Some Linear Models for Estimating the Motion of Rigid Bodies with Applications to Geometric Quality Assurance

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Abstract

A geometrical method to assess the quality of a part is to sample points on the surface of the part and to bring an ideal computer representation of the part as close as possible to the sampled locations. The points are sampled with a Coordinate Measuring Machine (CMM) that gives the coordinates, with respect to the machine's own three dimensional system of axis, of the sampled locations. Computer Assisted Design (CAD) gives the ideal representation of the part. The matching involves estimating a rotation and a translation vector characterizing the rigid body transformation needed to go from the computer model to the sampled locations. The sum of the squared residual distances between the sampled locations and the fitted computer part is a measure of the quality of the part. This paper investigates the statistical properties of this method when the surface of the part is made of planar regions. Estimating the translation vector and the rotation matrix is shown to be "locally" equivalent to fitting a linear model to the localization data. Three components of the residual sum of squared distances are identified. They measure within planar region variability, the orientation conformity of the planar regions, and the size discrepancies of the regions. Diagnostics for linear models are adapted to yield statistical tests for specific geometric failures of

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a part. The developments use first order asymptotic expansions of the estimators and of the sum of squared residuals for the local linear model, as the errors associated with the sampled locations go to 0.

KEY WORDS: Computer Assisted Design, Coordinate Measuring Machine, Directional Data, Regression Diagnostics, Rotations, Spherical Regression.

1 Introduction

This paper investigates the match between measurements taken on the surface of a three dimensional object and a theoretical representation of the object in a computer file. In an industrial setting, the computer file contains the specifications for the object, or part, derived through computer assisted design (CAD). Measurements on the surface of the part are taken with a coordinate measuring machine (CMM) probe; they consist of (x, y, z) coordinates with respect to a system of axis internal to the CMM. The CMM readings contain both measurement errors and manufacture errors. Measurement errors depend on the resolution of the probe which according to Chapman, Chen, and Kim (1995) is of the order of 10^{-4} mm. Manufacture errors are present when the part does meet CAD specifications.

To assess the quality of the part is to determine how well the CMM readings match CAD specifications. This is done by estimating, using orthogonal least squares, a rigid body transformation involving a translation vector T and a rotation matrix R, to go from the CAD to the CMM axis system. Once the transformation is estimated, to each CMM measurement is associated a CAD predicted value. The sum of the squared distances between observed and predicted measurements is a natural statistic to evaluate the quality of the part (Caskey et al, 1990). Chen and Chen (1992, 1997) investigated the statistical properties of this statistic. They suggested that its distribution could be well approximated by a chi-square with degrees of freedom equal to the number of CMM measurements taken on the part minus 6, the number of estimated parameters.

Statistical analysis of CMM data is considered in Kurfess and Banks (1990), Dowling (1992), and Dowling, Griffin, Tsui and Zhou (1993, 1997) among others. Chapman, Chen and Kim (1995) proposed to evaluate the conformity of a part by using directional features only. They characterized the orientation of a planar region with a unit vector orthogonal to the region. A part is declared acceptable if the theoretical CAD unit vectors can be matched to the CMM unit vectors, calculated with the localization data, by a simple rotation obtained through spherical regression (Rivest, 1989). They used diagnostics for spherical regression to identify planar surfaces whose orientation is defective. Rivest (1995) proposed adding a second step, for the assessment of within planar surface variability, to their analysis.

The CAD model is constructed in Section 2 together with a simple orthogonal least squares algorithm for estimating the motion parameters. Section 3 derives a local linear model that determines the distribution of the estimators when the errors are small. Using the terminology of Peddada and Chang (1996), Section 3 estimates the motion of rigid bodies for non homologous data since locations of the part cannot be matched exactly to CAD locations. The sum of the squared residuals, properly normalized, is shown to converge to a chi-square distribution as conjectured by Chen and Chen (1992). Section 4 identifies three components in the sum of the squared residuals. There is one component for variability orthogonal to the planar regions, one for orientation conformity, and one for size deficiencies. The orientation component is a generalization of Chapman, Chen and Kim (1995) conformity statistic. Section 5 shows how to use diagnostics for the associated local linear model to identify faulty features of a part. Diagnostics for orientation, size and planarity are constructed. The proposed methodology is used in Section 6 to construct statistical tools to assess the simple extrusion considered by Hulting (1995). A numerical example is also presented. Finally, note that an estimation problem similar to the one studied here is considered by Chang (1988).

2 Least Squares Estimation of the Parameters

Suppose that the surface of the part consists of m planar regions $\{S_1, \dots, S_m\}$. If the part is a cube, m is equal to 6 while for the diamond pin considered by Chapman, Chen, and Kim (1995), m is equal to 9. Let the 3×1 vectors y_{ij}, $j = 1, \dots n_i$ denote the coordinates of the n_i CMM readings in planar region i. We assume that $n_i > 2$ for each i. This section investigates the estimation of the rigid body transformation (T, R), where T is translation vector and R is a rotation, that provides the best match between CMM readings and the CAD file. The parametrization of planar regions and of rotations are first reviewed, then a least squares algorithm for estimating (T, R) is presented. The following notation is used throughout the paper:

- If v is a unit vector let its orthogonal complement $v_{(.)} = [v_{(1)}; v_{(2)}]$ be a 3×2 matrix containing a basis for the vector space orthogonal to v such that v, $v_{(1)}$ and $v_{(2)}$ form a right-hand rule oriented orthonormal basis.

- A skew-symmetric matrix A is a square matrix satisfying $A^t = -A$ ("t" denotes the transpose of a matrix). To the vector $u = (u_1, u_2, u_3)^t$ one associates the 3×3 skew-symmetric matrix U defined by

$$U = \begin{pmatrix} 0 & -u_3 & u_2 \\ u_3 & 0 & -u_1 \\ -u_2 & u_1 & 0 \end{pmatrix}.$$

If v is a 3×1 vector with associated skew-symmetric matrix V, then Uv denotes the exterior product of u and v. It is a vector orthogonal to both u and v. One has $Uv = -Vu$ where V is the skew-symmetric matrix associated to v; this is used extensively in the paper. When u is a unit vector, the skew-symmetric matrix U can conveniently be expressed in terms of its orthogonal complement $u_{(.)}$ as,

$$U = u_{(.)} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} u_{(.)}^t = u_{(2)} u_{(1)}^t - u_{(1)} u_{(2)}^t.$$

- If A is a skew-symmetric matrix of the A_{ij}'s, then let $a = (-A_{23}, A_{13}, -A_{12})^t$ be the component vector of A. It is clear that A is the skew-symmetric matrix associated to a. Thus there is a 1-1 correspondence between 3×3 skew-symmetric matrices and 3×1 component vectors.

2.1 Parametrization of Planar Regions

Plane i, defined as the plane in R^3 containing S_i, is determined by a pair (b_i, v_i) where v_i is a unit vector orthogonal to the plane and b_i is the signed distance between the CAD origin and plane i. Thus $b_i v_i$ is the vector of coordinates of the projection of the CAD origin in plane i. A parametric representation of plane i is easily constructed. Let $v_{i(.)}$ be a 3×2 orthogonal complement to v_i, then plane i is the set $\{b_i v_i + v_{i(.)} x : x \text{ in } R^2\}$. Since S_i is included in plane i, the points on the surface of the part in the CAD file are a subset of $\cup\{b_i v_i + v_{i(.)} x : x \text{ in } R^2\}$.

2.2 Parametrization of Rotations with Skew-symmetric Matrices

The set of 3×3 rotations, sometimes denoted $SO(3)$, is a Lie group and the set of 3×3 skew-symmetric matrices is the associated Lie algebra (Warner, 1983, p. 84). This Lie algebra provides a convenient parametrization of the rotations (Chang, 1986; Rivest, 1989). If A is 3×3 skew-symmetric with component vector a, then $A^2 = -a^t a I + a a^t$, and it is easily shown that

$$\exp(A) = I + A + \frac{1}{2}A^2 + \frac{1}{3!}A^3 + \ldots = \cos(\theta)I + \frac{\sin(\theta)}{\theta} A + \frac{1 - \cos(\theta)}{\theta^2} a a^t.$$

This is a rotation of angle $\theta = (a^t a)^{1/2}$ around axis $a/(a^t a)^{1/2}$.

In the engineering literature most papers investigating rotations uses a quaternion parametrization, see for instance, Kanatani (1993). The quaternion representation of a rotation is a unit vector in R^4 , $q = (\cos(\theta/2),\ \sin(\theta/2)a_1/\theta,\ \sin(\theta/2)a_2/\theta,\ \sin(\theta/2)a_3/\theta)^t$, where $a = (a_1, a_2, a_3)^t$ is the component vector of the skew-symmetric matrix A. The main advantage of the skew-symmetric parametrization is to yield a simple description of neighborhoods of rotations. Rotations close to R can be written $R\exp(A)$ where the components of A are small. For such A's, one has $\exp(A) \approx I + A$ and $R(I + A)$ parameterizes the rotations in an infinitesimal neighborhood of R.

2.3 Least Squares Fitting

Assuming that the planar region on which a CMM reading is taken can be identified with certainty, the model for the data is

$$y_{ij} = T + R(b_i v_i + v_{i(.)} x_{ij}) + \tau_{ij}, \tag{1}$$

where the unknown parameters are (T, R) and x_{ij}, $i = 1, \ldots, m \quad j = 1, \ldots, n_i$. The b_i's and the rotation matrices $[v_i; v_{i(1)}; v_{i(2)}]$ are known CAD specifications and τ_{ij} represent residual errors. The following notation, pertaining to model (1), is used throughout the paper,

- X_i be the $n_i \times 2$ matrix whose i^{th} row is given by x_{ij}^t;
- 1_i be a $n_i \times 1$ vector of 1's;
- $M_i = I - 1_i 1_i^t / n_i$ be the centering matrix for planar region i;
- $\varepsilon_{i\bullet}$ be a $n_i \times 1$ vector whose j^{th} element is given by $\varepsilon_{ij} = \tau_{ij}^t R v_i$, this is the component of the error that is orthogonal to the surface of planar region i.

The orthogonal least squares estimates of the parameters are the values minimizing $\sum \|y_{ij} - T - R(b_i v_i + v_{i(.)} x_{ij})\|^2$, where $\|\cdot\|$ denotes the Euclidean distance. For a given (i, j) and for (T, R) fixed, consider the calculation of the optimal x_{ij}. This is a classical linear least squares problem. The X-matrix is $R v_{i(.)}$ and the "dependent" variable is $y_{ij} - T - R b_i v_i$. The minimizing x_{ij} is given by $v_{i(.)}^t R^t (y_{ij} - T)$ and the residual vector is $(I - R v_{i(.)} v_{i(.)}^t R^t)(y_{ij} - T - R b_i v_i) = R v_i (v_i^t R^t y_{ij} - v_i^t R^t T - b_i)$, since $v_{i(.)} v_{i(.)}^t = I - v_i v_i^t$. The signed length of the residual vector $(v_i^t R^t y_{ij} - v_i^t R^t T - b_i)$ represents the distance, in direction $R v_i$, between a data vector and its CAD predicted value. This is an orthogonal distance since $R v_i$ is the direction orthogonal to the ith planar region of the object. The signs of the residuals, $\{v_i^t R^t y_{ij} - v_i^t R^t T - b_i\}$, depend on the CAD parametrization. Changing v_i to $-v_i$ changes the signs of all the residuals for planar region i.

The estimation of (T, R) requires the minimization of the sum of the squared distances,

$$\sum_{ij} (v_i^t R^t y_{ij} - v_i^t R^t T - b_i)^2. \tag{2}$$

A least squares algorithm for minimizing (2) is easily constructed using the skew-symmetric parametrization. Let R_k be the rotation at the k^{th} iteration. Write $R_{k+1} = R_k \exp(A_k) \approx R_k(I + A_k)$. To find the optimal A_k and the corresponding T_{k+1}, the translation parameter estimate at iteration $k+1$, minimize

$$\sum \{v_i^t (I - A) R_k^t y_{ij} - v_i^t R^t T - b_i\}^2 = \sum \{v_i^t R_k^t y_{ij} - b_i + a^t V_i R_k^t y_{ij} - v_i^t R^t T\}^2,$$

where a is the component vector of A and V_i is the skew-symmetric matrix corresponding to v_i. The minimizing $(a, R^t T)$ is equal to the least squares estimate of the regression of $\{v_i^t R_k^t y_{ij} - b_i\}$ on $\{(y_{ij}^t R_k V_i, v_i^t)^t\}$. In other words $R_{k+1} = R_k \exp(A_k)$ where the component vector of A_k and $R_{k+1}^t T_{k+1}$ are obtained by regressing $\{v_i^t R_k^t y_{ij} - b_i\}$ on $\{(y_{ij}^t R_k V_i, v_i^t)^t\}$. This is a Newton-Raphson algorithm; in the numerical results presented in Section 6, it converged smoothly to the least squares estimate for any choice of initial value. Let $SS_R = \sum (v_i^t \hat{R}^t y_{ij} - v_i^t \hat{R}^t \hat{T} - b_i)^2$ denote the sum of the squared residuals for model (1). This is the sum of the squared distances between the CMM sample points and their CAD predicted values.

Suppose now that one changes the origin of the CAD coordinates. Let w, w in R^3, be the new origin. Since, for any $i, w = v_i v_i^t w + v_{i(.)} v_{i(.)}^t w$, with respect to this new origin, model (1) becomes

$$y_{ij} = T + Rw + R[(b_i - v_i^t w) v_i + v_{i(.)}(x_{ij} - v_{i(.)}^t w)] + \tau_{ij}. \tag{3}$$

Let $\hat{R}_N$ and $\hat{T}_N$ denote the least squares estimates of the parameters for this new CAD parametrization. One easily shows that $\hat{R}_N = \hat{R}$ and $\hat{T}_N = \hat{T} + \hat{R}w$, furthermore the sums of the squared residuals are the same for the two parametrizations. Thus reparametrizing the CAD model does not change the results of the analysis.

3 First Order Approximations to the Least Squares Estimates

If, in model (1), the errors orthogonal to the planar surfaces, $\{\varepsilon_{ij} : i = 1, \ldots, m; j = 1, \ldots, n_i\}$ are null then the orthogonal least squares estimates are equal to the true values of the parameters. Since the errors are usually small one can approximate their contributions to the estimates by carrying out Taylor series expansions around the true values. Such expansions are carried out in this section. In all cases considered, a local linear model describes the first order contributions of the errors to the estimates. Such small errors sometimes occur when analyzing directional data. This section extends the methods used for the analysis of small errors directional data, sometimes called large kappa asymptotic (Watson, 1983; Chang, 1988; and Rivest, 1989), to the estimation of the motion of rigid bodies. Expansions are first presented for descriptive statistics involving one planar region only. We assume that the errors τ_{ij} in model (1) are small, or $O(\sigma)$.

3.1 A Local Linear Model for one Planar Region

Consider the n_i points, with coordinates y_{ij}, sampled on the ith planar surface. These points should be approximately coplanar. The direction of this plane is characterized by the unit vector orthogonal to the plane. An estimate $\hat{u}_i$ of this unit vector is given by the eigenvector corresponding to the smallest eigenvalue of the sum of squares and cross-products matrix, $\sum_j (y_{ij} - \bar{y}_{i.})(y_{ij} - \bar{y}_{i.})^t$ (Schomaker et al.,1959, Scheringer, 1971). Furthermore $\hat{\lambda}_i$, the smallest eigenvalue of this matrix, characterizes the clustering of the points around the estimated plane.

If the points are exactly coplanar, that is $\varepsilon_{ij} = 0$ for $i = 1, ..., n_i$, then $\hat{\lambda}_i = 0$ and $\hat{u}_i = Rv_i$. The first order, or $O(\sigma)$, contribution of the ε_{ij}'s to $\hat{\lambda}_i$ and $\hat{u}_i$ involve the regression of $\varepsilon_{i\bullet}$ on $[1_i; X_i]$. One has (Rivest, 1995)

$$\begin{aligned} \hat{u}_i &= R[v_i + v_{i(.)}(X_i^t M_i X_i)^{-1} X_i^t M_i \varepsilon_{i\bullet}] + O(\sigma^2) && (4) \\ \hat{\lambda}_i &= \varepsilon_{i\bullet}^t \{M_i - M_i X_i [X_i^t M_i X_i]^{-1} X_i^t M_i\} \varepsilon_{i\bullet} + O(\sigma^3). && (5) \end{aligned}$$

Thus $\hat{u}_i$ is related to the least squares estimates of the parameters for X_i while $\hat{\lambda}_i$ is approximately equal to the sum of the squared residuals for the regression of $\varepsilon_{i\bullet}$ on $[1_i; X_i]$. Chapman (1995) provides an alternative approach to the above expansions.

3.2 A Local Linear Model for R and T

First order approximations to the least squares estimators of the rotation matrix and of the translation parameter are now presented. The least squares estimate of R is $\hat{R} = R\exp(\hat{A}) = R(I+\hat{A})+O(\sigma^2)$, where $\hat{A}$ is a skew-symmetric matrix while that of T is $\hat{T} = T+\hat{t}$ where $\hat{t}$ is a 3×1 vector of $O(\sigma)$ components. Consider rotations $R\exp(A) \approx R(I+A)$ and translation vectors $T+t$ where the components of A and t are $O(\sigma)$. According to (1), for such rotations and translation vectors, (2), the sum of squares for the estimation of (T, R), is equal to

$$\begin{aligned}
&\sum[v_i^t(I - A + O(\sigma^2))R^t\{T + Rv_ib_i + Rv_{i(.)}x_{ij} + \tau_{ij} - T - t\} - b_i)]^2 \\
&\quad = \sum[v_i^tR^t\tau_{ij} - v_i^tAv_{i(.)}x_{ij} - v_i^tR^tt + O(\sigma)^2]^2 \\
&\quad = \sum[\varepsilon_{ij} + a^tV_iv_{i(.)}x_{ij} - t^tRv_i]^2 + O(\sigma)^3
\end{aligned} \tag{6}$$

where V_i is the skew-symmetric matrix whose component vector is v_i, as defined in Section 2. A first order approximation to $(\hat{a}, \hat{t})$, where $\hat{a}$ is the component vector of $\hat{A}$, can therefore be derived using standard least squares. Consider a regression model with 6 dependent variables, given for the (i, j) data point by the entries of v_i and of $-V_iv_{i(.)}x_{ij}$. The design matrix X for this regression is $(\sum n_i) \times 6$, with the n_i rows for planar region i equal to $[X_iv_{i(.)}^tV_i; 1_iv_i^t]$. Thus,

$$\begin{pmatrix} \hat{a} \\ R^t\hat{t} \end{pmatrix} = (X^tX)^{-1}X^t\varepsilon_{\bullet\bullet} + O(\sigma^2).$$

where $\varepsilon_{\bullet\bullet}$ is the $(\sum n_i) \times 1$ vector obtained by stacking the $\varepsilon_{i\bullet}$'s. The next lemma collects some useful results on X.

Lemma 1

Let Z be a $(\sum n_i) \times 3$ matrix whose n_i rows for planar region i are given by $[M_iX_iv_{i(.)}^tV_i]$, $w_i = V_i^tv_{i(.)}\bar{x}_{i.}$, and C be a $(\sum n_i) \times 6$ matrix whose n_i rows for planar region i are given by $[1_iw_i^t; 1_iv_i^t]$. Then $X = [Z; 0] + C$, furthermore the columns of Z are orthogonal to those of C.

An approximation for the sum of the squared residuals is easily obtained from the linear model representation,

$$SS_R = \sum_{ij}(v_i^t\hat{R}^ty_{ij} - v_i^t\hat{R}^t\hat{T} - b_i)^2 = \varepsilon_{\bullet\bullet}^t(I - X(X^tX)^{-1}X^t)\varepsilon_{\bullet\bullet} + O(\sigma^3). \tag{7}$$

3.3 Distributional Results under Normality

We now assume that $\{\varepsilon_{ij} : i = 1, \ldots, m; j = 1, \ldots, n_i\}$ are independent normal random variables with mean $E(\varepsilon_{ij}) = \mu_{ij}$ and variance σ^2, where the μ_{ij}'s are $O(\sigma)$ and σ is assumed to be small. The variance σ^2 is related to both measurement errors and minor manufacture errors. The means μ_{ij}'s are non null only for defective parts that differ substantially from CAD specifications. Let $\mu_{\bullet\bullet}$ stand for the $(\sum n_i) \times 1$ vector of the μ_{ij}'s. The distributions of the estimators and of the sum of squares for model (1) are given next. Let $N_p(\psi, \Sigma)$ denote the p-variate normal distribution with mean vector ψ and variance covariance matrix Σ and

$\chi^2_d(\delta^2)$ denote the non central chi-square distribution with d degrees of freedom and non-centrality parameter δ^2. Applying standard linear model theory to the local linear model presented in Section 3.2 leads to the following result.

Theorem 1

Let X be the $(\sum n_i) \times 6$ matrix defined in Lemma 1. Under the normality assumption, as σ goes to 0, one has

i. $\frac{1}{\sigma}\begin{pmatrix} \hat{a} \\ R^t\hat{t} \end{pmatrix} \sim N_6\left(\frac{(X^tX)^{-1}X^t\mu_{\bullet\bullet}}{\sigma}, (X^tX)^{-1}\right)$;

ii. $\frac{SS_R}{\sigma^2} \sim \chi^2_{\sum n_i - 6}(\delta^2_R)$ where $\delta^2_R = (\sum \mu^2_{ij} - \mu^t_{\bullet\bullet}X(X^tX)^{-1}X^t\mu_{\bullet\bullet})/\sigma^2$;

iii. $(\hat{R}, R^t\hat{t})$ and SS_R are asymptotically independent.

Theorem 1 provides a rigorous proof of Chen and Chen (1992) conjecture who proposed to approximate the distribution of SS_R by a χ^2 with $\sum n_i - 6$ degrees of freedom. This suggests to test conformity by rejecting a part if SS_R/σ_0^2 is larger that a suitably chosen critical value from the chi-square distribution with $\sum n_i - 6$ degrees of freedom and σ_0^2 is a tolerance bound. The normality assumption needed for the validity of such a test can be ascertained using the residuals $\{v_i^t\hat{R}^t y_{ij} - v_i^t\hat{R}^t\hat{T} - b_i : i = 1, \ldots, m; j = 1, \ldots, n_i\}$. The joint distribution of these residuals is the same, up to $O(\sigma^2)$ terms, as that of the residuals from linear model $y = X\beta + \varepsilon_{\bullet\bullet}$. Since, as shown in Section 2, the residuals are well defined up to a sign change, graphical assessments of the normality assumption should be carried out with half normal plots. Further residual diagnostics are proposed in Section 5.

4 A Decomposition of the Sum of the Squared Residual Distances

This section identifies three components in the sum of squared residuals SS_R: one for variability about the planar region, one for orientation conformity, and one for size deficiencies. These three elements are related to characteristics that are looked at when assessing a part (Tsui, 1995). In some instances it might be appropriate to set component specific tolerance levels, rather than one overall level based on SS_R. Indeed, the orientation component of SS_R generalizes the tolerancing statistic of Chen, Chapman and Kim (1995). Distributional results useful for setting component specific tolerances are derived in this section.

The proposed decomposition involves a second estimator of R, say $\hat{R}_1$, defined as the rotation minimizing $\sum\{(Rv_i - \hat{u}_i)^t(y_{ij} - \bar{y}_{i.})\}^2$. Properties of $\hat{R}_1$ as an estimator of R are discussed after the statement and the proof of the following.

Proposition 1

The residual sum of squares satisfies $SS_R = SS_P + SS_O + SS_S + O(\sigma^3)$ where

$$
\begin{aligned}
SS_P &= \sum_i \hat{\lambda}_i\,; \\
SS_O &= \sum_{ij}\{(\hat{R}_1 v_i - \hat{u}_i)^t(y_{ij} - \bar{y}_{i.})\}^2\,; \\
SS_S &= \sum_{ij}\{(\hat{R}v_i - \hat{u}_i)^t(y_{ij} - \bar{y}_{i.})\}^2 - \sum_{ij}\{(\hat{R}_1 v_i - \hat{u}_i)^t(y_{ij} - \bar{y}_{i.})\}^2 \\
&\quad + \sum_i n_i(v_i^t\hat{R}^t\bar{y}_{i.} - v_i^t\hat{R}^t\hat{T} - b_i)^2,
\end{aligned}
$$

where $\hat{u}_i$ and $\hat{\lambda}_i$ are defined in (4) and (5). The indices P, O, and S stand for planar region, orientation, and size respectively.

Proof: Observe that

$$
\sum_{ij}(v_i^t\hat{R}^t y_{ij} - v_i^t\hat{R}^t\hat{T} - b_i)^2 = \sum_{ij}\{v_i^t\hat{R}^t(y_{ij} - \bar{y}_{i.})\}^2 + \sum_i n_i(v_i^t\hat{R}^t\bar{y}_{i.} - v_i^t\hat{R}^t\hat{T} - b_i)^2,
$$

Furthermore,

$$
\begin{aligned}
\sum_{ij}\{v_i^t\hat{R}^t(y_{ij} - \bar{y}_{i.})\}^2 &= \sum_{ij}\{(\hat{R}v_i - \hat{u}_i)^t(y_{ij} - \bar{y}_{i.})\}^2 + \sum_{ij}\{\hat{u}_i^t(y_{ij} - \bar{y}_{i.})\}^2 \\
&+ \; 2\sum_{ij}\{(\hat{R}v_i - \hat{u}_i)^t(y_{ij} - \bar{y}_{i.})\hat{u}_i^t(y_{ij} - \bar{y}_{i.})\}.
\end{aligned}
$$

The result is proved by verifying that:

$$
\begin{aligned}
&\sum_{ij}\{\hat{u}_i^t(y_{ij} - \bar{y}_{i.})\}^2 = \sum_i \hat{u}_i^t\left\{\sum_j (y_{ij} - \bar{y}_{i.})(y_{ij} - \bar{y}_{i.})^t\right\}\hat{u}_i = \sum_i \hat{\lambda}_i, \\
&\sum_{ij}\{(\hat{R}v_i - \hat{u}_i)^t(y_{ij} - \bar{y}_{i.})\hat{u}_i^t(y_{ij} - \bar{y}_{i.})\} = \sum_i \hat{\lambda}_i(v_i^t\hat{R}^t\hat{u}_i - 1),
\end{aligned}
$$

The expansions derived Section 3 show that both, $\hat{\lambda}_i$ and $(v_i^t\hat{R}^t\hat{u}_i - 1)$, are $O(\sigma^2)$. The products $\hat{\lambda}_i(v_i^t\hat{R}^t\hat{u}_i - 1)$ are therefore $O(\sigma^4)$; they are negligible with respect to the other terms in the sums.

Q.E.D.

The first term of this decomposition measures variability normal to the planar regions. It is large when some surfaces of the part are rough, irregular or curved. The second term reflects the extent to which the estimated orientations of the planar regions, characterized by $\hat{u}_i$ defined by (4), can be matched to the CAD specifications. The third term is related to size. It is important when the distances between the CAD origin and some of the planar regions of the part are not equal to the prescribed b_i's.

To motivate $\hat{R}_1$ as an estimator of R, consider a generalization of model (1) where the distances b_i's are unknown except for the first three regions which serve as baselines (these first three regions are chosen such that v_1, v_2, and v_3 are linearly independent). This enlarged model has $m+3$ parameters. From Proposition 1, the least squares estimator of R is $\hat{R}_1$ while parameters T and b_i, $i = 4, \ldots, m$, are estimated by solving

$$v_i^t \hat{R}_1^t \bar{y}_{i.} - v_i^t \hat{R}_1^t T - b_i = 0, \text{ for } i = 1, \ldots, m.$$

In this enlarged model, there are no degrees of freedom left for size. The sum of the squared residuals, $\sum \hat{\lambda}_i + \sum \{(\hat{R}_1 v_i - \hat{u}_i)^t (y_{ij} - \bar{y}_{i.})\}^2 + O(\sigma^3)$, has two components, one for variability normal to the surfaces of the part and one for orientation. SS_S is the difference between two sums of squared residuals, that for model (1) minus that for the extended model defined above. Seen from a linear model perspective, this is the regression sum of squares for testing that the b_i's are the true distances between the planar regions and the CAD origin.

From (5), one can write $SS_P = \varepsilon_{\bullet\bullet}^t M_W \varepsilon_{\bullet\bullet} + O(\sigma^3)$ where

$$M_P = \text{bdiag}(M_i - M_i X_i (X_i^t M_i X_i)^{-1} X_i^t M_i)$$

and $\text{bdiag}(B_i)$ is a block diagonal matrix where B_i is the block for planar region i. Similar expansions for SS_O and SS_S are derived next.

Proposition 2

First order expansions for SS_O and SS_S are given by:

i. $SS_O = \varepsilon_{\bullet\bullet}^t M_O \varepsilon_{\bullet\bullet} + O(\sigma^3)$,
where $M_O = \text{bdiag}(M_i X_i (X_i^t M_i X_i)^{-1} X_i^t M_i) - Z(Z^t Z)^{-1} Z^t$ and Z is defined in Lemma 1.

ii. $SS_S = \varepsilon_{\bullet\bullet}^t M_S \varepsilon_{\bullet\bullet} + O(\sigma^3)$,
where $M_S = \mathrm{bdiag}(I - M_i) - X(X^tX)^{-1}X^t + Z(Z^tZ)^{-1}Z^t$.

Proof: In view of (7), it suffices to prove i. Let $R_1 = R\exp(A_1)$ where A_1 is a skew-symmetric matrix with $O(\sigma)$ components and let a_1 be the component vector of A_1. Using (4) and (1), simple manipulations lead to

$$\sum\{(R_1v_i - \hat{u}_i)^t(y_{ij} - \bar{y}_{i.})\}^2 = \sum_{ij}\{a_1^tV_i^tv_{i(.)}(x_{ij} - \bar{x}_{i.}) - (x_{ij} - \bar{x}_{i.})^t(X_i^tM_iX_i)^{-1}X_i^tM_i\varepsilon_{i\bullet}\}^2 + O(\sigma^3).$$

An approximate value for the minimizing a_1 is obtained using least squares. It is given by

$$\begin{aligned}\hat{a}_1 &= \left\{\sum_i V_i^tv_{i(.)}X_i^tM_iX_iv_{i(.)}^tV_i\right\}^{-1}\sum_i V_i^tv_{i(.)}X_i^tM_i\varepsilon_{i\bullet} + O(\sigma^2)\\ &= (Z^tZ)^{-1}Z^t\varepsilon_{\bullet\bullet} + O(\sigma^2),\end{aligned}$$

where Z is defined in Lemma 1. The sum of the squared residuals is

$$SS_O = \sum_i \varepsilon_{i\bullet}^tM_iX_i(X_i^tM_iX_i)^{-1}X_i^tM_i\varepsilon_{i\bullet} - \varepsilon_{\bullet\bullet}^tZ(Z^tZ)^{-1}Z^t\varepsilon_{\bullet\bullet}.$$

These two terms are equal to the two components for SS_O given by i).

Q.E.D.

Suppose that n measurements are taken on each planar surface, at evenly spaced points on a circle of radius 1. This is the sampling scheme proposed by Chapman, Chen, and Kim (1995). One has

$$\sum_j(y_{ij} - \bar{y}_{i.})(y_{ij} - \bar{y}_{i.})^t = \frac{n}{2}Rv_{i(.)}v_{i(.)}^tR^t + O(\sigma) = \frac{n}{2}R(I - v_iv_i^t)R^t + O(\sigma).$$

Since $R_1 = R(I + A_1) + O(\sigma^2)$, considering (4), $v_i^tR^t(R_1v_i - \hat{u}_i)$ is $O(\sigma^2)$. Therefore

$$\sum_{ij}\{(R_1v_i - \hat{u}_i)^t(y_{ij} - \bar{y}_{i.})\}^2 = \frac{n}{2}\sum_i(R_1v_i - \hat{u}_i)^t(R_1v_i - \hat{u}_i) + O(\sigma^3) = n\sum_i(1 - v_i^tR_1^t\hat{u}_i) + O(\sigma^3).$$

Rotation $\hat{R}_1$ is then, up to $O(\sigma^3)$ terms, obtained by maximizing $\sum v_i^tR^t\hat{u}_i$. This is the spherical regression estimator used by Chapman, Chen and Kim (1995). Thus $\hat{R}_1$ can be looked at as a generalization of the spherical regression estimator to situations where the sampling schemes differ from one planar region to the next. Also, SS_O is equivalent, under Chapman, Chen, and Kim's (1995) sampling scheme, to their conformity statistic. The next proposition identifies the instances where the estimates $\hat{R}$ and $\hat{R}_1$ are identical, up to $O(\sigma^2)$ terms.

Proposition 3

If there exists a CAD origin w such that, with respect to this origin, $\bar{x}_{i.} = 0$ for each i, then $\hat{R} = \hat{R}_1 + O(\sigma^2)$ and a reparametrization of the linear model of Proposition 1 in terms of $(a, R^t t + Wa)$ yields a design matrix with orthogonal components for rotation and for translation, where W is the skew-symmetric matrix corresponding to w. The design matrix for the new parametrization is $X_N = [Z; C_N]$, where Z is defined in Lemma 1, C_N is a $(\sum n_i) \times 3$ matrix whose rows for planar region i are given by $1_i v_i^t$.

Proof: According to (3), the hypothesis implies that $\bar{x}_{i.} = v_{i(.)}^t w$ for each i. In (6), one has $a^t V_i v_{i(.)} x_{ij} = a^t V_i v_{i(.)} (x_{ij} - \bar{x}_{i.}) + a^t V_i v_{i(.)} v_{i(.)}^t w_0$. Using $v_{i(.)} v_{i(.)}^t = I - v_i v_i^t$ yields $a^t V_i v_{i(.)} v_{i(.)}^t w = -a^t W v_i$. Putting this back in (6) one obtains

$$\sum [\varepsilon_{ij} + a^t V_i v_{i(.)} (x_{ij} - \bar{x}_{i.}) - (a^t W + t^t R) v_i]^2 + O(\sigma^3).$$

The first term of this expression is the sum of squared residuals for a linear model with design matrix X_N. Since X_N has orthogonal components, the minimizing a is given by $\hat{a} = (Z^t Z)^{-1} Z^t \varepsilon_{\bullet\bullet}$. This is identical, up to $O(\sigma^2)$ terms, to the expansion for $\hat{a}_1$ obtained in Proposition 2.

Q.E.D.

A sampling scheme for which $\bar{x}_{i\cdot}$ is null for each planar region, with a proper choice of the CAD origin, is said to be *symmetric*. Symmetric designs are only possible on relatively simple objects such as cubes and simplexes. For a design to be symmetric, the points on each planar surface have to be sampled in a symmetric fashion around the projection of the CAD origin on the corresponding plane. For many objects, such as the diamond pin of Chapman, Chen and Kim (1995), it is not possible to find a point whose projection on plane i is close to the center of S_i for each i. A two dimensional illustration of this phenomenon is presented in Figure 1. The projections of O_1 belong to the central parts of A and D and to the boundaries of B and C; the opposite is true for O_2.

Proposition 4

If the errors ε_{ij}'s are independent and normally distributed with the same variance σ^2, then, as σ goes to 0, SS_P/σ^2, SS_O/σ^2, and SS_S/σ^2 converge to independent chi-square distributions with respectively $\sum n_i - 3m$, $2m - 3$, and $m - 3$ degrees of freedom and non centrality

Figure 1: Selection of the CAD origin in a two dimensional diamond pin. Two possible origins O_1 and O_2 are shown with their projections on 4 regions

parameters given by $\mu_{\bullet\bullet}^t M_P \mu_{\bullet\bullet}/\sigma^2$, $\mu_{\bullet\bullet}^t M_O \mu_{\bullet\bullet}/\sigma^2$, and $\mu_{\bullet\bullet}^t M_S \mu_{\bullet\bullet}/\sigma^2$.

Proof: By construction it is clear that $M_P + M_O + M_S = I - X(X^tX)^{-1}X^t$. To complete the proof, it suffices to demonstrate that M_P, M_O, and M_S are idempotent matrices orthogonal to one another. Only the proof that M_S is idempotent will be presented, the other arguments are similar. Since, $I - M_i = 1_i 1_i^t/n_i$, it is clear that $\text{bdiag}(I - M_i)Z = 0$ thus $\text{bdiag}(I - M_i) + Z(Z^tZ)^{-1}Z^t$ is idempotent. To prove that M_S is idempotent, consider $\{\text{bdiag}(I - M_i) + Z(Z^tZ)^{-1}Z^t\}X$. As shown in Lemma 1, one can write X as $[Z; 0] + C$ where the n_i rows of C for planar region i are equal to $[1_i w_i^t; 1_i v_i^t]$. One has $Z(Z^tZ)^{-1}Z^tC = 0$, $Z(Z^tZ)^{-1}Z^t[Z; 0] = [Z; 0]$ and $\text{bdiag}(I - M_i)C = C$. Combining all these results together proves that $\{\text{bdiag}(I - M_i) + Z(Z^tZ)^{-1}Z^t\}X = X$ and that M_S is idempotent.

Q.E.D.

Fortunately, there is no need to actually calculate $\hat{R}_1$ to carry out the decomposition of Proposition 1. It suffices to calculate residuals for each component. If $r_{\bullet\bullet}$ stands for the $(\sum n_i) \times 1$ vector of residuals, $\{v_i^t R^t y_{ij} - v_i^t \hat{R}^t \hat{T} - b_i\}$, then the planar surface residuals are defined as $r_{\bullet\bullet P} = \hat{M}_P\, r_{\bullet\bullet}$ when $\hat{M}_P$ is an estimate of M_P obtained by replacing the unknown x_{ij}'s by their estimates obtained in Section 2.3, $\hat{x}_{ij} = v_{i(.)}^t(\hat{R}^t y_{ij} - \hat{T})$. Since the residuals are $O(\sigma)$, $\hat{M}_P r_{\bullet\bullet} = M_P r_{\bullet\bullet} + O(\sigma^2)$ and estimating the x's does not change the first order properties of the residuals. The residuals for orientation and for size, $r_{\bullet\bullet O}$ and $r_{\bullet\bullet S}$, are calculated in a similar way. The sum of squares for one particular component is estimated by the sum of the squares of the corresponding residuals. The calculations can be simplified by noting that $r_{\bullet\bullet}$ is orthogonal to the design matrix X. Therefore, $X^t r_{\bullet\bullet} = Z^t r_{\bullet\bullet} = 0$. This yields simple formulas for SS_S and SS_O: $SS_S = \sum_i (\sum_j r_{ij})^2/n_i + O(\sigma^3)$ while SS_O is sum of the predicted values of the m regressions of $M_i r_{i\bullet}$ on $M_i X_i$.

The hypothesis, made at the beginning of Section 2, that $n_i > 2$ for each i is needed for the decomposition of Proposition 1 to hold. It ensures that $\hat{\lambda}_i$ is non trivial. Note however that Theorem 1 still holds when some of the n_i's are less than 3.

5 Residual Diagnostics

When a part does not meet the tolerance criterion, one would like to identify the features that made the part defective. Chapman, Chen and Kim (1995) used the diagnostics of spherical regression to identify planar surfaces whose orientation is defective while Hulting (1995) suggests fitting "manufacture part models" which are generalizations of (1) that include parameters for possible defects. This section shows how to apply standard linear model diagnostics to the local linear model of Section 3 to identify defective features. Further diagnostics for the estimation of rigid bodies are discussed by Chang and Ko (1995).

A defect can be expressed as a non-null mean vector, $\mu_{\bullet\bullet} = D\gamma$ where D is a $(\sum n_i \times d)$ full column rank matrix related to the faulty feature and γ is some unknown parameter. A simple test (see Cook and Weisberg, 1982, p. 44) for the hypothesis $H_0 : \gamma = 0$ is given by reject H_0 at level α if

$$\frac{r_{\bullet\bullet}^t D(D^t\{I - X(X^tX)^{-1}X^t\}D)^{-1}D^t r_{\bullet\bullet}/d}{\{SS_R - r_{\bullet\bullet}^t D(D^t\{I - X(X^tX)^{-1}X^t\}D)^{-1}D^t r_{\bullet\bullet}\}/(\sum n_i - 6 - d)} > F_{d,\sum n_i - 6 - d,\alpha,}$$

where $F_{d,n,\alpha}$ denotes the upper α quantile from an F distribution with d and n degrees of freedom. When D is mostly related to one of the three components identified in Proposition 3, that is when D belongs to the column space of one of the three M matrix defined in Section 4, component specific diagnostics are easily constructed by replacing, in the F-statistic, SS_R and $I - X(X^tX)^{-1}X^t$ by the appropriate variance component and M matrix. Note also that in an enlarged model featuring the defect, the least squares estimate of γ is given by

$$\hat{\gamma} = (D^t\{I - X(X^tX)^{-1}X^t\}D)^{-1}D^t r_{\bullet\bullet}.$$

A simple method to construct the matrix D starts with calculating the CAD coordinates of the sampled points on planar region i, $b_i v_i + v_{i(.)} x_{ij}$. Next, one applies the geometrical transformation characterizing the defect to these points. Then μ_{ij} is equal to the distance between the transformed point for (i, j) and its projection on planar region i. Applications of this technique to the construction of diagnostics for size, orientation and surface roughness are now presented.

5.1 Size Diagnostics

Suppose that the true signed distance between planar region i and the origin is given by $b_i + \gamma$. In other words, all the points on planar surface i are translated by γv_i. For this defect, $\mu_{i\bullet} = \gamma 1_i$ while $\mu_{k\bullet} = 0$ when $k \neq i$. The D-matrix for a size deficiency in planar region is given by $D_{S,i}$, a $(\sum n_i) \times 1$ vector of 0's except for the n_i entries for planar region i which are equal to 1. Since $M_O D_{S,i} = M_P D_{S,i} = 0$, this diagnostic is a component of SS_S. One has $D_{S,i}^t r_{\bullet\bullet} = \sum_j r_{ij}$ and

$$D_{S,i}^t[I - X(X^tX)^{-1}X^t]D_{S,i} = n_i\{1 - n_i[w_i^t, v_i^t](X^tX)^{-1}[w_i, v_i]\};$$

for symmetric designs, this simplifies to $n_i(1 - n_i v_i^t(\sum n_j v_j v_j^t)^{-1} v_i)$. The "externally" standardized residual for this problem is

$$t_i = \frac{\sum_j r_{ij}}{\sqrt{n_i \hat{\sigma}_i^2 \{1 - n_i(w_i^t, v_i^t)(X^t X)^{-1}(w_i^t, v_i^t)^t\}}} \tag{8}$$

where

$$\hat{\sigma}_i^2 = \frac{1}{\sum_i n_i - 7} \left\{ SS_R - \frac{\left(\sum_j r_{ij}\right)^2}{n_i\{1 - n_i(w_i^t, v_i^t)(X^t X)^{-1}(w_i^t, v_i^t)^t\}} \right\}.$$

Comparing statistic t_i to critical values of the t-distribution with $\sum n_i - 7$ degrees of freedom yields a formal test for a size failure of the ith region. If the size variance differs from the surface variance or the orientation variance, one can replace SS_R by SS_S in $\hat{\sigma}_i^2$. This reduces the degrees of freedom to $m - 4$; it provides a size diagnostic unaffected by orientation or within surface variability.

5.2 Orientation Diagnostics

Suppose now that the ith planar region underwent a rotation of angle $(\gamma_1^2 + \gamma_2^2)^{1/2}$ about axis $(\gamma_1 v_{i(1)} + \gamma_2 v_{i(2)})/(\gamma_1^2 + \gamma_2^2)^{1/2}$. When γ_1 and γ_2 are small, or $O(\sigma)$, this rotation can be written as $I + \gamma_1 V_{i(1)} + \gamma_2 V_{i(2)} + o(\sigma)$, where $V_{i(k)}$ is, for $k = 1, 2$, the skew symmetric-matrix corresponding to $v_{i(k)}$. Neglecting $o(\sigma)$ terms, one has

$$\mu_{ij} = v_i^t(I + \gamma_1 V_{i(1)} + \gamma_2 V_{i(2)})(b_i v_i + v_{i(.)} x_{ij}) - b_i$$

Since $v_i^t V_{i(1)} v_{i(.)} = (0, 1)$ and $v_i^t V_{i(2)} v_{i(.)} = (-1, 0)$, $\mu_{ij} = \gamma_1 x_{ij2} - \gamma_2 x_{ij1}$ where x_{ij1} and x_{ij2} are the two elements of x_{ij}. The D-matrix for an orientation failure, $D_{O,i}$, has 2 columns; all its rows are null except for those associated with planar region i which are equal to X_i. One has $M_P D_{O,i} = 0$ and the corresponding defect is related to orientation and, to a lesser extent, to size. Indeed, for symmetric designs, $M_S D_{0,i} = 0$. A diagnostic involving only the orientation sum of squares is easily constructed. One has

$$D_{O,i}^t M_O D_{O,i} = X_i^t M_i X_i - X_i^t M_i X_i v_{i(.)}^t V_i (Z^t Z)^{-1} V_i^t v_{(.)} X_i^t M_i X_i \tag{9}$$

and a $F_{2,2m-5}$ statistic to test for an orientation defect in planar region i is

$$F_i = \frac{r_{\bullet\bullet O}^t D_{O,i}(D_{O,i}^t M_O D_{O,i})^{-1} D_{O,i}^t r_{\bullet\bullet O}/2}{[SS_O - r_{\bullet\bullet O}^t D_{O,i}(D_{O,i}^t M_O D_{O,i})^{-1} D_{O,i}^t r_{\bullet\bullet O}]/(2m-5)}.$$

This generalizes Chapman, Chen and Kim's (1995) diagnostic to arbitrary sampling designs within each planar region.

5.3 Surface Diagnostics

Within each surface, there is one degree of freedom for size and 2 for orientation; $n_i - 3$ degrees of freedom are left for surface evaluation. A diagnostic for failure of surface i to be planar involving only SS_P is given by:

$$F_i = \frac{\hat{\lambda}_i/(n_i - 3)}{\{SS_P - \hat{\lambda}_i\}/\{\sum n_j - n_i - 3(m-1)\}};$$

its null distribution is a F with $n_i - 3$ and $\{\sum n_j - n_i - 3(m-1)\}$ degrees of freedom.

6 Example

The sampling design of Hulting (1995) for a simple extrusion is presented in Figure 2. There are 4 surfaces and measurements are taken on each one using the same design. One has $v_1 = v_3 = (1,0,0)^t$ and $v_2 = v_4 = (0,1,0)^t$ and $b_1 = b_2 = -b_3 = -b_4 = b$ say. The vectors of $v_{1(.)}$ and $v_{3(.)}$ are $v_{1(1)} = v_{3(1)} = (0,1,0)^t$ and $v_{1(2)} = v_{3(2)} = (0,0,1)^t$ while $v_{2(1)} = v_{4(1)} = (1,0,0)^t$ and $v_{2(2)} = v_{4(2)} = (0,0,-1)^t$. With this choice of orthogonal complements, $v_{i(2)}$ is related to the z-coordinate for $i = 1,2,3,4$. It is convenient to take the CAD origin as the center of the extrusion. The center of each rectangular region acts as the origin for the planar coordinates. With the proposed $v_{i(.)}$'s, matrix X_i is the same for the four regions,

$$X_i^t = \begin{pmatrix} d & d & d & -d & -d & -d \\ -c & 0 & c & -c & 0 & c \end{pmatrix}.$$

The v_i's are coplanar so that the third entry of R^tT is not estimable; it can be set equal to 0. All the previous results apply with a design matrix X having 5 columns. The last two columns of X now involve $v_{1\#} = v_{3\#} = (1,0)^t$ for planar region 1 and 3 and $v_{2\#} = v_{4\#} = (0,1)^t$ for planar region 2 and 4. There are 5 parameters to estimate. For each $i, \bar{x}_{i.} = 0$; thus this design is symmetric. According to Proposition 1 there are 19 degrees of freedom associated with SS_R. The matrix X is given in Table 1.

Figure 2: CAD Specifications For the Extrusion with the Locations of the 24 Measurement Points with their Identification.

Id. number	X					Planar region
18&21	0	-c	-d	1	0	1&3
10&13	0	0	-d	1	0	1&3
2&5	0	c	-d	1	0	1&3
17&22	0	-c	d	1	0	1&3
9&14	0	0	d	1	0	1&3
1&6	0	c	d	1	0	1&3
3&8	-c	0	d	0	1	2&4
11&16	0	0	d	0	1	2&4
19&24	c	0	d	0	1	2&4
4&7	-c	0	-d	0	1	2&4
12&15	0	0	-d	0	1	2&4
20&23	c	0	-d	0	1	2&4

Table 1. Design Matrix for the Local Linear Model for the Extrusion

The coordinates of the 24 measurements to be taken on the extrusion are provided in the CAD system of axis. Since the measurements are performed by the CMM, before taking the measurements a reference frame is first established to go from the CAD to the CMM coordinates. This frame is subject to errors, so the actual X matrix is not exactly that given in Table 1. Using the matrix of Table 1 to construct diagnostics is valid as long as the errors in establishing the reference frame are small. We make this assumption in this section and use the matrix of Table 1 to construct diagnostics. From Table 1, one finds

$$X^tX = 12 \begin{pmatrix} 2c^2/3 & 0 & 0 & 0 & 0 \\ 0 & 2c^2/3 & 0 & 0 & 0 \\ 0 & 0 & 2d^2 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

6.1 Distribution of the Residuals

The row of X for a measurement taken in planar surface 1 or 3 is given by $u = [0, x_2, -x_1, 1, 0]^t$ where (x_1, x_2) denotes the coordinates of the measurements in the planar surface. Therefore,

$$u^t(X^tX)^{-1}u = \frac{1}{12}\left(1 + \frac{3x_2^2}{2c^2} + \frac{x_1^2}{2d^2}\right),$$

and the residual variance, $(1-u^t(X^tX)^{-1}u)\sigma^2$, takes two values. When $x_2 = 0$, i.e. for points in cross section 2, the residual variance is $7\sigma^2/8$; for points in cross sections 1 and 3, $|x_2| = c$, thus the residual variance is $3\sigma^2/4$. Points at the end of the extrusion have smaller residual variances; this was to be expected since these point have more leverage, as measured by $u^t(X^tX)^{-1}u$, when fitting the localization parameters. The results for measurements taken on planar surfaces 2 and 4 are similar.

The diagnostic for size, presented in Section 5.1 is easily calculated. Since the design is symmetric, one has $n_i(1 - n_i v_{i\#}^t(\sum n_i v_{i\#} v_{i\#}^t)^{-1} v_{i\#}) = 3$ for any i. Furthermore, $t_i = \sum_j r_{ij}/\sqrt{3\hat{\sigma}_i^2}$, where

$$\hat{\sigma}_i^2 = \frac{1}{18}\left\{ SS_R - \frac{1}{3}\left(\sum_j r_{ij}\right)^2 \right\}.$$

It has a t-distribution with 18 degrees of freedom.

The orientation diagnostics are easily constructed. It is easy to show that $D_{O,i} r_{\bullet\bullet}$ involves two contrasts. The first one, c_1, compares cross sections 1 and 3 within planar region i, the other, c_2 contrasts the two sides ($x_{ij1} = d$ versus $x_{ij1} = -d$) of the region. Furthermore one has

$$D_{O,i}^t M_O D_{O,i} = D_{O,i}^t (I - X(X^tX)^{-1}X^t) D_{O,i} = \begin{pmatrix} 9d^2/2 & 0 \\ 0 & 2c^2 \end{pmatrix}.$$

The F-statistic of Section 5.2 is easily evaluated since

$$r_{\bullet\bullet O}^t D_{O,i} (D_{O,i}^t M_O D_{O,i})^{-1} D_{O,i}^t r_{\bullet\bullet O} = \frac{2c_1^2}{9} + \frac{c_2^2}{2}.$$

6.2 A Bending Diagnostic

Suppose, as in Hulting (1995), that the extrusion is bent. Assume that cross section 1 has undergone a rotation about an axis orthogonal to $(0,0,1)^t$. As in Section 5.2, this rotation can be expressed as $I + \gamma_1 V_1 + \gamma_2 V_2$, where γ_1 and γ_2 are $O(\sigma)$. For data points 1,2,4,and 6, in planar regions 1 and 3, the μ_{ij}'s are given by:

$$\mu_{ij} = v_1^t (I + \gamma_1 V_1 + \gamma_2 V_2)(b_i v_1 + x_{ij} v_2 + c v_{1(2)}) - b_i = -\gamma_2 c,$$

while for points 3,4,7, and 8 in planar regions 2 and 4, $\mu_{ij} = -\gamma_1 c$. Thus, for this problem in $D^t r_{\bullet\bullet} = c(r_1 + r_2 + r_5 + r_6, r_3 + r_4 + r_7 + r_8)^t$ (indices refer to identification numbers); furthermore,

$$D^t (I - X(X^tX)^{-1}X^t) D = c^2 \begin{pmatrix} 2/3 & 0 \\ 0 & 2/3 \end{pmatrix}.$$

The F-statistic of Section 5 is easily constructed. Assuming that cross section 3 had undergone a rotation would lead to the same statistic. Since $r_{\bullet\bullet}$ is orthogonal to X, the two contrasts for a bending of cross section 3 are equal to minus the corresponding contrasts for cross section 1.

6.3 A Numerical Example

To illustrate the techniques proposed in this paper, extrusions were manufactured according to the specifications of Figure 2, with $b = 7/8$ inch (all the measurement of this section are reported in inches) in the Department of Mechanical Engineering of Université Laval. Table 2 presents the data for two extrusions. Extrusion 1 should have no defect while a gap of 0.005 inch has been built in one of the planar region of extrusion 2.

ID	Extrusion 1			Extrusion 2		
1	0.87612	-0.81671	-0.06296	0.87351	-0.78456	-0.06352
2	0.87563	-0.08721	-0.06298	0.87363	-0.08478	-0.06141
3	0.78827	0.00017	-0.07817	0.772	0.00011	-0.09247
4	0.09602	-6e-05	-0.07728	0.07174	0.00012	-0.09123
5	-5e-05	-0.07891	-0.10538	8e-05	-0.06915	-0.09123
6	0.00134	-0.76398	-0.10546	-0.00041	-0.76559	-0.09353
7	0.07932	-0.87501	-0.06973	0.77544	-0.87492	-0.08443
8	0.80166	-0.87474	-0.07062	0.07293	-0.87451	-0.08331
9	0.87609	-0.81553	-3.17946	0.87313	-0.83259	-2.97102
10	0.87551	-0.06977	-3.17919	0.87325	-0.07346	-2.96864
11	0.8204	-0.00296	-3.13869	0.79951	0.00478	-2.97858
12	0.08282	-0.00321	-3.13782	0.0668	0.0049	-2.97729
13	-0.0006	-0.04304	-3.15029	0.00028	-0.04229	-3.19577
14	0.00053	-0.78735	-3.18677	-0.00052	-0.78163	-3.20809
15	0.04958	-0.87864	-3.04785	0.8168	-0.87079	-3.03297
16	0.79838	-0.8784	-3.04889	0.06799	-0.8702	-3.03161
17	0.87503	-0.81616	-5.72296	0.87034	-0.81674	-5.72515
18	0.87478	-0.06877	-5.72262	0.87067	-0.0645	-5.72252
19	0.81032	-0.00548	-5.72305	0.81136	0.0089	-5.70738
20	0.07983	-0.00579	-5.72234	0.06282	0.00918	-5.70607
21	-0.0013	-0.06503	-5.71309	0.00172	-0.03892	-5.70956
22	0.00028	-0.81995	-5.71336	0.00119	-0.809	-5.71205
23	0.04631	-0.88065	-5.69485	0.81266	-0.86542	-5.69705
24	0.80585	-0.88039	-5.69567	0.06172	-0.86479	-5.69582

Table 2. Data Collected on two Extrusions.

The sampling design was approximately the same as that given in Figure 2, except that the CMM was not programmed to sample the points. Sampling was done manually; this explains some of the irregularity in the sampled locations. The algorithm of Section 2.3, with the identity matrix as starting value converged in 2 iterations only for both extrusions. The sums of squares for the two extrusions are given in Table 3.

Extrusion	$SS_R \times 10^6$	$SS_P \times 10^6$	$SS_O \times 10^6$	$SS_S \times 10^6$
1	2.96	0.94	1.30	0.72
2	41.47	3.88	11.09	26.50

Table 3. Sums of squares for the two extrusions.

From Table 3, it is clear that the 2 extrusions differ; orientation and size appear to be the components responsible for this difference. To find out the planar surfaces responsible for the deficiencies of the second extrusion, we calculated the diagnostics for size and orientation using the formulae of Section 6.1. This gives approximate results only; exact diagnostics, calculated with an estimated design matrix X, could have been obtained using the general formulae of Section 5. However approximate diagnostics are much easier to calculate and to interpret.

The t_{18} statistics for size in extrusion 2 are given by 5.60 and 0.24 for planar region 1&3 and 2&4 respectively. Thus, the distance between planar regions 1 and 3 is not 0.875. Since $\sum_j r_{1j}/3 = -0.003$, an estimate of the true distance is 0.872. The $F_{2,3}$ diagnostics for orientation are ∞, 0.29, 199.83, and 0.23 for planar regions 1 to 4. One F-statistic is reported as ∞ because its denominator is negative. This is possible since approximate diagnostics are calculated. The contrast defined in Section 6.1 as c_1 is responsible for the large F-statistics. This suggests that one of planar surfaces 1 and 3 has undergone a small rotation about axis $(0, 1, 0)^t$. This agrees with the way in which extrusion 2 was manufactured. While polishing the third planar region, one end of the extrusion was tilted upward by 0.005 inch. Thus, at the tilted end, the distance between planar regions 1 and 3 is about 0.870 inch. With this modification, the distance between planar regions 1 and 3 is less than 7/8 inch and the orientation of planar region 1 with respect to planar region 3 is defective.

To investigate the quality of the approximations derived in this work, data were generated for 1000 extrusions according to the specifications of Figure 2. The sampling errors were independent, with variances equal to 10^{-6}. The expected squared residuals, multiplied by

10^6, ranged between 0.84 and 0.95 for the sample points with identification numbers between 9 and 16 and between 0.67 and 0.81 for the others. These are close to the theoretical values of 0.875 for the central cross-section and of 0.75 for the others derived in Section 6.1. The F-statistic for bending was also calculated for these 1000 repetitions. Its distribution matched $F_{2,17}$ distribution very well. The estimates of the probabilities of being above the 90^{th}, 95^{th}, 99^{th} percentiles of the $F_{2,17}$ are respectively given by 0.105, 0.053, and 0.008 respectively. This concurs with the findings of Chen and Chen (1997) who noticed that, for many objects, the chi-square distribution approximates the distribution of SS_R/σ^2 quite well.

7 Discussion

This paper has shown how to use linear model's techniques to assess geometric integrity. The derivations are based on a local linear model underlying the estimation of the translation vector and of the rotation matrix needed to match the CMM data to the CAD model. All the distributional results of the paper rely on the assumption that the errors orthogonal to the planar regions are independent and normally distributed.

The framework proposed in this paper for the analysis of CMM data has many applications. For instance, Dowling et al (1993) argue that the errors within each planar surface are correlated. Further modeling of these errors could be carried out by fitting spatial models to the surface residuals using residual maximum likelihood (REML) methods. Also, residual plots could suggest alternatives to the normal distribution for the errors. Since the expansions of Section 2 and 3 are valid for any error distribution, they provide a firm ground on which to investigate CMM data.

It would be of interest to generalize the results of this paper to non planar regions. Linear, cylindrical and regions with varying curvature are common features of many parts. It is not clear, at present, whether the first order contributions of the errors to the estimates can still be described using local linear models in this general setting.

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