

Preface

These lecture notes are based on a course (Advanced Topics in Differential Equations) given in Spring 2010 at the Courant Institute of Mathematical Sciences. The notes describe aspects of mathematical modeling, analysis, computer simulation, and visualization in the mathematical sciences and engineering that involve singular perturbations. There is a large literature devoted to singular perturbation methods for ordinary and partial differential equations, but there are not many studies that deal with difference equations, Volterra integral equations, and purely nonlinear gradient systems where there is no dominant linear part. It is the purpose here to present sufficient rigorous methods and examples to position the reader to investigate singular perturbation problems in such equations. This work is based on the books *Analysis and Simulation of Chaotic Systems* [19], *Random Perturbation Methods with Applications in Science and Engineering* [44], and *Weakly Connected Neural Networks* [23], where there are several hundred references and more scholarly treatments of the literature. In some cases here, original manuscripts are referenced when the results are not available elsewhere in the more recent literature. Some of the examples in [19, 23, 44] are reproduced here, some are taken from cited literature, and some are new.

Often mathematical models are quite complicated and may involve time scales that put them beyond the reach of convenient computer simulations. But simple approximation methods can often extract important information from them. For example, basic mechanisms of enzyme reactions are complex and take place on widely separated time scales, but they have been described by a single differential equation (the Michaelis-Menten equation (5.26)) that identifies three useful parameters (the saturation constant, uptake velocity, and a dimensionless small parameter ε , which is a ratio of concentrations). The model identifies these critical parameters that are experimentally observable and that are used to characterize the reaction. Another example is Semenov's theory of explosion limits, in which a single differential equation can be extracted from over twenty chemical rate equations that model rapid chain branched reactions, and it identifies combinations of pressure and temperature that will result in an explosion.

Mathematical analysis of dynamical systems is based on *analytical methods* such as iterations, perturbations, and transformations of variables and on *geometrical methods*, such as singularity manifolds, hyperbolic structures, phase planes, and isocline topology. Geometrical methods are elegant and help us visualize dynamical processes, but analytical methods can deal with a broader range of problems, for example, those including random perturbations, external forcing over

unbounded time horizons, and bifurcations. Analytical methods also help us to make direct connections between models, experiments, and computer simulations.

As humans, we occupy regions in space and time that are between very small and very large and very slow and very fast. These intermediate space and time scales are perceptible to us, but mathematical analysis has helped us to perceive scales that are beyond our senses. For example, it is very difficult to “understand” electric and magnetic fields. Instead, our intuition is based on solutions to Maxwell’s equations. Fluid flows are quite complicated and often not accessible to experimental observations, but our knowledge is shaped by the solutions of the Navier-Stokes equations. Spin waves in thin ferromagnetic films occur on space scales of nanometers and time scales of gigahertz, but design is based on solutions of Schrödinger’s equation. We may often combine multiple time and space scales together with mathematical methods to unravel such complex dynamics. While realistic mathematical models of physical or biological processes may be complicated, there are mathematical methods that extract simplifications from them that capture essential aspects of the phenomena being modeled. These simpler models are often referred to as being *canonical models*.

We also live with varying levels of logical rigor in the mathematical sciences that range from complete detailed proofs in sharply defined mathematical structures to using mathematics to probe other structures where its validity is not known. Hopefully in those cases the results can be justified a posteriori.

The word *perturbation* causes some problems. For example, *perturb* means to throw into confusion, but its purpose here is to relate to a simpler situation. Identifying perturbations usually involves identifying critical parameters. Done right, parameters should be dimensionless numbers that result from scalings, such as using ratios of eigenvalues of linear problems. Parameter identification in problems might involve difficult mathematical preprocessing. However, once this is done, basic perturbation methods may be used to understand the perturbed problem in terms of solutions to the unperturbed problem. Basic perturbation methods used here are based on implicit function theorems, stability analysis, averaging, and stochastic approximations. Adaptations of these methods to various other problems are also described here. Two particularly useful perturbation methods are the method of averaging and the quasi-static state approximation (QSSA).

Perturbations usually involve a dimensionless scaling parameter, say denoted by ε , and perturbation methods typically make a statement that is valid as $\varepsilon \rightarrow 0$. But determining the actual size of errors is usually not feasible in most applications. How could such results be useful? Consider a problem whose solution is given by the series

$$f(\varepsilon) = \sum_{n=0}^{\infty} \varepsilon^n,$$

which converges for ε sufficiently small. Convergence tests from calculus show that in fact this series converges for $|\varepsilon| < 1$. Analytic continuation of this function

is also possible; in fact, the series can be summed with the result

$$f(\varepsilon) = \frac{1}{1 - \varepsilon},$$

which is well-defined for all real and complex numbers $\varepsilon \neq 1$. The point here is that even though the solution $f(\varepsilon)$ may be calculated only for ε near 0, that calculation may give global information. The validity of the approximation may be extended by summing, as in this case, or by creating a rational function approximation based on the series, as in Padé's approximation.

As a rough guide to terminology, a problem whose solution can be constructed in a power series in ε is referred to as being a *regular perturbation* problem. On the other hand, typical solutions of dynamical systems involve functions of the form $\exp(a/\varepsilon)$, where a may be real or complex, and these are referred to as being *singular perturbation* problems since this function has an essential singularity at $\varepsilon = 0$.

Computer simulations have enabled us to study models beyond the reach of mathematical analysis. For example, mathematical methods provide a language for modeling and some information, such as basic structure, existence, uniqueness, and stability, about their solutions. Then well-executed computer algorithms and visualizations can provide further qualitative and quantitative information about solutions. The computer simulations presented here describe and illustrate several critical computer experiments that have produced important and interesting results.

Analysis and computer simulations of mathematical models are important parts of understanding physical and biological phenomena. The knowledge created in modeling, analysis, simulation, and visualization reveals secrets of the processes being modeled.

Iteration is another mathematical method that complements perturbation methods. Iterations are mathematical procedures that begin with a state of the system and repetitively update it according to some algorithm. The same rule is applied to each new state, and so a sequence of iterates results. An important example is Newton's method for finding the zeros of a function, which continues to be the paradigm for iterative equation solving. However, chaotic behavior that is not detectable by perturbation methods can occur even when quite simple functions are iterated. On the other hand, while it may be difficult to extract precise information from iteration of a complicated system, iteration underlies most of the proofs of validity of perturbations in these notes.

Averaging is in the spirit of the Riemann-Lebesgue lemma and Birkhoff's ergodic theorems. A system may be subject to oscillatory or random external forcing, or the system itself might be intrinsically oscillatory. Mixing of oscillatory modes either through nonlinearity or through feedback can create quite complicated dynamics. The method of averaging extracts the slow modulation of a rapidly oscillating evolution, and the errors made are usually of higher order in the ratio of frequency-to-amplitude time scales. In the case of random perturbations, averaging is based on the law of large numbers and the central limit theorem. The first

gives the mean value of solutions, and the second describes the dispersion of the approximation.

There is a duality between quasi-static state approximations (QSSA) and stability features of a system. The stability of physical systems is often described using energy methods for gradient systems. These methods have been extended to more general gradient or gradientlike dynamical systems by Lyapunov and others. The most important stability concept used here is that of *stability under persistent disturbances*. This idea explains why mathematical results obtained for minimal models can often describe behavior of systems that are operating in irregular or noisy environments. For example, think of a metal bowl having a lowest point in it. A marble placed in the bowl will eventually move to the minimum point. If the bowl is now dented with many small craters or if small holes are put in it, the marble will still move to near where the minimum of the original bowl had been, and the degree of closeness can be determined from the size of the dents and holes. The dents and the holes introduce irregular disturbances to the system, but the dynamics of the marble are similar in both the simple (ideal) bowl and the imperfect (realized) bowl.

Stability under persistent disturbances is sometimes confused with structural stability. The two are quite different. Structural stability is a concept introduced to describe systems whose behavior changes only slightly when the system is slightly perturbed. Hyperbolic structures are particularly important examples of this. However, it is exactly significant changes in response to slight perturbations that are often the only things observable in experiments: Did something change? Stability under persistent disturbances carries the theory through such changes: For example, the differential equation

$$\dot{x} = ax - x^3 + \varepsilon f(t),$$

where f is bounded and integrable, ε is small, and a is another parameter, occurs in many models throughout these notes. When $\varepsilon = 0$ and a increases through the value $a = 0$, the structure of static state solutions changes dramatically from having only one real static state to having three. This example is an important canonical model in many applications, but it is not structurally stable at $a = 0$. Still, the system with $\varepsilon = 0$ is a gradient system (viz., $\dot{x} = -\nabla G(x)$ where $G(x) = x^4/4 - ax^2/2$) for a neighborhood of $x = 0$, $a = 0$. So, the system is stable under persistent disturbances. Note that while the equation depends smoothly on a , new static states when $a > 0$ are $\pm\sqrt{a}$, which have branch points at $a = 0$.

The two major topics studied in these notes are constructing approximate solutions to mathematical models and simulating those models in a computer. Each has its uses, its strengths, and its shortcomings. Our mathematical analysis builds mostly on perturbation and iteration methods: They are often difficult to use, but once they are understood, they can provide information about systems that is not otherwise available. Understanding them can facilitate computer simulations by identifying critical parameter regimes and extracting accurate approximations from them. Also, analytical methods can make sense of the behavior of noisy systems where computation is limited to one sample path at a time, and they can go beyond

the edge of practical computability in dealing with very fast processes (e.g., rapid chemical reactions) and small quantities (e.g., spin-torque nano-oscillator calculations).

Computer simulations have replaced much of the work formerly done by applied mathematicians (often as graduate students). There is a variety of sophisticated software packages, such as MATLAB, that solve singular perturbation problems in ways that do not require much knowledge of the system being solved. Simulations describe solutions of a mathematical model by describing sample trajectories of the process being modeled. Sample paths can be processed in a variety of ways by plotting, calculating ensemble statistics, and so on. On the other hand, simulations do not easily describe the dependence of solutions on model parameters, especially when they are noisy, nor are their stability, accuracy, and reliability always assured. They do not deal well with chaotic behavior or unexpected irregular or abrupt changes in a solution. The methods developed in these notes provide a more highly nuanced understanding of singular perturbation problems. There have been many successes for computer simulation to date—for example, the discovery and analysis of solitons—but there are some notable systems that are beyond the reach of today’s computing power and algorithms.

There are both geometrical and analytical theories of singular perturbation problems for ordinary differential equations that are based on invariant manifolds. In rough terms, one approach is due to J. Hadamard, which is based on iteration of manifolds in nonlinear problems. The other is due to O. Perron [4], who developed an analytic theory of manifolds for the Volterra integral equations describing similar problems. We follow Perron’s approach here for several reasons: First, the topological approach is generally not constructive and not directly useful for computation, while a main purpose in these notes is to provide algorithms for constructing approximate solutions and for computing solutions to singular perturbation problems. The approach here is based on the constructive asymptotic methods in [14, 19] and can lead to quasi-static manifolds that have interesting analytic features, such as branch points. Second, the approach taken here enables us to extend the asymptotic expansions for differential equations to solve comparable problems for systems of difference equations, for systems involving random noise, and for systems of Volterra integro-differential equations that are (to date) beyond the reach of the topological approach. Finally, more general methods in [19] are based on Lyapunov functions and were developed for systems satisfying less restrictive conditions than those required by center manifold theorems (e.g., see [19]), and they are in the spirit of stability under persistence disturbances, which we develop and use here.

There are many combinations of behavior that are not included in what is done in these notes. For example, a system could have a rapid oscillation for each point on a slow manifold, rather than having only a rapid transient to it. In general, if the slow variables have been identified and separated in the model, then we may freeze the slow variables and observe what the remainder of the system wants to do.

For example, consider the system

$$\frac{dx}{dt} = \varepsilon f(t, x, y, \varepsilon), \quad \frac{dy}{dt} = g(t, x, y, \varepsilon).$$

Since the slow variables (x) are separated out in this model, we may freeze them by simply setting $\varepsilon = 0$. Then we consider the rest of the system,

$$\frac{dy}{dt} = g(t, x_0, y, 0),$$

to see where the solutions will go. Suppose they go to a solution

$$y \rightarrow Y_0(t, x_0)$$

as $t \rightarrow \infty$. Next, we return to the slow system using this result:

$$\frac{dx_0}{dt} = \varepsilon f(t, x_0, Y_0(t, x_0), 0).$$

If Y_0 is a static state, then this problem is a candidate for the QSSA methods in Part II. However, if the function Y is a periodic or quasi-periodic function of the fast time variable t , or if it is an ergodic random process, then other methods must be used, perhaps some of the methods in Part I. There remain many unresolved problems of this kind, however.

The exercises are graded roughly in increasing difficulty in each chapter. Some are quite straightforward illustrations of material in the text, and others are quite lengthy projects requiring extensive mathematical analysis or computer simulation.

These notes were designed for a graduate level course in applied mathematics. Readers must have some degree of familiarity with methods of ordinary differential equations, for example, from a course based on Coddington and Levinson [4] or a similar level text. Students should also be competent with matrix methods and be able to use standard reference texts such as [47]. There are several books that provide background information on singular perturbation methods, which are listed in [19], where the context and literature of singular perturbations is presented. Standard references for the random perturbation theories developed and used here are in [6, 8, 38, 44]. Computer simulations in these notes use MATLAB, but any other scientific computing language may be used. While MATLAB is convenient and provides good graphical resources, it is an interpretive language, so greater computational speed may be realized using compiled languages, such as FORTRAN and C++.

Finally, there are many important and related topics in dynamical systems that are not touched on here. These notes are limited to revealing constructive methods based on implicit function theorems and iteration methods for differential, difference, and integral equations that are widely used today. It is designed for a one-semester course for students in applied mathematics, and it is not meant to be a general presentation of dynamical systems. As a result, many significant developments of analytical, topological, and geometrical methods for dynamical systems that give deep insight to their structure and behavior are not mentioned. On the

other hand, there are several topics not usually studied in standard dynamical systems texts that are presented here in some depth, such as difference equations and Volterra integral equations in both random and deterministic settings.

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