

Lecture 15

Phenotypic Evolution Models

Bruce Walsh. jbwalsh@u.arizona.edu. University of Arizona.

Notes from a short course taught June 2006 at University of Aarhus

The notes for this lecture were last corrected on 24 June 2006. Please email me any errors.

Quantitative-genetic models are often applied to problems in ecology and evolution, for example to model trait evolution under sexual selection, the evolution of life history traits, or long term evolution using species data from the fossil record. Such models, wherein the only genetic details appear through an initial covariance matrix, are often called **phenotypic evolution models**, as their main focus is to follow changes in the phenotypic mean. Provided we are willing to assume the distribution of phenotypes and breeding values remains multivariate normal, we can also follow changes in the covariance matrix as well.

This Lecture concludes our discussion of selection. We start with several univariate (single trait) examples before moving to a general discussion of the features of the multivariate model under general gaussian fitness functions. We conclude by reviewing vector calculus and matrix derivatives, applying this machinery to prove several previous results as well as a few key evolutionary theorems.

UNIVARIATE GAUSSIAN FITNESS FUNCTIONS

Response Under Normalizing Selection

While double-truncation is the common model of artificial stabilizing selection, the standard model for stabilizing selection in natural populations is to assume **normalizing** (or **nor-optimal**) selection (Weldon 1895, Haldane 1954),

$$W(z) = \exp\left(-\frac{(z-\theta)^2}{2\omega}\right) \quad (15.1)$$

The optimal value is $z = \theta$, and the strength of selection is given by ω . If $\omega \gg \sigma^2$, fitness falls off slowly and selection is weak, while if $\omega \ll \sigma^2$ selection is strong. If phenotypes are normally distributed before selection with mean μ and variance σ^2 , after selection phenotypes remain normally distributed with new mean and variance

$$\mu^* = \mu + \frac{\sigma^2}{\sigma^2 + \omega}(\theta - \mu) \quad \text{and} \quad \sigma_*^2 = \sigma^2 - \frac{\sigma^4}{\sigma^2 + \omega} \quad (15.2a)$$

This follows as a special case of the general Gaussian fitness function, which we examine shortly. Note that we cannot write $\sigma_*^2 = \kappa \sigma^2$ (as we did in Lecture 9 to obtain simpler expressions for the change in variance), as here κ is no longer a constant, but rather a function of σ^2 . However, under this model the distribution of genotypes remains normal after selection and hence parent-offspring regressions remain linear throughout. Thus, we can apply the breeders' equation to predict changes in the mean and Equation 9.38a to predict changes in the variance (under the infinitesimal model). Here,

$$S = \frac{\sigma^2}{\sigma^2 + \omega}(\theta - \mu) \quad \text{and} \quad \delta(\sigma_{z^*}^2) = -\frac{\sigma^4}{\sigma^2 + \omega} \quad (15.2b)$$

Note that the change in variance is independent of μ . The change in mean is thus given by

$$R(t) = h^2(t) S(t) = h^2(t) \frac{\sigma_z^2(t) [\theta - \mu(t)]}{\sigma_z^2(t) + \omega} \quad (15.3)$$

implying that the mean converges to θ . From Equation 9.38a, the change in the disequilibrium contribution is given by

$$d(t+1) = \frac{d(t)}{2} - \frac{h^4(t)}{2} \frac{\sigma_z^4(t)}{\sigma_z^2(t) + \omega} = \frac{d(t)}{2} - \frac{1}{2} \left[\frac{(\sigma_a^2 + d_t)^2}{\sigma_z^2 + d(t) + \omega} \right] \quad (15.4)$$

Note that both directional and stabilizing selection can simultaneously occur with normalizing selection — if $\mu \neq \theta$, the mean also changes under selection. The change in mean is given by the breeders equation with the appropriate heritability, the change in variance is obtained from the change in the disequilibrium contribution.

Example 15.1. Suppose normalizing selection occurs on a normally distributed character with $\sigma_z^2 = 100$, $h^2 = 0.5$, and $\omega = 200$. The dynamics of the disequilibrium contribution follow

$$d(t+1) = \frac{d(t)}{2} - \frac{1}{2} \frac{(50 + d(t))^2}{300 + d(t)}$$

implying at equilibrium that $d(t+1) = d(t) = \tilde{d}$, giving

$$\tilde{d}(\sigma_z^2 + \tilde{d} + \omega) + (\sigma_A^2 + \tilde{d})^2 = \tilde{d}(300 + \tilde{d}) + (\tilde{d} + 50)^2 = 0$$

solving this quadratic equation gives $\tilde{d} = -6.46$, hence $\tilde{h}^2 = (50 - 6.46)/(100 - 6.46) = 0.465$. Most of this reduction in heritability occurs in the first few generations.

Generation	0	1	2	3	4	5	∞
d_t	0	-4.17	-5.64	-6.16	-6.35	-6.42	-6.46
$\sigma_A^2(t)$	50.00	45.83	44.37	43.84	43.65	43.58	43.54
$h^2(t)$	0.50	0.48	0.47	0.47	0.47	0.47	0.47

Thus, under the infinitesimal model, the distribution reaches equilibrium with the phenotypes (before selection) normally distributed with mean θ and variance $\tilde{\sigma}_z^2 = 100 - 6.46 = 93.54$.

Application: Charlesworth's Model of the Cost of Phenotypic Selection

Evolutionary biologists are often obsessed with the **substitutional load**, essentially the *cost* of evolution — what fraction of the population must be eliminated by selection each generation in order to account for a given rate of evolution. To quote Charlesworth (1984)

"It would obviously be a serious embarrassment to neo-Darwinists if these loads turned out to be so high as to be incompatible with the survival of the species"

Charlesworth examined the cost of selection on a phenotypic trait by assuming a Gaussian fitness function (Equation 15.1) with $\theta = 0$. Departures from $\mu = 0$ result in directional selection, while stabilizing selection is occurring even when $\mu = 0$. With this fitness function, the mean fitness is easily computed (see below for the multivariate case) to be

$$\bar{W} = \frac{\omega}{\sqrt{\sigma_z^2 + \omega}} \exp\left(-\frac{\mu^2}{2(\sigma_z^2 + \omega)}\right) \quad (15.5)$$

We can also write this in a slightly different form, by recalling Equation 15.2b,

$$S = -\frac{\sigma_z^2 \mu}{\sigma_z^2 + \omega}, \quad \text{so that} \quad i^2 = \frac{S^2}{\sigma_z^2} = \frac{\sigma_z^2 \mu^2}{(\sigma_z^2 + \omega)^2} \quad (15.6a)$$

where i is the selection intensity. Substituting Equation 15.6a into 15.5 gives

$$\bar{W} = \frac{\omega}{\sqrt{\sigma_z^2 + \omega}} \exp\left(-i^2 \frac{(\sigma_z^2 + \omega)}{2\sigma_z^2}\right) \quad (15.6b)$$

The total load L is

$$L = 1 - \bar{W} = 1 - \frac{\omega}{\sqrt{\sigma_z^2 + \omega}} \exp\left(-i^2 \frac{(\sigma_z^2 + \omega)}{2\sigma_z^2}\right) \quad (15.7a)$$

Charlesworth partitioned the total load as $L = L_s + L_d$, with a load contribution from direction selection L_d and a load contribution L_s from stabilizing selection. Note that if $\mu = 0$ (population at the optimum), all of the selection is due to stabilizing selection, and the resulting load is

$$L_s = 1 - \sqrt{\frac{\omega}{\sigma_z^2 + \omega}} \quad (15.7b)$$

The directional selection load is given by $L - L_s$, the total load minus the stabilizing selection load, or

$$L_d = \sqrt{\frac{\omega}{\sigma_z^2 + \omega}} \left(1 - \exp\left[-i^2 \frac{(\sigma_z^2 + \omega)}{2\sigma_z^2}\right]\right) \quad (15.7c)$$

If the term in the exponent is small, using $\exp(-x) \simeq 1 - x$ gives

$$L_d \simeq \frac{i^2}{2} \sqrt{\frac{\omega(\sigma_z^2 + \omega)}{\sigma_z^4}} \quad (15.7d)$$

We often expect the selection intensity to vary. In this case, since $E[i^2] = \bar{i}^2 + \sigma_i^2$, where σ_i^2 is the variance in selection intensity, Equation 15.7d becomes

$$L_d \simeq \frac{\bar{i}^2 + \sigma_i^2}{2} \sqrt{\frac{\omega(\sigma_z^2 + \omega)}{\sigma_z^4}} \quad (15.7e)$$

Charlesworth noted that many of the parameters in Equation 15.7e can be estimated from a fossil sequence. Letting $\Delta\mu$ and $\sigma^2(\Delta\mu)$ be the mean and variance of the observed rate of change per generation, then

$$E(i) = \bar{i} = \frac{E[R]}{h^2\sigma_z} = \frac{\Delta\mu}{h^2\sigma_z}, \quad \text{implying} \quad \bar{i}^2 = \frac{(\Delta\mu)^2}{h^4\sigma_z^2} \quad (15.8a)$$

and likewise

$$\sigma_i^2 = \frac{\sigma^2(R)}{h^4\sigma_z^2} = \frac{\sigma^2(\Delta\mu)}{h^4\sigma_z^2} \quad (15.8b)$$

Thus for fossil data (which gives us σ_z^2 , $\Delta\mu$, and $\sigma^2(\Delta\mu)$) we can compute the directional and stabilizing load for various values of h^2 and strength of stabilizing selection ω/σ_z^2 , as the expected directional and stabilizing load can be estimated as

$$E[L_d] \simeq \frac{(\Delta\mu)^2 + \sigma^2(\Delta\mu)}{2h^4\sigma_z^2} \sqrt{\frac{\omega}{\sigma_z^2} \left(1 + \frac{\omega}{\sigma_z^2}\right)} \quad (15.9a)$$

and

$$E[L_s] \simeq 1 - \sqrt{\frac{\omega/\sigma_z^2}{1 + \omega/\sigma_z^2}} \quad (15.9b)$$

Example 15.2. As an example of computing a load, consider thoracic width in the radiolarian *Pseudocubus verma*. Here $\Delta\mu = 0.169 \times 10^{-7}$, $\sigma^2(\Delta\mu) = 2 \times 10^{-10}$, and $\sigma_z = 0.1217$. Taking $h^2 = 0.5$, then the estimated loads (under various assumptions about the strength ω/σ_z^2 of stabilizing selection) are as follows:

ω/σ_z^2	L_d	L_s
100	$1.84 \cdot 10^{-4}$	$4.96 \cdot 10^{-3}$
50	$9.20 \cdot 10^{-6}$	$9.85 \cdot 10^{-3}$
10	$1.91 \cdot 10^{-5}$	$4.66 \cdot 10^{-2}$
5	$1.00 \cdot 10^{-5}$	$8.71 \cdot 10^{-2}$
2	$4.47 \cdot 10^{-6}$	0.184

While the stabilizing load may be considerable (for example if $\omega/\sigma_z^2 = 5$, 8.7% of the population is culled each generation by stabilizing selection). However, for all of the hypothesized ω/σ_z^2 values, the directional selection load is extremely small. Hence directional selection is not a major burden for this species.

Application: Drift vs. Selection in the Fossil Record

In a classic paper, Lande (1976) looked at divergence in the fossil record, asking if the observed amount of divergence was more consistent with drift or selection. Recall (Lecture 7) that we previously developed tests for whether an observed long-term pattern was either too fast or too slow to be accounted for by drift alone. As promised in that Lecture, we now turn to asking how much selection is required to generate the observed pattern.

Lande assumed truncation selection, with individuals b standard deviations above the mean being culled. This is a model of weak selection, and Lande's question was what value of b can account for the observed pattern. Recalling Equation 1.12a, we can show that the population mean after selection becomes

$$\mu_* = \mu - \frac{\sigma_z}{\sqrt{2\pi}} \exp(-b^2/2) \quad (15.10a)$$

giving the selection differential as

$$S = -\frac{\sigma_z}{\sqrt{2\pi}} \exp(-b^2/2) \quad (15.10b)$$

Note that if $b < 0$, then truncation is on the smallest individuals and response increases the mean. Assuming heritability remains largely unchanged, the absolute value of the expected response over t generations is given by

$$|\mu_t - \mu| = \frac{th^2\sigma_z}{\sqrt{2\pi}} \exp(-b^2/2) \quad (15.10c)$$

Solving for b gives

$$|\hat{b}| = \sqrt{-2 \ln \left(\frac{\sqrt{2\pi} |\mu_t - \mu|}{\sigma_z h^2 t} \right)} = \sqrt{-2 \ln \left(\frac{\sqrt{2\pi}}{h^2 t} d \right)} \quad (15.11)$$

where $d = |\mu_t - \mu|/\sigma_z$ is the total divergence, expressed in units of phenotypic standard deviations.

Example 15.3. Once again, let's return to Reyment's foraminifer data (Examples 7.10 and 7.11). Here $d = 1.49$, $t = 5 \times 10^5$ generations, and we assume $h^2 = 0.3$, giving

$$b = \sqrt{-2 \ln \left(\frac{\sqrt{2\pi}}{0.3 \cdot 5 \times 10^5} 1.49 \right)} = 4.60$$

For a unit normal, $\Pr(U > 4.6) = 2.067 \times 10^{-6}$. Hence, each generation only removing two out of every million is sufficient selection to generate the observed change.

MULTIVARIATE GAUSSIAN FITNESS FUNCTIONS

Selection generally introduces non-normality even if the initial distribution is Gaussian. Ideally, we would like to have a class of fitness functions that allows us to model any combination of directional, convex, concave, and correlational selection and yet still preserves normality. The **Gaussian fitness function**,

$$\begin{aligned} W(\mathbf{z}) &= \exp\left(\boldsymbol{\alpha}^T \mathbf{z} - \frac{1}{2}(\mathbf{z} - \boldsymbol{\theta})^T \mathbf{W}(\mathbf{z} - \boldsymbol{\theta})\right) \\ &= \exp\left(\sum_i \alpha_i z_i - \frac{1}{2} \sum_i \sum_j (z_i - \theta_i)(z_j - \theta_j) W_{ij}\right) \end{aligned} \quad (15.12)$$

where \mathbf{W} is a symmetric matrix, is one such class. While this dates back to Weldon (1895) and Haldane (1954), this slightly more general form is due to Felsenstein (1977).

Directional selection occurs when $\boldsymbol{\alpha} \neq \mathbf{0}$ and/or $\boldsymbol{\mu} \neq \boldsymbol{\theta}$, while the elements of \mathbf{W} measure quadratic selection. If \mathbf{W} is a diagonal matrix, then $W_{ii} > 0$ implies convex selection on z_i about an optimal value of θ_i , while $W_{ii} < 0$ implies concave selection about θ_i . The larger the magnitude of W_{ii} , the stronger selection. As we saw in Lecture 14, some care must be taken in interpreting the nature of the fitness surface when \mathbf{W} has non-zero off-diagonal elements. Note from our discussions on the canonical axes of a quadratic form (Lecture 14) that, provided \mathbf{W}^{-1} exists, we can always transform the original vector of characters \mathbf{z} to a new vector \mathbf{y} such that this matrix is now diagonal with the diagonal elements being the eigenvalues of \mathbf{W} . The signs of these eigenvalues indicate whether selection is convex or concave (positive eigenvalues indicate convex selection, negative eigenvalues concave selection), while their magnitudes indicate the strength of selection (the larger the magnitude, the stronger the effect). If \mathbf{W} has k zero eigenvalues, the fitness surface has no curvature (is a plane) in k dimensions.

Phenotypes and Breeding Values Remain MVN After Selection

To see that the gaussian fitness function preserves normality, first note that if $p(\mathbf{z})$ is the phenotypic distribution before selection, then the phenotypic distribution after selection is

$$p^*(\mathbf{z}) = \frac{p(\mathbf{z}) W(\mathbf{z})}{\int p(\mathbf{z}) W(\mathbf{z}) d\mathbf{z}} = c p(\mathbf{z}) W(\mathbf{z})$$

where c is a constant such that $\int p^*(\mathbf{z}) d\mathbf{z} = 1$. If the vector of phenotypic values before selection $\mathbf{z} \sim \text{MVN}(\boldsymbol{\mu}, \mathbf{P})$, the distribution of phenotypes after selection is

$$\begin{aligned} p^*(\mathbf{z}) &= c p(\mathbf{z}) W(\mathbf{z}) \\ &= c \exp\left(\boldsymbol{\alpha}^T \mathbf{z} - \frac{1}{2}(\mathbf{z} - \boldsymbol{\theta})^T \mathbf{W}(\mathbf{z} - \boldsymbol{\theta})\right) \cdot \exp\left(-\frac{1}{2}(\mathbf{z} - \boldsymbol{\mu})^T \mathbf{P}^{-1}(\mathbf{z} - \boldsymbol{\mu})\right) \\ &= c \exp\left(\boldsymbol{\alpha}^T \mathbf{z} - \frac{1}{2}[(\mathbf{z} - \boldsymbol{\theta})^T \mathbf{W}(\mathbf{z} - \boldsymbol{\theta}) + (\mathbf{z} - \boldsymbol{\mu})^T \mathbf{P}^{-1}(\mathbf{z} - \boldsymbol{\mu})]\right) \end{aligned} \quad (15.13a)$$

If this distribution is Gaussian, it can be written as

$$p^*(\mathbf{z}) = (2\pi)^{-n/2} |\mathbf{P}^*|^{-1/2} \exp\left(-\frac{1}{2}(\mathbf{z} - \boldsymbol{\mu}^*)^T (\mathbf{P}^*)^{-1} (\mathbf{z} - \boldsymbol{\mu}^*)\right) \quad (15.13b)$$

where $\boldsymbol{\mu}^*$ and \mathbf{P}^* are the mean vector and phenotypic covariance matrix after selection. By matching terms in Equations 15.13a/b and doing a little algebra we find that these two distributions are indeed identical, with

$$\boldsymbol{\mu}^* = \mathbf{P}^*(\mathbf{P}^{-1}\boldsymbol{\mu} + \mathbf{W}\boldsymbol{\theta} + \boldsymbol{\alpha}) \quad (15.14a)$$

and

$$\mathbf{P}^* = (\mathbf{P}^{-1} + \mathbf{W})^{-1} \quad (15.14b)$$

If \mathbf{W}^{-1} exists, we can alternatively write \mathbf{P}^* as

$$\mathbf{P}^* = \mathbf{W}^{-1}(\mathbf{W}^{-1} + \mathbf{P})^{-1}\mathbf{P} \quad (15.14c)$$

$$= \mathbf{P}(\mathbf{W}^{-1} + \mathbf{P})^{-1}\mathbf{W}^{-1} \quad (15.14d)$$

These follow from standard matrix identities (e.g., Searle 1982) and will prove useful in further analysis of this model. Note that since \mathbf{P}^* is a covariance matrix, it must be positive-definite. This is always the case if \mathbf{W} is non-negative definite, but can fail if \mathbf{W} has at least one sufficiently large negative eigenvalue, as would occur with sufficiently strong disruptive selection on at least one character. In this case, the Gaussian fitness function is not appropriate (in effect, it means for at least one character, fitness approaches infinity as that character gets arbitrarily large or small at a faster rate than the frequency of that character value approaches zero, resulting in a mean population fitness of infinity).

Finally, it will be useful to have an expression for the mean population fitness under Gaussian selection, which is a function of the mean vector and covariance matrix. By definition,

$$\bar{W}(\boldsymbol{\mu}, \mathbf{P}) = \int W(\mathbf{z}) p(\mathbf{z}) d\mathbf{z}$$

To compute this integral, we use the standard trick of expressing this as a probability distribution times a function independent of \mathbf{z} . Since

$$\int (2\pi)^{-n/2} |\mathbf{P}^*|^{-1/2} \exp\left(-\frac{1}{2}(\mathbf{z} - \boldsymbol{\mu}^*)^T (\mathbf{P}^*)^{-1} (\mathbf{z} - \boldsymbol{\mu}^*)\right) d\mathbf{z} = 1$$

we find (after a little algebra) that when $\mathbf{z} \sim \text{MVN}$,

$$\bar{W}(\boldsymbol{\mu}, \mathbf{P}) = \sqrt{\frac{|\mathbf{P}^*|}{|\mathbf{P}|}} \cdot \exp\left(-\frac{1}{2} \left[\boldsymbol{\theta}^T \mathbf{W} \boldsymbol{\theta} + \boldsymbol{\mu}^T \mathbf{P}^{-1} \boldsymbol{\mu} - (\boldsymbol{\mu}^*)^T (\mathbf{P}^*)^{-1} \boldsymbol{\mu}^* \right]\right) \quad (15.15a)$$

Using Equation 15.14a, we can alternately express the term in the exponent as

$$\boldsymbol{\theta}^T \mathbf{W} \boldsymbol{\theta} + \boldsymbol{\mu}^T \mathbf{P}^{-1} (\mathbf{I} - \mathbf{P}^* \mathbf{P}^{-1}) \boldsymbol{\mu} - 2 \cdot \mathbf{b}^T \mathbf{P}^* \mathbf{P}^{-1} \boldsymbol{\mu} - \mathbf{b}^T (\mathbf{P}^*)^{-1} \mathbf{b} \quad (15.15b)$$

where $\mathbf{b} = \mathbf{W}\boldsymbol{\theta} + \boldsymbol{\alpha}$, and we have used $\mathbf{b}^T \mathbf{P}^{-1} \boldsymbol{\mu} = (\mathbf{b}^T \mathbf{P}^{-1} \boldsymbol{\mu})^T = \boldsymbol{\mu}^T \mathbf{P}^{-1} \mathbf{b}$.

The careful reader will observe that we have only shown that vector \mathbf{z} **phenotypes** remains Gaussian-distributed. Our main interest is how selection changes the distribution of the vector of *additive genetic values* \mathbf{g} as these determine the between-generation change. Provided $\mathbf{z} = \mathbf{g} + \mathbf{e}$, where \mathbf{g} and \mathbf{e} are independent and MVN, then the distribution of additive genetic values after selection also remains MVN. To see this, consider the expected fitness of an individual with additive genetic value \mathbf{g} ,

$$w(\mathbf{g}) = \int w(\mathbf{z}) p(\mathbf{z} | \mathbf{g}) d\mathbf{z}$$

The conditional distribution of \mathbf{z} given \mathbf{g} is $\mathbf{z} | \mathbf{g} = (\mathbf{g} + \mathbf{e}) | \mathbf{g} \sim \text{MVN}(\mathbf{g}, \mathbf{E})$, as phenotypes are distributed around their genotypic value \mathbf{g} according to the distribution of environmental values, which is $\text{MVN}(\mathbf{0}, \mathbf{E})$. Using the same approach leading to Equation 15.13, we can see that $w(\mathbf{g})$ is also of a Gaussian form and hence $p^*(\mathbf{g}) = w(\mathbf{g}) p(\mathbf{g})$ is also Gaussian.

The Selection Differential and Gradient

To conclude, let us combine these results with those obtained in Lecture 13 for the multivariate breeders' equation to examine changes in the vector of means and the covariance matrix. Consider changes in mean first. Since the distribution of additive genetic and phenotypic values remains Gaussian, then from the breeders' equation the expected change in the mean in generation t is $\mathbf{R}_t = \mathbf{G}_t \mathbf{P}_t^{-1} \mathbf{S}_t$. Noting that $\mathbf{S}_t = \boldsymbol{\mu}_t^* - \boldsymbol{\mu}_t$, from Equations 15.14a-c, we have

$$\begin{aligned} \mathbf{S}_t &= \mathbf{W}^{-1} (\mathbf{W}^{-1} + \mathbf{P}_t)^{-1} \mathbf{P}_t (\mathbf{P}_t^{-1} \boldsymbol{\mu}_t + \mathbf{W}\boldsymbol{\theta} + \boldsymbol{\alpha}) - \boldsymbol{\mu}_t \\ &= \mathbf{W}^{-1} (\mathbf{W}^{-1} + \mathbf{P}_t)^{-1} (\boldsymbol{\mu}_t + \mathbf{P}_t \mathbf{W}\boldsymbol{\theta} + \mathbf{P}_t \boldsymbol{\alpha}) - \boldsymbol{\mu}_t \end{aligned}$$

Using the identity

$$\mathbf{I} = \mathbf{W}^{-1} (\mathbf{W}^{-1} + \mathbf{P})^{-1} (\mathbf{W}^{-1} + \mathbf{P}) \mathbf{W} = \mathbf{W}^{-1} (\mathbf{W}^{-1} + \mathbf{P})^{-1} (\mathbf{I} + \mathbf{P}\mathbf{W})$$

this reduces to

$$\begin{aligned} \mathbf{S}_t &= \mathbf{W}^{-1} (\mathbf{W}^{-1} + \mathbf{P}_t)^{-1} (\boldsymbol{\mu}_t + \mathbf{P}_t \mathbf{W}\boldsymbol{\theta} + \mathbf{P}_t \boldsymbol{\alpha}) - \mathbf{W}^{-1} (\mathbf{W}^{-1} + \mathbf{P}_t)^{-1} (\mathbf{I} + \mathbf{P}_t \mathbf{W}) \boldsymbol{\mu}_t \\ &= \mathbf{W}^{-1} (\mathbf{W}^{-1} + \mathbf{P}_t)^{-1} ([\mathbf{I} - \mathbf{I} - \mathbf{P}_t \mathbf{W}] \boldsymbol{\mu}_t + \mathbf{P}_t \mathbf{W}\boldsymbol{\theta} + \mathbf{P}_t \boldsymbol{\alpha}) \\ &= \mathbf{W}^{-1} (\mathbf{W}^{-1} + \mathbf{P}_t)^{-1} \mathbf{P}_t (\mathbf{W}(\boldsymbol{\theta} - \boldsymbol{\mu}_t) + \boldsymbol{\alpha}) \end{aligned} \quad (15.16a)$$

At equilibrium $\hat{\mathbf{S}} = \mathbf{0}$. Assuming \mathbf{W} and \mathbf{P} are nonsingular, this implies $\mathbf{W}(\boldsymbol{\theta} - \hat{\boldsymbol{\mu}}) + \boldsymbol{\alpha} = \mathbf{0}$, giving

$$\hat{\boldsymbol{\mu}} = \boldsymbol{\theta} + \mathbf{W}^{-1} \boldsymbol{\alpha} \quad (15.16b)$$

Surprisingly, this equilibrium value is independent of the additive genetic and phenotypic covariance matrices (provided \mathbf{G} and \mathbf{P} are nonsingular) and simply depends on the elements of the fitness function. This interesting result was first noted by Zeng (1988) for a slightly different fitness function.

Likewise, the selection gradient for the general Gaussian fitness model becomes

$$\boldsymbol{\beta}_t = \mathbf{P}_t^{-1} \mathbf{S}_t = \mathbf{P}_t^{-1} \mathbf{W}^{-1} (\mathbf{W}^{-1} + \mathbf{P}_t)^{-1} \mathbf{P}_t (\mathbf{W}(\boldsymbol{\theta} - \boldsymbol{\mu}_t) + \boldsymbol{\alpha}) \quad (15.17)$$

The Within-Generation Change in \mathbf{G}

Turning now to the change in \mathbf{G} , we first note that

$$\begin{aligned} \mathbf{P}^* &= \mathbf{P} (\mathbf{P} + \mathbf{W}^{-1})^{-1} \mathbf{W}^{-1} = \mathbf{P} (\mathbf{P} + \mathbf{W}^{-1})^{-1} ([\mathbf{P} + \mathbf{W}^{-1}] - \mathbf{P}) \\ &= \mathbf{P} - \mathbf{P} (\mathbf{P} + \mathbf{W}^{-1})^{-1} \mathbf{P} \end{aligned} \quad (15.18a)$$

Thus

$$\mathbf{P}^{-1} (\mathbf{P}^* - \mathbf{P}) \mathbf{P}^{-1} = - (\mathbf{W}^{-1} + \mathbf{P})^{-1} \quad (15.18b)$$

Substituting this result into our result from Example 14.3, $\mathbf{G}^* - \mathbf{G} = \mathbf{G}\mathbf{P}^{-1}(\mathbf{P}^* - \mathbf{P})\mathbf{P}^{-1}\mathbf{G}$, gives

$$\mathbf{G}^* = \mathbf{G} - \mathbf{G}(\mathbf{W}^{-1} + \mathbf{P})^{-1}\mathbf{G} \quad (15.18c)$$

Changes in \mathbf{G} Under the General Infinitesimal Model

Equation 15.18c gives the *within-generation* change in \mathbf{G} . How much of this change is transferred to the next generation?

Recall Bulmer's treatment for the univariate case (Lecture 9), wherein all changes in variances occur due to gametic-phase disequilibrium d_t changing the additive variance. In this case, $\sigma_A^2(t) = \sigma_A^2(0) + d_t$, and hence $\sigma_z^2(t) = \sigma_z^2(0) + d_t$. Moving to multiple characters, disequilibrium is now measured by the matrix $\mathbf{D}_t = \mathbf{G}_t - \mathbf{G}_0$. Thus D_{ij} is the change in the additive genetic covariance between characters i and j induced by disequilibrium. Likewise, the phenotypic covariance matrix is given by $\mathbf{P}_t = \mathbf{P}_0 + \mathbf{D}_t$. Tallis (1987, Tallis and Leppard 1988) extend Bulmer's result to multiple characters, showing that

$$\Delta\mathbf{D}_t = \frac{1}{2}(\mathbf{G}_t\mathbf{P}_t^{-1}(\mathbf{P}_t^* - \mathbf{P}_t)\mathbf{P}_t^{-1}\mathbf{G}_t - \mathbf{D}_t) \quad (15.19)$$

where \mathbf{P}^* is the phenotypic covariance matrix after selection but before random mating. The regression argument leading to Equation 15.19 assumes linearity and homoscedasticity, hence strongly relies on the assumption that the joint distribution of additive genetic and phenotypic values is multivariate normal and remain so after selection.

We can also express Equation 15.19 in terms of the quadratic and directional selection gradients, γ and β . Recalling the definitions of \mathbf{C} , β , and γ (Lecture 14), we have

$$\mathbf{P}^* - \mathbf{P} = \mathbf{C} - \mathbf{S}\mathbf{S}^T$$

Hence

$$\begin{aligned} \mathbf{P}^{-1}(\mathbf{P}^* - \mathbf{P})\mathbf{P}^{-1} &= \mathbf{P}^{-1}(\mathbf{C} - \mathbf{S}\mathbf{S}^T)\mathbf{P}^{-1} \\ &= \mathbf{P}^{-1}\mathbf{C}\mathbf{P}^{-1} - (\mathbf{P}^{-1}\mathbf{S})(\mathbf{P}^{-1}\mathbf{S})^T \\ &= \gamma - \beta\beta^T \end{aligned} \quad (15.20)$$

Substituting into Equation 15.19 gives

$$\Delta\mathbf{D}_t = \frac{1}{2}(\mathbf{G}_t(\gamma_t - \beta_t\beta_t^T)\mathbf{G}_t - \mathbf{D}_t) \quad (15.21a)$$

Finally, recalling 14.16b, we can also express this as

$$\Delta\mathbf{D}_t = \frac{1}{2}(\mathbf{G}_t^* - \mathbf{G}_t) - \frac{\mathbf{D}_t}{2} \quad (15.21b)$$

where \mathbf{G}_t^* is the additive genetic covariance in generation t after selection but before random mating. Note from Equation 15.18c, that when the fitness function is multivariate normal (Equation 15.12),

$$\Delta\mathbf{D}_t = -\frac{1}{2}\left[\mathbf{G}(\mathbf{W}^{-1} + \mathbf{P})^{-1}\mathbf{G} + \frac{\mathbf{D}_t}{2}\right] \quad (15.21c)$$

Equation 15.21b shows that only half of the disequilibrium deviation in \mathbf{G} from the previous generation \mathbf{D}_t is passed onto the next generation and only half the within-generation change induced

by selection in that generation, as is expected since the infinitesimal mode assumes unlinked loci and hence each in generation recombination removes half of the present disequilibrium. The disequilibrium component converges to

$$\widehat{\mathbf{D}} = \widehat{\mathbf{G}} (\widehat{\boldsymbol{\gamma}} - \widehat{\boldsymbol{\beta}} \widehat{\boldsymbol{\beta}}^T) \widehat{\mathbf{G}} = (\mathbf{G}_0 + \widehat{\mathbf{D}}) (\widehat{\boldsymbol{\gamma}} - \widehat{\boldsymbol{\beta}} \widehat{\boldsymbol{\beta}}^T) (\mathbf{G}_0 + \widehat{\mathbf{D}}) \quad (15.22)$$

Where have place carrots over $\boldsymbol{\gamma}$ and $\boldsymbol{\beta}$ to remind the reader that these depend on \mathbf{P} , and hence on \mathbf{D} .

Hence, provided the joint distribution of additive genetic and phenotypic values remains multivariate normal, the equations for change in the mean and variance are $\mathbf{R}_t = \Delta \boldsymbol{\mu}_t = \mathbf{G}_t \boldsymbol{\beta}_t$ and $\Delta \mathbf{G}_t = \Delta \mathbf{D}_t$, with $\Delta \mathbf{D}_t$ given by Equation (15.21).

Example 15.4. Suppose only quadratic selection is acting on the two characters z_1 and z_2 , with

$$w(\mathbf{z}) = a - 0.25(z_1 - \mu_{z_1})^2 + 0.35(z_1 - \mu_{z_1})(z_2 - \mu_{z_2}) - 0.125(z_2 - \mu_{z_2})^2$$

Recalling that (Equation 14.11a) that the b_{ij} term in the quadratic corresponds to $\gamma_{ii}/2$ when $i = j$, otherwise it corresponds to γ_{ij} , the resulting matrix of quadratic selection gradients is

$$\boldsymbol{\gamma} = \begin{pmatrix} -0.50 & 0.35 \\ 0.35 & -0.25 \end{pmatrix}$$

Assume the unselected base population has additive genetic covariance matrix

$$\mathbf{G}_0 = \begin{pmatrix} 0.5 & 0.0 \\ 0.0 & 0.5 \end{pmatrix}$$

Starting at linkage equilibrium, $\mathbf{D}_0 = \mathbf{0}$, so that after one generation of selection

$$\begin{aligned} \mathbf{D}_1 &= \frac{1}{2} \mathbf{G}_0 \boldsymbol{\gamma} \mathbf{G}_0 = \frac{1}{2} \begin{pmatrix} 0.5 & 0.0 \\ 0.0 & 0.5 \end{pmatrix} \begin{pmatrix} -0.50 & 0.35 \\ 0.35 & -0.25 \end{pmatrix} \begin{pmatrix} 0.5 & 0.0 \\ 0.0 & 0.5 \end{pmatrix} \\ &= \begin{pmatrix} 0.063 & 0.044 \\ 0.044 & -0.031 \end{pmatrix} \end{aligned}$$

giving

$$\mathbf{G}_1 = \mathbf{G}_0 + \mathbf{D}_1 = \begin{pmatrix} 0.5 - 0.063 & 0.0 + 0.044 \\ 0.0 + 0.044 & 0.5 - 0.031 \end{pmatrix} = \begin{pmatrix} 0.437 & 0.044 \\ 0.044 & 0.469 \end{pmatrix}$$

Subsequent iterations give

$$\mathbf{G}_2 = \begin{pmatrix} 0.427 & 0.051 \\ 0.051 & 0.464 \end{pmatrix} \quad \text{and} \quad \mathbf{G}_5 = \begin{pmatrix} 0.425 & 0.052 \\ 0.052 & 0.462 \end{pmatrix}$$

with the equilibrium values given by

$$\widehat{\mathbf{G}} = \begin{pmatrix} 0.425 & 0.052 \\ 0.052 & 0.462 \end{pmatrix} \quad \text{and} \quad \widehat{\mathbf{D}} = \begin{pmatrix} -0.075 & 0.052 \\ 0.052 & -0.038 \end{pmatrix}$$

As with the univariate case, essentially all of the change occurs in the first two generations. Note that as we change \mathbf{G}_0 , we also change $\widehat{\mathbf{D}}$. Hence

$$\mathbf{G}_0 = \begin{pmatrix} 0.50 & -0.25 \\ -0.25 & 0.50 \end{pmatrix} \rightarrow \widehat{\mathbf{G}} = \begin{pmatrix} 0.383 & -0.146 \\ -0.146 & 0.407 \end{pmatrix}, \quad \widehat{\mathbf{D}} = \begin{pmatrix} -0.117 & 0.104 \\ 0.104 & -0.093 \end{pmatrix}$$

while

$$\mathbf{G}_0 = \begin{pmatrix} 0.50 & 0.25 \\ 0.25 & 0.50 \end{pmatrix} \rightarrow \widehat{\mathbf{G}} = \begin{pmatrix} 0.461 & 0.261 \\ 0.261 & 0.495 \end{pmatrix}, \quad \widehat{\mathbf{D}} = \begin{pmatrix} -0.039 & 0.011 \\ 0.011 & -0.005 \end{pmatrix}$$

Long-term Response: Balance Between Directional and Stabilizing Selection.

Zeng (1988) examined the long-term response (under the infinitesimal model) under a balance between direction and stabilizing selection. For modeling ease, assume stabilizing selection occurs first, followed by directional selection. Stabilizing selection occurs via the multivariate gaussian fitness function,

$$W(\mathbf{z}) = \exp\left(-\frac{1}{2}(\mathbf{z} - \boldsymbol{\theta})^T \mathbf{W}(\mathbf{z} - \boldsymbol{\theta})\right) \quad (15.23a)$$

Following stabilizing selection, directional selection is applied to some linear combination of characters by truncation selection on $y = \sum_{i=1}^n b_i z_i = \mathbf{b}^t \mathbf{z}$ where some of the b_i may be zero. From Equation 15.14c, the phenotypic variance-covariance matrix following stabilizing selection is $\mathbf{P}^* = \mathbf{W}^{-1}(\mathbf{W}^{-1} + \mathbf{P})^{-1}\mathbf{P}$ giving the variance on the index as

$$\sigma_I^2 = \mathbf{b}^T \mathbf{P}^* \mathbf{b} = \mathbf{b}^T \mathbf{W}^{-1}(\mathbf{W}^{-1} + \mathbf{P})^{-1} \mathbf{P} \mathbf{b} \quad (15.23b)$$

At equilibrium

$$\hat{\boldsymbol{\mu}} = \boldsymbol{\theta} + \mathbf{W}^{-1} \mathbf{b} \frac{i}{\sigma_I} \quad (15.24a)$$

If selection is relatively weak so that the amount of disequilibrium generated is very small then $\hat{\mathbf{P}} = \mathbf{P}$. Notice that this equilibrium solution is independent of the genetic covariance structure. In particular, note that if \mathbf{W} is diagonal (no selection on combinations of characters) then for the i th character,

$$\hat{\mu}_i = \theta_i + \frac{b_i}{W_{ii}} \left(\frac{i}{\sigma_I}\right) \quad (15.24b)$$

so that the long-term evolution of each character is independent unless at least one genetic correlation is perfect (so that \mathbf{G} is singular).

Long-term Response: The Infinitesimal Model with Drift and Mutation.

It is straightforward to extend many of our previous results on the interaction of drift, selection, and mutation to multivariate traits, provide we are willing to assume the infinitesimal model. Consider drift first. Let \mathbf{G}_t be the genetic covariance matrix in generation t . If \mathbf{G}_t changes strictly by drift, then $\mathbf{G}_t = \mathbf{G}_0(1 - f_t)$ where f_t is the inbreeding coefficient at time t ,

$$1 - f_t = \left(1 - \frac{1}{2N_e}\right)^t$$

Hence, the expected change after t generations of selection and drift is

$$\begin{aligned} \boldsymbol{\mu}_t - \boldsymbol{\mu}_0 &= \sum_{k=0}^t \mathbf{G}_k \boldsymbol{\beta} = \sum_{k=0}^t (1 - f_k) \mathbf{G}_0 \boldsymbol{\beta} \\ &= \mathbf{G}_0 \boldsymbol{\beta} \sum_{k=0}^t \left(1 - \frac{1}{2N_e}\right)^k \\ &\simeq 2N_e (1 - e^{-t/2N_e}) \mathbf{G}_0 \boldsymbol{\beta} \end{aligned} \quad (15.25)$$

Taking the limit of Equation 15.25 (i.e., letting $t \rightarrow \infty$), the selection limit is

$$\mathbf{R}_\infty = 2N_e \mathbf{G}_0 \boldsymbol{\beta} = 2N_e \mathbf{R}_0 \quad (15.26)$$

This generalizes Robertson's univariate result, with the selection limit (assuming no mutational input) simply being $2N_e$ times the initial response.

Now let's consider mutational input. Let \mathbf{U} be the matrix of per-generation input to the additive genetic variances and covariance. As with the univariate case, the covariance matrix under drift-mutation equilibrium is given by

$$\widehat{\mathbf{G}} = 2N_e \mathbf{U} \quad (15.27)$$

Under the assumptions of the infinitesimal model (so that selection is sufficiently weak that the dynamics of changes in allele frequencies are completely driven by drift and mutation), the additive genetic variance-covariance matrix at generation t is

$$\mathbf{G}_t = \widehat{\mathbf{G}} + (\mathbf{G}_0 - \widehat{\mathbf{G}}) e^{-t/2N_e} \quad (15.28)$$

giving the cumulative response to t generations of constant directional selection β as

$$\mathbf{R}_t = \boldsymbol{\mu}_t - \boldsymbol{\mu}_0 = \beta \left[t\widehat{\mathbf{G}} + 2N_e(1 - e^{-t/2N_e}) (\mathbf{G}_0 - \widehat{\mathbf{G}}) \right] \quad (15.27a)$$

DERIVATIVES OF VECTORS AND VECTOR-VALUED FUNCTIONS

The **gradient** (or **gradient vector**) of a scalar function f of a vector \mathbf{x} is obtained by taking partial derivatives of the function with respect to each variable. In matrix notation, the gradient operator is the column vector

$$\nabla_{\mathbf{x}}[f] = \frac{\partial f}{\partial \mathbf{x}} = \begin{pmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \\ \vdots \\ \frac{\partial f}{\partial x_n} \end{pmatrix}$$

The gradient at point \mathbf{x}_o corresponds to a vector indicating the direction of steepest ascent of the function at that point (the multivariate slope of f at the point \mathbf{x}_o). For example $f(\mathbf{x}) = \mathbf{x}^T \mathbf{x}$ has gradient vector $2\mathbf{x}$. At the point \mathbf{x}_o , $\mathbf{x}^T \mathbf{x}$ locally increases most rapidly if we change \mathbf{x} in the same direction as the vector going from point \mathbf{x}_o to point $\mathbf{x}_o + 2\delta \mathbf{x}_o$, where δ is a small positive value.

For a vector \mathbf{a} and a matrix \mathbf{A} of constants, it can easily be shown (e.g., Morrison 1976, Graham 1981, Searle 1982) that

$$\nabla_{\mathbf{x}} [\mathbf{a}^T \mathbf{x}] = \nabla_{\mathbf{x}} [\mathbf{x}^T \mathbf{a}] = \mathbf{a} \quad (15.29a)$$

$$\nabla_{\mathbf{x}} [\mathbf{A}\mathbf{x}] = \mathbf{A}^T \quad (15.29b)$$

Turning to quadratic forms, if \mathbf{A} is symmetric, then

$$\nabla_{\mathbf{x}} [\mathbf{x}^T \mathbf{A}\mathbf{x}] = 2 \cdot \mathbf{A}\mathbf{x} \quad (15.29c)$$

$$\nabla_{\mathbf{x}} [(\mathbf{x} - \mathbf{a})^T \mathbf{A}(\mathbf{x} - \mathbf{a})] = 2 \cdot \mathbf{A}(\mathbf{x} - \mathbf{a}) \quad (15.29d)$$

$$\nabla_{\mathbf{x}} [(\mathbf{a} - \mathbf{x})^T \mathbf{A}(\mathbf{a} - \mathbf{x})] = -2 \cdot \mathbf{A}(\mathbf{a} - \mathbf{x}) \quad (15.29e)$$

Taking $\mathbf{A} = \mathbf{I}$, Equation 15.29c implies

$$\nabla_{\mathbf{x}} [\mathbf{x}^T \mathbf{x}] = \nabla_{\mathbf{x}} [\mathbf{x}^T \mathbf{I}\mathbf{x}] = 2 \cdot \mathbf{I}\mathbf{x} = 2 \cdot \mathbf{x} \quad (15.29f)$$

Two final useful identities follow from the chain rule of differentiation,

$$\nabla_{\mathbf{x}} [\exp[f(\mathbf{x})]] = \exp[f(\mathbf{x})] \cdot \nabla_{\mathbf{x}} [f(\mathbf{x})] \quad (15.29g)$$

$$\nabla_{\mathbf{x}} [\ln[f(\mathbf{x})]] = \frac{1}{f(\mathbf{x})} \cdot \nabla_{\mathbf{x}} [f(\mathbf{x})] \quad (15.29h)$$

Example 15.5. Writing the MVN distribution as

$$\varphi(\mathbf{x}) = a \exp\left(-\frac{1}{2} \cdot (\mathbf{x} - \boldsymbol{\mu})^T \mathbf{V}_{\mathbf{x}}^{-1} (\mathbf{x} - \boldsymbol{\mu})\right)$$

where $a = \pi^{-n/2} |\mathbf{V}_{\mathbf{x}}|^{-1/2}$, then from Equation 15.29g,

$$\nabla_{\mathbf{x}} [\varphi(\mathbf{x})] = \varphi(\mathbf{x}) \cdot \nabla_{\mathbf{x}} \left[\left(-\frac{1}{2}\right) \cdot (\mathbf{x} - \boldsymbol{\mu})^T \mathbf{V}_{\mathbf{x}}^{-1} (\mathbf{x} - \boldsymbol{\mu}) \right]$$

Applying Equation 15.29d gives

$$\nabla_{\mathbf{x}} [\varphi(\mathbf{x})] = -\varphi(\mathbf{x}) \cdot \mathbf{V}_{\mathbf{x}}^{-1} (\mathbf{x} - \boldsymbol{\mu}) \quad (15.30a)$$

Note here that $\varphi(\mathbf{x})$ is a scalar and hence its order of multiplication does not matter, while the order of the other variables (being matrices) is critical. Similarly, we can consider the MVN as a function of the mean vector $\boldsymbol{\mu}$, in which case Equation 15.29e implies

$$\nabla_{\boldsymbol{\mu}} [\varphi(\mathbf{x}, \boldsymbol{\mu})] = \varphi(\mathbf{x}, \boldsymbol{\mu}) \cdot \mathbf{V}_{\mathbf{x}}^{-1} (\mathbf{x} - \boldsymbol{\mu}) \quad (15.30b)$$

Example 15.6. Lande (1979) showed that $\nabla_{\boldsymbol{\mu}} [\ln \bar{W}(\boldsymbol{\mu})] = \boldsymbol{\beta}$ when phenotypes are multivariate normal. Hence, the increase in mean population fitness is maximized if mean character values change in the same direction as the vector $\boldsymbol{\beta}$. To see this, from Equation 15.29h we have $\nabla_{\boldsymbol{\mu}} [\ln \bar{W}(\boldsymbol{\mu})] = \bar{W}^{-1} \nabla_{\boldsymbol{\mu}} [\bar{W}(\boldsymbol{\mu})]$. Writing mean fitness as $\bar{W}(\boldsymbol{\mu}) = \int W(\mathbf{z}) \varphi(\mathbf{z}, \boldsymbol{\mu}) d\mathbf{z}$ and taking the gradient through the integral gives

$$\nabla_{\boldsymbol{\mu}} [\ln \bar{W}(\boldsymbol{\mu})] = \nabla_{\boldsymbol{\mu}} \left[\int \frac{W(\mathbf{z})}{\bar{W}} \varphi(\mathbf{z}, \boldsymbol{\mu}) d\mathbf{z} \right] = \int w(\mathbf{z}) \nabla_{\boldsymbol{\mu}} [\varphi(\mathbf{z}, \boldsymbol{\mu})] d\mathbf{z}$$

If individual fitnesses are themselves functions of the population mean (are frequency-dependent), then a second integral appears as we can no longer assume $\nabla_{\boldsymbol{\mu}} [w(\mathbf{z})] = 0$ (see Equation 14.5b). Applying Equation 15.30b, we can rewrite this integral as

$$\begin{aligned} \int w(\mathbf{z}) \nabla_{\boldsymbol{\mu}} [\varphi(\mathbf{z}, \boldsymbol{\mu})] d\mathbf{z} &= \int w(\mathbf{z}) \varphi(\mathbf{z}) \mathbf{P}^{-1} (\mathbf{z} - \boldsymbol{\mu}) d\mathbf{z} \\ &= \mathbf{P}^{-1} \left(\int \mathbf{z} w(\mathbf{z}) \varphi(\mathbf{z}) d\mathbf{z} - \boldsymbol{\mu} \int w(\mathbf{z}) \varphi(\mathbf{z}) d\mathbf{z} \right) \\ &= \mathbf{P}^{-1} (\boldsymbol{\mu}^* - \boldsymbol{\mu}) = \mathbf{P}^{-1} \mathbf{S} = \boldsymbol{\beta} \end{aligned}$$

which follows since the first integral is the mean character value after selection and the second equals one as $E[w] = 1$ by definition.

Example 15.7. Compute $\nabla_{\boldsymbol{\mu}} [\ln \bar{W}(\boldsymbol{\mu}, \mathbf{P})]$ for the generalized Gaussian fitness function (Equation 15.12). From Equations 15.29g and 15.15a, we have

$$\nabla_{\boldsymbol{\mu}} [\ln \bar{W}(\boldsymbol{\mu}, \mathbf{P})] = \nabla_{\boldsymbol{\mu}} \left[\ln \left(\frac{|\mathbf{P}^*|}{|\mathbf{P}|} \right) \right] - \frac{1}{2} \cdot \nabla_{\boldsymbol{\mu}} [f(\boldsymbol{\mu})] = -\frac{1}{2} \cdot \nabla_{\boldsymbol{\mu}} [f(\boldsymbol{\mu})]$$

where $f(\boldsymbol{\mu})$ is given by Equation 15.15b and \mathbf{P}^* by Equation 15.18a (the first term is zero because \mathbf{P} and \mathbf{P}^* are independent of $\boldsymbol{\mu}$). Ignoring terms of f not containing $\boldsymbol{\mu}$ since the gradient of these (with respect to $\boldsymbol{\mu}$) is zero,

$$\nabla_{\boldsymbol{\mu}} [f(\boldsymbol{\mu})] = \nabla_{\boldsymbol{\mu}} [\boldsymbol{\mu}^T \mathbf{P}^{-1} (\mathbf{I} - \mathbf{P}^* \mathbf{P}^{-1}) \boldsymbol{\mu}] - 2 \cdot \nabla_{\boldsymbol{\mu}} [\mathbf{b}^T \mathbf{P}^{-1} \boldsymbol{\mu}]$$

where $\mathbf{b} = \mathbf{W}\boldsymbol{\theta} + \boldsymbol{\alpha}$. Applying Equations 15.29b/c,

$$\begin{aligned} \nabla_{\boldsymbol{\mu}} [\boldsymbol{\mu}^T \mathbf{P}^{-1} (\mathbf{I} - \mathbf{P}^* \mathbf{P}^{-1}) \boldsymbol{\mu}] &= 2 \cdot \mathbf{P}^{-1} (\mathbf{I} - \mathbf{P}^* \mathbf{P}^{-1}) \boldsymbol{\mu} \\ \nabla_{\boldsymbol{\mu}} [\mathbf{b}^T \mathbf{P}^{-1} \boldsymbol{\mu}] &= (\mathbf{b}^T \mathbf{P}^{-1})^T = \mathbf{P}^{-1} \mathbf{b} \end{aligned}$$

Hence,

$$\nabla_{\boldsymbol{\mu}} [\ln \bar{W}(\boldsymbol{\mu}, \mathbf{P})] = \mathbf{P}^{-1} [(\mathbf{P}^* \mathbf{P}^{-1} - \mathbf{I}) \boldsymbol{\mu} + \mathbf{b}] \quad (15.31a)$$

Using the definitions of \mathbf{P}^* and \mathbf{b} , we can (eventually) express this as

$$\nabla_{\boldsymbol{\mu}} [\ln \bar{W}(\boldsymbol{\mu}, \mathbf{P})] = \mathbf{P}^{-1} \mathbf{W}^{-1} (\mathbf{W}^{-1} + \mathbf{P})^{-1} \mathbf{P} (\mathbf{W}(\boldsymbol{\theta} - \boldsymbol{\mu}) + \boldsymbol{\alpha}) \quad (15.31b)$$

showing (from Equation 15.16a) that when $\mathbf{z} \sim \text{MVN}$, this gradient equals $\mathbf{P}^{-1} \mathbf{S} = \boldsymbol{\beta}$.

The Hessian Matrix, Local Maxima/minima, and Multidimensional Taylor Series

In univariate calculus, local extrema of a function occur when the slope (first derivative) is zero. The multivariate extension of this is that the gradient vector is zero, so that the slope of the function with respect to all variables is zero. A point \mathbf{x}_e where this occurs is called a **stationary** or **equilibrium** point, and corresponds to either a local maximum, minimum, saddle point or inflection point. As with the calculus of single variables, determining which of these is true depends on the second derivative. With n variables, the appropriate generalization is the **hessian** matrix

$$\mathbf{H}_{\mathbf{X}}[f] = \nabla_{\mathbf{X}} \left[\left(\nabla_{\mathbf{X}} [f] \right)^T \right] = \frac{\partial^2 f}{\partial \mathbf{x} \partial \mathbf{x}^T} = \begin{pmatrix} \frac{\partial^2 f}{\partial x_1^2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_1 \partial x_n} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{pmatrix} \quad (15.32)$$

This matrix is symmetric, as mixed partials are equal under suitable continuity conditions, and measures the local curvature of the function.

Example 15.8. Compute $\mathbf{H}_{\mathbf{X}} [\varphi(\mathbf{x})]$, the hessian matrix for the multivariate normal distribution. Recalling from Equation 15.30a that $\nabla_{\mathbf{X}} [\varphi(\mathbf{x})] = -\varphi(\mathbf{x}) \cdot \mathbf{V}_{\mathbf{X}}^{-1} (\mathbf{x} - \boldsymbol{\mu})$, we have

$$\begin{aligned} \mathbf{H}_{\mathbf{X}} [\varphi(\mathbf{x})] &= \nabla_{\mathbf{X}} \left[\left(\nabla_{\mathbf{X}} [\varphi(\mathbf{x})] \right)^T \right] \\ &= -\nabla_{\mathbf{X}} [\varphi(\mathbf{x}) \cdot (\mathbf{x} - \boldsymbol{\mu})^T \mathbf{V}_{\mathbf{X}}^{-1}] \\ &= -\nabla_{\mathbf{X}} [\varphi(\mathbf{x})] \cdot (\mathbf{x} - \boldsymbol{\mu})^T \mathbf{V}_{\mathbf{X}}^{-1} - \varphi(\mathbf{x}) \cdot \nabla_{\mathbf{X}} [(\mathbf{x} - \boldsymbol{\mu})^T \mathbf{V}_{\mathbf{X}}^{-1}] \\ &= \varphi(\mathbf{x}) \cdot \left(\mathbf{V}_{\mathbf{X}}^{-1} (\mathbf{x} - \boldsymbol{\mu})(\mathbf{x} - \boldsymbol{\mu})^T \mathbf{V}_{\mathbf{X}}^{-1} - \mathbf{V}_{\mathbf{X}}^{-1} \right) \end{aligned} \quad (15.33a)$$

Likewise,

$$\mathbf{H}_{\boldsymbol{\mu}} [\varphi(\mathbf{x}, \boldsymbol{\mu})] = \varphi(\mathbf{x}, \boldsymbol{\mu}) \cdot \left(\mathbf{V}_{\mathbf{x}}^{-1} (\mathbf{x} - \boldsymbol{\mu})(\mathbf{x} - \boldsymbol{\mu})^T \mathbf{V}_{\mathbf{x}}^{-1} - \mathbf{V}_{\mathbf{x}}^{-1} \right) \quad (15.33b)$$

To see how the hessian matrix determines the nature of equilibrium points, a slight digression on the multidimensional Taylor series is needed. Consider the Taylor series of a function of n variables $f(x_1, \dots, x_n)$ expanded about the point \mathbf{y} ,

$$f(\mathbf{x}) \simeq f(\mathbf{y}) + \sum_{i=1}^n (x_i - y_i) \frac{\partial f}{\partial x_i} + \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n (x_i - y_i)(x_j - y_j) \frac{\partial^2 f}{\partial x_i \partial x_j} + \dots$$

where all partials are evaluated at \mathbf{y} . In matrix form, the second-order Taylor expansion of $f(\mathbf{x})$ about \mathbf{x}_o is

$$f(\mathbf{x}) \simeq f(\mathbf{x}_o) + \nabla^T (\mathbf{x} - \mathbf{x}_o) + \frac{1}{2} (\mathbf{x} - \mathbf{x}_o)^T \mathbf{H} (\mathbf{x} - \mathbf{x}_o) \quad (15.34)$$

where ∇ and \mathbf{H} are the gradient and hessian with respect to \mathbf{x} evaluated at \mathbf{x}_o , e.g.,

$$\nabla \equiv \nabla_{\mathbf{x}} [f] \Big|_{\mathbf{x}=\mathbf{x}_o} \quad \text{and} \quad \mathbf{H} \equiv \mathbf{H}_{\mathbf{x}} [f] \Big|_{\mathbf{x}=\mathbf{x}_o}$$

At an equilibrium point \mathbf{x}_o , $\nabla = 0$, and Equation 15.34 implies

$$f(\mathbf{x}) - f(\mathbf{x}_o) \simeq \frac{1}{2} (\mathbf{x} - \mathbf{x}_o)^T \mathbf{H} (\mathbf{x} - \mathbf{x}_o)$$

so that the nature of local changes about the equilibrium point depend on quadratic products involving \mathbf{H} . From our discussion in Lecture 14, the behavior of this quadratic product is a function of the eigenvalues of \mathbf{H} .

Example 15.9. Consider the following demonstration (due to Lande 1979) that mean population fitness increases. Expanding the log of mean fitness in a Taylor series around the current population mean $\boldsymbol{\mu}$ gives the change in mean population fitness as

$$\Delta \ln \bar{W}(\boldsymbol{\mu}) = \ln \bar{W}(\boldsymbol{\mu} + \mathbf{R}) - \ln \bar{W}(\boldsymbol{\mu})$$

Which follows since the new mean is the old mean plus the response, $\mathbf{R} + \boldsymbol{\mu}$. Now expand $\ln \bar{W}(\boldsymbol{\mu} + \mathbf{R})$ about the value $\mathbf{x}_o = \boldsymbol{\mu}$ using Equation 15.34, so that $(\mathbf{x} - \mathbf{x}_o)$ is just \mathbf{R} giving

$$\Delta \ln \bar{W}(\boldsymbol{\mu}) \simeq \left[\ln \bar{W}(\boldsymbol{\mu}) + \left(\nabla_{\boldsymbol{\mu}} [\ln \bar{W}(\boldsymbol{\mu})] \right)^T \mathbf{R} + \frac{1}{2} \mathbf{R}^T \mathbf{H}_{\boldsymbol{\mu}} [\ln \bar{W}(\boldsymbol{\mu})] \mathbf{R} \right] - \ln \bar{W}(\boldsymbol{\mu})$$

assuming that second and higher-order terms can be neglected (as would occur with weak selection and the population mean away from an equilibrium point), then

$$\Delta \ln \bar{W}(\boldsymbol{\mu}) \simeq \left(\nabla_{\boldsymbol{\mu}} [\ln \bar{W}(\boldsymbol{\mu})] \right)^T \mathbf{R}$$

Assuming that the joint distribution of phenotypes and additive genetic values is MVN, then $\nabla_{\boldsymbol{\mu}} [\ln \bar{W}(\boldsymbol{\mu})] = \boldsymbol{\beta} = \mathbf{G}^{-1} \mathbf{R}$. Substituting gives

$$\Delta \ln \bar{W}(\boldsymbol{\mu}) \simeq (\mathbf{G}^{-1} \mathbf{R})^T \mathbf{R} = (\mathbf{R})^T \mathbf{G}^{-1} \mathbf{R} \geq 0$$

since \mathbf{G} is a variance-covariance matrix and hence is non-negative definite. Thus under these conditions, mean population fitness always increases, although since $\mathbf{R} \neq \nabla_{\boldsymbol{\mu}} [\ln \bar{W}(\boldsymbol{\mu})]$ fitness does not increase in the fastest possible manner.

Lecture 15 Problems

1. Consider a trait under stabilizing selection with fitness parameters $\theta = 10$ and $\omega = 10$. The trait starts off at $\mu = 0$, $\sigma_z^2 = 100$, and $\sigma_A^2 = 50$ with no initial disequilibrium ($d(0) = 0$). Follow how this population changes over 20 generations. Compute the mean (remember $\mu(t+1) = R(t) + \mu(t)$), disequilibrium $d(t)$, $\sigma_z^2(t)$, $\sigma_A^2(t)$ and $h^2(t)$. *Hint:* The easy way to do this problem is to use Equations 15.3 and 15.4 in a spread sheet to iterate over the 20 generations.

Solutions to Lecture 15 Problems

1. From Equation 15.3, we have

$$\mu(t+1) = \mu(t) + h^2(t) \frac{\sigma_z^2(t) [\theta - \mu(t)]}{\sigma_z^2(t) + \omega} = \mu(t) + \left(\frac{50 + d(t)}{100 + d(t)} \right) \frac{[100 + d(t)] [0 - \mu(t)]}{110 + d(t)}$$

while Equation 15.4 gives

$$d(t+1) = \frac{d(t)}{2} - \frac{1}{2} \left[\frac{(\sigma_A^2 + d_t)^2}{\sigma_z^2 + d(t) + \omega} \right] = \frac{d(t)}{2} - \frac{1}{2} \left[\frac{(50 + d(t))^2}{110 + d(t)} \right]$$

Starting with $\mu(0) = 10$ and $d(0) = 0$,

t	μ	d	σ_z^2	σ_A^2	h^2
0	10.00	0.00	100.00	50.00	0.50
1	5.45	-11.36	88.64	38.64	0.44
2	3.32	-13.25	86.75	36.75	0.42
3	2.06	-13.60	86.40	36.40	0.42
4	1.28	-13.67	86.33	36.33	0.42
5	0.80	-13.69	86.31	36.31	0.42
6	0.50	-13.69	86.31	36.31	0.42
7	0.31	-13.69	86.31	36.31	0.42
8	0.19	-13.69	86.31	36.31	0.42
9	0.12	-13.69	86.31	36.31	0.42
10	0.07	-13.69	86.31	36.31	0.42
11	0.05	-13.69	86.31	36.31	0.42
12	0.03	-13.69	86.31	36.31	0.42
13	0.02	-13.69	86.31	36.31	0.42
14	0.01	-13.69	86.31	36.31	0.42
15	0.01	-13.69	86.31	36.31	0.42
16	0.00	-13.69	86.31	36.31	0.42
17	0.00	-13.69	86.31	36.31	0.42
18	0.00	-13.69	86.31	36.31	0.42
19	0.00	-13.69	86.31	36.31	0.42
20	0.00	-13.69	86.31	36.31	0.42