The EUMETSAT Network of Satellite Application Facilities

O3M SAF

Ozone and Atmospheric Chemistry Monitoring

Fast Optimal Retrieval on Layers for IASI

ALGORITHM THEORETICAL BASIS DOCUMENT

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Reference document

- SAF/O3M/ULB/FORLI_SFTIC

TABLE OF CONTENTS

1. FOREWORD

The Fast Optimal/Operational Retrieval on Layers for IASI (FORLI) is a dedicated radiative transfer and retrieval software for IASI. It was developed at the Université Libre de Bruxelles (ULB; Hurtmans et al., 2012) in collaboration with LATMOS/IPSL, with the objective to provide global concentration distributions of atmospheric trace gases. For the inversion step, it relies on a scheme based on the widely used Optimal Estimation theory (Rodgers, 2000). Three versions of the software have currently been set-up to process IASI level 1C radiances in near-real-time, for vertical profile retrievals of CO, O_3 and HNO_3. These three versions are to be implemented at the EUMETSAT CAF in the frame of the O3M SAF CDOP-2 (O3M SAF CDOP-2 Agreement Signed on March 2012), to enhance the suite of trace gas products provided by the O3MSAF.

2. METHODS

2.1 Forward model

2.1.1 General formulation

2.1.1.1 Ray tracing for upward flux

The Ray-tracing defines for off-nadir geometries the light path *s* versus the altitude *z*. The sphericity of the Earth is explicitly accounted for in FORLI by including a local radius of curvature for the Earth $R_{\oplus}$ and the index of refraction of air. The elementary path is then written as

$$ds = \frac{n(z)(z+R_{\oplus})dz}{\sqrt{n^2(z)(z+R_{\oplus})^2 - R_{\oplus}^2 n^2(z_G)\sin(\theta)}} \qquad (1)$$

where $n(z)$ is the index of refraction of air at altitude z and θ the zenithal angle at the surface. The altitude dependency of $n(z)$ is expressed through the variation of temperature, pressure and humidity and is modeled using the Birch and Downs formulation (Birch and Downs, 1994). The index of refraction is considered wavenumber independent in the IASI spectral range. In order to calculate the path along the line of sight, Eq. (1) is integrated using a numerical method, as no analytical closed form exists.

2.1.1.2 Radiative transfer

Local thermodynamic equilibrium is assumed.
The monochromatic upwelling radiance at TOA is then calculated as

$$L^{\uparrow}(\tilde{v};\theta,z) = L^{\uparrow}(\tilde{v};\theta,0)\,\tau(\tilde{v};\theta,0,z) + \int_0^z J(\tilde{v},\mathbf{\Omega},z')\frac{\partial\tau(\tilde{v};\theta,z',z)}{\partial z'}dz' \qquad (2)$$

where $L^{\uparrow}(\tilde{v};\theta,0)$ is the radiance at the start of the light path at wavenumber $\tilde{v}$, $\tau(\tilde{v};\theta,z',z)$ is the transmittance from altitudes z' to z.

Atmospheric source term

$J(\tilde{v},\mathbf{\Omega},z')$, the atmospheric source term, is expressed in FORLI by the black-body emission function $B(\tilde{v},T)$ as a non-scattering medium is assumed.

Transmittance

The transmittance $\tau(\tilde{v};\theta,z',z)$ in equation (2) is related to the absorption coefficient κ by:

$$\tau(\tilde{v};\theta,z',z) = \exp\left[-\int_{z'}^{z}\sum_j \kappa_j(\tilde{v};z'')\rho_j(z'')\frac{\partial s(\theta,z'')}{\partial z''}dz''\right] \qquad (3)$$

where j refers to a given gaseous species, $\rho_j(z'')$ is the molecular density of that species at altitude z'', and $s(\theta,z'')$ is the curvilinear path determined by the ray tracing. The absorption coefficient κ contains absorption features described by single spectral lines and broadband formulations (e.g. continua).

Earth's source radiance

$L^{\uparrow}(\tilde{\nu};\theta,0)$, the Earth source radiance in equation (2) is calculated as:

$$L^{\uparrow}(\tilde{\nu};\theta,0)=\epsilon(\tilde{\nu})B(T_{\text{skin}})+(1-\epsilon(\tilde{\nu}))L_0^{\downarrow\dagger}(\tilde{\nu})+\alpha(\tilde{\nu})L_0^{\downarrow\star}(\tilde{\nu}) \quad (4)$$

where $\epsilon(\tilde{\nu})$ is the surface emissivity, $B(T_{\text{skin}})$ is the ground black-body Planck function at the ground temperature T_{skin} ;

$$L_0^{\downarrow\dagger}(\tilde{\nu})=\frac{1}{\pi}\int_0^{2\pi}d\phi\int_0^{\pi/2}d\theta\, L_0^{\downarrow}(\tilde{\nu};\theta)\sin(\theta)\cos(\theta) \quad (5)$$

is the mean radiance associated to the total downward flux reaching the surface, integrated upon all the geometries considering a Lambertian surface; $\alpha(\tilde{\nu})L_0^{\downarrow\star}(\tilde{\nu})$ is the fraction of sun light that is retro-reflected in the direction of the sounding beam, which depends on the sun azimuthal angle and the surface effective reflectivity $\alpha(\tilde{\nu})$. In FORLI both contribution from Lambertian and specular reflections are explicitly taken into account, following:

$$\alpha(\tilde{\nu})=((1-\epsilon(\tilde{\nu}))\mu_{\delta 0}+\rho\mu_{glint})6.7995\times 10^{-5} \quad (6)$$

With

$$\mu_{\delta 0}=\frac{\cos\theta^{\star}}{\pi} \quad (7)$$

$$\mu_{glint}=\frac{\cos\theta+\cos\theta^{\star}}{\sqrt{2[1+\sin\theta^{\star}\sin\theta\cos(\phi-\phi^{\star})-\cos\theta\cos\theta^{\star}]}} \quad (8)$$

where θ , $\theta^{\star}$, ϕ and $\phi^{\star}$ are the sun and satellite zenithal and azimuthal angles respectively, and where ρ in equation (6) is the effective reflectivity for specular reflection; the last factor on the right hand side of that equation is the solar solid angle. Note that $L_0^{\downarrow\star}(\tilde{\nu})$ in equation (4) is modeled by a Planck blackbody function at 5700 K, without including spectral lines.

2.1.2 Numerical approximations

2.1.2.1 Radiative transfer in a layered atmosphere

A discretized layered atmosphere is considered. The convention adopted here is to label the levels from 0 to N for altitudes starting from ground to the TOA, with an atmospheric layer bounded by two levels. The layer index is then ranging from 1 to N. For each layer, average parameters $(e.g.\ \overline{T}_i,\overline{P}_i,\ldots)$ are computed.

Light path

Equation (1) is integrated for each layer using a Gauss-Kronrod quadrature scheme.

Partial columns

For each layer, the partial column of each molecule j is computed using

$$PC_{i,j} = \int_{z_i}^{z_i+1} \rho_j(z) \frac{ds(z)}{dz} dz \qquad (9)$$

where $\rho_j(z)$ is the molecular density (in molecule/cm^3).

Earth's source radiance

$L^{\uparrow}(\tilde{\nu};\theta,0)$ is evaluated using two recursions similar to equation (4), the first being to approximate the downward flux $L_0^{\downarrow\dagger}(\tilde{\nu})$. This is achieved by computing an effective downward radiance with an zenithal angle of 53.5°, which approximates the integral within a few percent for $\epsilon \gtrsim 0.9$ (Turner, 2004).

Layer transmittance and radiance

Equation (2) is discretized using a recursive representation evaluated successively for each layer $i = 1 \ldots N$:

$$L_i^{\uparrow} = \overline{B_i} + (L_{i-1}^{\uparrow} - \overline{B_i})\tilde{\tau}_i \qquad (10)$$

where $\overline{B_i}$ is the Planck function for layer i at the average temperature $\overline{T_i}$ and $\tilde{\tau}_i = \tau(\tilde{\nu}; z_i, z_{i-1})$ is the effective transmittance of that layer.

Effective transmittances are computed for each layer using a formulation close to the analytical form equation (3), but using the average parameters:

$$\tilde{\tau}_i = \exp\left[-\sum_j PC_{i,j} \sum_l \kappa_{j,l}(\tilde{\nu}; \overline{T_i}, \overline{P_i})\right] \qquad (11)$$

where i refers to the layer; j, to the molecular species; and l, to the spectral line when relevant. For water vapor, the water concentration enters in the line shapes definition, and we should rigorously write $\kappa_{j,l}(\tilde{\nu}; \overline{T_i}, \overline{P_i}, \mathrm{VMR}_{j,i})$.

Multiplication factors

FORLI works with unit less multiplying factors $M_{i,j}$ instead of the partial columns $PC_{i,j}$ themselves (see also section 2 of SAF/O3M/ULB/ForliTECHv01). The multiplying factors are applied on the *a priori* profiles. Therefore equation (11) becomes:

$$\tilde{\tau}_i = \exp\left[-\sum_{j=\text{fitted}} M_{i,j} PC_{i,j} \sum_l \kappa_{j,l}(\tilde{\nu}; \overline{T_i}, \overline{P_i}) - \sum_{j=\text{fixed}} PC_{i,j} \sum_l \kappa_{j,l}(\tilde{\nu}; \overline{T_i}, \overline{P_i})\right] \qquad (12)$$

where the sum runs over the fitted molecules and the j--fixed molecules.

State vector

The total state vector includes the multiplying factors $M_{i,j}$ and T_{skin}.

2.2 Inverse model

2.2.1 Calculation of derivatives

All the derivatives of the direct model relative to the state vector are computed analytically. For the sake of clarity, dependencies in wavenumber and angles are omitted hereafter.

– For the derivatives $(\partial L_N^{\uparrow} / \partial M_{kj})$:

$$\frac{\partial L_N^{\uparrow}}{\partial M_{k,j}} = \frac{\partial L_N^{\uparrow}}{\partial \tilde{\tau}_k} \frac{\partial \tilde{\tau}_k}{\partial M_{k,j}} \tag{13}$$

with

$$\frac{\partial \tilde{\tau}_k}{\partial M_{k,j}} = -PC_{k,j} \sum_l \kappa_{j,l}(\tilde{\nu}; \overline{T}_i, \overline{P}_i) \tilde{\tau}_k . \qquad (14)[1]$$

and, for $k = 1 \ldots N$:

$$\frac{\partial L_N^{\uparrow}}{\partial \tilde{\tau}_k} = \prod_{j=k+1}^{N} \tilde{\tau}_j \frac{\partial L_k^{\uparrow}}{\partial \tilde{\tau}_k} \tag{15}$$

with

$$\frac{\partial L_k^{\uparrow}}{\partial \tilde{\tau}_k} = \prod_{j=1}^{k-1} \tilde{\tau}_j \frac{\partial L_0^{\uparrow}}{\partial \tilde{\tau}_k} . \tag{16}$$

– For the Earth source radiance:

$$\frac{\partial L_0^{\uparrow}}{\partial \tilde{\tau}_k} = (1-\epsilon) \frac{\partial L_0^{\downarrow \dagger}}{\partial \tilde{\tau}_k} + \alpha \frac{\partial L_0^{\downarrow \star}}{\partial \tilde{\tau}_k} . \tag{17}$$

with:

$$\frac{\partial L_0^{\downarrow \dagger}}{\partial \tilde{\tau}_k} = \prod_{j=1}^{k-1} \tilde{\tau}_j^{\dagger} \frac{\partial \tilde{\tau}_k^{\dagger}}{\partial \tilde{\tau}_k} (L_{k+1}^{\downarrow \dagger} - \overline{B}_k) \tag{18}$$

where we use $L_N^{\downarrow \dagger} = 0$, and $\tilde{\tau}_k^{\dagger}$ being the transmittance for the geometry with an effective angle.

– For the sun downward radiance:

$$\frac{\partial L_0^{\downarrow \star}}{\partial \tilde{\tau}_k} = \prod_{j=1, \neq k}^{N} \tilde{\tau}_j^{\dagger} \frac{\partial \tilde{\tau}_k^{\dagger}}{\partial \tilde{\tau}_k} L_N^{\downarrow \star} \tag{19}$$

where $L_N^{\downarrow \star} = B(T^{\star})$ is the sun radiance, and $\tilde{\tau}_k^{\star}$ the transmittance for the geometry with the solar zenithal angle.

[1] Note that an extra term for water vapor containing the derivative of κ vs. $M_{k,j}$ is included.

– For surface temperature:

$$\frac{\partial L_N^{\uparrow}}{\partial T_{\text{skin}}} = \frac{\partial L_N^{\uparrow}}{\partial L_0^{\uparrow}} \frac{\partial L_0^{\uparrow}}{\partial T_{\text{skin}}} = \prod_{j=1}^{N} \tilde{\tau}_j \left[\epsilon \frac{\partial B(T_{\text{skin}})}{\partial T_{\text{skin}}} \right]. \quad (20)$$

2.2.2 Optimal estimation

2.2.2.1 General formulation

The inverse problem is solved in FORLI using the Optimal Estimation Method (Rodgers, 2000). For the forward model, equation (2) can be written in a general way as:

$$\mathbf{y} = \mathbf{F}(\mathbf{x};\mathbf{b}) + \boldsymbol{\eta} \quad (21)$$

where $\mathbf{y}$ is the measurement vector containing the measured radiance, $\mathbf{x}$ is the state vector, $\mathbf{b}$ represents other fixed parameters (air temperature, pressure, instrumental parameters...), $\boldsymbol{\eta}$ is the measurement noise and $\mathbf{F}$ the forward radiative transfer function. Based on an *a priori* state $\mathbf{x}_a$ and considering a linear problem, the retrieved state $\hat{\mathbf{x}}$, is given by

$$\hat{\mathbf{x}} = \mathbf{x}_a + (\mathbf{K}^T \mathbf{S}_\eta^{-1} \mathbf{K} + \mathbf{S}_a^{-1})^{-1} \mathbf{K}^T \mathbf{S}_\eta^{-1} (\mathbf{y} - \mathbf{K}\mathbf{x}_a) \quad (22)$$

with $\mathbf{S}_\eta$ and $\mathbf{S}_a$ being the noise and a priori variance-covariance matrices respectively, and where $\mathbf{K}$ is the Jacobian of the forward model $\mathbf{F}$, the rows of which contain the derivatives of the spectrum with respect to the retrieved variables. In FORLI equation (22) is iteratively repeated using a Gauss-Newton method until convergence is achieved. For iteration j :

$$\mathbf{x}_{j+1} = \mathbf{x}_a + (\mathbf{K}_j^T \mathbf{S}_\eta^{-1} \mathbf{K}_j + \mathbf{S}_a^{-1})^{-1} \mathbf{K}_j^T \mathbf{S}_\eta^{-1} [\mathbf{y} - \mathbf{F}(\mathbf{x}_j) + \mathbf{K}(\mathbf{x}_j - \mathbf{x}_a)]. \quad (23)$$

2.2.2.2 Averaging kernel an gain matrices

The averaging kernel matrix is calculated as:

$$\mathbf{A} = \mathbf{G}\mathbf{K} \quad (24)$$

With $\mathbf{G}$ the gain matrix, whose rows are the derivatives of the retrieved state with respect to the spectral points:

$$\mathbf{G} = (\mathbf{K}^T \mathbf{S}_\eta^{-1} \mathbf{K} + \mathbf{S}_a^{-1})^{-1} \ \mathbf{K}^T \mathbf{S}_\eta^{-1}. \quad (25)$$

2.2.2.3 Error variance-covariance matrix

The variance-covariance matrix $\hat{\mathbf{S}}$ representing the total statistical error after the retrieval, is:

$$\hat{\mathbf{S}} = (\mathbf{K}^T \mathbf{S}_\eta^{-1} \mathbf{K} + \mathbf{S}_a^{-1})^{-1}. \quad (26)$$

2.3 Processing steps

2.3.1 Initialisation

Read spectrum

Get $\vec{y}$ on the wavenumberh grid defined by $\delta\tilde{\nu}$ and $\tilde{\nu}_{\text{start}}$ to $\tilde{\nu}_{\text{end}}$, check validity

Read model

Read altitude grid $z_i \; i=1\ldots N$. Put pressure, temperature, humidity and the volume mixing ratio of trace gases $j=1\ldots M$ on the altitude grid ($\vec{P}_N, \vec{T}_N, \vec{Q}_N$ and $\text{VMR}_{[N\times M]}$), check validity.

Build S_a

Read error covariance matrix $S_{a[N\times N]}$ from file, cut out entries below z_G. Calculate inverse $S_a{}^{-1}{}_{[N\times N]}$ Check validity.

Multiplication factors

Initialise the multiplicative factors $\overrightarrow{\text{MF}}$ and $\overrightarrow{\text{MF}}_a$ for all target species and set the cost function.

Index of refraction of air

Compute the function of the index of refraction of air $n(z)$.

Variables within the layer

Compute $T_i(z)$, $P_i(z)$, $Q_i(z)$, $\text{VMR}_{i,j}(z)$ from $\vec{T}$, $\vec{P}$, $\vec{Q}$, VMR

2.3.2 Ray tracing for upward flux

Path length in layer i

$$l_i = \int_{z_i}^{z_{i+1}} \frac{\mathrm{ds}(z)}{\mathrm{dz}} \mathrm{dz} \tag{27}$$

Molecular density of species j in layer i:

$$\rho_j(z) = \text{VMR}_{i,j}(z)\text{MF}_j(z)\frac{P_i(z)}{k_B T_i(z)} \tag{28}$$

Average parameters for layer i

$$<T>_i = \frac{\mathcal{T}_i}{l_i} \quad \text{where } \mathcal{T}_i = \int_{z_i}^{z_i+1} T_i(z)\frac{\mathrm{ds}(z)}{\mathrm{dz}}\mathrm{dz} \tag{29}$$

$$<P>_i = \frac{\mathcal{P}_i}{l_i} \quad \text{where } \mathcal{P}_i = \int_{z_i}^{z_i+1} P_i(z)\frac{\mathrm{ds}(z)}{\mathrm{dz}}\mathrm{dz} \tag{30}$$

$$<Q>_i = \frac{\mathcal{RH}_i}{l_i} \quad \text{where } \mathcal{RH}_i = \int_{z_i}^{z_i+1} Q_i(z)\frac{\mathrm{ds}(z)}{\mathrm{dz}}\mathrm{dz} \tag{31}$$

Partial column for species j in layer i:

The partial column $<\text{PC}^{\uparrow}>_{[N\times M]}$ for each layer i and molecule j is calculated using equation (9). The partial air column $<\vec{PC}^{\uparrow}_{\text{air}}>_{[N]}$ for each layer i is calculated as:

$$<PC^{\uparrow}_{air}>_i = \int_{z_i}^{z_i+1} \frac{P_i(z)}{kT_i(z)}\frac{ds(z)}{dz}\mathrm{dz} \tag{32}$$

2.3.3 Ray tracing for downward flux

Path length in layer i

The path length is calculated using equation (1) with θ=53.5 and the path length along the line of sight $\vec{l}_N$ is calculated for each layer i using equation (27).

Partial column for species j in layer i *:*

The partial column $< \mathrm{PC}^{\downarrow} >_{[N\times M]}$ for each layer i and molecule j is calculated using eq. (9) and the partial air column $< \overrightarrow{\mathrm{PC}}_{\mathrm{air}}^{\downarrow} >_{[N]}$ for each layer i using eq. (32).

2.3.4 Radiance and derivatives

Absorption coefficient in layer i

$\kappa_{i,j}(\tilde{\nu}, < T >_i, < P >_i, < Q >_i, j)$, is taken from pre-calculated lookup tables

Transmittance for layer i

The effective upward transmittance $\vec{\tau}_N^{\uparrow}$:

$$\tau_i^{\uparrow} = \exp\left[-\sum_{j=\text{fitted}} \mathrm{MF}_{i,j} < \mathrm{PC}^{\uparrow} >_{i,j} \sum_l \kappa_{j,l} - \sum_{j=\text{fixed}} < \mathrm{PC}^{\uparrow} >_{i,j} \sum_l \kappa_{j,l} \right]. \quad (33)$$

The effective downward transmittance $\vec{\tau}_N^{\downarrow}$ is calculated as:

$$\tau_i^{\downarrow} = \exp\left[-\sum_{j=\text{fitted}} \mathrm{MF}_{i,j} < \mathrm{PC}^{\downarrow} >_{i,j} \sum_l \kappa_{j,l} - \sum_{j=\text{fixed}} < \mathrm{PC}^{\downarrow} >_{i,j} \sum_l \kappa_{j,l} \right]. \quad (34)$$

Layer radiance

The radiance L measured at the sounder is recursively calculated following:

$$L_N^{\downarrow} = 0 \quad (35)$$

$$L_i^{\downarrow} = (L_{i+1}^{\downarrow} - B(< T >_{i+1}))\tau_{i+1}^{\downarrow} + B(< T >_{i+1}) \quad \text{until } L_0^{\downarrow} \text{ is reached.} \quad (36)$$

$$L_0^{\uparrow} = \epsilon B(T_G) + (1-\epsilon) L_0^{\downarrow} \quad (37)$$

$$L_i^{\uparrow} = (L_{i-1}^{\uparrow} - B(< T >_i))\tau_i^{\uparrow} + B(< T >_i) \quad \text{until } L_N^{\uparrow} = L \text{ is reached.} \quad (38)$$

Derivatives

– For upward transmittance over the multiplication factors:

$$\mathcal{D}_{k,j}^1 \equiv \frac{\partial \tau_k^{\uparrow}}{\partial \mathrm{MF}_{k,j}} = - < PC^{\uparrow} >_{k,j} \sum_l \kappa_{j,l} \tau_k^{\uparrow} \quad (39)$$

– For effective downward radiance over the upward transmittance:

$$\mathcal{D}_k^2 \equiv \frac{\partial L_0^{\downarrow}}{\partial \tau_k^{\uparrow}} = \prod_{j=1}^{k-1} \tau_j^{\downarrow} \exp\left(- \frac{< \mathrm{PC}_{\mathrm{air}}^{\downarrow} >_k}{< \mathrm{PC}_{\mathrm{air}}^{\uparrow} >_k} \right) \times \left(L_{k+1}^{\downarrow} - B(< T >_k) \right) \quad (40)$$

$$L_N^{\downarrow} = 0.$$

– For effective upward radiance over the upward transmittance is calculated as:

$$\mathcal{D}_k^3 \equiv \frac{\partial L_0^{\uparrow}}{\partial \tau_k^{\uparrow}} = (1-\epsilon)\mathcal{D}_k^2 \tag{41}$$

– For the upward radiance over the upward transmittance:

$$\mathcal{D}_k^4 \equiv \prod_{j=1}^{k-1} \tau_j^{\uparrow} \mathcal{D}_k^3 \tag{42}$$

– For the effective upward radiance over the upward transmittance is calculated as:

$$\mathcal{D}_k^5 \equiv \prod_{j=k+1}^{N} \tau_j^{\uparrow} \mathcal{D}_k^4 \tag{43}$$

– For effective upward radiation at TOA for each species j and layer k over the multiplicative factor:

$$K_{k,j} \equiv \mathcal{D}_k^5 \mathcal{D}_{k,j}^1 \tag{44}$$

– For skin temperature using eq (20)

All is stored in $\mathbf{K}_{[N\times M+X]}$

Surface reflectivity

Estimate effective reflectivity from $\vec{y}$ at short wavenumber end.

Convolution with the instrumental line shape:

$$\vec{L}_{[N]}^{\uparrow} \leftarrow \vec{L}_{[N]}^{\uparrow} \otimes ILS$$

$$\mathbf{K}_{[N\times M+X]} \leftarrow \mathbf{K}_{[N\times M+X]} \otimes ILS \tag{45}$$

2.3.5 Inversion

Calculation of new multiplication factors

$$\mathrm{W}_1 = \mathrm{S}_\eta^{-1}\mathrm{K}$$
$$\mathrm{W}_2 = \mathrm{S}_a^{-1} + \mathrm{K}^T\mathrm{W}_1$$
$$\overrightarrow{w_1} = \mathrm{K}(\overrightarrow{\mathrm{MF}} - \overrightarrow{\mathrm{MF}_a})^T$$
$$\overrightarrow{w_2} = \mathrm{W}_1^T[\vec{y} - \vec{L} + \overrightarrow{w_1}]$$
$$\mathrm{W}_3 = \mathrm{W}_2^{-1}$$
$$\mathrm{d}\vec{\mathrm{M}}\mathrm{F} = \mathrm{W}_3\overrightarrow{w_2}$$

Set $\vec{\mathrm{M}}\mathrm{F}_{new} = \vec{\mathrm{M}}\mathrm{F} + \mathrm{d}\vec{\mathrm{M}}\mathrm{F}$

Cost function

$$Cost_{\mathrm{new}} = (\vec{y}-\vec{L})^T \mathrm{S}_\eta^{-1}(\vec{y}-\vec{L}) + \left((\mathrm{MF}_{\mathrm{new}} - \mathrm{MF}_a)^T\right)^T \mathrm{S}_\mathrm{a}^{-1}\left((\mathrm{MF}_{\mathrm{new}} - \mathrm{MF}_a)^T\right) \tag{46}$$

$\hat{S}$ is calculated using equation (26).

The stepsize is calculated:

$$d = \sqrt{\left((\overrightarrow{\mathrm{MF}} - \overrightarrow{\mathrm{MF}_{\mathrm{new}}})^T \right)^T \ \hat{\mathbf{S}}^{-1} \left((\mathrm{MF} - \mathrm{MF}_{\mathrm{new}})^T \right)} \qquad (47)$$

Check for convergence:

If convergence is not achieve and the difference in cost functions too large set $\overrightarrow{\mathrm{MF}_a} = \overrightarrow{\mathrm{MF}_{\mathrm{new}}}$ $Cost = Cost_{\mathrm{new}}$ and loop.

2.3.6 Outputs

- Retrieved partial columns in layers using equation (9).
- Averaging kernels matrix using equation (24).
- Total statistical error matrix using equation (26).

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ACRONYMS

CAF: Central Application Facility at EUMETSAT
CDOP-2: second Continuous Development and Operations Phase (CDOP-2)
IASI: Infrared Atmospheric Sounding Interferometer
FORLI: Fast Optimal Retrievals on Layers for IASI
LATMOS: Laboratoire Atmosphères, Milieux, Observations Spatiales
O3M SAF: Ozone and Atmospheric Composition Monitoring Satellite Application Facility
PC: Partial Column
TOA: Top Of the Atmosphere
VMR: Volume Mixing Ratio
ULB: Université Libre de Bruxelles