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A randomization method for the calculation of covariation in multiple nonlinear relations: illustrated with the example of goal-directed movements

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Abstract. A randomization method is developed for the calculation of covariation between multiple variables that are linked nonlinearly to a dependent variable. Covariation is a phenomenon often invoked in the study of movement coordination to capture the fact that in coordinated movement the outcome shows greater than expected consistency from the variability in the component processes. However, in most cases, the problem is that more than two variables covary in a nonlinear fashion, which makes quantification with the bivariate linear covariation and correlation coefficient inapplicable. This paper presents a generalization of the calculation of linear bivariate covariance using a variant of a randomization method that is based on the comparison between the empirically measured variability in the outcome and a covariation-free variability. The latter can be estimated by permuting data sets. A generalized correlation coefficient is derived, and it is shown how errors of estimation can be quantified. The permutation method can also quantify partial multiple nonlinear covariation. The calculations are illustrated in a numerical example of an arm-reaching task. However, the method is applicable to all cases where the internal organization of a nonlinear system of multiple variables needs to be quantified. The relation and applicability of the permutation method compared to other methods using regression and principal component analysis are discussed and illustrated with a numerical example.

1 Organization and coordination measured in terms of covariation

Biological systems are constantly confronted with new and unpredictable situations in the environment. In addition, internal processes are generally assumed to be subjected to multiple sources of perturbations or noise. Due to these multiple external and internal unpredictable influences, it has been stated that a biological system can never be in exactly the same state twice. In the study of control and coordination of movements, it has become widely acknowledged that it is impossible for a human actor to perform exactly the same movement twice (Bernstein 1967). In light of this variability over repeated executions of the "same" movement, it is astonishing that goal-directed actions still show reliable movement outcomes over repeated performances. For example, when a person reaches for a cup using his/her entire arm, the configuration of the arm and finger joints at the moment of grasping and the involved joint angles will be slightly different every time. And yet the cup is reliably and safely grasped each time. It can therefore be expected that the joint angles are systematically related such that deviations in one joint are counteracted by compensatory changes in the other joint, leading to a relatively invariant endpoint position of the hand. In more general terms, there are constraints among the component processes of the system that compensate for deviations and reduce variability, thereby increasing the probability of a desired result.

The effect of such compensatory processes can be assessed by comparing the variability of the result (grasping the cup safely) with the variability that would be expected from the variability of the component processes (the individual joint angles of the arm). The reduction of result variability, however, can only be estimated if there is a reference value that captures the result if the system had *not* used compensatory processes. From the set of component variables the variability of the corresponding task solutions must be calculated. Thus, if the empirically measured variability for a given desired result is lower than this reference value, then this indicates that the system shows organization or "control" to achieve the result.

The degree of control or coordination can be quantified as the difference between the empirically measured result variability and the variability expected from independent component processes. In the following, we

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will develop a method for quantifying this aspect in nonlinear systems with multiple variables.

2 Covariance for the calculation of coordination in motor control studies

In studies on movement coordination, covariation has been frequently discussed as a signature for control. A considerable number of studies have quantified covariation between component variables with the goal of revealing fundamental motor control processes (Voigt 1933; Bernstein 1967; Arutyunyan et al. 1968,1969; Hughes and Abbs 1976; Lacquanti and Soechting 1982; Lee et al. 1982; Abbs et al. 1984; Abbs 1986; Anderson and Pitcairn 1986; Cordo 1988,1990; Darling and Cooke 1987a,b; Darling et al. 1988; McDonald et al. 1989; Bootsma and van Wieringen 1990; Loosch 1990,1995; van Emmerik 1992; Vereijken et al. 1992; Darling and Stephenson 1993; Gutman et al. 1993; Newell 1993; Stimpel 1993; Trillhose 1996; Loosch and Tamme 1998; Scholz and Schöner 1999; Scholz et al. 2000). However, in many cases, the methods used for the estimation of covariation were problematic. Most frequently bivariate linear covariance was the statistic used, although in most cases nonlinear relations between the variables existed. To circumvent this problem and still apply a bivariate linear covariance calculation, it has become common to transform nonlinear relations into linear ones by transforming one or both data streams on the basis of the known nonlinear functional relations. For example, the logarithmic transform is frequently applied to linearize data that relate in an exponential fashion. This transformation, however, is necessarily nonlinear and changes the interval scale of the original data. The transformed data are no longer on an interval scale and therefore violate an essential prerequisite for the application of covariance calculations (Elzinga 1985).

Similarly, it has not been possible to calculate covariance for multiple covariation, i.e., covariation among more than two variables, even if they form a linear relation. Note that the calculation of a covariance matrix only gives the complete list of pairwise covariations without summarizing them into a single value that expresses the covariation among all variables. The method of multiple regression is similarly not suited for this problem. Multiple regression addresses a fundamentally different issue, namely, how the linear combination of several predictors accounts for the variability in a criterion variable. Of only secondary importance are the relations among the predictors that are determined by pairwise covariations yielding pairwise correlation coefficients. To reveal the advantages and shortcomings of these methods, Appendix C compares several methods with the method presented in this paper. It will be evident that the multiple regression methods fail when the covariance is not between the predictors and the dependent measure but between the predictors themselves.

Another method proposed recently by Schöner, Scholz, and colleagues is the uncontrolled manifold method (UCM), which also aims at quantifying the variance of several variables with respect to a specific outcome (Schöner 1995; Scholz and Schöner 1999; Scholz et al. 2000). By using a linear approximation, this method determines the subspace of all variable combinations that lead to a defined goal state, i.e., the null space. The variability of the data is then split into two components, one that lies parallel ($\|$UCM) and one that lies orthogonal ($\perp$UCM) to the null space. The degree of covariation is then determined by comparing the relative contributions of these two components of variability. The comparison of methods in Appendix C will show that this method fails when certain prerequisites for the relation between variables and the specific outcome are not met.

To summarize, although there is wide interest and a range of applications for estimating covariation as an indicator for compensatory control processes, what has been missing is a method of calculating covariation in complex, i.e., multiple nonlinear, relations. The aim of the present paper is to develop a generalization of the statistical method for the calculation of covariance with the goal of measuring covariation for multiple nonlinear relations. We will illustrate and discuss the method with an example in movement control. However, the method is applicable to any data set with equivalent questions.

3 A generalized method for the calculation of covariation

Covariation between two series of variables $X = (x_1, \ldots, x_n)$ and $Y = (y_1, \ldots, y_n)$ shall be defined as the case where the deviations of pairwise related values (x_i, y_i) of their respective mean values $\bar{x}$ and $\bar{y}$ are related in a systematic way. Positive covariation exists when deviations of both variables have the same sign, i.e., the x-value below average is systematically paired with a y-value below average. For negative covariation below-average values are paired with above-average values. The common method of determining covariation between two variables is the calculation of covariance:

$$cov(x, y) = \frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y}) \tag{1}$$

Note that *covariation* refers to a generalized case, whereas *covariance* is the specific method for the bivariate linear case.

In order to generalize the calculation of covariation, let us begin by reformulating Eq. 1 to an equivalent expression, assuming a known relation between the two input variables x and y and the output variable c. Let us consider the linear relationship $c = x + y$. In this simple case, we can use standard linear statistics to obtain an equation for calculating the covariance between x and y with respect to c. Calculating the variance of the sum of two variables s^2_{x+y}, the covariance between x and y, $cov(x, y)$ is one component, as follows:

$$s^2_{x+y} = s^2_x + s^2_y + 2cov(x, y) \tag{2}$$

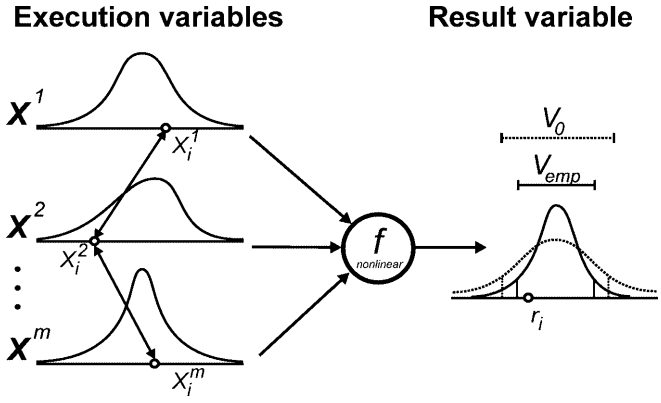

Fig. 1. Overview of the notation and the logic of the permutation method. For explanation of the notation see text

Rearranging Eq. 2 we get:

$$cov(x,y) = \frac{1}{2}\left(s_{x+y}^2 - \left(s_x^2 + s_y^2\right)\right) \tag{3}$$

s_{x+y}^2 denotes the variance that can be empirically measured in the actual result as the consequence of the co-occurrence of the two processes. In the following, this will be referred to as the empirically measured result variability V_{emp}. The second term, $(s_x^2 + s_y^2)$, is the variability in the result that would be observed if the covariance were zero. This quantity will be referred to as covariation-free result variability with the symbol V_0. Hence, we can rewrite Eq. 3 in shortened notation as:

$$cov(x,y) = \frac{1}{2}\left(V_{\text{emp}} - V_0\right) \tag{4}$$

On the basis of this equation we can now generalize the calculation of covariation beyond the specific case of linear and bivariate covariance. First, we discard the limitation of the bivariate case and assume an arbitrary finite number of m variables $X^1, X^2, \ldots, X^m$ (for an overview of the notation and the method see Fig. 1). Each of these m variables has n observations x_i^k, where the superscript k denotes to which variable it belongs and the index i ($i = 1, 2, \ldots, n$) denotes values from the same performance repetition. The overall result r_i is obtained by a potentially nonlinear function f. For the application of the following method it is necessary that this transfer function f is known. Note that this prerequisite is equally present in other comparable calculation methods. For instance, the application of covariance and linear multiple regression implies that f is linear. Similarly, the structure of f is known when calculating nonlinear multiple regression. For the comparison of different methods in Appendix C, nonlinear regression, Jacobian, and uncontrolled manifold, we calculated covariation with respect to the known outcome using f equally for all methods (see Appendix C).

The overall result r_i can now be written as

$$r_i = f\left(x_i^1, x_i^2, \ldots, x_i^m\right) \tag{5}$$

A variability measure V can be defined and used to capture the dispersion V_{emp} of the empirically measured result variables $r_1, r_2, \ldots, r_n$ for the m different execution variables $X^1, X^2, \ldots, X^m$, each with n repetitions, as follows:

$$V_{\text{emp}} = V(r_1, \ldots, r_n) = V\left(f(x_1^1, x_1^2, \ldots, x_1^m), f(x_2^1, x_2^2, \ldots, x_2^m), \ldots, f(x_n^1, x_n^2, \ldots, x_n^m)\right) \tag{6}$$

or in shortened notation:

$$V_{\text{emp}} = V_f(X^1, \ldots, X^m) \tag{7}$$

Using this notation and following Eq. 4, covariation COV can be formally expressed as:

$$COV\left(X^1, X^2, \ldots, X^m\right) = \frac{1}{2}\left(V_{\text{emp}} - V_0\right) \tag{8}$$

Note the capital letters in COV are used to distinguish this generalized concept from covariance cov defined in Eq. 1. In order to compute cov two quantities must be known: the empirical result variability V_{emp} and the covariation-free result variability V_0. According to Eq. 6, V_{emp} can be calculated either from the known series of results $(r_i, r_2, \ldots, r_n)$ or, since the functional relation f is known, from the measured data sets of the variables $X^1, X^2, \ldots, X^m$, where $X^k = \{x_1^k, \ldots, x_n^k\}$.

The problem with using Eq. 8 evidently lies in determining V_0. In the following, a method shall be developed that makes this possible. If this missing quantity can be estimated, it will become possible to calculate covariation for cases that have thus far been excluded, i.e., for multiple nonlinear relations. Before the formal derivation, the idea will be illustrated with a numerical example.

4 Example of a multiple nonlinear relation: multijoint pointing movements

Let us consider a three-joint arm movement confined to the horizontal plane (Fig. 2). The shoulder joint is located at the origin of the reference system ($x = 0$; $y = 0$), the joint angles for shoulder, elbow, and wrist are denoted by α, β, and γ, respectively. The segment lengths of upper arm, forearm, and hand are denoted by a, b, and c, respectively. The limb segment lengths used for the exemplary calculations were: $a = 40$ cm, $b = 40$ cm, and $c = 20$ cm. The task is to point with the tip of the hand to a target located at $x = 20$ cm, $y = 40$ cm. The results are the performed endpoint positions x, y associated with the respective sets of joint angles α, β, and γ. For the three-segment link α, β, and γ obey the following relations:

$$x = a\cos(\alpha) + b\cos(\alpha - \beta + \pi) + c\cos(\alpha - \beta - \gamma + 2\pi) \tag{9}$$

$$y = a\sin(\alpha) + b\sin(\alpha - \beta + \pi) + c\sin(\alpha - \beta - \gamma + 2\pi) \tag{10}$$

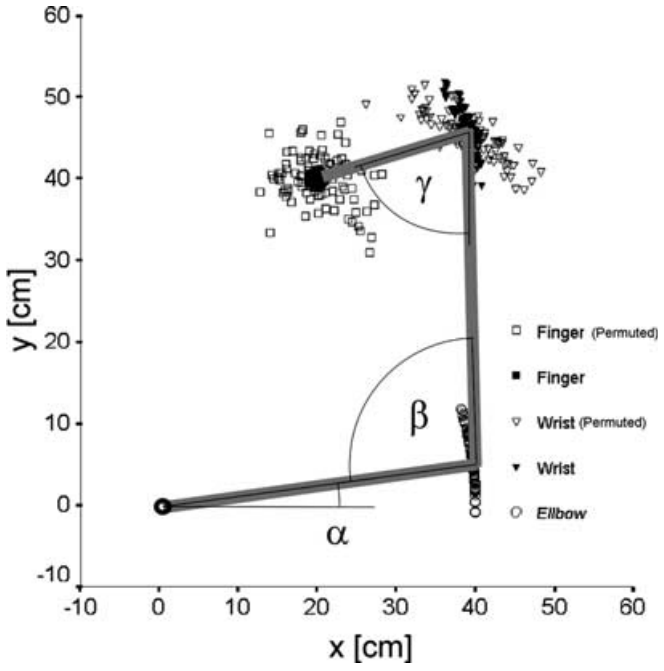

Fig. 2. Coordinates of the shoulder, elbow, and wrist of a three-joint arm model. The *markers* show the position coordinates of repeated executions. *Filled symbols* show the subset of 100 samples that showed covariation. *Open symbols* show the positions for the case where covariation is eliminated by the permutation method

The relation between joint angles and endpoint position is evidently nonlinear and redundant. As demonstrated in many previous studies, due to this redundancy a person performing this pointing task never repeats the movement and achieves the same endpoint position with exactly identical joint angles. For simplicity, the following example considers only endpoint positions and not the trajectories of the pointing task.

A data set of 10,000 values per angle was generated where each angle variable had stochastically independent normally distributed dispersions. The values used to generate the data in Fig. 2 were: mean $\alpha = 10°$, $s_\alpha = 5°$; mean $\beta = 90°$, $s_\beta = 10°$; mean $\gamma = 75°$, $s_\gamma = 20°$. From these data 10,000 triplets were formed. Out of these the 100 angle triplets were selected that had the smallest errors from the *x*-*y* target. In Fig. 2, the *x*-*y* endpoint coordinates of these 100 runs are represented by the filled dots. As we selected the most accurate runs, the contributing joint angles should therefore show more covariation than if Eqs. 9 and 10 were solved by using randomly matched angles. How can this covariation be estimated?

The calculation of pairwise linear covariance between joint angles and correlation coefficients yields the following values: $\rho_{\alpha,\beta} = 0.966$; $\rho_{\alpha,\gamma} = 0.977$; $\rho_{\beta,\gamma} = 0.954$. The problem is which, if any, of these three values should represent their covariation. On the other hand, for applying Eq. 8 it is necessary to know the magnitude of the end result variability when removed of its covariation V_0. In the present example, one option would be to use the variability in the results of the original 10,000 triplets that were created by independent drawings from normal distributions. This, however, does not yield a valid estimate, as the mean and variance of the selected data set are different from those of the original data set due to the selection. The goal is to determine result variability of a data set whose distribution properties are identical to those of the original data set. However, such a reference value does not exist in real situations.

A solution to this problem is provided by the so-called randomization methods (Manly 1997). With these methods such a reference value can be generated from the same sample set $(\alpha_i, \beta_i, \gamma_i)$ by removing the relations between the triplets. A new subset is created from the same 100 joint-angle triplets in which the sequence of each of the variables α, β, and γ is permuted separately. In Table 1, this is exemplified with the ten best values out of the set of 100 data triplets. Entering these new angle triplets $(\alpha_i^*, \beta_i^*, \gamma_i^*)$ into Eqs. 9 and 10, new *x*-*y* end positions (x_i^*, y_i^*) and their variability V_0 can be calculated (see Table 1). To this end, a method is needed that can calculate a single value that represents the variability

Table 1. The ten best trials from the arm simulation data, taken from a total number of 10,000 runs. The left columns show the original data; the right columns show the permuted data for the β- und γ-data sets. The bottom row lists the result variability as variance (s^2) in the individual variables and as bivariate variable error BVE (Hancock et al. 1995). The superscripts denote the number of the run in the original data set

Original data					Permuted data				
α [deg]	β [deg]	γ [deg]	x [cm]	y [cm]	α [deg]	β [deg]	γ [deg]	$x*$ [cm]	$y*$ [cm]
17.27^{1}	104.45^{1}	56.53^{1}	20.11	39.99	17.27^{1}	97.11^{10}	85.86^{6}	11.76	46.31
8.16^{2}	97.65^{2}	73.76^{2}	20.09	39.91	8.16^{2}	92.06^{6}	72.04^{3}	17.08	37.30
9.42^{3}	98.43^{3}	72.04^{3}	19.85	40.05	9.42^{3}	88.44^{5}	92.57^{5}	12.06	42.89
7.11^{4}	96.83^{4}	75.54^{4}	20.15	39.86	7.11^{4}	104.45^{1}	56.53^{1}	26.85	35.81
-1.26^{5}	88.44^{5}	92.57^{5}	19.80	39.91	-1.26^{5}	100.65^{8}	75.54^{4}	28.27	37.37
1.74^{6}	92.06^{6}	85.86^{6}	20.24	39.88	1.74^{6}	98.97^{7}	66.07^{8}	25.85	35.15
9.95^{7}	98.97^{7}	69.95^{7}	20.05	39.73	9.95^{7}	95.96^{9}	73.76^{2}	17.85	39.90
12.54^{8}	100.65^{8}	66.07^{8}	19.73	39.95	12.54^{8}	97.65^{2}	75.18^{10}	16.81	41.80
6.07^{9}	95.96^{9}	77.31^{9}	20.20	39.80	6.07^{9}	98.43^{3}	69.95^{7}	22.37	38.12
8.00^{10}	97.11^{10}	75.18^{10}	19.73	40.15	8.00^{10}	96.83^{4}	77.31^{9}	19.37	40.77
Result variability of *original data*		s^2	0.0353	0.0129	Result variability of *permuted data*		s^2	30.96	10.86
		BVE	**0.22**				BVE	**6.42**	

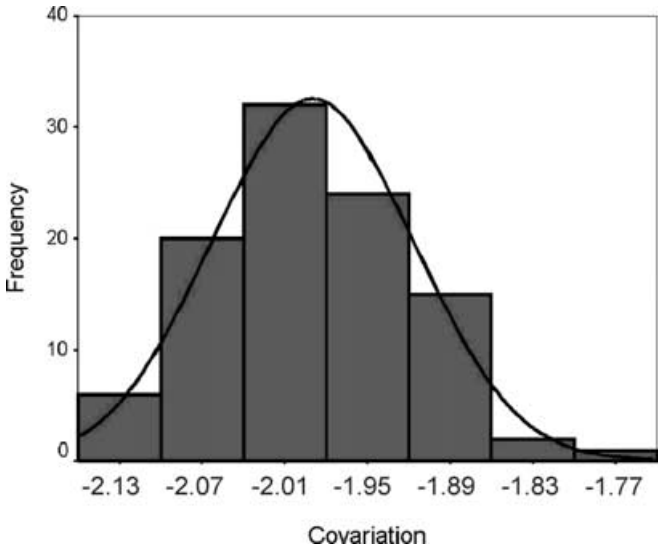

Fig. 3. Histogram of covariation values for repeated runs of the permutation method ($n = 100$). The computed values vary around a mean of -1.99 with a standard deviation of $s_{COV} = 0.09$. The *fitted curve* represents the normal distribution for the same mean and standard deviation

from the two-dimensional x-y result vector. In this case, V_{emp} and V_0 were calculated from the two data sets with a bivariate variable error measure BVE that combines the variable errors of two independent variables x and y into one quantity by the Pythagorean relation: $BVE = \left(s_x^2 + s_y^2\right)^{0.5}$ (Hancock 1995).

It is possible that even in this randomized set there are still pairings between angle values that have covariation "by chance." It is therefore important to estimate to what degree V_0 is influenced by these chance covariations. Therefore, this permutation was repeated 100 times yielding 100 covariation estimates calculated with Eq. 8, where V_{emp} and V_0 are expressed by BVE. In Fig. 3, the 100 covariation results are presented in a histogram. The mean value of covariation COV is -1.99.

To be able to estimate the variance of the values after repeated application of the permutation method, it is important to not only compare this to the mean value of the 10,000 triplets resulting from the permutation runs, but also to consider the results of the individual permutation runs. These covariation values have a standard deviation s_{COV} of 0.09. Note that this becomes the error estimate for one run of the permutation method. To evaluate how strongly this chance covariation influences the interpretation of the result, the meaning of the covariation $COV = -1.99$ needs to be clarified.

First, it will be tested to see whether the value is significantly different from zero. The covariation values from the repeated runs have a normal distribution around their mean verified by the Kolmogorov-Smirnov test: $Z = 0.752$, $p = 0.624$ and are represented by the solid curve in Fig. 3. A one-sample t-test confirms that the distribution of 100 covariation values from the permutation runs differs from zero. The t-value is 221.7, which is highly significant for a sample of 100 ($p < .001$). Although significant, taken by itself the absolute value of COV is without meaning. A more quantitative interpretation is possible only when the magnitude of COV is normalized to that portion of the variability that is uninfluenced by covariation, i.e., the "covariation-free variability." This is the rationale underlying the calculation of the correlation coefficient and will be developed for the multivariate case in the next sections. Presently we may note simply that $COV = -1.99$ corresponds to a generalized correlation coefficient $R = -0.83$, according to Eq. 18. The fact that R and COV are negative corresponds to the expectation that the variability in the end result is reduced by covariation, i.e., systematic compensatory processes have occurred.

5 A permutation method to determine covariation-free variability

In this section, the calculation steps of the example will be developed formally and the generalized correlation coefficient R will be defined. The core idea of the method is that covariation is eliminated by removing the relatedness of co-occurring values by permutation (Maguire et al. 1989b). Yet after this permutation it is still possible that values are correlated by chance and lead to a compensation or amplification of target deviations. Hence, the central question is which combination of values should serve as the reference value that eliminates all such influences. The most comprehensive method is to use all possible combinations of the original variables and then calculate the end results and their variability. Formally, this means: if $X^1, X^2, \ldots, X^m$ are the execution variables, then the variability of the end result V of all combinations of values is obtained by the product set $P = X^1 \times X^2 \times \cdots \times X^m$. The variability of the end result V_f of the product set P is the covariation-free variability V_0.

$$V_0 = V_f(P) \tag{11}$$

In Appendix A, we prove for the bivariate case that the covariation-free variance in the result is identical to the variance of the product set P. Equation 11 is a generalization of the bivariate covariance calculation and includes this as a special case.

A generalization of the calculation method for covariance to nonlinear multiple relations now becomes possible and meaningful. The variance of the result values, obtained from all possible combinations of variable values, can serve as a measure for V_0. In the arm movement example above, the product set P has 100^3 different combinations, and exact calculations can still be performed. However, in other studies there may be 80 measurements of 12 different variables, which obviously makes the calculation procedure of these 80^{12} possible combinations and their variability too cumbersome. In cases where P becomes too large, V_0 can be estimated from a subset of P. This method of estimating covariation in multiple nonlinear relations will be referred to as permutation method. Since in this case the entire set P is not considered, the computations only provide an estimate and it is necessary to systematically evaluate the quality of this estimate. This evaluation becomes

possible when the permutation method is performed repeatedly and generates new subsets of the product set. Considering the variance of the V_0 values, a confidence interval can be given for the estimate (Maguire et al. 1989b).

In sum, if the function f between execution (input) and result (output) variables is known, then the covariation-free variability V_0 can be calculated either directly by using P or indirectly by using several sample sets that are permuted. In Sect. 6, we will show how to apply this method to the example of the arm movement. We will also demonstrate how the accuracy of the method can be influenced so that a desired confidence interval is achieved.

6 The correlation coefficient in multiple nonlinear relations

To derive a multiple nonlinear correlation coefficient, we begin with the bivariate linear case. According to the known formula, the correlation coefficient ρ is calculated from the covariance:

$$\rho = \frac{cov(x,y)}{s_x s_y} \tag{12}$$

To generalize ρ a corresponding formulation for $s_x s_y$ must be found. Rearranging Eq. 12 we get

$$cov(x,y) = \rho s_x s_y \tag{13}$$

If Eq. 13 is inserted into Eq. 2 we get:

$$s^2_{x+y} = s^2_x + s^2_y + \rho 2 s_x s_y \tag{14}$$

For the case of maximal negative correlation $\rho = -1$, the variance in the result s^2_{x+y} attains its minimum value, indicating that compensatory covariation $2s_x s_y$ has its maximum effect. For the case of no covariation $\rho = 0$, s^2_{x+y} becomes $s^2_x + s^2_y$. When $\rho = 1$, the contribution of covariance to s^2_{x+y} is positive and variance in the result attains its maximal value.

Hence, in the linear case the term $2s_x s_y$ describes the maximal difference between V_{emp} and V_0, denoted by $\Delta V_{\max}$. Using this notation a generalized correlation coefficient R can be defined as

$$R = \frac{2COV}{\Delta V_{\max}} \tag{15}$$

In contrast to the linear case, $\Delta V_{\max}$ does not have to be symmetric around V_0. V_{emp} for maximal positive correlation need not have the same distance to V_0 as for maximal negative correlation. In Appendix B, this is demonstrated with a simple example. In the following sections we discuss a solution to this problem.

7 Calculation of the covariation-dependent influence on result variability $\Delta V_{\max}$

The logic of calculating R requires the normalization of the covariance by the maximal effect $\Delta V_{\max}$ that covariation can achieve. How strongly the variability in the result can be influenced by covariation is dependent on the task as expressed by its functional relation f. Therefore, the value of $\Delta V_{\max}$ must be determined for each case. There are two possibilities for doing this.

(1) A theory-based determination of $\Delta V_{\max}$

Referring back to the arm movement example, two important facts must be considered. First, perfect task performance requires zero variability over repetitions. Second, the system is redundant and can display compensatory deviations. Therefore, the minimally possible variability $V_{\min}$ is zero and the following holds:

$$\Delta V_{\max} = V_0 - V_{\min} = V_0 \tag{16}$$

and Eq. 15 can be written as

$$R = \frac{2COV}{V_0} \tag{17}$$

or equivalently

$$R = \frac{V_{\text{emp}}}{V_0} - 1 \tag{18}$$

If the task-required variability is not zero, as for instance when the arm points to a target area instead of a point, or the system is not redundant, the calculation of $V_{\min}$ must take this into account. When the covariation is positive, the normalization of COV uses the distance between V_0 and the variability in the end result produced by maximal positive covariation $V_{\max}$:

$$R = \frac{2COV}{V_{\max} - V_0} \tag{19}$$

Whether and how this value can be determined is different for each case. We therefore refrain from a discussion of these possibilities.

(2) Computational determination

An estimate of the maximal effect of covariation on the result variability $\Delta V_{\max}$ can also be obtained on the basis of the data alone. To this end, those permutations of the execution variables X^k must be found that yield the largest and the smallest result variability. This can be achieved by exhaustively computing the variances of all permutations of X^k. Equivalently, one can calculate the product set P of all X^k and draw all subsets T_j $(j = 1, 2, \ldots)$ such that in each T_j a member from each set of X^k occurs exactly once. With this condition it is ensured that each subset T_j is a potential result of a permutation of X^k. If one determines $V_f(T_j)$ for all subsets and determines the maximum $V_f(T_j)_{\max}$ and minimum $V_f(T_j)_{\min}$, then the following holds for negative covariation:

$$R^{-} = \frac{2COV}{V_0 - V_f(T_j)_{\min}} \tag{20}$$

for positive covariation:

$$R^{+} = \frac{2COV}{V_f(T_j)_{\max} - V_0} \tag{21}$$

Like the determination of V_0, it often happens that the calculation of all subsets T_j becomes numerically too cumbersome. In contrast to the calculation of covariation, using only subsets does not necessarily render converging estimates.

8 Calculation of partial multiple nonlinear covariations and correlations

At this point another advantage of the proposed method should be mentioned. With only a few modifications of the permutation method, partial covariations and correlations can also be calculated. When applying this method, it is not necessary that all data sets be permuted simultaneously. It is possible to permute only a subset of data, or even only one data series, or to permute several data sets in the same way, and thereby maintain the relatedness among selected subsets of data. In this way, covariation can be eliminated in a targeted fashion and quantified with respect to the empirically measured variability.

In the movement example, we permuted only the sequence of the wrist angles γ; the pairs of the other two angles α, β were kept constant. In this case, we obtained a partial covariation value of $COV = -1.52$, which corresponded to a partial correlation coefficient R of -0.79. If the angles for wrist and elbow were kept constant and only shoulder angles were permuted, $COV = -1.83$ and $R = -0.82$.

9 Summary of the calculation steps

Step 1: Prerequisites for the method – determining f and V

For the application of the method two conditions must be satisfied. (1) As already mentioned above, the functional relation f between the execution and the result variables must be known. (2) The results of the statistic V that is used to capture the variability estimates must have an interval scale. The calculation of the correlation coefficient requires V to have a relational scale so that a quotient can be calculated (see Eq. 15). The original data themselves do not have to satisfy any particular condition.

Step 2: Measuring the relevant variables

For repeated performances i there must be one measurement x_i for each variable X^m.

Step 3: Calculating V_{emp}

From the data sets of the execution variables $X = X^1, X^2, \ldots, X^k$ a result r_i can be calculated for each run i from knowing f or the transfer function. From their variability, V_{emp} can be calculated:

$$V_{\text{emp}} = V_f(X) \tag{22}$$

This procedure is preferred to the direct measurement of results and their variabilities as it cannot be excluded that the noted differences between V_0 and V_{emp} are partly produced by different measurement errors in execution and result variables. This recommendation, however, is based on the assumption that different measurement errors lead to a larger error in the result than potential inaccuracies and approximations in the model and the function f.

Step 4: Determining V_0

For each variable X the indices i of the run are permuted separately to generate new data sets: $X^* = X^{1^*}, X^{2^*}, \ldots, X^{m^*}$. In analogy to step 3, V_0 can be calculated:

$$V_0 = V_f(X^*) \tag{23}$$

If one wants to calculate partial covariations, then values of the individual data sets whose covariation are *not* of interest must be permuted in the same way.

As V_0 is only an estimate derived from the permuted data sets, the accuracy of this estimate must be calculated. Therefore, the permutations are repeated multiple times and the standard error σ for a single run is calculated. If the estimation error must be below a certain boundary ε, the permutation must be repeated n times, where n is calculated as follows:

$$n > \frac{\sigma}{\varepsilon^2} \tag{24}$$

Assuming that we want to obtain the covariation of the arm movement task with an accuracy of ± 1 standard deviation and $\varepsilon = 0.1$, we must perform at least nine permutation runs given the standard deviation of covariation $s = 0.09 (n > 0.09/0.01 = 9)$.

Step 5: Calculation of covariation

From the now known values for V_{emp} and V_0 covariation can be calculated applying Eq. 8.

Step 6: Determining $\Delta V_{\max}$

The maximal effect of covariation onto the result variability can be calculated theoretically or by computation. Note that it must be taken into account that this value can differ for positive and negative covariations.

Step 7: Calculation of the correlation coefficient

Knowing the values for COV and ΔV_{max} the correlation coefficient R can be calculated following Eq. 15.

10 Discussion

The organization and order of a system with many degrees of freedom is equivalent to the existence of constraints among component variables or processes. In biological systems, such internal constraints lead to the observation that the output is different from what would be expected from the random combination of its component variables. Goal-directed coordinated behavior of a biological system is governed by such constraints among the component processes. Conversely, it can be said that control in behavior resides in establishing such covariation among component variables. In the present paper, we developed a method that can quantify such control or organization. It should be pointed out that our method does not present another inferential statistic that assesses the probability at which a result must be ascribed to chance. Rather it presents a quantification of the covariation inherent in a set of variables. To further emphasize: our method is not an *inferential* statistical method but, it *describes* the relation between two data sets.[1]

One of the essential prerequisites – and apparent limitations – for applying the permutation method is that the functional relation, or transfer function, between the execution (input) and the result (output) variables must be known. The projection from the set of relevant component variables into the result space, performed for the measured data set or the permuted set of variables, is at the core of the permutation method. Explicit knowledge of the functional relation, however, is not a shortcoming specific to the permutation method but is required for all other quantifications of covariation. (For a comparison of the methods with a concrete numerical example see Appendix C.)

For instance, when computing the commonly used bivariate covariance and correlation coefficient, a linear functional relation is assumed. Evidently it is possible that in many cases where linear covariance is zero, other nonlinear relations exist. Note that a regression even with a more appropriate nonlinear function is not identical to covariation. While regression is a unidirectional projection from one variable (x) to the other (y), covariation estimates in a symmetric fashion how the two variables covary with respect to a third output variable r. In a bivariate linear or also nonlinear, e.g., polynomial regression, the residual or error variance is determined in only one of the variables, typically y, but differs for x and y. In contrast, determining covariance or covariation yields a "residual" symmetrically from all input variables. Similarly, in multiple nonlinear regression methods, e.g., the Levenberg-Marquardt algorithm (Press et al. 1989), the conceptual core is different: what is tested is the fit of a hypothesized function that connects several input variables, and their parameterization is optimized. For instance, when fitting a sphere into a three-dimensional cloud of data points, the parameter's radius and center of sphere are determined by an optimization method. In contrast, the permutation method would test the degree of covariation between the input variables when a sphere with specific parameter values for radius and center is given. In the same spirit, the residual variance of a regression could be interpreted, where zero variance corresponds to perfect covariation. However, as the regression does not give a reference value for covariation-free variance, the degree of covariation cannot be estimated.

In the case where the analytical function between component and result variables is not known, a transfer function can, for example, be approximated by using different curve-fitting techniques or a neural network. For instance, Ritter et al. (1989) developed a network that learns the relations between task parameters and representations of joint configurations. For a similar coordinate transformation, Kawato and colleagues (1988) proposed a network for the inverse dynamic transformation that associated a desired kinematic representation with joint torques. Clearly, a number of different network models are available that are designed to estimate the functional relations between coordinates (see also Jordan 1990). These transfer functions can then be used in the permutation method to project execution (input) variables into result (output) variables.

As it is necessary to establish an analytical or approximated transfer function, the effect of variability in all the component variables can be compared in the result space. Due to this property, the permutation method has advantages over another method that is similar in spirit although different in its original motivation. The uncontrolled manifold method (UCM), as proposed by Schöner, Scholz, and colleagues, similarly tests the effect of component variables with respect to a given task variable (Schöner 1995; Scholz and Schöner 1999; Scholz et al. 2000). In one study, the authors investigated a shooting movement with a laser pistol performed by the entire arm and measured the position of the laser beam for aiming accuracy and the seven joint angles of the arm as their execution variables. Their analysis tested the contribution of variance in joint angles onto the laser beam position on the target. In the 7D joint-angle space, the null space (the manifold in which variation has no effect on the task variable) was determined. In order to compare the variance within this manifold with the variance that has an effect on the result, the eigenvectors of the manifold were determined and variances (eigenvalues) parallel and orthogonal to the uncontrolled manifold were determined. Variance parallel to the manifold is interpreted as uncontrolled variance and variance orthogonal to this manifold as controlled. This comparison of variances can be made

[1] If one wanted to test whether covariation is different from zero, that is, perform an inferential statistical test, one can assume that all covariation values have a normal distribution and its standard deviations give a confidence interval. This confidence interval could be used to assess whether the determined value of covariation is statistically different from zero.

only if the space of the component variables is homogeneous. This is the case only if the component variables have the same dimensions, e.g., degrees. A second, potentially confounding, factor is when the variances are not of the same scale. If this is not the case or no adjustments are made, the variance in a value with a small range is underestimated (as can be seen in Appendix C). For the permutation method these issues do not play a role because comparisons are made only in result space, where differential contributions of the execution variables are faithfully represented. Another difference between the UCM method and the permutation method is that the UCM method assumes linearity in estimating the controlled and uncontrolled variance. Such linearization is not necessary for the permutation method, as the evaluation of variances is performed in result space.

The permutation method is not limited to any specific measure of dispersion, such as the standard deviations. Every dispersion measure that captures the distance between two or more values of the result variable can be used. For instance, in our arm movement example, two variables, x and y, captured the results that were combined in the bivariate variable error (BVE). Whenever such a compound dispersion measure can be defined, situations can be analyzed in which the result is expressed in any number of variables. For instance, if the output of a multivariable system, e.g., some dynamical system, is a trajectory, then the desired or average trajectory can be determined and distances between two trajectories expressed in terms of a root mean square measure. In this sense, it becomes evident that the permutation method can also be used for estimating robustness of input parameters in a dynamical model that generates a trajectory.

One more practical concern should be mentioned. As the calculation of covariance is based on the comparison between two variances, a confounding problem may arise when the data sets have different measurement errors. For instance, data collection of the arm's end position is associated with different errors than measurements of the joint angles. Then the difference between the empirical result variability and covariation-free variability may at least partially be caused by these different measurement errors. This problem can be circumvented as the permutation method also offers the possibility of computing the empirical result variability from the execution variables. To this end, the variability of the set of results should be calculated from the unpermuted set of X^k.

The method has a wide range of applications. From the arm movement example it may be concluded that the method is only applicable to situations where the result is only a single data point. However, the method can be equally applied when a sequence of points is produced, such as in a trajectory. To this end, the desired trajectory can be parsed into points that represent important landmarks. For each such landmark the effect of covariation can be estimated. In the same spirit, Scholz et al. (2000) applied the UCM method to evaluate a control variable in the pistol-shooting task. The average performed trajectory was parsed into ten points, and for each point variability in the null space and the direction orthogonal was estimated. What must be kept in mind is that each point on the trajectory is assumed to be a target for the executing variables, which is not necessarily the case. Under this same strong assumption the present method can also be applied to estimate covariation along landmarks in the trajectories.

In conclusion, we developed a permutation method for the calculation of covariation among multiple variables that are linked nonlinearly to a dependent variable. In the derivation, we generalized from the bivariate linear case, such that covariance and the correlation coefficient is a special case of our nonlinear multiple covariance and correlation coefficient. The permutation method is a variant of the Monte Carlo method, which has already been applied for many biological problems (Manly 1997). For illustration we used an example from the study of movement coordination where covariation has often been invoked to capture order and control in goal-directed movements.

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Appendix A

Proof: calculation of linear bivariate covariance is a special case of the permutation method

To demonstrate that the permutation method is a generalization of the calculation of covariance, it must be shown that the covariation-free variability V_0 is identical to the variability obtained when the result variability is determined by the product set P from the execution variables X^k. Following Eq. 2, the variance of the sum of two variables $A = \{a_1, a_2, \ldots, a_n)$ and $B = \{b_i, b_2, \ldots, b_n\}$ whose individual variances s_a^2 and s_b^2 and the covariation can be computed. Following Eq. 2 this is:

$$V_0 = s_a^2 + s_b^2 \tag{25}$$

If V_0 is calculated with the permutation method, then the set of all value combinations must be considered. In the bivariate case, this is the product set $A \times B$. Without limitation of generality, it can be assumed that the mean values of the two data sets are zero: $\bar{a} = \bar{b} = 0$. To permit comparison with the covariance calculation, we use the simple example where the result values r_i are the sum of the two execution parameters $r_i = a_i + b_i$. The variance $s_{A\times B}^2$ in the result across all combinations of values is:

$$s_{A\times B}^2 = \frac{\sum_{AxB} (r_m - \bar{r})^2}{n^2} = \frac{\sum_{AxB} \left(a_i + b_j - (\bar{a} + \bar{b})\right)^2}{n^2} \tag{26}$$

As $\bar{a} = \bar{b} = 0$, it follows that

$$s^2_{A\times B} = \frac{\sum\limits_{A\times B} a_i^2}{n^2} + \frac{\sum\limits_{A\times B} b_j^2}{n^2} + \frac{\sum\limits_{A\times B} 2a_i b_j}{n^2} \tag{27}$$

and

$$\sum_{A\times B} a_i^2 = n\sum_{u=1}^{n} (a_u - 0)^2 = n^2 s_a^2$$

and the same holds for $\sum\limits_{AxB} b_j^2$.

Therefore:

$$s^2_{A\times B} = s_a^2 + s_b^2 + \frac{\sum\limits_{A\times B} 2a_i b_j}{n^2} \tag{28}$$

With the following rearranging of terms it can be shown that the right summand is zero:

$$\begin{aligned}\sum_{A\times B} 2a_i b_j =& 2(a_1 b_1 + \cdots + a_n b_{k-1} + a_1 b_k \\ &+ \cdots + a_n b_k + a_1 b_{k+1} + \cdots + a_n b_n)\end{aligned} \tag{29}$$

The respective summands with the same b-values can be collected, yielding:

$$\sum_{A\times B} 2a_i b_j = 2(b_1 \sum_{z=1}^{n} a_z + \cdots + b_n \sum_{z=1}^{n} a_z) = 0 \tag{30}$$

as

$$\bar{a} = \frac{1}{n}\sum_{z=1}^{n} a_z = 0$$

Therefore, with consideration of (A1), we can write:

$$s^2_{A\times B} = s_a^2 + s_b^2 + 0 = V_0$$

Hence, the proof is complete.

Appendix B

Proof: the absolute value of the maximal positive covariation $\Delta V^+_{\max}$ is different from the maximal negative covariation $\Delta V^-_{\max}$

Let us assume two data sets with three samples each: $X^1 = \{0,0,1\}$ *and* $X^2 = \{0,9,0\}$. From one pair of values (x_i^1, x_i^2), $(i = 1,\ldots,3)$ the result r_i can be calculated with the function $f : y_i = x_i^1 x_i^2$. The product set $P = X^1 \times X^2$ includes the elements {(0,0), (0,0), (0,0), (0,9), (0,9), (1,9), (0,0), (0,0), (1,0)}. The set of all results determined by f is $Y = \{0, 0, 0, 0, 0, 9, 0, 0, 0\}$, with a mean value of 1. If standard deviations are used as the dispersion measure, then $s(Y) = 2.83$. Following the permutation method, the covariation-free result variability corresponds to the variability of the set, that is, $V_0 = s(Y) = 2.83$.

To determine the maximum negative covariation we must select the values of the two sets that have minimum variability in the result. In our example, there are many combinations that lead to a result variability of 0, e.g., $X^1 = \{0,9,0\}$ and $X^2 = \{0,0,1\}$, yield $Y = \{0,0,0\}$, with $V(Y) = 0$. $\Delta V^-_{\max}$ can be calculated from the difference: $\Delta V^-_{\max} = V_0 - 0 = 2.83$. In analogy, for the computation of $\Delta V^+_{\max}$, pairings of values must be selected that have the highest variability in the result. This occurs, for example, when $X^1 = \{0,0,9\}$ and $X^2 = \{0,0,1\}$, and $Y = \{0,0,9\}$, and $V(Y) = 3.83$. This means that $\Delta V^+_{\max} = V_{\max} - V_0 = 3.83 - 2.83 = 1$. This example demonstrates that the values of $\Delta V^+_{\max}$ and $\Delta V^-_{\max}$ can indeed be different.

Appendix C

Comparison of different methods to calculate multiple nonlinear covariation or correlation

For the following comparison between methods the following nonlinear relation f between three input variables x, y, and z, and one output variable c will serve as the example:

$$c = f(x,y,z) = x^2 + y^2 - z \tag{31}$$

Let us assume c is a constant. If all input triplets (x, y, z) that satisfy f are plotted, a paraboloid is obtained. Real data very rarely satisfy this relation exactly. Hence, we assume c is approximated with a remaining distance of ε. For simplicity we set $c = 0$ and write:

$$\varepsilon = x^2 + y^2 - z \tag{32}$$

where the variance of the ε-values is a measure for the size of the errors. Some of the methods use the Jacobian matrix, which requires the specification of a point in the space of input variables at which the Jacobian can be computed. In Eq. 32 the point $(0,0,0)$ is a solution of the equation at which the Jacobian is calculated. At $(0,0,0)$ the two partial derivatives $\partial f/\partial x$ and $\partial f/\partial y$ of this function are zero. The Jacobian has the value of $(0,0,-1)$ at this point.

For the task function Eq. 32 five data sets were created that contained different amounts of covariation and error variance. Each set consisted of 100 data points. Then five different methods of calculating covariance will be applied and their validity in estimating this known covariance will be compared. In all cases, the variance is used as error measure V.

The first data set, DS-0, contains only triplets of input values that exactly satisfy Eq. 32. While the x-values and y-values are normally distributed ($\bar{x} = \bar{y} = 0, s_x = s_y = 1.5$) and stochastically independent of each other, z is chosen to exactly obtain an output of $c = 0$. Hence, the covariation is perfect and thus all methods should give a correlation coefficient of either 1 or -1, depending on whether the specific method takes the sign into account.

The second data set, DS-10, is based on the same x-values and y-values as DS-0, but the output variance is not zero but has a variance of ε, as expressed in Eq. 32. For DS-10 the z-values were so chosen ($z = x^2 + y^2 - \varepsilon$)

Table 2. Summary of results of the computation of covariation and correlation of five selected methods

Data set Predicted correlation coefficient R		DS-0 −1	DS-10 −0.95	DS-50 0.71	DS-100 0	DS-100xy $\neq 0$
1. Linear regression	R	0.362	0.367	0.807	**0.095**	0.102
2. Nonlinear regression	R	**1**	**0.95**	**0.81**	**0.00**	0.00
3. Jacobian matrix	V_0R	**37.6**	**40.43**	**93.66**	51.34	81.66
		−1	**−0.90**	**−0.66**	0.79	0
4. UCM	$\parallel$ UCM	1.74	1.74	1.74	1.34	
	$\perp$UCM	6.13	6.35	9.68	9.04	9.04
5. Randomization	V_{emp}	**0**	**3.92**	**31.31**	**91.92**	**81.66**
	V_0	**70.9**	**82.7**	**133.86**	**92.80**	**130.46**
	R	**−1**	**−0.95**	**−0.76**	**−0.01**	**−0.37**

that the variance of the ε-values was 10% and the variance of $(x^2 + y^2)$ was 90% of the variance of the z-values. By this choice, the covariation is 90% of the total variance. The squared correlation coefficient should reflect this ratio, and a correlation coefficient of $0.9^{0.5} = 0.949$ (or -0.949) should be obtained.

The third data set, DS-50, was constructed like the second one; however, more error variance was added so that the variance of ε-values is of equal magnitude as the variance of the z-values. Consequently, the expected value for the correlation coefficient is $0.5^{0.5} = 0.707$.

In the fourth data set, DS-100, all input variables were generated independently and formed into triplets in a random fashion. Thus, 100% of the variance of the z-values are error variance, that is, variance of the ε-values. Consequently, we expect a correlation coefficient of zero.

In the fifth data set, DS-100xy, the x-values were generated so that for all triplets the following relation held: $x^2 + y^2 = 36$. The z-values vary independently of x and y with $\bar{z} = 0, s_z = 9$. Under these conditions the correlation coefficient cannot be given in advance. The relation between variables x and y, however, should reduce the error variance (variance of ε-values), which should lead to a correlation coefficient different from zero.

Each of these data sets was evaluated with five different methods that tested the data sets for their covariance and correlation:

1) Multiple linear regression with the regression equation $z = \mathrm{a}x + \mathrm{b}y + \mathrm{d}$, where a, b, and d are constants.

2) Multiple nonlinear regression with the following equation, which is equivalent to Eq. 32 if $c = 0$.

$$z = x^2 + y^2 \tag{33}$$

This method was performed using the procedure of the software SPSS 10.0, which uses a variant of Levenberg-Marquardt nonlinear regression (a detailed description of the procedures used can be found at http://www.spss.com/tech/stat/ index.htm).

3) Calculation of the Jacobian matrix. The expected result variability V_0 can be estimated from the variability of the input variables by taking partial derivatives at the selected point of the input variables. The partial derivatives are then multiplied with the variability values of the respective variables (Sust 1997).

4) The method of computing the uncontrolled manifold (UCM) Scholz and Schöner (1999). The variance is separated into two components, one parallel to the null space (spanned by $(1, 0, 0)$ and $(0, 1, 0)$ and one orthogonal to the direction of the null space (spanned by $(0, 0, 1)$). Note that to ensure comparability between the different methods, the calculation of directions parallel and orthogonal to the null space was determined using the Jacobian of the function f. Relevant with respect to the covariation is the ratio between the two components. Covariation is present when $\parallel$UCM/$\perp$UCM > 1 (Scholz and Schöner 1999) or $\parallel$UCM $\gg \perp$UCM (Scholz et al. 2000).

5) The permutation method as presented in the paper.

The application of the five methods rendered the results that are summarized in Table 2. The second row lists the results that should be obtained based on the known covariation and correlation in the constructed data sets. The bold numbers highlight the results of the various methods that agree with the predicted results. As expected, the linear regression method fails. The resulting correlation values produce correlation coefficients that do not even agree with the rank order of the expected values. Similarly as expected, the nonlinear regression produces correct coefficients as long as the relation between predictor $(x + y)$ and the dependent variable (z) is evaluated. Covariation between the predictor variables (x, y) cannot be calculated accurately.

In our example at (0, 0, 0), the Jacobian method relies exclusively on s_z^2 since two partial derivatives are zero. Therefore, this method renders correct values only if s_z^2 – by happenstance – is close to V_0. Note, if all partial derivates were zero, the estimate of V_0 would be zero and, thus, the correlation coefficient R would be infinite (see Eq. 15) irrespective of the variability of the input variables.

The UCM method fails if one follows the criteria stated to define covariation: $\parallel$UCM/$\perp$UCM > 1, or $\parallel$UCM $\gg \perp$UCM. Even when perfect covariation is present, we obtain $\parallel$UCM $< \perp$UCM, which is taken as an indication for the absence of covariation. The stated criteria hold only when the linearization provides a sufficient approximation. This would, for instance, be the case if the dispersions of the x- and y-values were smaller (s_x, $s_y < 1$) than they are in the given example. The method begins to give more veridical results when $s_x, s_y \leq 0.35$. Further critical prerequisites of the method are mentioned in the discussion section.

The present randomization method successfully predicts the known values of covariation and correlation.

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