

Supplementary Material: Advection, diffusion and delivery over a network.

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In the Supplementary Material we detail the mathematical machinery involved in solving the advection, diffusion and delivery equation over a network. In Section A we describe how to solve the particular case of stepwise constant initial conditions. In Section B we show how to calculate the concentration of resource that leaves its initial edge over the time step in question. In Section C we show how to calculate the concentration of resource that remains in the edge in which it started, and in Section D we describe how to calculate the total quantity of resource in each section of the network. Finally, in Section E we describe the Gaver-Stehfest algorithm for inverting our solutions from Laplace space into the time domain.

SOLVING ADVECTION, DIFFUSION AND DELIVERY IN LAPLACE SPACE

We are interested in calculating how the quantity of resource in a network changes over time, given that the resource decays or is delivered out of the network at a given rate, and is subject to advection and diffusion. In other words, we wish to solve a system of equations defined over a network, where the resource in edge ij of the network is governed by an equation of the form

$$\frac{\partial q_{ij}}{\partial t} + R_{ij}q_{ij} + u_{ij}\frac{\partial q_{ij}}{\partial x} - D_{ij}\frac{\partial^2 q_{ij}}{\partial x^2} = 0, \quad (1)$$

where q_{ij} is the quantity of resource per unit length, u_{ij} is the mean velocity, D_{ij} is the dispersion coefficient and R_{ij} is the rate at which a unit of resource is lost, or delivered out of the network. As we are interested in the case where the advective velocities u_{ij} may vary over several orders of magnitude, it is convenient to operate in Laplace space, and invert our solutions back into the time domain by using the Gaver-Stehfest algorithm. Note that after taking Laplace transforms $\mathcal{L}(q_{ij}(x, t)) = \int_0^\infty q_{ij}(x, t)e^{-st} dt = Q_{ij}(x, s)$, the fundamental Equation (1) becomes

$$(s + R_{ij})Q_{ij} + u_{ij}\frac{\partial Q_{ij}}{\partial x} - D_{ij}\frac{\partial^2 Q_{ij}}{\partial x^2} = q_{ij}(x, 0). \quad (2)$$

Also note that as in the Main Text, for each edge ij and every $s > 0$ we let

$$\alpha_{ij}(s) = \sqrt{u_{ij}^2 + 4D_{ij}(s + R_{ij})},$$

$$g_{ij} = \frac{u_{ij}l_{ij}}{2D_{ij}} \quad \text{and} \quad h_{ij}(s) = \frac{\alpha_{ij}(s)l_{ij}}{2D_{ij}}.$$

A. Stepwise constant initial conditions

We are interested in calculating how the quantity of resource in a network changes over time, given that the resource is subject to the fundamental Equation (1). In particular, it is convenient to consider a stepwise constant initial condition, as we can then calculate how the total quantity of resource in each segment of the network has changed by time t . The first step in this calculation is to find the Laplace transform of the concentrations at each node $\bar{C}(s)$. As we have seen, to calculate $\bar{C}(s)$ we must first find $\mathbf{M}_{ij}(s)$ and $\tilde{\mathbf{Y}}(s)$, which do not depend on the initial condition. For each sample point s and each edge ij we must also calculate $\beta_{ij}(s)$ and $\beta_{ji}(s)$, which capture the effect of the initial condition $q_{ij}(x, 0)$. In particular, we start this subsection by considering the case where the initial condition is

$$q_{ij}(x, 0) = \begin{cases} k & \text{if } \frac{n-1}{N}l_{ij} \leq x < \frac{n}{N}l_{ij} \\ 0 & \text{otherwise,} \end{cases}$$

where $n \leq N$, before moving on to consider the more general case of stepwise constant initial conditions. For the sake of clarity we drop the subscripts ij from l_{ij} , N_{ij} , R_{ij} , α_{ij} , g_{ij} and h_{ij} , and ignore the dependence on s of the terms α_{ij} and h_{ij} . Now, to find a particular solution to the fundamental Equation (2) we use the method of

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variation of parameters. This tells us that

$$f(x, s, q_{ij}(y, 0)) = \frac{e^{(g-h)\frac{x}{l}}}{\alpha} \int_0^x e^{(h-g)\frac{y}{l}} q_{ij}(y, 0) dy - \frac{e^{(g+h)\frac{x}{l}}}{\alpha} \int_0^x e^{-(g+h)\frac{y}{l}} q_{ij}(y, 0) dy. \quad (3)$$

Equation (3) tells us that for the given initial condition

$$\begin{aligned} f(l, s, q_{ij}) &= -\frac{ke^{g+h}}{\alpha} \int_{\frac{n-1}{N}l}^{\frac{n}{N}l} e^{-(g+h)\frac{x}{l}} dx \\ &\quad + \frac{ke^{g-h}}{\alpha} \int_{\frac{n-1}{N}l}^{\frac{n}{N}l} e^{(h-g)\frac{x}{l}} dx, \\ &= \frac{2Dke^{g+h}}{\alpha(u+\alpha)} \left(e^{-\frac{n}{N}(g+h)} - e^{-\frac{(n-1)}{N}(g+h)} \right) \\ &\quad - \frac{2Dke^{g-h}}{\alpha(u-\alpha)} \left(e^{\frac{n}{N}(h-g)} - e^{\frac{(n-1)}{N}(h-g)} \right). \end{aligned} \quad (4)$$

As in the Main Text we let

$$\beta_{ij}(s) \equiv \frac{-\alpha_{ij}(s)e^{-g_{ij}}}{2 \sinh(h_{ij}(s))} f(l, s, q_{ij}(y, 0)). \quad (5)$$

Substituting Equation (4) into Equation (5) gives us

$$\begin{aligned} \beta_{ij}(s) &= \frac{ke^{\frac{1-n}{N}g}}{4(s+R) \sinh(h)} \times \\ &\quad \left[e^{\frac{N-n}{N}h} \left(e^{\frac{h}{N}} - e^{-\frac{g}{N}} \right) (\alpha - u) \right. \\ &\quad \left. + e^{\frac{n-N}{N}h} \left(e^{-\frac{h}{N}} - e^{-\frac{g}{N}} \right) (\alpha + u) \right]. \end{aligned} \quad (6)$$

Recall that $f(x, s, q_1+q_2) = f(x, s, q_1) + f(x, s, q_2)$. Since Equation (5) is linear, it follows that if the initial condition contains several blocks of resource, each block makes its own separate contribution to $\beta_{ij}(s)$ and $\beta_{ji}(s)$. Let $x_0 = 0, x_1 = \frac{l}{N}, x_2 = \frac{2l}{N}, \dots, x_N = l$, and suppose that for all $1 \leq n \leq N$ we have

$$q_{ij}(x, 0) = k_{ij}^{(n)} \quad \text{for all } x_{n-1} < x < x_n. \quad (7)$$

Given such a stepwise constant initial condition, we can calculate $\beta_{ij}(s)$ by summing the contribution of each of the blocks of resource. That is to say, in the case of stepwise constant initial conditions, Equation (6) becomes

$$\begin{aligned} \beta_{ij}(s) &= \sum_{n=1}^N \frac{k_{ij}^{(n)} e^{\frac{1-n}{N}g}}{4(s+R) \sinh(h)} \times \\ &\quad \left[e^{\frac{N-n}{N}h} \left(e^{\frac{h}{N}} - e^{-\frac{g}{N}} \right) (\alpha - u) \right. \\ &\quad \left. + e^{\frac{n-N}{N}h} \left(e^{-\frac{h}{N}} - e^{-\frac{g}{N}} \right) (\alpha + u) \right]. \end{aligned} \quad (8)$$

We can find $\beta_{ji}(s)$ by using the above formula, substituting $-g_{ij}$ for g_{ji} , $-u_{ij}$ for u_{ji} and $k_{ij}^{(N-n+1)}$ for $k_{ji}^{(n)}$. It follows that where $g = g_{ij}$ and $u = u_{ij}$

$$\begin{aligned} \beta_{ji}(s) &= \sum_{n=1}^N \frac{k_{ij}^{(N-n+1)} e^{\frac{n-1}{N}g}}{4(s+R) \sinh(h)} \times \\ &\quad \left[e^{\frac{N-n}{N}h} \left(e^{\frac{h}{N}} - e^{\frac{g}{N}} \right) (\alpha + u) \right. \\ &\quad \left. + e^{\frac{n-N}{N}h} \left(e^{-\frac{h}{N}} - e^{\frac{g}{N}} \right) (\alpha - u) \right]. \end{aligned} \quad (9)$$

B. Resource that leaves its initial edge

If a particle leaves edge ij and reaches node i or j over the relevant time scale, it contributes to $\beta_{ij}(s)$ or $\beta_{ji}(s)$, and hence it contributes to our solution $C_i(s)$, $C_j(s)$ and $\mathcal{L}(\hat{q}_{ij}(x, t)) = \hat{Q}_{ij}(x, s)$. On the other hand, at time 0 none of the resource has reached the nodes, so the initial condition $\hat{q}_{ij}(x, 0) = 0$. It follows that the value of $\hat{Q}_{ij}(x, s)$ is related to the boundary conditions $X_{ij}(s)$ and $X_{ji}(s)$ by the Main Text Equation (MT-18). In other words, we can find $\hat{Q}_{ij}(x, s)$ by effectively considering an initially empty network, where resource is introduced at the nodes at a rate which exactly matches the rate at which resource reaches the nodes in the case where the network has the given non-zero initial condition. The propagation matrix described by Equation (MT-35) also accounts for the impact of any inlet nodes, in the case where resource is being added to the network.

We can therefore use Equations (MT-35), (8) and (9) to find $\bar{C}(s) = \{C_1(s), \dots, C_m(s)\}$, and in the case where the cross-sectional areas are constant, we can express $\hat{Q}_{ij}(x, s)$ in terms of the boundary conditions $X_{ij} = S_{ij}C_i(s)$ and $X_{ji} = S_{ij}C_j(s)$. In fact, we have

$$\begin{aligned} \hat{Q}_{ij}(x, s) &= S_{ij}C_i(s) \frac{\sinh(\frac{l-x}{l}h)}{\sinh(h)} e^{\frac{x}{l}g} \\ &\quad + S_{ij}C_j(s) \frac{\sinh(\frac{x}{l}h)}{\sinh(h)} e^{\frac{x-l}{l}g}, \end{aligned} \quad (10)$$

where the subscripts ij have been omitted for clarity. Since $\mathcal{L}(\int \hat{q}_{ij}(x, t) dx) = \int \hat{Q}_{ij}(x, s) dx$, we can find $\int \hat{q}_{ij}(x, t) dx$ by letting $s = \ln 2/t, \dots, N \ln 2/t$, calculating $\int \hat{Q}_{ij}(x, s) dx$ for each of these values of s , and applying the Gaver-Stehfest algorithm (see Section E).

As in Equation (7), we suppose that edge ij is divided into N_{ij} sections of equal length, and for the sake of clarity we drop the subscripts ij from D_{ij} , l_{ij} and N_{ij} . We let $y_{ij}^{(n)}(t)$ denote the mean value of $\hat{q}_{ij}(x, t)$ in the n th section of edge ij , and note that by definition

$$y_{ij}^{(n)}(t) = \frac{N}{l} \int_{\frac{n-1}{N}l}^{\frac{n}{N}l} \hat{q}_{ij}(x, t) dx. \quad (11)$$

Defining $Y_{ij}^{(n)}(s) \equiv \mathcal{L}(y_{ij}^{(n)}(t))$ we have

$$\begin{aligned} Y_{ij}^{(n)}(s) &= \frac{N}{l} \int_{\frac{n-1}{N}l}^{\frac{n}{N}l} \hat{Q}_{ij}(x, s) dx \\ &= \frac{ND}{l \sinh(h)} \left[\frac{X_{ij}e^h - X_{ji}e^{-g}}{u - \alpha} e^{(g-h)\frac{x}{l}} \right. \\ &\quad \left. + \frac{X_{ji}e^{-g} - X_{ij}e^{-h}}{u + \alpha} e^{(g+h)\frac{x}{l}} \right]_{\frac{n-1}{N}l}^{\frac{n}{N}l}, \end{aligned}$$

which implies that

$$\begin{aligned} Y_{ij}^{(n)}(s) &= \eta_{ij}(s)(\alpha + u) \times \\ &\quad \left[X_{ij} \left(e^{\frac{n-1}{N}(g-h)} - e^{\frac{n}{N}(g-h)} \right) + X_{ji} \times \right. \\ &\quad \left. \left(e^{\frac{n-N}{N}g - \frac{n+N}{N}h} - e^{\frac{n-N-1}{N}g - \frac{n+N-1}{N}h} \right) \right] \\ &+ \eta_{ij}(s)(\alpha - u) \times \\ &\quad \left[X_{ij} \left(e^{\frac{n-1}{N}g - \frac{2N-n+1}{N}h} - e^{\frac{n}{N}g - \frac{2N-n}{N}h} \right) \right. \\ &\quad \left. + X_{ji} \left(e^{\frac{n-N}{N}(g+h)} - e^{\frac{n-N-1}{N}(g+h)} \right) \right], \quad (12) \end{aligned}$$

$$\text{where } \eta_{ij}(s) = \frac{N_{ij}e^{h_{ij}}(s)}{4(s + R_{ij})l_{ij} \sinh(h_{ij}(s))}. \quad (13)$$

C. Resource that remains in its initial edge

Over the time scale t , not all of the resource will leave the edge in which it started. To find $\tilde{q}_{ij}(x, t)$, the quantity of resource that has not left edge ij , we must solve the advection, diffusion, delivery problem for each separate edge ij , where nodes i and j are absorbing boundaries and the initial condition $\tilde{q}_{ij}(x, 0) = q_{ij}(x, 0)$. The resulting solution accounts for those particles which do not reach a node in the relevant time-scale. In particular, we consider the case where the initial condition is stepwise constant, as in Equation (7).

The fundamental Equation (1) tells us that for each edge

$$\frac{\partial}{\partial t} \tilde{q}_{ij} = D_{ij} \frac{\partial^2}{\partial x^2} \tilde{q}_{ij} - u_{ij} \frac{\partial}{\partial x} \tilde{q}_{ij} - R_{ij} \tilde{q}_{ij}. \quad (14)$$

Furthermore, we are looking for a real valued function such that $\tilde{q}_{ij}(0, t) = 0$ and $\tilde{q}_{ij}(l_{ij}, t) = 0$ for all t . These conditions imply that we can express $\tilde{q}_{ij}(x, t)$ in the following form:

$$\begin{aligned} \tilde{q}_{ij}(x, t) &= e^{\frac{u_{ij}}{2D_{ij}}x} \sum_{m=1}^{\infty} A^m e^{\lambda_{ij}^m t} \sin\left(\frac{m\pi x}{l_{ij}}\right), \\ \text{where } \lambda_{ij}^m &= -\left(m^2 \frac{D_{ij}\pi^2}{l_{ij}^2} + \frac{u_{ij}^2}{4D_{ij}} + R_{ij}\right). \quad (15) \end{aligned}$$

The parameters A^m can be found by taking Fourier transforms. More specifically, we know that $\tilde{q}_{ij}(x, 0) = q_{ij}(x, 0)$, so

$$\begin{aligned} \sum_{n=1}^{\infty} A^m \sin\left(\frac{m\pi x}{l_{ij}}\right) &= q_{ij}(x, 0) e^{-g_{ij} \frac{x}{l_{ij}}} \quad \text{and} \\ \int_0^l \sin\left(\frac{m\pi x}{l_{ij}}\right) \sin\left(\frac{n\pi x}{l_{ij}}\right) dx &= \begin{cases} 0 & \text{if } m \neq n, \\ \frac{l_{ij}}{2} & \text{if } m = n. \end{cases} \end{aligned}$$

It follows that for every positive integer m ,

$$A^m = \frac{2}{l_{ij}} \int_0^{l_{ij}} \sin\left(\frac{m\pi x}{l_{ij}}\right) q_{ij}(x, 0) e^{-g_{ij} \frac{x}{l_{ij}}} dx.$$

In particular, consider the case where the initial condition is stepwise constant, and of the form described by Equation (7). Dropping some of the subscripts ij for clarity, we have

$$\begin{aligned} A^m &= \mu_{ij}^m \sum_{n=1}^N k_{ij}^{(n)} \left[e^{-g \frac{x}{l}} \times \right. \\ &\quad \left. \left(\frac{-g}{\pi m} \sin\left(\frac{m\pi x}{l}\right) - \cos\left(\frac{m\pi x}{l}\right) \right) \right]_{\frac{n-1}{N}l}^{\frac{n}{N}l} \\ &= \mu_{ij}^m \left(k_{ij}^{(1)} - k_{ij}^{(N)} e^{-g} (-1)^m \right) \\ &\quad + \mu_{ij}^m \sum_{n=1}^{N-1} \left[e^{-\frac{g}{N}n} \left(k_{ij}^{(n+1)} - k_{ij}^{(n)} \right) \times \right. \\ &\quad \left. \left(\frac{g}{\pi m} \sin\left(\frac{mn\pi}{N}\right) + \cos\left(\frac{mn\pi}{N}\right) \right) \right], \quad (16) \end{aligned}$$

where

$$\mu_{ij}^m = \frac{8D_{ij}^2 \pi m}{u_{ij}^2 l_{ij}^2 + 4D_{ij}^2 \pi^2 m^2}. \quad (17)$$

We are now in a position to find

$$z_{ij}^{(n)}(t) = \frac{N}{l} \int_{\frac{n-1}{N}l}^{\frac{n}{N}l} \tilde{q}_{ij}(x, t) dx,$$

as Equation (15) implies that

$$\begin{aligned} z_{ij}^{(n)}(t) &= \frac{N}{l} \int_{\frac{n-1}{N}l}^{\frac{n}{N}l} e^{\frac{g x}{l}} \sum_{m=1}^{\infty} A^m e^{\lambda_{ij}^m t} \sin\left(\frac{m\pi x}{l}\right) dx \\ &= \frac{N}{2} e^{g \frac{n}{N}} \sum_{m=1}^{\infty} \mu_{ij}^m A^m e^{\lambda_{ij}^m t} \left[\frac{g}{\pi m} \times \right. \\ &\quad \left(\sin\left(\frac{mn\pi}{N}\right) - e^{-\frac{g}{N}} \sin\left(\frac{m(n-1)\pi}{N}\right) \right) \\ &\quad \left. + \left(e^{-\frac{g}{N}} \cos\left(\frac{m(n-1)\pi}{N}\right) - \cos\left(\frac{mn\pi}{N}\right) \right) \right]. \quad (18) \end{aligned}$$

Note that $\mu_{ij}^m \rightarrow \frac{2}{\pi m}$ as $m \rightarrow \infty$, and likewise $A^m \in O(m^{-1})$. In contrast $e^{\lambda_{ij}^m t}$ tends to zero much

more rapidly. Indeed, we note that

$$\begin{aligned} \sum_{m=\Omega'}^{\infty} e^{\lambda_{ij}^m t} &= e^{-\left(\frac{u^2}{4D}+R\right)t} \sum_{m=\Omega'}^{\infty} e^{-\frac{D\pi^2 t}{l^2} m^2} \\ &< \frac{e^{-\left(\frac{u^2}{4D}+R\right)t}}{\Omega'} \int_{\Omega'}^{\infty} x e^{-\frac{D\pi^2 t}{l^2} x^2} dx \\ &< \frac{l^2}{2\Omega'\pi^2 D t} e^{\lambda_{ij}^{\Omega'} t}. \end{aligned} \quad (19)$$

It follows that the relative error

$$\left| \frac{\sum_{m=1}^{\infty} e^{\lambda_{ij}^m t} - \sum_{m=1}^{\Omega'} e^{\lambda_{ij}^m t}}{\sum_{m=1}^{\infty} e^{\lambda_{ij}^m t}} \right| < \frac{\sum_{m=\Omega'}^{\infty} e^{\lambda_{ij}^m t}}{\sum_{m=1}^{\infty} e^{\lambda_{ij}^m t}} < \epsilon$$

whenever we have

$$e^{\lambda_{ij}^{\Omega'} t} < \epsilon \frac{2\Omega'\pi^2 D_{ij} t}{l_{ij}^2} \sum_{m=1}^{\Omega'} e^{\lambda_{ij}^m t}. \quad (20)$$

We can therefore be confident that if we truncate the sum in Equation (18) at $m = \Omega'$, the relative errors in our estimates for $z_{ij}^{(n)}(t)$ will be smaller than ϵ provided that Ω' satisfies Equation (20). Also note that Equation (15) tells us that if $D_{ij} t > l_{ij}^2$ then $e^{\lambda_{ij}^m t}$ decreases rapidly, so Ω' does not need to be large unless $D_{ij} t \ll l_{ij}^2$. Furthermore, if $u_{ij}^2 t^2 > l_{ij}^2$ then most of the resource will leave edge ij over the time scale t , and $\tilde{q}_{ij}(x, t)$ will only make a small contribution to the total value of $q_{ij}(x, t)$.

D. Calculating the total quantity of resource in each segment of a network

Suppose that we wish to calculate the mean concentration per unit length in each segment of a network at time t , such that each part of our final answer has a relative error $\epsilon < 10^{-0.45\Omega}$, where Ω is an even integer. The first step is to set $s = \Omega \ln 2/t$, and apply Equations (8) and (9) to find $\beta_{ij}(s)$ and $\beta_{ji}(s)$ for each edge ij . We then compute $\mathbf{M}(s)$ and $\bar{p}(s)$, and employ the BiCGStab algorithm to find $\bar{C}(s_{\Omega})$, starting with the initial guess that for each i ,

$$C_i(s_{\Omega}) \approx \frac{\tau}{\Omega \ln 2} c_i(0) = \frac{\tau}{\Omega \ln 2} \frac{\sum_j k_{ij}^{(1)}}{\sum_j S_{ij}(0)}. \quad (21)$$

This initial guess for the value of $\bar{C}(s_{\Omega})$ would be correct if the concentration at the nodes was constant, and making such a guess can help to speed up the process of finding the true value of $\bar{C}(s_{\Omega})$. At each step, when we have identified $\bar{C}(s)$ such that $\mathbf{M}(s)\bar{C}(s) = \bar{p}(s)$, we store the vector $\bar{C}(s)$ and repeat for $s = s_{\Omega-1}, \dots, s_1$, where $s_n = n \ln 2/t$. The only difference is that for subsequent applications of the BiCGStab algorithm, we can take advantage of the approximation

$$C_i(s_n) \approx \frac{n+1}{n} C_i(s_{n+1}). \quad (22)$$

This is generally a better initial guess than that provided by Equation (21), so the BiCGStab algorithm converges on the solution more rapidly. Given $C_i(s_n)$ and $C_j(s_n)$, we can use Equation (12) to calculate $Y_{ij}^{(m)}(s_n)$ for each section in the edge ij . Having found $Y_{ij}^{(m)}(s_n)$ for each $1 \leq n \leq \Omega$, we can apply the Gaver-Stehfest algorithm to obtain $y_{ij}^{(m)}(t)$ (see Section E), and we repeat this process for each edge in the network.

Finally, for each edge ij we can use Equations (15), (17) and (16) to calculate a sequence of values for $e^{\lambda_{ij}^m t}$, μ_{ij}^m and A^m until we reach an integer Ω' such that $e^{\lambda_{ij}^{\Omega'} t}$ satisfies Equation (20). We then employ Equation (18) to find $z_{ij}^{(1)}(t), \dots, z_{ij}^{(N_{ij})}(t)$ (the mean quantity of resource in ij that has not reached a node), and note that for each section of the network the mean quantity of resource per unit length

$$k_{ij}^{(n)}(t) = y_{ij}^{(n)}(t) + z_{ij}^{(n)}(t). \quad (23)$$

E. Inverting from Laplace space

We have seen that we can calculate a sequence of real valued sample points in Laplace space, and we wish to calculate the corresponding value at a given point in time. Under these circumstances it is appropriate and efficient to apply the Gaver-Stehfest algorithm [1–6]. The key idea behind this algorithm (and other, related algorithms) is the notion of constructing a sequence of linear combinations of exponential functions, in order to form a weighted delta convergent sequence [1–6]. That is to say, we consider a sequence of functions $\delta_n(x, t)$ such that for any function q that is continuous at t , we have

$$\int_0^{\infty} \delta_n(v, t) q(v) dv = t \tilde{q}_n(t), \quad (24)$$

where $\tilde{q}_n(t) \rightarrow q(t)$ as $n \rightarrow \infty$. As we shall see, there are weighted delta convergent sequences of functions such that $\delta_n(v, t)$ is of the form

$$\delta_n(v, t) = \sum_{i=1}^n \omega_i e^{-\frac{\theta_i v}{t}}, \quad (25)$$

where $\theta_i > 0$ for all i , and the terms θ_i and ω_i do not depend on t . Now, if we suppose that our function q does not increase exponentially, then the Laplace transform $Q(s) = \int_0^{\infty} e^{-sv} q(v) dv$ is well defined for all positive numbers s . Hence the existence of $Q(s)$ for all positive s is a reasonable assumption, given the context in which our functions q arise. Assuming that $Q(s)$ is well defined for all positive numbers s , Equations (24) and (25) imply that

$$\begin{aligned} \tilde{q}_n(t) &= \frac{1}{t} \int_0^{\infty} \sum_{i=1}^n \omega_i e^{-\frac{\theta_i v}{t}} q(v) dv \\ &= \frac{1}{t} \sum_{i=1}^n \omega_i Q\left(\frac{\theta_i}{t}\right). \end{aligned}$$

Gaver [7] employed the sequence of functions

$$\delta_n(v, t) = \ln 2 \frac{(2n)!}{n!(n-1)!} (1 - e^{-\frac{v \ln 2}{t}})^n (e^{-\frac{v \ln 2}{t}})^n,$$

but the resulting terms $\tilde{q}^n(t)$ converge to $q(t)$ logarithmically slowly. Gaver also showed that the quantity $\tilde{q}^n(t) - q(t)$ can be expanded in terms of inverse powers of n , which enabled him to accelerate the convergence of his original sequence of approximations [7]. The most useful formula for finding an accurate estimate of $q(t)$ based on a linear combination of the Gaver estimates was derived by Stehfest [4], who stated that

$$q(t) \approx \tilde{q}_\Omega(t) = \frac{\ln 2}{t} \sum_{n=1}^{\Omega} \kappa_n Q\left(n \frac{\ln 2}{t}\right), \quad \text{where} \quad (26)$$

$$\kappa_n = (-1)^{n+\Omega/2} \sum_{k=\lceil(n+1)/2\rceil}^{\min(n, \Omega/2)} \frac{k^{\Omega/2} (2k)!}{(\Omega/2 - k)! k! (n - k)! (2k - n)!},$$

and Ω is even. Note that the terms κ_n can be extremely large, and that the value of κ_n depends on the parameter Ω . Furthermore, increasing the parameter Ω increases the accuracy of our estimate $q(t) \approx \tilde{q}_\Omega(t)$, provided that

we have sufficient system precision to utilize the exact values for κ_n .

The Gaver-Stehfest algorithm is very efficient and accurate, but it requires high system precision for the weights κ_n if it is to yield accurate estimates for $q(t)$. Indeed, if we wish to produce an estimate of $q(t)$ that is accurate to N significant digits, we must calculate the values of κ_n with an accuracy of about $2.5N$ significant digits [1, 2]. Fortunately, to calculate $q(t)$ accurately we do not require such a disproportionately high level of accuracy in the values of $Q(s)$.

If the transform $Q(s)$ has all its singularities on the negative real axis, and if the function $q(t)$ is infinitely differentiable for all $t > 0$, extensive experimentation [1, 2] indicates that the relative error

$$\left| \frac{q(t) - \tilde{q}_\Omega(t)}{q(t)} \right| \approx 10^{-0.45\Omega} \quad (27)$$

provided that the values κ_n have been calculated with sufficient precision [1, 2]. If the function q does not satisfy the above conditions $\tilde{q}_\Omega(t)$ may converge to $q(t)$ rather more slowly, but as a rule of thumb setting $\Omega = 10$ and using standard double precision for the weights κ_n will ensure that the Gaver-Stehfest algorithm produces inversions that are accurate to at least three significant digits.

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