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# Multivariate Process Capability Indices: A Directional Approach

Miroslav Šiman<sup>a</sup>

<sup>a</sup> Institute of Information Theory and Automation of the ASCR, Prague, Czech Republic Accepted author version posted online: 17 Jan 2014.Published online: 22 Apr 2014.

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### Multivariate Process Capability Indices: A Directional Approach

MIROSLAV ŠIMAN

Institute of Information Theory and Automation of the ASCR, Prague, Czech Republic

We propose a unified, universal, natural, and very intuitive way how to obtain new multivariate and tool wear extensions of univariate process capability indices by means of projection pursuit. We also illustrate the methodology in detail of the popular precision and accuracy indices, generalize the latter in a few different ways in the same spirit, add some personal insight, discuss the computational issues involved, and demonstrate the advantages of our approach in a small data example.

Keywords Process capability index; Projection pursuit; Quantile regression.

Mathematics Subject Classification Primary 62P30; Secondary 62H99.

#### 1. Introduction

Process capability indices (PCIs) were introduced for evaluating the acceptability of manufacturing processes, and since they have become essential for any quality improvement program.

In the standard univariate case, we assume that there is only one important stochastic feature  $Y \in \mathbb{R}$  of the output and that we have an idea about the optimal target value  $T \in \mathbb{R}$  of the process as well as about the range  $\mathcal{T} = [LSL, USL]$  of all its conforming output values. The goal of PCIs is to quantify how much Y meets our expectations, and many univariate PCIs have already been proposed and thoroughly investigated for this purpose. Naturally, they are often based on the scalar quantities T, USL, and LSL as well as on some parameters of the distribution  $\mathcal{L}(Y)$  of Y; see Pearn and Kotz (2006) or Kotz and Lovelace (1998) for a survey.

Those books also briefly summarize current proposals of PCIs in the multivariate context, where we have to deal with a stochastic vector process characteristic  $\mathbf{Y} \in \mathbb{R}^m$ , with its optimal target value  $\mathbf{T} \in \mathbb{R}^m$  and with the tolerance region  $\mathcal{T} \subset \mathbb{R}^m$  of all conforming values of  $\mathbf{Y}$ . These proposals often assume a special shape of  $\mathcal{T}$  or a special distribution of  $\mathbf{Y}$  such as normal or elliptical, employ variance matrices and related Mahalanobis distances

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Address correspondence to Miroslav Šiman, Institute of Information Theory and Automation of the ASCR, Pod Vodárenskou věží 4, CZ-182 08, Prague, 8, Czech Republic. E-mail: siman@utia.cas.cz and principal or axial vectors, use ellipsoids, and consider either their volumes or their largest inflated copies still contained in the tolerance region.

Of all these ideas, it is only that of considering some directions that seems somewhat related to our approach of employing all directions at all in the projection pursuit methodology, see, e.g., Friedman (1987) and Huber (1985), that we use to generalize univariate PCIs to the multivariate and regression/tool wear context in a systematic way and without any limiting assumptions on T and the distribution of **Y**.

The only other work combining projection pursuit methodology with process capability indices is probably that of He et al. (2007), written in Chinese. After examining its formulae and English abstract, we still believe that our contribution is substantially different for it is partly based on some very recent results, discusses *general* PCIs in the *general* multivariate and *regression* context, proposes no less than four different multivariate generalizations of the accuracy index, presents much of unique personal insight, and does not use projections of the tolerance region.

In what follows, we present basic definitions and notation in Sec. 2, introduce the multivariate generalization of PCIs in Sec. 3, illustrate it on precision and accuracy indices in Secs. 3.1 and 3.2, describe the regression (multivariate) generalization in Sec. 4, briefly discuss the computational aspects in Sec. 5, and conclude with a simple data example in Sec. 6.

#### 2. Definitions and Notation

Let us consider a multivariate product or process  $\mathbf{Y} \in \mathbb{R}^m$ ,  $m \ge 1$ , whose engineering specification is given by a convex and compact tolerance region  $\mathcal{T} \subset \mathbb{R}^m$  and by a target value  $\mathbf{T} \in \mathcal{T}$  in the interior of  $\mathcal{T}$ . The convexity assumption on  $\mathcal{T}$  is satisfied by all the common tolerance regions of elliptical and polyhedral shapes, and it guarantees that any segment linking  $\mathbf{T} \in \mathcal{T}$  with any  $\mathbf{y} \in \mathcal{T}$  lies in  $\mathcal{T}$ , which is often highly desirable. The compactness of  $\mathcal{T}$  is not limiting at all because its boundary  $\partial \mathcal{T}$  is too negligible to have any effect, and everything real and material is bounded anyway.

Furthermore, we will always assume  $\mathbf{T} = \mathbf{0}$  without any loss of generality as we can always shift the coordinate system accordingly. And if the target value  $\mathbf{T} = \mathbf{0}$  is given, then any  $\mathbf{u} \in S^{m-1} := {\mathbf{u} \in \mathbb{R}^m, \|\mathbf{u}\| = 1}$  leads to the unique point  $L_{\mathbf{u}}$  on  $\partial \mathcal{T}$  of the form  $r_{\mathbf{u}}\mathbf{u}$  for some  $r_{\mathbf{u}} > 0, r_{\mathbf{u}} = \|L_{\mathbf{u}} - \mathbf{T}\| = \|L_{\mathbf{u}}\|$ .

Finally, we will consider an auxiliary univariate process  $Z \in \mathbb{R}$  with the target value T = 0 in the tolerance interval [LSL, USL], and we will assume that  $C = C(\mathcal{L}(Z), LSL, USL, T)$  is an arbitrary univariate PCI whose value, roughly speaking, decreases with the worsening behavior/capability of Z. Usually, C depends on the distribution  $\mathcal{L}(Z)$  of Z only through a few of its scalar characteristics such as moments or quantiles.

#### 3. Multivariate Extension

We suggest to generalize *C* to the multivariate index  $C_M$  for  $\mathbf{Y} \in \mathbb{R}^m$  with target  $\mathbf{T} = \mathbf{0}$  by means of the projection pursuit:

$$C_M = \inf_{\mathbf{u} \in \mathcal{S}^{m-1}} C(\mathcal{L}(\mathbf{u}'\mathbf{Y}), -r_{-\mathbf{u}}, r_{\mathbf{u}}, 0).$$
(1)

In other words,  $C_M$  is the least favorable of all values of C computed from projections  $\mathbf{u}'\mathbf{Y}$ ,  $\mathbf{u} \in S^{m-1}$ , with [LSL, USL] replaced with  $[-r_{-\mathbf{u}}, r_{\mathbf{u}}]$ . Of course, this coefficient might also be scaled or shifted by a suitable constant if it were found more convenient, which

holds for any other PCI as well. Furthermore, new multivariate PCIs could be obtained by combining a few of such multivariate indices into a single one, which is already a common practice in the univariate setting. For example, one might generalize  $C_{pk}^*$  on p. 184 in Pearn and Kotz (2006) to  $C_{pk,M}^* = C_{p,M}^*(1 - k_{a,M})$  with  $C_{p,M}^*$  and any version of  $k_{a,M}$  considered below, and possibly also with  $C_{p,M}^*$  replaced with the multivariate precision index of Šiman (2014).

If the infimum in (1) is achieved for a vector  $\mathbf{d} \in S^{m-1}$ , i.e.,  $C_M = C(\mathcal{L}(\mathbf{d}'\mathbf{Y}), -r_{-\mathbf{d}}, r_{\mathbf{d}}, 0)$ , then such a critical direction **d** indicates where the problems with capability are the most serious, which is also an interesting piece of information.

Note as well that the index naturally degenerates to the univariate case for  $S^0 = \{-1, 1\}$ , and that many distributional parameters influencing common univariate PCIs are the same for processes *Z* and -Z if indeed T = 0. In fact, many univariate process capability indices can easily be rewritten in the form of  $C_M$  for m = 1, which makes their multivariate generalization very straightforward.

#### 3.1 Example 1: Multivariate Precision Index

For example, the univariate precision index  $C_p^*$ , discussed on p. 183 of Pearn and Kotz (2006), can be rewritten as follows:

$$C_p^* = \min\left\{\frac{USL - T}{3\sqrt{\operatorname{var}(Y)}}, \frac{T - LSL}{3\sqrt{\operatorname{var}(Y)}}\right\} = \inf_{\mathbf{u}\in\mathcal{S}^0} \frac{r_{\mathbf{u}}}{3\sqrt{\operatorname{var}(\mathbf{u}'\mathbf{Y})}}.$$

Consequently, it could be generalized to the multivariate context as

$$C_{p,M}^* = \inf_{\mathbf{u}\in\mathcal{S}^{m-1}}\frac{r_{\mathbf{u}}}{3\sqrt{\operatorname{var}(\mathbf{u}'\mathbf{Y})}}$$

Still, we continue to prefer the multivariate precision index introduced in the accompanying paper Šiman (2014) because we are deeply convinced that any precision index should be independent of the target value.

#### 3.2 Example 2: Multivariate Accuracy Indices

We believe that process accuracy is well defined only with respect to a given target and that it should depend on the process only through its parameter of location. In the setting considered above, with  $\mathbf{Y} \in \mathbb{R}^m$  and  $\mathbf{T} = \mathbf{0}$ , we therefore propose the following definition of multivariate accuracy index  $k_{a,M}$  of  $\mathbf{Y}$ :

$$k_{a,M} = \sup_{\mathbf{u}\in\mathcal{S}^{m-1}} \frac{\mathbf{u}'\boldsymbol{\mu}}{r_{\mathbf{u}}},\tag{2}$$

where  $\mu$  stands for a location parameter of **Y**. This definition works for any sensible choice of  $\mu$  and falls into the general framework introduced above for  $\mu = E\mathbf{Y}$  when  $\mathbf{u}'\mu = E\mathbf{u}'\mathbf{Y}$ . Nevertheless, other location parameters might be employed as well. For example, we would recommend to set  $\mu$  equal to an affine equivariant multivariate median of **Y** whenever there is no a priori information about the distribution of **Y** available; see Small (1990) for an inspiration. Furthermore, this index could be modified in several ways, for example

$$k_{a,M}^{I} = \sup_{\mathbf{u}\in\mathcal{S}^{m-1}} \frac{\mathbf{u}'\boldsymbol{\mu}}{0.5(r_{\mathbf{u}} + r_{-\mathbf{u}})}, \quad k_{a,M}^{II} = \sup_{\mathbf{u}\in\mathcal{S}^{m-1}} \frac{|\mathbf{u}'\boldsymbol{\mu}|}{r_{\mathbf{u}}}, \quad \text{or} \quad k_{a,M}^{III} = \frac{\sup_{\mathbf{u}\in\mathcal{S}^{m-1}} \mathbf{u}'\boldsymbol{\mu}}{\inf_{\mathbf{u}\in\mathcal{S}^{m-1}} r_{\mathbf{u}}} \quad (3)$$

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where the last two alternatives might be found useful for processes whose output is expected to be conforming even when it is reversed (taken with the opposite sign) or rotated arbitrarily. Each index in (2) and (3) is defined as a *supremum* over all directions because the univariate index C behind it, i.e. the version for m = 1, *increases* with the worsening capability of the underlying process.

If  $\mu = EY$ , then  $k_{a,M}^{I}$  degenerates to index k in the univariate case if the midpoint of the tolerance interval is zero. Similarly, both  $k_{a,M}^{II}$  and  $k_{a,M}^{III}$  always reduce to index  $k^*$  for m = 1; see p. 31 and p. 184 of Pearn and Kotz (2006) for the indices k and  $k^*$ , respectively. To the best of our limited knowledge of PCIs, the most natural index  $k_{a,M}$  has not yet been considered in the literature even in the univariate case.

Note that these definitions virtually ignore the precision of the process and avoid any complicated inflating of some level sets or quantile regions. As the univariate accuracy index  $C_a$  is currently defined as 1 - k, we might also subtract  $k_{a,M}$ ,  $k_{a,M}^I$ ,  $k_{a,M}^{II}$ , and  $k_{a,M}^{III}$  from 1 to obtain its direct multivariate counterparts.

#### 4. Regression Extension

The multivariate index introduced in the previous section could be generalized easily even to the regression setup where **Y** is accompanied with a stochastic vector of regressors  $\mathbf{X} \in \mathbb{R}^{p}$ , simply by considering the conditional distribution of the projections instead. Indeed,

$$C_R = \inf_{\mathbf{u}\in\mathcal{S}^{m-1}} C(\mathcal{L}(\mathbf{u}'\mathbf{Y}|\mathbf{X}), -r_{-\mathbf{u}}, r_{\mathbf{u}}, 0)$$

is such a very natural regression multivariate index of Y generalizing  $C_M$  to the regression context. In other words,  $C_R$  can be obtained from  $C_M$  by replacing the distribution of projections  $\mathcal{L}(\mathbf{u}'\mathbf{Y})$  with its conditional counterpart  $\mathcal{L}(\mathbf{u}'\mathbf{Y}|\mathbf{X})$ . While conditional means and variances can be easily obtained from the least squares regression, conditional quantilebased characteristics naturally follow from the quantile regression approach, introduced in Koenker and Bassett (1978) and masterly reviewed in Koenker (2005). The latter approach is very appealing both from the computational point of view and because it does not require any limiting moment assumptions. Consequently, it might be beneficial to redefine all common process capability indices in terms of reasonable quantiles (despite the resulting possible mild increase in their sample variability), by replacing their moment-based distributional parameters with their quantile-based equivalents under the assumption of normality; see, e.g., p. 143 of Kotz and Lovelace (1998) for such an approach. For example, the mean could be replaced with the median or with the midpoint of an interquantile range, the standard deviation with a scaled interquantile range, and both skewness and kurtosis with their quantile-based counterparts presented in White et al. (2010) and Kim and White (2004). Although the choice of quantiles for this purpose is usually only a matter of convention, the extreme quantiles should be avoided at any cost since their precise estimation from small to moderate data samples is next to impossible.

Note that the multivariate accuracy indices described above might be generalized to the regression context by replacing  $\mu = \mu(\mathcal{L}(\mathbf{Y}))$  with  $\mu(\mathcal{L}(\mathbf{Y}|\mathbf{X}))$ . Needless to say that there are also affine equivariant regression multivariate medians indicated in the literature; see, e.g., Hallin et al. (2010) or Paindaveine and Šiman (2011) and references therein.

#### 5. Computational Aspects

In the empirical case, the suprema and infima in the definitions of  $C_M$  and  $C_R$  could always be approximated accurately by corresponding maxima and minima over a finite but dense grid of equispaced directions  $\mathbf{u} \in S^{m-1}$ , which provides a clue how to compute these coefficients in practice. Furthermore, the empirical (regression) quantiles of projections  $\mathbf{u}'\mathbf{Y}$  can be obtained analytically for all  $\mathbf{u} \in S^{m-1}$  by means of parametric programming, see Paindaveine and Šiman (2011, 2014). In fact, even some statistics based on projection pursuit can be computed exactly despite the infimum or supremum involved, see Šiman (2011), which might be true for some special indices  $C_M$  or  $C_R$  as well. In any case,  $C_{p,M}^*$ ,  $k_{a,M}$ ,  $k_{a,M}^I$ ,  $k_{a,M}^{II}$ , and  $k_{a,M}^{III}$  can be calculated trivially if  $\mathcal{T}$  is a hypersphere centered at  $\mathbf{T} = \mathbf{0}$ , i.e., if  $r_{\mathbf{u}}$  is constant on  $S^{m-1}$ .

#### 6. Practical Example

In this section, we illustrate the application and benefits of our methodology by applying it to a small data example.

Assume the target  $\mathbf{T} = 0$  and the tolerance region  $\mathcal{T}$  in the form of a convex quadrilateral given by vertices [8, 0], [0, 8], [-8, 0], and [0, -16]. Suppose that n = 100 observations  $\mathbf{Y}_1, \dots, \mathbf{Y}_n$  of the bivariate process  $\mathbf{Y}$  can be represented as a random sample drawn from the multivariate normal distribution with independent components  $N(\mathbf{m}, \mathbb{V})$  with  $\mathbf{m} = (0.5, 2)'$  and  $\mathbb{V} = \text{diag}(1, 2)$ ; see Fig. 1. If  $\mathbf{T}$  were different from  $\mathbf{0}$ , we would shift the coordinate system and consider new observations  $\mathbf{Y}_1 - \mathbf{T}, \dots, \mathbf{Y}_n - \mathbf{T}$  with zero target and the tolerance region  $\mathcal{T} - \mathbf{T}$  instead.



**Figure 1.** This figure partly explains the proposed methodology for an example of n = 100 (light gray) observations  $Y_1, \ldots, Y_n$  of (the output of) a manufacturing process  $\mathbf{Y}$ , represented here by a random sample from the multivariate normal distribution  $N(\mathbf{m}, \mathbb{V})$  with  $\mathbf{m} = (0.5, 2)'$  and  $\mathbb{V} = \text{diag}(1, 2)$ . We further assume zero target  $\mathbf{T} = \mathbf{0}$  and the tolerance region  $\mathcal{T}$  (with its thick black border  $\partial \mathcal{T}$ ) in the form of the convex quadrilateral given by vertices [8, 0], [0, 8], [-8, 0], and [0, -16]. The picture also displays points  $\boldsymbol{\mu} = (Y_1 + \cdots + Y_n)/n$ ,  $\mathbf{A} = L_{\mathbf{u}}$ ,  $\mathbf{B} = L_{-\mathbf{u}}$ ,  $\mathbf{P} = L_{\mathbf{v}}$ , and  $\mathbf{Q} = L_{\mathbf{w}}$ , where  $\mathbf{u} = (-0.62, 0.78)'$ ,  $\mathbf{v} = (0.51, 0.86)'$ , and  $\mathbf{w} = (0.59, 0.81)'$  are the critical directions where the extreme in the definition of  $C_{p,M}^*$ ,  $k_{a,M}$ , and  $k_{a,M}^l$  is achieved, respectively. The line segments  $\langle \mathbf{0}, A \rangle$ ,  $\langle \mathbf{0}, B \rangle$ ,  $\langle \mathbf{0}, P \rangle$ , and  $\langle \mathbf{0}, Q \rangle$  are of length  $r_{\mathbf{u}}, r_{-\mathbf{u}}, r_{\mathbf{v}}$ , and  $r_{\mathbf{w}}$ , in that order. The small black dots on the line segment  $\langle A, B \rangle$  stand for the projections of observations  $\mathbf{Y}_1, \ldots, \mathbf{Y}_n$  onto the line with directional vector  $\mathbf{u}$ .

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How can we compute the multivariate generalization of a univariate capability index  $C = C(\mathcal{L}(Z), LSL, USL, 0)$  of process Z with target 0 and tolerance interval [LSL, USL]? Ideally, we would consider each direction  $\mathbf{u} \in S^{m-1}$ , use it to compute the univariate index C from the scalar process of projections  $\mathbf{u}'\mathbf{Y}_i$ , i = 1, ..., n, with zero target and the tolerance interval [LSL, USL] =  $[-r_{-\mathbf{u}}, r_{\mathbf{u}}]$ , and find the infimum of all such values (if C decreases with deteriorating capability). In practice, we usually cannot work with infinite numbers of directions, and this is why we typically employ only a large dense subset of them (or use parametric programming if it is possible).

In our empirical bivariate example, we considered  $N_{\phi} = 360,000$  equispaced directions  $\mathbf{u}_i = (\cos(i/N_{\phi}), \sin(i/N_{\phi}))', i = 0, \dots, N_{\phi} - 1$ , which made the error caused by the finite-sample approximation truly negligible. Then,

$$r_{\mathbf{u}_{i}} = \begin{cases} 8/((1,1)\mathbf{u}_{i}), & 0 \le i < N_{\phi}/4 \\ 8/((-1,1)\mathbf{u}_{i}), & N_{\phi}/4 \le i < N_{\phi}/2 \\ -16/((2,1)\mathbf{u}_{i}), & N_{\phi}/2 \le i < 3N_{\phi}/4 \\ -16/((-2,1)\mathbf{u}_{i}), & 3N_{\phi}/4 \le i < N_{\phi} \end{cases}$$
(4)

 $\mu = (Y_1 + \dots + Y_n)/n = (0.64, 2.16)'$ , and

$$k_{a,M} \doteq \max_{i=0,\dots,N_{\phi}-1} \left\{ \frac{\mathbf{u}_i' \boldsymbol{\mu}}{r_{\mathbf{u}_i}} \right\} = 0.37$$
(5)

was achieved for  $\mathbf{u}_{59263} = (0.51, 0.86)'$ . The other indices such as  $C_{p,M}^*$  or  $k_{a,M}^I$  can be computed quite analogously:  $C_{p,M}^* \doteq 1.45$  was achieved for  $\mathbf{u}_{128679} = (-0.62, 0.78)'$  and  $k_{a,M}^I \doteq 0.31$  was achieved for  $\mathbf{u}_{53638} = (0.59, 0.81)'$ .

That clearly shows that it is not generally enough to examine only a few orthonormal directions (semiaxial directions, principal vectors, and the like) as is typically done in practice nowadays. For example, if we considered only four semiaxial directions (1, 0)', (0, 1)', (-1, 0)' and (0, -1)', i.e., if  $N_{\phi} = 4$ , then we would obtain the same critical vector (0, 1)' for all the three indices considered, for which the univariate process capability indices behind  $k_{a,M}$ ,  $C_{p,M}^*$ , and  $k_{a,M}^I$  are equal to quite different values 0.27, 2.00, and 0.18, respectively. See also Fig. 1 for a graphical illustration of this data example.

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