CHAPTER 6

Summary and Conclusions

6.1 Summary

This dissertation has successfully addressed the problem of the evaluation, design and sensitivity analysis of a set of colour scanning filters. The approach of Vrhel and Trussell to the colour correction problem [38, 39] was shown to present a problem in filter design which is similar to the problem of obtaining tristimulus values. Similarly, the problem of signature determination in satellite imaging was shown to be parallel to the problem of determination of tristimulus values. The commonality among these problems indicated the need for a broader framework for the evaluation of a set of filters, and hence for the design of a set of filters. Chapter 3 presented a data-independent measure and data-dependent measures which evaluate a set of filters from within the broader framework. Simulations on various data sets were reported, and the results implied that the measures were good indicators of the mean square error for corrected data.

Chapter 4 dealt with the use of the data-independent measure as an optimization criterion in the design of sets of scanning filters. The results obtained were very encouraging, and filter sets with high values of the data-independent measure were obtained. Given the filter designs, Eastman Kodak and Barr Associates responded with closest filters that they were able to manufacture. These filters were also presented in Chapter 4.

A sensitivity analysis of the filters with respect to filter fabrication errors was presented in Chapter 5. The second differential was used for an estimate of the change in the data-independent measure and the mean square ΔE_{Lab} error over the data set due to filter fabrication errors, and to thus provide a bound on these errors. Simulations indicated that the bounds provided reasonable estimates of the change in the mean square ΔE_{Lab} error and in the data-independent measure.

6.2 Contributions

The major contributions of this dissertation are:

1. A data-independent measure was developed to evaluate a set of three or more scanning filters which span a space of dimension three or larger. The measure was derived directly from the mean square fundamental error over a data set consisting of spectra with independent, identically distributed components, and was shown to be a generalization of Neugebauer's q-factor. Simulations indicated that this measure predicts accurately the mean square fundamental error, the mean square tristimulus error and the mean ΔE_{Lab} error over a data set if the data are corrected. Unlike other existing measures, the measure may be used in applications like colour correction where the space to be spanned is in general of dimension larger than three.

2. The data-independent measure was extended to a set of data-dependent measures based on mean square tristimulus errors. In the experiments performed, the average ΔE_{Lab} error was monotonic as a function of the data-dependent measures.

3. The data-independent measure was used to choose the set of three best filters from an existing set of filters. The filters were installed in a scanner at the Imaging Concepts Laboratory, Eastman Kodak, where they performed far better than an existing set of filters which was chosen using another evaluation criterion.

4. The data-independent measure was used as an optimization criterion to design filters that could be fabricated. The filters were modelled as smooth non-negative functions like the gaussian. This lead to a parametrized optimization problem which was easily solved through existing optimization algorithms. The results were extremely good.

5. The gradient of the mean square ΔE_{Lab} error was used to trim the best parametrized filters obtained, in order to obtain filters thatwere closer to optimal with respect to perceptual error. The results indicated that such trimming decreases the mean square ΔE_{Lab} error considerably. Filter sets with slightly higher values of the data-independent measure were also obtained through trimming with respect to the gradient of the data-independent measure.

6. The second differential of the data-independent measure and of the mean square ΔE_{Lab} error with respect to filter transmissivities provided a basis for the sensitivity analysis of filter designs. Bounds on the largest allowable error at all wavelengths and at a single wavelength given a maximum allowable change in the measure or the mean square ΔE_{Lab} error were derived and tested.

6.3 Directions for Further Research

In research the solution of a particular problem often leads to further questions and the definition of directions for further research. The work presented in this dissertation indicated that the following additional topics and problems would be worth pursuing.

1. The method of filter design to obtain realizable filters that span a certain space has only been implemented for three-dimensional spaces in this dissertation. The design procedure may be extended easily to spaces of more than three dimensions, particularly for applications like colour correction and satellite imaging.

2. The requirement of 'most orthogonal' filters may be imposed during the design procedure to obtain 'most orthogonal' filters with a large value of the data-independent measure.

3. The set of acceptable colour scanning filters are all members of the intersection of the two sets:

   The set of smooth filters shown to be convex in Chapter 4,

   $$C_s = \{\mathbf{M} = [\mathbf{m}_1, \ldots .\mathbf{m}_r] | \mathbf{m}_i(j+1) + \mathbf{m}_i(j-1) - 2\mathbf{m}_i(j) \leq \delta; 1 \leq i \leq r; 2 \leq j \leq N-1\}$$

   and the set of filter sets consisting of non-negative filters with large enough measures,

   $$C_{\nu n} = \{\mathbf{M} | \nu(\mathbf{A}_L, \mathbf{M}_H) \geq 1 - \delta, \mathbf{M}_{ij} \geq 0\}$$

   It was shown n Chapter 4 that the set

   $$C_\nu = \{\mathbf{M} | \nu(\mathbf{A}_L, \mathbf{M}_H) \geq 1 - \delta\}$$

is not convex. It appears that the constraint of non-negativity could result in a convex set, $C_{\nu n}$. As a good physically realizable set would lie in the intersection of the two sets

$$\mathbf{M} \in C_{\nu n} \cap C_s$$

the method of Projection Onto Convex Sets (POCS) [1, 32] or the more general Method of Successive Projections (MOSP) [4] could be used profitably in scanning filter design. It would be worthwhile to determine if the set $C_{\nu n}$ is convex.

4. Further analysis and experimental work could provide a bound on the euclidean norm of the error vector $vec\ d\mathbf{M}$, such that for all error vectors with euclidean norm smaller than the bound the second differential would provide an accurate estimate of the change in measure or mean square ΔE_{Lab} error.

5. The sensitivity analysis presented may be used to provide a criterion for the design of 'least sensitive' filters. The sensitivity analysis provides an explicit formula for the relationship between eigenvalues of the matrix $\mathcal{H}$ and maximum allowable fabrication errors. The matrix $\mathcal{H}$ may itself be directly related to the set of scanning filters $\mathbf{M}$, and this relationship may be used to define least sensitive filters.

6.4 Conclusions

The vector space approach has proved very useful as a framework for the design and analysis of optimal colour scanning filters. It allows the extension of the problem of the determination of tristimulus values to the problem of the determination of s-stimulus values ($s \geq 3$). The data-independent measure developed to evaluate a set of three or more filters that are to span a space of dimension three or larger proves very useful as a coarse optimization criterion, and as a coarse measure of the performance of a set of colour scanning filters. The data-independent measure may be used as an optimization criterion to produce very good filter sets which are non-negative and smooth, and hence physically realizable. The gradient of the filter sets with respect to the data-independent measure or the mean square ΔE_{Lab} error provides a means of improving the performance of the designed filters considerably while maintaining the smooth nature of the curves and hence their realizability. The second differential provides a reasonable estimate of the change in the data-independent measure and in the mean square ΔE_{Lab} error, and hence provides good estimates of the maximum allowable error in filter fabrication. The method of designing colour scanning filters and estimating their sensitivity may be used to produce exceptionally good results when the scanner characteristic is available and the space that is required to be spanned is known.

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Appendix

Theorem 1. Given scanning filter measurements $\mathbf{M}_H^T\mathbf{f}$ *and correlation matrix* $\mathbf{R} = E[\mathbf{f}\mathbf{f}^T]$*, the linear minimum mean square error estimate of the s-stimulus values* $\mathbf{t} = \mathbf{V}^T\mathbf{f}$ *is*

$$\hat{\mathbf{t}} = (\mathbf{V}^T\mathbf{R}\mathbf{M}_H(\mathbf{M}_H^T\mathbf{R}\mathbf{M}_H)^-)(\mathbf{M}_H^T\mathbf{f})$$

and the mean square error of this estimate is

$$E[||\mathbf{t} - \hat{\mathbf{t}}||^2] = Trace(\mathbf{V}^T\mathbf{R}\mathbf{V} - \mathbf{V}^T\mathbf{R}\mathbf{M}_H(\mathbf{M}_H^T\mathbf{R}\mathbf{M}_H)^-\mathbf{M}_H^T\mathbf{R}\mathbf{V})$$

where $\mathbf{X}^-$ *represents the generalized inverse or the g-inverse of matrix* $\mathbf{X}$ *[26]*

Proof:

Let $\hat{\mathbf{t}} = \mathbf{B}\mathbf{M}_H^T\mathbf{f}$ be a linear estimate. Then,

$$E[||\mathbf{t} - \hat{\mathbf{t}}||^2] = E[(\mathbf{V}^T\mathbf{f} - \mathbf{B}\mathbf{M}_H^T\mathbf{f})^T(\mathbf{V}^T\mathbf{f} - \mathbf{B}\mathbf{M}_H^T\mathbf{f})]$$

is the mean-square error of the linear estimate. To simplify manipulation the above mean square error may be written as:

$$E[||\mathbf{t} - \hat{\mathbf{t}}||^2] = E[Trace(\mathbf{V}^T\mathbf{f} - \mathbf{B}\mathbf{M}_H^T\mathbf{f})(\mathbf{V}^T\mathbf{f} - \mathbf{B}\mathbf{M}_H^T\mathbf{f})^T]$$

which is

$$E[||\mathbf{t} - \hat{\mathbf{t}}||^2] = Trace(\mathbf{V}^T - \mathbf{B}\mathbf{M}_H^T)\mathbf{R}(\mathbf{V}^T - \mathbf{B}\mathbf{M}_H^T)^T$$

which may be rewritten as

$$E[||\mathbf{t} - \hat{\mathbf{t}}||^2] = Trace(\mathbf{V}^T\mathbf{R}\mathbf{V} - \mathbf{B}\mathbf{M}_H^T\mathbf{R}\mathbf{V} - \mathbf{V}^T\mathbf{R}\mathbf{M}_H\mathbf{B}^T + \mathbf{B}\mathbf{M}_H^T\mathbf{R}\mathbf{M}_H\mathbf{B}^T)$$

As $Trace\mathbf{XYZ} = Trace\mathbf{ZXY}$ [21, pg. 10],

$$E[||\mathbf{t} - \hat{\mathbf{t}}||^2] = Trace(\mathbf{V}^T\mathbf{R}\mathbf{V} - 2\mathbf{B}\mathbf{M}_H^T\mathbf{R}\mathbf{V} + \mathbf{B}\mathbf{M}_H^T\mathbf{R}\mathbf{M}_H\mathbf{B}^T) \qquad (.1)$$

Differentiating the above expression gives

$$\frac{\partial E[||\mathbf{t} - \hat{\mathbf{t}}||^2]}{\partial \mathbf{B}} = 2\mathbf{V}^T\mathbf{R}\mathbf{M}_H - 2\mathbf{B}\mathbf{M}_H^T\mathbf{R}\mathbf{M}_H$$

A necessary condition for expression (.1) to have a minimum at $\mathbf{B} = \mathbf{B}_0$ is [27]

$$2\mathbf{V}^T\mathbf{R}\mathbf{M}_H - 2\mathbf{B}_0\mathbf{M}_H^T\mathbf{R}\mathbf{M}_H = \mathbf{0}$$

which implies that

$$\mathbf{B}_0\mathbf{M}_H^T\mathbf{R}\mathbf{M}_H = \mathbf{V}^T\mathbf{R}\mathbf{M}_H$$

All solutions of the above equation are of the form

$$\mathbf{B}_0 = \mathbf{V}^T\mathbf{R}\mathbf{M}_H(\mathbf{M}_H^T\mathbf{R}\mathbf{M}_H)^- \qquad (.2)$$

where $(\mathbf{M}_H^T\mathbf{R}\mathbf{M}_H)^-$ is the generalized inverse (g-inverse) [26] of $\mathbf{M}_H^T\mathbf{R}\mathbf{M}_H$. In general, $\mathbf{B}_0$ is not unique because $(\mathbf{M}_H^T\mathbf{R}\mathbf{M}_H)^-$ is not unique. When $\mathbf{M}_H^T\mathbf{R}\mathbf{M}_H$ is non-singular, the g-inverse is unique and $(\mathbf{M}_H^T\mathbf{R}\mathbf{M}_H)^- = (\mathbf{M}_H^T\mathbf{R}\mathbf{M}_H)^{-1}$. In either case, the value of $\hat{\mathbf{t}}_1 = \mathbf{B}_0\mathbf{M}_H^T\mathbf{f}$ is unique (see Theorem 7). The Hessian of the error expression is [27]

$$\frac{\partial^2 E[||\mathbf{t} - \hat{\mathbf{t}}||^2]}{\partial^2 \mathbf{B}} = -2\mathbf{M}_H^T\mathbf{R}\mathbf{M}_H$$

which is the negative of a quadratic form for all solutions of the form of equation(.2). This implies that all solutions of the form (.2) give local minima for the error expression [27]. Substituting (.2) in the error expression (.1), gives

$$E[||\mathbf{t} - \hat{\mathbf{t}}||^2] = Trace(\mathbf{V}^T\mathbf{R}\mathbf{V} - 2\mathbf{V}^T\mathbf{R}\mathbf{M}_H(\mathbf{M}_H^T\mathbf{R}\mathbf{M}_H)^-\mathbf{M}_H^T\mathbf{R}\mathbf{V} +$$

$$\mathbf{V}^T\mathbf{R}\mathbf{M}_H(\mathbf{M}_H^T\mathbf{R}\mathbf{M}_H)^-\mathbf{M}_H^T\mathbf{R}\mathbf{M}_H(\mathbf{M}_H^T\mathbf{R}\mathbf{M}_H)^-\mathbf{M}_H^T\mathbf{R}\mathbf{V})$$

The properties of the g-inverse imply that [26]

$$(\mathbf{M}_H^T\mathbf{R}\mathbf{M}_H)^-\mathbf{M}_H^T\mathbf{R}\mathbf{M}_H(\mathbf{M}_H^T\mathbf{R}\mathbf{M}_H)^- = (\mathbf{M}_H^T\mathbf{R}\mathbf{M}_H)^-$$

and

$$E[||\mathbf{t} - \hat{\mathbf{t}}||^2] = Trace(\mathbf{V}^T\mathbf{R}\mathbf{V} - \mathbf{V}^T\mathbf{R}\mathbf{M}_H(\mathbf{M}_H^T\mathbf{R}\mathbf{M}_H)^-\mathbf{M}_H^T\mathbf{R}\mathbf{V}) \qquad (.3)$$

Theorem 2. The reconstruction error, or the error between the true and the reconstructed fundamental, $\mathbf{e} = \mathbf{V}(\mathbf{V}^T\mathbf{V})^-(\mathbf{t} - \hat{\mathbf{t}})$, *is* $\mathbf{0}$ *for every* $\mathbf{R}$ *if and only if* $R(\mathbf{M}_H) \supseteq R(\mathbf{V})$.

Proof:

To prove the 'if' portion of the theorem, note that

$$R(\mathbf{M}_H) \supseteq R(\mathbf{V})$$

implies that

$$\mathbf{V} = \mathbf{M}_H\mathbf{X}$$

for some matrix $\mathbf{X}$. Substituting the above in equation (.3) gives

$$E[||\mathbf{t} - \hat{\mathbf{t}}||^2] = 0$$

which implies that $\mathbf{t} = \hat{\mathbf{t}}$, which implies that $\mathbf{e} = \mathbf{0}$.

To prove the 'only if' portion, note that

$$\mathbf{e} = \mathbf{0} \; for \; every \; \mathbf{R} \Rightarrow \mathbf{e} = \mathbf{0} \; for \; \mathbf{R} = \mathbf{I}$$

which implies that (from Theorem 1)

$$\mathbf{e} = \mathbf{V}(\mathbf{V}^T\mathbf{V})^{-1}(\mathbf{V}^T - \mathbf{V}^T\mathbf{M}_H(\mathbf{M}_H^T\mathbf{M}_H)^-\mathbf{M}_H^T)\mathbf{f} = P_V(\mathbf{I} - P_{M_H})\mathbf{f} = \mathbf{0} \quad (.4)$$

Showing that $R(\mathbf{M}_H) \supseteq R(\mathbf{V})$is equivalent to showing that

$$Null(\mathbf{V}) \supseteq Null(\mathbf{M}_H).$$

In the special case where R($\mathbf{V}$) is the HVSS, this means that the 'black space' of the Human Visual System includes the 'black space' of the scanning filters. Let $\mathbf{f}$ lie in the black space of the scanning filters, $\mathbf{f} \epsilon Null(\mathbf{M}_H)$. This implies that [26]

$$P_{M_H}\mathbf{f} = \mathbf{0}$$

From equation (.4) this implies that

$$P_V\mathbf{f} = \mathbf{0}$$

and $\mathbf{f} \epsilon Null(\mathbf{V})$ [26]. This completes the proof.

Theorem 3. $E[||\mathbf{e}||^2] = Trace(\mathbf{N}^T\mathbf{RN} - \mathbf{N}^T\mathbf{RM}_H(\mathbf{M}_H^T\mathbf{RM}_H)^-\mathbf{M}_H^T\mathbf{RN})$ *when* $\mathbf{N}$ *represents an orthonormal basis for* $R(\mathbf{V})$ *and* $E[\mathbf{ff}^T] = \mathbf{R}$.

Proof:

From the definition of the reproduction error $\mathbf{e}$ in Theorem 2, the mean of the sum of the squares of the reproduction (or fundamental) error components, or the mean-square reproduction (or fundamental) error, is:

$$E[||\mathbf{e}||^2] =$$

$$E[Trace\mathbf{NN}^T(\mathbf{I} - \mathbf{RM}_H(\mathbf{M}_H^T\mathbf{RM}_H)^-\mathbf{M}_H^T)\mathbf{ff}^T(\mathbf{I} - \mathbf{M}_H(\mathbf{M}_H^T\mathbf{RM}_H)^-\mathbf{M}_H^T\mathbf{R})\mathbf{NN}^T]$$

Using the fact that $Trace(\mathbf{XYZ}) = Trace(\mathbf{ZXY})$ and $\mathbf{N}^T\mathbf{N} = \mathbf{I}$, the above equation is

$$E[||\mathbf{e}||^2] =$$

$$E[Trace\mathbf{N}^T(\mathbf{I} - \mathbf{RM}_H(\mathbf{M}_H^T\mathbf{RM}_H)^-\mathbf{M}_H^T)\mathbf{ff}^T(\mathbf{I} - \mathbf{M}_H(\mathbf{M}_H^T\mathbf{RM}_H)^-\mathbf{M}_H^T\mathbf{R})\mathbf{N}]$$

which can be expanded and rewritten as:

$$E[||\mathbf{e}||^2] \; = \; Trace(\mathbf{N}^T\mathbf{R}\mathbf{N} \; - \; 2\mathbf{N}^T\mathbf{R}\mathbf{M}_H(\mathbf{M}_H^T\mathbf{R}\mathbf{M}_H)^-\mathbf{M}_H^T\mathbf{R}\mathbf{N}$$

$$+\mathbf{N}^T\mathbf{R}\mathbf{M}_H(\mathbf{M}_H^T\mathbf{R}\mathbf{M}_H)^-(\mathbf{M}_H^T\mathbf{R}\mathbf{M}_H)(\mathbf{M}_H^T\mathbf{R}\mathbf{M}_H)^-\mathbf{M}_H^T\mathbf{R}\mathbf{N})$$

if $E[\mathbf{f}\mathbf{f}^T] \; = \; \mathbf{R}$. Clearly, the above equation is

$$E[||\mathbf{e}||^2] \; = \; Trace(\mathbf{N}^T\mathbf{R}\mathbf{N} \; - \; \mathbf{N}^T\mathbf{R}\mathbf{M}_H(\mathbf{M}_H^T\mathbf{R}\mathbf{M}_H)^-\mathbf{M}_H^T\mathbf{R}\mathbf{N}) \qquad (.5)$$

Theorem 4 $\quad 0 \; \leq \; E[||\mathbf{e}||^2] \; \leq \; Trace \; P_V\mathbf{R} \; \leq \; Trace \; \mathbf{R}$

Proof:

$E[||\mathbf{e}||^2]$ is the expected value of a non-negative quantity and is hence non-negative. Further, the second term in equation (.5), $\mathbf{N}^T\mathbf{R}\mathbf{M}_H(\mathbf{M}_H^T\mathbf{R}\mathbf{M}_H)^-\mathbf{M}_H^T\mathbf{R}\mathbf{N}$, is of the form $\mathbf{N}^T\mathbf{R}\mathbf{M}_H\mathbf{X}^-(\mathbf{N}^T\mathbf{R}\mathbf{M}_H^T)^T$ where $\mathbf{X}$ is a quadratic form. This implies that the term is positive semi-definite [12]. This implies that

$$Trace(\mathbf{N}^T\mathbf{R}\mathbf{M}_H(\mathbf{M}_H^T\mathbf{R}\mathbf{M}_H)^-\mathbf{M}_H^T\mathbf{R}\mathbf{N}) \; \geq \; 0$$

and

$$0 \; \leq \; E[||\mathbf{e}||^2] \; \leq \; Trace \; \mathbf{N}^T\mathbf{R}\mathbf{N}$$

Further, from $P_V \; = \; \mathbf{N}\mathbf{N}^T$, and the fact that $Trace(\mathbf{XYZ}) \; = \; Trace(\mathbf{ZXY})$,

$$Trace\mathbf{N}^T\mathbf{R}\mathbf{N} \; = \; Trace \; P_V\mathbf{R} \leq Trace\mathbf{R}$$

from [12]. Hence,

$$0 \; \leq \; E[||\mathbf{e}||^2] \; \leq \; Trace \; P_V\mathbf{R} \; \leq Trace\mathbf{R}$$

Theorem 5. $E[||\mathbf{e}||^2] \; = \; \sigma^2(\sum_{i=1}^{\alpha}(1 \; - \; \lambda_i^2(\mathbf{O}^T\mathbf{N}))) \quad = \; \sigma^2 Trace(P_V \; - \; P_V P_{M_H})$ *when*

$E[\mathbf{f}\mathbf{f}^T] = \mathbf{R} = \sigma^2\mathbf{I}$, $\mathbf{N}$ *is an orthonormal basis for* $R(\mathbf{V})$ *and* $\mathbf{O}$ *is an orthonormal basis for* $R(\mathbf{M}_H)$.

Proof:

Substituting $\mathbf{R} = \sigma^2\mathbf{I}$ in equation (.5) gives

$$E[||\mathbf{e}||^2] = \sigma^2 Trace(\mathbf{N}^T\mathbf{N} - \mathbf{N}^T\mathbf{M}_H(\mathbf{M}_H^T\mathbf{M}_H)^{-}\mathbf{M}_H^T\mathbf{N}).$$

which may be rewritten as

$$E[||\mathbf{e}||^2] = \sigma^2(\alpha - Trace\mathbf{N}^T P_{M_H}\mathbf{N}). \quad (.6)$$

Using $P_{M_H} = \mathbf{O}\mathbf{O}^T$, the above equation may be rewritten as

$$E[||\mathbf{e}||^2] = \sigma^2 Trace(\mathbf{I}_\alpha - \mathbf{N}^T\mathbf{O}\mathbf{O}^T\mathbf{N}).$$

where $\mathbf{I}_\alpha$ is the α-dimensional identity matrix. This simplifies to

$$E[||\mathbf{e}||^2] = \sigma^2(\sum_{i=1}^{\alpha}(1 - \lambda_i^2(\mathbf{O}^T\mathbf{N})))$$

where $\lambda_i(\mathbf{O}^T\mathbf{N})$ denotes the i^{th} singular value of $\mathbf{O}^T\mathbf{N}$. Equation (.6) may also be rewritten as

$$E[||\mathbf{e}||^2] = \sigma^2 Trace(P_V - P_V P_{M_H})$$

using $Trace\mathbf{XYZ} = Trace\mathbf{ZXY}$ and $P_V = \mathbf{N}\mathbf{N}^T$.

Theorem 6. $\sum_{i=1}^{\alpha}\lambda_i^2(\mathbf{O}^T\mathbf{N}) = \sum_{i=1}^{\beta} q(\mathbf{o}_i)$.

Proof:

The proof follows from simple matrix algebra:

$$\sum_{i=1}^{\alpha}\lambda_i^2(\mathbf{O}^T\mathbf{N}) = Trace(\mathbf{O}^T\mathbf{N}\mathbf{N}^T\mathbf{O}) = Trace(\mathbf{O}^T\mathbf{N}\mathbf{N}^T\mathbf{N}\mathbf{N}^T\mathbf{O})$$

$$= Trace(P_V(\mathbf{O}))^T P_V(\mathbf{O}) \;=\; \sum_{i=1}^{\beta} ||P_V(\mathbf{o}_i)||^2 \;=\; \sum_{i=1}^{\beta} ||\mathbf{o}_i||^2 q(\mathbf{o}_i) \;=\; \sum_{i=1}^{\beta} q(\mathbf{o}_i)$$

Theorem 7 Given a non-singular correlation matrix $\mathbf{R}$*, let* $<\mathbf{x}, \mathbf{y}>' = \mathbf{x}\mathbf{R}^{-1}\mathbf{y}$ *define an inner-product. Let* P'_X *define the projection operator with respect to the norm* $||.||'$*. Then,* $\widehat{P_V}\mathbf{f}_1 = P_V\mathbf{R}\mathbf{M}_H(\mathbf{M}_H^T\mathbf{R}\mathbf{M}_H)^-\mathbf{M}_H^T = P_V P'_{RM_H}\mathbf{f}$*. Further, this implies that* $\hat{\mathbf{t}} = \mathbf{V}^T P_V P'_{RM_H}\mathbf{f}$*, and hence that the expressions for* $\widehat{P_V}\mathbf{f}_1$ *and* $\hat{\mathbf{t}}_1$ *are well-defined.*

Proof:

To show that $\widehat{P_V}\mathbf{f}_2 = P_V P'_{RM_H}\mathbf{f}$ the following lemma is needed.

Lemma 7.1 $P'_X = \mathbf{X}(\mathbf{X}^T\mathbf{R}^{-1}\mathbf{X})^-\mathbf{X}^T\mathbf{R}^{-1}$

Proof: Let $P'_X(\mathbf{m}) = \hat{\mathbf{m}}$. Then $\hat{\mathbf{m}} \in R(\mathbf{X})$, and $\hat{\mathbf{m}} = \mathbf{X}\hat{\mathbf{a}}$ for some $\hat{\mathbf{a}}$.

$$<\mathbf{m} - \hat{\mathbf{m}},\, \mathbf{m} - \hat{\mathbf{m}}>' \;\leq\; <\mathbf{m} - \mathbf{x},\, \mathbf{m} - \mathbf{x}>' \;\; \textit{for all } \mathbf{x} \in R(\mathbf{X})$$

implies that

$$(\mathbf{m} - \mathbf{X}\mathbf{a})^T\mathbf{R}^{-1}(\mathbf{m} - \mathbf{X}\mathbf{a})$$

has a minimum at $\mathbf{a} = \hat{\mathbf{a}}$. Differentiating this with respect to $\mathbf{a}$ and setting the result to zero gives

$$2\mathbf{X}^T\mathbf{R}^{-1}(\mathbf{m} - \mathbf{X}\mathbf{a}) = \mathbf{0}$$

A necessary condition for the minimum is that it must satisfy the above equation. A minimum exists because the minimum represents the projection of a point in a finite-dimensional Hilbert space onto a subspace [12]. Hence the required minimum is of the form

$$\hat{\mathbf{m}} = \mathbf{X}(\mathbf{X}^T\mathbf{R}^{-1}\mathbf{X})^-\mathbf{X}^T\mathbf{R}^{-1}\mathbf{m}$$

This gives a well-defined value for $\hat{\mathbf{m}}$ [26]. The result follows.

Theorem 8. $d(\nu(\mathbf{A}_L, \mathbf{M}_H)) = \frac{2Trace(\mathbf{M}_H^T\mathbf{M}_H)^{-1}\mathbf{M}_H^T P_V(\mathbf{I} - P_{M_H})\mathbf{H}d\mathbf{M}}{3}$

Proof:

The following laws of matrix differentials are used to obtain the required differentials:

$$
\begin{aligned}
d(a\mathbf{X}) &= ad\mathbf{X} \\
d(\mathbf{AX}) &= \mathbf{A}d\mathbf{X} \\
d(\mathbf{XY}) &= \mathbf{X}d\mathbf{Y} + d\mathbf{XY} \\
d(Trace\mathbf{X}) &= Trace\ d\mathbf{X} \\
d(\mathbf{X}^{-1}) &= -\mathbf{X}^{-1}(d\mathbf{X})\mathbf{X}^{-1} \\
d(\mathbf{X}^T) &= (d\mathbf{X})^T
\end{aligned} \tag{.7}
$$

Using the above rules,

$d(\nu(\mathbf{A}_L, \mathbf{M}_H)) =$

$$
(Trace(\mathbf{NN}^T(d\mathbf{M}_H(\mathbf{M}_H^T\mathbf{M}_H)^{-1}\mathbf{M}_H^T -
$$
$$
\mathbf{M}_H(\mathbf{M}_H^T\mathbf{M}_H)^{-1}((d\mathbf{M}_H)^T\mathbf{M}_H + \mathbf{M}_H^T d\mathbf{M}_H)(\mathbf{M}_H^T\mathbf{M}_H)^{-1})\mathbf{M}_H^T +
$$
$$
\mathbf{M}_H(\mathbf{M}_H^T\mathbf{M}_H)^{-1}(d\mathbf{M}_H)^T)))/3
$$

Using $Trace\mathbf{X} = Trace\mathbf{X}^T$, and $Trace\mathbf{XYZ} = Trace\mathbf{ZXY}$ and expanding the above equation gives

$d(\nu(\mathbf{A}_L, \mathbf{M}_H)) =$

$$
\frac{Trace(2((\mathbf{M}_H^T\mathbf{M}_H)^{-1}\mathbf{M}_H P_V - (\mathbf{M}_H^T\mathbf{M}_H)^{-1}\mathbf{M}_H P_V P_{M_H})d\mathbf{M}_H)}{3} \tag{.8}
$$

the result follows from $d\mathbf{M}_H = \mathbf{H}d\mathbf{M}$.

Theorem 9 If $\mathbf{K}$ *is such that*

$$
vec\ d\mathbf{M} = vec\ d\mathbf{M}^T\mathbf{K}
$$

and,

$$\mathcal{A} = \frac{2}{3}\{\mathbf{H}(-(\mathbf{M}_H^T\mathbf{M}_H)^{-1} \oplus (\mathbf{I} - P_{M_H})P_V(\mathbf{I} - P_{M_H})$$

$$+ (\mathbf{M}_H^T\mathbf{M}_H)^{-1}\mathbf{M}_H^T P_V \mathbf{M}_H(\mathbf{M}_H^T\mathbf{M}_H)^{-1} \oplus (\mathbf{I} - P_{M_H})$$

$$+ 2\mathbf{K}(\mathbf{I} - P_{M_H})P_V\mathbf{M}_H(\mathbf{M}_H^T\mathbf{M}_H)^{-1} \oplus (\mathbf{M}_H^T\mathbf{M}_H)^{-1}\mathbf{M}_H^T)\mathbf{H}\}$$

Let

$$\mathcal{H} = \frac{\mathcal{A}^T + \mathcal{A}}{2}$$

then, $d^2\nu = -\,vec\; d\mathbf{M}^T\mathcal{H} vec\; d\mathbf{M}$

Proof:

Differentiating equation (.8) using the rules in equations (.7),

$d^2(\nu(\mathbf{A}_L, \mathbf{M}_H)) =$

$$\frac{2}{3}Trace\{-(\mathbf{M}_H^T\mathbf{M}_H)^{-1}d\mathbf{M}_H^T\mathbf{M}_H(\mathbf{M}_H^T\mathbf{M}_H)^{-1}\mathbf{M}_H^T P_V(\mathbf{I} - P_{M_H})d\mathbf{M}_H \tag{.9}$$

$$-(\mathbf{M}_H^T\mathbf{M}_H)^{-1}\mathbf{M}_H^T d\mathbf{M}_H(\mathbf{M}_H^T\mathbf{M}_H)^{-1}\mathbf{M}_H^T P_V(\mathbf{I} - P_{M_H})d\mathbf{M}_H \tag{.10}$$

$$+ (\mathbf{M}_H^T\mathbf{M}_H)^{-1}d\mathbf{M}_H^T P_V(\mathbf{I} - P_{M_H})d\mathbf{M}_H \tag{.11}$$

$$- (\mathbf{M}_H^T\mathbf{M}_H)^{-1}\mathbf{M}_H^T P_V d\mathbf{M}_H(\mathbf{M}_H^T\mathbf{M}_H)^{-1}\mathbf{M}_H^T d\mathbf{M}_H \tag{.12}$$

$$+ (\mathbf{M}_H^T\mathbf{M}_H)^{-1}\mathbf{M}_H^T P_V\mathbf{M}_H(\mathbf{M}_H^T\mathbf{M}_H)^{-1}d\mathbf{M}_H^T\mathbf{M}_H(\mathbf{M}_H^T\mathbf{M}_H)^{-1}\mathbf{M}_H^T d\mathbf{M}_H \tag{.13}$$

$$+ (\mathbf{M}_H^T\mathbf{M}_H)^{-1}\mathbf{M}_H^T P_V\mathbf{M}_H(\mathbf{M}_H^T\mathbf{M}_H)^{-1}\mathbf{M}_H^T d\mathbf{M}_H(\mathbf{M}_H^T\mathbf{M}_H)^{-1}\mathbf{M}_H^T d\mathbf{M}_H \tag{.14}$$

$$- (\mathbf{M}_H^T\mathbf{M}_H)^{-1}\mathbf{M}_H^T P_V\mathbf{M}_H(\mathbf{M}_H^T\mathbf{M}_H)^{-1}d\mathbf{M}_H^T d\mathbf{M}_H\} \tag{.15}$$

Combining the terms (.9) and (.11) above gives:

$$(\mathbf{M}_H^T\mathbf{M}_H)^{-1}d\mathbf{M}_H^T(\mathbf{I} - P_{M_H})P_V(\mathbf{I} - P_{M_H})d\mathbf{M}_H \tag{.16}$$

Terms (.13) and (.15) combined give:

$$- \ (\mathbf{M}_H^T\mathbf{M}_H)^{-1}\mathbf{M}_H^T P_V \mathbf{M}_H (\mathbf{M}_H^T\mathbf{M}_H)^{-1} d\mathbf{M}_H^T (\mathbf{I} \ - \ P_{M_H}) d\mathbf{M}_H \qquad (.17)$$

Terms (.12) and (.14) combined give:

$$- \ (\mathbf{M}_H^T\mathbf{M}_H)^{-1}\mathbf{M}_H^T P_V (\mathbf{I} \ - \ P_{M_H}) d\mathbf{M}_H (\mathbf{M}_H^T\mathbf{M}_H)^{-1}\mathbf{M}_H^T d\mathbf{M}_H \qquad (.18)$$

Term (.18) is identical to term (.10) as $Trace\ \mathbf{XYZ} \ = \ Trace\mathbf{ZXY}$. From the above simplifications the expression for the second differential of the data-independent measure is the sum of terms (.10), (.16), (.17) and (.18):

$d^2(\nu(\mathbf{A}_L, \mathbf{M}_H)) \ =$

$$\frac{2}{3}Trace\{(\mathbf{M}_H^T\mathbf{M}_H)^{-1} d\mathbf{M}_H^T (\mathbf{I} \ - \ P_{M_H}) P_V (\mathbf{I} \ - \ P_{M_H}) d\mathbf{M}_H$$

$$- \ (\mathbf{M}_H^T\mathbf{M}_H)^{-1}\mathbf{M}_H^T P_V \mathbf{M}_H (\mathbf{M}_H^T\mathbf{M}_H)^{-1} d\mathbf{M}_H^T (\mathbf{I} \ - \ P_{M_H}) d\mathbf{M}_H$$

$$- \ 2(\mathbf{M}_H^T\mathbf{M}_H)^{-1}\mathbf{M}_H^T P_V (\mathbf{I} \ - \ P_{M_H}) d\mathbf{M}_H (\mathbf{M}_H^T\mathbf{M}_H)^{-1}\mathbf{M}_H^T d\mathbf{M}_H\}$$

Notice that each term in the expression for the second differential is of the form $Trace\mathbf{X}d\mathbf{M}\mathbf{Y}d\mathbf{M}^T$ or $Trace\mathbf{X}d\mathbf{M}\mathbf{Y}d\mathbf{M}$. Each expression may be simplified to the form $(vecd\mathbf{M})^T\mathbf{Z}vecd\mathbf{M}$ using the following formulae [21, pg. 192-193]:

$$Trace\mathbf{B}d\mathbf{X}^T\mathbf{C}d\mathbf{X} \ = \ (dvec\mathbf{X})^T(\mathbf{B}^T \oplus \mathbf{C})dvec\mathbf{X} \qquad (.19)$$

and

$$Trace\mathbf{B}d\mathbf{X}\mathbf{C}d\mathbf{X} \ = \ (dvec\mathbf{X})^T\mathbf{K}(\mathbf{B}^T \oplus \mathbf{C})dvec\mathbf{X} \qquad (.20)$$

Using the above equations, the second differential of the data-independent measure may be written as:

$d^2(\nu(\mathbf{A}_L, \mathbf{M}_H)) \ =$

$$\frac{2}{3}Trace\{(vecd\mathbf{M}_H)^T(\mathbf{M}_H^T\mathbf{M}_H)^{-1} \oplus (\mathbf{I} \ - \ P_{M_H}) P_V (\mathbf{I} \ - \ P_{M_H}) vec\ d\mathbf{M}_H$$

$$- (vecd\mathbf{M}_H)^T(\mathbf{M}_H^T\mathbf{M}_H)^{-1}\mathbf{M}_H^T P_V \mathbf{M}_H(\mathbf{M}_H^T\mathbf{M}_H)^{-1} \oplus (\mathbf{I} \; - \; P_{M_H})vec\ d\mathbf{M}_H$$

$$- 2(vecd\mathbf{M}_H)^T\mathbf{K}(\mathbf{I} \; - \; P_{M_H})P_V\mathbf{M}_H(\mathbf{M}_H^T\mathbf{M}_H)^{-1} \oplus (\mathbf{M}_H^T\mathbf{M}_H)^{-1}\mathbf{M}_H^T vec\ d\mathbf{M}_H\}$$

From which

$$d^2(\nu(\mathbf{A}_L, \mathbf{M}_H)) \;=\; -\,(vec\ d\mathbf{M})^T \mathcal{A} vecd\mathbf{M})$$

Further,

$$d^2\nu \;=\; \frac{1}{2}\{(vecd\mathbf{M})^T\mathcal{A}vecd\mathbf{M} \;+\; (vecd\mathbf{M})^T\mathcal{A}^T vecd\mathbf{M}\}$$

from which the result follows.

Theorem. 10 Let

$$\mathbf{\Theta} \;=\; (\mathbf{M}_H^T\mathbf{R}\mathbf{M}_H)^{-1}$$

$$\mathbf{\Psi} \;=\; \mathbf{I} \;-\; \mathbf{M}_H(\mathbf{M}_H^T\mathbf{R}\mathbf{M}_H)^{-1}\mathbf{M}_H^T\mathbf{R}$$

$$\mathbf{\Lambda} \;=\; 2\begin{bmatrix} \frac{500(a-a_1)}{9(x^5x_n)^{1/3}} & 0 & 0 \\ 0 & \frac{116(L-L_1) \; - \; 500(a-a_1) \; + \; 200(b-b_1)}{9(y^5y_n)^{1/3}} & 0 \\ 0 & 0 & \frac{-200(b-b_1)}{9(z^5z_n)^{1/3}} \end{bmatrix}$$

and

$$\mathcal{G} \;=\; 2\mathbf{R}\mathbf{A}(\mathbf{\Omega}\mathbf{\Upsilon}^T\mathbf{\Upsilon}\mathbf{\Omega} \;-\; \mathbf{\Lambda})\mathbf{A}^T\mathbf{R}$$

Then the second differential of the mean square ΔE_{Lab} *error is* $(vecd\mathbf{M})^T\mathcal{H}vecd\mathbf{M}$ *where*

$$\mathcal{H} \;=\; \frac{1}{2}(\mathcal{A} \;+\; \mathcal{A}^T)$$

and

$$\mathcal{A} \;=\; (\mathbf{H}[(\mathbf{\Theta} \oplus \mathbf{\Psi}^T(\frac{\sum_{\mathbf{f}}\mathbf{\Xi}}{n})\mathbf{\Psi}) \;+\; \frac{2}{n}\sum_{\mathbf{f}}(\mathbf{K}\mathbf{\Psi}^T\mathcal{G}\mathbf{M}_H\mathbf{\Theta} \oplus \mathbf{\Theta}\mathbf{M}_H^T\mathbf{f}\mathbf{f}^T\mathbf{\Psi})$$

$$+ \;\frac{1}{n}\sum_{\mathbf{f}}(\mathbf{\Theta}\mathbf{M}_H^T\mathcal{G}\mathbf{M}_H\mathbf{\Theta} \oplus \mathbf{\Psi}^T\mathbf{f}\mathbf{f}^T\mathbf{\Psi}) \;+\; \frac{1}{n}\sum_{\mathbf{f}}(\mathbf{\Theta}\mathbf{M}_H^T\mathbf{f}\mathbf{f}^T\mathbf{M}_H\mathbf{\Theta} \oplus \mathbf{\Psi}^T\mathcal{G}\mathbf{\Psi})$$

$$-2\ (\mathbf{KRM}_H\mathbf{\Theta} \oplus \mathbf{\Theta M}_H^T(\frac{\sum_{\mathbf{f}} \mathbf{\Xi}}{n})\mathbf{\Psi})\ -\ (\mathbf{\Theta M}_H^T(\frac{\sum_{\mathbf{f}} \mathbf{\Xi}}{n})\mathbf{M}_H\mathbf{\Theta} \oplus \mathbf{R\Psi})]\mathbf{H})$$

Proof: Differentiating the expression for the first differential of the mean square ΔE_{Lab} error

$$d(\frac{\sum_{\mathbf{f}} \Delta E_{Lab}^2(\mathbf{f})}{n})\ =$$

$$Trace(\mathbf{M}_H^T\mathbf{RM}_H)^{-1}\mathbf{M}_H^T(\frac{\sum_{\mathbf{f}} \mathbf{\Xi}(\mathbf{f})}{n})(\mathbf{I}\ -\ \mathbf{M}_H(\mathbf{M}_H^T\mathbf{RM}_H)^{-1}\mathbf{M}_H^T\mathbf{R})d\mathbf{M}_H \qquad (.21)$$

term by term using the laws of matrix differentials stated in (.7) gives:

$$d^2 f\ =\ d^2\frac{\sum_{\mathbf{f}} \Delta E_{Lab}^2(\mathbf{f})}{n}\ =$$

$$Trace\{(\mathbf{M}_H^T\mathbf{RM}_H)^{-1}d\mathbf{M}_H^T(\frac{\sum_{\mathbf{f}} \mathbf{\Xi}}{n})(\mathbf{I}\ -\ \mathbf{M}_H(\mathbf{M}_H^T\mathbf{RM}_H)^{-1}\mathbf{M}_H^T\mathbf{R})d\mathbf{M}_H \qquad (.22)$$

$$-\ \{(\mathbf{M}_H^T\mathbf{RM}_H)^{-1}(d\mathbf{M}_H^T\mathbf{RM}_H)(\mathbf{M}_H^T\mathbf{RM}_H)^{-1}\mathbf{M}_H^T(\frac{\sum_{\mathbf{f}} \mathbf{\Xi}}{n}) \qquad (.23)$$

$$(\mathbf{I}\ -\ \mathbf{M}_H(\mathbf{M}_H^T\mathbf{RM}_H)^{-1}\mathbf{M}_H^T\mathbf{R})d\mathbf{M}_H\}$$

$$-\ \{(\mathbf{M}_H^T\mathbf{RM}_H)^{-1}(\mathbf{M}_H^T\mathbf{R}d\mathbf{M}_H)(\mathbf{M}_H^T\mathbf{RM}_H)^{-1}\mathbf{M}_H^T(\frac{\sum_{\mathbf{f}} \mathbf{\Xi}}{n}) \qquad (.24)$$

$$(\mathbf{I}\ -\ \mathbf{M}_H(\mathbf{M}_H^T\mathbf{RM}_H)^{-1}\mathbf{M}_H^T\mathbf{R})d\mathbf{M}_H\}$$

$$+\ (\mathbf{M}_H^T\mathbf{RM}_H)^{-1}\mathbf{M}_H^T(\frac{\sum_{\mathbf{f}} d\mathbf{\Xi}}{n})(\mathbf{I}\ -\ \mathbf{M}_H(\mathbf{M}_H^T\mathbf{RM}_H)^{-1}\mathbf{M}_H^T\mathbf{R})d\mathbf{M}_H \qquad (.25)$$

$$+\ (\mathbf{M}_H^T\mathbf{RM}_H)^{-1}\mathbf{M}_H^T(\frac{\sum_{\mathbf{f}} \mathbf{\Xi}}{n})(\ -\ d\mathbf{M}_H(\mathbf{M}_H^T\mathbf{RM}_H)^{-1}\mathbf{M}_H^T\mathbf{R})d\mathbf{M}_H \qquad (.26)$$

$$+\ \{(\mathbf{M}_H^T\mathbf{RM}_H)^{-1}\mathbf{M}_H^T(\frac{\sum_{\mathbf{f}} \mathbf{\Xi}}{n}) \qquad (.27)$$

$$(\mathbf{M}_H(\mathbf{M}_H^T\mathbf{RM}_H)^{-1}(d\mathbf{M}_H^T\mathbf{RM}_H)(\mathbf{M}_H^T\mathbf{RM}_H)^{-1}\mathbf{M}_H^T\mathbf{R})d\mathbf{M}_H\}$$

$$+ \ \{(\mathbf{M}_H^T\mathbf{R}\mathbf{M}_H)^{-1}\mathbf{M}_H^T(\frac{\sum_{\mathbf{f}} \boldsymbol{\Xi}}{n}) \tag{.28}$$

$$(\mathbf{M}_H(\mathbf{M}_H^T\mathbf{R}\mathbf{M}_H)^{-1}(\mathbf{M}_H^T\mathbf{R}d\mathbf{M}_H)(\mathbf{M}_H^T\mathbf{R}\mathbf{M}_H)^{-1}\mathbf{M}_H^T\mathbf{R})d\mathbf{M}_H\}$$

$$+ \ (\mathbf{M}_H^T\mathbf{R}\mathbf{M}_H)^{-1}\mathbf{M}_H^T(\frac{\sum_{\mathbf{f}} \boldsymbol{\Xi}}{n})(- \mathbf{M}_H(\mathbf{M}_H^T\mathbf{R}\mathbf{M}_H)^{-1}d\mathbf{M}_H^T\mathbf{R})d\mathbf{M}_H \tag{.29}$$

Combining terms (.22) and (.23) of the expression for the second differential gives:

$$\boldsymbol{\Theta}d\mathbf{M}_H^T\boldsymbol{\Psi}^T(\frac{\sum_{\mathbf{f}} \boldsymbol{\Xi}}{n})\boldsymbol{\Psi}d\mathbf{M}_H \tag{.30}$$

Combining terms (.24), (.26) and (.28) gives

$$- \ 2\ \boldsymbol{\Theta}(\mathbf{M}_H^T\mathbf{R}d\mathbf{M}_H)\boldsymbol{\Theta}\mathbf{M}_H^T(\frac{\sum_{\mathbf{f}} \boldsymbol{\Xi}}{n})\boldsymbol{\Psi}d\mathbf{M}_H \tag{.31}$$

Combining terms (.27) and (.29) gives:

$$- \quad \boldsymbol{\Theta}\mathbf{M}_H^T(\frac{\sum_{\mathbf{f}} \boldsymbol{\Xi}}{n})\mathbf{M}_H\boldsymbol{\Theta}d\mathbf{M}_H^T\mathbf{R}\boldsymbol{\Psi}d\mathbf{M}_H \tag{.32}$$

Further, from the definition

$$\boldsymbol{\Xi}(\mathbf{f}) \ = \ \mathbf{f}\mathbf{c}^T(\mathbf{f})\boldsymbol{\Upsilon}\boldsymbol{\Omega}(\mathbf{f})\mathbf{A}^T\mathbf{R} \ + \ \mathbf{R}\mathbf{A}\boldsymbol{\Omega}(\mathbf{f})\boldsymbol{\Upsilon}^T\mathbf{c}(\mathbf{f})\mathbf{f}^T$$

the first differential of the matrix Ξ is

$$d\boldsymbol{\Xi} \ = \ \mathbf{f}d(\mathbf{c}^T\boldsymbol{\Upsilon}\boldsymbol{\Omega})\mathbf{A}^T\mathbf{R} \ + \ \mathbf{R}\mathbf{A}d(\boldsymbol{\Omega}\boldsymbol{\Upsilon}^T\mathbf{c})\mathbf{f}^T$$

The above differentiation is made easier by the following observation:

$$\mathbf{c}^T\boldsymbol{\Upsilon}\boldsymbol{\Omega} \ =$$

$$2[\frac{500(a-a_1)}{3(x^2x_n)^{1/3}}, \ \frac{116(L-L_1)-500(a-a_1)+200(b-b_1)}{3(y^2y_n)^{1/3}}, \ \frac{-200(b-b_1)}{3(z^2z_n)^{1/3}}]$$

Differentiating the above expression term-by-term gives:

$$d\frac{500(a-a_1)}{3(x^2x_n)^{1/3}} = \frac{500(x^2x_n)^{1/3}da \; - \; \frac{2}{3}500(a-a_1)(x^{-1/3}x_n^{1/3})dx}{3(x^2x_n)^{2/3}}$$

$$d\frac{116(L-L_1) - 500(a-a_1) + 200(b-b_1)}{3(y^2y_n)^{1/3}} =$$

$$\{(y^2y_n)^{1/3}(116dL - 500da + 200db)$$

$$-\frac{2}{3}(y^{-1/3}y_n^{1/3})(116(L-L_1) - 500(a-a_1) + 200(b-b_1))dy\}/3(y^2y_n)^{2/3}$$

and,

$$d\frac{-200(b-b_1)}{3(z^2z_n)^{1/3}} = \frac{-200(z^2z_n)^{1/3}db \; + \; \frac{2}{3}200(b-b_1)(z^{-1/3}z_n^{1/3})dz}{3(z^2z_n)^{2/3}}$$

This gives an expression for the required differential:

$$d(\mathbf{c}^T\boldsymbol{\Upsilon}\boldsymbol{\Omega})^T = 2\begin{bmatrix} 0 & \frac{500}{3(x^2x_n)^{1/3}} & 0 \\ \frac{116}{3(y^2y_n)^{1/3}} & \frac{-500}{3(y^2y_n)^{1/3}} & \frac{200}{3(y^2y_n)^{1/3}} \\ 0 & 0 & \frac{-200}{3(z^2z_n)^{1/3}} \end{bmatrix} d\mathcal{F}(\hat{\mathbf{t}})$$

$$-4\begin{bmatrix} \frac{500(a-a_1)}{9(x^5x_n)^{1/3}} & 0 & 0 \\ 0 & \frac{116(L-L_1) \; - \; 500(a-a_1) \; + \; 200(b-b_1)}{9(y^5y_n)^{1/3}} & 0 \\ 0 & 0 & \frac{-200(b-b_1)}{9(z^5z_n)^{1/3}} \end{bmatrix} d\hat{\mathbf{t}}$$

This implies that

$$d(\mathbf{c}^T\boldsymbol{\Upsilon}\boldsymbol{\Omega})^T = = 2(\boldsymbol{\Omega}\boldsymbol{\Upsilon}^T\boldsymbol{\Upsilon}\boldsymbol{\Omega} \; - \; \boldsymbol{\Lambda})d\hat{\mathbf{t}}$$

and

$$d\Xi = 2(\mathbf{RA}(\boldsymbol{\Omega}\boldsymbol{\Upsilon}^T\boldsymbol{\Upsilon}\boldsymbol{\Omega} \; - \; \boldsymbol{\Lambda})d\hat{\mathbf{t}}\mathbf{f}^T \; + \; \mathbf{f}d\hat{\mathbf{t}}^T(\boldsymbol{\Omega}\boldsymbol{\Upsilon}^T\boldsymbol{\Upsilon}\boldsymbol{\Omega} \; - \; \boldsymbol{\Lambda})\mathbf{A}^T\mathbf{R}) \qquad (.33)$$

Using the expression for $d\hat{\mathbf{t}}$ in equation (4.22) gives:

$$d\Xi = \mathcal{G}d\mathbf{M}_H\boldsymbol{\Theta}\mathbf{M}_H^T\mathbf{ff}^T \; - \; \mathcal{G}\mathbf{M}_H\boldsymbol{\Theta}\mathbf{M}_H^T\mathbf{R}d\mathbf{M}_H\boldsymbol{\Theta}\mathbf{M}_H^T\mathbf{ff}^T \qquad (.34)$$

$$- \mathcal{G}\mathbf{M}_H\boldsymbol{\Theta}d\mathbf{M}_H^T\mathbf{R}\mathbf{M}_H\boldsymbol{\Theta}\mathbf{M}_H^T\mathbf{ff}^T \ + \ \mathcal{G}\mathbf{M}_H\boldsymbol{\Theta}d\mathbf{M}_H^T\mathbf{ff}^T$$

$$+ \ \mathbf{ff}^T\mathbf{M}_H\boldsymbol{\Theta}d\mathbf{M}_H^T\mathcal{G} - \mathbf{ff}^T\mathbf{M}_H\boldsymbol{\Theta}d\mathbf{M}_H^T\mathbf{R}\mathbf{M}_H\boldsymbol{\Theta}\mathbf{M}_H^T\mathcal{G}$$

$$- \ \mathbf{ff}^T\mathbf{M}_H\boldsymbol{\Theta}\mathbf{M}_H^T\mathbf{R}d\mathbf{M}_H\boldsymbol{\Theta}\mathbf{M}_H^T\mathcal{G} \ + \ \mathbf{ff}^Td\mathbf{M}_H\boldsymbol{\Theta}\mathbf{M}_H^T\mathcal{G}$$

Combining the above terms pairwise gives:

$$d\Xi \ = \ \mathcal{G}\boldsymbol{\Psi}d\mathbf{M}_H\boldsymbol{\Theta}\mathbf{M}_H^T\mathbf{ff}^T \ + \ \mathcal{G}\mathbf{M}_H\boldsymbol{\Theta}d\mathbf{M}_H^T\boldsymbol{\Psi}^T\mathbf{ff}^T \ +$$

$$\mathbf{ff}^T\mathbf{M}_H\boldsymbol{\Theta}d\mathbf{M}_H^T\boldsymbol{\Psi}^T\mathcal{G} \ - \ \mathbf{ff}^T\boldsymbol{\Psi}d\mathbf{M}_H\boldsymbol{\Theta}\mathbf{M}_H^T\mathcal{G}$$

Term (.25) in the expression for the second differential is:

$$\frac{\sum_{\mathbf{f}}}{n}Trace\boldsymbol{\Theta}\mathbf{M}_H^T\mathcal{G}\boldsymbol{\Psi}d\mathbf{M}_H\boldsymbol{\Theta}\mathbf{M}_H^T\mathbf{ff}^T\boldsymbol{\Psi}d\mathbf{M}_H \ +$$

$$\frac{\sum_{\mathbf{f}}}{n}Trace\boldsymbol{\Theta}\mathbf{M}_H^T\mathcal{G}\mathbf{M}_H\boldsymbol{\Theta}d\mathbf{M}_H^T\boldsymbol{\Psi}^T\mathbf{ff}^T\boldsymbol{\Psi}d\mathbf{M}_H \ +$$

$$\frac{\sum_{\mathbf{f}}}{n}Trace\boldsymbol{\Theta}\mathbf{M}_H^T\mathbf{ff}^T\mathbf{M}_H\boldsymbol{\Theta}d\mathbf{M}_H^T\boldsymbol{\Psi}^T\mathcal{G}\boldsymbol{\Psi}d\mathbf{M}_H \ +$$

$$\frac{\sum_{\mathbf{f}}}{n}Trace\boldsymbol{\Theta}\mathbf{M}_H^T\mathbf{ff}^T\boldsymbol{\Psi}d\mathbf{M}_H\boldsymbol{\Theta}\mathbf{M}_H^T\mathcal{G}\boldsymbol{\Psi}d\mathbf{M}_H$$

The first and fourth terms are identical in the above expression and the expression for the second differential may be rewritten as the sum of the above expressions and expressions (.30), (.31), and (.32):

$$d^2\frac{\sum_{\mathbf{f}}\Delta E_{Lab}^2(\mathbf{f})}{n} \ = \ \boldsymbol{\Theta}d\mathbf{M}_H^T\boldsymbol{\Psi}^T(\frac{\sum_{\mathbf{f}}\Xi}{n})\boldsymbol{\Psi}d\mathbf{M}_H \ + \tag{.35}$$

$$\frac{2}{n}\sum_{\mathbf{f}}Trace\boldsymbol{\Theta}\mathbf{M}_H^T\mathcal{G}\boldsymbol{\Psi}d\mathbf{M}_H\boldsymbol{\Theta}\mathbf{M}_H^T\mathbf{ff}^T\boldsymbol{\Psi}d\mathbf{M}_H \ +$$

$$\frac{1}{n}\sum_{\mathbf{f}}Trace\boldsymbol{\Theta}\mathbf{M}_H^T\mathcal{G}\mathbf{M}_H\boldsymbol{\Theta}d\mathbf{M}_H^T\boldsymbol{\Psi}^T\mathbf{ff}^T\boldsymbol{\Psi}d\mathbf{M}_H \ +$$

$$\frac{1}{n}\sum_{\mathbf{f}} Trace \mathbf{\Theta} \mathbf{M}_H^T \mathbf{f}\mathbf{f}^T \mathbf{M}_H \mathbf{\Theta} d\mathbf{M}_H^T \mathbf{\Psi}^T \mathcal{G} \mathbf{\Psi} d\mathbf{M}_H +$$

$$-2\ \mathbf{\Theta}(\mathbf{M}_H^T \mathbf{R} d\mathbf{M}_H)\mathbf{\Theta}\mathbf{M}_H^T(\frac{\sum_{\mathbf{f}} \mathbf{\Xi}}{n})\mathbf{\Psi} d\mathbf{M}_H$$

$$-\ \mathbf{\Theta}\mathbf{M}_H^T(\frac{\sum_{\mathbf{f}} \mathbf{\Xi}}{n})\mathbf{M}_H \mathbf{\Theta} d\mathbf{M}_H^T \mathbf{R}\mathbf{\Psi} d\mathbf{M}_H$$

Using equations (.19) and (.20), expression .35 may be rewritten as

$$d^2\frac{\sum_{\mathbf{f}} \Delta E_{Lab}^2(\mathbf{f})}{n} = (vecd\mathbf{M}_H)^T(\mathbf{\Theta} \oplus \mathbf{\Psi}^T(\frac{\sum_{\mathbf{f}} \mathbf{\Xi}}{n})\mathbf{\Psi})vecd\mathbf{M}_H +$$

$$(vecd\mathbf{M}_H)^T(\frac{2}{n}\sum_{\mathbf{f}} 2\mathbf{K}\mathbf{\Psi}^T\mathcal{G}\mathbf{M}_H\mathbf{\Theta} \oplus \mathbf{\Theta}\mathbf{M}_H^T\mathbf{f}\mathbf{f}^T\mathbf{\Psi})vecd\mathbf{M}_H +$$

$$(vecd\mathbf{M}_H)^T(\frac{1}{n}\sum_{\mathbf{f}} \mathbf{\Theta}\mathbf{M}_H^T\mathcal{G}\mathbf{M}_H\mathbf{\Theta} \oplus \mathbf{\Psi}^T\mathbf{f}\mathbf{f}^T\mathbf{\Psi})vecd\mathbf{M}_H +$$

$$(vecd\mathbf{M}_H)^T(\frac{1}{n}\sum_{\mathbf{f}} \mathbf{\Theta}\mathbf{M}_H^T\mathbf{f}\mathbf{f}^T\mathbf{M}_H\mathbf{\Theta} \oplus \mathbf{\Psi}^T\mathcal{G}\mathbf{\Psi})vecd\mathbf{M}_H$$

$$-2\ (vecd\mathbf{M}_H)^T(\mathbf{K}\mathbf{R}\mathbf{M}_H\mathbf{\Theta} \oplus \mathbf{\Theta}\mathbf{M}_H^T(\frac{\sum_{\mathbf{f}} \mathbf{\Xi}}{n})\mathbf{\Psi})vecd\mathbf{M}_H +$$

$$-\ (vecd\mathbf{M}_H)^T(\mathbf{\Theta}\mathbf{M}_H^T(\frac{\sum_{\mathbf{f}} \mathbf{\Xi}}{n})\mathbf{M}_H\mathbf{\Theta} \oplus \mathbf{R}\mathbf{\Psi})vecd\mathbf{M}_H$$

and,

$$d^2 f = (vecd\mathbf{M})^T \mathcal{A} vecd\mathbf{M}$$

where

$$\mathcal{A} = (\mathbf{H}(\mathbf{\Theta} \oplus \mathbf{\Psi}^T(\frac{\sum_{\mathbf{f}} \mathbf{\Xi}}{n})\mathbf{\Psi}\mathbf{H})$$

$$+\ \frac{2}{n}\sum_{\mathbf{f}} \mathbf{H}2\mathbf{K}\mathbf{\Psi}^T\mathcal{G}\mathbf{M}_H\mathbf{\Theta} \oplus \mathbf{\Theta}\mathbf{M}_H^T\mathbf{f}\mathbf{f}^T\mathbf{\Psi})\mathbf{H}$$

$$+ (\frac{1}{n}\sum_{\mathbf{f}} \mathbf{H\Theta M}_H^T \mathcal{G} \mathbf{M}_H \mathbf{\Theta} \oplus \mathbf{\Psi}^T \mathbf{ff}^T \mathbf{\Psi H})$$

$$+ (\frac{1}{n}\sum_{\mathbf{f}} \mathbf{H\Theta M}_H^T \mathbf{ff}^T \mathbf{M}_H \mathbf{\Theta} \oplus \mathbf{\Psi}^T \mathcal{G} \mathbf{\Psi H})$$

$$-2\ \mathbf{H}(K_{qn}\mathbf{RM}_H\mathbf{\Theta} \oplus \mathbf{\Theta M}_H^T(\frac{\sum_{\mathbf{f}} \mathbf{\Xi}}{n})\mathbf{\Psi H})$$

$$-\ (\mathbf{H\Theta M}_H^T(\frac{\sum_{\mathbf{f}} \mathbf{\Xi}}{n})\mathbf{M}_H\mathbf{\Theta} \oplus \mathbf{R\Psi H})$$

The result follows.