Simultaneous Nadir Overpasses

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The purpose of these notes is to derive the equations provided by TT, so I can understand the current thinking, and the limitations, and then to suggest possible ways forward.

1 Current method

1.1 Data and regression model

Consider a set of radiance measurements made by (i) a reference instrument, $L^{\mathrm{r}}_{i(k)}$, and (ii) a target instrument, $L^{\mathrm{t}}_{i(k)}$ (i is the measurement number for channel k). It is desired that the target instrument should have the same characteristics as the reference instrument (ideally that it should produce the same profile as the reference instrument when looking at the same scene under the same conditions). A calibration procedure is to be performed to allow this. It is assumed (for now at least) that the two instruments share the same set of channels, and that they are measuring the atmosphere at the same place and time.

Suppose that the following is a reasonable model of how the parallel measurements are related:

$$L^{\mathrm{t}}_{i(k)} = a^{\mathrm{r}}_{(k)} + b^{\mathrm{r}}_{(k)} L^{\mathrm{r}}_{i(k)} + \nu_{i(k)}, \tag{1}$$

where $a^{\mathrm{r}}_{(k)}$ and $b^{\mathrm{r}}_{(k)}$ are channel-dependent parameters, and ν_i is the mismatch between the measurement from the target instrument, $L^{\mathrm{t}}_{i(k)}$, and that from the processed version of the reference instrument, $a^{\mathrm{r}}_{(k)} + b^{\mathrm{r}}_{(k)} L^{\mathrm{r}}_{i(k)}$. Assume that $\left\langle \nu_{i(k)} \right\rangle = 0$ and that $\left\langle \nu^2_{i(k)} \right\rangle = {\sigma^{\mathrm{t}}_{i(k)}}^2$, where $\langle \bullet \rangle$ means take the expectation over a large number of imagined repeated measurements.

Inverting (1) (and ignoring the mismatch term since it is unknowable) gives

$$\hat{L}^{\mathrm{t}}_{i(k)} \equiv L^{\mathrm{r}}_{i(k)} \approx \frac{L^{\mathrm{t}}_{i(k)}}{b^{\mathrm{r}}_{(k)}} - \frac{a^{\mathrm{r}}_{(k)}}{b^{\mathrm{r}}_{(k)}}. \tag{2}$$

Posing the equation this way round allows us to define the calibration: $\hat{L}^{\mathrm{t}}_{i(k)}$ is defined as the calibrated version of the target radiances.

1.2 Posing the least-squares problem

Suppose that we have n pieces of data for each of $L^{\mathrm{r}}_{i(k)}$ and, $L^{\mathrm{t}}_{i(k)}$, i.e. $1 \leq i \leq n$ and let these be organised in vectors $\mathbf{l}^{\mathrm{r}}_{(k)}$ and $\mathbf{l}^{\mathrm{t}}_{(k)}$. Furthermore, let

$$\mathbf{x}_{(k)} = \begin{pmatrix} a^{\mathrm{r}}_{(k)} \\ b^{\mathrm{r}}_{(k)} \end{pmatrix}. \tag{3}$$

Equation (1) may then be written as

$$\mathbf{l}^{\mathrm{t}}_{(k)} = \mathbf{H}_{(k)} \mathbf{x}_{(k)} + \boldsymbol{\nu}_{(k)}, \tag{4}$$

where

$$\mathbf{H}_{(k)} = \begin{pmatrix} 1 & L^{\mathrm{r}}_{1(k)} \\ 1 & L^{\mathrm{r}}_{2(k)} \\ \vdots & \vdots \\ 1 & L^{\mathrm{r}}_{n(k)} \end{pmatrix} = \begin{pmatrix} \mathbf{1} & \mathbf{l}^{\mathrm{r}}_{(k)} \end{pmatrix}. \tag{5}$$

The usual interpretation of (1) and (4) is that $\mathbf{l}^{\mathrm{r}}_{i(k)}$ is known perfectly, but $\mathbf{l}^{\mathrm{t}}_{(k)}$ is not (errors in $\mathbf{l}^{\mathrm{t}}_{(k)}$ are described by $\boldsymbol{\nu}_{(k)}$).

We form the following least squares problem:

$$J_{(k)}[\mathbf{x}_{(k)}] = \frac{1}{2}\left(\mathbf{l}^{\mathrm{t}}_{(k)} - \mathbf{H}_{(k)}\mathbf{x}_{(k)}\right)^{\mathrm{T}} \mathbf{R}^{-1}_{(k)} \left(\mathbf{l}^{\mathrm{t}}_{(k)} - \mathbf{H}_{(k)}\mathbf{x}_{(k)}\right). \tag{6}$$

There may be one such cost function for each channel, k, considered.

1.3 Solving the least-squares problem

The minimum is this cost function is the $\mathbf{x}_{(k)}$ that makes this stationary (i.e. the first derivative zero):

$$\nabla J_{(k)} = -\mathbf{H}^{\mathrm{T}}_{(k)}\mathbf{R}^{-1}_{(k)}\left(\mathbf{l}^{\mathrm{t}}_{(k)} - \mathbf{H}_{(k)}\mathbf{x}^{\mathrm{optimal}}_{(k)}\right) = 0, \tag{7}$$

which rearranges to

$$\mathbf{x}^{\mathrm{optimal}}_{(k)} = \left(\mathbf{H}^{\mathrm{T}}_{(k)}\mathbf{R}^{-1}_{(k)}\mathbf{H}_{(k)}\right)^{-1}\mathbf{H}^{\mathrm{T}}_{(k)}\mathbf{R}^{-1}_{(k)}\mathbf{l}^{\mathrm{t}}_{(k)}. \tag{8}$$

Assuming that $\mathbf{R}_{(k)}$ is diagonal (diagonal elements ${\sigma^{t}_{i(k)}}^{2}$), and using (5) gives the following parts of (8):

$$\begin{aligned}
\left(\mathbf{H}^{\mathrm{T}}_{(k)}\mathbf{R}^{-1}_{(k)}\mathbf{H}_{(k)}\right)^{-1} &= \frac{1}{s^{1}s^{\mathrm{rr}} - s^{\mathrm{r}2}}\begin{pmatrix} s^{1} & -s^{\mathrm{r}} \\ -s^{\mathrm{r}} & s^{\mathrm{rr}} \end{pmatrix}, &(9)\\
\mathbf{H}^{\mathrm{T}}_{(k)}\mathbf{R}^{-1}_{(k)}\mathbf{l}^{\mathrm{t}}_{(k)} &= \begin{pmatrix} s^{\mathrm{rt}} \\ s^{\mathrm{t}} \end{pmatrix}, &(10)
\end{aligned}$$

where s^{1}, s^{r}, s^{rr}, s^{t}, and s^{rt} are shorthand for terms that are calculable from the data (we drop the channel (k) subscript for convenience):

$$\begin{aligned}
s^{1} = \sum_{i} {\sigma^{\mathrm{t}}_{i(k)}}^{-2},\ s^{\mathrm{r}} = \sum_{i} L^{\mathrm{r}}_{i(k)}{\sigma^{\mathrm{t}}_{i(k)}}^{-2},\ s^{\mathrm{rr}} = \sum_{i} {L^{\mathrm{r}}_{i(k)}}^{2}{\sigma^{\mathrm{t}}_{i(k)}}^{-2},\\
s^{\mathrm{t}} = \sum_{i} L^{\mathrm{t}}_{i(k)}{\sigma^{\mathrm{t}}_{i(k)}}^{-2},\ s^{\mathrm{rt}} = \sum_{i} L^{\mathrm{r}}_{i(k)}L^{\mathrm{t}}_{i(k)}{\sigma^{\mathrm{t}}_{i(k)}}^{-2}.
\end{aligned} \tag{11}$$

Putting this together in (8) leads to

$$\mathbf{x}^{\mathrm{optimal}}_{(k)} = \begin{pmatrix} a^{\mathrm{r}}_{(k)} \\ b^{\mathrm{r}}_{(k)} \end{pmatrix} = \frac{1}{s^{1}s^{\mathrm{rr}} - s^{\mathrm{r}2}}\begin{pmatrix} s^{1} & -s^{\mathrm{r}} \\ -s^{\mathrm{r}} & s^{\mathrm{rr}} \end{pmatrix}\begin{pmatrix} s^{\mathrm{rt}} \\ s^{\mathrm{t}} \end{pmatrix}. \tag{12}$$

1.4 Uncertainty of the solution

In addition to the optimal set of parameters, the least squares problem also estimates the error covariance of the parameters. This is the inverse of the Hessian (second derivative) of the cost function. The Hessian is

$$\nabla^{2} J_{(k)} = \mathbf{H}^{\mathrm{T}}_{(k)}\mathbf{R}^{-1}_{(k)}\mathbf{H}_{(k)}, \tag{13}$$

so the inverse Hessian is simply (9). In particular, the variances of $a^{\mathrm{r}}_{(k)}$ and $b^{\mathrm{r}}_{(k)}$ are

$$\begin{aligned}
\sigma^{2}_{a^{\mathrm{r}}_{(k)}} &= \frac{s^{1}}{s^{1}s^{\mathrm{rr}} - s^{\mathrm{r}2}}, &(14)\\
\sigma^{2}_{b^{\mathrm{r}}_{(k)}} &= \frac{s^{\mathrm{rr}}}{s^{1}s^{\mathrm{rr}} - s^{\mathrm{r}2}}, &(15)
\end{aligned}$$

and the error cross covariance is

$$c_{a^{\mathrm{r}}_{(k)}b^{\mathrm{r}}_{(k)}} = \frac{-s^{\mathrm{r}}}{s^{1}s^{\mathrm{rr}} - s^{\mathrm{r}2}}. \tag{16}$$

1.5 Uncertainty in the target radiances post calibration (i.e. in use)

Consider (2). Performing a first-order error analysis for errors in $\hat{L}^{\mathrm{t}}_{i(k)}$ (denoted $\delta\hat{L}^{\mathrm{t}}_{i(k)}$):

$$\begin{aligned}
\delta\hat{L}^{\mathrm{t}}_{i(k)} &\approx \frac{\partial\hat{L}^{\mathrm{t}}_{i(k)}}{\partial L^{\mathrm{t}}_{i(k)}}\delta L^{\mathrm{t}}_{i(k)} + \frac{\partial\hat{L}^{\mathrm{t}}_{i(k)}}{\partial b^{\mathrm{r}}_{(k)}}\delta b^{\mathrm{r}}_{(k)} + \frac{\partial\hat{L}^{\mathrm{t}}_{i(k)}}{\partial a^{\mathrm{r}}_{(k)}}\delta a^{\mathrm{r}}_{(k)}, \\
&= \frac{1}{b^{\mathrm{r}}_{(k)}}\delta L^{\mathrm{t}}_{i(k)} + \left(-\frac{L^{\mathrm{t}}_{i(k)}}{{b^{\mathrm{r}}_{(k)}}^2} + \frac{a^{\mathrm{r}}_{(k)}}{{b^{\mathrm{r}}_{(k)}}^2}\right)\delta b^{\mathrm{r}}_{(k)} - \frac{1}{b^{\mathrm{r}}_{(k)}}\delta a^{\mathrm{r}}_{(k)}.
\end{aligned}$$

The variance is then:

$$\begin{aligned}
\left\langle{\delta\hat{L}^{\mathrm{t}}_{i(k)}}^2\right\rangle &= \frac{1}{{b^{\mathrm{r}}_{(k)}}^2}\underbrace{\left\langle{\delta L^{\mathrm{t}}_{i(k)}}^2\right\rangle}_{{\sigma^{\mathrm{t}}_{i(k)}}^2} + 2\left(-\frac{L^{\mathrm{t}}_{i(k)}}{{b^{\mathrm{r}}_{(k)}}^3} + \frac{a^{\mathrm{r}}_{(k)}}{{b^{\mathrm{r}}_{(k)}}^3}\right)\underbrace{\left\langle\delta L^{\mathrm{t}}_{i(k)}\delta b^{\mathrm{r}}_{(k)}\right\rangle}_{0} - 2\frac{1}{{b^{\mathrm{r}}_{(k)}}^2}\underbrace{\left\langle\delta L^{\mathrm{t}}_{i(k)}\delta a^{\mathrm{r}}_{(k)}\right\rangle}_{0} \\
&+ \left(-\frac{L^{\mathrm{t}}_{i(k)}}{{b^{\mathrm{r}}_{(k)}}^2} + \frac{a^{\mathrm{r}}_{(k)}}{{b^{\mathrm{r}}_{(k)}}^2}\right)^2\underbrace{\left\langle{\delta b^{\mathrm{r}}_{(k)}}^2\right\rangle}_{\sigma^2_{b^{\mathrm{r}}_{(k)}}} - 2\left(-\frac{L^{\mathrm{t}}_{i(k)}}{{b^{\mathrm{r}}_{(k)}}^3} + \frac{a^{\mathrm{r}}_{(k)}}{{b^{\mathrm{r}}_{(k)}}^3}\right)\underbrace{\left\langle\delta b^{\mathrm{r}}_{(k)}\delta a^{\mathrm{r}}_{(k)}\right\rangle}_{c_{a^{\mathrm{r}}_{(k)}b^{\mathrm{r}}_{(k)}}} + \frac{1}{{b^{\mathrm{r}}_{(k)}}^2}\underbrace{\left\langle{\delta a^{\mathrm{r}}_{(k)}}^2\right\rangle}_{\sigma^2_{a^{\mathrm{r}}_{(k)}}}, \\
&= \frac{1}{{b^{\mathrm{r}}_{(k)}}^2}\left[{\sigma^{\mathrm{t}}_{i(k)}}^2 + \left(a^{\mathrm{r}}_{(k)} - L^{\mathrm{t}}_{i(k)}\right)^2\sigma^2_{b^{\mathrm{r}}_{(k)}} + \sigma^2_{a^{\mathrm{r}}_{(k)}} - \frac{2}{b^{\mathrm{r}}_{(k)}}\left(a^{\mathrm{r}}_{(k)} - L^{\mathrm{t}}_{i(k)}\right)c_{a^{\mathrm{r}}_{(k)}b^{\mathrm{r}}_{(k)}}\right]. \qquad (17)
\end{aligned}$$

Equation (17) is slightly different from TT's equation. Some of the differences are in details (possibly algebraic errors), but one difference (the ${\sigma^{\mathrm{t}}_{i(k)}}^2$ term) is present because here we account for random error in the target measurements.

2 Issues

TT's listed issues with the conventional method are reproduced as follows (some of my thoughts are given in italics).

1. Assumes relationship is linear, some detectors are non-linear at cold temperatures.
   (a) *By "cold temperatures" if you mean low brightness temperatures, then assuming that any non-linear effects are weak over the adjustments by the calibration, then it is possible to do a separate calibration for different bins of brightness temperatures, providing that enough data are available.*
   (b) *If you mean the temperature of the detector, then I need to know more about how detectors work. I would presume that detectors are kept very cold to minimise spurious signals emanating from the spacecraft itself.*
2. Assumes no uncertainty in any observations. Both observations have observation error covariances – still waiting for new FCDR files with target covariances.
   (a) *The analysis here does account for random error in the target measurements (${\sigma^{\mathrm{t}}_{i(k)}}^2$), but not in the reference measurements. See point 6 below.*
   (b) *The above neglects errors between channels (k). Accounting for errors between channels results in similar equations, but would require a rethink. More in Sect. 4.*
3. Assumes if the difference between the target and environment areas is with 3σ of environment area to be consistent.
4. No accounting for representativeness or collocation uncertainty of the independent measurements.
   (a) *This is the big problem.*
5. Error-in-variables (EIV) models provide a more suitable approach. However are non-trivial.

6. Substitution of OLS [*ordinary least squares*] minimisation for EIV method such as orthogonal distance regression (ODR) would account for uncertainties in observations but not collocation uncertainty.
   (a) *More of this in Sect. 3 below.*
7. Can data assimilation provide a framework to account for all uncertainties in the system and propagate the correlation structures within the uncertainties?
   (a) *Almost certainly the methods used in DA can be applied here to some degree. More of this to follow.*

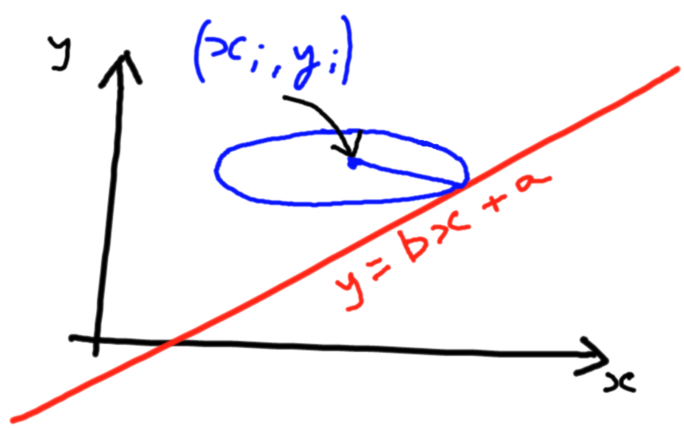
Some issues of my own are as follows (perhaps just categories of problems of the type 4 above).

1. Cloud contamination issues (if the reference has cloud but the target does not, or vice-versa).
2. Surface differences between target scene and reference scene (for channels that see the surface).

3 Considering observation errors of both instruments

3.1 Posing the least-squares problem when errors are present for both instruments

Suppose that each measurement of the target radiance has error variance ${\sigma^{\mathrm{t}}_{i(k)}}^2$, and additionally that each measurement of the reference radiance has error radiance ${\sigma^{\mathrm{r}}_{i(k)}}^2$ (before we had assumed that the latter is zero). We ask the question, "What is the distance between a measurement pair $(L^{\mathrm{r}}_{i(k)}, L^{\mathrm{t}}_{i(k)})$ and the straight line $L^{\mathrm{t}}_{(k)} = a^{\mathrm{r}}_{(k)} + b^{\mathrm{r}}_{(k)} L^{\mathrm{r}}_{(k)}$ where the distance is specified in multiples of the error standard deviations of each measurement?" (see Fig. – $(L^{\mathrm{r}}_{(k)}, L^{\mathrm{t}}_{(k)}) \to (x, y)$ in the Fig.)



The scaled distance between an arbitrary point on the line $(L^{\mathrm{r}}_{(k)}, L^{\mathrm{t}}_{(k)}) = (L^{\mathrm{r}}_{(k)}, a^{\mathrm{r}}_{(k)} + b^{\mathrm{r}}_{(k)} L^{\mathrm{r}}_{(k)})$ and the measurement $(L^{\mathrm{r}}_{i(k)}, L^{\mathrm{t}}_{i(k)})$ is $d_{i(k)}$:

$$d^2_{i(k)} = \frac{(L^{\mathrm{r}}_{(k)} - L^{\mathrm{r}}_{i(k)})^2}{{\sigma^{\mathrm{r}}_{i(k)}}^2} + \frac{(a^{\mathrm{r}}_{(k)} + b^{\mathrm{r}}_{(k)} L^{\mathrm{r}}_{(k)} - L^{\mathrm{t}}_{i(k)})^2}{{\sigma^{\mathrm{t}}_{i(k)}}^2}. \tag{18}$$

Finding the $L^{\mathrm{r}}_{(k)}$ that minimises this:

$$\frac{dd^2_{i(k)}}{dL^{\mathrm{r}}_{(k)}} = 2\frac{L^{\mathrm{r}}_{(k)} - L^{\mathrm{r}}_{i(k)}}{{\sigma^{\mathrm{r}}_{i(k)}}^2} + 2\frac{(a^{\mathrm{r}}_{(k)} + b^{\mathrm{r}}_{(k)} L^{\mathrm{r}}_{(k)} - L^{\mathrm{t}}_{i(k)}) b^{\mathrm{r}}_{(k)}}{{\sigma^{\mathrm{t}}_{i(k)}}^2}.$$

The derivative is zero when $L^{\mathrm{r}}_{(k)} = L^{\mathrm{r0}}_{(k)}$:

$$L^{\mathrm{r0}}_{(k)} = \frac{L^{\mathrm{r}}_{i(k)} {\sigma^{\mathrm{t}}_{i(k)}}^2 + (L^{\mathrm{t}}_{i(k)} b^{\mathrm{r}}_{(k)} - a^{\mathrm{r}}_{(k)} b^{\mathrm{r}}_{(k)}) {\sigma^{\mathrm{r}}_{i(k)}}^2}{{\sigma^{\mathrm{t}}_{i(k)}}^2 + {b^{\mathrm{r}}_{(k)}}^2 {\sigma^{\mathrm{r}}_{i(k)}}^2}, \tag{19}$$

making the shortest scaled distance between the $(L^{\rm r}_{i(k)}, L^{\rm t}_{i(k)})$ and the straight line from (18) (after some algebra):

$$d^2_{i(k)} = \frac{\left(L^{\rm t}_{i(k)} - L^{\rm r}_{i(k)} b^{\rm r}_{(k)} - a^{\rm r}_{(k)}\right)^2}{{\sigma^{\rm t}_{i(k)}}^2 + {b^{\rm r}_{(k)}}^2 {\sigma^{\rm r}_{i(k)}}^2}.$$

Notice that in the case when ${\sigma^{\rm r}_{i(k)}}^2 = 0$ the problem reduces to the case discussed in Sect. 1. The cost function is the sum of contributions from all measurement pairs:

$$J_{(k)}(a^{\rm r}_{(k)}, b^{\rm r}_{(k)}) = \frac{1}{2}\sum_i d^2_{i(k)} = \frac{1}{2}\sum_i \frac{\left(L^{\rm t}_{i(k)} - L^{\rm r}_{i(k)} b^{\rm r}_{(k)} - a^{\rm r}_{(k)}\right)^2}{{\sigma^{\rm t}_{i(k)}}^2 + {b^{\rm r}_{(k)}}^2 {\sigma^{\rm r}_{i(k)}}^2}. \tag{20}$$

The aim is to find the $a^{\rm r}_{(k)}$ and $b^{\rm r}_{(k)}$ that minimise this cost function. This cost function is non-linear in $b^{\rm r}_{(k)}$, making it more difficult to solve than (6), but below is my suggested method.

3.2 Solving the least-squares problem when errors are present for both instruments

This suggested solution is iterative (not sure if it will converge).

1. Solve the problem in Sect. 1 when errors are present for $\mathbf{l}^{\rm t}_{(k)}$ only. This gives a first guess ($p = 0$) for the value of $\mathbf{x}^{p=0}_{(k)}$, defined in a similar way to (3), i.e.

$$\mathbf{x}^p_{(k)} = \begin{pmatrix} a^{{\rm r},p}_{(k)} \\ b^{{\rm r},p}_{(k)} \end{pmatrix}. \tag{21}$$

2. Set $p = 1$. This is the iteration number.

3. Solve a similar problem for iteration p as follows. Define the following cost function (c.f. (6)):

$$J^p_{(k)}[\mathbf{x}^p_{(k)}] = \frac{1}{2}\left(\mathbf{l}^{\rm t}_{(k)} - \mathbf{H}_{(k)}\mathbf{x}^p_{(k)}\right)^{\rm T} {\mathbf{R}^p_{(k)}}^{-1} \left(\mathbf{l}^{\rm t}_{(k)} - \mathbf{H}_{(k)}\mathbf{x}^p_{(k)}\right), \tag{22}$$

where $\mathbf{H}_{(k)}$ is defined in (5), and $\mathbf{R}^p_{(k)}$ is the diagonal matrix with elements ${\mathbf{R}^p_{(k)}}_{ii} = {\sigma^{\rm t}_{i(k)}}^2 + {b^{{\rm r},p-1}_{(k)}}^2 {\sigma^{\rm r}_{i(k)}}^2$ (the denominator in (20)). The solution at the pth iteration is similar to (8), i.e.

$$\mathbf{x}^p_{(k)} = \left(\mathbf{H}^{\rm T}_{(k)} {\mathbf{R}^p_{(k)}}^{-1} \mathbf{H}_{(k)}\right)^{-1} \mathbf{H}^{\rm T}_{(k)} {\mathbf{R}^p_{(k)}}^{-1} \mathbf{l}^{\rm t}_{(k)}. \tag{23}$$

The solution is similar to (12), but where s^1, $s^{\rm r}$, $s^{\rm rr}$, $s^{\rm t}$, and $s^{\rm rt}$ are (11), but where ${\sigma^{\rm t}_{i(k)}}^2 \rightarrow {\sigma^{\rm t}_{i(k)}}^2 + {b^{{\rm r},p-1}_{(k)}}^2 {\sigma^{\rm r}_{i(k)}}^2$.

4. If converged, stop. Otherwise, increment p and go to step 3.

3.3 Uncertainty of the solution when errors are present for both instruments

An approximation of the uncertainties in $\mathbf{x}^p_{(k)}$ can be found by assuming that errors are approximately Gaussian. In this case the variances of and covariance between errors in the best fit $a^{\rm r}_{(k)}$ and $b^{\rm r}_{(k)}$ are given as (14), (15), and (16), but with the modified versions of s^1, $s^{\rm r}$, $s^{\rm rr}$, $s^{\rm t}$, and $s^{\rm rt}$ as detailed in step 3 in the solution procedure. It is also possible to refine the Hessian calculation in (13) to allow for the $b^{{\rm r},p}_{(k)}$ in the denominator in this case.

4 Considering observation error covariances between channels

If there are error covariances between different channels then we need to solve the problem for all channels at once. Let us build on the case in Sect. 3 now when errors between channels are correlated. The channel index (k) will now be useful. We will consider K channels, and m measurements of each channel.

4.1 Starting to pose the least-squares problem for correlated observation errors and when errors are present for both instruments

The solution will be along the same lines as the algorithm in Sect. 3. Let us call the set of observations of different channels, but made at the same instant/scene/instrument an *observation packet* (for want of a better term) [in this sense each observation packet comprises a spectrum; let there be m observation packets]. Let i be the observation packet index ($1 \le i \le m$). Define the following objects:

- An observation packet for the reference instrument is $\mathbf{l}^{\mathrm{r}}$. This is a K-element vector. For a particular observation packet, i, this is denoted $\mathbf{l}_i^{\mathrm{r}}$.
- The associated observation packet for the target instrument is $\mathbf{l}^{\mathrm{t}}$. This is a K-element vector. For a particular observation packet this is denoted $\mathbf{l}_i^{\mathrm{t}}$.
- The $a_{(k)}^{\mathrm{r}}$-values (as in (1)) assembled into a vector is $\mathbf{a}$. This is a K-element vector.
- The $b_{(k)}^{\mathrm{r}}$-values (as in (1)) assembled into a vector is $\mathbf{b}$. This is a K-element vector. The diagonal matrix whose diagonal elements are those of $\mathbf{b}$ is $\mathbf{B} = \mathrm{diag}(\mathbf{b})$. This is a $K \times K$ matrix (used below).
- The regression model relating $\mathbf{l}^{\mathrm{r}}$ and $\mathbf{l}^{\mathrm{t}}$ is

$$\mathbf{l}^{\mathrm{t}} = \mathbf{a} + \mathbf{B}\mathbf{l}^{\mathrm{r}}. \tag{24}$$

  This represents the same regression model used before (1), but expressed for all channels in one expression. Eq. (24) itself does not mix-up regression coefficients between channels. This model may be thought of as existing in a $2K$-dimensional *parameter space* (K dimensions each for $\mathbf{a}$ and $\mathbf{b}$; compare this to the case in Sect. 1 where there were just two unknowns as we were considering each channel separately). N.B. The above formulation is different to that used before in (4), e.g. we do not here use a $\mathbf{H}$-matrix.
- The observation error covariance matrix for the reference instrument is $\mathbf{R}^{\mathrm{r}}$. This is a $K \times K$ matrix.
- The observation error covariance matrix for the target instrument is $\mathbf{R}^{\mathrm{t}}$. This is a $K \times K$ matrix.

Let the distance (in $2K$-dimensional *observation space*) of observation packet i ($\mathbf{l}_i^{\mathrm{r}}, \mathbf{l}_i^{\mathrm{t}}$) from an arbitrary point defined by ($\mathbf{l}^{\mathrm{r}}, \mathbf{l}^{\mathrm{t}}$) and weighted by the error covariances be d_i:

$$d_i^2 = \left(\mathbf{l}^{\mathrm{r}} - \mathbf{l}_i^{\mathrm{r}}\right)^{\mathrm{T}} \mathbf{R}^{\mathrm{r}\,-1} \left(\mathbf{l}^{\mathrm{r}} - \mathbf{l}_i^{\mathrm{r}}\right) + \left(\mathbf{l}^{\mathrm{t}} - \mathbf{l}_i^{\mathrm{t}}\right)^{\mathrm{T}} \mathbf{R}^{\mathrm{t}\,-1} \left(\mathbf{l}^{\mathrm{t}} - \mathbf{l}_i^{\mathrm{t}}\right),$$

(we have assumed that errors between those of $\mathbf{l}_i^{\mathrm{r}}$ and $\mathbf{l}_i^{\mathrm{t}}$ are correlated). Imposing the constraint (24) leaves us with

$$d_i^2 = \left(\mathbf{l}^{\mathrm{r}} - \mathbf{l}_i^{\mathrm{r}}\right)^{\mathrm{T}} \mathbf{R}^{\mathrm{r}\,-1} \left(\mathbf{l}^{\mathrm{r}} - \mathbf{l}_i^{\mathrm{r}}\right) + \left(\mathbf{a} + \mathbf{B}\mathbf{l}^{\mathrm{r}} - \mathbf{l}_i^{\mathrm{t}}\right)^{\mathrm{T}} \mathbf{R}^{\mathrm{t}\,-1} \left(\mathbf{a} + \mathbf{B}\mathbf{l}^{\mathrm{r}} - \mathbf{l}_i^{\mathrm{t}}\right). \tag{25}$$

(c.f. (18)). The value of the vector $\mathbf{l}^{\mathrm{r}}$ that minimises this distance is found by making (25) stationary:

$$\nabla_{\mathbf{l}^{\mathrm{r}}} d_i^2 = \mathbf{R}^{\mathrm{r}\,-1} \left(\mathbf{l}^{\mathrm{r}} - \mathbf{l}_i^{\mathrm{r}}\right) + \mathbf{B}\mathbf{R}^{\mathrm{t}\,-1} \left(\mathbf{a} + \mathbf{B}\mathbf{l}^{\mathrm{r}} - \mathbf{l}_i^{\mathrm{t}}\right) = 0,$$

which happens when

$$\mathbf{l}^{\mathrm{r}} = \left(\mathbf{R}^{\mathrm{r}\,-1} + \mathbf{B}\mathbf{R}^{\mathrm{t}\,-1}\mathbf{B}\right)^{-1} \left[\mathbf{R}^{\mathrm{r}\,-1}\mathbf{l}_i^{\mathrm{r}} - \mathbf{B}\mathbf{R}^{\mathrm{t}\,-1} \left(\mathbf{a} - \mathbf{l}_i^{\mathrm{t}}\right)\right], \tag{26}$$

(c.f. (19)). This is the value of $\mathbf{l}^{\mathrm{r}}$ that, when used with (24) to give the associated $\mathbf{l}^{\mathrm{t}}$ (for a *given* $\mathbf{a}$ and $\mathbf{b}$), gives a point in observation space $(\mathbf{l}^{\mathrm{r}}, \mathbf{l}^{\mathrm{t}})$ that is closest to the ith pair of observation packets $(\mathbf{l}^{\mathrm{r}}_i, \mathbf{l}^{\mathrm{t}}_i)$ (by allowing for the expected degree of uncertainty in the measurements). Now turn this problem around. Substitute (26) into (25), sum up the contributions for each pair of observation packets, and then determine the $\mathbf{a}$ and $\mathbf{b}$ that minimises the resulting cost function. First substitute (26) into (25) (this gets a bit messy, so we will do this in parts; it is possible to skip to (29) for the resulting expression for d_i^2 to avoid the details). The difference that appears in the first term of (25):

$$\begin{aligned}
\mathbf{l}^{\mathrm{r}} - \mathbf{l}^{\mathrm{r}}_i &= \left(\mathbf{R}^{\mathrm{r}-1} + \mathbf{B}\mathbf{R}^{\mathrm{t}-1}\mathbf{B}\right)^{-1} \left[\mathbf{R}^{\mathrm{r}-1}\mathbf{l}^{\mathrm{r}}_i - \mathbf{B}\mathbf{R}^{\mathrm{t}-1}\left(\mathbf{a} - \mathbf{l}^{\mathrm{t}}_i\right)\right] - \mathbf{l}^{\mathrm{r}}_i \\
&= \left(\mathbf{R}^{\mathrm{r}-1} + \mathbf{B}\mathbf{R}^{\mathrm{t}-1}\mathbf{B}\right)^{-1} \left[\cancel{\mathbf{R}^{\mathrm{r}-1}\mathbf{l}^{\mathrm{r}}_i} - \mathbf{B}\mathbf{R}^{\mathrm{t}-1}\left(\mathbf{a} - \mathbf{l}^{\mathrm{t}}_i\right) - \left(\cancel{\mathbf{R}^{\mathrm{r}-1}} + \mathbf{B}\mathbf{R}^{\mathrm{t}-1}\mathbf{B}\right)\mathbf{l}^{\mathrm{r}}_i\right] \\
&= \left(\mathbf{R}^{\mathrm{r}-1} + \mathbf{B}\mathbf{R}^{\mathrm{t}-1}\mathbf{B}\right)^{-1} \left[\mathbf{B}\mathbf{R}^{\mathrm{t}-1}\left(\mathbf{l}^{\mathrm{t}}_i - \mathbf{a}\right) - \mathbf{B}\mathbf{R}^{\mathrm{t}-1}\mathbf{B}\mathbf{l}^{\mathrm{r}}_i\right] \\
&= \left(\mathbf{R}^{\mathrm{r}-1} + \mathbf{B}\mathbf{R}^{\mathrm{t}-1}\mathbf{B}\right)^{-1} \mathbf{B}\mathbf{R}^{\mathrm{t}-1}\left[\mathbf{l}^{\mathrm{t}}_i - \mathbf{a} - \mathbf{B}\mathbf{l}^{\mathrm{r}}_i\right].
\end{aligned} \tag{27}$$

The difference that appears in the second term of (25):

$$\begin{aligned}
\mathbf{a} + \mathbf{B}\mathbf{l}^{\mathrm{r}} - \mathbf{l}^{\mathrm{t}}_i &= \mathbf{a} + \mathbf{B}\left(\mathbf{R}^{\mathrm{r}-1} + \mathbf{B}\mathbf{R}^{\mathrm{t}-1}\mathbf{B}\right)^{-1} \left[\mathbf{R}^{\mathrm{r}-1}\mathbf{l}^{\mathrm{r}}_i - \mathbf{B}\mathbf{R}^{\mathrm{t}-1}\left(\mathbf{a} - \mathbf{l}^{\mathrm{t}}_i\right)\right] - \mathbf{l}^{\mathrm{t}}_i \\
&= \mathbf{B}\left(\mathbf{R}^{\mathrm{r}-1} + \mathbf{B}\mathbf{R}^{\mathrm{t}-1}\mathbf{B}\right)^{-1} \Big[\left(\mathbf{R}^{\mathrm{r}-1} + \mathbf{B}\mathbf{R}^{\mathrm{t}-1}\mathbf{B}\right)\mathbf{B}^{-1}\mathbf{a} + \mathbf{R}^{\mathrm{r}-1}\mathbf{l}^{\mathrm{r}}_i - \mathbf{B}\mathbf{R}^{\mathrm{t}-1}\left(\mathbf{a} - \mathbf{l}^{\mathrm{t}}_i\right) \\
&\qquad - \left(\mathbf{R}^{\mathrm{r}-1} + \mathbf{B}\mathbf{R}^{\mathrm{t}-1}\mathbf{B}\right)\mathbf{B}^{-1}\mathbf{l}^{\mathrm{t}}_i\Big] \\
&= \mathbf{B}\left(\mathbf{R}^{\mathrm{r}-1} + \mathbf{B}\mathbf{R}^{\mathrm{t}-1}\mathbf{B}\right)^{-1} \Big[\mathbf{R}^{\mathrm{r}-1}\mathbf{B}^{-1}\mathbf{a} + \cancel{\mathbf{B}\mathbf{R}^{\mathrm{t}-1}\mathbf{a}} + \mathbf{R}^{\mathrm{r}-1}\mathbf{l}^{\mathrm{r}}_i - \cancel{\mathbf{B}\mathbf{R}^{\mathrm{t}-1}\mathbf{a}} + \cancel{\mathbf{B}\mathbf{R}^{\mathrm{t}-1}\mathbf{l}^{\mathrm{t}}_i} \\
&\qquad - \mathbf{R}^{\mathrm{r}-1}\mathbf{B}^{-1}\mathbf{l}^{\mathrm{t}}_i - \cancel{\mathbf{B}\mathbf{R}^{\mathrm{t}-1}\mathbf{l}^{\mathrm{t}}_i}\Big] \\
&= \mathbf{B}\left(\mathbf{R}^{\mathrm{r}-1} + \mathbf{B}\mathbf{R}^{\mathrm{t}-1}\mathbf{B}\right)^{-1} \left[\mathbf{R}^{\mathrm{r}-1}\mathbf{B}^{-1}\mathbf{a} + \mathbf{R}^{\mathrm{r}-1}\mathbf{l}^{\mathrm{r}}_i - \mathbf{R}^{\mathrm{r}-1}\mathbf{B}^{-1}\mathbf{l}^{\mathrm{t}}_i\right] \\
&= \mathbf{B}\left(\mathbf{R}^{\mathrm{r}-1} + \mathbf{B}\mathbf{R}^{\mathrm{t}-1}\mathbf{B}\right)^{-1} \mathbf{R}^{\mathrm{r}-1}\left[\mathbf{B}^{-1}\mathbf{a} + \mathbf{l}^{\mathrm{r}}_i - \mathbf{B}^{-1}\mathbf{l}^{\mathrm{t}}_i\right] \\
&= \mathbf{B}\left(\mathbf{R}^{\mathrm{r}-1} + \mathbf{B}\mathbf{R}^{\mathrm{t}-1}\mathbf{B}\right)^{-1} \mathbf{R}^{\mathrm{r}-1}\mathbf{B}^{-1}\left[\mathbf{a} + \mathbf{B}\mathbf{l}^{\mathrm{r}}_i - \mathbf{l}^{\mathrm{t}}_i\right] \\
&= -\mathbf{B}\left(\mathbf{R}^{\mathrm{r}-1} + \mathbf{B}\mathbf{R}^{\mathrm{t}-1}\mathbf{B}\right)^{-1} \mathbf{R}^{\mathrm{r}-1}\mathbf{B}^{-1}\left[\mathbf{l}^{\mathrm{t}}_i - \mathbf{a} - \mathbf{B}\mathbf{l}^{\mathrm{r}}_i\right].
\end{aligned} \tag{28}$$

Substituting (27) and (28) into (25) gives

$$\begin{aligned}
d_i^2 &= \left(\mathbf{l}^{\mathrm{r}} - \mathbf{l}^{\mathrm{r}}_i\right)^{\mathrm{T}} \mathbf{R}^{\mathrm{r}-1}\left(\mathbf{l}^{\mathrm{r}} - \mathbf{l}^{\mathrm{r}}_i\right) + \frac{1}{2}\left(\mathbf{a} + \mathbf{B}\mathbf{l}^{\mathrm{r}} - \mathbf{l}^{\mathrm{t}}_i\right)^{\mathrm{T}} \mathbf{R}^{\mathrm{t}-1}\left(\mathbf{a} + \mathbf{B}\mathbf{l}^{\mathrm{r}} - \mathbf{l}^{\mathrm{t}}_i\right) \\
&= \left[\mathbf{l}^{\mathrm{t}}_i - \mathbf{a} - \mathbf{B}\mathbf{l}^{\mathrm{r}}_i\right]^{\mathrm{T}} \mathbf{R}^{\mathrm{t}-1}\mathbf{B}\left(\mathbf{R}^{\mathrm{r}-1} + \mathbf{B}\mathbf{R}^{\mathrm{t}-1}\mathbf{B}\right)^{-1} \mathbf{R}^{\mathrm{r}-1} \times \\
&\qquad \left(\mathbf{R}^{\mathrm{r}-1} + \mathbf{B}\mathbf{R}^{\mathrm{t}-1}\mathbf{B}\right)^{-1} \mathbf{B}\mathbf{R}^{\mathrm{t}-1}\left[\mathbf{l}^{\mathrm{t}}_i - \mathbf{a} - \mathbf{B}\mathbf{l}^{\mathrm{r}}_i\right] + \\
&\quad \left[\mathbf{l}^{\mathrm{t}}_i - \mathbf{a} - \mathbf{B}\mathbf{l}^{\mathrm{r}}_i\right]^{\mathrm{T}} \mathbf{B}^{-1}\mathbf{R}^{\mathrm{r}-1}\left(\mathbf{R}^{\mathrm{r}-1} + \mathbf{B}\mathbf{R}^{\mathrm{t}-1}\mathbf{B}\right)^{-1} \mathbf{B}\mathbf{R}^{\mathrm{t}-1} \times \\
&\qquad \mathbf{B}\left(\mathbf{R}^{\mathrm{r}-1} + \mathbf{B}\mathbf{R}^{\mathrm{t}-1}\mathbf{B}\right)^{-1} \mathbf{R}^{\mathrm{r}-1}\mathbf{B}^{-1}\left[\mathbf{l}^{\mathrm{t}}_i - \mathbf{a} - \mathbf{B}\mathbf{l}^{\mathrm{r}}_i\right] \\
&= \left[\mathbf{l}^{\mathrm{t}}_i - \mathbf{a} - \mathbf{B}\mathbf{l}^{\mathrm{r}}_i\right]^{\mathrm{T}} \times \\
&\quad \Big\{\mathbf{R}^{\mathrm{t}-1}\mathbf{B}\left(\mathbf{R}^{\mathrm{r}-1} + \mathbf{B}\mathbf{R}^{\mathrm{t}-1}\mathbf{B}\right)^{-1} \mathbf{R}^{\mathrm{r}-1}\left(\mathbf{R}^{\mathrm{r}-1} + \mathbf{B}\mathbf{R}^{\mathrm{t}-1}\mathbf{B}\right)^{-1} \mathbf{B}\mathbf{R}^{\mathrm{t}-1} + \\
&\quad \mathbf{B}^{-1}\mathbf{R}^{\mathrm{r}-1}\left(\mathbf{R}^{\mathrm{r}-1} + \mathbf{B}\mathbf{R}^{\mathrm{t}-1}\mathbf{B}\right)^{-1} \mathbf{B}\mathbf{R}^{\mathrm{t}-1}\mathbf{B}\left(\mathbf{R}^{\mathrm{r}-1} + \mathbf{B}\mathbf{R}^{\mathrm{t}-1}\mathbf{B}\right)^{-1} \mathbf{R}^{\mathrm{r}-1}\mathbf{B}^{-1}\Big\} \\
&\quad \left[\mathbf{l}^{\mathrm{t}}_i - \mathbf{a} - \mathbf{B}\mathbf{l}^{\mathrm{r}}_i\right].
\end{aligned} \tag{29}$$

We now attempt to factorise the term in curly brackets.

4.2 Factorising the covariance matrix

Factorising the term in curly brackets in (29) (it is possible to skip the details here and go straight to the simplified form of the total cost function $J[\mathbf{a},\mathbf{b}] = \frac{1}{2}\sum_i d_i^2$ found as (33)):

$$\mathbf{R}^{\mathrm{t}-1}\mathbf{B}\left(\mathbf{R}^{\mathrm{r}-1}+\mathbf{B}\mathbf{R}^{\mathrm{t}-1}\mathbf{B}\right)^{-1}\mathbf{R}^{\mathrm{r}-1}\left(\mathbf{R}^{\mathrm{r}-1}+\mathbf{B}\mathbf{R}^{\mathrm{t}-1}\mathbf{B}\right)^{-1}\mathbf{B}\mathbf{R}^{\mathrm{t}-1}+$$
$$\mathbf{B}^{-1}\mathbf{R}^{\mathrm{r}-1}\left(\mathbf{R}^{\mathrm{r}-1}+\mathbf{B}\mathbf{R}^{\mathrm{t}-1}\mathbf{B}\right)^{-1}\mathbf{B}\mathbf{R}^{\mathrm{t}-1}\mathbf{B}\left(\mathbf{R}^{\mathrm{r}-1}+\mathbf{B}\mathbf{R}^{\mathrm{t}-1}\mathbf{B}\right)^{-1}\mathbf{R}^{\mathrm{r}-1}\mathbf{B}^{-1} \tag{30}$$

Note first what can be done with the following pattern of operators:

$$\begin{aligned}
\mathbf{B}^{-1}\mathbf{R}^{\mathrm{r}-1}\left(\mathbf{R}^{\mathrm{r}-1}+\mathbf{B}\mathbf{R}^{\mathrm{t}-1}\mathbf{B}\right)^{-1}\mathbf{B}\mathbf{R}^{\mathrm{t}-1} &= \\
\left(\left[\mathbf{B}\mathbf{R}^{\mathrm{t}-1}\right]^{-1}\left[\mathbf{R}^{\mathrm{r}-1}+\mathbf{B}\mathbf{R}^{\mathrm{t}-1}\mathbf{B}\right]\left[\mathbf{B}^{-1}\mathbf{R}^{\mathrm{r}-1}\right]^{-1}\right)^{-1} &= \\
\left(\mathbf{R}^{\mathrm{t}}\mathbf{B}^{-1}\left[\mathbf{R}^{\mathrm{r}-1}+\mathbf{B}\mathbf{R}^{\mathrm{t}-1}\mathbf{B}\right]\mathbf{R}^{\mathrm{r}}\mathbf{B}\right)^{-1} &= \\
\left(\mathbf{R}^{\mathrm{t}}+\mathbf{B}\mathbf{R}^{\mathrm{r}}\mathbf{B}\right)^{-1}, &
\end{aligned} \tag{31}$$

which can also be written as:

$$\left(\mathbf{R}^{\mathrm{r}-1}+\mathbf{B}\mathbf{R}^{\mathrm{t}-1}\mathbf{B}\right)^{-1} = \mathbf{R}^{\mathrm{r}}\mathbf{B}\left(\mathbf{R}^{\mathrm{t}}+\mathbf{B}\mathbf{R}^{\mathrm{r}}\mathbf{B}\right)^{-1}\mathbf{R}^{\mathrm{t}}\mathbf{B}^{-1}. \tag{32}$$

Identify (31) in each line of the expression to be factorised (30) (the underlined parts of the following):

$$\mathbf{R}^{\mathrm{t}-1}\mathbf{B}\left(\mathbf{R}^{\mathrm{r}-1}+\mathbf{B}\mathbf{R}^{\mathrm{t}-1}\mathbf{B}\right)^{-1}\mathbf{B}\underleftrightarrow{\mathbf{B}^{-1}\mathbf{R}^{\mathrm{r}-1}\left(\mathbf{R}^{\mathrm{r}-1}+\mathbf{B}\mathbf{R}^{\mathrm{t}-1}\mathbf{B}\right)^{-1}\mathbf{B}\mathbf{R}^{\mathrm{t}-1}}+$$
$$\underleftrightarrow{\mathbf{B}^{-1}\mathbf{R}^{\mathrm{r}-1}\left(\mathbf{R}^{\mathrm{r}-1}+\mathbf{B}\mathbf{R}^{\mathrm{t}-1}\mathbf{B}\right)^{-1}\mathbf{B}\mathbf{R}^{\mathrm{t}-1}}\mathbf{B}\left(\mathbf{R}^{\mathrm{r}-1}+\mathbf{B}\mathbf{R}^{\mathrm{t}-1}\mathbf{B}\right)^{-1}\mathbf{R}^{\mathrm{r}-1}\mathbf{B}^{-1}$$

So (30) becomes:

$$\mathbf{R}^{\mathrm{t}-1}\mathbf{B}\left(\mathbf{R}^{\mathrm{r}-1}+\mathbf{B}\mathbf{R}^{\mathrm{t}-1}\mathbf{B}\right)^{-1}\mathbf{B}\left(\mathbf{R}^{\mathrm{t}}+\mathbf{B}\mathbf{R}^{\mathrm{r}}\mathbf{B}\right)^{-1}+$$
$$\left(\mathbf{R}^{\mathrm{t}}+\mathbf{B}\mathbf{R}^{\mathrm{r}}\mathbf{B}\right)^{-1}\mathbf{B}\left(\mathbf{R}^{\mathrm{r}-1}+\mathbf{B}\mathbf{R}^{\mathrm{t}-1}\mathbf{B}\right)^{-1}\mathbf{R}^{\mathrm{r}-1}\mathbf{B}^{-1}.$$

Each term in (30) is symmetric (even though this is not obvious in the rewritten form). Transposing the first line of the above therefore does not change the equation, but reverses the order of the matrices (note that they are all symmetric):

$$\left(\mathbf{R}^{\mathrm{t}}+\mathbf{B}\mathbf{R}^{\mathrm{r}}\mathbf{B}\right)^{-1}\mathbf{B}\left(\mathbf{R}^{\mathrm{r}-1}+\mathbf{B}\mathbf{R}^{\mathrm{t}-1}\mathbf{B}\right)^{-1}\mathbf{B}\mathbf{R}^{\mathrm{t}-1}+$$
$$\left(\mathbf{R}^{\mathrm{t}}+\mathbf{B}\mathbf{R}^{\mathrm{r}}\mathbf{B}\right)^{-1}\mathbf{B}\left(\mathbf{R}^{\mathrm{r}-1}+\mathbf{B}\mathbf{R}^{\mathrm{t}-1}\mathbf{B}\right)^{-1}\mathbf{R}^{\mathrm{r}-1}\mathbf{B}^{-1}$$

Now use (32):

$$\begin{aligned}
&\left(\mathbf{R}^{\mathrm{t}}+\mathbf{B}\mathbf{R}^{\mathrm{r}}\mathbf{B}\right)^{-1}\mathbf{B}\mathbf{R}^{\mathrm{r}}\mathbf{B}\left(\mathbf{R}^{\mathrm{t}}+\mathbf{B}\mathbf{R}^{\mathrm{r}}\mathbf{B}\right)^{-1}\mathbf{R}^{\mathrm{t}}\mathbf{B}^{-1}\mathbf{B}\mathbf{R}^{\mathrm{t}-1}+\\
&\left(\mathbf{R}^{\mathrm{t}}+\mathbf{B}\mathbf{R}^{\mathrm{r}}\mathbf{B}\right)^{-1}\mathbf{B}\mathbf{R}^{\mathrm{r}}\mathbf{B}\left(\mathbf{R}^{\mathrm{t}}+\mathbf{B}\mathbf{R}^{\mathrm{r}}\mathbf{B}\right)^{-1}\mathbf{R}^{\mathrm{t}}\mathbf{B}^{-1}\mathbf{R}^{\mathrm{r}-1}\mathbf{B}^{-1} =\\
&\left(\mathbf{R}^{\mathrm{t}}+\mathbf{B}\mathbf{R}^{\mathrm{r}}\mathbf{B}\right)^{-1}\mathbf{B}\mathbf{R}^{\mathrm{r}}\mathbf{B}\left(\mathbf{R}^{\mathrm{t}}+\mathbf{B}\mathbf{R}^{\mathrm{r}}\mathbf{B}\right)^{-1}+\\
&\left(\mathbf{R}^{\mathrm{t}}+\mathbf{B}\mathbf{R}^{\mathrm{r}}\mathbf{B}\right)^{-1}\mathbf{B}\mathbf{R}^{\mathrm{r}}\mathbf{B}\left(\mathbf{R}^{\mathrm{t}}+\mathbf{B}\mathbf{R}^{\mathrm{r}}\mathbf{B}\right)^{-1}\mathbf{R}^{\mathrm{t}}\mathbf{B}^{-1}\mathbf{R}^{\mathrm{r}-1}\mathbf{B}^{-1} =\\
&\left(\mathbf{R}^{\mathrm{t}}+\mathbf{B}\mathbf{R}^{\mathrm{r}}\mathbf{B}\right)^{-1}\mathbf{B}\mathbf{R}^{\mathrm{r}}\mathbf{B}\left(\mathbf{R}^{\mathrm{t}}+\mathbf{B}\mathbf{R}^{\mathrm{r}}\mathbf{B}\right)^{-1}\left[\mathbf{I}+\mathbf{R}^{\mathrm{t}}\mathbf{B}^{-1}\mathbf{R}^{\mathrm{r}-1}\mathbf{B}^{-1}\right].
\end{aligned}$$

Note:

$$\left[\mathbf{I}+\mathbf{R}^{\mathrm{t}}\mathbf{B}^{-1}\mathbf{R}^{\mathrm{r}-1}\mathbf{B}^{-1}\right] = \left[\mathbf{B}\mathbf{R}^{\mathrm{r}}\mathbf{B}+\mathbf{R}^{\mathrm{t}}\right]\mathbf{B}^{-1}\mathbf{R}^{\mathrm{r}-1}\mathbf{B}^{-1}.$$

Therefore we can finish the factorisation:

$$\left(\mathbf{R}^{\mathrm{t}}+\mathbf{B}\mathbf{R}^{\mathrm{r}}\mathbf{B}\right)^{-1}\mathbf{B}\mathbf{R}^{\mathrm{r}}\mathbf{B}\left(\mathbf{R}^{\mathrm{t}}+\mathbf{B}\mathbf{R}^{\mathrm{r}}\mathbf{B}\right)^{-1}\left[\mathbf{B}\mathbf{R}^{\mathrm{r}}\mathbf{B}+\mathbf{R}^{\mathrm{t}}\right]\mathbf{B}^{-1}\mathbf{R}^{\mathrm{r}\,-1}\mathbf{B}^{-1}= \left(\mathbf{R}^{\mathrm{t}}+\mathbf{B}\mathbf{R}^{\mathrm{r}}\mathbf{B}\right)^{-1}.$$

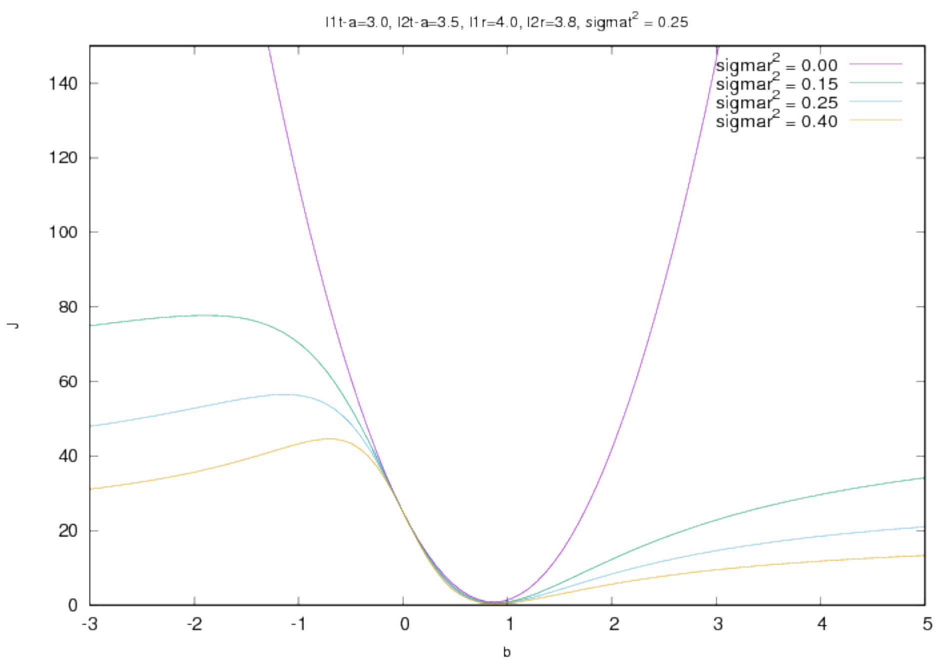
Thus, expression (30) may be replaced by the above. This is a worthwhile exercise to simplify the cost function!

4.3 Finishing posing the problem

The cost function found by sum of the squares of the observation packet distances from the set of straight lines (and dividing by 2 by convention):

$$J[\mathbf{a},\mathbf{b}]=\frac{1}{2}\sum_i d_i^2=\frac{1}{2}\sum_{i=1}^{m}\left[\mathbf{l}_i^{\mathrm{t}}-\mathbf{a}-\mathbf{B}\mathbf{l}_i^{\mathrm{r}}\right]^{\mathrm{T}}\left(\mathbf{R}^{\mathrm{t}}+\mathbf{B}\mathbf{R}^{\mathrm{r}}\mathbf{B}\right)^{-1}\left[\mathbf{l}_i^{\mathrm{t}}-\mathbf{a}-\mathbf{B}\mathbf{l}_i^{\mathrm{r}}\right], \tag{33}$$

where recall, $\mathbf{B}=\mathrm{diag}(\mathbf{b})$. As was found in the case when the errors between channels are uncorrelated (20), this problem is not quadratic due to the $\mathbf{B}$ defining the combined covariance matrix (just as for the uncorrelated case in Sect. 3). As an example, the Fig. plots $J[a,b]$ in the case of two pairs of observations of a single channel, for a fixed a for four possible values of $\sigma^{\mathrm{r}2}$ ($\mathbf{R}^{\mathrm{r}}{=}\sigma^{\mathrm{r}2}$) as shown in the key to the Fig. Changing $\sigma^{\mathrm{r}2}$ from zero results in a non-quadratic cost function with a less well-defined minimum, an aymmetric profile around the minimum, and a nearby maximum.



5 Allowing for non-coincidental scenes

Let us make the following assumptions and considerations.

1. Let us put aside for now serious inhomogeneities like the potentially varying presence of cloud in the target and reference scenes (e.g. by assuming clear skies in all scenes considered).
2. We have access to the following extra information concerning the scenes:
   (a) A radiative transfer model (RTM) that is capable of simulating the reference and target observation packets.
   (b) Reasonably accurate model profiles of geophysical variables that are needed by the RTM.

3. Assume that the reference and target instruments share the same RTM.

We will allow for deviations in the positions and viewing angles corresponding to the reference and target observation packets.

5.1 Proposal – a possible solution by adapting the approach already used

Take the following definitions:

- $\mathbf{x}^{\mathrm{r}}$ is the model's vertical profile for the scene of the reference instrument, with particular error $\delta\mathbf{x}^{\mathrm{r}}$. This is an n-element vector.
- θ^{r} is the viewing angle of the reference instrument's view. This is a scalar.
- $\mathbf{x}^{\mathrm{r}}_{\mathrm{true}}$ is the true version of $\mathbf{x}^{\mathrm{r}}$ ($\mathbf{x}^{\mathrm{r}}$ is the model version, which will be in error). This is an n-element vector.
- $\mathbf{l}^{\mathrm{r}}$ is an observation packet from the reference instrument, with particular error $\delta\mathbf{l}^{\mathrm{r}}$. This is a K-element vector.
- $\mathbf{l}^{\mathrm{r}}_{\mathrm{true}}$ is the noise-free observation packet that a perfect reference instrument would observe. This is a K-element vector.
- $\mathbf{x}^{\mathrm{t}}$ is the model's vertical profile seen by the target instrument, with particular error $\delta\mathbf{x}^{\mathrm{t}}$. This is an n-element vector.
- θ^{t} is the viewing angle of the target instrument's view. This is a scalar.
- $\mathbf{x}^{\mathrm{t}}_{\mathrm{true}}$ is the true version of $\mathbf{x}^{\mathrm{t}}$. This is an n-element vector.
- $\mathbf{l}^{\mathrm{t}}$ is an observation packet from the target instrument, with particular error $\delta\mathbf{l}^{\mathrm{t}}$. This is a K-element vector.
- $\mathbf{l}^{\mathrm{t}}_{\mathrm{true}}$ is the noise-free observation packet that a perfect target instrument would observe. This is a K-element vector.
- $\mathbf{h}(\mathbf{x}, \theta)$ is the RTM (assumed the same model for the target and reference instruments), with particular error $\boldsymbol{\epsilon}^{\mathbf{h}}$. This operator accepts an n-element vector, and a scalar as its input and has a K-element vector as its output.
- $\delta\mathbf{x}^{\mathrm{rt}}$ is the difference in modelled vertical profiles of reference and target instruments. This is an n-element vector.
- $\delta\theta^{\mathrm{rt}}$ is the difference in viewing angles of reference and target instruments. This is a scalar.

Some equations that we assume link these definitions:

$$
\begin{aligned}
\mathbf{x}^{\mathrm{r}} &= \mathbf{x}^{\mathrm{r}}_{\mathrm{true}} + \delta\mathbf{x}^{\mathrm{r}} \\
\mathbf{x}^{\mathrm{t}} &= \mathbf{x}^{\mathrm{t}}_{\mathrm{true}} + \delta\mathbf{x}^{\mathrm{t}} \\
\mathbf{h}(\mathbf{x}^{\mathrm{r}}_{\mathrm{true}}, \theta^{\mathrm{r}}) &= \mathbf{l}^{\mathrm{r}}_{\mathrm{true}} + \boldsymbol{\epsilon}^{\mathbf{h}}_1 \\
\mathbf{h}(\mathbf{x}^{\mathrm{t}}_{\mathrm{true}}, \theta^{\mathrm{t}}) &= \mathbf{l}^{\mathrm{t}}_{\mathrm{true}} + \boldsymbol{\epsilon}^{\mathbf{h}}_2 \\
\mathbf{l}^{\mathrm{r}} &= \mathbf{l}^{\mathrm{r}}_{\mathrm{true}} + \delta\mathbf{l}^{\mathrm{r}} \\
\mathbf{l}^{\mathrm{t}} &= \mathbf{l}^{\mathrm{t}}_{\mathrm{true}} + \delta\mathbf{l}^{\mathrm{t}} \\
\delta\mathbf{x}^{\mathrm{rt}} &= \mathbf{x}^{\mathrm{t}} - \mathbf{x}^{\mathrm{r}} \\
\delta\theta^{\mathrm{rt}} &= \theta^{\mathrm{t}} - \theta^{\mathrm{r}}.
\end{aligned}
$$

Let us assume that the overarching problem is now to regress the target instrument's observation to something that is as close as possible to $\mathbf{l}^{\mathrm{t}}_{\mathrm{true}}$. This, presumably, is the idea behind the current strategy

(Sect. 1), but where it is the reference instrument's data itself, $\mathbf{l}^{\mathrm{r}}$, that is a proxy for the 'truth'. Now develop an expression for $\mathbf{l}^{\mathrm{t}}_{\mathrm{true}}$ (using the above definitions and by linearising where necessary):

$$
\begin{aligned}
\mathbf{l}^{\mathrm{t}}_{\mathrm{true}} &= \mathbf{h}(\mathbf{x}^{\mathrm{t}}_{\mathrm{true}}, \theta^{\mathrm{t}}) - \boldsymbol{\epsilon}^{\mathbf{h}}_2 \\
&= \mathbf{h}(\mathbf{x}^{\mathrm{t}} - \delta\mathbf{x}^{\mathrm{t}}, \theta^{\mathrm{t}}) - \boldsymbol{\epsilon}^{\mathbf{h}}_2 \\
&\approx \mathbf{h}(\mathbf{x}^{\mathrm{t}}, \theta^{\mathrm{t}}) - \mathbf{H}_{\mathbf{x}^{\mathrm{t}},\theta^{\mathrm{t}}}\delta\mathbf{x}^{\mathrm{t}} - \boldsymbol{\epsilon}^{\mathbf{h}}_2 \\
&= \mathbf{h}(\mathbf{x}^{\mathrm{r}} + \delta\mathbf{x}^{\mathrm{rt}}, \theta^{\mathrm{r}} + \delta\theta^{\mathrm{rt}}) - \mathbf{H}_{\mathbf{x}^{\mathrm{t}},\theta^{\mathrm{t}}}\delta\mathbf{x}^{\mathrm{t}} - \boldsymbol{\epsilon}^{\mathbf{h}}_2 \\
&\approx \mathbf{h}(\mathbf{x}^{\mathrm{r}}, \theta^{\mathrm{r}}) + \mathbf{H}_{\mathbf{x}^{\mathrm{r}},\theta^{\mathrm{r}}}\delta\mathbf{x}^{\mathrm{rt}} + \mathbf{H}_{\theta^{\mathrm{r}},\mathbf{x}^{\mathrm{r}}}\delta\theta^{\mathrm{rt}} - \mathbf{H}_{\mathbf{x}^{\mathrm{t}},\theta^{\mathrm{t}}}\delta\mathbf{x}^{\mathrm{t}} - \boldsymbol{\epsilon}^{\mathbf{h}}_2 \\
&= \mathbf{h}(\mathbf{x}^{\mathrm{r}}_{\mathrm{true}} + \delta\mathbf{x}^{\mathrm{r}}, \theta^{\mathrm{r}}) + \mathbf{H}_{\mathbf{x}^{\mathrm{r}},\theta^{\mathrm{r}}}\delta\mathbf{x}^{\mathrm{rt}} + \mathbf{H}_{\theta^{\mathrm{r}},\mathbf{x}^{\mathrm{r}}}\delta\theta^{\mathrm{rt}} - \mathbf{H}_{\mathbf{x}^{\mathrm{t}},\theta^{\mathrm{t}}}\delta\mathbf{x}^{\mathrm{t}} - \boldsymbol{\epsilon}^{\mathbf{h}}_2 \\
&\approx \mathbf{h}(\mathbf{x}^{\mathrm{r}}_{\mathrm{true}}, \theta^{\mathrm{r}}) + \mathbf{H}_{\mathbf{x}^{\mathrm{r}},\theta^{\mathrm{r}}}\delta\mathbf{x}^{\mathrm{r}} + \mathbf{H}_{\mathbf{x}^{\mathrm{r}},\theta^{\mathrm{r}}}\delta\mathbf{x}^{\mathrm{rt}} + \mathbf{H}_{\theta^{\mathrm{r}},\mathbf{x}^{\mathrm{r}}}\delta\theta^{\mathrm{rt}} - \mathbf{H}_{\mathbf{x}^{\mathrm{t}},\theta^{\mathrm{t}}}\delta\mathbf{x}^{\mathrm{t}} - \boldsymbol{\epsilon}^{\mathbf{h}}_2 \\
&= \mathbf{l}^{\mathrm{r}}_{\mathrm{true}} + \boldsymbol{\epsilon}^{\mathbf{h}}_1 + \mathbf{H}_{\mathbf{x}^{\mathrm{r}},\theta^{\mathrm{r}}}\delta\mathbf{x}^{\mathrm{r}} + \mathbf{H}_{\mathbf{x}^{\mathrm{r}},\theta^{\mathrm{r}}}\delta\mathbf{x}^{\mathrm{rt}} + \mathbf{H}_{\theta^{\mathrm{r}},\mathbf{x}^{\mathrm{r}}}\delta\theta^{\mathrm{rt}} - \mathbf{H}_{\mathbf{x}^{\mathrm{t}},\theta^{\mathrm{t}}}\delta\mathbf{x}^{\mathrm{t}} - \boldsymbol{\epsilon}^{\mathbf{h}}_2 \\
&= \mathbf{l}^{\mathrm{r}} - \delta\mathbf{l}^{\mathrm{r}} + \boldsymbol{\epsilon}^{\mathbf{h}}_1 + \mathbf{H}_{\mathbf{x}^{\mathrm{r}},\theta^{\mathrm{r}}}\delta\mathbf{x}^{\mathrm{r}} + \mathbf{H}_{\mathbf{x}^{\mathrm{r}},\theta^{\mathrm{r}}}\delta\mathbf{x}^{\mathrm{rt}} + \mathbf{H}_{\theta^{\mathrm{r}},\mathbf{x}^{\mathrm{r}}}\delta\theta^{\mathrm{rt}} - \mathbf{H}_{\mathbf{x}^{\mathrm{t}},\theta^{\mathrm{t}}}\delta\mathbf{x}^{\mathrm{t}} - \boldsymbol{\epsilon}^{\mathbf{h}}_2, \qquad (34)
\end{aligned}
$$

where the Jacobians are

$$
\begin{aligned}
\mathbf{H}_{\mathbf{x}_0,\theta_0} &= \left.\frac{\partial \mathbf{h}}{\partial \mathbf{x}}\right|_{\mathbf{x}_0,\theta_0} && \text{a } K \times n \text{ matrix} \\
\mathbf{H}_{\theta_0,\mathbf{x}_0} &= \left.\frac{\partial \mathbf{h}}{\partial \theta}\right|_{\theta_0,\mathbf{x}_0}. && \text{a } K \times 1 \text{ matrix}
\end{aligned}
$$

Equation (34) shows how the reference measurement, $\mathbf{l}^{\mathrm{r}}$, is related to the object that we actually want to regress to, $\mathbf{l}^{\mathrm{r}}_{\mathrm{true}}$ (the current approach ignores all of the correction terms on the right hand side of (34)). The idea now is to understand which of the other terms we know or can estimate, which we only know the statistics of, and which we have little idea of.

$$
\mathbf{l}^{\mathrm{t}}_{\mathrm{true}} = \underbrace{\mathbf{l}^{\mathrm{r}} + \mathbf{H}_{\mathbf{x}^{\mathrm{r}},\theta^{\mathrm{r}}}\delta\mathbf{x}^{\mathrm{rt}} + \mathbf{H}_{\theta^{\mathrm{r}},\mathbf{x}^{\mathrm{r}}}\delta\theta^{\mathrm{rt}}}_{\text{known/calculable}} + \underbrace{-\delta\mathbf{l}^{\mathrm{r}} + \mathbf{H}_{\mathbf{x}^{\mathrm{r}},\theta^{\mathrm{r}}}\delta\mathbf{x}^{\mathrm{r}} - \mathbf{H}_{\mathbf{x}^{\mathrm{t}},\theta^{\mathrm{t}}}\delta\mathbf{x}^{\mathrm{t}}}_{\text{statistics known}} + \underbrace{\boldsymbol{\epsilon}^{\mathbf{h}}_1 - \boldsymbol{\epsilon}^{\mathbf{h}}_2}_{\text{known unknowns}}. \qquad (35)
$$

- The "known/calculable" terms comprise the reference measurement, the linear correction due to the non-coincident scenes, and the linear correction due to the non-coincident viewing angles.
- The "statistics known" terms comprise the reference measurement error, the state error in the reference scene, and the state error in the target scene.
- The "known unknown" terms comprise the RTM errors at the reference and target scenes, which I assume have unknown statistics.

This method would work in practice by finding $\mathbf{a}, \mathbf{b}$ by minimising (33) using the following information:

- $\mathbf{l}^{\mathrm{r}}_i$ in (33) would be replaced by the effective reference measurement packet $\mathbf{l}^{\mathrm{r}}_i + \mathbf{H}_{\mathbf{x}^{\mathrm{r}},\theta^{\mathrm{r}}}\delta\mathbf{x}^{\mathrm{rt}}_i + \mathbf{H}_{\theta^{\mathrm{r}},\mathbf{x}^{\mathrm{r}}}\delta\theta^{\mathrm{rt}}_i$.
- $\mathbf{l}^{\mathrm{t}}_i$ in (33) is still $\mathbf{l}^{\mathrm{t}}_i$.
- $\mathbf{R}^{\mathrm{r}}$ in (33) would be replaced by the effective reference error covariance (the covariance of the "statistics known" terms):

$$
\begin{aligned}
&\left\langle \delta\mathbf{l}^{\mathrm{r}}\delta\mathbf{l}^{\mathrm{r}\,\mathrm{T}} \right\rangle + \left\langle (\mathbf{H}_{\mathbf{x}^{\mathrm{r}},\theta^{\mathrm{r}}}\delta\mathbf{x}^{\mathrm{r}})(\mathbf{H}_{\mathbf{x}^{\mathrm{r}},\theta^{\mathrm{r}}}\delta\mathbf{x}^{\mathrm{r}})^{\mathrm{T}} \right\rangle + \left\langle (\mathbf{H}_{\mathbf{x}^{\mathrm{t}},\theta^{\mathrm{t}}}\delta\mathbf{x}^{\mathrm{t}})(\mathbf{H}_{\mathbf{x}^{\mathrm{t}},\theta^{\mathrm{t}}}\delta\mathbf{x}^{\mathrm{t}})^{\mathrm{T}} \right\rangle \\
&\quad + \left\langle (\mathbf{H}_{\mathbf{x}^{\mathrm{r}},\theta^{\mathrm{r}}}\delta\mathbf{x}^{\mathrm{r}})(\mathbf{H}_{\mathbf{x}^{\mathrm{t}},\theta^{\mathrm{t}}}\delta\mathbf{x}^{\mathrm{t}})^{\mathrm{T}} \right\rangle + \left\langle (\mathbf{H}_{\mathbf{x}^{\mathrm{t}},\theta^{\mathrm{t}}}\delta\mathbf{x}^{\mathrm{t}})(\mathbf{H}_{\mathbf{x}^{\mathrm{r}},\theta^{\mathrm{r}}}\delta\mathbf{x}^{\mathrm{r}})^{\mathrm{T}} \right\rangle,
\end{aligned}
$$

  noting that $\left\langle \delta\mathbf{l}^{\mathrm{r}}\delta\mathbf{l}^{\mathrm{r}\,\mathrm{T}} \right\rangle$ is the original $\mathbf{R}^{\mathrm{r}}$. We have assumed that:

  - $\delta\mathbf{l}^{\mathrm{r}}$ is uncorrelated with $\delta\mathbf{x}^{\mathrm{r}}$ and $\delta\mathbf{x}^{\mathrm{t}}$,
  - correlations between $\delta\mathbf{x}^{\mathrm{r}}$ and $\delta\mathbf{x}^{\mathrm{t}}$cannot be neglected,
  - model errors $\boldsymbol{\epsilon}^{\mathbf{h}}_1$ and $\boldsymbol{\epsilon}^{\mathbf{h}}_2$ are negligible.

- $\mathbf{R}^{\mathrm{t}}$ in (33) is still $\mathbf{R}^{\mathrm{t}}$.

Terms like $\left\langle\left(\mathbf{H}_{\mathbf{x}^{\mathrm{r}},\theta^{\mathrm{r}}}\delta\mathbf{x}^{\mathrm{r}}\right)\left(\mathbf{H}_{\mathbf{x}^{\mathrm{r}},\theta^{\mathrm{r}}}\delta\mathbf{x}^{\mathrm{r}}\right)^{\mathrm{T}}\right\rangle$ can be written in the form $\mathbf{H}_{\mathbf{x}^{\mathrm{r}},\theta^{\mathrm{r}}}\left\langle\delta\mathbf{x}^{\mathrm{r}}\delta\mathbf{x}^{\mathrm{r}\mathrm{T}}\right\rangle\mathbf{H}^{\mathrm{T}}_{\mathbf{x}^{\mathrm{r}},\theta^{\mathrm{r}}}$ only if the result is insensitive to the linearisation state of the linear operators. The linear operators (in this example $\mathbf{H}_{\mathbf{x}^{\mathrm{r}},\theta^{\mathrm{r}}}$) depend upon a linearisation state (in this example $\mathbf{x}^{\mathrm{r}},\theta^{\mathrm{r}}$). The difficulty now is to estimate terms like $\left\langle\left(\mathbf{H}_{\mathbf{x}^{\mathrm{r}},\theta^{\mathrm{r}}}\delta\mathbf{x}^{\mathrm{r}}\right)\left(\mathbf{H}_{\mathbf{x}^{\mathrm{r}},\theta^{\mathrm{r}}}\delta\mathbf{x}^{\mathrm{r}}\right)^{\mathrm{T}}\right\rangle$. This may be achieved by having a large number of vertical model profiles of proxy errors representative of the conditions present at the reference and target scenes (e.g. the right season, latitude, cloud conditions, low/high surface pressure, land/sea, etc). It will be simpler (and may even be adequate) to take an average of the covariances. There are well-used methods to compute proxy errors (the particular one will depend upon the data available to the user).

5.2 Summary

Equation (33) with the above adaptations becomes:

$$J[\mathbf{a},\mathbf{b}] = \frac{1}{2}\sum_{i=1}^{m}\left[\mathbf{l}_i^{\mathrm{t}} - \mathbf{a} - \mathbf{B}\left\{\mathbf{l}^{\mathrm{r}} + \mathbf{H}_{\mathbf{x}^{\mathrm{r}},\theta^{\mathrm{r}}}\delta\mathbf{x}^{\mathrm{rt}} + \mathbf{H}_{\theta^{\mathrm{r}},\mathbf{x}^{\mathrm{r}}}\delta\theta^{\mathrm{rt}}\right\}\right]^{\mathrm{T}}\left(\mathbf{R}^{\mathrm{t}} + \mathbf{B}\mathbf{R}^{\mathrm{r}}\mathbf{B}\right)^{-1}[\bullet]\,. \tag{36}$$

6 Options for solving the total least squares problem

Minimizing a "total least squares problem" (36) (or in a more generic form (33)) is generally regarded as considerably more difficult than an "ordinary least squares problem" (where the errors are on the dependent variable only). There are a number of options:

1. Minimize the problem by assuming that the problem may be thought of as a sequence of ordinary least squares problems – see eg. Sect. 3.2. Code for this has already been made.
2. Solve the problem with a 'numerical analysis' approach. This poses the problem in terms of a singular value decomposition – see Sect. 7.
3. Use the approach used by many physicists, e.g. [3, 4] – see Sect. (8).

7 Solving the total least squares problem using the numerical analysis approach

It is claimed [1] that the total least squares problem can be solved using the following procedure. We first use the following symbols (consider the scalar case first):

$$\boldsymbol{\beta} = \begin{pmatrix} b \\ a \end{pmatrix}, \qquad \mathbf{X} = \begin{pmatrix} x_1 & 1 \\ \vdots & \vdots \\ x_n & 1 \end{pmatrix}, \qquad \mathbf{y} = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}, \tag{37}$$

where the x_i are different measurements of the reference measurement (the analogy of $\mathbf{l}^{\mathrm{r}} + \mathbf{H}_{\mathbf{x}^{\mathrm{r}},\theta^{\mathrm{r}}}\delta\mathbf{x}^{\mathrm{rt}} + \mathbf{H}_{\theta^{\mathrm{r}},\mathbf{x}^{\mathrm{r}}}\delta\theta^{\mathrm{rt}}$ in (36) but in the scalar case), the $y_i$are different measurement of the target instrument (the analogy of $\mathbf{l}_i^{\mathrm{t}}$ but in the scalar case), and b and a are the regression coefficients (analogies of $\mathbf{b}$ and $\mathbf{a}$ respectively but in the scalar case). The multivariate case will be dealt with later if a satisfactory solution can be found using this approach[1].

[1] In fact I think that this approach is unsuitable for the problem in hand, so this section can be ignored if required. See Sect. 7.2 for the reasons.

7.1 The basis of the numerical analysis approach

The model relating these variables is

$$\mathbf{y} \approx \mathbf{X}\boldsymbol{\beta},$$

where the approximation accounts for the fact that $\mathbf{y}$ and $\mathbf{X}$ are in error. The errors are accounted for by allowing residuals in these quantities ($\Delta\mathbf{y}$ and $\Delta\mathbf{X}$ respectively) leading to

$$\mathbf{y} + \Delta\mathbf{y} = (\mathbf{X} + \Delta\mathbf{X})\,\boldsymbol{\beta}. \tag{38}$$

The idea now is to find the smallest $\Delta\mathbf{y}$ and $\Delta\mathbf{X}$ that satisfy the above[2].This will be done through a singular value decomposition. The matrix to be decomposed in this way is found from (38):

$$((\mathbf{X} + \Delta\mathbf{X}) \,\square\, (\mathbf{y} + \Delta\mathbf{y})) \begin{pmatrix} \boldsymbol{\beta} \\ -1 \end{pmatrix} = 0, \tag{39}$$

where the light square reminds us that the two matrices are not multiplied, but are block matrices (this is only used in situations that are ambiguous in this respect). The matrix $(\mathbf{X}\square\mathbf{y})$ – of dimension $n \times 3$ – has the following singular value decomposition

$$(\mathbf{X}\square\mathbf{y}) = \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^{\mathrm{T}}. \tag{40}$$

Assuming that the rank of $(\mathbf{X}\square\mathbf{y})$ is 3, $\mathbf{U}$ is the $n \times 3$ orthogonal matrix ($\mathbf{U}^{\mathrm{T}}\mathbf{U} = \mathbf{I}_3$) of left singular vectors, $\mathbf{V}$ is the 3×3 orthogonal matrix of right singular vectors ($\mathbf{V}^{\mathrm{T}}\mathbf{V} = \mathbf{I}_3$), and $\boldsymbol{\Sigma}$ is the ordered 3×3 diagonal matrix of singular values (ordered in the sense that the largest singular value is positioned in $\boldsymbol{\Sigma}_{11}$, and the smallest in $\boldsymbol{\Sigma}_{33}$). Let us look for the modification matrix $(\Delta\mathbf{X}\square\Delta\mathbf{y})$ such that $(\mathbf{X}\square\mathbf{y}) + (\Delta\mathbf{X}\square\Delta\mathbf{y})$ has the same singular vectors as $(\mathbf{X}\square\mathbf{y})$, and has the same singular values apart from the smallest one which is replaced by 0. To see this, consider $\mathbf{U}$, $\mathbf{V}$, and $\boldsymbol{\Sigma}$ partitioned in the following way:

$$\begin{aligned} \mathbf{U} &= (\mathbf{U_X}\square\mathbf{u_y}) \\ \boldsymbol{\Sigma} &= \begin{pmatrix} \boldsymbol{\Sigma}_\mathbf{X} & 0 \\ 0 & \Sigma_\mathbf{y} \end{pmatrix} \\ \mathbf{V} &= \begin{pmatrix} \mathbf{V_{XX}} & \mathbf{v_{XY}} \\ \mathbf{v}^{\mathrm{T}}_\mathbf{YX} & V_\mathbf{YY} \end{pmatrix}, \end{aligned} \tag{41}$$

where $\mathbf{U_X}$ is the $n \times 2$ submatrix, $\mathbf{u_y}$ is the n element vector comprising the last column of $\mathbf{U}$, $\boldsymbol{\Sigma}_\mathbf{X}$ is 2×2, $\Sigma_\mathbf{y}$ is scalar, $\mathbf{V_{XX}}$ is 2×2, $\mathbf{v_{XY}}$ is a 2-element column vector, $\mathbf{v}^{\mathrm{T}}_\mathbf{YX}$ is a 2-element row vector, and $V_\mathbf{YY}$ is a scalar. The singular value decomposition (40) in this form is

$$(\mathbf{X}\square\mathbf{y}) = (\mathbf{U_X}\square\mathbf{u_y}) \begin{pmatrix} \boldsymbol{\Sigma}_\mathbf{X} & 0 \\ 0 & \Sigma_\mathbf{y} \end{pmatrix} \begin{pmatrix} \mathbf{V}^{\mathrm{T}}_\mathbf{XX} & \mathbf{v_{YX}} \\ \mathbf{v}^{\mathrm{T}}_\mathbf{XY} & V_\mathbf{YY} \end{pmatrix}, \tag{42}$$

and the singular value decomposition of $(\mathbf{X}\square\mathbf{y}) + (\Delta\mathbf{X}\square\Delta\mathbf{y})$ is

$$(\mathbf{X} + \Delta\mathbf{X}\square\mathbf{y} + \Delta\mathbf{y}) = (\mathbf{U_X}\square\mathbf{u_y}) \begin{pmatrix} \boldsymbol{\Sigma}_\mathbf{X} & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \mathbf{V}^{\mathrm{T}}_\mathbf{XX} & \mathbf{v_{YX}} \\ \mathbf{v}^{\mathrm{T}}_\mathbf{XY} & V_\mathbf{YY} \end{pmatrix},$$

by design (as a result of the strategy mentioned above). This means that

$$(\Delta\mathbf{X}\square\Delta\mathbf{y}) = -\,(\mathbf{U_X}\square\mathbf{u_y}) \begin{pmatrix} 0 & 0 \\ 0 & \Sigma_\mathbf{y} \end{pmatrix} \begin{pmatrix} \mathbf{V}^{\mathrm{T}}_\mathbf{XX} & \mathbf{v_{YX}} \\ \mathbf{v}^{\mathrm{T}}_\mathbf{XY} & V_\mathbf{YY} \end{pmatrix}. \tag{43}$$

Note the following properties of the singular vectors:

$$\begin{aligned} \mathbf{U}^{\mathrm{T}}\mathbf{U} &= \mathbf{I}_3 \\ &= \begin{pmatrix} \mathbf{U}^{\mathrm{T}}_\mathbf{X} \\ \mathbf{u}^{\mathrm{T}}_\mathbf{y} \end{pmatrix} (\mathbf{U_X}\square\mathbf{u_y}) \\ &= \begin{pmatrix} \mathbf{U}^{\mathrm{T}}_\mathbf{X}\mathbf{U_X} & \mathbf{U}^{\mathrm{T}}_\mathbf{X}\mathbf{u_y} \\ \mathbf{u}^{\mathrm{T}}_\mathbf{y}\mathbf{U_X} & \mathbf{u}^{\mathrm{T}}_\mathbf{y}\mathbf{u_y} \end{pmatrix} \\ &= \begin{pmatrix} \mathbf{I}_2 & 0 \\ 0 & 1 \end{pmatrix}, \end{aligned} \tag{44}$$

[2] I cannot currently prove that this procedure is exactly the same as the one in (36), but the equivalence appears to be claimed in other sources, e.g. [2].

$$
\begin{aligned}
\mathbf{V}^{\mathrm{T}}\mathbf{V} &= \mathbf{I}_3 \\
&= \begin{pmatrix} \mathbf{V}_{\mathbf{XX}}^{\mathrm{T}} & \mathbf{v}_{\mathbf{YX}} \\ \mathbf{v}_{\mathbf{XY}}^{\mathrm{T}} & V_{\mathbf{YY}} \end{pmatrix} \begin{pmatrix} \mathbf{V}_{\mathbf{XX}} & \mathbf{v}_{\mathbf{XY}} \\ \mathbf{v}_{\mathbf{YX}}^{\mathrm{T}} & V_{\mathbf{YY}} \end{pmatrix} \\
&= \begin{pmatrix} \mathbf{V}_{\mathbf{XX}}^{\mathrm{T}}\mathbf{V}_{\mathbf{XX}} + \mathbf{v}_{\mathbf{YX}}\mathbf{v}_{\mathbf{YX}}^{\mathrm{T}} & \mathbf{V}_{\mathbf{XX}}^{\mathrm{T}}\mathbf{v}_{\mathbf{XY}} + \mathbf{v}_{\mathbf{YX}}V_{\mathbf{YY}} \\ \mathbf{v}_{\mathbf{XY}}^{\mathrm{T}}\mathbf{V}_{\mathbf{XX}} + V_{\mathbf{YY}}\mathbf{v}_{\mathbf{YX}}^{\mathrm{T}} & \mathbf{v}_{\mathbf{XY}}^{\mathrm{T}}\mathbf{v}_{\mathbf{XY}} + V_{\mathbf{YY}}^2 \end{pmatrix} \\
&= \begin{pmatrix} \mathbf{I}_2 & 0 \\ 0 & 1 \end{pmatrix}. \qquad (45)
\end{aligned}
$$

Expanding (43) gives

$$
\begin{aligned}
(\Delta\mathbf{X} \square \Delta\mathbf{y}) &= -\left(\mathbf{U}_{\mathbf{X}} \square \mathbf{u}_{\mathbf{y}}\right) \begin{pmatrix} 0 & 0 \\ \Sigma_{\mathbf{y}}\mathbf{v}_{\mathbf{XY}}^{\mathrm{T}} & \Sigma_{\mathbf{y}}V_{\mathbf{YY}} \end{pmatrix} \\
&= -\left(\mathbf{u}_{\mathbf{y}}\Sigma_{\mathbf{y}}\mathbf{v}_{\mathbf{XY}}^{\mathrm{T}} \square \mathbf{u}_{\mathbf{y}}\Sigma_{\mathbf{y}}V_{\mathbf{YY}}\right) \\
&= -\mathbf{u}_{\mathbf{y}}\Sigma_{\mathbf{y}}\left(\mathbf{v}_{\mathbf{XY}}^{\mathrm{T}} \square V_{\mathbf{YY}}\right). \qquad (46)
\end{aligned}
$$

This can be rewritten by first noting that (42) can be written – using orthogonality (45) – as

$$
\begin{aligned}
(\mathbf{X} \square \mathbf{y}) \begin{pmatrix} \mathbf{V}_{\mathbf{XX}} & \mathbf{v}_{\mathbf{XY}} \\ \mathbf{v}_{\mathbf{YX}}^{\mathrm{T}} & V_{\mathbf{YY}} \end{pmatrix} &= \left(\mathbf{U}_{\mathbf{X}} \square \mathbf{u}_{\mathbf{y}}\right) \begin{pmatrix} \mathbf{\Sigma}_{\mathbf{X}} & 0 \\ 0 & \Sigma_{\mathbf{y}} \end{pmatrix} \\
&= \left(\mathbf{U}_{\mathbf{X}}\mathbf{\Sigma}_{\mathbf{X}} \square \mathbf{u}_{\mathbf{y}}\Sigma_{\mathbf{y}}\right).
\end{aligned}
$$

The second column of the above is

$$
(\mathbf{X} \square \mathbf{y}) \begin{pmatrix} \mathbf{v}_{\mathbf{XY}} \\ V_{\mathbf{YY}} \end{pmatrix} = \mathbf{u}_{\mathbf{y}}\Sigma_{\mathbf{y}},
$$

which can be substituted into (46)

$$
(\Delta\mathbf{X} \square \Delta\mathbf{y}) = -(\mathbf{X} \square \mathbf{y}) \begin{pmatrix} \mathbf{v}_{\mathbf{XY}} \\ V_{\mathbf{YY}} \end{pmatrix} \left(\mathbf{v}_{\mathbf{XY}}^{\mathrm{T}} \square V_{\mathbf{YY}}\right).
$$

Now act from the right with the column vector as indicated in the following, and then use orthogonality (45)

$$
\begin{aligned}
(\Delta\mathbf{X} \square \Delta\mathbf{y}) \begin{pmatrix} \mathbf{v}_{\mathbf{XY}} \\ V_{\mathbf{YY}} \end{pmatrix} &= -(\mathbf{X} \square \mathbf{y}) \begin{pmatrix} \mathbf{v}_{\mathbf{XY}} \\ V_{\mathbf{YY}} \end{pmatrix} \left(\mathbf{v}_{\mathbf{XY}}^{\mathrm{T}} \square V_{\mathbf{YY}}\right) \begin{pmatrix} \mathbf{v}_{\mathbf{XY}} \\ V_{\mathbf{YY}} \end{pmatrix}. \\
&= -(\mathbf{X} \square \mathbf{y}) \begin{pmatrix} \mathbf{v}_{\mathbf{XY}} \\ V_{\mathbf{YY}} \end{pmatrix},
\end{aligned}
$$

so

$$
(\mathbf{X} + \Delta\mathbf{X} \square \mathbf{y} + \Delta\mathbf{y}) \begin{pmatrix} \mathbf{v}_{\mathbf{XY}} \\ V_{\mathbf{YY}} \end{pmatrix} = 0.
$$

Divide by $-V_{\mathbf{YY}}$ (assuming that it is non-zero)

$$
(\mathbf{X} + \Delta\mathbf{X} \square \mathbf{y} + \Delta\mathbf{y}) \begin{pmatrix} -\mathbf{v}_{\mathbf{XY}}/V_{\mathbf{YY}} \\ -1 \end{pmatrix} = 0.
$$

Comparing this with (39), we get

$$
\boldsymbol{\beta} = -\mathbf{v}_{\mathbf{YX}}/V_{\mathbf{YY}}. \qquad (47)
$$

7.2 Some thoughts on the numerical analysis approach

There are some difficulties that I have with this approach to solving the total least squares problem.

1. I cannot prove that the above solution is formally equivalent to minimizing functions like (33).
2. How are the error covariance matrices of the measurements incorporated in this approach? Does it effectively assume that the errors are iid (identical and independently distributed)?
3. How should the multivariate aspect of the problem be introduced?
4. The $\mathbf{X}$ matrix as defined in (37) has a constant second column (comprised of 1s), yet the method implies that there is a correction potentially to all components $\mathbf{X}$ (called $\Delta\mathbf{X}$), which includes changes to the second column. As it stands there appears to be no constraint to enforce the second column of $\Delta\mathbf{X}$ to be zero. In my mind this is a show-stopper for this method.

8 Solving the total least squares problem using the approach developed by physicists

We will follow the method described in [3]. This is based on a problem of finding one gradient and one intercept (a 2-dimensional problem). Our problem is multivariate, so we first transform the single problem of $2K$ dimensions problem to K 2-dimensional problems. We will refer to (33) in how to do this[3].

8.1 Reminder of the problem

Equation (33) is

$$J[\mathbf{a},\mathbf{b}] = \frac{1}{2}\sum_i d_i^2 = \frac{1}{2}\sum_{i=1}^{m}\left[\mathbf{l}_i^{\mathrm{t}} - \mathbf{a} - \mathbf{B}\mathbf{l}_i^{\mathrm{r}}\right]^{\mathrm{T}}\left(\mathbf{R}^{\mathrm{t}} + \mathbf{B}\mathbf{R}^{\mathrm{r}}\mathbf{B}\right)^{-1}\left[\mathbf{l}_i^{\mathrm{t}} - \mathbf{a} - \mathbf{B}\mathbf{l}_i^{\mathrm{r}}\right],$$

where $\mathbf{l}_i^{\mathrm{t}}$ is one source of information (K elements) with error covariance $\mathbf{R}^{\mathrm{t}}$, and $\mathbf{l}_i^{\mathrm{r}}$ is the other source (K elements) with error covariance $\mathbf{R}^{\mathrm{r}}$.

8.2 Reducing to a number of separate problems

Multiplying $\mathbf{l}_i^{\mathrm{t}}$ and $\mathbf{l}_i^{\mathrm{r}}$ by $\mathbf{R}^{\mathrm{t}\,-1/2}$ and $\mathbf{R}^{\mathrm{r}\,-1/2}$ respectively yields variables (indicated with a hat) whose errors are iid:

$$\begin{aligned}\hat{\mathbf{l}}_i^{\mathrm{t}} &= \mathbf{R}^{\mathrm{t}\,-1/2}\mathbf{l}_i^{\mathrm{t}},\\ \hat{\mathbf{l}}_i^{\mathrm{r}} &= \mathbf{R}^{\mathrm{r}\,-1/2}\mathbf{l}_i^{\mathrm{r}}.\end{aligned} \tag{48}$$

Each component of these vectors can then be treated independently. The error variances of each component is unity, so the weights $W(x_i)$ and $W(y_i)$ in [3] are all unity (where his x_i is our $\hat{\mathbf{l}}_i^{\mathrm{r}}$ and his y_i is our $\hat{\mathbf{l}}_i^{\mathrm{t}}$). Let us consider the kth component of $\hat{\mathbf{l}}_i^{\mathrm{t}}$ and $\hat{\mathbf{l}}_i^{\mathrm{r}}$ (denoted as $\hat{l}_i^{\mathrm{t}}$ and $\hat{l}_i^{\mathrm{r}}$ respectively, and dropping a k label for brevity). The problem that we solve is to find the best fit $\hat{a}$ and $\hat{b}$ such that $\hat{l}_i^{\mathrm{t}} \approx \hat{b}\hat{l}_i^{\mathrm{r}} + \hat{a}$, where $\hat{l}_i^{\mathrm{t}}$ and $\hat{l}_i^{\mathrm{r}}$ each have error variances of unity.

8.3 Developing the solution in [3]

8.3.1 Straight from paper in our notation and with unit weights

All summations are from $i = 1$ to $i = m$.

- Solve the following equation $f(\hat{b}) = \hat{b}^3 - 3\alpha\hat{b}^2 + 3\beta\hat{b} - \gamma = 0$.
- $\alpha = 2/(3\delta)\sum W_i^2 U_i V_i$.
- $\beta = 1/(3\delta)\left(\sum W_i^2 V_i^2 - \sum W_i U_i^2\right)$.
- $\gamma = -1/\delta\sum W_i U_i V_i$.
- $\delta = \sum W_i^2 U_i^2$.
- $W_i = 1/(\hat{b}^2 + 1)$.
- $U_i = \hat{l}_i^{\mathrm{r}} - \left\langle \hat{l}^{\mathrm{r}} \right\rangle$.
- $V_i = \hat{l}_i^{\mathrm{t}} - \left\langle \hat{l}^{\mathrm{t}} \right\rangle$.
- $\left\langle \hat{l}_i^{\mathrm{r}} \right\rangle = \sum W_i \hat{l}_i^{\mathrm{r}} / \sum W_i$.

[3] In the full problem (36) is actually the relevant cost function to minimize (since it accounts for the differences in positions of the two instruments in each measurement). The two cost functions have the same form, and are related by following the prescription in Sect. (5.1).

- $\left\langle \hat{l}_i^{\mathrm{t}} \right\rangle = \sum W_i \hat{l}_i^{\mathrm{t}} / \sum W_i$.
- Then from $\hat{b}$ we compute $\hat{a} = \left\langle \hat{l}_i^{\mathrm{t}} \right\rangle - \hat{b} \left\langle \hat{l}_i^{\mathrm{r}} \right\rangle$.

Notice that although $f(\hat{b})$ appears to be a cubic equation, there is a $\hat{b}$ dependence to W_i. We shall see though things simplify below, showing that the overall problem reduces to a quadratic problem.

8.3.2 Subsitute for W_i

- Solve the following equation $f(\hat{b}) = \hat{b}^3 - 3\alpha\hat{b}^2 + 3\beta\hat{b} - \gamma = 0$.
- $\alpha = 2/(3\delta) \sum U_i V_i / (\hat{b}^2 + 1)^2$.
- $\beta = 1/(3\delta) \left(\sum V_i^2 / (\hat{b}^2 + 1)^2 - \sum U_i^2 / (\hat{b}^2 + 1) \right)$.
- $\gamma = -1/\delta \sum U_i V_i / (\hat{b}^2 + 1)$.
- $\delta = \sum U_i^2 / (\hat{b}^2 + 1)^2$.

8.3.3 Substitute for δ

- Solve the following equation $f(\hat{b}) = \hat{b}^3 - 3\alpha\hat{b}^2 + 3\beta\hat{b} - \gamma = 0$.
- $\alpha = 2/3 \sum U_i V_i / \sum U_i^2$.
- $\beta = 1/3 \left(\sum V_i^2 / \sum U_i^2 - (\hat{b}^2 + 1) \sum U_i^2 / \sum U_i^2 \right) = 1/3 \left(\sum V_i^2 / \sum U_i^2 - (\hat{b}^2 + 1) \right)$.
- $\gamma = -(\hat{b}^2 + 1) \sum U_i V_i / \sum U_i^2$.

8.3.4 Substitute α, β, and γ into the cubic-like equation

$$\begin{aligned}
f(\hat{b}) &= \hat{b}^3 - 2\frac{\sum U_i V_i}{\sum U_i^2}\hat{b}^2 + \left(\frac{\sum V_i^2}{\sum U_i^2} - (\hat{b}^2 + 1) \right) \hat{b} + (\hat{b}^2 + 1) \frac{\sum U_i V_i}{\sum U_i^2} \\
&= \hat{b}^3 - 2\frac{\sum U_i V_i}{\sum U_i^2}\hat{b}^2 + \frac{\sum V_i^2}{\sum U_i^2}\hat{b} - (\hat{b}^2 + 1)\hat{b} + (\hat{b}^2 + 1) \frac{\sum U_i V_i}{\sum U_i^2} \\
&= \hat{b}^3 - 2\frac{\sum U_i V_i}{\sum U_i^2}\hat{b}^2 + \frac{\sum V_i^2}{\sum U_i^2}\hat{b} - \hat{b}^3 - \hat{b} + \hat{b}^2 \frac{\sum U_i V_i}{\sum U_i^2} + \frac{\sum U_i V_i}{\sum U_i^2} \\
&= -\frac{\sum U_i V_i}{\sum U_i^2}\hat{b}^2 + \left(\frac{\sum V_i^2}{\sum U_i^2} - 1 \right) \hat{b} + \frac{\sum U_i V_i}{\sum U_i^2} = 0 \\
g(\hat{b}) = \sum U_i^2 f(\hat{b}) &= -\sum U_i V_i \hat{b}^2 + \left(\sum V_i^2 - \sum U_i^2 \right) \hat{b} + \sum U_i V_i = 0.
\end{aligned}$$

The cubic term is zero by cancellation.

8.3.5 Find the roots

The roots of $g(\hat{b})$ are as follows:

$$\hat{b} = \frac{\left(\sum V_i^2 - \sum U_i^2 \right) \pm \sqrt{\left(\sum V_i^2 - \sum U_i^2 \right)^2 + 4 \left(\sum U_i V_i \right)^2}}{2 \sum U_i V_i}.$$

There are, perhaps surprisingly two roots (which are real). These are, presumably, both equivalent best fit solutions. This procedure is repeated for all components of $\hat{\mathbf{l}}_i^{\mathrm{t}}$ and $\hat{\mathbf{l}}_i^{\mathrm{r}}$ to yield components of vectors $\hat{\mathbf{a}}$ and $\hat{\mathbf{b}}$.

8.4 Transform to the original variables

We require a transform between $\mathbf{l}_i^{\mathrm{t}}$ and $\mathbf{l}_i^{\mathrm{r}}$ (rather than between $\hat{\mathbf{l}}_i^{\mathrm{t}}$ and $\hat{\mathbf{l}}_i^{\mathrm{r}}$). The transform between $\hat{\mathbf{l}}_i^{\mathrm{t}}$ and $\hat{\mathbf{l}}_i^{\mathrm{r}}$ is

$$\hat{\mathbf{l}}_i^{\mathrm{t}} = \hat{\mathbf{B}}\hat{\mathbf{l}}_i^{\mathrm{r}} + \hat{\mathbf{a}},$$

where $\hat{\mathbf{B}} = \mathrm{diag}(\hat{\mathbf{b}})$. Using (48) yields

$$\begin{aligned} \mathbf{R}^{\mathrm{t}\,-1/2}\mathbf{l}_i^{\mathrm{t}} &= \hat{\mathbf{B}}\mathbf{R}^{\mathrm{r}\,-1/2}\mathbf{l}_i^{\mathrm{r}} + \hat{\mathbf{a}} \\ \mathbf{l}_i^{\mathrm{t}} &= \mathbf{R}^{\mathrm{t}\,1/2}\hat{\mathbf{B}}\mathbf{R}^{\mathrm{r}\,-1/2}\mathbf{l}_i^{\mathrm{r}} + \mathbf{R}^{\mathrm{t}\,1/2}\hat{\mathbf{a}} \\ &= \mathbf{B}\mathbf{l}_i^{\mathrm{r}} + \mathbf{a} \qquad (49) \\ \text{where } \mathbf{B} &= \mathbf{R}^{\mathrm{t}\,1/2}\hat{\mathbf{B}}\mathbf{R}^{\mathrm{r}\,-1/2} \qquad (50) \\ \text{and } \mathbf{a} &= \mathbf{R}^{\mathrm{t}\,1/2}\hat{\mathbf{a}}. \qquad (51) \end{aligned}$$

Note that here the matrix that multiplies $\mathbf{l}_i^{\mathrm{r}}$ (the matrix $\mathbf{B}$) is no longer diagonal.

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