Laplace Transform Methods

ChE 132A handout

(Adapted from Graham and Rawlings (2022).)

Laplace transforms are highly useful for solving linear ordinary and partial differential equations. Their usefulness stems from the following feature: taking a Laplace transform of a (linear) ordinary differential equation (ODE) converts it into an algebraic equation, which is usually much easier to solve than the starting ODE. Similarly taking the Laplace transform of a (linear) partial differential equation (PDE) converts it into an ODE, which is again easier to solve than the starting PDE.

1 Brief Multivariable Calculus Review

1.1 Leibniz Rule for Differentiating an Integral

The Leibniz rule gives the derivative of an integral whose limits and integrand all depend on the differentiation variable

$$\frac{d}{dt}\int_{a(t)}^{b(t)} f(t,t')\ \mathrm{d}t' = \frac{db}{dt}f(t,b) - \frac{da}{dt}f(t,a) + \int_{a(t)}^{b(t)} \frac{\partial f}{\partial t}(t,t')\ \mathrm{d}t' \tag{1}$$

The three contributions, labeled ①–③ in Figure 1, arise from: ① the upper limit moving, ② the lower limit moving, and ③ the change in the integrand with t.

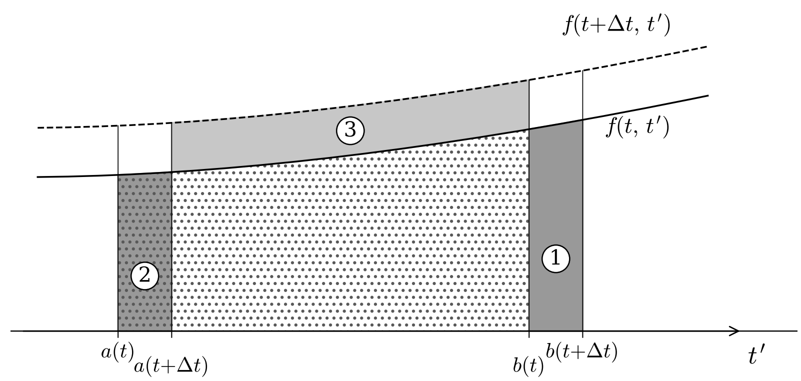

Figure 1: Geometric interpretation of the three contributions to the Leibniz rule (1).

1.2 Exchanging the Order of Integration

Consider the triangular region $T = \{(t,t') : 0 \le t' \le t,\ t \ge 0\}$ shown in Figure 2. Slicing T with a vertical strip of width $\mathrm{d}t$ at fixed t (integrating t' from 0 to t), or equivalently with a horizontal strip of height $\mathrm{d}t'$ at fixed t' (integrating t from t' to ∞), gives the same area element $\mathrm{d}A = \mathrm{d}t'\ \mathrm{d}t$. Therefore

$$\iint_T f(t,t')\ \mathrm{d}A = \int_0^\infty \int_0^t f(t,t')\ \mathrm{d}t'\ \mathrm{d}t = \int_0^\infty \int_{t'}^\infty f(t,t')\ \mathrm{d}t\ \mathrm{d}t' \tag{2}$$

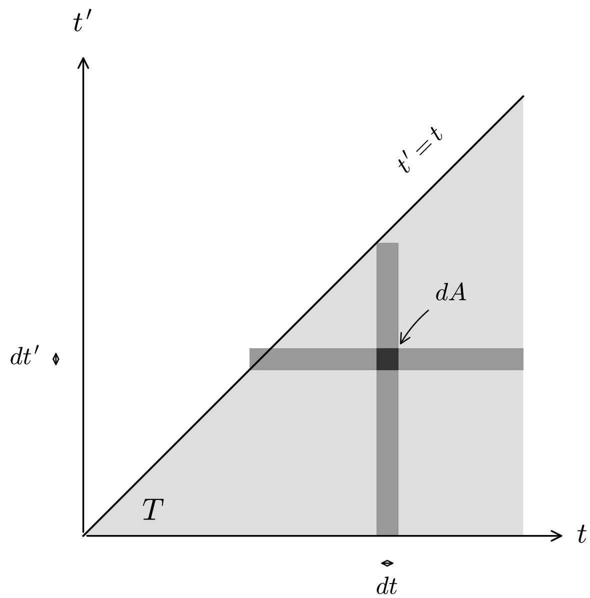

Figure 2: Triangular region T for exchanging the order of integration in (2). A vertical strip (width $\mathrm{d}t$, integrating t' from 0 to t) and a horizontal strip (height $\mathrm{d}t'$, integrating t from t' to ∞) share the small area element $\mathrm{d}A$.

2 Laplace Transform Definition and Properties

Definition. Consider functions of time $f(t)$ that vanish for $t < 0$. If there exists a real constant $c > 0$ such that $f(t)e^{-ct} \to 0$ sufficiently fast as $t \to \infty$, we can define the Laplace transform of $f(t)$, denoted $\overline{f}(s)$, for all complex-valued s such that $\mathrm{Re}(s) \geq c$

$$\mathcal{L}(f(t)) = \int_0^\infty e^{-st} f(t)\ \mathrm{d}t = \overline{f}(s), \qquad \mathrm{Re}(s) \geq c \tag{3}$$

The inverse formula is given by

$$\mathcal{L}^{-1}(\overline{f}(s)) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} e^{st}\overline{f}(s)\ \mathrm{d}s = f(t), \qquad t \geq 0 \tag{4}$$

Properties.

1. **Linearity.** For every scalar α, β and functions $f(t), g(t)$,

$$\mathcal{L}\{\alpha f(t) + \beta g(t)\} = \alpha\overline{f}(s) + \beta\overline{g}(s)$$

   The inverse transform is also linear

$$\mathcal{L}^{-1}\{\alpha\overline{f}(s) + \beta\overline{g}(s)\} = \alpha f(t) + \beta g(t)$$

2. **Transform of derivatives.**

$$\mathcal{L}\left(\frac{\mathrm{d}f(t)}{\mathrm{d}t}\right) = s\overline{f}(s) - f(0)$$

$$\mathcal{L}\left(\frac{\mathrm{d}^2 f(t)}{\mathrm{d}t^2}\right) = s^2\overline{f}(s) - sf(0) - f'(0)$$
$$\mathcal{L}\left(\frac{\mathrm{d}^n f(t)}{\mathrm{d}t^n}\right) = s^n\overline{f}(s) - s^{n-1}f(0) - s^{n-2}f'(0) - \cdots - sf^{(n-2)}(0) - f^{(n-1)}(0)$$

3. **Transform of an integral.**
$$\mathcal{L}\left(\int_0^t f(t')\ \mathrm{d}t'\right) = \frac{1}{s}\overline{f}(s)$$

4. **Derivative of the transform with respect to s.**
$$\mathcal{L}\big(t^n f(t)\big) = (-1)^n \frac{\mathrm{d}^n\overline{f}(s)}{\mathrm{d}s^n}$$

5. **Time delay and s-delay.**
$$\mathcal{L}(f(t-a)H(t-a)) = e^{-as}\overline{f}(s), \qquad \mathcal{L}(e^{at}f(t)) = \overline{f}(s-a)$$
where the Heaviside or unit step function is defined as
$$H(t) = \begin{cases} 0, & t < 0 \\ 1, & 0 < t \end{cases}$$

6. **Laplace convolution theorem.**
$$\mathcal{L}\left(\int_0^t f(t')g(t-t')\ \mathrm{d}t'\right) = \overline{f}(s)\overline{g}(s), \qquad \mathcal{L}\left(\int_0^t f(t-t')g(t')\ \mathrm{d}t'\right) = \overline{f}(s)\overline{g}(s)$$

7. **Final value theorem.**
$$\lim_{s\to 0} s\overline{f}(s) = \lim_{t\to\infty} f(t)$$
if and only if $s\overline{f}(s)$ is bounded for all $\mathrm{Re}(s) \geq 0$.

8. **Initial-value theorem.**
$$\lim_{s\to\infty} s\overline{f}(s) = \lim_{t\to 0^+} f(t)$$

We can readily compute the Laplace transform of many simple $f(t)$ by using the definition and performing the integral. In this fashion we can construct Table 1 of Laplace transform pairs. Such tables prove useful in solving differential equations.

3 Ordinary Differential Equations

Example 3.1 (A forced first-order differential equation)**.** Consider the first-order differential equation with forcing term
$$\frac{\mathrm{d}x}{\mathrm{d}t} = ax + bu(t), \qquad x(0) = x_0$$
Use the Laplace transform to find $x(t)$ for any forcing $u(t)$.

Table 1: Small table of Laplace transform pairs. A more extensive table is found at the end of this handout.

$f(t)$	$\overline{f}(s)$
$\delta(t)$	1
1	$\dfrac{1}{s}$
t	$\dfrac{1}{s^2}$
$t^n,\ -1 < n$	$\dfrac{\Gamma(n+1)}{s^{n+1}}$
$\cos \omega t$	$\dfrac{s}{s^2+\omega^2}$
$\sin \omega t$	$\dfrac{\omega}{s^2+\omega^2}$
$\sinh \omega t$	$\dfrac{\omega}{s^2-\omega^2}$
$\cosh \omega t$	$\dfrac{s}{s^2-\omega^2}$
e^{at}	$\dfrac{1}{s-a}$
te^{at}	$\dfrac{1}{(s-a)^2}$
$e^{at}\cos \omega t$	$\dfrac{s-a}{(s-a)^2+\omega^2}$
$e^{at}\sin \omega t$	$\dfrac{\omega}{(s-a)^2+\omega^2}$

Solution. Taking the Laplace transform, substituting the initial condition, and solving for $\overline{x}(s)$, give

$$s\overline{x}(s) - x_0 = a\overline{x}(s) + b\overline{u}(s)$$

so

$$\overline{x}(s) = \frac{x_0}{s-a} + b\frac{\overline{u}(s)}{s-a}$$

We can invert the first term directly using Table 1, and the second term using the table and the convolution theorem, giving

$$x(t) = x_0 e^{at} + b\int_0^t e^{a(t-t')}u(t')\ \mathrm{d}t'$$

We see the effect of the initial condition x_0 and the forcing term $u(t)$. If $a < 0$ so the system is asymptotically stable, the effect of the initial condition decays exponentially with time. The forcing term affects the solution through the convolution of u with the time-shifted exponential. □

Example 3.2 (Particle motion)**.** Consider the motion of a particle of mass m connected to a spring with spring constant K and experiencing an applied force $F(t)$ as depicted in Figure 3.

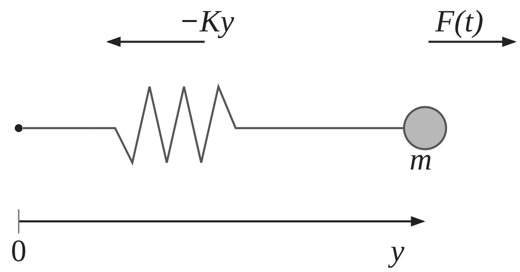

Figure 3: Particle of mass m at position y experiences spring force $-Ky$ and applied force $F(t)$.

Let y denote the displacement from the origin and model the spring as applying force $F_s = -Ky$. Newton's equation of motion for this system is then

$$m\frac{\mathrm{d}^2 y}{\mathrm{d}t^2} = F - Ky$$

We require two boundary conditions for this second-order differential equation. If we assume the particle is initially at rest at the origin, then the boundary conditions are both specified at $t = 0$ and these initial conditions are

$$y(0) = 0, \qquad \frac{\mathrm{d}y}{\mathrm{d}t}(0) = 0$$

If we divide by the mass of the particle we can express the model as

$$\frac{\mathrm{d}^2 y}{\mathrm{d}t^2} + k^2 y = f$$

with

$$y(0) = 0, \qquad \frac{\mathrm{d}y}{\mathrm{d}t}(0) = 0, \qquad k^2 = \frac{K}{m}, \qquad f = \frac{F}{m}$$

Take the Laplace transform of the model and find the position of the particle versus time $y(t)$, for arbitrary applied force $f(t)$.

Solution. Taking the Laplace transform of the equation of motion and substituting in the two initial conditions gives

$$s^2\overline{y}(s) - sy(0) - y'(0) + k^2\overline{y}(s) = \overline{f}(s)$$

so that

$$s^2\overline{y}(s) + k^2\overline{y}(s) = \overline{f}(s)$$

Solving this equation for $\overline{y}(s)$ gives

$$\overline{y}(s) = \frac{\overline{f}(s)}{s^2 + k^2}$$

We see the transform is the product of two functions of s. The inverse of each of these is available

$$\mathcal{L}^{-1}(\overline{f}(s)) = f(t), \qquad \mathcal{L}^{-1}\left(\frac{1}{s^2 + k^2}\right) = \frac{1}{k}\sin kt$$

The first follows by the definition of $\overline{f}(s)$ and the second follows from Table 1. Using the convolution theorem then gives

$$y(t) = \frac{1}{k}\int_0^t f(t')\sin k(t-t')\ \mathrm{d}t'$$

We see that the particle position is a convolution integral of the applied force with the sine function. The reader may wish to check that this solution indeed satisfies the differential equation and both initial conditions as claimed. □

Example 3.3 (Sets of coupled first-order differential equations)**.** Consider next the inhomogeneous constant-coefficient system

$$\frac{\mathrm{d}x}{\mathrm{d}t} = Ax + Bu(t), \qquad x(0) = x_0$$

in which $x \in \mathbb{R}^n$, $u \in \mathbb{R}^m$, $A \in \mathbb{R}^{n\times n}$, $B \in \mathbb{R}^{n\times m}$. In systems and control applications, x is known as the state vector and u is the manipulated variable vector. Use Laplace transforms to find $x(t)$ for this problem.

Solution. Again taking the Laplace transform, substituting the initial condition, and solving for $\overline{x}(s)$ gives

$$s\overline{x}(s) - x_0 = A\overline{x}(s) + B\overline{u}(s)$$

$$(sI - A)\overline{x}(s) = x_0 + B\overline{u}(s)$$

$$\overline{x}(s) = (sI-A)^{-1}x_0 + (sI-A)^{-1}B\overline{u}(s)$$

We next require the matrix version of the Laplace transform pair

$$e^{at} \longleftrightarrow \frac{1}{s-a}, \qquad e^{At} \longleftrightarrow (sI-A)^{-1}$$

which can be checked by applying the definition of the Laplace transform. Using this result and the convolution theorem gives

$$x(t) = e^{At}x_0 + \int_0^t e^{A(t-t')}Bu(t')\ \mathrm{d}t'$$

Notice we cannot move the constant matrix B outside the integral as we did in the scalar case because the indices in the matrix multiplications must conform as shown below

$$x(t)_{n\times 1} = (e^{At})_{n\times n}(x_0)_{n\times 1} + \int_0^t \left(e^{A(t-t')}\right)_{n\times n}(B)_{n\times m}(u(t'))_{m\times 1}\ \mathrm{d}t'$$

□

4 Application to Process Control

Because the Laplace transform converts linear differential equations into algebraic equations, it is particularly useful in chemical process dynamics and feedback control. Consider the liquid-level process shown in Figure 4. A tank receives an inflow $d(t)$—the *disturbance*, arriving from an upstream process unit that we cannot control—and discharges through an outflow $u(t)$ that we can manipulate. The liquid volume $v(t)$ is the quantity we wish to automatically regulate so that we do not accidentally overflow the tank or empty the tank and cavitate the pump.

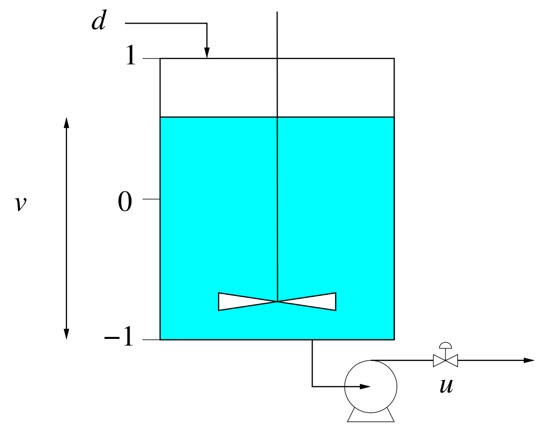

Figure 4: Liquid-level process. The inflow $d(t)$ is the disturbance; the outflow $u(t)$ is the manipulated variable; $v(t)$ is the liquid volume to be controlled.

A mass balance on the tank (assuming constant liquid density) gives the first-order linear ODE

$$\frac{d}{dt}v(t) = d(t) - u(t), \qquad v(0) = 0 \tag{5}$$

Taking the Laplace transform and solving for $\overline{v}(s)$

$$\overline{v}(s) = \frac{1}{s}\,\overline{d}(s) - \frac{1}{s}\,\overline{u}(s) \tag{6}$$

Transfer functions and block diagrams. The output $\overline{v}(s)$ in (6) is a linear combination of the two input transforms, each weighted by the *transfer function* $1/s$. We represent this compactly as the *block diagram* in Figure 5. Each box multiplies the entering signal by the transfer function written inside it; the circle is a *summer* that adds its inputs with the sign shown at each arrow. A positive sign is normally assumed if no sign is given.

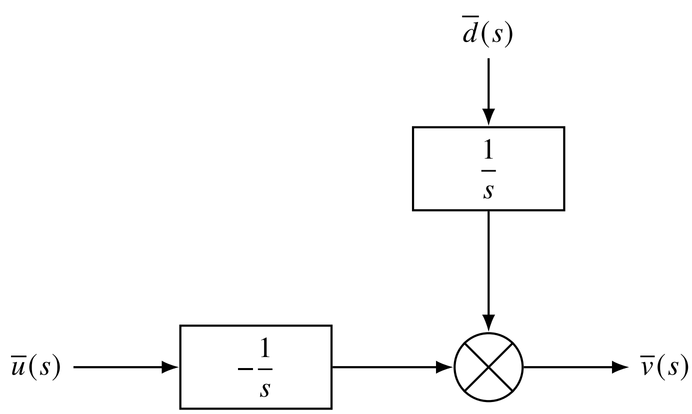

Figure 5: Block diagram for the liquid-level process. Each $1/s$ block is an integrator; the summer combines the disturbance and manipulated-variable contributions.

Equation (6) makes explicit what the mass balance implies: the tank volume is the time-integral of the net inflow $(d - u)$. A sustained imbalance $d \neq u$ causes the volume to rise or fall without bound—the integrating character of the tank is captured directly by the $1/s$ transfer function.

5 Partial Differential Equations

Next we illustrate the solution of several linear PDEs with Laplace transforms. For a user with some experience, Laplace transforms are probably the most powerful method for solving linear, low-dimensional PDEs in closed form. After taking the Laplace transform of a PDE, usually with respect to the time variable, the result is a linear ODE in the transform function. We can often solve this ODE. To perform the inverse transform, we then require some inverse formulas for transforms with singularities. We develop these inverse formulas next and then solve some example PDEs.

Let the transform function

$$\overline{f}(s) = \frac{\overline{p}(s)}{\overline{q}(s)}$$

have singularities at the zeros of $\overline{q}(s)$, which is assumed to have m simple zeros

$$\overline{q}(s) = 0 \qquad s = s_1, s_2, \ldots, s_m$$

The inverse of this Laplace transform is given by the following formula

$$f(t) = \sum_{n=1}^{m} a_n e^{s_n t}, \qquad a_n = \frac{\overline{p}(s_n)}{\overline{q}'(s_n)} \tag{7}$$

which is usually called the *Heaviside expansion theorem*. When $\overline{p}(s)$ and $\overline{q}(s)$ are polynomials, the coefficients a_n can be derived using partial fractions. But the result applies to more general cases as well.

When the zeros of $\overline{q}(s)$ are higher than first order, $f(t)$ is a linear combination of products of polynomials and exponentials of time, and the coefficients are more complex. Let the zero s_n have order r_n, $n = 1, 2, \ldots, m$. Then the inverse is given by

$$f(t) = \sum_{n=1}^{m} e^{s_n t} \sum_{i=1}^{r_n} a_{ni} t^{i-1} \tag{8}$$

The coefficients a_{ni}, for $i = 1, \ldots, r_n$, $n = 1, 2, \ldots, m$, are given by

$$a_{ni} = \frac{\phi^{(r_n - i)}(s_n)}{(r_n - i)!\,(i-1)!}$$

in which

$$\phi(s) = (s - s_n)^{r_n} \frac{\overline{p}(s)}{\overline{q}(s)}$$

and $\phi^{(i)}(s_n)$ denotes the i-th derivative of $\phi(s)$ evaluated at $s = s_n$.

Next we use Laplace transforms to solve the reaction-diffusion equation. We will see that the transform has only simple zeros and we will use (7) for calculating the inverse.

Example 5.1 (Reaction and diffusion in a membrane)**.** The following model describes diffusion through a membrane in which component A decomposes by a first-order reaction. The membrane initially has zero concentration of A. At $t = 0$ the concentration at the side of the membrane at $x = 0$ is abruptly raised to concentration c_{A0} and the other side is maintained at zero concentration

$$\text{PDE} \quad \frac{\partial c_A}{\partial t} = D_A \frac{\partial^2 c_A}{\partial x^2} - K c_A$$

$$\text{BC1} \quad c_A(0,t) = c_{A0}, \qquad t > 0$$
$$\text{BC2} \quad c_A(L,t) = 0, \qquad t > 0$$
$$\text{IC} \quad c_A(x,0) = 0, \qquad 0 < x < L$$

(a) Define the dimensionless variables

$$c = \frac{c_A}{c_{A0}}, \qquad z = \frac{x}{L}, \qquad \tau = \frac{tD_A}{L^2}, \qquad k = \frac{KL^2}{D_A}$$

and show that the model reduces to

$$\text{PDE} \quad \frac{\partial c}{\partial \tau} = \frac{\partial^2 c}{\partial z^2} - kc$$
$$\text{BC1} \quad c(0,\tau) = 1, \qquad \tau > 0$$
$$\text{BC2} \quad c(1,\tau) = 0, \qquad \tau > 0$$
$$\text{IC} \quad c(z,0) = 0, \qquad 0 < z < 1$$

in which $k = KL^2/D_A$ is the only dimensionless parameter appearing in the problem. This dimensionless parameter is known as the Thiele number or Thiele modulus in the chemical reaction engineering literature. It indicates the ratio of the reaction rate to the diffusion rate.

(b) Take the Laplace transform of your model (also the boundary conditions). Solve the resulting differential equation and boundary conditions for $\overline{c}(z,s)$ and show that

$$\overline{c}(z,s) = \frac{\sinh\!\left(\sqrt{s+k}\,(1-z)\right)}{s\,\sinh\sqrt{s+k}}$$

(c) Apply the final-value theorem to $\overline{c}(z,s)$ to find the steady-state solution $c_s(z)$.

(d) Take the limit of this solution as $k \to 0$ for the zero-reaction case. Does your solution satisfy the diffusion equation?

(e) Sketch the solution $c_s(z)$ for a range of k values and show the effect of reaction on the steady-state concentration profile.

(f) Let $\overline{p}(s) = \sinh\!\left(\sqrt{s+k}\,(1-z)\right)$ and $\overline{q}(s) = s\,\sinh\sqrt{s+k}$, and find the zeros s_n of $\overline{q}(s)$. Also find the value of $\overline{p}(s_n)/\overline{q}'(s_n)$ at the zeros of $\overline{q}(s)$. The following formulas may be helpful:

$$\cosh(iu) = \cos u, \qquad \sinh(iu) = i\sin u$$

(g) Invert the transform and find $c(z,\tau)$. Check that the solution satisfies the PDE and boundary conditions.

Solution. **(a)** Inserting the defined dimensionless variables in the PDE gives

$$D_A \frac{c_{A0}}{L^2}\frac{\partial c}{\partial \tau} = D_A \frac{c_{A0}}{L^2}\frac{\partial^2 c}{\partial z^2} - Kc_{A0}c$$

and rearranging gives

$$\frac{\partial c}{\partial \tau} = \frac{\partial^2 c}{\partial z^2} - \frac{KL^2}{D_A}c$$

so

$$\frac{\partial c}{\partial \tau} = \frac{\partial^2 c}{\partial z^2} - kc$$

Inserting the dimensionless variables in the boundary and initial conditions gives

$$c_{A0}c(z,\tau) = c_{A0}, \qquad z = 0,\ \tau > 0$$

$$c_{A0}c(z,\tau) = 0, \qquad zL = L,\ \tau > 0$$

$$c_{A0}c(z,\tau) = 0, \qquad 0 < zL < L,\ \tau = 0$$

which simplify to

$$c(z,\tau) = 1, \qquad z = 0,\ \tau > 0$$

$$c(z,\tau) = 0, \qquad z = 1,\ \tau > 0$$

$$c(z,\tau) = 0, \qquad 0 < z < 1,\ \tau = 0$$

(b) Taking the Laplace transform of the PDE and boundary conditions gives

$$s\overline{c}(z,s) - c(z,0) = \frac{\mathrm{d}^2\overline{c}}{\mathrm{d}z^2} - k\overline{c}$$

so that

$$\frac{\mathrm{d}^2\overline{c}}{\mathrm{d}z^2} - (k+s)\overline{c} = 0$$

with transformed boundary conditions

$$\overline{c}(1,s) = 0, \qquad \overline{c}(0,s) = \frac{1}{s}$$

The solution of the ODE can be written

$$\overline{c}(z,s) = a\cosh\left(\sqrt{s+k}(1-z)\right) + b\sinh\left(\sqrt{s+k}(1-z)\right)$$

and we use the two boundary conditions to find the constants a and b. We have

$$0 = a, \qquad \frac{1}{s} = b\ \sinh\sqrt{s+k}$$

so

$$b = \frac{1}{s\ \sinh\sqrt{s+k}}$$

which gives

$$\overline{c}(z,s) = \frac{\sinh\left(\sqrt{s+k}(1-z)\right)}{s\ \sinh\sqrt{s+k}}$$

(c) Applying the final-value theorem gives

$$c_s(z) = \lim_{s\to 0} s\overline{c}(z,s) = \lim_{s\to 0}\frac{\sinh\left(\sqrt{s+k}(1-z)\right)}{\sinh\sqrt{s+k}}$$

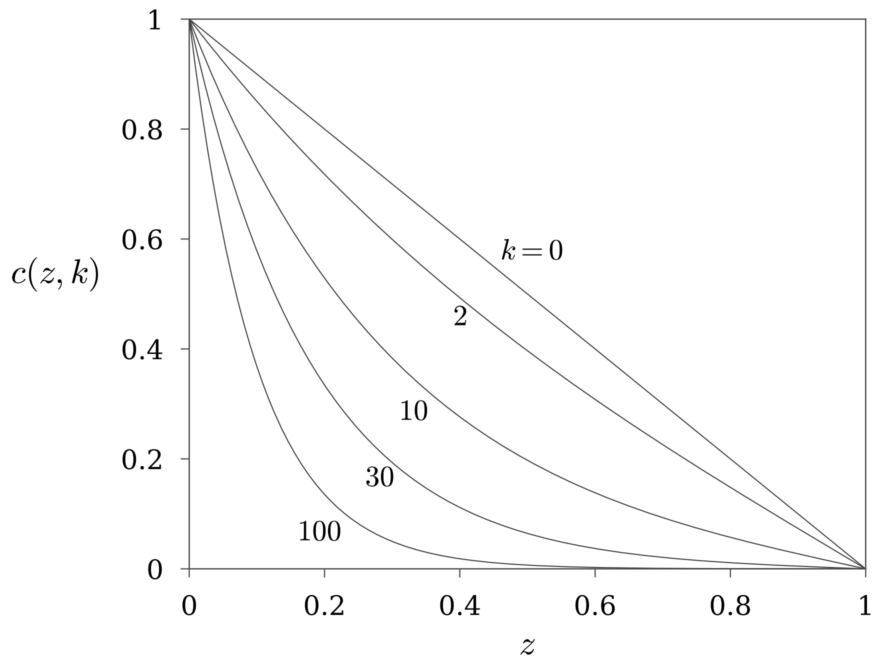

Figure 6: Concentration versus membrane penetration distance for different reaction rate constants.

and therefore

$$c_s(z) = \frac{\sinh\big(\sqrt{k}(1-z)\big)}{\sinh\sqrt{k}}$$

(d) Using the fact that $\sinh x \approx x$ for small x gives

$$\lim_{k\to 0} c_s(z) = \frac{\sqrt{k}(1-z)}{\sqrt{k}} = 1 - z$$

Yes, the solution satisfies the steady-state diffusion equation and boundary conditions

$$\frac{\mathrm{d}^2 c_s(z)}{\mathrm{d}z^2} = 0, \qquad c_s(0) = 1, \qquad c_s(1) = 0$$

(e) The concentration profile $c_s(z)$ versus z for a variety of rate constants k is given in Figure 6. We see that a large reaction rate constant prevents species A from diffusing very far into the membrane.

(f) Since the zeros of $\sin u$ are $u = \pm n\pi$, $n = 0, 1, 2, \ldots$, the zeros of $\sinh u$ are $u = \pm n\pi i$, $n = 0, 1, 2, \ldots$. The zeros of $\sinh\sqrt{k+s}$ are given by

$$s_n = -(n^2\pi^2 + k),$$

and for these roots, we have $\sqrt{s_n + k} = n\pi i$, in which we choose the positive square root. Therefore the zeros of the denominator $\overline{q}(s)$ are

$$s = \{\, 0,\ -(n^2\pi^2 + k)\,\}, \qquad n = 0, 1, 2, \ldots$$

These are simple zeros so the inversion formula in (7) is applicable. Differentiating $\overline{q}(s)$ and evaluating $\overline{q}'(s)$ at the zeros gives

$$\overline{q}'(s) = \sinh\sqrt{s+k} + \frac{s\cosh\sqrt{s+k}}{2\sqrt{s+k}}$$

$$\overline{q}'(0) = \sinh\sqrt{k}$$
$$q'\big(-(n^2\pi^2 + k)\big) = -\frac{(n^2\pi^2 + k)(-1)^n}{2n\pi i}$$

Evaluating $\overline{p}(s)$ at the zeros gives

$$\overline{p}(0) = \sinh\big(\sqrt{k}(1-z)\big), \qquad p\big(-(n^2\pi^2 + k)\big) = i \sin n\pi(1-z)$$

(g) Putting these terms together in (7) gives

$$c(z,\tau) = \frac{\sinh\big(\sqrt{k}(1-z)\big)}{\sinh\sqrt{k}} + \sum_{n=0}^{\infty}(-1)^n \frac{2n\pi}{n^2\pi^2 + k} \sin\big(n\pi(1-z)\big)e^{-(n^2\pi^2+k)\tau}$$

Noticing the $n = 0$ term vanishes, we can rewrite the solution as

$$c(z,\tau) = \frac{\sinh\big(\sqrt{k}(1-z)\big)}{\sinh\sqrt{k}} - 2\sum_{n=1}^{\infty} \frac{(-1)^{n+1} n\pi}{n^2\pi^2 + k} \sin\big(n\pi(1-z)\big)e^{-(n^2\pi^2+k)\tau} \tag{9}$$

□

Exercises

Exercise 1 (Differentiating integrals).

Taken from (Graham and Rawlings, 2022, Exercise 2.11).

Use the Leibniz rule for differentiating integrals to solve the following two problems.

(a) Check that the solution to the differential equation

$$\frac{dy}{dt} + p(t)\,y = q(t)$$

with initial condition $y(0) = y_0$ is

$$y(t) = e^{-\int_0^t p(t')\,\mathrm{d}t'} \left[\int_0^t q(t'')\, e^{\int_0^{t''} p(\tau)\,\mathrm{d}\tau}\, \mathrm{d}t'' + y_0 \right]$$

Remember to show the solution satisfies both the differential equation and initial condition.

(b) Derive a Leibniz rule for differentiating the double integral

$$f(t) = \int_{a(t)}^{b(t)} \int_{c(t,p)}^{d(t,p)} h(t,p,s)\ \mathrm{d}s\ \mathrm{d}p$$

Your answer should not contain the derivatives of any integrals.

Exercise 2 (Convolution theorem).

Taken from (Graham and Rawlings, 2022, Exercise 2.12).

Use the definition of the Laplace transform to derive the convolution theorem

$$\mathcal{L}\left\{ \int_0^t f(t')\, g(t-t')\ \mathrm{d}t' \right\} = \overline{f}(s)\,\overline{g}(s)$$

Exercise 3 (Final-value and initial-value theorems).

Taken from (Graham and Rawlings, 2022, Exercise 2.13).

Two useful theorems are the final- and initial-value theorems

$$\lim_{t\to\infty} f(t) = \lim_{s\to 0}\ s\overline{f}(s)$$

if and only if $|s\overline{f}(s)| < \infty$ for all s such that $\mathrm{Re}(s) \geq 0$; otherwise $\lim_{t\to\infty} f(t)$ does not exist; and

$$\lim_{t\to 0^+} f(t) = \lim_{s\to\infty}\ s\overline{f}(s)$$

(a) The conditions on $s\overline{f}(s)$ for the final-value theorem are *crucial*. For the functions below, state which satisfy the conditions and give their final values.

(a) $\dfrac{1}{s}$

(b) $\dfrac{1}{s^2}$

(c) $\dfrac{1}{s(s-a)}, \quad \text{Re}(a) > 0$

(d) $\dfrac{1}{s(s+a)}, \quad \text{Re}(a) > 0$

(b) What are the initial values, $f(0^+)$?

(c) Invert each of the transforms to get $f(t)$ and check your results.

Exercise 4 (Network of four isomerization reactions).

Taken from (Graham and Rawlings, 2022, Exercise 2.14).

Consider the set of reversible, first-order reactions

$$A \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} B \underset{k_{-2}}{\overset{k_2}{\rightleftharpoons}} C \underset{k_{-3}}{\overset{k_3}{\rightleftharpoons}} D \underset{k_{-4}}{\overset{k_4}{\rightleftharpoons}} E$$

taking place in a well-mixed, batch reactor. The reactions are all elementary with corresponding first-order rate expressions. Let the concentration of the species be arranged in a column vector $c = \begin{bmatrix} c_A & c_B & c_C & c_D & c_E \end{bmatrix}^T$.

(a) Write the mass balance for the well-mixed, batch reactor of constant volume $dc/dt = Kc$. What is K for this problem?

(b) What is the solution of this mass balance for initial condition $c(0) = c_0$? What calculation do you do to find out if this solution is stable?

(c) Determine the rank of matrix K. Hint: focus on the rows of K. Justify your answer. From the fundamental theorem of linear algebra, what is the dimension of the null space of K?

(d) What is the condition for a steady-state solution of the model? Is the steady state unique? Why or why not?

Exercise 5 (Network of first-order chemical reactions).

Taken from (Graham and Rawlings, 2022, Exercise 2.15).

Consider the generalization of Exercise 4 to the following set of n reversible, first-order reactions

$$A_1 \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} A_2 \underset{k_{-2}}{\overset{k_2}{\rightleftharpoons}} A_3 \underset{k_{-3}}{\overset{k_3}{\rightleftharpoons}} \cdots \underset{k_{-(n-1)}}{\overset{k_{n-1}}{\rightleftharpoons}} A_n$$

taking place in a well-mixed, batch reactor. The reaction rate for the ith reaction is $r_i = k_i c_{A_i} - k_{-i} c_{A_{i+1}}$. Let the concentration of the species be arranged in a column vector $c = \begin{bmatrix} c_{A_1} & c_{A_2} & \cdots & c_{A_n} \end{bmatrix}^T$.

(a) Write the mass balance for the well-mixed, batch reactor of constant volume $dc/dt = \cdots$.

(b) What is the solution of this mass balance for initial condition $c(0) = c_0$?

(c) What is the steady-state solution of the model? Is the steady state unique? Why or why not?

(d) What calculation would you do to decide if the steady state is stable?

Exercise 6 (Differentiating a Laplace transform).

Taken from (Graham and Rawlings, 2022, Exercise 2.16).

Establish property 4 of the Laplace transform properties, which states for $n \geq 1$

$$\frac{d\overline{f}(s)}{ds} = -\mathcal{L}\{t\, f(t)\}$$

Exercise 7 (Partial fraction expansion).

Taken from (Graham and Rawlings, 2022, Exercise 3.24).

We often teach inversion of Laplace transforms by so-called partial fraction expansion. For example, given

$$\overline{f}(s) = \frac{1}{(s-a)(s-b)(s-c)}, \qquad a \neq b \neq c$$

note that $a \neq b \neq c$ ensures a, b, and c are simple zeros of the denominator polynomial.

The function $\overline{f}(s)$ is first written as a summation of simpler fractions

$$\frac{1}{(s-a)(s-b)(s-c)} = \frac{A}{s-a} + \frac{B}{s-b} + \frac{C}{s-c} \tag{10}$$

and the coefficients A, B, and C are determined. Then the inverse is simply

$$f(t) = Ae^{at} + Be^{bt} + Ce^{ct}$$

(a) Determine A, B, and C in the partial expansion approach and determine $f(t)$.

(b) Apply (7) with $\overline{p}(s) = 1$ and $\overline{q}(s) = (s-a)(s-b)(s-c)$, and find $f(t)$ using (7). Which method do you prefer and why? Notice that (7) can be applied when the denominator $\overline{q}(s)$ is more general than a polynomial, as shown in Example 3.15.

Exercise 8 (Leibniz rule application).

Let

$$F(t) = \int_0^{t^2} e^{-(t-\tau)}\, d\tau$$

(a) Compute $\dfrac{dF}{dt}$ using the Leibniz rule.

(b) Simplify your final answer as much as possible.

Exercise 9 (Laplace transforms of polynomials and exponentials).

Compute the Laplace transform of each function:

(a) $f(t) = 3 + 2t$

(b) $f(t) = e^{-2t}$

(c) $f(t) = te^{-2t}$

(d) Use your answers to compute $\mathcal{L}\{3 + 2t + te^{-2t}\}$

Exercise 10 (Solving ODE with Laplace transforms).

Solve using Laplace transforms:

$$\frac{dx}{dt} + 2x = 4, \quad x(0) = 1$$

(a) Take the Laplace transform and solve for $\overline{x}(s)$

(b) Invert to find $x(t)$

(c) Identify the steady-state value and check it makes sense from the ODE

Exercise 11 (Solving another ODE with Laplace transforms).

Solve using Laplace transforms:

$$\frac{dy}{dt} - y = e^{t}, \quad y(0) = 0$$

(a) Take the Laplace transform and solve for $\overline{y}(s)$

(b) Invert to find $y(t)$

Exercise 12 (Solving a second-order ODE with Laplace transforms).

Solve the following second-order differential equation using Laplace transforms:

$$\frac{d^2x}{dt^2} + 4\frac{dx}{dt} + 3x = e^{-t}, \quad x(0) = 0, \quad x'(0) = 1$$

(a) Take the Laplace transform of the equation and solve for $\overline{x}(s)$

(b) Perform partial fraction decomposition on $\overline{x}(s)$

(c) Invert the transform to find $x(t)$

Exercise 13 (Steady-state reaction diffusion in a membrane).

Rather than solve the transient problem as in Example 5.1, let's consider the steady-state version of diffusion through a membrane in which component A decomposes by first-order reaction. We then have the steady-state reaction-diffusion equation

$$D_A \frac{d^2}{dx^2} c_A - K c_A = 0$$

Let's assume the boundary conditions to be the same as in Example 5.1, which are

$$c_A(0) = c_{A0} \qquad c_A(L) = 0$$

(a) Nondimensionalize this equation using the dimensionless variables defined in Example 5.1 and show that it becomes

$$\frac{d^2}{dz^2} c - kc = 0 \qquad c(0) = 1 \quad c(1) = 0$$

How is the parameter k defined? Show that it is dimensionless. Notice that there is only a single dimensionless parameter in this problem. How many physical parameters did we start with?

(b) Now let's choose two linearly independent solutions to this second-order ODE. Let's call them $y_1(z)$ and $y_2(z)$. Rather than guess among the pairs $y_1 = e^{\sqrt{k}z}$ and $y_2 = e^{-\sqrt{k}z}$, or $y_1 = \cosh(\sqrt{k}z)$ and $y_2 = \sinh(\sqrt{k}z)$, etc., let's try to save ourselves some work. Can you think of a pair where one of them is zero at $z = 0$ $y_1(0) = 0$ and the other is zero at $z = 1$, $y_2(1) = 0$. That will often simplify the algebra of satisfying the boundary conditions.

Hint: think about a function of $(1 - z)$ as well as a function of z when you select the pair of linearly independent solutions.

(c) After making your choice of y_1 and y_2, set $c(z) = ay_1(z) + by_2(z)$ and find a and b from the two boundary conditions.

(d) Make a plot of your solution $c(z; k)$ for $z \in [0, 1]$ for several values of your parameter k. Describe what happens for small and large values of k. Connect that behavior to the reaction-diffusion process taking place in the membrane.

Exercise 14 (Steady-state reaction diffusion with nonzero end conditions).

Consider the previous exercise, Exercise 13. Let's say we decide to change the boundary condition at the right end of the membrane to $c_A(L) = c_L$, where $c_L \geq 0$ is not necessarily zero. Use the same dimensionless variables as in Example 5.1,

$$z = x/L \qquad c = c_A/c_0$$

(a) Nondimensionalize the equation and boundary conditions and show that

$$\frac{d^2 c}{dz^2} - kc = 0 \qquad c(0) = 1 \quad c(1) = \rho \tag{11}$$

What is ρ? Notice that the ODE is still homogeneous — only the right boundary condition has changed.

(b) Use the same linearly independent pair y_1, y_2 from Exercise 13 and set $c(z) = ay_1(z) + by_2(z)$. Find a and b from the two boundary conditions. Check that you recover the solution of Exercise 13 when $\rho = 0$.

(c) Make a plot of $c(z; k, \rho)$ for $z \in [0, 1]$ for several values of ρ at fixed k. Describe what happens as $\rho \to 1$. What is the physical situation in the membrane when $\rho = 1$?

Exercise 15 (The Laplace transform can also solve BVPs).

The classic use case of the Laplace transform is to solve initial value problems (IVPs), but with a little ingenuity, we can stretch it to solve boundary value problems (BVPs) as well. Consider again the membrane reaction-diffusion problem of Exercise 14. The dimensionless boundary value is given by (11)

$$\frac{d^2c}{dz^2} - kc = 0 \qquad c(0) = 1 \quad c(1) = \rho$$

Let's consider extending the function $c(z)$ to be the value we seek for $z \in [0, 1]$ and define $c(z) = 0$ for $z \in (1, \infty)$. So now $c(z)$ is defined on the usual entire positive real axis, and we can take its Laplace transform.

(a) Take the Laplace transform of the ODE and BCs, and show that the transform is

$$\overline{c}(s) = \frac{s + c_z(0)}{s^2 - k}$$

Notice that the *unknown* first derivative at $z = 0$ appears, and we have not been able to use our boundary condition at $z = 1$ yet. OK, the first rule of using Laplace transforms in these situations is:

Do Not Panic!

(b) Just leave the $c_z(0)$ term as an unknown constant and invert the transform.

(c) Now that you are back in the z-domain, apply the second boundary condition at $z = 1$ and solve for $c_z(0)$ and show that

$$c_z(0) = \sqrt{k}\,\frac{\rho - \cosh\sqrt{k}}{\sinh\sqrt{k}}$$

(d) Substitute that result back into your $c(z)$ expression and show that

$$c(z) = \frac{\sinh\sqrt{k}\cosh(\sqrt{k}\,z) - \cosh\sqrt{k}\sinh(\sqrt{k}\,z)}{\sinh\sqrt{k}} + \rho\,\frac{\sinh(\sqrt{k}\,z)}{\sinh\sqrt{k}}$$

(e) What hyperbolic addition formula can you use to simplify the numerator of the first term and what does that give for the final solution $c(z)$.

Exercise 16 (Two chemical reactions in series).

Consider the following two irreversible reactions taking place in a well-stirred batch reactor[1]

$$\mathrm{A} \xrightarrow{k_1} \mathrm{B} \tag{12}$$

$$\mathrm{B} \xrightarrow{k_2} \mathrm{C} \tag{13}$$

[1]Taken from Rawlings and Ekerdt (2020).

Reactant A decomposes to form an intermediate B that can further react to form a final product C. Let the reaction rates be given by simple first-order rate expressions in the corresponding reactants,

$$r_1 = k_1 c_A, \qquad r_2 = k_2 c_B$$

Write down the mass balances for components A, B, and C in terms of the reaction rates. The initial concentrations are specified constants, c_{A0}, c_{B0}, c_{C0}.

(a) Noting that species C does not show up in the balances for species A and B, take the Laplace transform of the mass balance for A, and show that

$$\overline{c}_A(s) = \frac{c_{A0}}{s + k_1}$$

(b) Take the Laplace transform of the mass balance for B and show that

$$\overline{c}_B(s) = \frac{c_{B0}}{s + k_2} + \frac{k_1 c_{A0}}{(s + k_1)(s + k_2)}$$

(c) Invert the transform of A.

(d) Use partial fractions and invert the transform of B.

(e) Finally, what is $c_C(t)$. Note that you do not have to solve its mass balance. Look back at your three species balances. What combination of c_A, c_B, c_C is invariant (does not change with time) for this reaction network? Find $c_C(t)$ from the value of this invariant at $t = 0$.

(f) Make a single plot showing $c_A(t), c_B(t), c_C(t)$ versus time starting with only A at the initial time. What are the final concentrations of A, B, and C, for these irreversible reactions. Adjust k_1 and k_2 to see their effect on the dynamics of the species concentrations.

Laplace Transform Table

The Laplace transform pairs used in the text are collected below.

Larger table of Laplace transforms. Page numbers refer to Graham and Rawlings (2022).

	$f(t)$	$\overline{f}(s)$	**page**
1	$\alpha f(t) + \beta g(t)$	$\alpha \overline{f}(s) + \beta \overline{g}(s)$	106
2	$\dfrac{\mathrm{d} f(t)}{\mathrm{d}t}$	$s\overline{f}(s) - f(0)$	107
3	$\dfrac{\mathrm{d}^2 f(t)}{\mathrm{d}t^2}$	$s^2\overline{f}(s) - sf(0) - f'(0)$	107
4	$\dfrac{\mathrm{d}^n f(t)}{\mathrm{d}t^n}$	$s^n\overline{f}(s) - \sum_{i=1}^{n} s^{n-i} f^{(i-1)}(0)$	107
5	$\int_0^t f(t')\, \mathrm{d}t'$	$\dfrac{1}{s}\overline{f}(s)$	107
6	$t^n f(t)$	$(-1)^n \dfrac{\mathrm{d}^n \overline{f}(s)}{\mathrm{d}s^n}$	107, 228
7	$f(t-a)H(t-a)$	$e^{-as}\overline{f}(s)$	108
8	$e^{at} f(t)$	$f(s-a)$	108
9	$\int_0^t f(t')g(t-t')\, \mathrm{d}t'$	$\overline{f}(s)\overline{g}(s)$	108, 227
10	$\lim_{t\to 0^+} f(t)$ (initial value theorem)	$\lim_{s\to\infty} s\overline{f}(s)$	108, 227
11	$\lim_{t\to\infty} f(t)$ (final value theorem)	$\lim_{s\to 0} s\overline{f}(s)^\dagger$	108, 227
12	$H(t)$	$\dfrac{1}{s}$	109
13	$\delta(t)$	1	115
14	$\delta^{(n)}(t), \quad n \geq 0$	s^n	115
15	t	$\dfrac{1}{s^2}$	109
16	$t^n, \quad n > -1$	$\dfrac{\Gamma(n+1)}{s^{n+1}}$	109
17	e^{at}	$\dfrac{1}{s-a}$	109
18	$e^{At}, \quad A \in \mathbb{R}^{n\times n}$	$(sI - A)^{-1}$	112
19	te^{at}	$\dfrac{1}{(s-a)^2}$	109

continued on next page

	$f(t)$	$\overline{f}(s)$	**page**
20	$\sin\omega t$	$\dfrac{\omega}{s^2+\omega^2}$	109
21	$\cos\omega t$	$\dfrac{s}{s^2+\omega^2}$	109
22	$\sinh\omega t$	$\dfrac{\omega}{s^2-\omega^2}$	109
23	$\cosh\omega t$	$\dfrac{s}{s^2-\omega^2}$	109
24	$e^{at}\sin\omega t$	$\dfrac{\omega}{(s-a)^2+\omega^2}$	109
25	$e^{at}\cos\omega t$	$\dfrac{s-a}{(s-a)^2+\omega^2}$	109
26	$\displaystyle\sum_{n=1}^{m}\frac{\overline{p}(s_n)}{\overline{q}'(s_n)}e^{s_n t}, \quad \overline{q}(s_n)$ simple zero	$\dfrac{\overline{p}(s)}{\overline{q}(s)}$	315
27	$\displaystyle\sum_{n=1}^{m}e^{s_n t}\sum_{i=1}^{r_n}a_{ni}t^{i-1}, \quad \overline{q}(s_n)$ zero of order r_n	$\dfrac{\overline{p}(s)}{\overline{q}(s)}*$	316
28	$\dfrac{k}{2\sqrt{\pi t^3}}\,e^{-k^2/(4t)}$	$e^{-k\sqrt{s}}, \quad k>0$	337
29	$\dfrac{1}{\sqrt{\pi t}}\,e^{-k^2/(4t)}$	$\dfrac{e^{-k\sqrt{s}}}{\sqrt{s}}, \quad k>0$	337
30	$\mathrm{erfc}\left(\dfrac{k}{2\sqrt{t}}\right)$	$\dfrac{e^{-k\sqrt{s}}}{s}, \quad k>0$	337
31	$\dfrac{e^{\alpha t}}{2\sqrt{\alpha}}\left\{e^{-k\sqrt{\alpha}}\,\mathrm{erfc}\left(\dfrac{k}{2\sqrt{t}}-\sqrt{\alpha t}\right)-e^{k\sqrt{\alpha}}\,\mathrm{erfc}\left(\dfrac{k}{2\sqrt{t}}+\sqrt{\alpha t}\right)\right\}$	$\dfrac{e^{-k\sqrt{s}}}{(s-\alpha)\sqrt{s}}, \quad k>0$	337
32	$\dfrac{2}{\sqrt{\pi}}\sqrt{t}\,e^{-k^2/(4t)}-k\ \mathrm{erfc}\left(\dfrac{k}{2\sqrt{t}}\right)$	$\dfrac{e^{-k\sqrt{s}}}{s\sqrt{s}}, \quad k>0$	551
33	$\dfrac{e^{\alpha t}}{2}\left\{e^{-k\sqrt{\alpha}}\,\mathrm{erfc}\left(\dfrac{k}{2\sqrt{t}}-\sqrt{\alpha t}\right)+e^{k\sqrt{\alpha}}\,\mathrm{erfc}\left(\dfrac{k}{2\sqrt{t}}+\sqrt{\alpha t}\right)\right\}$	$\dfrac{e^{-k\sqrt{s}}}{s-\alpha}, \quad k>0$	351
34	$\dfrac{1}{2t}e^{-k^2/(4t)}$	$K_0(k\sqrt{s}), \quad k>0$	338
35	$\dfrac{1}{k}e^{-k^2/(4t)}$	$\dfrac{K_1(k\sqrt{s})}{\sqrt{s}}, \quad k>0$	338
36	$\dfrac{\sinh(x\sqrt{k})}{\sinh\sqrt{k}}-2\displaystyle\sum_{n=1}^{\infty}\frac{(-1)^{n+1}n\pi}{n^2\pi^2+k}\sin(n\pi x)e^{-(n^2\pi^2+k)t}$	$\dfrac{\sinh(x\sqrt{s+k})}{s\ \sinh\sqrt{s+k}}$	321
37	$1-2\displaystyle\sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{n\pi x}\sin(n\pi x)e^{-n^2\pi^2 t}$	$\dfrac{\sinh(x\sqrt{s})}{xs\ \sinh\sqrt{s}}$	342
38	$1+2\displaystyle\sum_{n=1}^{\infty}(-1)^n\cos(n\pi x)e^{-n^2\pi^2 t}$	$\dfrac{\cosh(x\sqrt{s})}{\sqrt{s}\ \sinh\sqrt{s}}$	353
39	$1-2\displaystyle\sum_{n=0}^{\infty}\frac{(-1)^n}{(n+1/2)\pi}\cos((n+1/2)\pi x)e^{-((n+1/2)\pi)^2 t}$	$\dfrac{\cosh(x\sqrt{s})}{s\ \cosh\sqrt{s}}$	340

continued on next page

	$f(t)$	$\overline{f}(s)$	**page**
40	$1 - 2\sum_{n=1}^{\infty} \frac{1}{\alpha_n J_1(\alpha_n)} J_0(\alpha_n x) e^{-\alpha_n^2 t}, \quad J_0(\alpha_n) = 0$	$\frac{I_0(x\sqrt{s})}{s I_0(\sqrt{s})}$	342
41	$2\sum_{n=1}^{\infty} (-1)^{n+1} \sin(n\pi a)\sin(n\pi b)\cos(n\pi t)$	$\frac{\sinh(as)\sinh(bs)}{\sinh s}$	322
42	$2\sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n\pi} \sin(n\pi a)\sin(n\pi b)\sin(n\pi t)$	$\frac{\sinh(as)\sinh(bs)}{s\ \sinh s}$	348

† Final value exists if and only if $s\overline{f}(s)$ is bounded for $\mathrm{Re}(s) \geq 0$.

$$^{*}\ a_{ni} = \frac{\phi^{(r_n - i)}(s_n)}{(r_n - i)!(i-1)!}, \qquad \phi(s) = (s - s_n)^{r_n} \frac{\overline{p}(s)}{\overline{q}(s)}$$

References

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