DISCRETE MATHEMATICS

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In a traditional chemical engineering curriculum, the richness of discrete mathematics is not sufficiently used. Although selected numerical techniques for the solution of differential equation have received at least adequate attention in earlier texts[1,2] as well as in more recent works,[3-5] mathematics courses taught to chemical engineering students generally tend to put more emphasis on analytic approaches linked to continuous systems, and discrete techniques usually take second place.

In the domain of process dynamics and control, the importance of digital techniques has been reflected more perceptibly in the textbook literature. Sampled-data control, one of the most important applications of discrete mathematics, is routinely covered (but to a varying extent) in currently popular textbooks.[6-9] In spite of much progress in bringing discrete mathematics to the forefront, competence of the average chemical engineering student in this area still leaves much to be desired. The course described in this paper is an attempt to remedy this situation.

COURSE STRUCTURE

The purpose of a senior-level elective course, which also carries full credit as a graduate course for Master's degree candidates, is to increase the students' knowledge in discrete mathematics of interest to chemical engineers and to motivate students to make further excursions into this field on their own. The contents of this one-trimester exercise (thirteen weeks, thirty-six lectures), shown in Table 1, lean somewhat heavily to process dynamics and control, as a follow-up to a compulsory introductory course in that subject. Applications independent of process control are also emphasized, and discrete techniques allowing the numerical solution of a variety of problems (not necessarily related to process control) make up a small but still significant proportion of the course material.

At the beginning of the lectures, the students receive a set

TABLE 1
Topic Areas Covered in Course

1. Finite difference operators and systems • Application to discrete and continuous systems: numerical integration and solution of differential equations • Use of the E-operator, the state-transition matrix method, and z-transformation *(7 lectures)*
2. Open-loop linear (control) systems • Sampling and the starred Laplace transform • z-transformation • Digital convolution • Hold elements and signal reconstruction • Pulse transfer function • Inversion of z-transforms • Digital transfer functions • Digital filtering • Digital P, PI, PD, and PID controllers *(6 lectures)*
3. Closed-loop linear (control) systems • Closed-loop transfer functions and system stability via z-transforms and bilinear (r;w) transforms • Sampling instants and system stability • Elementary controller design: the minimal prototype/deadbeat response controller and the Dahlin controller • Digital control for load changes • Design of controllers via bilinear transform-based frequency response techniques *(10 lectures)*
4. Elements of nonlinear discrete and sampled-data control systems • Digital convolution and diagonal invariance *(3 lectures)*
5. Elements of discrete stochastic techniques • Markov-chain representation of discrete and continuous systems • Problem solution via linear algebra and z-transforms • Application to rate processes *(2 lectures)*
6. Intersample behavior • Advanced- and modified z-transforms • Intersample response via digital convolution • Treatment of process time-delay via modified z-transforms *(6 lectures)*
7. Review via a specific problem whose analysis is traced through the six topics listed above *(2 lectures)*

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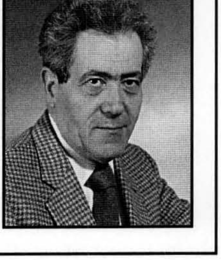

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TABLE 2
Illustration of Typical Problem Complexity

Level: low

A reactant decomposes in a batch reactor according to the rate law $dc/dt=-0.5c^{0.5}$ where c is in mol/dm^3 and t is in min. At zero time, c=1. Estimate the reactant concentration at equally spaced time intervals of 0.05 min by the RK-2 algorithm and compare the estimated values to the analytical solution.

Level: low

A continuous system is subjected to an impulse input of unit magnitude. The response is exp(-t) where t is time. The same system is exposed to a sampled ramp with unity slope. What is the system response?

Level: medium

Derive the quadrature formula in Eq. (1) via Taylor-series theory and the stipulation that the integral be approximated as A[f(a)+f(-a)]+Bf(0), where A, B, and a are a-priori indeterminate constants.[10]

Level: medium

Consider the infrared tracker problem in the text by Saucedo and Schiring,[11] Figure 9-35, page 418. The overall forward-branch transfer function is

$$G(s)=K[1-\exp(-0.1s)]/[s^2(s+3.5)]$$

with K=7. This is a unity-feedback system with an ideal sampler (T=0.1) following the comparator.

a) Is this system marginally stable according to the GM≥2; PM≥30° criterion?

b) What is the maximum value of K for marginal stability?

c) Why is a very poor marginal stability tolerated for this system?

Level: high

In the forward branch of a control system block diagram, the transfer function G(s)=20/[(s+1)(s+3)] is placed between two synchronized ideal samplers (T=0.5). The closed-loop system has a unity feedback. If we put a proportional controller in front of G(s), what is the region of stable controller gains?

Level: high

Analyze the 'recipe' for deadbeat-response controller design by Gupta and Hasdorff,[12] with generalized input $R(z)=Q_n(z^{-1})^{n+1}$, where Q_n is a finite polynomial in powers of z^{-1} such that there is no zero at z=1.

of solved problems of varying complexity, but there are no formal homework problem assignments. Encouraged throughout the entire course to explore various "take-offs" on problems in the handout set, students have ample opportunity to employ various computer facilities available to them on campus; every problem in the handout set, however, can be solved with a standard scientific calculator. A small sample of typical problems is shown in Table 2. Students are examined via a two-hour mid-term test and a three-hour final examination. The open-book/open-notes exams are designed to equally test the students' understanding of fundamental principles and their computational prowess.

FAST AND ACCURATE NUMERICAL INTEGRATION

A major principle reiterated in the course is the avoidance of a sledgehammer-against-the-fly application of numerical methods. A case in point is the quadrature formula[10]

$$\int_{-h}^{h} f(x)dx = h\left[5\,f\left(-h\sqrt{0.6}\right)+8\,f(0)+5\,f\left(h\sqrt{0.6}\right)\right]/9 \tag{1}$$

whose error, $h^7 f^{(vi)}(0)/15790$, guarantees an accurate value of integrals for *monotonic* functions whose sixth-order derivative is zero at the mid-interval of integration. If the integration interval is not symmetric around x=0, linear translation is first to be done. This integration formula seems to be unnoticed in the chemical engineering literature in spite of

TABLE 3
Illustration of a Simple Gaussian Quadrature (Eq. 1)

Problem • Estimate via Eq. (1) the numerical value of the integral of the function f(x)=exp(x) on the interval [0,1]. Compare to the analytical answer: exp(1)-1=1.71828 (to five-decimal accuracy).

Solution • The mid-point position being at x=0.5, we have for $f(-h\sqrt{0.6})$ the expression $0.5-0.5\sqrt{0.6}=0.11270$. Similarly, the expression $0.5+0.5\sqrt{0.6}=0.88730$ stands for $f(h\sqrt{0.6})$. Hence the integral is approximated by

$$\int_0^1 \exp(x)dx$$
$$\approx 0.5\left[5\exp(0.1127)+8\exp(0.5)+5\exp(0.88730)\right]/9$$
$$=1.71828$$

The error of estimation is 8×10^{-7} only!

its high accuracy and simplicity. Table 3 illustrates an application.

DISCRETE SOLUTION OF CONTINUOUS PROBLEMS

The handling of linear differential equations by linear algebraic structures is one of the best indications of the power of discrete mathematics (and the humble programmable calculator). As discussed in an earlier paper,[13] the Markov-chain model of chemical rate equations is particularly instructive in this respect. The treatment of a consecutive first-order decomposition process

$$A \Rightarrow B \Rightarrow C \quad (2)$$

with rate constants k_1 = 3.6/h (first step) and k_2 = 7.2/h (second step) is used for illustration. The analytical solution for species concentrations A and B with initial conditions A_o = 1 and B_o = 0 mol/dm^3

$$A = A_o \exp(-k_1 t) \quad (3a)$$

$$B = [k_1 A_o / (k_2 - k_1)][\exp(-k_1 t) - \exp(-k_2 t)] \quad (3b)$$

is contrasted with the Markov-chain model

$$A[n+1] = (1-k_1)A[n] \quad (4a)$$

$$B[n+1] = k_1 A[n] + (1-k_2)B[n] \quad (4b)$$

Equations (3a,3b) are obtained by solving analytically two differential mole balances, whereas Eqs. (4a,4b) are the Markov states obtained by post-multiplying the transitional probability matrix by the (n-1) state probability vector.[14] Close agreement is demonstrated in Table 4 in the case of one-second state intervals. The establishment of Eqs. (4a,4b) does *not* require calculus and/or conventional discretization of differential equations.

TABLE 4
Computation of Species Concentration in a First-Order Consecutive Reaction Scheme (Eq. 12)
A_o = 1 mol/dm^3; B_o = 0 mol/dm^3; k_1 = 3.6/h; k_2 = 7.2/h

Time(s) or stage number (n)	A(t) mol/dm^3 Eq.(3)	A(t) mol/dm^3 Eq.(4)	B(t) mol/dm^3 Eq.(3)	B(t) mol/dm^3 Eq.(4)
0	1	1	0	0
10	0.9900	0.9891	0.0098	0.0108
50	0.9512	0.9502	0.0464	0.0473
100	0.9048	0.9039	0.0861	0.0870
200	0.8187	0.8178	0.1484	0.1491
500	0.6065	0.6058	0.2386	0.2390
600	0.5488	0.5481	0.2476	0.2479
693	0.5001	0.4994	0.2500	0.2502
694	0.4995	0.4989	0.2500	0.2502
700	0.4966	0.4959	0.2500	0.2502
800	0.4493	0.4487	0.2474	0.2475
1000	0.3679	0.3673	0.2325	0.2325

Species B acquires its maximum value of ≈ 0.25 mol/dm^3 at $t = 0.001\ell n(2) \approx 693$s.

DIGITAL CONVOLUTION AND THE DIAGONAL INVARIANCE PRINCIPLE

For the computation of the output of a linear (control) system, the digital convolution equation

$$c[n] = \sum_{k=0}^{n} g[n-k]r[k] \quad (5)$$

is a particularly useful tool. In Eq. (5), g denotes the impulse response of the system, r is the input into the system, and n represents the state of the discrete time. The principle of diagonal invariance[15] recognizes an important structural aspect of Eq. (5) written in its expanded form:

$$c[n] = g[n]r[0] + g[n-1]r[1] + g[n-2]r[2] + \cdots + g[0]r[n] \quad (6)$$

namely that cross-multiplication of elements of the vectors g and r, with respect to a vertical symmetry line drawn between them, yields c[n] at any arbitrary value of n. This

TABLE 5
Analysis of a Nonlinear Closed-Loop Control System via Digital Convolution (Eq. 9)

n	g[n]	m[n]	c[n]	e[n]
0	0	1	0	0.3
1	0.1998	1	0.1998	0.1002
2	0.1740	-1	0.3738	-0.0738
3	0.0776	1	0.0518	0.2482
4	0.0304	1	0.1338	0.1662
5	0.0114	-1	0.3380	-0.0380
6	0.004239	1	0.0370	0.2630
7	0.001564	1	0.1282	0.1718
8	0.000576	-1	0.3359	-0.0359
9	0.000212	1	0.0362	0.2637
10	0.000078	1	0.1279	0.1721

property is especially useful in the case of a closed-loop system, were r[k] in Eq. (5) is replaced by e[k], *i.e.,* the k-th state value of the error. In the case of unity feedback, Eq. (5) is replaced by Eqs. (7a,7b):

$$c[n]=\sum_{k=0}^{n} g[n-k]e[k] \tag{7a}$$

$$e[n]=r[n]-c[n] \tag{7b}$$

(comparator equation)

Finally, if there is a nonlinear element placed between the comparator and the system, we have the equation set

$$c[n]=\sum_{k=0}^{n} g[n-k]m[k] \tag{8a}$$

$$m[n]=f\{e[n]\} \tag{8b}$$

$$e[n]=r[n]-c[n] \tag{8c}$$

where m=f(e) represents the nonlinear element. This well-known approach in signal processing, which may also be regarded as a one-dimensional illustration of the state transition matrix technique, offers an efficient alternative to the conventional z-transformation approach to linear problems and an elegant as well as efficient means of dealing with nonlinear problems.

Table 5 illustrates its application to the on-off control of a stirred-tank heater, discussed by Coughanowr[8] in terms of phase-plane analysis. A dimensionless on-off element with output magnitudes (-1,+1) is placed between an ideal sampler receiving the error signal and the process with transfer function $G_p(s) = 1/[(s+1)(s+2)]$. The process gain is arbitrarily set to unity, since the purpose of the exercise is only to show oscillatory behavior. This being a sample-data variant of the original problem, we also insert a zero-order hold with transfer function [1 - exp(-Ts)]/s between the controller output and $G_p(s)$. Defining $G(s)=G_p(s)/s$ and setting T=1, we obtain

$$g(t) = [1 + \exp(-2t) - 2\exp(-t)]/2$$

hence

$$g[0]=0 \tag{9a}$$

$$g[n]=1.71828\exp(-n)-3.1945\exp(-2n) \qquad n=1,2,\ldots \tag{9b}$$

upon some manipulation. Let the set-point be suddenly changed to 0.3 (from zero). The computation of the output proceeds as follows:

$$c[0]=g[0]m[0]=0$$

$$r[0]=0.3$$

$$m[0]=1$$

$$c[1]=g[1]m[0]+g[0]m[1]=0.1998$$

$$r[1]=0.1002$$

$$m[1]=1$$

$$c[2]=g[2]m[0]+g[1]m[1]+g[0]m[2]=0.3738$$

$$r[2]=-0.0738$$

$$m[2]=-1$$

etc.

The vertical line between the g-column and the m-column in Table 5 is the symmetry axis for diagonal invariance. Notice that g[0]m[k] element is zero regardless of the value of k, hence each c[n] value depends only on previous values m[0], m[1],... m[n-1]. As n increases, the output settles to a vanishingly small-amplitude oscillation, known as the chatter phenomenon.

FINAL REMARKS

No currently available textbook covers the entire course material, but several texts treat the contents of individual chapters. Students consulting the books by Stephanopoulos[6] and Coughanowr[8] seem to fare best in the course.

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Professor B.C. Kuo of the University of Illinois set me firmly on the path of "digital thinking" about thirty-five years ago. I hope that I transmit his enthusiasm to at least some of my students.

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