambert's book [29] five propositions about  
105 stiffness, each of them capturing some important aspects of it, are given. As matter  
106 of fact, it has been also stated that no universally accepted definition of stiffness  
107 exists [36].

108 There are, in the literature, other definitions based on other numerical difficulties,  
109 such as, for example, large Lipschitz constants or logarithmic norms [37], or non-  
110 normality of matrices [23]. Often is not even clear if stiffness refers to particular  
111 solutions (see, e.g. [25]) or to problems as a whole.

112 Sometimes one has the feeling that stiffness is becoming so broad to be nearly  
113 synonymous of difficult.

114 At the moment, even if the old intuitive definition relating stiffness to multiscale  
115 problems survives in most of the authors, the most successful definition seems to  
116 be the one based on particular effects of the phenomenon rather than on the phe-  
117 nomenon itself, such as, for example, the following almost equivalent items:

118 D4: *Stiff equations are equations where certain implicit methods . . . perform better,*  
119 *usually tremendous better, than explicit ones [11].*

120 D5: *Stiff equations are problems for which explicit methods don't work [21].*

121 D6: *If a numerical method with a finite region of absolute stability, applied to a*  
122 *system with any initial condition, is forced to use in a certain interval of inte-*  
123 *gration a step length which is excessively small in relation to the smoothness*  
124 *of the exact solution in that interval, then the system is said to be stiff in that*  
125 *interval [29].*

126 As usually happens, describing a phenomenon by means of its effects may not  
127 be enough to fully characterize the phenomenon itself. For example, saying that fire  
128 is what produces ash, would oblige firemen to wait for the end of a fire to see if the  
129 ash has been produced. In the same way, in order to recognize stiffness according  
130 to the previous definitions, it would be necessary to apply first one<sup>3</sup> explicit method  
131 and see if it works or not. Some authors, probably discouraged by the above de-  
132 feats in giving a rigorous definition, have also affirmed that a rigorous mathematical  
133 definition of stiffness is not possible [20].

134 It is clear that this situation is unacceptable for at least two reasons:

135  
136  
137 <sup>3</sup>It is not clear if one is enough: in principle the definition may require to apply all of them.  
138

- it is against the tradition of Mathematics, where objects under study have to be *precisely* defined;
- it is necessary to have the possibility to recognize *operatively* this class of problems, in order to increase the efficiency of the numerical codes to be used in applications.

Concerning the first item, our opinion is that, in order to gain in precision, it would be necessary to revise the concept of *stability* used in Numerical Analysis, which is somehow different from the homonym concept used in all the other fields of Mathematics, where stable are equilibrium points, equilibrium sets, reference solutions, etc., but not equations or problems<sup>4</sup> (see also [17] and [30]).

Concerning the second item, *operatively* is intended in the sense that the definition must be stated in terms of *numerically observable* quantities such as, for example, norms of vectors or matrices. It was believed that, seen from the applicative point of view, a formal definition of stiffness would not be strictly necessary: *Complete formality here is of little value to the scientist or engineer with a real problem to solve* [24].

Nowadays, after the great advance in the quality of numerical codes,<sup>5</sup> the usefulness of a formal definition is strongly recognized, also from the point of view of applications: *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* [6].

In this paper, starting from ideas already partially exposed elsewhere [2, 4, 26], we will try to unravel the question of the definition of stiffness and show that a precise and operative definition of it, which encompasses all the known facets, is possible.

In order to be as clear as possible, we shall start with the simpler case of initial value for a single linear equation and gradually we shall consider more general cases and, eventually, we shall synthesize the results.

## 1.2 The Asymptotic Stability Case

For initial value problems for ODEs, the concept of stability concerns the behavior of a generic solution  $y(t)$ , in the neighborhood of a reference solution  $\bar{y}(t)$ , when the initial value is perturbed. When the problem is linear and homogeneous, the difference,  $e(t) = y(t) - \bar{y}(t)$ , satisfies the same equation as  $\bar{y}(t)$ . For nonlinear problems, one resorts to the linearized problem, described by the variational equation, which, essentially, provides valuable information only when  $\bar{y}(t)$  is asymptotically stable. Such a variational equation can be used to generalize to nonlinear problems the arguments below which, for sake of simplicity, concerns only the linear case.

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<sup>4</sup>Only in particular circumstances, for example in the linear case, it is sometimes allowed the language abuse: the nonlinear case may contain simultaneously stable and unstable solutions.

<sup>5</sup>A great deal of this improvement is due to the author of the previous sentence.

185 Originally, stiffness was almost always associated with initial value problems  
 186 having asymptotically stable equilibrium points (dissipative problems) (see, e.g.,  
 187 Dahlquist [13]). We then start from this case, which is a very special one. Its pecu-  
 188 liarities arise from the following two facts:<sup>6</sup>

- 189 • it is the most common in applications;
- 190 • there exists a powerful and fundamental theorem, usually called *Stability in the*  
 191 *first approximation Theorem* or *Poincaré-Liapunov Theorem*, along with its corol-  
 192 lary due to Perron<sup>7</sup>, which allows us to reduce the study of stability of critical  
 193 points, of a very large class of nonlinearities, to the study of the stability of the  
 194 corresponding linearized problems (see, e.g., [9, 27, 35, 38]).

196 The former fact explains the pressure of applications for the treatment of such  
 197 problems even before the computer age. The latter one provides, although not al-  
 198 ways explicitly recognized, the mathematical solid bases for the profitable and ex-  
 199 tensive use, in Numerical Analysis, of the linear test equation to study the fixed- $h$   
 200 stability of numerical methods.

201 We shall consider explicitly the case where the linearized problem is au-  
 202 tonomous, although the following definitions will take into account the more general  
 203 case.

204 Our starting case will then be that of an initial value problem having an asymp-  
 205 totically stable reference solution, whose representative is, in the scalar case,

$$206 \begin{aligned} 207 y' &= \lambda y, \quad t \in [0, T], \quad \operatorname{Re} \lambda < 0, \\ 208 y(0) &= \eta, \end{aligned} \quad (1.2.1)$$

209 where the reference solution (an equilibrium point, in this case) has been placed  
 210 at the origin. From what is said above, it turns out that it is not by chance that it  
 211 coincides with the famous test equation.

212  
 213 *Remark 1.1* It is worth observing that the above test equation is not less general  
 214 than  $y' = \lambda y + g(t)$ , which very often appears in the definitions of stiffness: the  
 215 only difference is the reference solution, which becomes  $\bar{y}(t) = \int_0^t e^{\lambda(t-s)} g(s) ds$ ,  
 216 but not the topology of solutions around it. This can be easily seen by introducing  
 217 the new variable  $z(t) = y(t) - \bar{y}(t)$  which satisfies exactly equation (1.2.1) and then,  
 218 trivially, must share the same stiffness. Once the solution  $z(t)$  of the homogeneous  
 219 equation has been obtained, the solution  $y(t)$  is obtained by adding to it  $\bar{y}(t)$  which,  
 220 in principle, could be obtained by means of a quadrature formula. This allows us to  
 221 conclude that if any stiffness is in the problem, this must reside in the homogeneous  
 222 part of it, i.e., in problem (1.2.1).  
 223

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224  
 225  
 226 <sup>6</sup>We omit, for simplicity, the other fact which could affect new definitions, i.e., the fact that the  
 227 solutions of the linear equation can be integrated over any large interval because of the equivalence,  
 228 in this case, between asymptotic and exponential stability.

229 <sup>7</sup>It is interesting to observe that the same theorem is known as the *Ostrowsky's Theorem*, in the  
 230 theory of iterative methods.

231 *Remark 1.2* We call attention to the interval of integration  $[0, T]$ , which depends on  
 232 our need for information about the solution, even if the latter exists for all values of  $t$ .  
 233 This interval must be considered as datum of the problem. This has been sometimes  
 234 overlooked, thus creating some confusion.

235  
 236 Having fixed problem (1.2.1), we now look for a mathematical tool which allows  
 237 us to state formally the intuitive concept, shared by almost all the definitions of  
 238 stiffness: i.e., we look for one or two parameters which tells us if in  $[0, T]$  the  
 239 solution varies rapidly or not. This can be done easily by introducing the following  
 240 two measures for the solution of problem (1.2.1):

$$241 \quad \kappa_c = \frac{1}{|\eta|} \max_{t \in [0, T]} |y(t)|, \quad \gamma_c = \frac{1}{|\eta|} \frac{1}{T} \int_0^T |y(t)| dt, \quad (1.2.2)$$

242 which, in the present case, assume the values:

$$243 \quad \kappa_c = 1, \quad \gamma_c = \frac{1}{|\operatorname{Re} \lambda| T} (1 - e^{\operatorname{Re} \lambda T}) \approx \frac{1}{|\operatorname{Re} \lambda| T} = \frac{T^*}{T},$$

244 where  $T^* = |\operatorname{Re} \lambda|^{-1}$  is the transient time. The two measures  $\kappa_c, \gamma_c$  are called *con-*  
 245 *ditioning parameters* because they measure the sensitivity of the solution subject to  
 246 a perturbation of the initial conditions in the infinity and in the  $l_1$  norm.

247 Sometimes, it would be preferable to use a lower value of  $\gamma_c$ , i.e.,

$$248 \quad \gamma_c = \frac{1}{|\lambda| T}. \quad (1.2.3)$$

249 This amounts to consider also the oscillating part of the solution (see also Re-  
 250 mark 1.5 below).

251 By looking at Fig. 1.1, one realizes at once that a rapid variation of the solution  
 252 in  $[0, T]$  occurs when  $\kappa_c \gg \gamma_c$ . It follows then that the parameter

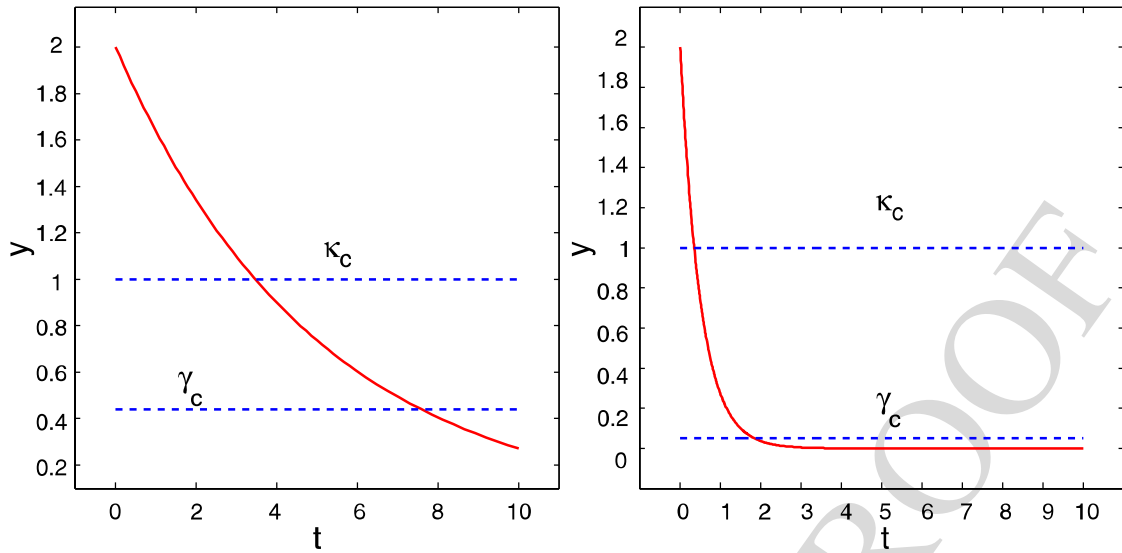
$$253 \quad \sigma_c = \frac{\kappa_c}{\gamma_c} \equiv \frac{T}{T^*}, \quad (1.2.4)$$

254 which is the ratio between the two characteristic times of the problem, is more sig-  
 255 nificant. Consequently, the definition of stiffness follows now trivially:

256 **Definition 1.3** The initial value problem (1.2.1) is *stiff* if  $\sigma_c \gg 1$ .

257 The parameter  $\sigma_c$  is called *stiffness ratio*.

258 *Remark 1.4* The width of the integration interval  $T$  plays a fundamental role in the  
 259 definition. This is an important point: some authors, in fact, believe that stiffness  
 260 should concern equations; some others believe that stiffness should concern prob-  
 261 lems, i.e., equations and data. We believe that both statements are partially correct:  
 262 stiffness concerns equations, integration time, and a set of initial data (not a specific  
 263 one of them). Since this point is more important in the non scalar case, it will be  
 264 discussed in more detail later.



**Fig. 1.1** Solutions and values of  $k_c$  and  $\gamma_c$  in the cases  $\lambda = -0.2$  (left plot) and  $\lambda = -2$  (right plot)

*Remark 1.5* When  $\sigma_c$  is defined according to (1.2.3), the definition of stiffness continues to be also meaningful in the case  $\text{Re } \lambda = 0$ , i.e., when the critical point is only marginally stable. In fact, let

$$\lambda = i\omega \equiv i \frac{2\pi}{T^*}.$$

Then,

$$\sigma_c = 2\pi \frac{T}{T^*},$$

and the definition encompasses also the case of *oscillating stiffness* introduced by some authors (e.g., [34]). Once again the stiffness is the ratio of two times. If information about the solution on the smaller time scale is needed, an adequately small stepsize should be used. It is worth noting that high oscillating systems (with respect to  $T$ ) fall in the class of problems for which explicit methods do not work, and then are stiff according to definitions D4–D6.

When  $\lambda = 0$ , then  $k_c = \gamma_c = \sigma_c = 1$ .

In the case  $\text{Re } \lambda > 0$  (i.e., the case of an unstable critical point), both parameters  $k_c$  and  $\gamma_c$  grow exponentially with time. This implies that small variations in the initial conditions will imply exponentially large variations in the solutions, both pointwise and on average: i.e., the problem is *ill conditioned*.

Of course, the case  $\text{Re } \lambda = 0$  considered above cannot be considered as representative of more difficult nonlinear equations, since linearization is in general not allowed in such a case.

The linearization is not the only way to study nonlinear differential (or difference) equations. The so called *Liapunov second method* can be used as well (see, e.g., [22, 27, 38]). It has been used, in connection with stiffness in [5, 13–17], al-

though not always explicitly named.<sup>8</sup> Anyway, no matter how the asymptotic stability of a reference solution is detected, the parameters (1.2.2) and Definition 1.3 continue to be valid. Later on, the problem of effectively estimating such parameters will also be discussed.

### 1.2.1 The Discrete Case

Before passing to the non scalar case, let us now consider the discrete case, where some interesting additional considerations can be made. Here, almost all we have said for the continuous case can be repeated. The first approximation theorem can be stated almost in the same terms as in the continuous case (see e.g. [28]).

Let the interval  $[0, T]$  be partitioned into  $N$  subintervals of length  $h_n > 0$ , thus defining the mesh points:  $t_n = \sum_{j=1}^n h_j$ ,  $n = 0, 1, \dots, N$ .

The linearized autonomous problem is now:

$$y_{n+1} = \mu_n y_n, \quad n = 0, \dots, N - 1, \quad y_0 = \eta, \quad (1.2.5)$$

where the  $\{\mu_n\}$  are complex parameters. The conditioning parameters for (1.2.5), along with the stiffness ratio, are defined as:

$$\begin{aligned} \kappa_d &= \frac{1}{|\eta|} \max_{i=0, \dots, N} |y_i|, & \gamma_d &= \frac{1}{|\eta|} \frac{1}{T} \sum_{i=1}^N h_i \max(|y_i|, |y_{i-1}|), \\ \sigma_d &= \frac{k_d}{\gamma_d}. \end{aligned} \quad (1.2.6)$$

This permits us to define the notion of *well representation* of a continuous problem by means of a discrete one.

**Definition 1.6** The problem (1.2.1) is *well represented* by (1.2.5) if

$$k_c \approx k_d, \quad (1.2.7)$$

$$\gamma_c \approx \gamma_d. \quad (1.2.8)$$

In the case of a constant mesh-size  $h$ ,  $\mu_n \equiv \mu$  and it easily follows that the condition (1.2.7) requires  $|\mu| < 1$ . It is not difficult to recognize the usual  $A$ -stability conditions for one-step methods (see Table 1.1). Furthermore, it is easily recognized that the request that condition (1.2.7) holds uniformly with respect to  $h\lambda \in \mathbb{C}^-$  implies that the numerical method producing (1.2.5) must be implicit.

What does condition (1.2.8) require more? Of course, it measures how faithfully the integral  $\int_0^T |y(t)| dt$  is approximated by the quadrature formula  $\sum_{i=1}^N h_i \cdot \max(|y_i|, |y_{i-1}|)$ , thus giving a sort of global information about the behavior of the

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<sup>8</sup>Often, it appears under the name of one-sided Lipschitz condition.



**Table 1.1** Condition (1.2.7) for some popular methods

Method	$\mu$	Condition
Explicit Euler	$1 + h\lambda$	$ 1 + h\lambda  < 1$
Implicit Euler	$\frac{1}{1-h\lambda}$	$ \frac{1}{1-h\lambda}  < 1$
Trapezoidal rule	$\frac{1+h\lambda/2}{1-h\lambda/2}$	$ \frac{1+h\lambda/2}{1-h\lambda/2}  < 1$

method producing the approximations  $\{y_i\}$ . One of the most efficient global strategies for changing the stepsize is based on monitoring this parameter [3, 4, 7, 8, 32, 33]. In addition to this, when finite precision arithmetic is used, then an interesting property of the parameter  $\gamma_d$  occurs [26]: if it is smaller than a suitably small threshold, this suggests that we are doing useless computations, since the machine precision has already been reached.

### 1.2.2 The non Scalar Case

In this case, the linearized problem to be considered is

$$y' = Ay, \quad t \in [0, T], \quad y(0) = \eta, \tag{1.2.9}$$

with  $A \in \mathbb{R}^{m \times m}$  and having all its eigenvalues with negative real part. It is clear from what was said in the scalar case that, denoting by  $\Phi(t) = e^{At}$  the fundamental matrix of the above equation, the straightforward generalization of the definition of the conditioning parameters (1.2.2) would lead to:

$$\kappa_c = \max_{t \in [0, T]} \|\Phi(t)\|, \quad \gamma_c = \frac{1}{T} \int_0^T \|\Phi(t)\| dt, \quad \sigma_c = \frac{\kappa_c}{\gamma_c}. \tag{1.2.10}$$

Indeed, these straight definitions *work most of the time*, as is confirmed by the following example, although, as we shall explain soon, not always.

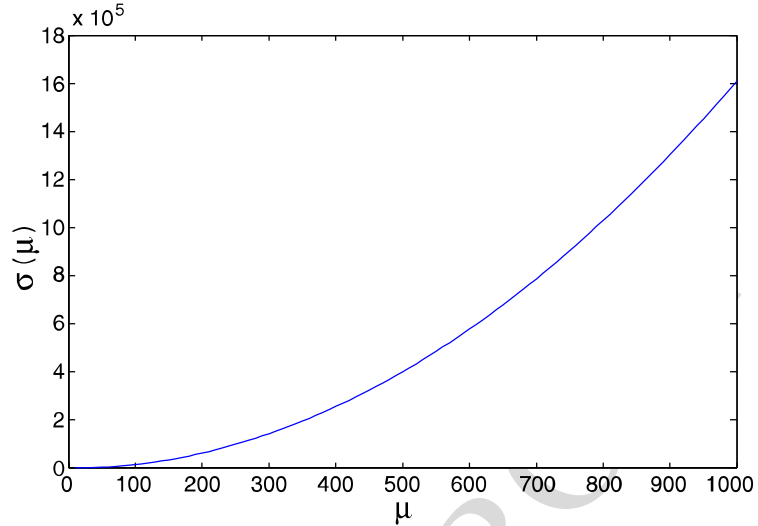
*Example 1.7* Let us consider the well-known Van der Pol's problem,

$$\begin{aligned} y_1 &= y_2, \\ y_2 &= -y_1 + \mu y_2(1 - y_1^2), \quad t \in [0, 2\mu], \\ y(0) &= (2, 0)^T, \end{aligned} \tag{1.2.11}$$

whose solution approaches a limit cycle of period  $T \approx 2\mu$ . It is also very well-known that, the larger the parameter  $\mu$ , the more difficult the problem is. In Fig. 1.2 we plot the parameter  $\sigma_c(\mu)$  (as defined in (1.2.10)) for  $\mu$  ranging from 0 to  $10^3$ . Clearly, stiffness increases with  $\mu$ .

Even though (1.2.10) works for this problem, this is not true in general. The problem is that the definition of stiffness as the ratio of two quantities may require a lower bound for the denominator. While the definition of  $\kappa_c$  remains unchanged, the definition of  $\sigma_c$  is more entangled. Actually, we need two different estimates of such a parameter:

**Fig. 1.2** Estimated stiffness ratio of Van der Pol's problem (1.2.11)



- an upper bound, to be used for estimating the conditioning of the problem in  $l_1$  norm;
- a lower bound, to be used in defining  $\sigma_c$  and, then, the stiffness.

In the definition given in [2, 4], this distinction was not made, even though the definition was (qualitatively) completed by adding

$$\text{“for at least one of the modes”}. \tag{1.2.12}$$

We shall be more precise in a moment. In the meanwhile, it is interesting to note that the clarification contained in (1.2.12) is already in one of the two definitions given by Miranker [34]:

*A system of differential equations is said to be stiff on the interval  $(0, \bar{t})$  if there exists a solution of that system a component of which has a variation on that interval which is large compared to  $\frac{1}{\bar{t}}$ ,*

where it should be stressed that the definition considers equations and not problems: this implies that the existence of largely variable components may appear for at least one choice of the initial conditions, not necessary for a specific one.

Later on, the definition was modified so as to translate into formulas the above quoted sentence (1.2.12). The following definitions were then given (see, e.g., [26]):

$$\begin{aligned} \kappa_c(T, \eta) &= \frac{1}{\|\eta\|} \max_{0 \leq t \leq T} \|y(t)\|, & \kappa_c(T) &= \max_{\eta} \kappa_c(T, \eta), \\ \gamma_c(T, \eta) &= \frac{1}{T\|\eta\|} \int_0^T \|y(t)\| dt, & \gamma_c(T) &= \max_{\eta} \gamma_c(T, \eta) \end{aligned} \tag{1.2.13}$$

and

$$\sigma_c(T) = \max_{\eta} \frac{\kappa_c(T, \eta)}{\gamma_c(T, \eta)}. \tag{1.2.14}$$

The only major change regards the definition of  $\sigma_c$ . Let us be more clear on this point with an example, since it leads to a controversial question in the literature: i.e.,

461 the dependence of stiffness from the initial condition. Let  $A = \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_m)$   
 462 with  $\lambda_i < 0$  and  $|\lambda_1| > |\lambda_2| > \dots > |\lambda_m|$ . The solution of problem (1.2.9) is  $y(t) =$   
 463  $e^{At}\eta$ .

464 If  $\sigma_c$  is defined according to (1.2.10), it turns out that  $\|e^{At}\| = e^{\lambda_m t}$  and, then,  
 465  $\gamma_c(T) \approx \frac{1}{T|\lambda_m|}$ . If, however, we take  $\eta = (1, 0, \dots, 0)^T$ , then  $y(t) = e^{\lambda_1 t}$  and  $\gamma_c(T)$   
 466 becomes  $\gamma_c(T) \approx \frac{1}{T|\lambda_1|}$ . Of course, by changing the initial point, one may activate  
 467 each one of the *modes*, i.e. the functions  $e^{\lambda_i t}$  on the diagonal of the matrix  $e^{At}$ ,  
 468 leaving silent the others. This is the reason for specifying, in the older definition,  
 469 the quoted sentence (1.2.12). The new definition (1.2.14), which essentially poses  
 470 as the denominator of the ratio  $\sigma_c$  the smallest value among the possible values of  
 471  $\gamma_c(T, \eta)$ , is more compact and complies with the needs of people working on the  
 472 construction of codes, who like more operative definitions. For the previous diagonal  
 473 example, we have that  $k_c$  continues to be equal to 1, while  $\gamma_c(T) = \frac{1}{T|\lambda_1|}$ .

474 Having got the new definition (1.2.14) of  $\sigma_c(T)$ , the definition of stiffness con-  
 475 tinues to be given by Definition 1.3 given in the scalar case, i.e., the problem (1.2.9)  
 476 is *stiff* if  $\sigma_c(T) \gg 1$ .

477 How does this definition reconcile with the most used definition of stiffness for  
 478 the linear case, which considers the “smallest” eigenvalue  $\lambda_m$  as well? The answer is  
 479 already in Miranker’s definition D3. In fact, usually the integration interval is chosen  
 480 large enough to provide complete information on the behavior of the solution. In this  
 481 case, until the slowest mode has decayed enough, i.e.  $T = 1/|\lambda_m|$ , which implies

$$482 \quad \sigma_c \left( T = \frac{1}{|\lambda_m|} \right) = \left| \frac{\lambda_1}{\lambda_m} \right|, \quad (1.2.15)$$

483 which, when much larger than 1, coincides with the most common definition of  
 484 stiffness in the linear case. However, let us insist on saying that if the interval of in-  
 485 tegration is much smaller than  $1/|\lambda_m|$ , *the problem may be not stiff* even if  $|\frac{\lambda_1}{\lambda_m}| \gg 1$ .

486 The controversy about the dependence of the definition of stiffness on the ini-  
 487 tial data is better understood by considering the following equation given in [29,  
 488 pp. 217–218]:

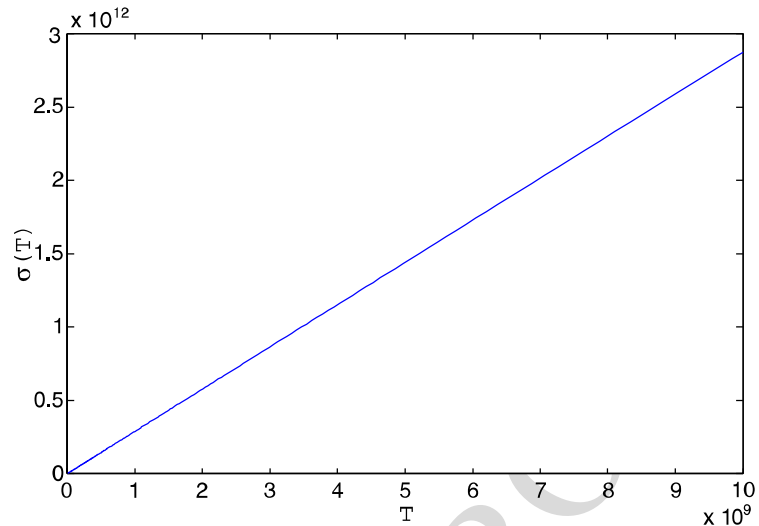
$$489 \quad \frac{d}{dt} \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = \begin{pmatrix} -2 & 1 \\ -1.999 & 0.999 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} + \begin{pmatrix} 2 \sin t \\ 0.999(\sin t - \cos t) \end{pmatrix},$$

490 whose general solution is

$$491 \quad \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = c_1 e^{-t} \begin{pmatrix} 1 \\ 1 \end{pmatrix} + c_2 e^{-0.001t} \begin{pmatrix} 1 \\ 1.999 \end{pmatrix} + \begin{pmatrix} \sin t \\ \cos t \end{pmatrix}.$$

492 The initial condition  $y(0) = (2, 3)^T$  requires  $c_2 = 0$  and, then, the slowest mode is  
 493 not activated: the solution rapidly reaches the reference solution. If this information  
 494 was known beforehand, one could, in principle, choose the interval of integration  
 495  $T$  much smaller than  $\frac{1}{0.001}$ . This, however, does not take into account the fact that  
 496 the computer uses finite precision arithmetic, which may not represent exactly the  
 497 initial condition. To be more precise, let us point out that the slowest mode is  
 498 not activated only if the initial condition is on the line  $y_2(0) - y_1(0) - 1 = 0$ . Any  
 499 irrational value of  $y_1(0)$  will not be well represented on the computer. This is enough  
 500  
 501  
 502  
 503  
 504  
 505  
 506

**Fig. 1.3** Estimated stiffness ratio of Robertson's problem (1.2.16)



to activate the silent mode. Of course, if one is sure that the long term contribution to the solution obtained on the computer is due to this kind of error, a small value of  $T$  can always be used. But it is rare that this information is known in advance. For this reason, we consider the problem to be stiff, since we believe that the definition of stiffness cannot distinguish, for example, between rational and irrational values of the initial conditions. Put differently, initial conditions are like a fuse that may activate stiffness.

We conclude this section by providing a few examples, which show that Definition 1.3, when  $\sigma_c$  is defined according to (1.2.14), is able to adequately describe the stiffness of nonlinear and/or non autonomous problems as well.

*Example 1.8* Let us consider the well-known Robertson's problem:

$$\begin{aligned}
 y_1 &= -0.04y_1 + 10^4 y_2 y_3, \\
 y_2 &= 0.04y_1 - 10^4 y_2 y_3 - 3 \times 10^7 y_2^2, \quad t \in [0, T], \\
 y_3 &= 3 \times 10^7 y_2^2, \\
 y(0) &= (1, 0, 0)^T.
 \end{aligned}
 \tag{1.2.16}$$

Its stiffness ratio with respect to the length  $T$  of the integration interval, obtained through the linearized problem and considering a perturbation of the initial condition of the form  $(0, \varepsilon, -\varepsilon)^T$ , is plotted in Fig. 1.3. As it is well-known, the figure confirms that for this problem stiffness increases with  $T$ .

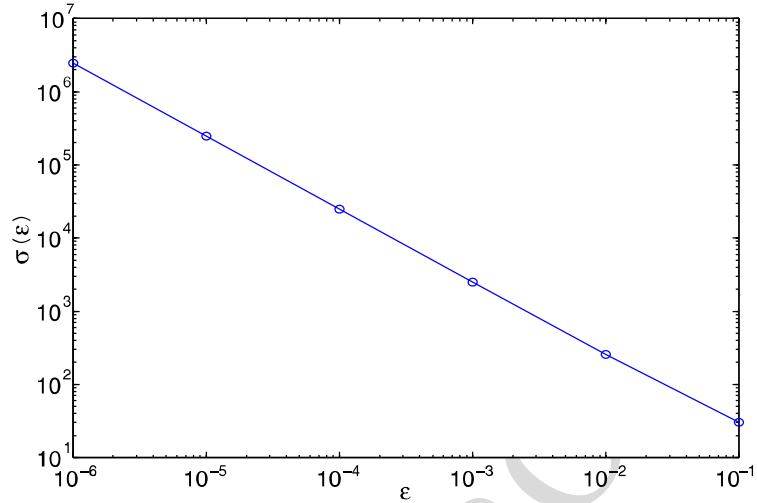
*Example 1.9* Let us consider the so-called Kreiss problem [21, p. 542], a linear and non autonomous problem:

$$y' = A(t)y, \quad t \in [0, 4\pi], \quad y(0) \text{ fixed}, \tag{1.2.17}$$

where

$$A(t) = Q^T(t)\Lambda Q(t), \tag{1.2.18}$$

**Fig. 1.4** Estimated stiffness ratio of the Kreiss problem (1.2.17)–(1.2.19)



and

$$Q(t) = \begin{pmatrix} \cos t & \sin t \\ -\sin t & \cos t \end{pmatrix}, \quad \Lambda_\epsilon = \begin{pmatrix} -1 & \\ & -\epsilon^{-1} \end{pmatrix}. \quad (1.2.19)$$

Its stiffness ratio with respect to the small positive parameter  $\epsilon$ , obtained by considering a perturbation of the initial condition of the form  $(-\epsilon, 1)^T$ , is plotted in Fig. 1.4. As one expects, the figure confirms that the stiffness of the problem behaves as  $\epsilon^{-1}$ , as  $\epsilon$  tends to 0.

*Example 1.10* Let us consider the following linear and non autonomous problem, a modification of problem (1.2.17), that we call “modified Kreiss problem”:<sup>9</sup>

$$y' = A(t)y, \quad t \in [0, 4\pi], \quad y(0) \text{ fixed}, \quad (1.2.20)$$

where

$$A(t) = Q_\epsilon^{-1}(t)P^{-1}\Lambda_\epsilon P Q_\epsilon(t), \quad (1.2.21)$$

and

$$P = \begin{pmatrix} -1 & 0 \\ 1 & 1 \end{pmatrix}, \quad Q_\epsilon(t) = \begin{pmatrix} 1 & \epsilon \\ e^{\sin t} & e^{\sin t} \end{pmatrix}, \quad \Lambda_\epsilon = \begin{pmatrix} -1 & \\ & -\epsilon^{-1} \end{pmatrix}. \quad (1.2.22)$$

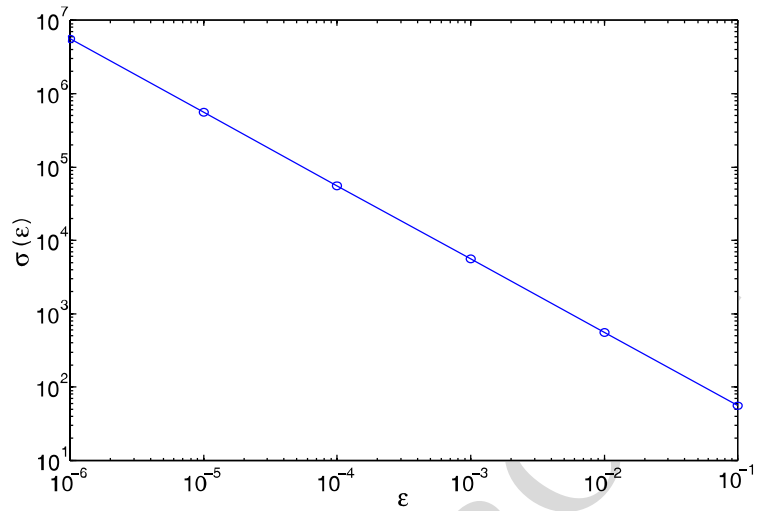
Its stiffness ratio with respect to the small positive parameter  $\epsilon$ , obtained by considering a perturbation of the initial condition of the form  $(-\epsilon, 1)^T$ , is shown in Fig. 1.5. Also in this case the stiffness of the problem behaves as  $\epsilon^{-1}$ , as  $\epsilon$  tends to 0.

*Remark 1.11* It is worth mentioning that, in the examples considered above, we numerically found that

$$\max_\eta \frac{\kappa_c(T, \eta)}{\gamma_c(T, \eta)}$$

<sup>9</sup>This problem has been suggested by J.I. Montijano.

**Fig. 1.5** Estimated stiffness ratio of the modified Kreiss problem (1.2.20)–(1.2.22)



is obtained by considering an initial condition  $\eta$  in the direction of the eigenvector of the Jacobian matrix (computed for  $t \approx t_0$ ) associated to the dominant eigenvalue. We note that, for an autonomous linear problem, if  $A$  is diagonalizable, this choice activates the *mode* associated with  $\lambda_1$ , i.e., the eigenvalue of maximum modulus of  $A$ .

### 1.2.3 The Non Scalar Discrete Case

As for the scalar case, what we said for the continuous problems can be repeated, *mutatis mutandis*, for the discrete ones. For brevity, we shall skip here the details for this case, also because they can be deduced from those described in the more general case discussed in the next section.

## 1.3 Boundary Value Problems (BVPs)

The literature about BVPs is far less abundant than that about IVPs, both in the continuous and in the discrete case. While there are countless books on the latter subject presenting it from many points of view (e.g., stability of motion, dynamical systems, bifurcation theory, etc.), there are many less books about the former. More importantly, the subject is usually presented as a by product of the theory of IVPs. This is not necessarily the best way to look at the question, even though many important results can be obtained this way. However, it may sometimes be more useful to look at the subject the other way around. Actually, the question is that IVPs are naturally a subclass of BVPs. Let us informally clarify this point without many technical details which can be found, for example, in [4].

IVPs transmit the initial information “from left to right”. Well conditioned IVPs are those for which the initial value, along with the possible initial errors, decay

645 moving from left to right. FVPs (Final Value problems) are those transmitting in-  
646 formation “from right to left” and, of course, well conditioning should hold when  
647 the time, or the corresponding independent variable, varies towards  $-\infty$ . More pre-  
648 cisely, considering the scalar test equation (1.2.1), the asymptotically stability for  
649 IVPs and FVPs requires  $\operatorname{Re} \lambda < 0$  and  $\operatorname{Re} \lambda > 0$ , respectively. BVPs transmit infor-  
650 mation both ways. Consequently, they cannot be scalar problems but vectorial of  
651 dimension at least two. We need then to refer to the test equation (1.2.9). It can be  
652 affirmed that a well conditioned linear BVP needs to have eigenvalues with both  
653 negative and positive real parts (*dichotomy*, see, e.g., [1, 4]). More precisely: the  
654 number of eigenvalues with negative real part has to match the amount of informa-  
655 tion transmitted “from left to right”, and the number of eigenvalues with positive  
656 real part has to match the amount of information traveling “from right to left”. For  
657 brevity, we shall call the above statement *continuous matching rule*. Of course, if  
658 there are no final conditions, then the problem becomes an IVP and, as we have  
659 seen, in order to be well conditioned, it must have all the eigenvalues with negative  
660 real part. In other words, the generalization of the case of asymptotically stable IVPs  
661 is the class of well conditioned BVPs *because both satisfy the continuous matching*  
662 *rule*. This is exactly what we shall assume hereafter.

663 Similar considerations apply to the discrete problems, where the role of the imag-  
664 inary axis is played by the unit circumference in the complex plane. It is not sur-  
665 prising that a numerical method will *well represent* a continuous autonomous linear  
666 BVP if the corresponding matrix has as many eigenvalues inside the unit circle as  
667 the number of initial conditions and as many eigenvalues outside the unit circle as  
668 the number of final conditions (*discrete matching rule*).

669  
670 *Remark 1.12* The idea that IVPs are a subset of BVPs is at the root of the class of  
671 methods called *Boundary Value Methods (BVMs)* which permits us, thanks to the  
672 discrete matching rule, to define high order and perfectly *A*-stable methods (i.e.,  
673 methods having the imaginary axis separating the stable and unstable domains),  
674 which *overcome the Dahlquist's barriers*, and are able to solve both IVPs and BVPs  
675 (see, e.g., [4]).

676  
677 *Remark 1.13* From this point of view, the popular *shooting method*, consisting of  
678 transforming a BVP into an IVP and then applying a good method *designed for*  
679 *IVPs*, does not appear to be such a good idea. As matter of fact, even a very well  
680 conditioned linear BVP, i.e. one which satisfies the continuous matching rule, will  
681 be transformed in a badly conditioned IVP, since the matrix of the continuous IVP  
682 shall, of course, contain eigenvalues with positive real part. This will prevent the  
683 discrete matching rule to hold.

### 684 685 686 **1.3.1 Stiffness for BVPs**

687  
688 Coming back to our main question, stiffness for BVPs is now defined by generaliz-  
689 ing the idea already discussed in the previous sections.  
690

As in the previous cases, we shall refer to linear problems, but the definitions will also be applicable to nonlinear problems as well. Moreover, according to what is stated above, we shall only consider the case where the problems are well conditioned (for the case of ill conditioned problems, the arguments are slightly more entangled, see e.g. [7]). Then, let us consider the linear and non autonomous BVP:

$$y' = A(t)y, \quad t \in [0, T], \quad B_0y(0) + B_1y(T) = \eta, \quad (1.3.1)$$

where  $y(t), \eta \in \mathbb{R}^m$  and  $A(t), B_0, B_1 \in \mathbb{R}^{m \times m}$ . The solution of the problem (1.3.1) is

$$y(t) = \Phi(t)Q^{-1}\eta,$$

where  $\Phi(t)$  is the fundamental matrix of the problem such that  $\Phi(0) = I$ , and  $Q = B_0 + B_1\Phi(T)$ , which has to be nonsingular, in order for (1.3.1) to be solvable.<sup>10</sup>

As in the continuous IVP case, the conditioning parameters are defined (see (1.2.13)) as:

$$\begin{aligned} \kappa_c(T, \eta) &= \frac{1}{\|\eta\|} \max_{0 \leq t \leq T} \|y(t)\|, & \kappa_c(T) &= \max_{\eta} \kappa_c(T, \eta), \\ \gamma_c(T, \eta) &= \frac{1}{T\|\eta\|} \int_0^T \|y(t)\| dt, & \gamma_c(T) &= \max_{\eta} \gamma_c(T, \eta). \end{aligned} \quad (1.3.2)$$

Consequently, the stiffness ratio is defined as (see (1.2.14)):

$$\sigma_c(T) = \max_{\eta} \frac{\kappa_c(T, \eta)}{\gamma_c(T, \eta)},$$

and the problem is stiff if  $\sigma_c(T) \gg 1$ . Moreover, upper bounds of  $\kappa_c(T)$  and  $\gamma_c(T)$  are respectively given by:

$$\kappa_c(T) \leq \max_{0 \leq t \leq T} \|\Phi(t)Q^{-1}\|, \quad \gamma_c(T) \leq \frac{1}{T} \int_0^T \|\Phi(t)Q^{-1}\| dt. \quad (1.3.3)$$

Thus, the previous definitions naturally extend to BVPs the results stated for IVPs. In a similar way, when considering the discrete approximation of (1.3.1), for the sake of brevity provided by a suitable one-step method over a partition  $\pi$  of the interval  $[0, T]$ , with subintervals of length  $h_i, i = 1, \dots, N$ , the discrete problem will be given by

$$y_{n+1} = R_n y_n, \quad n = 0, \dots, N-1, \quad B_0 y_0 + B_1 y_N = \eta, \quad (1.3.4)$$

whose solution is given by

$$y_n = \left( \prod_{i=0}^{n-1} R_i \right) Q_N^{-1} \eta, \quad Q_N = B_0 + B_1 \prod_{i=0}^{N-1} R_i.$$

---

<sup>10</sup>Observe that, in the case of IVPs,  $B_0 = I$  and  $B_1 = O$ , so that  $Q = I$ .



The corresponding discrete conditioning parameters are then defined by:

$$\kappa_d(\pi, \eta) = \frac{1}{\|\eta\|} \max_{0 \leq n \leq N} \|y_n\|, \quad \kappa_d(\pi) = \max_{\eta} \kappa_d(\pi, \eta), \tag{1.3.5}$$

$$\gamma_d(\pi, \eta) = \frac{1}{T\|\eta\|} \sum_{i=1}^N h_i \max(\|y_i\|, \|y_{i-1}\|), \quad \gamma_d(\pi) = \max_{\eta} \gamma_d(\pi, \eta),$$

and

$$\sigma_d(\pi) = \max_{\eta} \frac{\kappa_d(\pi, \eta)}{\gamma_d(\pi, \eta)}.$$

According to Definition 1.6, we say that the discrete problem<sup>11</sup> (1.3.4) well represents the continuous problem (1.3.1) if

$$\kappa_d(\pi) \approx \kappa_c(T), \quad \gamma_d(\pi) \approx \gamma_c(T). \tag{1.3.6}$$

*Remark 1.14* It is worth mentioning that innovative mesh-selection strategies for the efficient numerical solution of stiff BVPs have been defined by requiring the match (1.3.6) (see, e.g., [3, 4, 7, 8, 26]).

### 1.3.2 Singular Perturbation Problems

The numerical solution of singular perturbation problems can be very difficult because they can have solutions with very narrow regions of rapid variation characterized by boundary layers, shocks, and interior layers. Usually, the equations depend on a small parameter, say  $\varepsilon$ , and the problems become more difficult as  $\varepsilon$  tends to 0. It is not always clear, however, how the width of the region of rapid variation is related to the parameter  $\varepsilon$ . By computing the stiffness ratio  $\sigma_c(T)$ , we observe that singularly perturbed problems are stiff problems. Moreover, as the following examples show, the parameter  $\sigma_c(T)$  provides us also with information about the width of the region of rapid variation.

The examples are formulated as second order equations: of course, they have to be transformed into corresponding first order systems, in order to apply the results of the previous statements.

*Example 1.15* Let us consider the linear singularly perturbed problem:

$$\varepsilon y'' + ty' = -\varepsilon\pi^2 \cos(\pi t) - \pi t \sin(\pi t), \quad y(-1) = -2, \quad y(1) = 0, \tag{1.3.7}$$

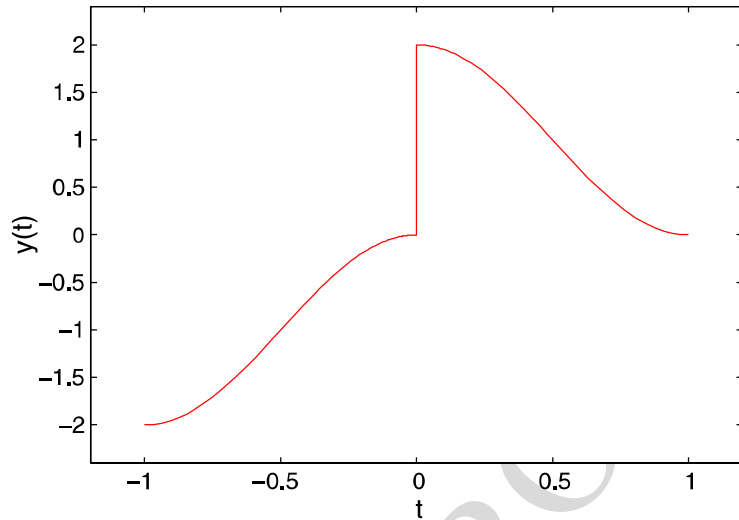
whose solution has, for  $0 < \varepsilon \ll 1$ , a turning point at  $t = 0$  (see Fig. 1.6). The exact solution is  $y(t) = \cos(\pi t) + \exp((t - 1)/\sqrt{\varepsilon}) + \exp(-(t + 1)/\sqrt{\varepsilon})$ .

In Fig. 1.7 we plot an estimate of the stiffness ratio obtained by considering two different perturbations of the boundary conditions of the form  $(1, 0)^T$  and  $(0, 1)^T$ .

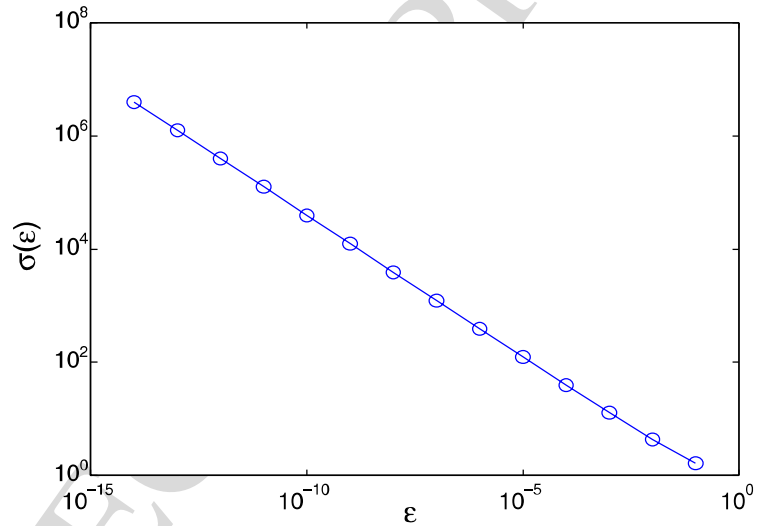
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<sup>11</sup>It is both defined by the used method and by the considered mesh.

**Fig. 1.6** Problem (1.3.7),  $\varepsilon = 10^{-8}$



**Fig. 1.7** Estimated stiffness ratio of problem (1.3.7)



The parameter  $\varepsilon$  varies from  $10^{-1}$  to  $10^{-14}$ . We see that the (estimated) stiffness parameter grows like  $\sqrt{\varepsilon^{-1}}$ .

*Example 1.16* Let us consider the following nonlinear problem:

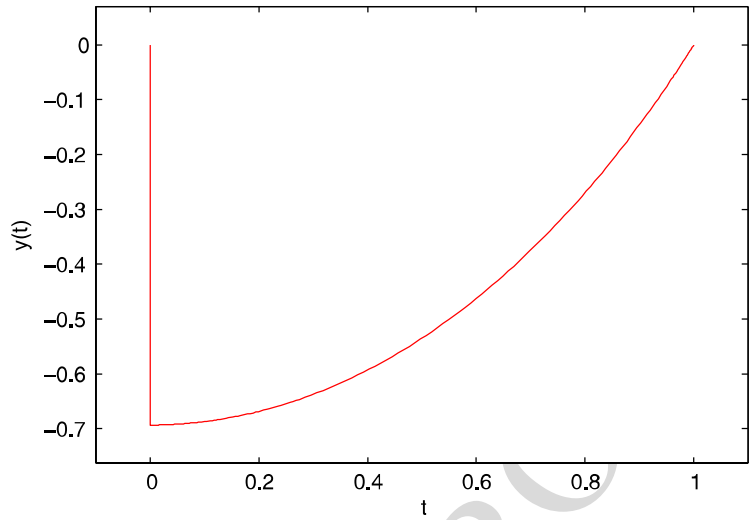
$$\varepsilon y'' + \exp(y)y' - \frac{\pi}{2} \sin\left(\frac{\pi t}{2}\right) \exp(2y) = 0, \quad y(0) = 0, \quad y(1) = 0. \quad (1.3.8)$$

This problem has a boundary layer at  $t = 0$  (see Fig. 1.8). In Fig. 1.9 we plot an estimate of the stiffness ratio obtained by considering two different perturbations of the boundary conditions of the form  $(1, 0)^T$  and  $(0, 1)^T$ . The parameter  $\varepsilon$  varies from 1 to  $10^{-8}$ . We see that the (estimated) stiffness parameter grows like  $\varepsilon^{-1/2}$ , as  $\varepsilon$  tends to 0.

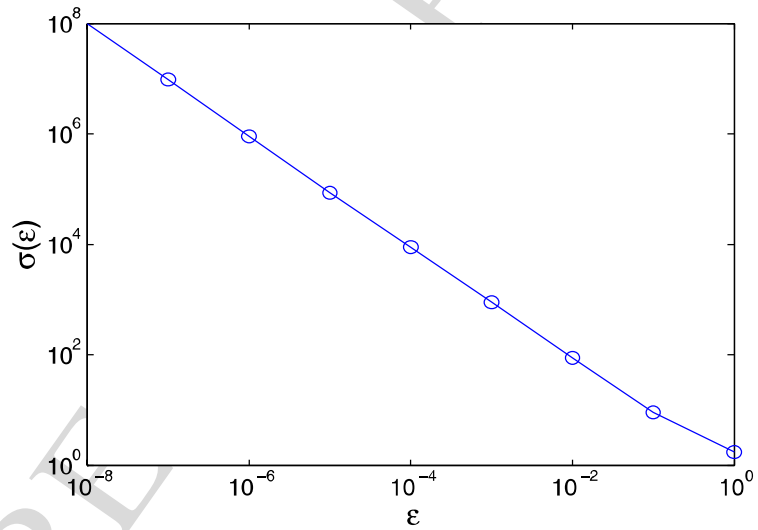
*Example 1.17* Let us consider the nonlinear Troesch problem:

$$y'' = \mu \sinh(\mu y), \quad y(0) = 0, \quad y(1) = 1. \quad (1.3.9)$$

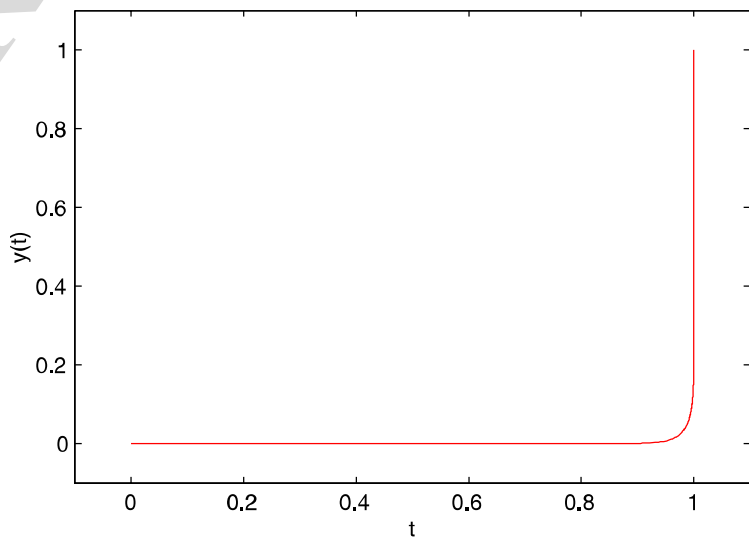
**Fig. 1.8** Problem (1.3.8),  $\varepsilon = 10^{-6}$



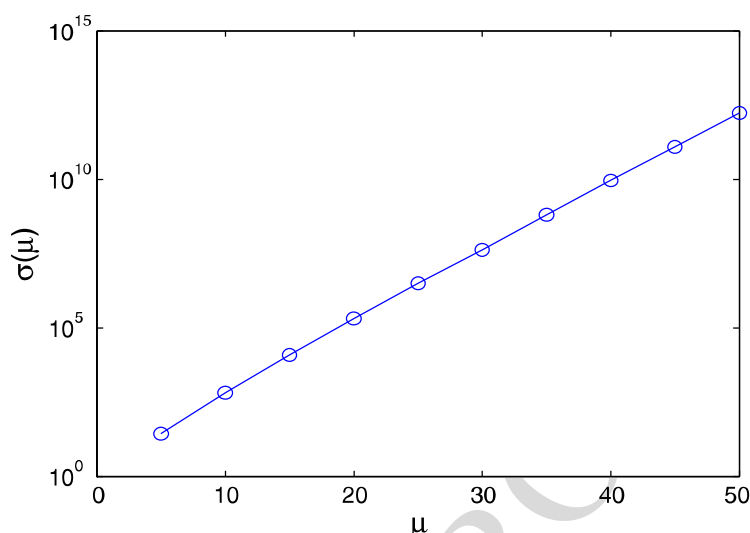
**Fig. 1.9** Estimated stiffness ratio of problem (1.3.8)



**Fig. 1.10** Troesch's problem (1.3.7),  $\mu = 50$



**Fig. 1.11** Estimated stiffness ratio of Troesch's problem (1.3.9)



This problem has a boundary layer near  $t = 1$  (see Fig. 1.10). In Fig. 1.11 we plot the estimate of the stiffness ratio obtained by considering two different perturbations of the boundary conditions of the form  $(1, 0)^T$  and  $(0, 1)^T$ . The parameter  $\mu$  is increased from 1 to 50 and, as expected, the stiffness ratio increases as well: for  $\mu = 50$ , it reaches the value  $1.74 \times 10^{12}$ .

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