

Lecture 14

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Lecture 13 examined selection response with multiple traits. Here we consider measuring selection on multivariate phenotypes in some detail, as this is a very popular exercise in modern evolutionary biology. Moving to multiple traits poses no changes in measuring fitnesses of *individuals* (Lecture 12), but does require us to provide the multivariate versions of the univariate differentials S and C and gradients β and γ . As might be expected, these are the matrix extensions of their univariate counterparts (Lecture 12).

SELECTION ON MULTIVARIATE PHENOTYPES: DIFFERENTIALS AND GRADIENTS

Lecture 12 described a variety of measures of univariate selection, with an emphasis on approximating the individual fitness function. In extending these methods to multiple characters, our main concern is the effect of phenotypic correlations. Our development is based on the multiple regression approach of Lande and Arnold (1983). Similar approaches based on path analysis have also been suggested (Maddox and Antonovics 1983, Mitchell-Olds 1987, Crespi and Bookstein 1988). These offer a complementary method of analysis as is discussed below.

The phenotype of an individual is now a vector $\mathbf{z} = (z_1, z_2, \dots, z_n)^T$ of n character values. Denote the mean vector and covariance matrix of \mathbf{z} before selection by $\boldsymbol{\mu}$ and \mathbf{P} , and by $\boldsymbol{\mu}^*$ and \mathbf{P}^* after selection (but before reproduction). To avoid additional complications, we examine only a single episode of selection.

Changes in the Mean Vector: The Directional Selection Differential, \mathbf{S}

The multivariate extension of the **directional selection differential** S is the vector

$$\mathbf{S} = \boldsymbol{\mu}^* - \boldsymbol{\mu}$$

whose i th element is S_i , the differential for character z_i . As with the univariate case, the Robertson-Price identity (Equation 12.8) holds, so that the elements of \mathbf{S} represent the covariance between character value and relative fitness, $S_i = \sigma(z_i, w)$. This immediately implies (Equation 12.5) that the opportunity for selection I (the population variance in **relative** fitness) bounds the range of S_i ,

$$\frac{|S_i|}{\sigma_{z_i}} \leq \sqrt{I} \quad (14.1)$$

As is illustrated in Figure 14.1, \mathbf{S} confounds the direct effects of selection on a character with the indirect effects due to selection on phenotypically correlated characters. Suppose character 1 is under direct selection to increase in value while character 2 is not directly selected. As Figure 14.1 shows, if z_1 and z_2 are uncorrelated, there is no within-generation change in μ_2 (the mean of z_2). However, if z_1 and z_2 are positively correlated, individuals with large values of z_1 also tend to have large values of z_2 , resulting in a within-generation increase in μ_2 . Conversely, if z_1 and z_2 are negatively correlated, selection to increase z_1 results in a within-generation decrease in μ_2 . Hence, a character not under selection can still experience a within-generation change in its phenotypic distribution due to selection on a phenotypically correlated character (indirect selection). Fortunately, the **directional selection gradient** $\boldsymbol{\beta} = \mathbf{P}^{-1}\mathbf{S}$ accounts for indirect selection due to phenotypic correlations, providing a less biased picture of the nature of directional selection acting on \mathbf{z} .

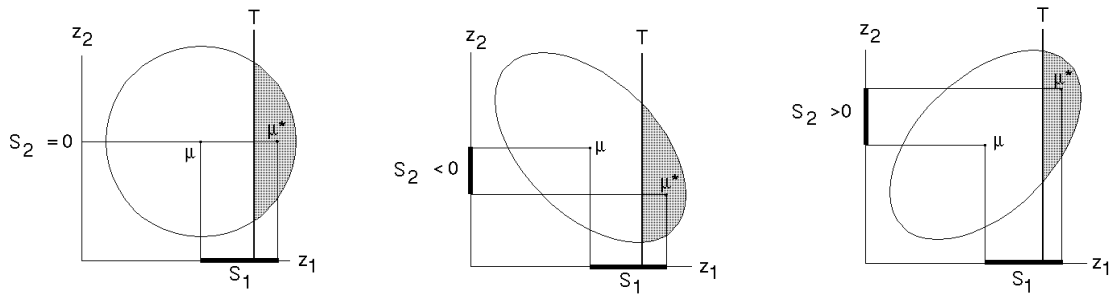


Figure 14.1. Selection on a character can result in a within-generation change in the mean of other phenotypically correlated characters not themselves under direct selection. Assume that character 1 is under simple truncation selection so that only individuals with $z_1 > T$ reproduce. **Left:** When z_1 and z_2 are uncorrelated, $S_2 = 0$. **Center:** When z_1 and z_2 are negatively correlated, $S_2 < 0$. **Right:** When z_1 and z_2 are positively correlated, $S_2 > 0$.

The Directional Selection Gradient β

As we will discuss shortly, the directional selection gradient β removes the effects of phenotypic correlations because it is a vector of partial regression coefficients. From multiple regression theory (Lecture 2), the vector of partial regression coefficients for predicting the value of y given a vector of observations \mathbf{z} is $\mathbf{P}^{-1} \boldsymbol{\sigma}(\mathbf{z}, y)$, where \mathbf{P} is the covariance matrix of \mathbf{z} , and $\boldsymbol{\sigma}(\mathbf{z}, y)$ is the vector of covariances between the elements of \mathbf{z} and the variable y . Since $\mathbf{S} = \boldsymbol{\sigma}(\mathbf{z}, w)$, it immediately follows that

$$\mathbf{P}^{-1} \boldsymbol{\sigma}(\mathbf{z}, w) = \mathbf{P}^{-1} \mathbf{S} = \boldsymbol{\beta} \quad (14.2)$$

is the vector of partial regression for the best linear regression of **relative** fitness w on phenotypic value \mathbf{z} , viz.,

$$w(\mathbf{z}) = a + \sum_{j=1}^n \beta_j z_j = a + \boldsymbol{\beta}^T \mathbf{z} \quad (14.3a)$$

Our main interest in this equation is the vector $\boldsymbol{\beta}$ of partial regression coefficients – the slopes for the individual z_i . There are several equivalent ways writing this expression and these various forms interchangeably appear in the literature. First, noting that the regression passes through the mean of w and the mean of \mathbf{z} , namely $(1, \boldsymbol{\mu})$,

$$w(\mathbf{z}) = 1 + \sum_{j=1}^n \beta_j (z_j - \mu_j) = 1 + \boldsymbol{\beta}^T (\mathbf{z} - \boldsymbol{\mu}) \quad (14.3b)$$

We can also translate the \mathbf{z} values before the analysis to set $\boldsymbol{\mu} = 0$, in which case

$$w(\mathbf{z}) = 1 + \sum_{j=1}^n \beta_j z_j = 1 + \boldsymbol{\beta}^T \mathbf{z} \quad (14.3c)$$

Since β_j is a partial regression coefficient, it represents the change generated in relative fitness by changing z_j while holding all other character values in \mathbf{z} constant — a one unit increase in z_j (holding all other characters constant) increases the expected relative fitness by β_j . Provided we can exclude the possibility of unmeasured characters influencing fitness that are phenotypically correlated with \mathbf{z} , a character under no directional selection has $\beta_j = 0$ — when all other characters are held constant, the best linear regression predicts no change in expected fitness as we change the value of z_j . Thus, $\boldsymbol{\beta}$ accounts for the effects of phenotypic correlations only among the **measured**

characters. Unmeasured traits under selection that are phenotypically correlated with those we measure and/or unmeasured environmental factors that influence both fitness and the values of our measured traits result in β being a biased measure of the amount of directional selection acting on each measured character.

Since $\mathbf{S} = \mathbf{P}\beta$, we have

$$S_i = \sum_{j=1}^n \beta_j P_{ij} = \beta_i P_{ii} + \sum_{j \neq i} \beta_j P_{ij} \quad (14.4)$$

illustrating that the directional selection differential confounds direct selection on that character with indirect contributions due to selection on phenotypically correlated characters. Equation 14.4 implies that if two characters are phenotypically uncorrelated ($P_{ij} = 0$), selection on one has no within-generation effect on the phenotypic mean of the other. However, recall from Lecture 13 that if i and j are *genetically* correlated (non-zero additive genetic covariance), then selection on one trait results in a correlated response in the other, *even if there is no phenotypic within-generation change in the mean*.

Directional Gradients, Fitness Surface Geometry and Selection Response

When phenotypes are multivariate normal, β provides a convenient descriptor of the geometry of both the individual and mean population fitness surfaces. Recall from vector calculus that the gradient vector $\nabla_{\mathbf{x}}f(\mathbf{x})$ is defined at

$$\nabla_{\mathbf{x}}f(\mathbf{x}) = \begin{pmatrix} \partial f / \partial x_1 \\ \partial f / \partial x_2 \\ \vdots \\ \partial f / \partial x_n \end{pmatrix}$$

Further recall that the gradient vector of a function points to the direction of change in the variables that will give the greatest (local) increase in the function. In Lecture 15 we will show that

$$\beta = \nabla_{\boldsymbol{\mu}}[\ln \bar{W}(\boldsymbol{\mu})] = \bar{W}^{-1} \cdot \nabla_{\boldsymbol{\mu}}[\bar{W}(\boldsymbol{\mu})] \quad (14.5a)$$

which holds provided fitnesses are frequency-independent (Lande 1976, 1979). In this case β is the gradient of **mean population** fitness with respect to the mean vector $\boldsymbol{\mu}$. Since β gives the direction of steepest increase in the mean population fitness surface, mean population fitness increases most rapidly when $\mathbf{R} = \beta$, i.e., when the between-generation change in means is in the same direction as the selection gradient. If fitnesses are frequency-dependent (individual fitnesses change as the population mean changes), then for $\mathbf{z} \sim \text{MVN}$,

$$\beta = \nabla_{\boldsymbol{\mu}}[\ln \bar{W}(\boldsymbol{\mu})] + \int \nabla_{\boldsymbol{\mu}}[w(\mathbf{z})] \phi(\mathbf{z}) d\mathbf{z} \quad (14.5b)$$

where the second term accounts for the effects of frequency-dependence and ϕ is the MVN density function (Lande 1976). Here β does not point in the direction of steepest increase in \bar{W} unless the second integral is zero.

If we instead consider the **individual fitness** surface $w(\mathbf{z})$, we can alternatively express β as the gradient of **individual fitnesses** averaged over the population distribution of phenotypes,

$$\beta = \int \nabla_{\mathbf{z}}[w(\mathbf{z})] \phi(\mathbf{z}) d\mathbf{z} \quad (14.6)$$

which holds provided $\mathbf{z} \sim \text{MVN}$ (Lande and Arnold 1983). To see this, using integration by parts gives

$$\int_{\mathbf{a}}^{\mathbf{b}} \nabla_{\mathbf{z}}[w(\mathbf{z})] \phi(\mathbf{z}) \, d\mathbf{z} = w(\mathbf{z}) \phi(\mathbf{z}) \Big|_{\mathbf{a}}^{\mathbf{b}} - \int_{\mathbf{a}}^{\mathbf{b}} \nabla_{\mathbf{z}}[\phi(\mathbf{z})] w(\mathbf{z}) \, d\mathbf{z}$$

Taking the limit as $\mathbf{a} \rightarrow -\infty$ and $\mathbf{b} \rightarrow \infty$, the first term on the right-hand side vanishes as $\phi(\mathbf{z}) \rightarrow 0$ when $\mathbf{z} \rightarrow \pm\infty$ (as the phenotypic distribution is assumed to be bounded). If $\mathbf{z} \sim \text{MVN}(\boldsymbol{\mu}, \mathbf{P})$, then we will show in Lecture 15 that

$$\nabla_{\mathbf{z}}[\phi(\mathbf{z})] = \phi(\mathbf{z}) \mathbf{P}^{-1} (\mathbf{z} - \boldsymbol{\mu})$$

Hence

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

Note from this derivation that Equation 14.6 holds regardless of whether fitness is frequency dependent or frequency independent.

Finally, while our focus has been on the role $\boldsymbol{\beta}$ plays in measuring phenotypic selection, it also plays an important role in the response to selection. If we can assume the breeders' equation holds, $\boldsymbol{\beta}$ is the only measure of phenotypic selection required to predict the response in mean as $\mathbf{R} = \mathbf{G}\boldsymbol{\beta}$. Cheverud (1984) makes the important point that although it is often assumed a set of phenotypically correlated traits responds to selection in a coordinated fashion, this is not necessarily the case. Since $\boldsymbol{\beta}$ removes the effects of phenotypic correlations, phenotypic characters will only respond as a group if they are all under direct selection or if they are **genetically** correlated, a point we discussed in detail in Lecture 13.

Changes in the Covariance Matrix: The Quadratic Selection Differential \mathbf{C}

Motivated by the univariate case wherein $C = \sigma[w, (z - \mu)(z - \mu)]$, define the multivariate **quadratic selection differential** to be a square ($n \times n$) matrix \mathbf{C} whose elements are the covariances between all pairs of quadratic deviations $(z_i - \mu_{z_i})(z_j - \mu_{z_j})$ and relative fitness w , viz.,

$$C_{ij} = \sigma[w, (z_i - \mu_{z_i})(z_j - \mu_{z_j})] \quad (14.7a)$$

As is derived below (Example 14.1), Lande and Arnold (1983) showed that

$$\mathbf{C} = \sigma[w, (\mathbf{z} - \boldsymbol{\mu})(\mathbf{z} - \boldsymbol{\mu})^T] = \mathbf{P}^* - \mathbf{P} + \mathbf{S}\mathbf{S}^T \quad (14.7b)$$

If no quadratic selection is acting, the covariance between each quadratic deviation and fitness is zero and $\mathbf{C} = \mathbf{0}$. In this case Equation 14.7b gives

$$P_{ij}^* - P_{ij} = -S_i S_j \quad (14.8)$$

demonstrating that the $S_i S_j$ term corrects C_{ij} for the change in covariance caused by directional selection alone.

Example 14.1. We wish to show $\mathbf{P}^* - \mathbf{P} = \sigma[w, (\mathbf{z} - \boldsymbol{\mu})(\mathbf{z} - \boldsymbol{\mu})^T] - \mathbf{S}\mathbf{S}^T$, which implies Equation 14.7b. From the definition of the variance-covariance matrix,

$$\begin{aligned} \mathbf{P} &= E [(\mathbf{z} - \boldsymbol{\mu})(\mathbf{z} - \boldsymbol{\mu})^T] = \int (\mathbf{z} - \boldsymbol{\mu})(\mathbf{z} - \boldsymbol{\mu})^T p(\mathbf{z}) \, d\mathbf{z} \\ \mathbf{P}^* &= E [(\mathbf{z}^* - \boldsymbol{\mu}^*)(\mathbf{z}^* - \boldsymbol{\mu}^*)^T] = \int (\mathbf{z} - \boldsymbol{\mu}^*)(\mathbf{z} - \boldsymbol{\mu}^*)^T p^*(\mathbf{z}) \, d\mathbf{z} \end{aligned}$$

where $p^*(\mathbf{z}) = w(\mathbf{z}) p(\mathbf{z})$ is the distribution of \mathbf{z} after selection (but before reproduction). Noting that $\boldsymbol{\mu}^* = \boldsymbol{\mu} + \mathbf{S}$,

$$\begin{aligned} (\mathbf{z} - \boldsymbol{\mu}^*)(\mathbf{z} - \boldsymbol{\mu}^*)^T &= (\mathbf{z} - \boldsymbol{\mu} - \mathbf{S})(\mathbf{z} - \boldsymbol{\mu} - \mathbf{S})^T \\ &= (\mathbf{z} - \boldsymbol{\mu} - \mathbf{S})(\mathbf{z} - \boldsymbol{\mu})^T - \mathbf{S}^T \\ &= (\mathbf{z} - \boldsymbol{\mu})(\mathbf{z} - \boldsymbol{\mu})^T - (\mathbf{z} - \boldsymbol{\mu})\mathbf{S}^T - \mathbf{S}(\mathbf{z} - \boldsymbol{\mu})^T + \mathbf{S}\mathbf{S}^T \end{aligned}$$

Since $\int \mathbf{z} p^*(\mathbf{z}) d\mathbf{z} = \boldsymbol{\mu}^*$ and $\int p^*(\mathbf{z}) d\mathbf{z} = 1$, we have that $\int \mathbf{S}\mathbf{S}^T p^*(\mathbf{z}) d\mathbf{z} = \mathbf{S}\mathbf{S}^T$,

$$\begin{aligned} \int (\mathbf{z} - \boldsymbol{\mu})\mathbf{S}^T p^*(\mathbf{z}) d\mathbf{z} &= (\boldsymbol{\mu}^* - \boldsymbol{\mu})\mathbf{S}^T = \mathbf{S}\mathbf{S}^T, \quad \text{and} \\ \int \mathbf{S}(\mathbf{z} - \boldsymbol{\mu})^T p^*(\mathbf{z}) d\mathbf{z} &= \mathbf{S}(\boldsymbol{\mu}^*)^T - \mathbf{S}\boldsymbol{\mu}^T = \mathbf{S}(\boldsymbol{\mu}^* - \boldsymbol{\mu})^T = \mathbf{S}\mathbf{S}^T \end{aligned}$$

Combining these results,

$$\begin{aligned} \mathbf{P}^* &= \int (\mathbf{z} - \boldsymbol{\mu})(\mathbf{z} - \boldsymbol{\mu})^T w(\mathbf{z}) p(\mathbf{z}) d\mathbf{z} - \mathbf{S}\mathbf{S}^T - \mathbf{S}\mathbf{S}^T + \mathbf{S}\mathbf{S}^T \\ &= E[w(\mathbf{z}) \cdot (\mathbf{z} - \boldsymbol{\mu})(\mathbf{z} - \boldsymbol{\mu})^T] - \mathbf{S}\mathbf{S}^T \end{aligned}$$

Since $E[w(\mathbf{z})] = 1$, we can write $\mathbf{P} = E[w(\mathbf{z})] \cdot \mathbf{P}$. Using the definition of \mathbf{P} then gives

$$\begin{aligned} \mathbf{P}^* - \mathbf{P} &= E[w(\mathbf{z}) \cdot (\mathbf{z} - \boldsymbol{\mu})(\mathbf{z} - \boldsymbol{\mu})^T] - \mathbf{S}\mathbf{S}^T - E[w(\mathbf{z})] \cdot E[(\mathbf{z} - \boldsymbol{\mu})(\mathbf{z} - \boldsymbol{\mu})^T] \\ &= \sigma[w(\mathbf{z}), (\mathbf{z} - \boldsymbol{\mu})(\mathbf{z} - \boldsymbol{\mu})^T] - \mathbf{S}\mathbf{S}^T \end{aligned}$$

with the last equality following from $\sigma(x, y) = E(x \cdot y) - E(x)E(y)$.

As was the case for \mathbf{S} , the fact that C_{ij} is a covariance immediately allows us to bound its range using the opportunity for selection. Since $\sigma^2(x, y) \leq \sigma^2(x)\sigma^2(y)$,

$$C_{ij}^2 \leq I \sigma^2[(z_i - \mu_{z_i})(z_j - \mu_{z_j})] \quad (14.9a)$$

When z_i and z_j are bivariate normal, then (Kendall and Stuart 1983),

$$\sigma^2[(z_i - \mu_{z_i})(z_j - \mu_{z_j})] = P_{ij}^2 + P_{ii}P_{jj} = P_{ij}^2(1 + \rho_{ij}^{-2}) \quad (14.9b)$$

where ρ_{ij} is the phenotypic covariance between z_i and z_j . Hence, for Gaussian-distributed phenotypes,

$$\left| \frac{C_{ij}}{P_{ij}} \right| \leq \sqrt{I} \sqrt{1 + \rho_{ij}^{-2}} \quad (14.10)$$

which is a variant of the original bound based on I suggested by Arnold (1986).

The Quadratic Selection Gradient, γ

Like \mathbf{S} , \mathbf{C} confounds the effects of direct selection with selection on phenotypically correlated characters. However, as was true for \mathbf{S} , these indirect effects can also be removed by a regression. Consider the best **quadratic** regression of relative fitness as a function of phenotypic value,

$$w(\mathbf{z}) = a + \sum_{j=1}^n b_j z_j + \frac{1}{2} \sum_{j=1}^n \sum_{k=1}^n \gamma_{jk} (z_j - \mu_j)(z_k - \mu_k) \quad (14.11a)$$

$$= a + \mathbf{b}^T \mathbf{z} + \frac{1}{2} (\mathbf{z} - \boldsymbol{\mu})^T \boldsymbol{\gamma} (\mathbf{z} - \boldsymbol{\mu}) \quad (14.11b)$$

Where the ij -th element of the matrix γ is γ_{ij} . Again, we can expression this in a simpler form by translating \mathbf{z} so all traits have mean zero, in which case

$$w(\mathbf{z}) = 1 + \mathbf{b}^T \mathbf{z} + \frac{1}{2} \mathbf{z}^T \gamma \mathbf{z} \quad (14.11c)$$

Using multiple regression theory (Lande and Arnold 1983), the matrix γ of quadratic partial regression coefficients is given by

$$\gamma = \mathbf{P}^{-1} \sigma[w, (\mathbf{z} - \boldsymbol{\mu})(\mathbf{z} - \boldsymbol{\mu})^T] \mathbf{P}^{-1} = \mathbf{P}^{-1} \mathbf{C} \mathbf{P}^{-1} \quad (14.12)$$

This is the **quadratic selection gradient** and (like β) removes the effects of phenotypic correlations, providing a more accurate picture of how selection is operating on the multivariate phenotype.

The vector of linear coefficients \mathbf{b} for the quadratic regression need not equal the vector of partial regression coefficients β obtained by assuming only a **linear** regression. Equation 12.21 shows (for the univariate case) that if the phenotypic distribution is skewed, b is a function of both S and C , while β is only a function of S . When phenotypes are multivariate normal, skew is absent and Lande and Arnold (1983) show that $\mathbf{b} = \beta$, recovering the multivariate version of the Pearson-Lande-Arnold regression,

$$w(\mathbf{z}) = 1 + \beta^T \mathbf{z} + \frac{1}{2} \mathbf{z}^T \gamma \mathbf{z} \quad (14.13)$$

Since the γ_{ij} are partial regression coefficients, they predict the change in expected fitness caused by changing the associated quadratic deviation while holding all other variables constant. Increasing $(z_j - \mu_j)(z_k - \mu_k)$ by one unit in such a way as to hold all other variables and pairwise combinations of characters constant, relative fitness is expected to increase by γ_{jk} for $j \neq k$ and by $\gamma_{jj}/2$ if $j = k$ (the difference arises because $\gamma_{jk} = \gamma_{kj}$, so that γ_{jk} appears twice in the regression unless $j = k$). The coefficients of γ thus describe the nature of selection on quadratic deviations from the mean for both single characters and pairwise combinations of characters. $\gamma_{ii} < 0$ implies fitness is expected to decrease as z_i moves away (in either direction) from its mean. As was discussed in Lecture 11, this is a necessary, *but not sufficient*, condition for stabilizing selection on character i . As a result, the term **convex selection** or **convex fitness surface** is often used with stabilizing selection restricted for when the fitness surface is *both convex and* the population distribution is under a peak in the fitness surface. Similarly, $\gamma_{ii} > 0$ implies fitness is expected to increase as i moves away from its mean (**concave selection**), again a necessary, but not sufficient conditional for disruptive selection. Turning to combinations of characters, non-zero values of γ_{jk} ($j \neq k$) suggests the presence of **correlation selection** — $\gamma_{jk} > 0$ suggests selection for a positive correlation between characters j and k , while $\gamma_{jk} < 0$ suggests selection for a negative correlation.

Example 14.2. Brodie (1992) examined one-year survivorship in the garter snake *Thamnophis ordinoides* in a population in Oregon. Over a three year period, 646 snakes were marked, 101 of which were eventually recaptured. Four morphological and behavior characters were measured — overall stripedness of the body color pattern (stripes), sprint speed, distance moved until an antipredator display performed, and number of reversals of direction during flight from predators (reversals). None of the β_i or γ_{ii} were significant. However, there was a significant quadratic association between striping pattern and number of reversals, with $\gamma_{ij} = -0.268 \pm 0.097$. As is shown in Figure 14.2, the best-fitting quadratic regression of individual fitness has a saddle point. Brodie suggests a biological explanation for selection favoring a negative correlation between these two characters. The presence of body stripes makes it difficult for predators to judge the speed of the snake, so frequent reversals would be disadvantageous. Conversely, when the body pattern is banded, blotched or spotted, detection of movement by visual predators is enhanced. In such individuals, frequent reversals can disrupt a visual search.

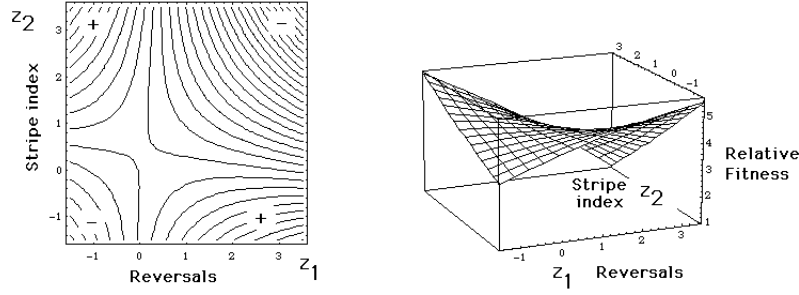


Figure 14.2. The fitness surface (measured as one-year survivorship) for z_1 (number of reversals) and z_2 (body stripe index) in the garter snake *Thamnophis ordinoides*. There is a significant correlational gradient between these two characters, with all other directional and quadratic gradients being nonsignificant. **Left:** Plotting lines of equal fitness, with peaks represented by a + and valleys by a - shows the best-fitting quadratic fitness surface has a saddle point. **Right:** Three-dimensional representation of the best-fitting quadratic fitness surface. The eigenvalues of γ are 0.256 and -0.290 , indicating roughly equal amounts of convex selection along one canonical axis (given by the index $0.77 \cdot z_1 - 0.64 \cdot z_2$) and concave selection along the other ($0.64 \cdot z_1 + 0.77 \cdot z_2$). Data from Brodie (1992).

Although it seems straightforward to infer the overall nature of selection by looking at these various pairwise combinations, this can give a very misleading picture about the geometry of the fitness surface. We discuss this problem and its solution shortly.

Finally, we can see the effects of phenotypic correlations in the quadratic selection differential. Solving for \mathbf{C} by post- and pre-multiplying γ by \mathbf{P} gives $\mathbf{C} = \mathbf{P} \gamma \mathbf{P}$, or

$$C_{ij} = \sum_{k=1}^n \sum_{\ell=1}^n \gamma_{k\ell} P_{ik} P_{\ell j} \quad (14.14)$$

showing that within-generation changes in phenotypic covariance, as measured by \mathbf{C} , are influenced by quadratic selection on phenotypically-correlated characters.

Quadratic Gradients, Fitness Surface Geometry and Selection Response

When phenotypes are multivariate-normally distributed, γ provides a measure of the average curvature of the **individual** fitness surface, as

$$\gamma = \int \mathbf{H}_{\mathbf{z}}[W(\mathbf{z})] \phi(\mathbf{z}) d\mathbf{z} \quad (14.15a)$$

where $\mathbf{H}_{\mathbf{z}}[f]$ denotes the Hessian matrix with respect to \mathbf{z} and is a multivariate measure of the quadratic curvature of a function (the ij -th element of $\mathbf{H}_{\mathbf{z}}[f]$ is $\partial^2 f / \partial z_i \partial z_j$). This result, due to Lande and Arnold (1983), can be obtained by an integration by parts argument similar to that used to obtain Equation 14.6, and holds for both frequency-dependent and frequency-independent fitnesses. When fitnesses are frequency-independent (again provided $\mathbf{z} \sim \text{MVN}$), γ provides a description of the curvature of the **log mean population** fitness surface, with

$$\mathbf{H}_{\boldsymbol{\mu}}[\ln \bar{W}(\boldsymbol{\mu})] = \gamma - \beta \beta^T \quad (14.15b)$$

In particular,

$$\frac{\partial \ln \bar{W}(\boldsymbol{\mu})}{\partial \mu_i \partial \mu_j} = \gamma_{ij} - \beta_i \beta_j \quad (14.15c)$$

This result is due to Lande (cited in Phillips and Arnold 1989) and points out that there are two sources for curvature in the mean fitness surface: $-\beta\beta^T$ from directional selection and γ from quadratic selection.

Finally, when the breeders' equation holds, γ and β are sufficient to describe phenotypic selection on the additive-genetic covariance matrix. From Example 14.3 (below), the difference between the additive genetic covariance \mathbf{G}^* after selection (but before reproduction) and the covariance matrix \mathbf{G} before selection is

$$\mathbf{G}^* - \mathbf{G} = \mathbf{G}\mathbf{P}^{-1}(\mathbf{P}^* - \mathbf{P})\mathbf{P}^{-1}\mathbf{G} \quad (14.16a)$$

We can express this in terms of gradients as follows:

$$\begin{aligned} \mathbf{G}^* - \mathbf{G} &= \mathbf{G}\mathbf{P}^{-1}(\mathbf{P}^* - \mathbf{P})\mathbf{P}^{-1}\mathbf{G} \\ &= \mathbf{G}\mathbf{P}^{-1}(\mathbf{C} - \mathbf{S}\mathbf{S}^T)\mathbf{P}^{-1}\mathbf{G} \\ &= \mathbf{G}(\mathbf{P}^{-1}\mathbf{C}\mathbf{P}^{-1} - (\mathbf{P}^{-1}\mathbf{S})(\mathbf{P}^{-1}\mathbf{S})^T)\mathbf{G} \\ &= \mathbf{G}(\gamma - \beta\beta^T)\mathbf{G} \end{aligned} \quad (14.16b)$$

Hence, the within-generation change in \mathbf{G} has a component from directional selection (β) and a second due from quadratic selection (γ),

$$\begin{aligned} \mathbf{G}^* - \mathbf{G} &= -\mathbf{G}\beta\beta^T\mathbf{G} + \mathbf{G}\gamma\mathbf{G} \\ &= -\mathbf{R}\mathbf{R}^T + \mathbf{G}\gamma\mathbf{G} \end{aligned} \quad (14.16c)$$

In terms of the change in covariance for two particular characters, this can be factored as

$$\begin{aligned} G_{ij}^* - G_{ij} &= -\left(\sum_{k=1}^n \beta_k G_{ik}\right)\left(\sum_{k=1}^n \beta_k G_{jk}\right) + \sum_{k=1}^n \sum_{\ell=1}^n \gamma_{k\ell} G_{ik} G_{\ell j} \\ &= -R_i \cdot R_j + \sum_{k=1}^n \sum_{\ell=1}^n \gamma_{k\ell} G_{ik} G_{\ell j} \end{aligned} \quad (14.16d)$$

Thus the within-generation change in the additive genetic variance of character i is given by

$$G_{ii}^* - G_{ii} = -(R_i)^2 + \sum_{k=1}^n \sum_{\ell=1}^n \gamma_{k\ell} G_{ik} G_{i\ell} \quad (14.16e)$$

Example 14.3. *This example is a technical derivation and can be skipped by the casual reader.* What is \mathbf{G}^* , the variance-covariance matrix of breeding values after selection (but before recombination and random mating) under the assumptions leading to the multivariate breeders' equation? From the definition of a covariance matrix,

$$\mathbf{G}^* = E\left((\mathbf{g} - \boldsymbol{\mu}^*)(\mathbf{g} - \boldsymbol{\mu}^*)^T\right)$$

where $\boldsymbol{\mu}^*$ is the vector of phenotypic means following selection. Using, respectively, Equation 13.14a, the matrix identity $(\mathbf{A}\mathbf{B}\mathbf{c})^T = \mathbf{c}^T\mathbf{B}^T\mathbf{A}^T$ (recalling that \mathbf{G} and \mathbf{P}^{-1} are symmetric), and expanding gives

$$\begin{aligned} \mathbf{G}^* &= E\left(\left[\mathbf{G}\mathbf{P}^{-1}(\mathbf{z} - \boldsymbol{\mu}^*) + \mathbf{e}\right]\left[\mathbf{G}\mathbf{P}^{-1}(\mathbf{z} - \boldsymbol{\mu}^*) + \mathbf{e}\right]^T\right) \\ &= E\left(\left[\mathbf{G}\mathbf{P}^{-1}(\mathbf{z} - \boldsymbol{\mu}^*) + \mathbf{e}\right]\left[(\mathbf{z} - \boldsymbol{\mu}^*)^T\mathbf{P}^{-1}\mathbf{G} + \mathbf{e}^T\right]\right) \\ &= E\left(\mathbf{G}\mathbf{P}^{-1}(\mathbf{z} - \boldsymbol{\mu}^*)(\mathbf{z} - \boldsymbol{\mu}^*)^T\mathbf{P}^{-1}\mathbf{G}\right) + E\left(\mathbf{G}\mathbf{P}^{-1}(\mathbf{z} - \boldsymbol{\mu}^*)\mathbf{e}^T\right) \\ &\quad + E\left(\mathbf{e}(\mathbf{z} - \boldsymbol{\mu}^*)^T\mathbf{P}^{-1}\mathbf{G}\right) + E(\mathbf{e}\mathbf{e}^T) \end{aligned}$$

Using Equation 2.16a and the independence of \mathbf{e} and \mathbf{z} , this reduces to

$$\mathbf{G}^* = \mathbf{G}\mathbf{P}^{-1}E((\mathbf{z} - \boldsymbol{\mu}^*)(\mathbf{z} - \boldsymbol{\mu}^*)^T)\mathbf{P}^{-1}\mathbf{G} + \mathbf{G}\mathbf{P}^{-1}E(\mathbf{z} - \boldsymbol{\mu}^*)E(\mathbf{e}^T) \\ + E(\mathbf{e})E((\mathbf{z} - \boldsymbol{\mu}^*)^T)\mathbf{P}^{-1}\mathbf{G} + E(\mathbf{e}\mathbf{e}^T)$$

This can be further simplified by noting that $E(\mathbf{e}) = \mathbf{0}$ and that $E[(\mathbf{z} - \boldsymbol{\mu}^*)(\mathbf{z} - \boldsymbol{\mu}^*)^T] = \mathbf{P}^*$ is the phenotypic variance-covariance matrix after selection. Finally, $E(\mathbf{e}\mathbf{e}^T) = \mathbf{V}_e$, giving

$$\mathbf{G}^* = \mathbf{G}\mathbf{P}^{-1}\mathbf{P}^*\mathbf{P}^{-1}\mathbf{G} + \mathbf{0} + \mathbf{0} + (\mathbf{G} - \mathbf{G}\mathbf{P}^{-1}\mathbf{G})$$

Writing $\mathbf{G}\mathbf{P}^{-1}\mathbf{G} = \mathbf{G}\mathbf{P}^{-1}\mathbf{P}\mathbf{P}^{-1}\mathbf{G}$ and factoring gives the within-generation change in the variance-covariance matrix of breeding values as

$$\mathbf{G}^* - \mathbf{G} = \mathbf{G}\mathbf{P}^{-1}\mathbf{P}^*\mathbf{P}^{-1}\mathbf{G} - \mathbf{G}\mathbf{P}^{-1}\mathbf{P}\mathbf{P}^{-1}\mathbf{G} \\ = \mathbf{G}\mathbf{P}^{-1}(\mathbf{P}^* - \mathbf{P})\mathbf{P}^{-1}\mathbf{G}$$

as obtained by Lande and Arnold (1983).

Summary

Table 14.1 (next page) summarizes the main features of differentials and gradients.

MULTIDIMENSIONAL QUADRATIC FITNESS REGRESSIONS

As noted in Lecture 11, in many cases approximating the individual fitness function by a quadratic may give a very distorted view of the true fitness surface (e.g., when multiple fitness peaks are present). With this caveat in mind, quadratic fitness surfaces are still quite useful. One advantage is that a quadratic is the simplest surface allowing for curvature. Further, when phenotypes are gaussian distributed, the coefficients in the quadratic regression also appear as the coefficients of equations for predicting evolutionary change (Table 14.1). We briefly review some statistical issues of fitting such regressions before examining the geometry of multivariate quadratic regressions, which can get rather involved.

Estimation, Hypothesis Testing and Confidence Intervals

Even if we can assume that a best-fit quadratic is a reasonable approximation of the individual fitness surface, we are still faced with a number of statistical problems. Unless we test for, and confirm, multivariate normality, β and γ must be estimated from separate regressions — β from the best linear regression, γ from the best quadratic regression. In either case, there are a large number of parameters to estimate — γ has $n(n+1)/2$ terms and β has n terms, for a total $n(n+3)/2$. With 5, 10, and 25 characters, this corresponds to 20, 65 and 350 parameters. The number of observations should greatly exceed $n(n+3)/2$ in order estimate these parameters with any precision.

A second problem is **multicollinearity** — if many of the characters being measured are highly correlated with each other, the phenotypic covariance matrix \mathbf{P} can be nearly singular, so that small errors in estimating \mathbf{P} result in large differences in \mathbf{P}^{-1} , which in turn gives a very large sampling variance for the estimate of β and γ . One possibility is to use principal components to extract a subset of the characters (measured as PCs, linear combinations of the characters) that explains most of the phenotypic variance of \mathbf{P} , and the perform fitness regressions using the first few PCs as the characters (Lande and Arnold 1983). This approach also reduces the problem of the number of parameters to estimate, but some have expressed concern that it risks the real possibility of removing the most important characters and PCs are often difficult to interpret biologically. While the first PC for morphological characters generally corresponds to a general measure of size, the others are often much more problematic. Finally, using PCs can spread the effects of selection on one character over several PCs, further complicating interpretation.

Table 14.1. Analogous features of directional and quadratic differentials and gradients.

Changes in Means (Directional Selection)	Changes in Covariances (Quadratic Selection)
Differentials measure the covariance between relative fitness and phenotype	
$S_i = \sigma [w, z_i]$	$C_{ij} = \sigma [w, (z_i - \mu_i)(z_j - \mu_j)]$
The opportunity for selection bounds the differential	
$\frac{ S_i }{\sigma(z_i)} \leq \sqrt{I}$ for any distribution of \mathbf{z}	$\left \frac{C_{ij}}{P_{ij}} \right \leq \sqrt{I} \sqrt{1 + \rho_{ij}^{-2}}$ provided $\mathbf{z} \sim \text{MVN}$
Differentials confound direct and indirect selection	
$\mathbf{S} = \boldsymbol{\mu}^* - \boldsymbol{\mu} = \mathbf{P}\boldsymbol{\beta}$	$\mathbf{C} = \mathbf{P}^* - \mathbf{P} + \mathbf{S}\mathbf{S}^T = \mathbf{P}\boldsymbol{\gamma}\mathbf{P}$
Gradients measure the amount of direct selection	
$\boldsymbol{\beta} = \mathbf{P}^{-1}\mathbf{S}$	$\boldsymbol{\gamma} = \mathbf{P}^{-1}\mathbf{C}\mathbf{P}^{-1}$
Gradients describe the slope and curvature of the mean population fitness surface, provided $\mathbf{z} \sim \text{MVN}$ and fitnesses are frequency-independent	
$\beta_i = \frac{\partial \ln \bar{W}(\boldsymbol{\mu})}{\partial \mu_i}$	$\gamma_{ij} = \frac{\partial^2 \ln \bar{W}(\boldsymbol{\mu})}{\partial \mu_i \partial \mu_j} + \beta_i \beta_j$
Gradients describe the average slope and average curvature of the individual fitness surface, provided $\mathbf{z} \sim \text{MVN}$	
$\beta_i = \int \frac{\partial w(\mathbf{z})}{\partial z_i} \phi(\mathbf{z}) d\mathbf{z}$	$\gamma_{ij} = \int \frac{\partial^2 w(\mathbf{z})}{\partial z_i \partial z_j} \phi(\mathbf{z}) d\mathbf{z}$
Gradients appear as coefficients in fitness regressions	
$w(\mathbf{z}) = a + \boldsymbol{\beta}^T(\mathbf{z} - \boldsymbol{\mu})$ $\boldsymbol{\beta}$ = slope of best linear fit	$w(\mathbf{z}) = a + \mathbf{b}^T(\mathbf{z} - \boldsymbol{\mu}) + \frac{1}{2}(\mathbf{z} - \boldsymbol{\mu})^T \boldsymbol{\gamma}(\mathbf{z} - \boldsymbol{\mu})$ $\boldsymbol{\gamma}$ = the quadratic coefficient of the best quadratic fit. $\mathbf{b} = \boldsymbol{\beta}$ when $\mathbf{z} \sim \text{MVN}$
Gradients appear as coefficients in evolutionary equations when $(\mathbf{z}, \mathbf{g}) \sim \text{MVN}$	
$\mathbf{R} = \mathbf{G}\boldsymbol{\beta}$	$\mathbf{G}^* - \mathbf{G} = \mathbf{G}(\boldsymbol{\gamma} - \boldsymbol{\beta}\boldsymbol{\beta}^T)\mathbf{G}$

An alternative option is that most traits we measure are themselves artificial, and we are naive to assume that they neatly correspond to the actual characters under selection. In such cases, a lower dimensional subspace of \mathbf{P} may contain most of the variation. As was the case for \mathbf{G} (Lecture 13), by considering such a subspace we are likely to gain a much better (and less biased) perspective on the nature of selection. We return to this point shortly.

Geometric Aspects

In spite of their apparent simplicity, multivariate quadratic fitness regressions have a rather rich geometric structure. Scaling characters so that they have mean zero, the general quadratic fitness regression can be written as

$$w(\mathbf{z}) = 1 + \sum_{i=1}^n b_i z_i + \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \gamma_{ij} z_i z_j = 1 + \mathbf{b}^T \mathbf{z} + \frac{1}{2} \mathbf{z}^T \boldsymbol{\gamma} \mathbf{z} \quad (14.17)$$

If $\mathbf{z} \sim \text{MVN}$, then $\mathbf{b} = \boldsymbol{\beta}$ (the vector of coefficients of the best *linear* fit). As an aside, if we regard Equation 14.17 as a second-order Taylor series approximation of $w(\mathbf{z})$, \mathbf{b} and $\boldsymbol{\gamma}$ can be interpreted as the gradient and hessian of individual fitness evaluated at the population mean (here $\boldsymbol{\mu} = \mathbf{0}$ by construction). The nature of curvature of Equation 14.17 is determined by the matrix $\boldsymbol{\gamma}$. Even though a quadratic is the simplest curved surface, its geometry can still be very difficult to visualize.

We start our exploration of this geometry by considering the gradient of this best-fit quadratic fitness surface. Taking the gradient of Equation 14.17 (Lecture 15 reviews these operations on matrices and vectors) gives

$$\nabla_{\mathbf{z}}[w(\mathbf{z})] = \mathbf{b} + \boldsymbol{\gamma} \mathbf{z} \quad (14.18)$$

Thus, at the point \mathbf{z} the direction of steepest ascent on the fitness surface (the direction in which to move in phenotype space to maximally increase individual fitness) is given by the vector $\mathbf{b} + \boldsymbol{\gamma} \mathbf{z}$ (when $\boldsymbol{\mu} = \mathbf{0}$).

Solving $\nabla_{\mathbf{z}}[w(\mathbf{z})] = \mathbf{0}$, a point \mathbf{z}_o is a candidate for a local extremum (stationary point) if $\boldsymbol{\gamma} \mathbf{z}_o = -\mathbf{b}$. When $\boldsymbol{\gamma}$ is nonsingular,

$$\mathbf{z}_o = -\boldsymbol{\gamma}^{-1} \mathbf{b} \quad (14.19a)$$

is the unique stationary point of this quadratic surface. Substituting into Equation 14.17, the expected individual fitness at this point is

$$w_o = a + \frac{1}{2} \mathbf{b}^T \mathbf{z}_o \quad (14.19b)$$

as obtained by Phillips and Arnold (1989). Since $\partial^2 w(\mathbf{z}) / \partial z_i \partial z_j = \gamma_{ij}$, the hessian of $w(\mathbf{z})$ is just $\boldsymbol{\gamma}$. Thus \mathbf{z}_o is a local minimum if $\boldsymbol{\gamma}$ is positive-definite (all eigenvalues are positive), a local maximum if $\boldsymbol{\gamma}$ is negative-definite (all eigenvalues are negative), or a saddle point if the eigenvalues differ in sign. If $\boldsymbol{\gamma}$ is singular (has at least one zero eigenvalue) then there is no unique stationary point. An example of this is seen in Figure 14.3 where there is a ridge (rather than a single point) of phenotypic values having the highest fitness value. The consequence of a zero eigenvalue is that the fitness surface has no curvature along the axis defined by the associated eigenvector. If $\boldsymbol{\gamma}$ has k zero eigenvalues, then the fitness surface has no curvature along k dimensions. Ignoring fitness change along these dimensions, the remaining fitness space has only a single stationary point, which is given by Equation 14.19a for $\boldsymbol{\gamma}$ and \mathbf{b} reduced to the $n - k$ dimensions showing curvature.

A Brief Digression: Orthonormal and Diagonalized Matrices

We need some additional matrix machinery at this point to further our discussion of the geometry of the quadratic fitness surface, which is defined by the geometry of the matrix $\boldsymbol{\gamma}$.

Matrix transformations consist of two basic operations, rotations (changes in the direction of a vector) and scalings (changes in its length). We can partition a matrix transformation into these two basic operations by using **orthonormal** matrices. Writing a square matrix \mathbf{U} as $\mathbf{U} = (\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_n)$ where each \mathbf{u}_i is an n dimensional column vector, \mathbf{U} is orthonormal if

$$\mathbf{u}_i^T \mathbf{u}_j = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}$$

In other words, each column of \mathbf{U} is independent from every other column and has unit length. Matrices with this property are also referred to as **unitary**, or **orthogonal** and satisfy

$$\mathbf{U}^T \mathbf{U} = \mathbf{U} \mathbf{U}^T = \mathbf{I} \quad (14.20a)$$

Hence,

$$\mathbf{U}^T = \mathbf{U}^{-1} \quad (14.20b)$$

The coordinate transformation induced by an orthonormal matrix has a very simple geometric interpretation in that it is a **rigid rotation** of the original coordinate system — all axes of the original coordinate are simply rotated by the same angle to create the new coordinate system. To see this, note first that orthonormal matrices preserve all inner products. Taking $\mathbf{y}_1 = \mathbf{U}\mathbf{x}_1$ and $\mathbf{y}_2 = \mathbf{U}\mathbf{x}_2$,

$$\mathbf{y}_1^T \mathbf{y}_2 = \mathbf{x}_1^T (\mathbf{U}^T \mathbf{U}) \mathbf{x}_2 = \mathbf{x}_1^T \mathbf{x}_2$$

A special case of this is that orthonormal matrices do not change the length of vectors, as $\|\mathbf{y}_1\| = \mathbf{y}_1^T \mathbf{y}_1 = \mathbf{x}_1^T \mathbf{x}_1 = \|\mathbf{x}_1\|$. If θ is the angle between vectors \mathbf{x}_1 and \mathbf{x}_2 , then following transformation by an orthonormal matrix,

$$\cos(\theta | \mathbf{y}_1, \mathbf{y}_2) = \frac{\mathbf{y}_1^T \mathbf{y}_2}{\sqrt{\|\mathbf{y}_1\| \|\mathbf{y}_2\|}} = \frac{\mathbf{x}_1^T \mathbf{x}_2}{\sqrt{\|\mathbf{x}_1\| \|\mathbf{x}_2\|}} = \cos(\theta | \mathbf{x}_1, \mathbf{x}_2)$$

and the angle between any two vectors remains unchanged following their transformation by the same orthonormal matrix.

A symmetric matrix \mathbf{A} (such as a variance-covariance matrix) can be **diagonalized** as

$$\mathbf{A} = \mathbf{U} \mathbf{\Lambda} \mathbf{U}^T \quad (14.21a)$$

where $\mathbf{\Lambda}$ is a diagonal matrix, and \mathbf{U} is an orthonormal matrix ($\mathbf{U}^{-1} = \mathbf{U}^T$). If λ_i and \mathbf{e}_i are the i th eigenvalue and its associated unit eigenvector of \mathbf{A} , then

$$\mathbf{\Lambda} = \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_n) = \begin{pmatrix} \lambda_1 & 0 & \dots & 0 \\ 0 & \lambda_2 & \dots & 0 \\ \vdots & & \ddots & \vdots \\ 0 & \dots & \dots & \lambda_n \end{pmatrix} \quad (14.21b)$$

and

$$\mathbf{U} = (\mathbf{e}_1, \mathbf{e}_2, \dots, \mathbf{e}_n) \quad (14.21c)$$

Geometrically, \mathbf{U} describes a rigid rotation of the original coordinate system while $\mathbf{\Lambda}$ is the amount by which unit lengths in the original coordinate system are scaled in the transformed system. Using Equation 14.21a, it is easy to show that

$$\mathbf{A}^{-1} = \mathbf{U} \mathbf{\Lambda}^{-1} \mathbf{U}^T \quad (14.22a)$$

$$\mathbf{A}^{1/2} = \mathbf{U} \mathbf{\Lambda}^{1/2} \mathbf{U}^T \quad (14.22b)$$

where the **square root matrix** $\mathbf{A}^{1/2}$ (which is also symmetric) satisfies $\mathbf{A}^{1/2} \mathbf{A}^{1/2} = \mathbf{A}$. Since $\mathbf{\Lambda}$ is diagonal, the i th diagonal elements of $\mathbf{\Lambda}^{-1}$ and $\mathbf{\Lambda}^{1/2}$ are λ_i^{-1} and $\lambda_i^{1/2}$ respectively, implying that if λ_i is an eigenvalue of \mathbf{A} , then λ_i^{-1} and $\sqrt{\lambda_i}$ are eigenvalues of \mathbf{A}^{-1} and $\mathbf{A}^{1/2}$. Note that Equations 14.22a/b imply that \mathbf{A} , \mathbf{A}^{-1} and $\mathbf{A}^{1/2}$ all have the same eigenvectors. Finally, using Equation 14.21a

we see that premultiplying \mathbf{A} by \mathbf{U}^T and then postmultiplying by \mathbf{U} gives a diagonal matrix whose elements are the eigenvalues of \mathbf{A} ,

$$\begin{aligned} \mathbf{U}^T \mathbf{A} \mathbf{U} &= \mathbf{U}^T (\mathbf{U} \mathbf{\Lambda} \mathbf{U}^T) \mathbf{U} = (\mathbf{U}^T \mathbf{U}) \mathbf{\Lambda} (\mathbf{U}^T \mathbf{U}) \\ &= \mathbf{\Lambda} \end{aligned} \tag{14.23}$$

As we will shortly see, the effect of using such a transformation is that (on this new scale) we remove all cross-product terms. Put another way, *on this new scale, there is no correlational selection.*

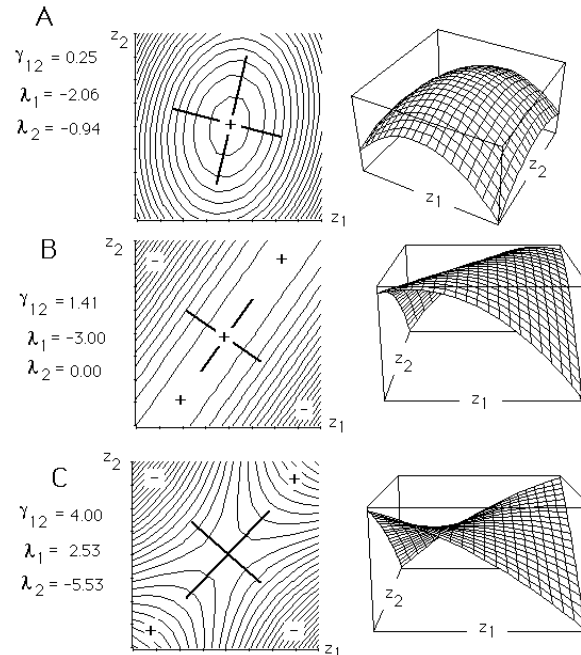


Figure 14.3. Three quadratic fitness surfaces, all of which have $\gamma_{11} = -2$ and $\gamma_{22} = -1$ and $\mathbf{b} = \mathbf{0}$ (i.e., no directional selection). On the left are curves of equal fitness values, with peaks being represented by a +, and valleys by a -. Axes of symmetry of the surface (the canonical or principal axes of γ) are denoted by the thick lines. These axes correspond to the eigenvectors of γ . On the right are three dimensional plots of individual fitness as a function of the phenotypic values of the characters z_1 and z_2 . **Top:** $\gamma_{12} = 0.25$. This corresponds to convex selection on both characters, with fitness falling off more rapidly (as indicated by the shorter distance between contour lines) along the z_1 axis than along the z_2 axis. **Middle:** $\gamma_{12} = \sqrt{2} \simeq 1.41$, in which case γ is singular. The resulting fitness surface shows a ridge in one direction with strong convex selection in the other. **Bottom:** When $\gamma_{12} = 4$, the fitness surface now shows a saddle point, with convex selection along one of the canonical axes of the fitness surface and concave selection along the other.

Canonical Transformation of γ

While the (quadratic) fitness surface curvature is completely determined by γ , it is easy to be misled about the actual nature of the fitness surface if one simply tries to infer it by inspection of γ , as the following example illustrates.

Example 14.4. Consider selection acting on two characters z_1 and z_2 . Suppose we find that $\gamma_{11} = -2$ and $\gamma_{22} = -1$, suggesting that the individual fitness surface has negative curvature in both z_1 and z_2 .

At first glance the picture this evokes is convex (stabilizing) selection on both z_1 and z_2 , with the convex selection surface perhaps rotated due to selection for correlations between z_1 and z_2 . The first caveat is that negative curvature, by itself, does not imply a local maximum. Even if γ is negative definite, the equilibrium point \mathbf{z}_0 may be *outside* of the observed range of population values and hence not currently applicable to the population being studied. A much more subtle point is that, as Figure 14.3 shows, the nature of the fitness surface is very dependent on the amount of selection for correlations between z_1 and z_2 . Figure 14.3 considers the surfaces associated with three different values of γ_{12} under the assumption that $\mathbf{b} = \mathbf{0}$. Note that although in all three cases $\gamma_{12} > 0$ (i.e., selection favors increased correlations between the phenotypic values of z_1 and z_2), the fitness surfaces are qualitatively very different. When $\gamma_{12} = 0.25$ (Figure 14.3A), the individual fitness surface indeed shows convex selection in both characters. However, when $\gamma_{12} = \sqrt{2} \simeq 1.42$ (Figure 14.3B), the fitness surface has a ridge in one direction, with convex selection in the other. When $\gamma_{12} = 4$ (Figure 14.3C), the fitness surface is a saddle, with convex selection along one axis and concave selection along the other. An especially troubling point is that if the standard error of γ_{12} is sufficiently large we would not be able to distinguish between these very different types of selection even if we could show that $\gamma_{11}, \gamma_{22} < 0$, and $\gamma_{12} > 0$.

Thus, even for two characters, visualizing the individual fitness surface is not trivial and can easily be downright misleading. The problem is that the cross-product terms (γ_{ij} for $i \neq j$) make the quadratic form difficult to interpret geometrically. Removing these terms by a change of variables so that the axes of new variables coincide with the axes of symmetry of the quadratic form (its canonical axes) greatly facilitates visualization of the fitness surface. From Equation 14.23, if we consider the matrix \mathbf{U} whose columns are the eigenvalues of γ , the transformation $\mathbf{y} = \mathbf{U}^T \mathbf{z}$ (hence $\mathbf{z} = \mathbf{U} \mathbf{y}$ since $\mathbf{U}^{-1} = \mathbf{U}^T$ as \mathbf{U} is orthonormal) removes all cross-product terms in the quadratic form, as

$$\begin{aligned}
 w(\mathbf{z}) &= a + \mathbf{b}^T \mathbf{U} \mathbf{y} + \frac{1}{2} (\mathbf{U} \mathbf{y})^T \gamma (\mathbf{U} \mathbf{y}) \\
 &= a + \mathbf{b}^T \mathbf{U} \mathbf{y} + \frac{1}{2} \mathbf{y}^T (\mathbf{U}^T \gamma \mathbf{U}) \mathbf{y} \\
 &= a + \mathbf{b}^T \mathbf{U} \mathbf{y} + \frac{1}{2} \mathbf{y}^T \mathbf{A} \mathbf{y} \\
 &= a + \sum_{i=1}^n \theta_i y_i + \frac{1}{2} \sum_{i=1}^n \lambda_i y_i^2
 \end{aligned} \tag{14.24}$$

where $\theta_i = \mathbf{b}^T \mathbf{e}_i$, $y_i = \mathbf{e}_i^T \mathbf{z}$, with λ_i and \mathbf{e}_i the eigenvalues and associated unit eigenvectors of γ . Alternatively, if a stationary point \mathbf{z}_0 exists (e.g., γ is nonsingular), the change of variables $\mathbf{y} = \mathbf{U}^T (\mathbf{z} - \mathbf{z}_0)$ further removes all linear terms (Box and Draper 1987), so that

$$w(\mathbf{z}) = w_o + \frac{1}{2} \mathbf{y}^T \mathbf{A} \mathbf{y} = w_o + \frac{1}{2} \sum_{i=1}^n \lambda_i y_i^2 \tag{14.25}$$

where $y_i = \mathbf{e}_i^T (\mathbf{z} - \mathbf{z}_0)$ and w_o is given by Equation 14.19b. Equation 14.24 is called the **A canonical form** and Equation 14.25 the **B canonical form** (Box and Draper 1987). Both forms represent a rotation of the original axis to the new set of axes (the canonical axes of γ) that align them with axes of symmetry of the quadratic surface. The B canonical form further shifts the origin to the stationary point \mathbf{z}_o . Since the contribution to individual fitness from $\mathbf{b}^T \mathbf{z}$ is a hyperplane, its effect is to tilt the fitness surface. The B canonical form “levels” this tilting, allowing us to focus entirely on the curvature (quadratic) aspects of the fitness surface.

The orientation of the quadratic surface is determined by the eigenvectors of γ while the eigenvalues of γ determine the nature and amount of curvature of the surface along each canonical axis.

Along the axis defined by y_i , the individual fitness function has positive curvature (is concave) if $\lambda_i > 0$, has negative curvature (is convex) if $\lambda_i < 0$, or has no curvature (is a plane) if $\lambda_i = 0$. The amount of curvature is indicated by the magnitude of λ_i , the larger $|\lambda_i|$ the more extreme the curvature.

An alternative way to think about this canonical transformation is that the original vector \mathbf{z} of n characters is transformed into a vector \mathbf{y} of n independent selection indices (Simms 1990). Directional selection on the index y_i is measured by θ_i , while quadratic selection is measured by λ_i .

Returning to Figure 14.3, we see that the axes of symmetry of the quadratic surface are the canonical axes of γ . For $\gamma_{12} = 0.25$, $\lambda_1 = -2.06$ and $\lambda_2 = -0.94$ so that the fitness surface is convex along each canonical axis, with more extreme curvature along the y_1 axis. When $\gamma = \sqrt{2}$, one eigenvalue is zero while the other is -3 , so that the surface shows no curvature along one axis (it is a plane), but is strongly convex along the other. Finally, when $\gamma_{12} = 4$, the two eigenvalues differ in sign, being -5.53 and 2.53 . This generates a saddle point with the surface being concave along one axis and convex along with other, with the convex curvature being more extreme.

If $\lambda_i = 0$, the fitness surface along y_i has no curvature, so that the fitness surface is a ridge along this axis. If $\theta_i = \mathbf{b}^T \mathbf{e}_i > 0$ this is a rising ridge (fitness increases as y_i increases), it is a falling ridge (fitness decrease as y_i increase) if $\theta_i < 0$, and is flat if $\theta_i = 0$. Returning to Figure 14.3B, the effect of \mathbf{b} is to tilt the fitness surface. Denoting values on the axis running along the ridge by y_1 , if $\theta_1 > 0$ the ridge rises so that fitness increases as y_1 increases. Even if γ is not singular, it may be nearly so, with some of the eigenvalues being very close to zero. In this case, the fitness surface shows little curvature along the axes given by the eigenvectors associated with these near-zero eigenvalues. From Equation 14.24, the fitness change along a particular axis (here given by \mathbf{e}_i) is $\theta_i y_i + (\lambda_i/2) y_i^2$. If $|\theta_i| \gg |\lambda_i|$, the curvature of the fitness surface along this axis is dominated by the effects of linear (as opposed to quadratic) selection. Phillips and Arnold (1989) present a nice discussion of several other issues relating to the visualization of multivariate fitness surfaces, while Box and Draper (1987) review the statistical foundations of this approach.

Strength of Selection: γ_{ii} Versus λ

We have seen that the γ_{ii} can potentially give a very misleading picture of the nature of quadratic selection, while the eigenvalues λ of γ provide an exact description of the true nature of selection. Blows and Brooks stress this point, noting that in an analysis of 19 studies that $|\gamma_{ii}|_{max} < |\lambda|_{max}$. Thus, studies (such as Kingsolver et al. 2001) that report weak values for quadratic selection are potentially biased, as they simply used γ_{ii} values, rather than the full geometry of γ , as described by the eigenvectors.

Example 14.5. Brooks and Endler (2001) examined four color traits in male guppies associated with sexual selection. The estimated γ matrix was

$$\gamma = \begin{pmatrix} 0.016 & -0.016 & -0.028 & 0.103 \\ -0.016 & 0.00003 & 0.066 & -0.131 \\ -0.028 & 0.066 & -0.011 & -0.099 \\ 0.103 & -0.131 & -0.099 & 0.030 \end{pmatrix}$$

Just considering the diagonal elements suggests evidence for weak concave selection ($\gamma_{44} = 0.030$, $\gamma_{11} = 0.016$), and some evidence for very weak convex selection ($\gamma_{33} = -0.011$). However, the eigenvalues of γ are 0.132, 0.006, -0.038, and -0.064. Of these only the leading eigenvalue is significant, with the amount of concave selection being over four times that suggested from the largest γ_{ii} value.

Subspaces of γ

Blows and Brooks (2003) note several advantages of focusing on estimating the λ_i versus the entire matrix of γ_{ij} , noting that there are n eigenvalues, and $n(n-1)/2$ elements in γ . Further, given

that many eigenvalues may be close to zero, a subspace of γ (as was the case for \mathbf{G} in Lecture 13) may essentially capture all of the relevant information on the quadratic fitness surface. Following Simms (1990) and Simms and Rausher (1993), Blows and Brooks suggest that estimation and hypothesis testing can occur by first obtaining the eigenvectors of γ , and then use these to generate the transformed variables $\mathbf{y} = \mathbf{U}^T \mathbf{z}$ in the quadratic regression given by Equation 14.24. The quadratic terms correspond to eigenvalues, and confidence intervals, as well as significance, can be conducted within the standard GLM framework (Lecture 2).

There has been considerable debate as to how γ and \mathbf{G} interact over long-term selection. One view is that γ comes to shape \mathbf{G} in that the two matrices become geometrically similar. Blows et al. (2004), building upon the results of Krzanowski (1979), suggest an approach for comparing the major subspaces of \mathbf{G} and γ . As was the case for \mathbf{G} (Lecture 13), form a matrix \mathbf{B} for a subset of k eigenvectors on γ by forming the matrix $\mathbf{B} = (\mathbf{e}_1, \dots, \mathbf{e}_k)$. Forming a similar matrix \mathbf{A} with $k \leq n/2$ leading eigenvectors of the $n \times n$ matrix \mathbf{G} , the two subspaces can be compared with the matrix

$$\mathbf{S} = \mathbf{A}^T \mathbf{B} \mathbf{B}^T \mathbf{A} \quad (14.26)$$

The eigenvalues of \mathbf{S} describes the angles between the orthogonal axes of \mathbf{A} and \mathbf{B} . Specifically, the smallest angle is given by $\cos^{-1} \sqrt{\lambda_1}$, where λ_1 is the leading eigenvalue of \mathbf{S} .

UNMEASURED CHARACTERS AND OTHER BIOLOGICAL CAVEATS

Even if we are willing to assume that the best-fitting quadratic regression is a reasonable approximation of the individual fitness surface, there are still a number of important biological caveats to keep in mind. For example, the fitness surface can change in both time and space, often over short spatial/temporal scales (e.g., Kalisz 1986, Stewart and Schoen 1987, Scheiner 1989, Jordan 1991), so that one estimate of the fitness surface may be quite different from another estimation at a different time and/or location. Hence, considerable care must be used before pooling data from different times and/or sites to improve the precision of estimates. When the data are such that selection gradients can be estimated separately for different times or areas, space/time by gradient interactions can be tested for in a straightforward fashion (e.g., Mitchell-Olds and Bergelson 1990).

Population structure can also influence fitness surface estimation in other ways. If the population being examined has overlapping generations, fitness data must be adjusted to reflect this (e.g., Stratton 1992). Likewise, if members in the population differ in their amount of inbreeding, measured characters and fitness may show a spurious correlation if both are affected by inbreeding depression (Willis 1993).

Perhaps the most severe caveat for the regression approach of estimating $w(z)$ is unmeasured characters — estimates of the amount of direct selection acting on a character are biased if that character is phenotypically correlated to unmeasured characters also under selection (Lande and Arnold 1983, Mitchell-Olds and Shaw 1987). Adding one or more of these unmeasured characters to the regression can change initial estimates of β and γ . Conversely, selection acting on unmeasured characters that are phenotypically *uncorrelated* with those being measured has no effect on estimates of β and γ .

The Bias due to Environmental Correlations Between Fitness and Characters

As mentioned before, environmental correlations between characters and fitness can bias estimates of how phenotypes influence fitness (Rausher 1992). Suppose plant size and total seed set in an annual plant are both influenced by the soil concentration of nitrogen, so that plants in nitrogen-rich soil have both large size and large seed set, while plants in nitrogen-poor soil have small size and small seed set. Thus, even though we may observe a positive correlation between plant size and seed set, size itself may have no effect on seed set.

To express this effect formally, decompose the phenotype of the i th character as $z_i = g_i + E_i$, where g represents the genetic contribution and E the environmental contribution (assume

no genotype \times environment interaction and that g and E are independent). Decomposing the covariance between phenotypic value and fitness gives

$$S_i = \sigma(w, z_i) = \sigma(w, g_i + E_i) = \sigma(w, g_i) + \sigma(w, E_i)$$

The first term is the covariance between genotypic value and fitness, while the second (which concerns us here) is the covariance between fitness and E_i the environmental deviation of z_i . Provided that E_i does not influence fitness other than through its effect on phenotype ($E_i \rightarrow z_i \rightarrow w$), the environmental covariance does not bias our view of the phenotype-fitness association. However, if E_i also has an effect on fitness **independent** of its effect on the phenotype (e.g., $E_i \rightarrow w$ without passing through z_i), this augments the covariance over that from the phenotypic effects on fitness alone. Following Rausher (1992), we use the method of path analysis (Appendix 1 of Lynch and Walsh) to examine the amount of bias created by such environmental correlations. Figure 14.5 shows a simplified version for two characters.

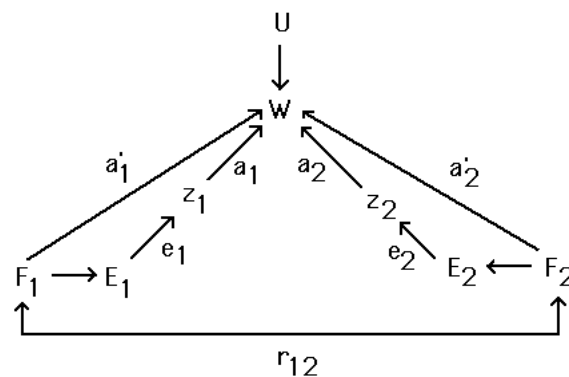


Figure 14.5. A path analysis model incorporating character-fitness correlations due to shared environmental effects. Here relative fitness w is determined by the phenotypic value of two characters (z_1 and z_2) and by three environmental values F_1 , F_2 , and U . See text for further details. After Rausher (1992).

Without loss of generality, assume that E_i is completely determined by the environmental factor F_i . We wish to decompose the correlation between E_i ($= F_i$) and w into a component due to the direct association between phenotype and fitness and a component due to association between environmental value and fitness *independent* of the phenotypic value. For two characters, the path diagram in Figure 14.5 shows four paths creating correlations between w and E_1 . The paths $F_1 \rightarrow E_1 \rightarrow z_1 \rightarrow w$ and $F_1 \leftrightarrow F_2 \rightarrow E_2 \rightarrow z_2 \rightarrow w$ represent the contribution of the environmental effects through their effect on phenotypes. The first path represents the phenotypic contribution through z_1 (with path coefficient product of $e_1 \cdot a_1$), the second the contribution from z_2 due to the correlation between environmental effects of z_1 and z_2 (path product = $r_{12} \cdot e_2 \cdot a_2$). The effects of the environment on fitness independent of phenotypic value are given by the two remaining paths, $F_1 \rightarrow w$ and $F_1 \leftrightarrow F_2 \rightarrow w$ (with products a_1' and $r_{12} \cdot a_2'$, respectively). Summing all four paths gives the correlation between fitness and the environmental deviation of character i as

$$\rho(w, E_i) = (e_1 \cdot a_i + r_{12} \cdot e_2 \cdot a_2) + (a_1' + r_{12} \cdot a_2')$$

This correlation can be expressed in terms of a covariance, with $\sigma(w, E_i) = \sigma(w) \cdot \sigma(E_i) \cdot \rho(w, E_i)$. The first term is the correlation generated by the path through the phenotype, while the second is the contribution to the correlation of E and w that is *independent* of the phenotype.

More generally, consider n characters where r_{ij} is the correlation between E_i and E_j , e_i the path coefficient for the effect of the environmental deviation on phenotype ($E_i \rightarrow z_i$), a_i the path coefficient for the effect of phenotype on fitness ($z_i \rightarrow w$), and a'_i the path coefficient for the effect of E_i on fitness, independent of phenotypic value ($E_i \rightarrow w$). In this case

$$\sigma(w, E_i) = \sigma(w) \cdot \sigma(E_i) \cdot \left(\left[e_i a_i + \sum_{j \neq i} r_{ij} e_j a_j \right] + \left[a'_i + \sum_{j \neq i} r_{ij} a'_j \right] \right) \quad (14.27a)$$

The contribution from the association of phenotypic value and fitness are given by the first set of terms (those involving a_i), while the second set (those involving a'_i) represents the contribution from associations of environmental values and fitness that are independent of phenotypic value. This set of terms alters the phenotype-fitness covariance over that created by the phenotypic influence on fitness alone. Subtracting off this additional covariance term, viz.,

$$S_i - \sigma(w) \cdot \sigma_E(z_i) \cdot \left(a'_i + \sum_{j \neq i} r_{ij} a'_j \right) \quad (14.27b)$$

removes this bias. Since we almost never have knowledge of the a'_i , the utility of Equation 14.27b is in exploring just how important these effects might be, given various assumptions. Rausher suggests an alternative method, based on regressing relative fitness on breeding values (rather than phenotypic value) to remove some of these sources of bias.

Lecture 14 Problems

1. Suppose the matrix \mathbf{A} can be diagonalized, e.g., $\mathbf{A} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^T$. Let λ_i denote the i th eigenvalue and \mathbf{e}_i the associated (unit) eigenvector of \mathbf{A} .

a: What is \mathbf{A}^2 ? What are the eigenvalues and eigenvectors?

b: What is \mathbf{A}^n , where n is an integer? What are the eigenvalues and eigenvectors?

2. Suppose you observe the following vector of phenotypic means before and after selection

$$\boldsymbol{\mu} = \begin{pmatrix} 10 \\ 20 \end{pmatrix}, \quad \boldsymbol{\mu}^* = \begin{pmatrix} 15 \\ 8 \end{pmatrix}$$

with phenotypic covariance matrices before and after selection of

$$\mathbf{P} = \begin{pmatrix} 40 & 20 \\ 20 & 100 \end{pmatrix}, \quad \mathbf{P}^* = \begin{pmatrix} 60 & -10 \\ -10 & 80 \end{pmatrix}$$

a: Compute the differentials \mathbf{S} and \mathbf{C} .

b: Compute the gradients β, γ .

c: What can you say about the nature of selection given a and b?

d: Compute the eigenvalues and eigenvectors of γ .

c: What can you say about the nature of selection given d?

Solutions to Lecture 14 Problems

1. a: $\mathbf{A}^2 = \mathbf{A}\mathbf{A} = (\mathbf{U}\mathbf{\Lambda}\mathbf{U}^T)(\mathbf{U}\mathbf{\Lambda}\mathbf{U}^T) = \mathbf{U}\mathbf{\Lambda}(\mathbf{U}^T\mathbf{U})\mathbf{\Lambda}\mathbf{U}^T = \mathbf{U}\mathbf{\Lambda}\mathbf{\Lambda}\mathbf{U}^T = \mathbf{U}\mathbf{\Lambda}^2\mathbf{U}^T$. Thus λ_i^2 is an eigenvalue of \mathbf{A}^2 and \mathbf{e}_i is its associated eigenvector.

b: Following from part a, we can write $\mathbf{A}^n = \mathbf{U}\mathbf{\Lambda}^n\mathbf{U}^T$, so that λ_i^n is an eigenvalue of \mathbf{A}^n and \mathbf{e}_i is its associated eigenvector.

2. a.

$$\mathbf{S} = \boldsymbol{\mu}^* - \boldsymbol{\mu} = \begin{pmatrix} 15 \\ 8 \end{pmatrix} - \begin{pmatrix} 10 \\ 20 \end{pmatrix} = \begin{pmatrix} 5 \\ -12 \end{pmatrix}$$

$$\mathbf{C} = \mathbf{P}^* - \mathbf{P} + \mathbf{S}\mathbf{S}^T = \begin{pmatrix} 60 & -10 \\ -10 & 80 \end{pmatrix} - \begin{pmatrix} 40 & 20 \\ 20 & 100 \end{pmatrix} + \begin{pmatrix} 5 \\ -12 \end{pmatrix} \begin{pmatrix} 5 & -12 \end{pmatrix} = \begin{pmatrix} 45 & -90 \\ -90 & 124 \end{pmatrix}$$

b:

$$\boldsymbol{\beta} = \mathbf{P}^{-1}\mathbf{S} = \begin{pmatrix} 40 & 20 \\ 20 & 100 \end{pmatrix}^{-1} \begin{pmatrix} 5 \\ -12 \end{pmatrix} = \begin{pmatrix} 0.206 \\ -0.161 \end{pmatrix}$$

$$\boldsymbol{\gamma} = \mathbf{P}^{-1}\mathbf{C}\mathbf{P}^{-1} = \begin{pmatrix} 40 & 20 \\ 20 & 100 \end{pmatrix}^{-1} \begin{pmatrix} -5 & 30 \\ 30 & -164 \end{pmatrix} \begin{pmatrix} 40 & 20 \\ 20 & 100 \end{pmatrix}^{-1} = \begin{pmatrix} 0.0663 & -0.0451 \\ -0.0451 & 0.0278 \end{pmatrix}$$

c: Visual inspection of $\boldsymbol{\gamma}$ suggests concave (disruptive) selection on trait 1 and trait 2, as well as selection for negative correlation between traits 1 and 2.

d: The eigenvalues and eigenvectors of $\boldsymbol{\gamma}$ are $\lambda_1 = 0.0962$, $\lambda_2 = -0.0020$, while the associated eigenvectors are

$$\mathbf{e}_1 = \begin{pmatrix} -0.834 \\ 0.551 \end{pmatrix}, \quad \mathbf{e}_2 = \begin{pmatrix} 0.551 \\ 0.834 \end{pmatrix}$$

e: There is convex selection along the axis defined by $-0.834 \cdot z_1 + 0.551 \cdot z_2$ and no (quadratic) selection along the axis defined by $0.551 \cdot z_1 + 0.834 \cdot z_2$.