Quality quantifier of indirect measurements

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Abstract: A quality quantifier, referred to as *measurement quality quantifier* (MQQ), is proposed for indirect measurements. It satisfies the property that the MQQ of the data fusion of two or more independent measurements is the sum of the MQQs of the individual measurements and can also be determined in absolute terms for ill-posed problems. It is calculated from the covariance and Jacobian matrices of the observations, but the same result is also obtained using the covariance and averaging kernel matrices of the retrieved quantities. In the case of measurements of a continuous distribution a quantifier that provides the information distribution can be derived from the MQQ. The proposed quantifiers are herewith used for the quality assessment of atmospheric ozone measurements performed by IASI and MIPAS instruments.

OCIS codes: (100.3190) Inverse problems; (120.0280) Remote sensing and sensors; (110.3055) Information theoretical analysis; (010.1280) Atmospheric composition; (000.3860) Mathematical methods in physics.

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1. Introduction

The quantification of the quality of indirect measurements is an important tool needed for the comparison of different experiments and for the identification of the strategy that provides the best information about a target set of parameters. In particular, the quality quantification is the very issue in the design of atmospheric measurements [1] where a choice among different proposed experiments has to be done with the purpose of maximizing the information on some atmospheric parameters.

Many observation systems are presently operating on board space-borne and airborne platforms, as well as from ground-based stations, providing complementary and redundant measurements of a variety of atmospheric parameters. The use of potential synergies among these observing systems is a key element for the full exploitation of current and future missions within an overall strategy in which the combination of data obtained with different sensors (data fusion) can provide target products of the best quality in terms of precision and accuracy, as well as spatial and temporal coverage and resolution [2–4]. In order to optimize the design of single and coordinated atmospheric measurements it is essential to have a quality parameter able to characterize consistently both the single measurements and the result of data fusion of several measurements.

For the quality quantification we would like to have a parameter that has some useful properties. The first property is that it has to increase when the errors of the target parameters decrease. The second property is that the quality quantifier of the data fusion of two or more independent measurements is the sum of the quality quantifiers of the individual measurements (we refer to this property as *additivity property*). In this paper, starting from these two basic properties we identify a parameter, that we call *measurement quality quantifier* (MQQ), and evaluate its performances.

Currently the quality quantification of measurements of atmospheric vertical profiles is often made using the *Shannon information content* [1]. This quantifier is used in the framework of the optimal estimation and evaluates the information gain brought by the measurement with respect to the a priori information. Consequently the value of the Shannon information content is a relative quality quantifier depending on the covariance matrix (CM) of the a priori profile and it cannot be adapted to quantify the absolute information coming from the observations in case of ill-posed problems. Furthermore, as illustrated in [4], the Shannon information content does not satisfies the additivity property for data fusion. Another quality quantifier recently introduced [5] is the *information load*. It describes the information brought by the observations with respect to a set of target parameters and we will show that it is closely linked with the MQQ introduced in this paper.

The MQQ of indirect measurements depends on type and number of the target parameters that we are estimating, therefore, in the case of indirect measurements of a continuous distribution, such as the vertical profiles of atmospheric constituents, the MQQ depends on

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the grid on which the distribution is represented. However, in the case of comparison of performances of two instruments that measure the vertical profile of an atmospheric parameter, the two retrieval analyses have in general different vertical grids and the MQQs calculated for the two instruments cannot be directly compared. In order to overcome this difficulty we derive from the MQQ a quantifier that for fine enough grids is independent of the grid. We refer to this quantifier as *grid normalized MQQ*. Because of this property, the value of this quantifier coincides with that obtained for an infinitely small grid step. Consequently the grid normalized MQQ has the property of providing the measurement quality of the vertical profile when it is represented by a continuous function of altitude.

In Section 2 we identify the MQQ for direct measurements and in Section 3 we extend the definition of MQQ to indirect measurements. In Section 4 we define the relative MQQ that quantifies the measurement quality in relation to the value of the measured quantity. In Section 5 we show how to calculate the MQQ from the diagnostic of the solution of a constrained retrieval. In Section 6 we face the problem of the quality quantification of indirect measurements of a continuous distribution and introduce the grid normalized MQQ. In Section 7 we provide some examples of applications in which the MQQ is used to evaluate the performances of the instruments IASI (Infrared Atmospheric Sounding Interferometer) [6] and MIPAS (Michelson Interferometer for Passive Atmospheric Sounding)) [7]. Finally in Section 8 we draw the conclusions.

2. Quality quantifier for direct measurements

The quality quantifier of indirect measurements must be a generalization of that used for direct measurements. For this reason, we first perform the identification of the quality quantifier in the case of direct measurements.

2.1 Direct measurement of a scalar quantity

We consider the direct measurement affected by Gaussian noise of a scalar quantity x and look for a quantifier that properly describes the measurement quality. The standard deviation σ of the Gaussian probability distribution of the value of the measured quantity represents the error of the measurement and, therefore, as stated in the introduction, we look for a quality quantifier of the measurement that decreases when σ increases.

In order to identify the expression for the quality quantifier we consider the case of performing two independent measurements of the same quantity x. We indicate the results of the two measurements with y_1 and y_2 that are characterized by the errors σ_1 and σ_2. On the basis of the additivity property stated in the introduction we require that the quality quantifier of the fusion of the two measurements is the sum of the quality quantifiers of the two original measurements. It is well known that the best estimation of x from the two measurements is obtained determining the x value that minimizes the chi-square function:

$$\chi^2(x) = \frac{(y_1 - x)^2}{\sigma_1^2} + \frac{(y_2 - x)^2}{\sigma_2^2}. \qquad (1)$$

The minimization of $\chi^2(x)$ provides the best estimation $\hat{x}$ of x given by:

$$\hat{x} = \frac{\frac{y_1}{\sigma_1^2} + \frac{y_2}{\sigma_2^2}}{\frac{1}{\sigma_1^2} + \frac{1}{\sigma_2^2}}, \qquad (2)$$

which is affected by an error σ that is related to σ_1 and σ_2 by the equation:

$$\frac{1}{\sigma^2} = \frac{1}{\sigma_1^2} + \frac{1}{\sigma_2^2}. \qquad (3)$$

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Equation (3) shows that the fusion of two independent measurements of the same quantity determines the sum of the inverse square errors of the two measurements. This result suggests that a good quality quantifier of the direct measurement of a scalar quantity is the inverse of the square error that we call *measurement quality quantifier* (MQQ) and indicate with Q.

2.2 Direct measurement of a vector quantity

Now we consider n direct measurements of a vector quantity $\mathbf{x}$ of n components. The values x_i of the n components of $\mathbf{x}$ are individually determined by the measurements $\hat{x}_i$ that have errors σ_i uncorrelated with each other. This condition can be described saying that the CM $\mathbf{S}_x$ of $\hat{\mathbf{x}}$ is a diagonal matrix:

$$\mathbf{S}_x = \begin{pmatrix} \sigma_1^{\ 2} & 0 & ... & 0 \\ 0 & \sigma_2^{\ 2} & ... & 0 \\ ... & ... & ... & ... \\ 0 & 0 & ... & \sigma_n^{\ 2} \end{pmatrix}. \tag{4}$$

We notice that the inverse matrix of $\mathbf{S}_x$ contains in the diagonal the MQQs of the components of $\mathbf{x}$:

$$\mathbf{S}_x^{\ -1} = \begin{pmatrix} 1/\sigma_1^{\ 2} & 0 & ... & 0 \\ 0 & 1/\sigma_2^{\ 2} & ... & 0 \\ ... & ... & ... & ... \\ 0 & 0 & ... & 1/\sigma_n^{\ 2} \end{pmatrix} = \begin{pmatrix} Q_1 & 0 & ... & 0 \\ 0 & Q_2 & ... & 0 \\ ... & ... & ... & ... \\ 0 & 0 & ... & Q_n \end{pmatrix}. \tag{5}$$

We can consider the direct measurement of a vector as the fusion of n independent measurements of n different quantities and, on the basis of the additivity property, we define the MQQ associated with the measurement of $\mathbf{x}$ as the sum of the MQQs of its components:

$$Q = \sum_{i=1}^{n} Q_i = tr(\mathbf{S}_x^{\ -1}), \tag{6}$$

where $tr(\ldots)$ denotes the trace of the matrix.

An expression has been found for the MQQ in the case of the direct measurement of a vector.

Of course, for the sum in Eq. (6) to have a physical meaning it is necessary that the components of $\mathbf{x}$ are dimensionally homogeneous.

3. Quality quantifier for indirect measurements

3.1 Indirect measurement of a scalar quantity

In the case of an indirect measurement of the scalar quantity x we observe another quantity y related to x by a model given by a function $F(x)$:

$$y = F(x) \tag{7}$$

and determine an estimate $\hat{x}$ of x from the inversion of Eq. (7).

In order to distinguish the estimate $\hat{x}$ from the experimental quantity y we call the former *the measurement of x* and indicate the latter as *the observation y*.

The error σ of $\hat{x}$ is calculated by propagating the error ε on y by means of an expansion of Eq. (7) at the first order:

$$\sigma = \frac{\varepsilon}{k}, \tag{8}$$

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where k is the derivative of $F(x)$ with respect to x calculated in $\hat{x}$. From Eq. (8) we obtain the expression of the MQQ of the indirect measurement of x:

$$Q = \frac{1}{\sigma^2} = \frac{k^2}{\varepsilon^2}. \tag{9}$$

Equation (9) shows that in the case of indirect measurements an important role is played by the derivative of the function relating the observation with the inferred quantity. This derivative expresses the sensitivity of the observation to the inferred quantity and, therefore, the measurement quality increases with it.

Now we consider the case of performing two independent observations y_1 and y_2 (characterized by errors ε_1 and ε_2) of the same quantity x. The two observations are related to x by means of two functions:

$$y_1 = F_1(x) \tag{10}$$

$$y_2 = F_2(x). \tag{11}$$

Since now we have two equations and only one unknown we cannot directly solve the inversion problem as done for the case of Eq. (7), indeed, because of the experimental errors the two equations can be incompatible. Analogously to what we did in the case of direct measurements we look for the value that minimizes the chi-square function:

$$\chi^2(x) = \frac{\left(y_1 - F_1(x)\right)^2}{\varepsilon_1^{\,2}} + \frac{\left(y_2 - F_2(x)\right)^2}{\varepsilon_2^{\,2}}. \tag{12}$$

The value $\hat{x}$ of x that minimizes $\chi^2(x)$ is the one that makes equal to zero the derivative of $\chi^2(x)$ with respect to x and, therefore, satisfies the following equation:

$$\frac{k_1\left(y_1 - F_1(\hat{x})\right)}{\varepsilon_1^{\,2}} + \frac{k_2\left(y_2 - F_2(\hat{x})\right)}{\varepsilon_2^{\,2}} = 0, \tag{13}$$

where k_1 and k_2 are the derivatives of $F_1(x)$ and $F_2(x)$ at $\hat{x}$.

Equation (13) determines $\hat{x}$ as a function of the observations y_1 and y_2 and from a first order expansion of this function we can calculate the error propagation from y_1 and y_2 into $\hat{x}$ and determine its error σ:

$$\sigma^2 = g_1^{\,2}\varepsilon_1^{\,2} + g_2^{\,2}\varepsilon_2^{\,2}, \tag{14}$$

where $g_1 = \left(\frac{\partial \hat{x}}{\partial y_1}\right)$ and $g_2 = \left(\frac{\partial \hat{x}}{\partial y_2}\right)$. Performing the derivatives of Eq. (13) with respect to y_1 and y_2 (neglecting the dependence of k_1 and k_2 on $\hat{x}$, that is assuming the linear approximation for $F_1(x)$ and $F_2(x)$ around the minimum of $\chi^2(x)$) we obtain two equations from which g_1 and g_2 can be determined. Substituting these values of g_1 and g_2 in Eq. (14) we obtain the equation:

$$Q = \frac{1}{\sigma^2} = \frac{k_1^{\,2}}{\varepsilon_1^{\,2}} + \frac{k_2^{\,2}}{\varepsilon_2^{\,2}}. \tag{15}$$

Comparing Eq. (15) and Eq. (9) we see that also in the case of indirect measurements the MQQ of the fusion of two independent measurements of the same quantity is equal to the sum of the MQQs of the two original measurements.

A long procedure has been followed to derive Eq. (15), but this will be useful for the understanding of the less intuitive result that is obtained in Section 3.2.

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3.2 Indirect measurement of a vector quantity

Now we consider the most general case of m indirect measurements of a vector quantity $\mathbf{x}$ made of n components. We represent the m observations with a vector $\mathbf{y}$ characterized by the CM $\mathbf{S}_y$ and the relationship between $\mathbf{x}$ and $\mathbf{y}$ is expressed by a function $\mathbf{F}(\mathbf{x})$ from $\mathbf{R}^n$ to $\mathbf{R}^m$ (including all the vectors made of ordered n-tuples and m-tuples of real numbers, respectively):

$$\mathbf{y} = \mathbf{F}(\mathbf{x}). \tag{16}$$

The measurement of $\mathbf{x}$ is given by the value $\hat{\mathbf{x}}$ which minimizes the chi-square function:

$$\chi^2(\mathbf{x}) = (\mathbf{y} - \mathbf{F}(\mathbf{x}))^T \mathbf{S}_y^{-1} (\mathbf{y} - \mathbf{F}(\mathbf{x})). \tag{17}$$

Imposing that the derivatives of $\chi^2(\mathbf{x})$ with respect to the components of $\mathbf{x}$ are equal to zero we find that the value $\hat{\mathbf{x}}$ must satisfy the following equation:

$$\mathbf{K}^T \mathbf{S}_y^{-1} (\mathbf{y} - \mathbf{F}(\hat{\mathbf{x}})) = \mathbf{0}, \tag{18}$$

where $\mathbf{K}$ is the Jacobian matrix of $\mathbf{F}(\mathbf{x})$ (including the partial derivatives of $\mathbf{F}(\mathbf{x})$ with respect to the elements of $\mathbf{x}$) calculated in $\hat{\mathbf{x}}$.

Equation (18) is a vector equation that corresponds to a system of n equations in n unknown. If the n equations are independent, Eq. (18) determines $\hat{\mathbf{x}}$ as a function of the observations $\mathbf{y}$ and we can calculate the error $\boldsymbol{\sigma}$ on $\hat{\mathbf{x}}$ by propagating the errors $\boldsymbol{\varepsilon}$ on $\mathbf{y}$:

$$\boldsymbol{\sigma} = \mathbf{G}\boldsymbol{\varepsilon}, \tag{19}$$

where $\mathbf{G}$ is the *gain matrix* $\mathbf{G} = \frac{\partial \hat{\mathbf{x}}}{\partial \mathbf{y}}$ (the matrix whose *ij*-th element is $G_{ij} = \frac{\partial \hat{x}_i}{\partial y_j}$). The CM $\mathbf{S}_x$ of $\hat{\mathbf{x}}$ is then given by:

$$\mathbf{S}_x = \langle \boldsymbol{\sigma}\boldsymbol{\sigma}^T \rangle = \mathbf{G}\mathbf{S}_y\mathbf{G}^T, \tag{20}$$

where $\langle ... \rangle$ denotes the mean value.

Performing the derivatives of Eq. (18) with respect to the components of $\mathbf{y}$ (neglecting the dependence of $\mathbf{K}$ on $\hat{\mathbf{x}}$, that is assuming the linear approximation of $\mathbf{F}(\mathbf{x})$ around the minimum of $\chi^2(\mathbf{x})$), we obtain the expression of $\mathbf{G}$:

$$\mathbf{G} = \left(\mathbf{K}^T \mathbf{S}_y^{-1} \mathbf{K}\right)^{-1} \mathbf{K}^T \mathbf{S}_y^{-1}. \tag{21}$$

Substituting Eq. (21) in Eq. (20) we obtain the expression for $\mathbf{S}_x$:

$$\mathbf{S}_x = \left(\mathbf{K}^T \mathbf{S}_y^{-1} \mathbf{K}\right)^{-1}. \tag{22}$$

Now, differently from the case discussed in Section 2.2, the matrix $\mathbf{S}_x$ is not diagonal, that is the errors in the elements of $\hat{\mathbf{x}}$ are correlated with each other. However, since $\mathbf{S}_x$ is a positive-definite symmetric matrix, it is possible to make it diagonal by an orthogonal transformation that identifies linear combinations of the elements of $\hat{\mathbf{x}}$ that are independent of each other. This means that it is possible to find an orthogonal matrix $\mathbf{U}$ for which the matrix $\boldsymbol{\Lambda} = \mathbf{U}^T \mathbf{S}_x \mathbf{U}$ is a diagonal matrix with positive diagonal elements $\lambda_1^2, \lambda_2^2, \ldots \lambda_n^2$ that are the eigenvalues of $\mathbf{S}_x$. $\boldsymbol{\Lambda}$ is the CM of the vector $\mathbf{U}^T \hat{\mathbf{x}}$, whose components represent the n uncorrelated quantities that have been determined by the observations, and the eigenvalues measure the square errors with which these components have been measured. Analogously to

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what we did for direct measurements, on the basis of the additivity property, we define the MQQ as the sum of the MQQs of the n uncorrelated components:

$$Q = \sum_{i=1}^{n} \frac{1}{\lambda_i^{\,2}} = tr(\mathbf{\Lambda}^{-1}) \tag{23}$$

and notice that Q is equal to the summation of the eigenvalues of $\mathbf{\Lambda}^{-1}$.

Since $\mathbf{\Lambda}^{-1} = \mathbf{U}^T \mathbf{S}_x^{\,-1} \mathbf{U}$ and considering that the trace of a matrix is invariant by orthogonal transformations, we obtain:

$$Q = tr(\mathbf{\Lambda}^{-1}) = tr(\mathbf{U}^T \mathbf{S}_x^{\,-1} \mathbf{U}) = tr(\mathbf{S}_x^{\,-1}). \tag{24}$$

Analogously to the case of direct measurements we can define the MQQ of indirect measurements as the trace of the inverse of the CM $\mathbf{S}_x$.

Substituting Eq. (22) in Eq. (24) we obtain the following expression for the MQQ of a vector determined with indirect observations $\mathbf{y}$:

$$Q = tr\left(\mathbf{K}^T \mathbf{S}_y^{\,-1} \mathbf{K}\right). \tag{25}$$

Equation (25) has been derived supposing that the n equations of Eq. (18) are independent of each other. If this assumption does not apply, it is not possible to calculate the inverse of $\mathbf{K}^T \mathbf{S}_y^{\,-1} \mathbf{K}$ that appears in Eqs. (21) and (22) and the retrieval is an ill-posed problem. However, we can still calculate the eigenvalues of $\mathbf{K}^T \mathbf{S}_y^{\,-1} \mathbf{K}$ and still define the MQQ as equal to the summation of these eigenvalues. Indeed when the retrieval is ill-posed some eigenvalues are equal to zero and this implies that the corresponding components of the vector $\mathbf{U}^{\mathrm{T}} \hat{\mathbf{x}}$ have not been measured and do not contribute to the MQQ. Nevertheless the MQQ can still be determined accounting for the measured components. Therefore, the quantity defined in Eq. (25) provides the MQQ of indirect measurements regardless of whether the inverse problem is well-posed or not.

3.3 General considerations

Having defined the MQQ as the trace of the inverse of the CM it has been possible to generalize the MQQ to ill-posed problems. Other definitions of quality quantifiers, as for example the *Shannon information content* [1], also use the inverse of the CM, but calculate instead the determinant of this matrix. In this case the generalization to ill-posed problems cannot be done because if some eigenvalues of the inverse of the CM are zero also the determinant is zero independently of the values of the others. Therefore, for ill-posed problems, the determinant of the inverse of the CM is not able to quantify the measurement quality on the basis of the errors of the measured components.

This conclusion can also be reached looking at the geometrical interpretation of the determinant and of the trace of a positive-semidefinite symmetric matrix. The determinant of the matrix represents the volume of the hypercuboid with lengths of the edges equal to the eigenvalues of the matrix. The trace of the matrix is the square diagonal of the hypercuboid with edges equal to the square root of the eigenvalues of the matrix. If one of the edges of the hypercuboid is zero then the hypercuboid becomes a hypercuboid of n-1 dimensions and the n-dimensional volume is zero. On the other hand, the diagonal of the (n-1)-hypercuboid is different from zero and its value depends on the lengths of the edges different from zero.

As a consequence of its definition the MQQ does not provide any information on how many components of the unknown vector have been measured. Indeed the same value of the MQQ can be obtained either measuring many components with large errors or measuring a few components with small errors. If for some reason it is preferable to measure more components giving less importance to the errors with which the components are measured it is useful to consider together with the MQQ also a quantifier of the number of measured components that can be identified in the degrees of freedom for signal [1]. Indeed, the MQQ cannot replace the existing quantifiers, it rather complements them with new and useful properties.

We notice that the matrix $\mathbf{K}^T\mathbf{S}_y^{-1}\mathbf{K}$ that we have used to define the MQQ is the *Fisher information matrix* [8] of the likelihood function $L(\mathbf{x}) = P(\mathbf{y}|\mathbf{x})$ (that is the conditional probability distribution to obtain **y** given **x**, considering $P(\mathbf{y}|\mathbf{x})$ as a function of **x**) when we assume a Gaussian distribution for $P(\mathbf{y}|\mathbf{x})$:

$$P(\mathbf{y}\,|\,\mathbf{x}) = \frac{1}{(2\pi)^{m/2}\left|\mathbf{S}_y\right|^{1/2}}\exp\left\{-\frac{1}{2}\left(\mathbf{y}-\mathbf{F}(\mathbf{x})\right)^T\mathbf{S}_y^{-1}\left(\mathbf{y}-\mathbf{F}(\mathbf{x})\right)\right\}, \qquad (26)$$

that is generally appropriate for describing the noise associated with experimental data. Indeed, the Fisher information matrix **F** relative to $L(\mathbf{x})$ is defined as:

$$\mathbf{F} = \int P(\mathbf{y}\,|\,\mathbf{x})\left(\frac{\partial \ln P(\mathbf{y}\,|\,\mathbf{x})}{\partial \mathbf{x}}\right)\left(\frac{\partial \ln P(\mathbf{y}\,|\,\mathbf{x})}{\partial \mathbf{x}}\right)^T d\mathbf{y} \qquad (27)$$

and substituting $\frac{\partial \ln P(\mathbf{y}\,|\,\mathbf{x})}{\partial \mathbf{x}} = \mathbf{K}^T\mathbf{S}_y^{-1}\left(\mathbf{y}-\mathbf{F}(\mathbf{x})\right)$ (derived from Eq. (26)) we obtain:

$$\mathbf{F} = \mathbf{K}^T\mathbf{S}_y^{-1}\left[\int P(\mathbf{y}\,|\,\mathbf{x})\left(\mathbf{y}-\mathbf{F}(\mathbf{x})\right)\left(\mathbf{y}-\mathbf{F}(\mathbf{x})\right)^T d\mathbf{y}\right]\mathbf{S}_y^{-1}\mathbf{K} = \mathbf{K}^T\mathbf{S}_y^{-1}\mathbf{K}, \qquad (28)$$

where we have exploited the fact that the expected value of $\left(\mathbf{y}-\mathbf{F}(\mathbf{x})\right)\left(\mathbf{y}-\mathbf{F}(\mathbf{x})\right)^T$ is the CM $\mathbf{S}_y$.

Therefore, Eq. (25) can also be written as:

$$Q = tr(\mathbf{F}) = \sum_{i=1}^{n} F_{ii}. \qquad (29)$$

Furthermore, since $\mathbf{S}_y$ is a positive-definite matrix, we have that:

$$F_{ii} = \left(\mathbf{K}^T\mathbf{S}_y^{-1}\mathbf{K}\right)_{ii} = \left(\mathbf{K}^T\mathbf{S}_y^{-1/2}\mathbf{S}_y^{-1/2}\mathbf{K}\right)_{ii} = \sum_{j=1}^{m}\left(\mathbf{S}_y^{-1/2}\mathbf{K}\right)_{ji}^{2} \geq 0, \qquad (30)$$

that is F_{ii} are not-negative quantities given by the sum of the square elements of the *i*-th column of the matrix $\mathbf{S}_y^{-1/2}\mathbf{K}$ and consequently from Eq. (29) it follows that the MQQ is the sum of all the square elements of the matrix $\mathbf{S}_y^{-1/2}\mathbf{K}$. Equations (29-30) show that the MQQ is written as the sum of *n* quantities greater than or equal to zero that we can interpret as the contributions to the total MQQ related to the measurements of the single elements of **x**. We refer to the contributions F_{ii} as the *MQQ components*.

We notice that the square root of the MQQ components F_{ii} is closely linked with the *information load* (defined as the square root of the diagonal elements of $\mathbf{K}^T\mathbf{K}$) introduced in [5] and therewith used to evaluate the amount and the spatial distribution of the information that is carried by MIPAS [7] observations about the target atmospheric parameters. Both the information load and the MQQ components quantify the quality of the measurement of the different unknowns of the retrieval, however, in this paper we prefer to use the latter because it takes into account the effect of $\mathbf{S}_y$ and has the additivity property.

Indeed the additivity property of the MQQ also applies to its components. This statement can be demonstrated in the following way. We consider two independent indirect measurements $\mathbf{y}_1$ (of m_1 elements) and $\mathbf{y}_2$ (of m_2 elements) of the set of parameters represented by the vector **x**. The measurements are characterized, respectively, by the Jacobian matrices $\mathbf{K}_1$ and $\mathbf{K}_2$ and by the CMs $\mathbf{S}_{y1}$ and $\mathbf{S}_{y2}$. In order to calculate the MQQ components F_{ii} of the data fusion of the two measurements we consider the two measurements as a single

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measurement $\mathbf{y} = \begin{pmatrix} \mathbf{y}_1 \\ \mathbf{y}_2 \end{pmatrix}$ (including $m_1 + m_2$ observations) with Jacobian matrix $\mathbf{K} = \begin{pmatrix} \mathbf{K}_1 \\ \mathbf{K}_2 \end{pmatrix}$ and CM $\mathbf{S}_y = \begin{pmatrix} \mathbf{S}_{y1} & \mathbf{0} \\ \mathbf{0} & \mathbf{S}_{y2} \end{pmatrix}$, where the notation $\begin{pmatrix} \mathbf{L} \\ \mathbf{M} \end{pmatrix}$ means the matrix (vector) obtained arranging the rows of the matrix (vector) **M** below the rows of the matrix (vector) **L**. Consequently $\mathbf{S}_y^{-1/2}\mathbf{K} = \begin{pmatrix} \mathbf{S}_{y1}^{-1/2}\mathbf{K}_1 \\ \mathbf{S}_{y2}^{-1/2}\mathbf{K}_2 \end{pmatrix}$ and, using Eq. (30), we obtain:

$$F_{ii} = \sum_{j=1}^{m_1+m_2} \left(\mathbf{S}_y^{-1/2}\mathbf{K}\right)_{ji}^2 = \sum_{j=1}^{m_1} \left(\mathbf{S}_{y1}^{-1/2}\mathbf{K}_1\right)_{ji}^2 + \sum_{j=1}^{m_2} \left(\mathbf{S}_{y2}^{-1/2}\mathbf{K}_2\right)_{ji}^2. \quad (31)$$

Equation (31) shows that the MQQ components F_{ii} of the data fusion are the sum of the MQQ components $(F_1)_{ii}$ and $(F_2)_{ii}$ of the two original measurements. This result can be extended to the data fusion of any number of measurements.

4. Relative quality quantifier

In order to understand the meaning of the MQQ components F_{ii} we explicitly write the expression of these terms:

$$F_{ii} = \sum_{l,j=1}^{m} K_{li} \left(S_y^{-1}\right)_{lj} K_{ji} \approx \sum_{l,j=1}^{m} \frac{\Delta y_l}{\Delta x_i} \left(S_y^{-1}\right)_{lj} \frac{\Delta y_j}{\Delta x_i} = \frac{1}{\left(\Delta x_i\right)^2} \sum_{l,j=1}^{m} \Delta y_l \left(S_y^{-1}\right)_{lj} \Delta y_j. \quad (32)$$

From Eq. (32) we see that F_{ii} represents the sum of the quadratic variations of the observations, weighted with the CM $\mathbf{S}_y$, that correspond to a variation Δx_i divided by the square of Δx_i.

Since from the experimental point of view in some cases the quantity that is relevant is $\frac{\Delta x_i}{x_i}$ rather then Δx_i, it can be useful to use a *relative MQQ* instead of the absolute MQQ defined in subsection 3.2. The definition of a relative quality quantifier can be deduced from Eq. (32) substituting the square absolute variation $(\Delta x_i)^2$ with the square relative variation $\left(\frac{\Delta x_i}{x_i}\right)^2$. We obtain the following expression for the dimensionless relative MQQ components:

$$F_{ii} x_i^2 = \frac{1}{\left(\frac{\Delta x_i}{x_i}\right)^2} \sum_{l,j=1}^{m} \Delta y_l \left(S_y^{-1}\right)_{lj} \Delta y_j. \quad (33)$$

Summing the relative MQQ components $F_{ii}x_i^2$ we can define a relative MQQ as equal to:

$$Q_r = \sum_{i=1}^{n} F_{ii} x_i^2. \quad (34)$$

5. The invariant of the retrieval problem

In the case of either an ill-posed or an ill-conditioned indirect measurement a constraint is used for the retrieval of the unknown and the CM of the retrieved estimate of **x** is no longer equal to the inverse of the Fisher matrix of the observations. Therefore, the Fisher matrix and the MQQ, which are defined by quantities (**K** and $\mathbf{S}_y$) characterizing the observations, can no longer be simply derived from the quantities characterizing the retrieval. In order to verify how the Fisher matrix can be calculated from the diagnostics that are generally distributed to

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the data user together with the retrieval products the mathematics of the constrained retrieval is briefly recalled.

In a constrained retrieval the estimation of the unknown is obtained minimizing a cost function $c(\mathbf{x})$ that is the sum of the chi-square function plus a constraint function $R(\mathbf{x})$:

$$c(\mathbf{x}) = (\mathbf{y} - \mathbf{F}(\mathbf{x}))^T \mathbf{S}_y^{-1} (\mathbf{y} - \mathbf{F}(\mathbf{x})) + R(\mathbf{x}). \quad (35)$$

The constraint function is used whenever the information contained in the observations is not sufficient to retrieve the unknown with acceptable errors.

Imposing the derivatives of $c(\mathbf{x})$ with respect to the components of $\mathbf{x}$ equal to zero we find that the value $\hat{\mathbf{x}}$ of $\mathbf{x}$ that minimizes $c(\mathbf{x})$ satisfies the following equation:

$$-2\mathbf{K}^T \mathbf{S}_y^{-1} (\mathbf{y} - \mathbf{F}(\hat{\mathbf{x}})) + \left. \frac{\partial R(\mathbf{x})}{\partial \mathbf{x}} \right|_{\mathbf{x}=\hat{\mathbf{x}}} = \mathbf{0}. \quad (36)$$

The vector $\hat{\mathbf{x}}$ is determined from Eq. (36) as a function of the observations $\mathbf{y}$ and is characterized by the CM $\mathbf{S}_x$ and by the averaging kernel matrix (AKM) that is defined as $\mathbf{A} = \frac{\partial \hat{\mathbf{x}}}{\partial \mathbf{x}}$ [1,9,10]. We can calculate the CM following the same procedure as in Subsection 3.2. We perform the derivatives of Eq. (36) with respect to the elements of $\mathbf{y}$ and solve the obtained equation with respect to the gain matrix $\mathbf{G}$, which turns out to be equal to:

$$\mathbf{G} = (\mathbf{K}^T \mathbf{S}_y^{-1} \mathbf{K} + \mathbf{R})^{-1} \mathbf{K}^T \mathbf{S}_y^{-1}, \quad (37)$$

where we have defined the matrix $\mathbf{R} = \frac{1}{2} \left. \frac{\partial^2 R(\mathbf{x})}{\partial \mathbf{x}^2} \right|_{\mathbf{x}=\hat{\mathbf{x}}}$.

Substituting Eq. (37) in Eq. (20) we obtain the expression for the CM of $\hat{\mathbf{x}}$:

$$\mathbf{S}_x = (\mathbf{K}^T \mathbf{S}_y^{-1} \mathbf{K} + \mathbf{R})^{-1} \mathbf{K}^T \mathbf{S}_y^{-1} \mathbf{K} (\mathbf{K}^T \mathbf{S}_y^{-1} \mathbf{K} + \mathbf{R})^{-1}. \quad (38)$$

We can see that in this case, because of the use of the constraint, the expression of $\mathbf{S}_x$ does not coincide with that given in Eq. (22). Therefore, now it is not correct to estimate the MQQ of the measurement calculating the trace of the inverse of $\mathbf{S}_x$ because this quantity contains the information that we have added with the constraint. In order to obtain the correct expression for the MQQ we need to consider also the AKM.

Using Eq. (37) we obtain the following expression for the AKM:

$$\mathbf{A} = \frac{\partial \hat{\mathbf{x}}}{\partial \mathbf{x}} = \frac{\partial \hat{\mathbf{x}}}{\partial \mathbf{y}} \frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \mathbf{G}\mathbf{K} = (\mathbf{K}^T \mathbf{S}_y^{-1} \mathbf{K} + \mathbf{R})^{-1} \mathbf{K}^T \mathbf{S}_y^{-1} \mathbf{K}. \quad (39)$$

In the case of a well-posed problem the matrix $\mathbf{K}^T \mathbf{S}_y^{-1} \mathbf{K}$ is invertible and consequently also the CM $\mathbf{S}_x$ expressed by Eq. (38) is invertible. In this case it is easy to verify that, because of Eqs. (38) and (39), the matrix $\mathbf{A}^T \mathbf{S}_x^{-1} \mathbf{A}$ is equal to the Fisher information matrix:

$$\mathbf{A}^T \mathbf{S}_x^{-1} \mathbf{A} = \mathbf{K}^T \mathbf{S}_y^{-1} \mathbf{K} = \mathbf{F}. \quad (40)$$

In the case of an ill-posed problem the matrix $\mathbf{K}^T \mathbf{S}_y^{-1} \mathbf{K}$ is not invertible, therefore, also the CM $\mathbf{S}_x$ is not invertible. However, we can consider the generalized inverse [11] of $\mathbf{S}_x$ that we indicate with $\mathbf{S}_x^{\#}$ and that can be calculated using the singular value decomposition. It is possible to demonstrate (see Appendix) that:

$$\mathbf{A}^T \mathbf{S}_x^{\#} \mathbf{A} = \mathbf{K}^T \mathbf{S}_y^{-1} \mathbf{K} = \mathbf{F}. \quad (41)$$

Equation (41) shows that, even if different constraints provide different solutions that have different CMs (Eq. (38)) and AKMs (Eq. (39)), the combination $\mathbf{A}^T\mathbf{S}_x^{\#}\mathbf{A}$ is an invariant independent from the constraint $R(\mathbf{x})$ and it provides the quantity from which we can calculate the MQQ:

$$Q = tr\left(\mathbf{K}^T\mathbf{S}_y^{-1}\mathbf{K}\right) = tr\left(\mathbf{A}^T\mathbf{S}_x^{\#}\mathbf{A}\right). \tag{42}$$

The result of Eq. (42) is rather general, but it does not apply when the constraint is seen as another measurement characterized by the CM $\mathbf{R}^{-1}$ and the solution is interpreted as the weighted mean of the two measurements (the actual measurement and the constraint). This is for instance the case of the "optimal estimation method". In this case the CM of $\hat{\mathbf{x}}$ is not given by Eq. (38) but by [1]:

$$\mathbf{S}_x = \left(\mathbf{K}^T\mathbf{S}_y^{-1}\mathbf{K} + \mathbf{R}\right)^{-1}, \tag{43}$$

that is always a not singular matrix.

Therefore, in the case of the optimal estimation method the invariant $\mathbf{F} = \mathbf{K}^T\mathbf{S}_y^{-1}\mathbf{K}$ from which we can calculate the MQQ is not given by Eq. (40) but, using Eqs. (39) and (43), is equal to:

$$\mathbf{F} = \mathbf{K}^T\mathbf{S}_y^{-1}\mathbf{K} = \left(\mathbf{K}^T\mathbf{S}_y^{-1}\mathbf{K} + \mathbf{R}\right)\mathbf{A} = \mathbf{S}_x^{-1}\mathbf{A}. \tag{44}$$

The Fisher matrix is an invariant of the retrieval process that, given the set of unknowns, characterizes the observations (through $\mathbf{K}$ and $\mathbf{S}_y$) and that, independently of the adopted constraint, can also be determined from the quantities that characterize the measurements (through $\mathbf{A}$ and $\mathbf{S}_x$). The existence of this invariant proves that the retrieval, if properly made and fully characterized, is a process that does not destroy any information.

6. Information distribution

In the case of indirect measurements of a continuous distribution, such as the vertical profiles of atmospheric constituents, since the MQQ defined by Eq. (42) depends on the set of unknowns that are retrieved, a different value of MQQ is obtained when the vertical profile is represented on a different vertical grid. Indeed, since to each element x_i of $\mathbf{x}$ is associated an altitude interval Δz_i, a variation of the parameter x_i determines a variation of the observations $\mathbf{y}$ proportional to the altitude interval Δz_i, and the element K_{ij} of $\mathbf{K}$ is proportional to Δz_j. Consequently the diagonal elements F_{ii} are proportional to Δz_i^2 and, as stated above, their values depend on the grid on which the vertical profile is represented. Also the MQQ (the sum of the F_{ii}) depends on the grid and in particular it approaches zero for very fine grids when Δz_i tend to zero.

We want to define a quality quantifier that tends to a finite value different from zero when Δz_i tend to zero, and, therefore, this value represents the measurement quality referred to the vertical profile represented as a continuous function of altitude. Since F_{ii} are proportional to Δz_i^2 we define the grid normalized MQQ components as:

$$f_i = \frac{F_{ii}}{\Delta z_i^2} \tag{45}$$

and call this quantity the *information distribution*.

If the vertical grid is fine enough to capture the vertical variation of the MQQ components, the f_i values in the neighborhood of each altitude are independent of the grid. Accordingly we can define the *grid normalized MQQ* as:

$$q = \sum_{i=1}^{n} f_i \Delta z_i, \tag{46}$$

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that in the limit of $\Delta z_i \to 0$ tends to the integral of the information distribution *f*(*z*) and provides an overall assessment of the quality of a distribution measurement (independently of the selected retrieval grid).

Following the argumentations described in Section 4 we can define the *relative information distribution* as $f_i x_i^2$ and the *grid normalized relative MQQ* as:

$$q_r = \sum_{i=1}^{n} f_i x_i^2 \Delta z_i, \tag{47}$$

Examples about the use of these quantifiers will be given in the next Section.

7. Some applications

7.1 Quality of IASI and MIPAS ozone measurements and of their data fusion

In this Subsection we use the quality quantifiers introduced in the previous sections to compare the quality of two co-located ozone measurements performed by IASI and MIPAS instruments and of their data fusion. The analysis of these two measurements as well as their data fusion is described in detail in [4]. We recall here the basic information needed to understand the quality comparison and refer to [4] for further details.

The IASI instrument [6], launched onboard the sun-synchronous polar orbiting satellite Metop-A (Metereological Operational) on 19 October 2006, is a nadir-viewing Fourier transform spectrometer for passive atmospheric sounding in the thermal infrared region from 645 to 2760 cm^{-1}. The retrieval of the ozone vertical profile was performed using a version of the MARC (Millimetre-wave Atmospheric-Retrieval Code) retrieval code [12] recently upgraded for the analysis of the REFIR (Radiation Explorer in the Far InfraRed) measurements [13,14] and subsequently optimized, in the frame of a project of the European Spatial Agency (ESA), for IASI measurements.

The MIPAS instrument [7], launched onboard the sun-synchronous polar orbiting satellite Envisat (ENVIronmental SATellite) on 1st March 2002 is a limb-viewing Fourier-transform spectrometer operating in the middle infrared between 685 and 2410 cm^{-1}. The retrieval of the ozone profile was performed using the ORM (Optimized Retrieval Model) [15–18] that is the scientific prototype of the ESA operational level 2 code.

Two co-located IASI and MIPAS measurements acquired on 4 July 2008 at the following geolocations: time (UTC) 9:57:00, latitude 21.83 N, longitude 5.88 W for the IASI measurement and time (UTC) 10:40:55, latitude 21.93 N, longitude 6.22 W for the MIPAS measurement have been used to perform a data fusion.

In Fig. 1 we report the components $F_{ii} x_i^2$ of the relative MQQ as a function of altitude for the IASI measurement, the MIPAS measurement and their data fusion. Since the two retrievals have been performed using the same retrieval grid (from 1 to 80 km of altitude at 1 km steps), the MQQ components provide an adequate parameter for the comparison. Figure 1 shows clearly that the MIPAS measurement contains information on the ozone profile between 15 and 60 km, while the IASI measurement contains information below 30 km with a minimum at 15 km. The data fusion contains information on the ozone profile between 1 and 60 km with a minimum around to 15 km where both instruments have a contribution to the relative MQQ that is very small. The oscillations in the line of the MIPAS measurement correspond to maxima of the information for tangent altitudes of the observations. The analysis of the MQQ components highlights the relative merits of the two measurements as well as the strength and the weakness of the product of their fusion.

The relative MQQ Q_r is 50156 for the IASI measurement, 125225 for the MIPAS measurement and 175381 for the data fusion, confirming again the additivity property of the MQQ parameter.

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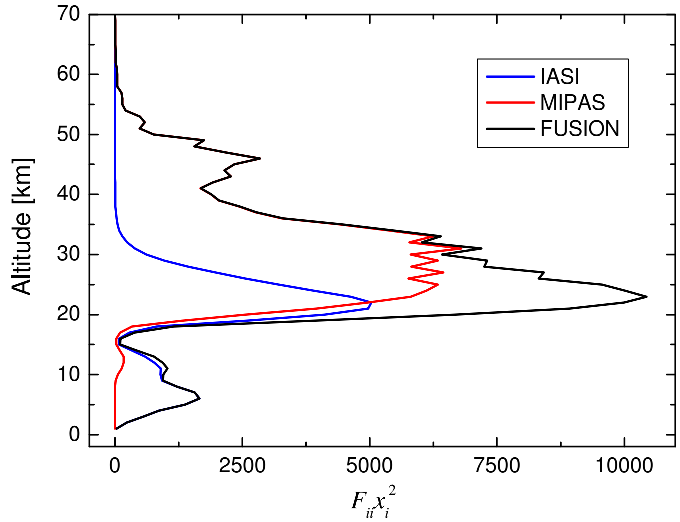

Fig. 1. Components $F_{ii}x_i^2$ of the relative MQQ as a function of altitude for the IASI measurement (blue line), the MIPAS measurement (red line) and their data fusion (black line).

A comparison of the quality of the measurements of IASI and MIPAS analyzed in this Subsection using the conventional quantifiers such as retrieval errors, Shannon information content and degrees of freedom for signal is reported in [4]. The results obtained in [4] depend on the CM of the a priori profile used in the analysis (in that case a climatological profile), on the other hand the results reported here quantify in absolute way the quality of the observations with respect to the retrieved parameters independently of any constraint that can be used in the retrieval.

7.2 Comparison of quality of MIPAS full and optimized resolution measurements

The MIPAS instrument onboard of Envisat from July 2002 to March 2004 has acquired measurements with an interferometer maximum path difference (MPD) equal to 20 cm, corresponding to a spectral resolution of 0.025 cm^{-1}. A limb sequence in the nominal observation mode was composed of 17 spectra that looked at different tangent altitudes from 6 to 68 km, with a step of 3 km in the troposphere and lower stratosphere and of up to 8 km in the high stratosphere. The measurements acquired between July 2002 and March 2004 are referred to as *full resolution* (FR) measurements.

After January 2005 the measurements were acquired with a reduced MPD equal to 8.2 cm. The interferograms acquired with reduced MPD are Fourier-transformed in spectra and re-sampled with a spectral resolution of 0.0625 cm^{-1}. In the nominal observation mode adopted after January 2005, a MIPAS limb scan consists of 27 spectra that look at different tangent altitudes from 7 to 72 km with a step of 1.5 km in the troposphere and lower stratosphere and of up to 4.5 km in the high stratosphere. The measurements acquired since January 2005 are referred to as *optimized resolution* (OR) measurements.

The ORM code performs the retrieval of the ozone profile fitting the simulated radiance to the observations in a selected set of spectral intervals (called "microwindows") [19] that contain the maximum information on ozone. Two different sets of microwindows have been selected for the ozone retrieval from FR and OR measurements, each set being optimized for the specific measurement scenario. The details about the measurement scenarios and the microwindow selection for FR and OR measurements can be found in [20].

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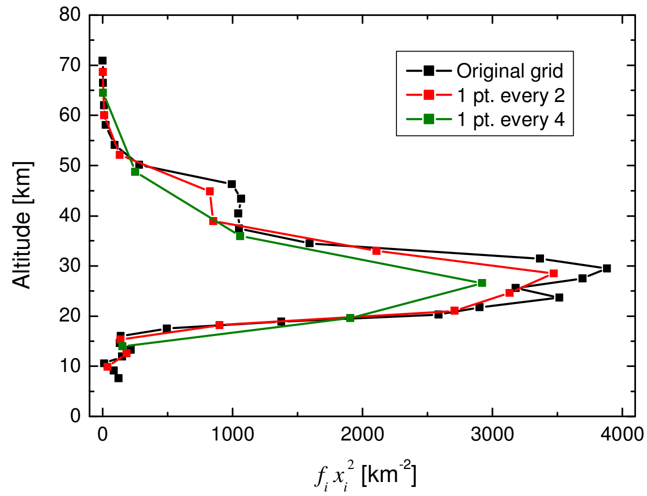

Fig. 2. Relative information distribution of an OR MIPAS measurement of ozone calculated for the original retrieval grid (black line and squares) and degrading the retrieval grid of a factor two (red line and squares) and of a factor four (green line and squares). The information distribution provides an assessment of the acquired information and weakly depends on the retrieval grid.

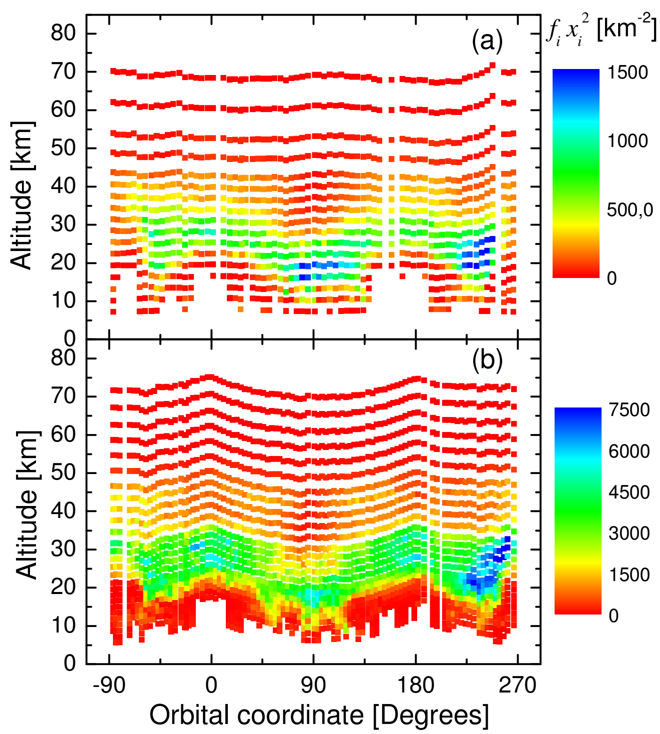

Fig. 3. Relative information distribution for orbit #8271 (a), acquired at FR, and for orbit #29184 (b), acquired at OR, as a function of altitude and orbital coordinate. Notice the factor five between the color scales for the two orbits.

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In this Subsection we compare the quality of MIPAS ozone FR and OR measurements. Since the retrieval grid adopted by ORM coincides with the observation tangent altitudes which are different for FR and OR measurements, we cannot directly compare the MQQ components, but we can compare the information distributions introduced in Section 6. Indeed, for enough fine grids, this quantifier is independent of the grid.

In order to verify this statement we report in Fig. 2 the relative information distribution for an OR MIPAS measurement of ozone calculated at the original retrieval grid as well as at the retrieval grids degraded by a factor two and by a factor four. We can see that degrading the retrieval grid by a factor two we lose some details of the distribution structure, but there is not a significant change in the values. A larger, but still contained, change is observed for a degradation by a factor four.

Since the FR retrieval grid is degraded with respect to the OR retrieval grid less than a factor two, the comparison of the information distributions provides a correct quality comparison of the measurements in the two scenarios.

We have calculated the relative information distributions for the two following Envisat orbits: orbit #8271 acquired on 29 September 2003 at FR and orbit #29184 acquired on 29 September 2007 at OR. In Fig. 3 we report the relative information distribution as a function of altitude and orbital coordinate for the two analyzed orbits. The orbital coordinate is defined as the value of the latitude in the hemisphere where the longitude is between 90° W and 90° E and 180° minus the latitude in the other hemisphere. Therefore, orbital coordinates of −90°, 0°, +90°, +180° and +270° correspond to the South pole, the equator, the North pole, the equator and the South pole, respectively. Figure 3 shows that the relative information distribution has a maximum between 15 and 35 km of altitude, depending on the orbital coordinate, with larger values between 225° and 270° for both FR and OR measurements. The FR orbit shows large values also close to the North pole. Figure 3a and Fig. 3b have color scales that differ by a factor five and, despite the overall similar appearance of the color distributions of the two figures, the quality of OR measurements is significantly better than that of FR measurements.

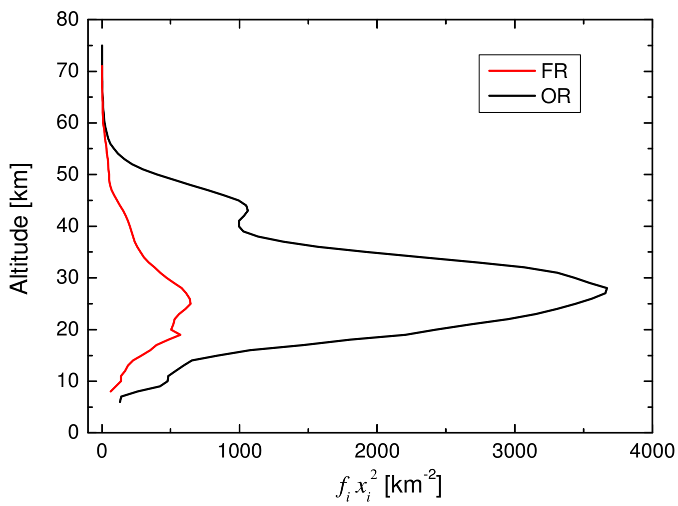

Fig. 4. Relative information distribution $f_i x_i^2$ as a function of altitude averaged along the orbit for FR measurements (orbit #8271 red line) and for OR measurements (orbit #29184 black line).

In order to visualize more clearly the quality difference of the two measurement scenarios in Fig. 4 we report the average along the orbit of the relative information distributions as a

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function of altitude. Figure 4 has been obtained interpolating the values reported in Fig. 3 on a common grid of 1 km steps and averaging the interpolated values along the orbits. The average grid normalized relative MQQs obtained integrating the curves reported in Fig. 4 are 13622 km^{-1} for the FR orbit and 75845 km^{-1} for the OR orbit, proving the improvement attained with the new measurement scenario.

Finally we remark the importance of having a grid independent quality quantifier which has made possible to quantify in absolute way the quality increase occurred passing from FR to OR MIPAS measurements. It is not possible to obtain this result with the conventional quantifiers such as retrieval errors, Shannon information content and degrees of freedom for signal, that only allow the comparison between retrievals represented on the same vertical grid.

8. Conclusion

We have identified a quality quantifier, referred to as MQQ, that can consistently be defined for both direct and indirect measurements of both scalar and vector quantities and that satisfies the additivity property. This means that the MQQ of the data fusion of two or more independent measurements is the sum of the MQQs of the individual measurements.

The MQQ is the only quality quantifier, defined for the characterization of the retrieval products, that has the additivity property. This makes the MQQ particularly useful in the context of data fusion activities and an important complement to the characterizations provided by other quality quantifiers.

For indirect measurements the quantifier is equal (see Eq. (25)) to the trace of the matrix $\mathbf{K}^T \mathbf{S}_y^{-1} \mathbf{K}$, which is the Fisher information matrix of the likelihood function, and can, differently from other information quantifiers such as the Shannon information content, be also defined in absolute terms for ill-posed inversion problems.

The Fisher matrix is calculated from quantities, such as the covariance and Jacobian matrices, that characterize the observations. However, in the case of an unconstrained retrieval the Fisher matrix is equal to the inverse of the CM of the retrieved measurements.

Furthermore, we have demonstrated that for a constrained retrieval, in which the constraint does not contain additional information, a combination of the CM and of the AKM of the retrieval is invariant to the constraint and is equal to the Fisher matrix. This invariant only depends on the CM of the observations and on the forward model and describes the information that the observations have about the unknown parameters. The MQQ is a function of this invariant and, therefore, has the property of being independent of the constraint that is used in the retrieval.

In the case of a constrained retrieval, in which the constraint contains additional information, a different combination of the products of the constrained retrieval must be used for the calculation of the Fisher matrix, the MQQ still being equal to the trace of the Fisher matrix.

The value of the MQQ depends on the set of unknowns, but a new set of unknowns that is obtained with an orthogonal transformation has the same MQQ as the original one. Given a set of unknowns each contributes to the total MQQ with its MQQ component (see Eq. (29)). The MQQ components quantify the quality of the measurement of the different unknowns of the retrieval and the MQQ is equal to the summation of the MQQ components.

The additivity property also applies to the MQQ components because the MQQ components of the data fusion of two measurements are equal to the sum of the MQQ components of the original measurements. This result can be extended to the data fusion of any number of measurements.

When the measured quantity is a continuous distribution, the MQQ components and the MQQ depend on the sampling grid of the distribution and the need arises of characterizing the observations independently of the selected grid. To this purposes a grid normalized MQQ and the grid normalized MQQ components have been defined. For the step of the sampling grid tending to zero the grid normalized MQQ components tend to the values of a finite function,

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which well characterizes the information distribution of the observations. The shape, and also the intensity, of the information distribution can also be reasonably captured with calculations made with relatively coarse values of the sampling grid (see Fig. 2).

As examples of the possible applications we have used the proposed quantifiers to evaluate the quality of the measurements of the ozone vertical profiles performed by the IASI and MIPAS instruments and of their data fusion. This analysis has identified the vertical ranges where IASI and MIPAS contain information about the ozone profile, assessing their complementarities, redundancies and common weaknesses, and has quantified the quality increase occurred when the measurement scenario of MIPAS was changed.

Appendix

We give the demonstration that in ill-posed retrievals, where the CM $\mathbf{S}_x$ is not invertible, we have:

$$\mathbf{A}^T\mathbf{S}_x^{\#}\mathbf{A} = \mathbf{K}^T\mathbf{S}_y^{-1}\mathbf{K}, \tag{A1}$$

where $\mathbf{S}_x^{\#}$ is the generalized inverse of $\mathbf{S}_x$ [11]. The generalized inverse of $\mathbf{S}_x$ can be calculated in the following way. Since $\mathbf{S}_x$ is a symmetric matrix we can find an orthogonal matrix $\mathbf{U}$ for which $\mathbf{S}_x = \mathbf{U\Lambda U}^T$ where $\mathbf{\Lambda}$ is a diagonal matrix with some diagonal values equal to zero. The generalized inverse of $\mathbf{S}_x$ is the matrix $\mathbf{S}_x^{\#} = \mathbf{U\Lambda}^{\#}\mathbf{U}^T$ where $\mathbf{\Lambda}^{\#}$ is the diagonal matrix whose diagonal elements are given by $\Lambda^{\#}_{ii}=1/\Lambda_{ii}$ if Λ_{ii} is different from zero and by $\Lambda^{\#}_{ii}=0$ if Λ_{ii} is equal to zero.

Multiplying the matrix $\mathbf{A}^T\mathbf{S}_x^{\#}\mathbf{A}$ times the identity matrix $\mathbf{I} = \left(\mathbf{K}^T\mathbf{S}_y^{-1}\mathbf{K}+\mathbf{R}\right)\left(\mathbf{K}^T\mathbf{S}_y^{-1}\mathbf{K}+\mathbf{R}\right)^{-1}$ on the left and on the right, we get:

$$\mathbf{A}^T\mathbf{S}_x^{\#}\mathbf{A} = \left(\mathbf{K}^T\mathbf{S}_y^{-1}\mathbf{K}+\mathbf{R}\right)\left(\mathbf{K}^T\mathbf{S}_y^{-1}\mathbf{K}+\mathbf{R}\right)^{-1}\mathbf{A}^T\mathbf{S}_x^{\#}\mathbf{A}\left(\mathbf{K}^T\mathbf{S}_y^{-1}\mathbf{K}+\mathbf{R}\right)^{-1}\left(\mathbf{K}^T\mathbf{S}_y^{-1}\mathbf{K}+\mathbf{R}\right). \tag{A2}$$

From Eqs. (38-39) we have the following relation between $\mathbf{A}$ and $\mathbf{S}_x$:

$$\mathbf{A}\left(\mathbf{K}^T\mathbf{S}_y^{-1}\mathbf{K}+\mathbf{R}\right)^{-1} = \mathbf{S}_x. \tag{A3}$$

Substituting Eq. (A3) and its transposed in Eq. (A2) and recalling that $\mathbf{S}_x$ is a symmetric matrix, we obtain:

$$\begin{aligned}\mathbf{A}^T\mathbf{S}_x^{\#}\mathbf{A} &= \left(\mathbf{K}^T\mathbf{S}_y^{-1}\mathbf{K}+\mathbf{R}\right)\mathbf{S}_x\mathbf{S}_x^{\#}\mathbf{S}_x\left(\mathbf{K}^T\mathbf{S}_y^{-1}\mathbf{K}+\mathbf{R}\right) = \\ &= \left(\mathbf{K}^T\mathbf{S}_y^{-1}\mathbf{K}+\mathbf{R}\right)\mathbf{S}_x\left(\mathbf{K}^T\mathbf{S}_y^{-1}\mathbf{K}+\mathbf{R}\right),\end{aligned} \tag{A4}$$

where we have used the property of the generalized inverse $\mathbf{S}_x\mathbf{S}_x^{\#}\mathbf{S}_x = \mathbf{S}_x$ [11].

Substituting Eq. (38) in Eq. (A4) we obtain Eq. (A1).

Acknowledgments

The study was conducted as part of the CTOTUS project that is supported by the POR program of the Tuscany Region within the CReO/FESR objectives 2007-2013. The forward and inverse models used in this work for MIPAS measurements have been optimized and tested in the frame of the project *Support to MIPAS Level 2 product validation* under ESA-ESRIN contract N. 21719/08/I-OL. The authors are grateful to Ugo Cortesi and Samuele Del Bianco for the support provided in the study for the data fusion of IASI and MIPAS measurements.

#158642 - $15.00 USD Received 23 Nov 2011; revised 19 Jan 2012; accepted 31 Jan 2012; published 16 Feb 2012