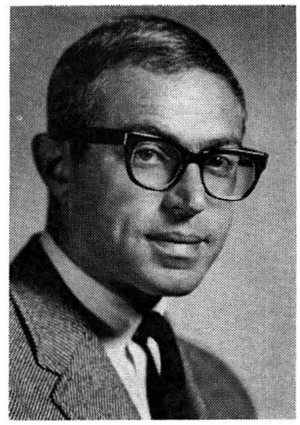
A Course in Control and Optimization

OPTIMAL CONTROL OF REACTION SYSTEMS



Leon Lapidus is professor and chairman of the chemical engineering department at Princeton University. He was educated at Syracuse University (BS and MS) and the University of Minnesota (PhD, '50). He teaches courses in analysis of transport phenomena and computational techniques and in numerical techniques in engineering analysis. His research interests lie in the areas of optimization, optimal control and stability of chemical reaction systems.

LEON LAPIDUS
Princeton University
Princeton, N. J. 08540

In this article we shall briefly outline some of the major topics covered in a graduate course in Optimal Control of Reaction Systems at Princeton. This course was originally started in 1955 as a full year of Numerical Analysis and has gradually evolved into its present form. This was achieved by the inclusion in 1959 of selected items (3 and 6 in Table II below) and the subsequent addition of more and more material until the present coverage resulted.

TABLE I—TEXTS RECOMMENDED FOR COURSE IN OPTIMAL CONTROL OF REACTION SYSTEMS

I- 1. Athans, M., and Falb, P. L., "Optimal Control", McGraw-Hill (1966).
I- 2. Bryson, A. E., and Ho, Y., "Applied Optimal Control", Blaisdell (1969).
I- 3. Koppel, L. B., "Introduction to Control Theory", Prentice-Hall (1968).
I- 4. Lapidus, L., and Luus, R., 'Optimal Control of Engineering Processes", Blaisdell (1967).
I- 5. Larson, R. E., "State Increment Dynamic Programming", Elsevier (1968).
I- 6. Lee, E. S., 'Quasilinearization and Invariant Imbedding", Academic Press (1968).
I- 7. Luenberger, D. G., "Optimization by Vector Space Methods", Wiley (1969).
I- 8. Ogata, K., "State Space Analysis of Control Systems", Prentice-Hall (1967).
I- 9. Roberts, S. M., "Dynamic Programming in Chemical Engineering and Process Control", Academic Press (1964).
I-10. Sage, A. P., "Optimum Systems Control", Prentice-Hall (1968).
I-11. Wilde, D. J., and Beightler, C. S., "Foundations of Optimization", Prentice-Hall (1967).

Table I lists a number of recommended texts which are used through the year and Table II gives some details on the explicit topics covered in the course. The main text references are I-2 and I-4, but all those shown in Table I are consulted at various points. Recent references have been included in Table II so that the reader or student has a convenient starting point for published material.

The course is devoted to the mathematical and numerical-computational aspects of the state-space or time-domain approach as distinguished from the frequency or transform domain. In general it covers deterministic problems although some stochastic control and the effects of noise are briefly treated near the end of the course. Extensive numerical and computer problems are given as exercises to allow the students to try their hand at applying the theory. As an example, the optimal control of a series of CSTR will be discussed in class and the same problem but with control delay will be given to the students to solve by a variety of algorithms. However, emphasis on complex physical reactions systems for complexity sake is kept to a minimum.

To give some perspective to the course objectives we present Figure 1 which is taken from an article of Kalman, Lapidus and Shapiro published in 1959 in the *Instn. Chem. Engrs. Journal.* Here we show an on-line adaptive (learning) computer connected directly to a process or system. Within the computer there are three main programs designated A, B and C. The function of program A is to carry out the optimal control of

TABLE II—COURSE OUTLINE FOR OPTIMAL CONTROL OF REACTION SYSTEMS

*1. **Numerical Concepts.** Vector-matrix manipulation, solution of O.D.E. and P.D.E., iteration methods and accelerating convergence and functional analysis. Refs.: Amundson, "Mathematical Methods in Chem. Eng.", Prentice-Hall (1966); Lapidus, "Digital Computation for Chem. Eng.", McGraw-Hill (1962); I-7 and I-8 of Table I.; Kantorovich, "Approximate Methods of Higher Analysis", Interscience (1958).*

*2. **Necessary and Sufficient Conditions for Minimum.** Hessian matrix, constraints, Lagrange multipliers and penalty functions. Refs.: I-2 and I-11 of Table I.

3. **Optimal Control Problem.** Definitions of systems, constraints, performance index and selection of optimal control. Refs.: I-1 and I-4 of Table I; Lapidus, *Chem. Eng. Prog.* **63**, No. 12, 64 (1967).

4. **Minimum Principle.** Continuous and discrete form of Minimum Principle, extensions, simplifications, numerical difficulties and advantages. Refs.: I-2, I-4 and I-10 of Table I; Gurel and Lapidus, *IEC Fund.* **7**, 617 (1968).

5. **Dynamic Programming and Invariant Imbedding.** Continuous and discrete form of dynamic programming, numerical solution of full nonlinear control problem, numerical solution of 2-point B.V. problems and numerical questions. Refs.: I-4, I-5, I-6 and I-9 of Table I; Seinfeld, *IEC Proc. Design and Devel.* **7**, 475, 479 (1968); Rothenberger, *AIChE Jrn.* **13**, 114 (1967).

6. **Linear-Quadratic Problem.** Solution of special control problem via Minimum Principle, dynamic programming and variational calculus. Continuous and discrete problems, Riccati equation and numerical questions. The ASP computer program. Refs.: I-4 and I-10 of Table I; Lapidus, *Chem. Eng. Prog.* **63**, No. 12, 64 (1967).

7. **Minimum Time Problem.** So ution via Minimum Principle, concept of switching times, bang-bang control and singular control. Connection to linear and nonlinear programming. Refs.: Lesser, *AIChE Jrn.* 12, 143 (1966); Flynn,*AIChE Jrn.* 15, 308 (1969); I-2, I-3 and I-4 of Table I.

8. **Optimal Control Algorithms.** Numerical algorithms for iteratively solving the full nonlinear control problem. First (gradient) and second variation methods including quasilinearization, neighborhood extremals, and the use of the linear-quadratic procedure. Constraints and penalty functions. Open and closed-loop solutions. Refs.: I-2 and I-4 of Table I.

9. **Suboptimal control.** Generation of closed-loop feedback approximate control of nonlinear systems. Refs.: Internal work only.

10. **Sensitivity Analysis. Performance and trajectory sensitivity, adaptive systems, parameter compensation, closed and open-loop algorithms. Refs.: Kokotivoc, *Int. Jrnl. Cont.* 9, 111 (1969); Sobral, *Proc* IEEE 56, 1644 (1968); Seinfeld, *Canad. Jrn. Chem. Eng.* 47, 212 (1969).

11. **Stability.** Single and multiple equilibrium points, limit cycles, lumped and distributed systems and Liapunov functions. Refs.: Storey, *Brit. Chem. Eng.* **13**, 1585 (1968); Aris, *Chem. Eng. Sci.* **24**, 149 (1969); Luss, *Chem. Eng. Sci.* **23**, 1237 (1968); Gurel, *IEC* **61**, No. 3, 30 (1969); Berger, *AIChE Jrn.* **14**, 558 (1968), **15**, 171 (1969).

12. **Control and Stability.** Linear quadratic problem and Liapunov functions, lumped and distributed systems, time-optional control and control algorithms. Refs.: I-3 and I-4 of Table I; Denn, *AIChE Jrn.* **13**, 926 (1967); Chant, *Canad. Jrn. Chem. Eng.* **46**, 376, (1968); Wang, *AIChE Jrn.* **14**, 934, 976 (1968).

13. **Control of Distributed Parameter Systems. Minimum Principle, dynamic programming, finite differencing, method of lines and control algorithms. Refs.: I-3 of Table I; Seinfeld, *Chem. Eng. Sci.* **23**, 1461 (1968); Denn, *IEC Fund.* **7**, 410 (1968); Seinfeld, *AIChE Jrn.* **15**, 57 (1969).

14. **Filtering, Parameter Estimation and Identification. Linear and nonlinear systems determination of parameters, black box representation and computational questions. Refs.: Bard, *Cat. Reviews* **2**, 67 (1968); Harris, *AIChE Jrn.* **13**, 291 (1967); Peterson, *Chem. Eng. Sci.* **21**, 655 (1966); I-6 of Table I.

* Depending on the background of the students.

** If enough time is available.

the process (issue commands to the various inputs) using the latest process measurements and taking into account the control objective and the dynamic model of the process. Program B continually analyses the process measurements to identify an accurate model of the process. Program C is used to generate and inject special calibrating signals into the process such that they do not significantly disturb the process; yet they perturb the process in such a way that useful information can be obtained by means of sophisticated data evaluation techniques. Feedback between the programs is also allowed to increase the efficiency of the overall operation.

Within this simple appearing arrangement we have all of the features of the publicized learning computer which can build its own mathematical model of a process and then carry out any prescribed form of control. The present course is directed, as much as feasible, to detailing the mathematics of these different features. Because of the current state of technology, Program A receives the major emphasis although Programs B and C are discussed (14 of Table II).

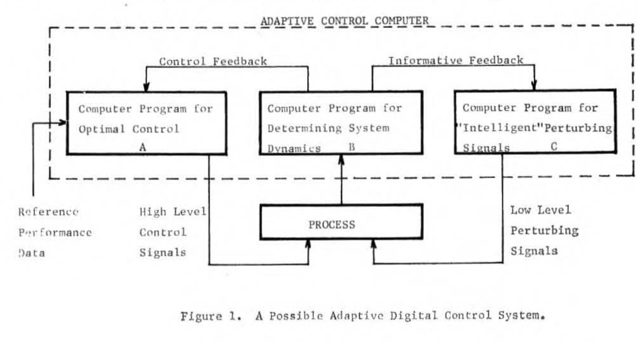


Figure 1. A Possible Adaptive Digital Control System.

The course is devoted to the mathematical and numerical-computational aspects of the state-space or time domain approach as distinguished from the frequency domain.

INTRODUCTORY MATERIAL

Because of the wide background of students who take this course it is necessary to first present certain introductory topics which are then used throughout the year. These include the complete vector-matrix notation and its uses such as evaluating the transition matrix and the pseudo-inverse, the numerical solution of ordinary and partial differential equations, the fundamental properties of convergence algorithms and some basic material on functional analysis. The solution of equations and the numerical stability of these solutions is necessary because they are an integral portion of all control algorithms and must be done correctly. Further, convergence algorithms are used throughout the entire course to actually obtain the optimal control.

In addition to these numerical concepts it may be necessary to present some preliminary details on the necessary and sufficient conditions for an unconstrained minimum of a multivariable function, the influence and effects of constraints and the use of Lagrange multipliers and penalty functions to handle constraints. These items, which can be developed for a simple two-variable function, can be carried over directly to the most complicated control problem. As such the concepts are absolutely necessary throughout the course.

TABLE III DEFINITION OF OPTIMAL DETERMINISTIC CONTROL PROBLEM

1. General Form	
Given:	
1. $\dot{\mathbf{x}}(t) = \mathbf{f}(\mathbf{x},\mathbf{u})$	System Model
2. $\mathbf{x}(t_o)$	Initial State
3. Control and State Constraints	
4. Final Time Conditions (t_f)	
5. $I = \phi[\mathbf{x}(t_f),t_f] + \int_{t_o}^{t_f} J[\mathbf{x}(t),\mathbf{u}(t)]dt$	Scalar Index
2. Linear-Quadratic Form.	
1. $\dot{\mathbf{x}}(t) = \mathbf{A}\mathbf{x} + \mathbf{B}\mathbf{u}$	Linear System
2, 3, and 4 are same	
5. $I = \mathbf{x}(t_f)'\mathbf{S}\mathbf{x}(t_f) + \int_{t_o}^{t_f}[\mathbf{x}'\mathbf{Q}\mathbf{x} + \mathbf{u}'\mathbf{R}\mathbf{u}]dt$	Quadratic Scalar Index

Find $u(t)$, $t_o \le t \le t_f$, such that I is minimized subject to constraints of 1-4.

MAIN TOPICS

With these preliminaries in hand the next step in the course is to define the optimal control problem (see 1 of Table III) and to detail the minimum principle and the techniques of dynamic programming and invariant imbedding as general methods of solving the problem. Here it is very important to give numerical examples and to illustrate both the positive and negative features of these solution methods.

The linear-quadratic problem (see 2 in Table III) is then treated in detail using the minimum principle, dynamic programming and variational calculus. This is important because the techniques developed form the basis for all 2nd order algorithms for solving the full nonlinear control problem. Because of the availability of the ASP computer program (see I-4) to numerically solve this linear-quadratic problem a number of different exercises are given to the students.

The minimum-time problem is then solved via the minimum principle and the connection to linear and nonlinear programming detailed. Computational considerations and the singular case are stressed. This area is interesting since it connects to programming methods and is applicable to the analysis of many reactor systems.

Next we discuss a wide variety of computational algorithms for solving the nonlinear control problem without and with constraints. These methods include the gradient (first variation) approach and the second variation including quasilinearization. Much of this analysis can be connected directly to the special linear-quadratic case already treated. In addition, consideration is given to a form of suboptimal control which is easily developed and yields a closed-loop type of approximate control. At the same time sensitivity considerations are employed to indicate the influence of parameter uncertainties and to generate iterative methods for the optimal control.

Since many reaction systems exhibit the features of stability and instability we then turn to a detailed discussion of the concepts of trajectory paths in the neighborhood (or global) of an equilibrium point. This leads directly into an analysis of multiple equilibrium points, non-uniqueness of solutions of nonlinear equations, limit cycles and Liapunov functions. In particular the Liapunov function approach is extended to distributed parameter systems and to provide convenient algorithms for minimum-time and suboptimal control.

The extension of many of the above ideas may now be used advantageously to analyze the control of distributed parameter systems. Here we treat the control problem in its normal form or carry out a partial type of lumping (finite differencing) to convert the system to sets of ordinary differential equations. In both cases a variety of possible control algorithms following from the minimum principle and dynamic programming are developed.

Finally we consider the identification problem either in its full complexity where no apriori information about the reaction system is known or where a model is available but the parameters must be adjusted to fit experimental data (parameter estimation). Here we turn to the linear-quadratic case treated as a filtering problem, carry out nonlinear last-square regression and fit the system data with generalized orthogonal polynomials. Questions such as the noise involved in the inputs and on the measurement are of importance.

AMUNDSON on Math (Cont'd from p. 177)

and some comments must be made and analogies are drawn with finite vector systems.

The object of such a course should be to present methods for new problems. If a problem has been solved once then the engineer should use it. But with a new problem there is no one to tell him when the problem is properly posed. Has the model been drawn so it makes mathematical sense and how does one test whether it does? Whether a solution fits certain physical and chemical requirements will be determined by comparison with experiment, but this comparison is meaningless if the model is not self-consistent.

There is frequent confusion in the minds of beginning graduate students on what is mathematics and what is not mathematics, and, if such a course serves no other function, this question should be answered for him. All of our problems as engineers are physically motivated and the translation of a problem into mathematical terms is **not** mathematics. The generation of the appropriate mathematical model is the job of a good engineer and whether conclusions drawn from the model agree with experiment is the test of how good an engineer he is. If the model does not agree with the experiments, one of two things may be at fault. Either the model was poorly drawn in that it does not describe the physical situation or the model is incomplete or inconsistent. Once the model is put to paper a mathematical problem must be solved. The engineer must somehow convince himself either by intuition or rigorous mathematical argument that the mathematical problem is properly posed. The old argument that the problem is a physical one and therefore possesses a unique solution is a useful argument but not infallible, since only nature solves physical problems and she is quite capable of giving a non-unique solution. The argument also betrays an unrealistic confidence in the engineer for it assumes that he has translated the physical problem into mathematical language **exactly**, a most unlikely event. This is really a very complicated problem, for in the course of the solution certain changes or approximations in the model, both physical and mathematical, are made and these should be examined in some detail to insure that the structure has not been destroyed.

If the model does not agree with the experiments . . . either the model was poorly drawn . . . or it is incomplete or inconsistent.

In conclusion, such a graduate course should not only teach techniques but it should also give the student a feel for what he is doing and what is involved. It has been frequently asserted that we teach only mathematics and neglect engineering. On the contrary, we are trying to teach the student the proper place and function of mathematics, showing not only its strengths but also the pitfalls which may befall the unwary and the uninstructed.

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