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Estimation of errors in color measurement using multivariate statistics

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Abstract

Usually color coordinates of a colorimetric controlled process are located in an ellipsoid in the color space. These ellipsoids are usually not aligned to the coordinate axes. Their shape and orientation depend on the variances and covariances of the data. In such cases multivariate statistics has to be applied to describe the scattering around the mean color. Instead of ΔE the Mahalanobis distance is a superior measure for the statistical distance in color space. On this basis the errors in a measuring process have been estimated. The examples presented include the detection of outliers, the precision and time stability of the spectrophotometer, with the use of electronic references.

Scattering of color coordinates

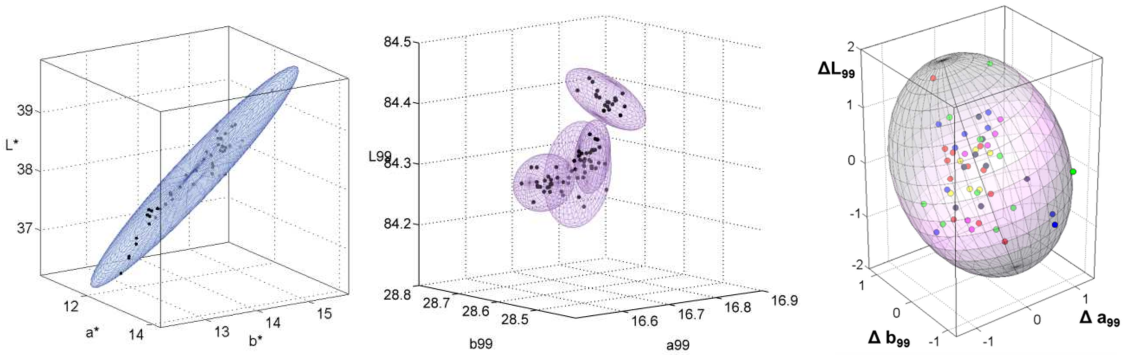


Fig. 1: Typical scattering of color coordinates around an average color in different processes (from left to right): scattering of color coordinates on a wood surface [1], 4 color standard cards RAL1021 rape yellow [2], industrial coatings of RAL-colors [3].

Usually scattering of data is expected in any measuring or controlling process (Fig. 1). Color measurement or a process monitored by color measurement results in a cloud of data with a certain shape in the color space. Only in case of equally scaled, equally weighted, and independent coordinate axes isotropic scattering results in a spherical data cloud (Fig. 2). Color coordinates, e.g. CIELAB-coordinates, are scaled to the visual sensation of the human eye and are a priori not independent. These are the reasons that even a stochastic scattering of process data results in an anisotropic cloud of data that is rotated against coordinate axes. In other words, color measurement data randomly dispersed around an average color result in an ellipsoidally shaped cloud rotated against the L^*,a^*,b^*-axes rather than in a spherical one (Fig. 2, bottom).

Two color measurements that occur with the same probability in a process generally result in two color loci with different Euclidian distances ΔE^*_{ab} from the average color of the process (Fig. 3). As a consequence ΔE^*_{ab} is not an adequate measure to describe a color measurement process.

Therefore control of color specification has to be discerned from process control. ΔE^*_{ab} is a parameter for the description of visual perception of color differences. It is not sufficient to monitor the production or a measuring process. In the following, the Mahalanobis distance [4, 5] is used to describe the weighted statistical distance of a measurement relative to the process average.

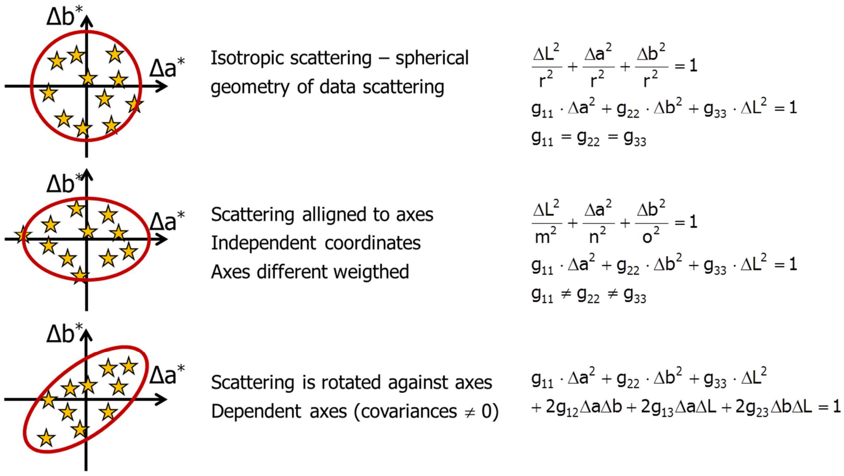


Fig. 2: Geometry of scattering of 3-dimensional data.

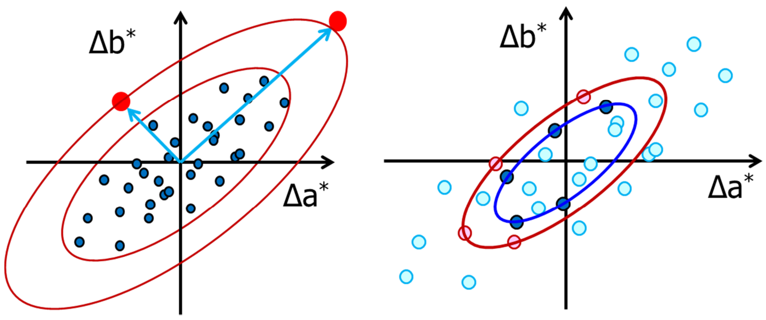


Fig. 3: The data dispersion is described by an ellipsoid. Data points located on the surface of the same ellipsoid have the same Mahalanobis distance from the average (left). As the ellipsoid radius is proportional to the probability, all points on the same ellipsoid occur with the same statistical probability (right).

Multivariate statistical methods for the description of scattering of color coordinates

CIELAB color coordinates are calculated from the tristimulus values X,Y,Z. Tristimulus values are derived from overlapping regions in the reflection spectrum and are not independent. Therefore covariances are different from zero. As previously mentioned, color spaces are designed on the basis of visual sensation aiming on uniformity in color differences, and a spherical dispersion is not expected. For this reason multivariate statistics have to be applied.

The best fitted method to describe the scattering of color loci is to use an ellipsoid that encloses a defined amount of measured color coordinates, e.g. 95% or 99%. In multivariate statistics an ellipsoid that encloses a certain number of data of the population is called a prognosis ellipsoid. To calculate the prognosis ellipsoid the average color coordinates, variances v_{ik} (with i=k, Eq. 1) and covariances v_{ik} (with i≠k, Eq. 2) of all coordinates are calculated and listed in the covariance matrix V (Eq. 3). The coefficients g_{ik} of the equation of the prognosis ellipsoid (Eq. 5) are the elements of the inverted covariance matrix G (Eq. 4). The size of the prognosis ellipsoid for a certain confidence level (1-α) is estimated by either the quantile of the Fisher- or the Beta-distribution (Eq. 6) with n is the number of measurements, 3 as number of dimensions (coordinate axes), and (1-α) as confidence level. In our investigation we used the F-distribution (Eq. 6).

Eq. 1
$$v_{11} = \mathrm{var}(a^*) = \frac{1}{n-1}\sum_{i=1}^{n}\left(a_i^* - \overline{a^*}\right)^2$$

Eq. 2
$$v_{12} = v_{21} = \mathrm{cov}(a^*, b^*) = \frac{1}{n-1}\sum_{i=1}^{n}\left(a_i^* - \overline{a^*}\right)\cdot\left(b_i^* - \overline{b^*}\right)$$

Eq. 3 $$\mathbf{V} = \begin{pmatrix} v_{11} & v_{12} & v_{13} \\ v_{21} & v_{22} & v_{23} \\ v_{31} & v_{32} & v_{33} \end{pmatrix}$$

Eq. 4 $$\mathbf{G} = \mathbf{V}^{-1} = \begin{pmatrix} g_{11} & g_{21} & g_{31} \\ g_{12} & g_{22} & g_{32} \\ g_{13} & g_{23} & g_{33} \end{pmatrix}$$

Eq. 5 $$g_{11} \cdot \left(a^* - \overline{a^*}\right)^2 + g_{22} \cdot \left(b^* - \overline{b^*}\right)^2 + g_{33} \cdot \left(L^* - \overline{L^*}\right)^2 + 2 \cdot g_{12} \cdot \left(a^* - \overline{a^*}\right) \cdot \left(b^* - \overline{b^*}\right) + 2 \cdot g_{23} \cdot \left(b^* - \overline{b^*}\right) \cdot \left(L^* - \overline{L^*}\right) + 2 \cdot g_{13} \cdot \left(a^* - \overline{a^*}\right) \cdot \left(L^* - \overline{L^*}\right) = T^2$$

Eq. 6 $$T^2 \approx \frac{p(n+1)\cdot(n-1)}{n\cdot(n-3)} \cdot F_{(3,n-3,1-\alpha)} \quad \text{or} \quad T^2 \approx \frac{(n-1)^2}{n} \cdot B_{(3/2,(n-3-1)/2,1-\alpha)}$$

Mahalanobis distance as statistical distance for the process control – T²-Chart

T^2 is the square Mahalanobis distance and a synonym for Hoteling's T^2 [4]. In Eq. 5 T^2 is used as a square ellipsoid radius. An ellipsoid radius is not an Euclidian distance. It represents the extension of the ellipsoid dependent on the direction (Fig. 3). In case of s Hotelling's T^2-statistics it is used as a weighted statistical distance from the center point (average). The weighting factors are the coefficients g_{ik} of the ellipsoid equation (Eq. 5) that are deduced from the process scattering.

The population is estimated by the prognosis ellipsoid with the confidence level e.g. $(1-\alpha)=0.99$. In this case a data point outside of the prognosis ellipsoid is an outlier with an error probability of $\alpha=0.01$. Consequently the corresponding T^2-value might be used as an upper control limit (**UCL**) for the process and for the detection of outliers.

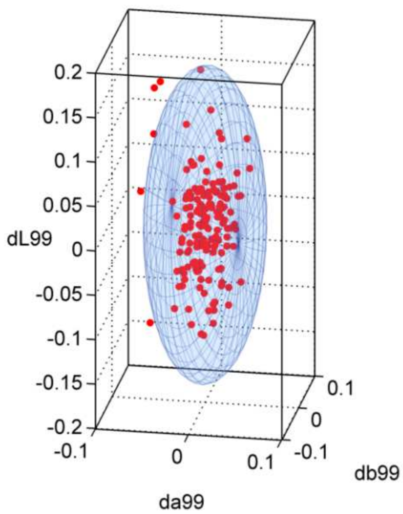


Fig. 4: Scattering of data with prognosis ellipsoid of a stable production in the difference coordinate system of the DIN99 color space with the average color as center point. Each data point is a mean value of 20 measurements at different locations of the sample. The prognosis ellipsoid has a confidence level of $(1-\alpha)=0.99$ revealing five outliers.

Detection of outliers

Usually only a sample containing n color measurements from the basic population is available. Assuming a steady state process a sample taken to derive the **UCL** is called historical data set (**HDS**).

The parameters of the population have to be estimated from this sample. This sample may contain outliers which are not elements of the population which obeys a certain statistical distribution. For the detection of outliers one calculates the sample mean, the covariance matrix and the **UCL** (according to Eq. 6). If T^2 of a data point has a value greater than the **UCL**, it is an outlier and has to be purged from the preliminary dataset. With the remaining observations, new estimates for the mean value and the covariance matrix are calculated. For a second pass through the data also the **UCL** has to be recalculated for the remaining number of observations. Again, all detected outliers are removed and the process is repeated until a homogenous set of data is obtained (Fig. 5) [4]. If a confidence level of $(1-\alpha)=0.99$ is defined, an observation with a T^2 higher than the **UCL** is an outlier with an error probability of 0.01 (=1%). In statistical process control the remaining data is the basis for definition of the **UCL**, the covariance matrix V and the average color for all following observations.

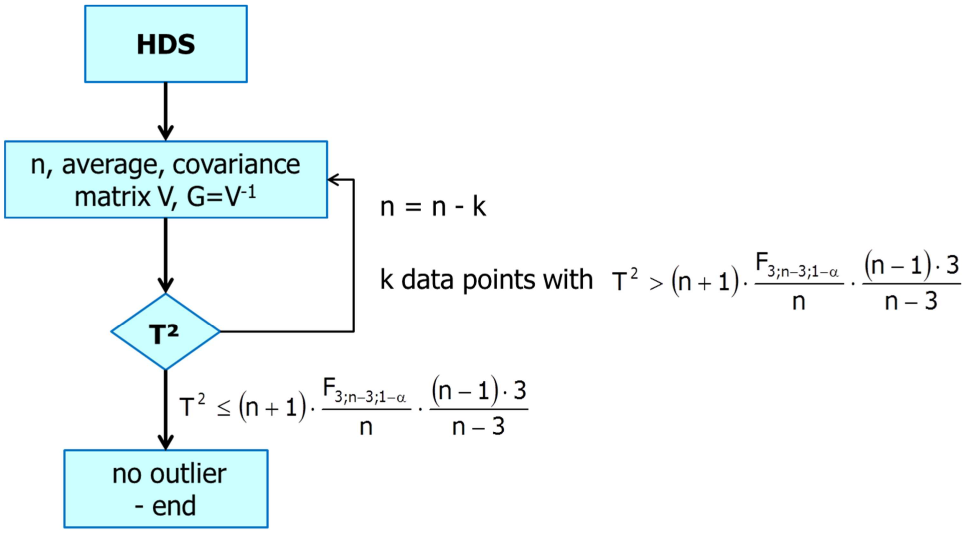


Fig. 5: Flow chart for the elimination of outliers from a historical data set (**HDS**).

Estimation of errors using electronically stored reference data

To obtain the capability of a production or measurement process, the knowledge of errors in measurement is important. In some cases specifications are very close to the gauge of uncertainty of the color measurement process. To cut down costs, time and personnel, companies use electronically stored color coordinates as references. Usually spectrophotometers demand a reference and a sample for the measurement, and detect the color difference between both. As a reference either a physical color standard or a defined L*,a*,b*-value is used. In this work the estimation of adjacent errors using electronically stored references was performed.

As the CIELAB color space is not visually uniform for small color differences ($\Delta E^*ab < 5$) it is preferable to use the DIN99 color space [6]. DIN99 is uniform for small color differences and hence it is possible to compare the errors of different colors in DIN99 coordinates. In CIELAB one may only compare color differences from non-Euclidian calculations like color differences based on CIE2000, CIE94 or CMC [7–9]. Only in the three dimensional DIN99 color coordinates (ΔL_{99}, Δa_{99}, Δb_{99}) it is possible to visualize the dispersion of measured color coordinates. When using any of the color difference formulae the problem is transferred into a one dimensional color difference scale (ΔE) and the possibility of visualization in a three dimensional color space is lost. Therefore we used the DIN99 color space in this work. The DIN99 color space is also the basis for the color tolerances of uniform colors for automotive coatings as specified in the DIN 6172-1 [10].

For the estimation of errors we used 8 samples. 4 of which have been RAL color cards (RAL3000 flame red, RAL3015 light pink, RAL5010 gentian blue, RAL5024 pastel blue). The others were home-made scratch resistant and cleanable color reference samples in the vicinity of the used RAL colors, labeled as anchor standards.

Our basic approach was to measure the set of color standard samples at 20 days within two month and compare the color coordinates. The color coordinates of each observation were treated as if they were absolute values.

One measurement approach (procedure **A**) was to calibrate the instrument, followed by 5 measurements of absolute color coordinates L*,a*,b*, on random positions, on each color sample in random order of samples. This approach represents a practice in educated industrial labs (others sometimes remain at one or three measurements on each sample).

The other approach (procedure **B**) includes calibration of the instrument, 40 subsequent blind measurements to warm up the instrument, anew calibration followed by 20 measurements at random positions on each sample. This procedure represents an approach to explore the maximum limits of precision, when using a spectrophotometer together with electronically stored references.

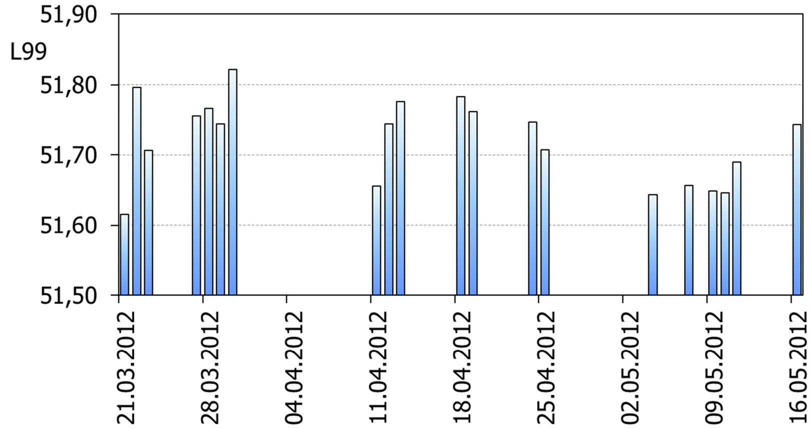


Fig. 6: Example for a time series, L_{99} value of the anchor standard in the vicinity of flame red (Datacolor SF600+, d/8, SPIN).

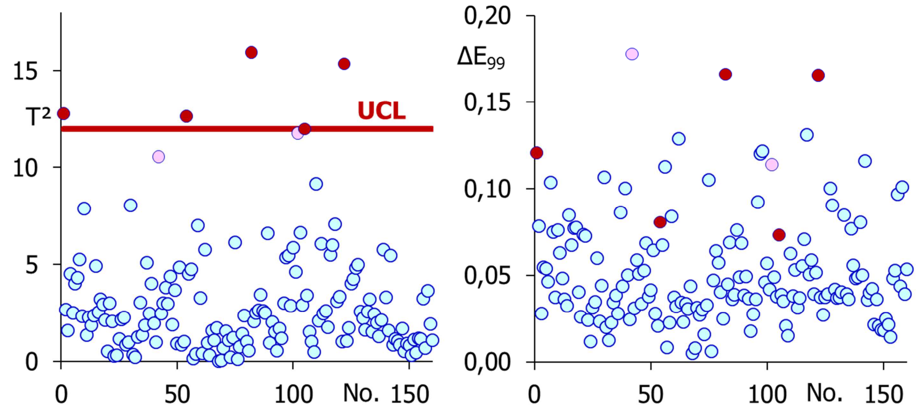
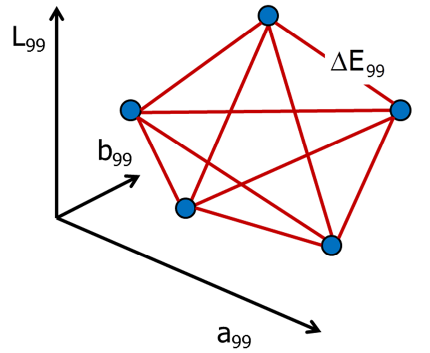


Fig. 7: T^2-Chart for the elimination of outliers (left), with outliers in the 1st cycle (pink), outliers eliminated in the 2nd cycle (red) und the upper control limit after the 2nd cycle. The chart of ΔE_{99} reveals that the elimination of outliers is not useful to take a color difference as a criterion.

In both procedures, measurements were done on 20 days, within a period of 2 month. In the first step, color coordinates of each sample were transformed into DIN99 coordinates and the average color coordinates were calculated for each time series. In the second step, color differences of each mean value to the average coordinates of a time series were calculated and for all samples within procedures **A** or **B** transferred to the difference coordinate system ΔL_{99}, Δa_{99}, Δb_{99}. This leads to the dispersion of color coordinates within procedure **A**, or within **B**, respectively.

On both data sets, form procedure **A** and from procedure **B**, the outliers were eliminated according to the procedure shown in Fig. 5. In case of procedure **B** (20 measurements) 7 outliers were eliminated in two cycles (s. Fig. 4, Tab. 1). Fig. 4 shows the dispersion of the data set of procedure **B** including the outliers. The ellipsoid in Fig. 4 was calculated for the covariance matrix and the Mahalanobis distance T^2 for a confidence level of $(1-\alpha)=0.99$ after the 2nd cycle. Applying the outlier elimination to the

$$\Delta E_{99k} = \sqrt{\left(\Delta L_{99,i} - \Delta L_{99,k}\right)^2 + \left(\Delta L_{99,i} - \Delta L_{99,k}\right)^2 + \left(\Delta L_{99,i} - \Delta L_{99,k}\right)^2}$$



$$\begin{pmatrix} (\Delta E_{99})_{1,1} & \cdots & \cdots & \cdots & (\Delta E_{99})_{1,k} \\ & 0 & \vdots & (\Delta E_{99})_{i,k} & \vdots \\ & & 0 & \vdots & \vdots \\ & & & 0 & \vdots \\ & & & & (\Delta E_{99})_{i,i} \end{pmatrix}$$

Fig. 8: Determination of the distance matrix with the elements $\Delta E_{99,ik}$.

In a first step the distance matrix of each procedure was calculated. In a data set with 160 elements 12720 color distances ΔE are present. Statistical analysis of one half of the distance matrix of procedure **B** provided a standard distribution of color differences (Fig. 9, left). The 0.95-quantile of the color distances had a magnitude of ΔE_{99} = 0.18 (Tab. 1). That means, if one measures according to the procedure **B**, the uncertainty is in this magnitude with a confidence level of 95%. In other words, in average every 20th observation has a higher error.

In case of procedure **A** it was not possible to fit any simple distribution to the data set containing all observations as it seems to contain elements of different populations. In this case, the parameters were derived from a fitted function (Tab. 1).

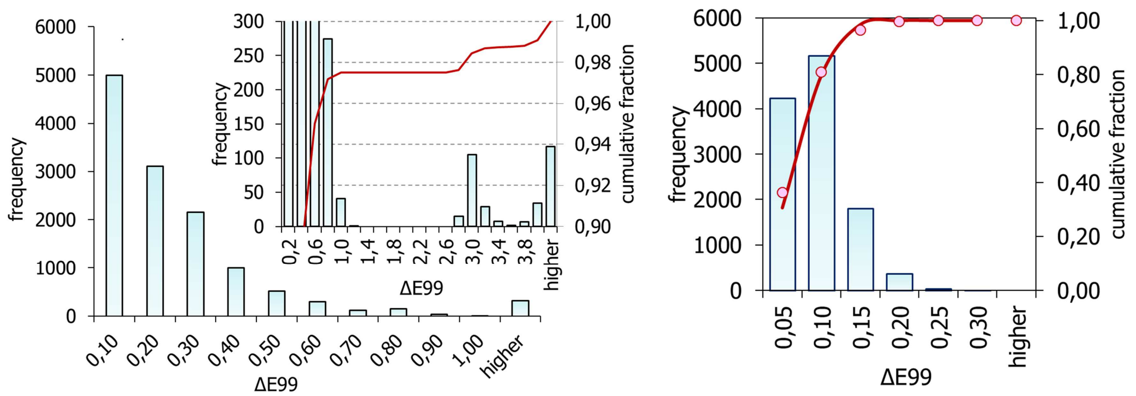


Fig. 9: Analysis of distance matrices of procedure **A** (5 measurements) including all 160 data points (left), and procedure **B** after elimination of outliers (20 measurements, left).

After elimination of the outliers the parameters like median and the 0.95 and 0.99 quantiles of the data sets of procedure **A** and **B** were approximately equal (Tab. 1). This is a necessary constraint if the data sets of both procedures belong to the same population.

The uncertainty of ΔE_{99} for procedure **A** was derived from the dataset including the outliers, as usually outliers are not eliminated according to the above described procedure (Fig. 5). The uncertainty of color difference for a confidence level of 95% had the magnitude of ΔE_{99} = 0.60 (Tab. 1). That means, in average every 20th observation has a higher error.

Tab. 1: Statistical parameters for the errors in ΔE_{99}, for procedures **A** and **B**, for the basic data sets and for data sets without the outliers.

		procedure **A** 5 measurements	procedure **B** 20 measurements
data set including outliers 160 datapoints	maximum ΔE_{99}	6.71	0.31
	median ΔE_{99}	0.15	0.07
	95%-quantil of ΔE_{99}	0.60	0.18
	99%-quantil of ΔE_{99}	4.00	0.23
data set after elimination of outliers	elimination cycles	12	2
	eliminated data points	30	7
	95%-quantil of ΔE_{99}	0.12	0.13
	99%-quantil of ΔE_{99}	0.14	0.16

Conclusions

Analysis of color measurements is a typical problem of multivariate statistics: Usually color coordinates of a colorimetric controlled process are located in an ellipsoid in the color space. These ellipsoids are usually not aligned to the coordinate axes. Their shape and orientation depend on the variances and covariances of the data. In such cases multivariate statistics has to be applied to describe the scattering around the mean color. Instead of ΔE a superior measure for the statistical distance in color space is the Mahalanobis distance.

On this basis the errors in a measuring process using electronically stored references have been estimated. The example included the detection of outliers and the precision with a spectrophotometer and color samples in the lab.

When color coordinates, derived from the average of 5 measurements on a typical sample, are compared to an electronic reference, an uncertainty in the color difference of $\Delta E99 = 0.60$ has to be taken into account. To derive the process capability the magnitude of the uncertainty has to be compared with the specification. A capable process should have a specification that's magnitude is at least twice as high. This might be fulfilled in the architectural applications but not for high end products. In the German automotive industry for the color tolerance of coatings is in the magnitude of $\Delta E99 \leq 0.3$ for the batch samples [10].

Literature

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