Optimal Control of Transitions between Nonequilibrium Steady States

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$$\dot{x} = -\frac{k(t)}{\gamma} x + \eta(t)$$

When $k(t)$ is held fixed, a straightforward application of variational calculus demonstrates that a straight-line protocol in $v(t)$ is *exactly* optimal and agrees with the predictions of the linear response approximation [Eq. (4)]. In Ref. [11], the average Y-value was measured for three distinct experimental trials involving protocols with constant k. As summarized in Fig. 2, the optimal protocol, namely the naive straight line in the case of constant k, shows significantly reduced Y-value compared with the protocols used in each experimental trial. However, in terms of testing the performance of the optimal protocols [Eq. (8)], $k_f \neq k_i$ is the more general case.

As in the case of finding globally optimal protocols, the problem of finding optimal straight line protocols simplifies dramatically in $(\xi, \ )$ coordinates. Using Eq. (7), we find.

$$< Y >_{\Lambda} \approx \beta\gamma^3 \ {}_0^{\tau} dt[1+b^2 \ {}^2(t)]\left(\frac{d}{dt}\right)^2, \qquad (9)$$

for

$$b \equiv 2\beta\gamma^2 \frac{k_f v_i - k_i v_f}{k_f - k_i} \qquad (10)$$

The Euler-Lagrange equation implies

$$\frac{d}{dt} = \frac{\frac{1}{\tau} \ {}_0^{f} dz \quad 1+b^2 z^2}{1+b^2 \ {}^2(t)}, \qquad (11)$$

which determines an implicit expression for (t):

$$2b\left(\frac{t}{\tau}\right) \ {}_0^{f} dz \quad 1+b^2z^2 = b(\ (t) \quad 1+b^2 \ {}^2(t)$$

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Furthermore, the relatively simple model system we treat in this manuscript represents a new frontier for the analytical solution of optimal protocols under the inverse diffusion tensor approximation. For significantly more complicated models of greater biological interest, a simple general approach (in lieu of a search for an analytical solution) would be a fully numerical method, involving the calculation of the inverse diffusion tensor at a grid of points in control parameter space, analogous to the approach in [19].

Finally, there remains the important open question of what quantity or quantities are to be optimized in faithful models of biological processes. In this paper, we made the choice of optimizing the Y-value which has been experimentally studied in this particular model system [11] and may be optimized by the same geometric framework as in [4]. These qualities were advantageous to begin a clear and mathematically tractable first step towards optimization of steady state transitions.

However, it is possible and perhaps likely that a properly defined average dissipated heat will be the biologically relevant quantity to optimize rather than the Y-value. We anticipate that a geometric approach to optimization will be applicable to these more general systems and notions of heat production in a relevant regime of parameter values and protocol durations. However, a

The line element corresponding to the metric in Eq. (27) is

$$ds^2 = \frac{\gamma}{4k^4} \quad k + 4\beta(\gamma v)^2 \quad dk^2 - 2\beta v\left(\frac{\gamma}{k}\right)^3 dk\ dv + \beta\frac{\gamma^3}{k^2}dv^2. \quad (28)$$

To find the explicit coordinate transformation making the Euclidean geometry manifest, we write the line element as

$$ds^2 = \beta\gamma^3\{[d\left(\frac{v}{k}\right)]^2 + (\frac{dk}{2\sqrt{\beta\gamma}k^{\frac{3}{2}}})^2\} \quad (29)$$

This suggests the coordinate transformation $\xi = \frac{v}{k}$, $\quad = \frac{1}{\gamma\sqrt{\beta k}}$, so that

$$ds^2 = \beta\gamma^3(d\xi^2 + d\quad^2). \quad (30)$$

In this coordinate system, geodesics are straight lines of constant speed. To find optimal protocols in (k,v) space, one simply transforms the coordinates of the endpoints into $(\xi,\ )$ space, connects these points by a straight line, and uses the inverse transformation to map the line onto a curve in (k,v) space. This follows from the invariance of the geodesic equation [16]. Explicitly, the optimal protocol joining (k_i,v_i) and (k_f,v_f) is

$$k(t) = [\frac{1}{\sqrt{k_i}}(1-T) + \frac{1}{\quad k_f}T]^{-2}, \quad (31\ )$$

$$v(t) = k(t)[\frac{v_i}{k_i}(1-T) + T\frac{v_f}{k_f}], \quad (31b\ )$$

where $T = \frac{t}{\tau}$.

We validate the optimality of the geodesics [Eq. (31)] numerically via the Fokker-Planck equation [12],

$$\frac{\partial}{\partial t} = \frac{k(t)}{\gamma}\frac{\partial}{\partial x}(x\quad) + v(t)\frac{\partial}{\partial x} + \frac{1}{\beta\gamma}\frac{\partial^2}{\partial x^2} \quad (32)$$

In full generality, the mean Y-value as a functional of the protocol $\ (t) = (k(t),v(t))$ is

$$_0^{\tau} dt[-\frac{\dot{k}}{2k} - \frac{\beta}{2}\left(\frac{\gamma v}{k}\right)^2\dot{k} + \frac{\beta}{2}\dot{k}\langle x^2\rangle_{\Lambda} + \beta\gamma\dot{v}\langle x\rangle_{\Lambda} + \beta\gamma^2\frac{v}{k}\dot{v}] \quad (33)$$

Here angled brackets denote averages over the nonequilibrium probability density $\ (x,t)$.

By integrating Eq. (32) against x and x^2, we find a system of equations for relevant nonequilibrium averages:

$$\frac{d}{dt}\langle x\rangle_{\Lambda} = -\frac{k(t)}{\gamma}\langle x\rangle_{\Lambda} - v(t), \quad (34\ )$$

$$\frac{d}{dt}\langle x^2\rangle_{\Lambda} = -\frac{2k(t)}{\gamma}\langle x^2$$