1 Local expansion of the fitness surface

Suppose that $\rho(t) \geq 0$ is a weighting function on $[0, \infty)$ so that fitness is a function of $L^2(\rho)$ distance of the impulse response from optimal. With $h_0(t) = C_0 e^{tA_0} B_0$ a representative of the optimal set:

$$\begin{aligned} D(A,B,C)^2 &:= \int_0^\infty \rho(t) \left| h_A(t) - h_0(t) \right|^2 dt \\ &:= \int_0^\infty \rho(t) \left| C e^{At} B - C_0 e^{A_0 t} B_0 \right|^2 dt \\ &= \int_0^\infty \rho(t) \operatorname{tr} \left\{ \left(C e^{At} B - C_0 e^{A_0 t} B_0 \right)^T \left(C e^{At} B - C_0 e^{A_0 t} B_0 \right) \right\} dt \\ &= \int_0^\infty \rho(t) \operatorname{tr} \left\{ \left(C e^{At} B - C_0 e^{A_0 t} B_0 \right) \left(C e^{At} B - C_0 e^{A_0 t} B_0 \right)^T \right\} dt, \end{aligned} \tag{1}$$

where $\operatorname{tr} X$ denotes the trace of a square matrix X. How does this change as we perturb about (A_0, B_0, C_0)? First we differentiate with respect to A, keeping $B = B_0$ and $C = C_0$ fixed. Since

$$\frac{d}{du} e^{(A+uZ)t} |_{u=0} = \int_0^t e^{As} Z e^{A(t-s)} ds, \tag{2}$$

we have that

$$\begin{aligned} \frac{d}{du} D(A+uZ, B_0, C_0)^2 |_{u=0} &= 2 \int_0^\infty \rho(t) \operatorname{tr} \left\{ C_0 \left(\int_0^t e^{As} Z e^{A(t-s)} ds \right) B_0 B_0^T \left(e^{At} - e^{A_0 t} \right)^T C_0^T \right\} dt \\ &= 2 \int_0^\infty \rho(t) \operatorname{tr} \left\{ C_0 \left(\int_0^t e^{As} Z e^{A(t-s)} ds \right) B_0 \left(h_A(t) - h_0(t) \right)^T \right\} dt \end{aligned} \tag{3}$$

and, by differentiating this and supposing that A is on the optimal set, i.e., $h_A(t) = h_0(t)$, (so without loss of generality, $A = A_0$):

$$\begin{aligned} \mathcal{H}^{A,A}(Y,Z) &:= \frac{1}{2} \frac{d}{du} \frac{d}{dv} D(A_0 + uY + vZ, B_0, C_0)^2 |_{u=v=0} \\ &= \int_0^\infty \rho(t) \operatorname{tr} \left\{ C_0 \left(\int_0^t e^{A_0 s} Y e^{A_0 (t-s)} ds \right) B_0 B_0^T \left(\int_0^t e^{A_0 s} Z e^{A_0 (t-s)} ds \right)^T C_0^T \right\} dt. \end{aligned} \tag{4}$$

The function $\mathcal{H}$ will define a quadratic form. To illustrate the use of this, suppose that B and C are fixed. By defining Δ_{ij} to be the matrix with a 1 in the (i,j)th slot and 0 elsewhere, the coefficients of the quadratic form is

$$H_{ij,k\ell}(A) := \mathcal{H}(\Delta_{ij}, \Delta_{k\ell}). \tag{5}$$

We could use this to get the quadratic approximation to D near the optimal set. To do so, it'd be nice to have a way to compute the inner integral above. Suppose that we diagonalize $A = U \Lambda U^{-1}$. Then

$$\int_0^t e^{As} Z e^{A(t-s)} ds = \int_0^t U e^{\Lambda s} U^{-1} Z U e^{\Lambda (t-s)} U^{-1} ds \tag{6}$$

Now, notice that

$$\begin{aligned} \int_0^t e^{s\lambda_i} e^{(t-s)\lambda_j} ds &= \frac{e^{t\lambda_i} - e^{t\lambda_j}}{\lambda_i - \lambda_j} && \text{if} \quad i \neq j \\ &= t e^{t\lambda_i} && \text{if} \quad i = j \end{aligned} \tag{7}$$

Therefore, defining

$$\begin{aligned} X_{ij}(t,Z) &= \left(U^{-1} Z U \right)_{ij} \frac{e^{t\lambda_i} - e^{t\lambda_j}}{\lambda_i - \lambda_j} && \text{if} \quad i \neq j \\ &= \left(U^{-1} Z U \right)_{ii} t e^{t\lambda_i} && \text{if} \quad i = j \end{aligned} \tag{8}$$

moving the U and U^{-1} outside the integral and integrating we get that

$$\int_0^t e^{As} Z e^{A(t-s)} ds = UX(t,Z)U^{-1}. \tag{9}$$

This implies that

$$D(A_0 + \epsilon Z)^2 \approx \frac{1}{2}\epsilon^2 \int_0^\infty \rho(t) \operatorname{tr}\left\{CUX(t,Z)U^{-1}BB^T(U^{-1})^T X(t,Z)^T U^T C^T\right\} dt. \tag{10}$$

To compute the $n^2 \times n^2$ matrix H, we see that if $Z = \Delta_{k\ell}$, then

$$\begin{aligned} X_{ij}^{k\ell}(t) &= (U^{-1})_{\cdot k} U_{\ell \cdot} \frac{e^{t\lambda_i} - e^{t\lambda_j}}{\lambda_i - \lambda_j} && \text{if} \quad i \neq j \\ &= (U^{-1})_{\cdot k} U_{\ell \cdot} t e^{t\lambda_i} && \text{if} \quad i = j \end{aligned} \tag{11}$$

where $U_{k\cdot}$ is the kth row of U, and so

$$H_{ij,k\ell}(A) = \int_0^\infty \rho(t) \operatorname{tr}\left\{CUX^{ij}(t)U^{-1}BB^T(U^{-1})^T X^{k\ell}(t)^T U^T C^T\right\} dt. \tag{12}$$

This implies that

$$D(A_0 + \epsilon Z)^2 \approx \frac{1}{2}\epsilon^2 \sum_{ijk\ell} H_{ij,k\ell}(A_0) Z_{ij} Z_{k\ell}. \tag{13}$$

By section **??**, if we set $\Sigma = \sigma^2 I$ and $U = H$, then a population at $A_0 + Z$ experiences a restoring force of strength $(I + \sigma^2 H^{-1})^{-1} Z$ (treating Z as a vector and H as an operator on these). If σ^2 is small compared to H^{-1} then this is approximately $-\sigma^2 H^{-1} Z$. This suggests that the population mean follows an Ornstein-Uhlenbeck process, as described (in different terms) in Hansen and Martins [1996].

More generally, B and C may also change. To extend this we need the remaining second derivatives of D^2. First, in B:

$$\begin{aligned} \mathcal{H}^{B,B}(Y,Z) &:= \frac{1}{2}\frac{d}{du}\frac{d}{dv} D(A_0, B_0 + uY + vZ, C_0)|_{u=v=0} \\ &= \frac{1}{2}\int_0^\infty \rho(t) \operatorname{tr}\left\{C_0 e^{tA_0} \frac{d}{du}\frac{d}{dv}(uY + vZ)(uY + vZ)^T|_{u=v=0} e^{tA_0^T} C_0^T\right\} dt \\ &= \frac{1}{2}\int_0^\infty \rho(t) \operatorname{tr}\left\{C_0 e^{tA_0} \left(YZ^T + ZY^T\right) e^{tA_0^T} C_0^T\right\} dt. \end{aligned} \tag{14}$$

Next, in C:

$$\begin{aligned} \mathcal{H}^{B,B}(Y,Z) &:= \frac{1}{2}\frac{d}{du}\frac{d}{dv} D(A_0, B_0, C_0 + uY + vZ)|_{u=v=0} \\ &= \frac{1}{2}\int_0^\infty \rho(t) \operatorname{tr}\left\{B_0 e^{tA_0^T} \frac{d}{du}\frac{d}{dv}(uY + vZ)^T(uY + vZ)|_{u=v=0} e^{tA_0} B_0\right\} dt \\ &= \frac{1}{2}\int_0^\infty \rho(t) \operatorname{tr}\left\{B_0 e^{tA_0^T} \left(YZ^T + ZY^T\right) e^{tA_0} B_0\right\} dt. \end{aligned} \tag{15}$$

Now, the mixed derivatives in B and C:

$$\begin{aligned} \mathcal{H}^{B,C}(Y,Z) &:= \frac{1}{2}\frac{d}{du}\frac{d}{dv} D(A_0, B_0 + uY, C_0 + vZ)|_{u=v=0} \\ &= \int_0^\infty \rho(t) \operatorname{tr}\left\{Y e^{tA_0^T} C_0^T Z e^{tA_0} B_0\right\} dt. \end{aligned} \tag{16}$$

In A and B

$$\begin{aligned}\mathcal{H}^{A,B}(Y,Z) &:= \frac{1}{2}\frac{d}{du}\frac{d}{dv}D(A_0+uY,B_0+vZ,C_0)|_{u=v=0} \\ &= \int_0^\infty \rho(t)\,\mathrm{tr}\left\{C_0\left(\int_0^t e^{sA_0}Ye^{(t-s)A_0}ds\right)B_0Z^Te^{tA_0}C_0\right\}dt,\end{aligned} \tag{17}$$

and finally in A and C:

$$\begin{aligned}\mathcal{H}^{A,C}(Y,Z) &:= \frac{1}{2}\frac{d}{du}\frac{d}{dv}D(A_0+uY,B_0,C_0+vZ)|_{u=v=0} \\ &= \int_0^\infty \rho(t)\,\mathrm{tr}\left\{C_0\left(\int_0^t e^{sA_0}Ye^{(t-s)A_0}ds\right)B_0B_0e^{tA_0}Z\right\}dt.\end{aligned} \tag{18}$$

Together, numerical computation of these expressions, along with estimates of genetic covariance within a population, allow precise predictions of evolutionary dynamics of a particular system. The approximation should be good as long as the second-order Taylor approximation holds.

References

Thomas F. Hansen and Emilia P. Martins. Translating between microevolutionary process and macroevolutionary patterns: The correlation structure of interspecific data. *Evolution*, 50(4):1404–1417, 1996. ISSN 00143820, 15585646. URL http://www.jstor.org/stable/2410878.