Individual Sections of the Book

Inverse Problems: Exercices

With *mathematica*, *matlab*, and *scilab* solutions

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March 12, 2007

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4.3 The Gomos Instrument in the Envisat Satellite

As explained in Tamminen (2004), the GOMOS (Global Ozone Monitoring by Occultation on Stars) satellite is one of the 10 instruments onboard the ESA’s Envisat satellite (see figure 4.21), which, in a polar sun-synchronous orbit at about 800 km above the Earth, is targeted on studying the Earth’s environment. The main objective of GOMOS is to measure the atmospheric composition and especially the ozone concentration in the stratosphere and mesosphere with high vertical resolution. In addition to ozone (O$_3$), the UV–visible spectrometer (250–675 nm) can be used to detect also NO$_2$, NO$_3$, aerosols, and neutral density. The GOMOS instrument uses the stellar occultation technique. The measurement principle is quite simple: the stellar spectrum measured through the atmosphere is compared with the reference spectrum measured above the atmosphere (see figure 4.22). Due to the absorption and scattering in the atmosphere the light measured through the atmosphere is attenuated and the attenuation is proportional to the amount of constituents in the atmosphere. The measurements are repeated at different tangential altitudes to obtain vertical profiles of the concentrations of different atmospheric constituents. Each occultation consists of about 70–100 spectra measured at different tangential altitudes and each spectrum includes measurements at 1416 different wavelengths.

4.3.1 Simplified Theory

Assume we only use one star, whose spectrum, measured far from Earth’s atmosphere, is $S^0(\lambda)$. The spectrum $S^\text{n}(\lambda)$ of the $n$-th ray $R^n$ (a ray possibly passing through the atmosphere) can be computed as

$$ S^\text{n}(\lambda) = S^0(\lambda) \exp \left[ - \int_{R^n} d\ell \sum_{\text{gas}} a_{\text{gas}}(\lambda) \rho_{\text{gas}}(z(\ell), \theta(\ell), \phi(\ell)) \right] , $$

where the coefficient $a_{\text{gas}}(\lambda)$ measured in the laboratory, represents the capacity of each gas in absorbing the signal in a given wavelength, and $\rho(z, \theta, \phi)$ is the concentration (assumed small) of a given gas at point $(z, \theta, \phi)$ in the atmosphere. The integral is along the ray path, and $d\ell$ represents the length element along the ray path. The path of each ray is, of course, refracted by the atmosphere, but, to simplify this numerical example we shall assume below that that rays are straight.

One introduces the spectral ratio

$$ T^\text{n}(\lambda) \equiv \frac{S^\text{n}(\lambda)}{S^0(\lambda)} , $$

and, because we prefer Cartesian parameters, the logarithmic spectral ratio

$$ t^\text{n}(\lambda) \equiv \log T^\text{n}(\lambda) = \log \frac{S^\text{n}(\lambda)}{S^0(\lambda)} . $$

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4 I borrowed the idea of this exercise from a dissertation of Johanna Tamminen (2004), posted in the web. This short section (i.e., section ??) is obtained by “copy and paste” from her text. But I develop the formulas of the sections below in my way—and adapt them to a simplified version of the GOMOS experiment—and use the simple least-squares technique instead of the Monte Carlo Markov chain used by Tamminen.

5 Two infra-red channels are used to detect O$_2$ and H$_2$O.

6 The concentration is not a Cartesian parameter, but let us avoid this complication here.
4.3 The Gomos Instrument in the Envisat Satellite

Figure 4.21: The ENVISAT satellite, with its ten instruments.

Equation (4.20) then gives

\[
\begin{align*}
t_n^\nu (\lambda) &= - \int \! d\ell \sum_{\text{gas}} \alpha_{\text{gas}}^{\nu} (\lambda) \ \rho_{\text{gas}}^{\nu} (z(\ell), \theta(\ell), \phi(\ell)),
\end{align*}
\]

which is our basic equation, solving the forward modeling problem.

We shall see in the course, that it is possible to set the inverse problem taking as an unknown the function \(\rho(z, \theta, \varphi)\), but let us use here a simplified approach, where the Earth’s atmosphere is divided into a certain number of three-dimensional cells. We can then write

\[
\begin{align*}
t_n^\nu (\lambda) &= - \sum_p \sum_q \sum_r \ell_{n pqr} \sum_{\text{gas}} \alpha_{\text{gas}}^{\nu} (\lambda) \ \rho_{\text{gas}}^{\nu} (pqr),
\end{align*}
\]

where the indices \(\{p, q, r\}\) identify the cells (the index \(p\) may represent the altitude of a cell, the index \(q\) its latitude, and the index \(r\) its longitude), where \(\ell_{n pqr}\) is the length of the \(n\)-th ray inside the cell \(\{p, q, r\}\), and where \(\rho_{\text{gas}}^{\nu} (pqr)\) represents the concentration of each gas inside each cell (these quantities are now our basic unknowns). To prepare for subsequent notations, let us from now just write \(g\) instead of “gas”. Our last equation then becomes

\[
\begin{align*}
t_n^\nu (\lambda) &= - \sum_p \sum_q \sum_r \sum_g \ell_{n pqr} \alpha_g^{\nu} (\lambda) \ \rho_g^{\nu} (pqr),
\end{align*}
\]

Equivalently, we can write

\[
\begin{align*}
t_n^\nu (\lambda) &= - \sum_p \sum_q \sum_r \sum_g \ell_{n pqr} \alpha_g^{\nu} (\lambda) \ \rho_g^{\nu} (pqr),
\end{align*}
\]

i.e.,

\[
\begin{align*}
t_n^\nu (\lambda) &= + \sum_p \sum_q \sum_r \sum_g K_{n pqr}^{\nu g} \rho_g^{\nu} (pqr),
\end{align*}
\]

where I have introduced the coefficients

\[
K_{n pqr}^{\nu g} = - \ell_{n pqr}^{\nu} \alpha_g^{\nu} (\lambda),
\]
Equation (4.27) expresses a linear relation between the observable parameters \( \{ d_i \} \equiv \{ t^n(\lambda_\nu) \} \) and the model parameters \( \{ m_\mu \} \equiv \{ \rho^g_{pqr} \} \), a relation that, below, shall be written using the two following forms:

\[
d_i = \sum_\mu G_{i\mu} m_\mu ; \quad d = G m .
\]

(4.29)

4.3.2 Simplified Problem

To simplify this numerical problem, let us disregard the variation of the gas concentration as a function of latitude and longitude, by assuming that it depends only on height (see figure 4.22). Equation (4.27) then becomes

\[
t^n(\lambda_\nu) = + \sum_p \sum_g K_{vp}^g \rho^g_p ,
\]

(4.30)

with the coefficients

\[
K_{vp}^g = - \ell_p^m a^g(\lambda_\nu) .
\]

(4.31)

The index \( p \) is the same as above (it represents the \( p \)-th layer of the atmosphere).

Figure 4.22: As a first approximation, disregarding the variation of the concentration of different gases as a function of longitude and latitude, one may use the GOMOS instrument to measure the variation as function of height (figure adapted from Tamminen, 2004).

4.3.3 Numerical Application

Executable notebook at
http://www.ipgp.jussieu.fr/~tarantola/exercices/chapter_04/GOMOS.nb

For the numerical application, we shall just consider two atmospheric layers and three gases in each layer (see figure 4.23), so we have six model parameters. We shall assume that we measure two rays, and, for each ray, the spectral amplitude at two wavelengths, so we have four observations. We have less observations than model parameters, but the explicit use of some a priori information makes this issue irrelevant.

The linear system (4.30) now becomes, explicitly,

\[
\begin{pmatrix}
  t^1(\lambda_1) \\
  t^1(\lambda_2) \\
  t^2(\lambda_1) \\
  t^2(\lambda_2)
\end{pmatrix} = \begin{pmatrix}
  K_{11}^{11} & K_{11}^{12} & K_{12}^{11} & K_{12}^{12} & K_{11}^{13} & K_{12}^{13} \\
  K_{21}^{11} & K_{21}^{12} & K_{22}^{11} & K_{22}^{12} & K_{21}^{13} & K_{22}^{13} \\
  K_{21}^{11} & K_{21}^{12} & K_{22}^{11} & K_{22}^{12} & K_{21}^{13} & K_{22}^{13} \\
  K_{21}^{21} & K_{21}^{22} & K_{22}^{21} & K_{22}^{22} & K_{21}^{23} & K_{22}^{23}
\end{pmatrix} \begin{pmatrix}
  \rho_1^1 \\
  \rho_2^1 \\
  \rho_1^2 \\
  \rho_2^2 \\
  \rho_1^3 \\
  \rho_2^3
\end{pmatrix} .
\]

(4.32)
4.3 The Gomos Instrument in the Envisat Satellite

Figure 4.23: Artificial numerical example, in an imaginary Earth (small globe and large atmosphere). Two rays available, with two wavelengths observed for each ray (four data values). Two atmospheric layers, with three gases in each layer (six model parameters).

Let us introduce the vector \( \mathbf{d} \) representing the four observable quantities,

\[
\mathbf{d} = \begin{pmatrix}
t^1(\lambda_1) \\
t^1(\lambda_2) \\
t^2(\lambda_1) \\
t^2(\lambda_2)
\end{pmatrix},
\]

the vector \( \mathbf{m} \) representing the six model parameters,

\[
\mathbf{m} = \begin{pmatrix}
\rho^1_1 \\
\rho^2_1 \\
\rho^1_2 \\
\rho^2_2 \\
\rho^1_3 \\
\rho^2_3
\end{pmatrix},
\]

and the “sensitivity” matrix

\[
\mathbf{G} = 
\begin{pmatrix}
K_{11}^{11} & K_{12}^{11} & K_{11}^{12} & K_{12}^{12} & K_{11}^{13} & K_{12}^{13} \\
K_{21}^{11} & K_{22}^{11} & K_{21}^{12} & K_{22}^{12} & K_{21}^{13} & K_{22}^{13} \\
K_{21}^{21} & K_{22}^{21} & K_{21}^{22} & K_{22}^{22} & K_{21}^{23} & K_{22}^{23} \\
K_{21}^{23} & K_{22}^{23} & K_{21}^{23} & K_{22}^{23} & K_{21}^{22} & K_{22}^{22}
\end{pmatrix},
\]

so we can write the forward modeling relation (4.32) as

\[
\mathbf{d} = \mathbf{G} \mathbf{m}.
\]

Using equation (4.31), we can explicitly write the sensitivity matrix:

\[
\mathbf{G} = 
\begin{pmatrix}
-a a^1(\lambda_1) & -2 b a^1(\lambda_1) & -a a^2(\lambda_1) & -2 b a^2(\lambda_1) & -a a^3(\lambda_1) & -2 b a^3(\lambda_1) \\
-a a^1(\lambda_2) & -2 b a^1(\lambda_2) & -a a^2(\lambda_2) & -2 b a^2(\lambda_2) & -a a^3(\lambda_2) & -2 b a^3(\lambda_2) \\
0 & -c a^1(\lambda_1) & 0 & -c a^2(\lambda_1) & 0 & -c a^3(\lambda_1) \\
0 & -c a^1(\lambda_2) & 0 & -c a^2(\lambda_2) & 0 & -c a^3(\lambda_2)
\end{pmatrix}.
\]
Assume that laboratory measurements have provided the constants
\[
\begin{align*}
\alpha_1(\lambda_1) &= 0.07 \text{ m}^{-1} ; \quad \alpha_1(\lambda_2) = 0.13 \text{ m}^{-1} \\
\alpha_2(\lambda_1) &= 0.05 \text{ m}^{-1} ; \quad \alpha_2(\lambda_2) = 0.20 \text{ m}^{-1} \\
\alpha_3(\lambda_1) &= 0.09 \text{ m}^{-1} ; \quad \alpha_3(\lambda_2) = 0.15 \text{ m}^{-1}
\end{align*}
\]

(4.38)

that describe the absorption properties of each of our three gases, for each of our two wavelengths. The geometry of the experiment is as indicated in figure 4.23, so we have the following lengths,
\[
a = 10.5 \text{ m} \quad ; \quad b = 4.2 \text{ m} \quad ; \quad c = 11.2 \text{ m} .
\]

(4.39)

We enter these values in the computer as follows

(* I wish that Mathematica knows what a Meter or a Second are *)

\[
< < \text{Miscellaneous`PhysicalConstants} \>
\]

and

(* Introducing the matrix G *)

\[
G = \{\{-s_1 A_1[L1], -2 t_1 A_1[L1], -s_1 A_2[L1], -2 t_1 A_2[L1], -s_1 A_3[L1], -2 t_1 A_3[L1]\},
\{ -s_1 A_1[L2], -2 t_1 A_1[L2], -s_1 A_2[L2], -2 t_1 A_2[L2], -s_1 A_3[L2], -2 t_1 A_3[L2]\},
\{0, -s_2 A_1[L1], 0, -s_2 A_2[L1], 0, -s_2 A_3[L1]\},
\{0, -s_2 A_1[L2], 0, -s_2 A_2[L2], 0, -s_2 A_3[L2]\}\};
\]

\[
s_1 = 10.5 \text{ Meter} ; \quad t_1 = 4.2 \text{ Meter} ; \quad s_2 = 11.2 \text{ Meter} ;
\]

\[
A_1[L1] = 0.07/\text{Meter} ; \quad A_1[L2] = 0.13/\text{Meter} ; \quad A_2[L1] = 0.05/\text{Meter} ;
\]

\[
A_2[L2] = 0.20/\text{Meter} ; \quad A_3[L1] = 0.09/\text{Meter} ; \quad A_3[L2] = 0.15/\text{Meter} ;
\]

We then obtain the following numerical matrix
\[
G = \begin{pmatrix}
-0.735 & -0.588 & -0.525 & -0.420 & -0.945 & -0.756 \\
-1.365 & -1.092 & -2.100 & -1.680 & -1.575 & -1.260 \\
0 & -0.784 & 0 & -0.560 & 0 & -1.008 \\
0 & -1.456 & 0 & -2.240 & 0 & -1.680
\end{pmatrix} .
\]

(4.40)

For the numerical exercise, assume that the prior values of the model parameters are as follows (see the left of figure 4.24),
\[
\begin{align*}
m^1_{\text{prior}} &= 0.019 \pm 0.015 \\
m^2_{\text{prior}} &= 0.019 \pm 0.015 \\
m^3_{\text{prior}} &= 0.021 \pm 0.015 \\
m^4_{\text{prior}} &= 0.021 \pm 0.015 \\
m^5_{\text{prior}} &= 0.025 \pm 0.006 \\
m^6_{\text{prior}} &= 0.016 \pm 0.006 ,
\end{align*}
\]

(4.41)

this defines what in the course has been denoted \( m_{\text{prior}} \) and the covariance matrix \( C_{\text{prior}} \). For the computer this makes
4.3 The Gomos Instrument in the Envisat Satellite

\[ \text{(* Introducing the prior information *)} \]
\[
\begin{align*}
\mathbf{m}_{\text{prior}} &= \{0.019, 0.019, 0.021, 0.021, 0.025, 0.016\}; \\
\text{sigma}[1] &= 0.015; \quad \text{sigma}[2] = 0.015; \quad \text{sigma}[3] = 0.015; \\
\text{sigma}[4] &= 0.015; \quad \text{sigma}[5] = 0.006; \quad \text{sigma}[6] = 0.006; \\
\text{C}_{\text{prior}} &= \text{DiagonalMatrix}\{\text{sigma}[1]^2, \text{sigma}[2]^2, \text{sigma}[3]^2, \text{sigma}[4]^2, \text{sigma}[5]^2, \text{sigma}[6]^2\};
\end{align*}
\]

Finally, assume that the results of our measurements can be expressed as follows:

\[
\begin{align*}
\mathbf{d}_{\text{obs}}^1 &= -0.085 \pm 0.002 \\
\mathbf{d}_{\text{obs}}^2 &= -0.177 \pm 0.002 \\
\mathbf{d}_{\text{obs}}^3 &= -0.040 \pm 0.002 \\
\mathbf{d}_{\text{obs}}^4 &= -0.084 \pm 0.002.
\end{align*}
\]

This defines what in the course has been denoted \( \mathbf{d}_{\text{obs}} \) and the covariance matrix \( \mathbf{C}_{\text{obs}} \). For the computer

\[ \text{(* Introducing the observations *)} \]
\[
\begin{align*}
\mathbf{d}_{\text{obs}} &= \{-0.085, -0.177, -0.040, -0.084\}; \\
\mathbf{C}_{\text{obs}} &= \text{sigmad}^{-2}\text{IdentityMatrix}[4]; \\
\text{sigmad} &= 0.002;
\end{align*}
\]

From this point on, we can just apply the formulas demonstrated in class. The posterior covariance matrix is

\[
\begin{align*}
\mathbf{C}_{\text{post}}^{-1} &= \mathbf{G}^T \mathbf{C}_{\text{obs}}^{-1} \mathbf{G} + \mathbf{C}_{\text{prior}}^{-1},
\end{align*}
\]

and the posterior values of the model parameters are obtained as

\[
\begin{align*}
\mathbf{m}_{\text{post}} &= \mathbf{C}_{\text{post}}\left(\mathbf{G}^T \mathbf{C}_{\text{obs}}^{-1} \mathbf{d}_{\text{obs}} + \mathbf{C}_{\text{prior}}^{-1} \mathbf{m}_{\text{prior}}\right).
\end{align*}
\]

The two lines of code are

\[ \text{(* Using the linear least squares formulas *)} \]
\[
\begin{align*}
\mathbf{C}_{\text{post}} &= \text{Inverse}[\text{Transpose}[\mathbf{G}].\text{Inverse}[\mathbf{C}_{\text{obs}}].\mathbf{G} + \text{Inverse}[\mathbf{C}_{\text{prior}}]]; \\
\mathbf{m}_{\text{post}} &= \mathbf{C}_{\text{post}}.(\text{Transpose}[\mathbf{G}].\text{Inverse}[\mathbf{C}_{\text{obs}}].\mathbf{d}_{\text{obs}} + \text{Inverse}[\mathbf{C}_{\text{prior}}].\mathbf{m}_{\text{prior}});
\end{align*}
\]

With this, one obtains the posterior solution and the following posterior uncertainties, represented at the right of figure 4.24 (the prior values are also included, for discussion):

\[
\begin{align*}
\mathbf{m}_{\text{post}}^1 &= 0.028 \pm 0.008 \quad; \quad (\mathbf{m}_{\text{prior}}^1 = 0.019 \pm 0.015) \\
\mathbf{m}_{\text{post}}^2 &= 0.022 \pm 0.007 \quad; \quad (\mathbf{m}_{\text{prior}}^2 = 0.019 \pm 0.015) \\
\mathbf{m}_{\text{post}}^3 &= 0.016 \pm 0.004 \quad; \quad (\mathbf{m}_{\text{prior}}^3 = 0.021 \pm 0.015) \\
\mathbf{m}_{\text{post}}^4 &= 0.011 \pm 0.003 \quad; \quad (\mathbf{m}_{\text{prior}}^4 = 0.021 \pm 0.015) \\
\mathbf{m}_{\text{post}}^5 &= 0.027 \pm 0.005 \quad; \quad (\mathbf{m}_{\text{prior}}^5 = 0.025 \pm 0.006) \\
\mathbf{m}_{\text{post}}^6 &= 0.017 \pm 0.005 \quad; \quad (\mathbf{m}_{\text{prior}}^6 = 0.016 \pm 0.006).
\end{align*}
\]
We shall also discuss in class the posterior correlation matrix:

\[
\rho = \begin{pmatrix}
1 & -0.16 & -0.70 & +0.29 & -0.69 & -0.04 \\
-0.16 & 1 & +0.25 & -0.66 & -0.05 & -0.80 \\
-0.70 & +0.25 & 1 & -0.51 & +0.01 & +0.07 \\
+0.29 & -0.66 & -0.51 & 1 & +0.09 & +0.10 \\
-0.69 & -0.05 & +0.01 & +0.09 & 1 & -0.01 \\
-0.04 & -0.80 & +0.07 & +0.10 & -0.01 & 1
\end{pmatrix}
\] (4.46)

Figure 4.24: Prior and posterior information on the model parameters.

4.3.4 Question:
What should we do if the lengths \(a\), \(b\), and \(c\) had significant uncertainties?

4.3.5 References