Appendix D. Covariance matrices

Although the concepts presented below apply identically to vector fields, for brevity present discussion is limited to simple vectors.

Consider a two-component force vector response $\boldsymbol{F}$:

$$\boldsymbol{F}_j = \begin{bmatrix} F_{xj} & F_{yj} \end{bmatrix}^\top \tag{D.1}$$

where j indexes the responses, and there are a total of J responses. After computing the mean force vector $\overline{\boldsymbol{F}}$ as:

$$\overline{\boldsymbol{F}} = \begin{bmatrix} \overline{F_x} \\ \\ \overline{F_y} \end{bmatrix} = \frac{1}{J} \sum_{j=1}^{J} \overline{\boldsymbol{F}}_j \tag{D.2}$$

the covariance matrix $\boldsymbol{W}$ can be assembled as follows:

$$\boldsymbol{W} = \begin{bmatrix} W_{xx} & W_{xy} \\ \\ W_{yx} & W_{yy} \end{bmatrix} \tag{D.3}$$

where the elements of $\boldsymbol{W}$ are:

$$W_{xx} = \frac{1}{J-1} \sum_{j=1}^{J} (F_{xj} - \overline{F}_x)^2 \tag{D.4}$$

$$W_{yy} = \frac{1}{J-1} \sum_{j=1}^{J} (F_{yj} - \overline{F}_y)^2 \tag{D.5}$$

$$W_{xy} = W_{yx} = \frac{1}{J-1} \sum_{j=1}^{J} (F_{xj} - \overline{F}_x)(F_{yj} - \overline{F}_y) \tag{D.6}$$

Thus the diagonal elements W_{xx} and W_{yy} are the intra-component variances (i.e. squared standard deviations), and the off-diagonal elements W_{xy} and W_{yx} are the inter-component covariances between F_x and F_y over multiple responses. Importantly, changes in F_x and F_y are completely uncorrelated if and only if W_{xy}=0.

One contention of this paper is that separate (univariate) analysis of F_x and F_y is biased when testing non-directed hypotheses. The main reason is that F_x analysis considers only W_{xx} and F_y analysis considers only W_{yy}. This is equivalent to assuming W_{xy}=0, an assumption which may not be valid (Appendix B).

A geometric interpretation of $\boldsymbol{W}$ is useful both for visualizing vector variance (Fig.S3) and for appreciating canonical correlation analysis (Appendix E). Consider that $\boldsymbol{W}$ represents an ellipse whose geometry is defined by the solutions to the eigenvalue problem:

$$\boldsymbol{W}\boldsymbol{v} = \lambda\boldsymbol{v} \tag{D.7}$$

Here $\boldsymbol{v}$ and λ are the eigenvectors and eigenvalues, respectively, and there are two unique eigensolutions unless both ($W_{xx} = W_{yy}$) and ($W_{xy} = 0$), in which case there is only one eigensolution and $\boldsymbol{W}$ represents a circle. When there are two solutions the eigenvectors represent the ellipse axes (or equivalently: principal axes), and the eigenvalues represent the axes' lengths (or variance in the direction of the principal axes). An equivalent interpretation is that <u>one eigenvector of $\boldsymbol{W}$ represents the direction of maximum variance</u> within the dataset. This means that we can rotate our original coordinate system xy to a new coordinate system $x'y'$ so that variance along the new x' axis is the maximum possible variance obtainable for all possible x'.