Identification of Vertical Profiles of Radar Reflectivity for Hydrological Applications Using an Inverse Method. Part I: Formulation

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ABSTRACT

The vertical variability of reflectivity in the radar beam is one of the main sources of error in estimating rainfall intensity. This vertical variability, which has several origins, is characterized globally by a function called "vertical profile of reflectivity." The impact of this vertical profile of reflectivity on the radar measurement is quantified by incorporating this function in the radar equation. It is then possible to specify the influence of the characteristics of the radar, the distance, and the vertical profile on errors in estimating rain rates at the ground level. A method for determining the vertical profile of reflectivity is then described. This procedure requires the use of radar images from at least two different elevation angles. It is based on the evolution of the ratio of reflectivities (reflectivity at high elevation divided by reflectivity at a lower elevation angle) versus distance. The ratio evolution is closely related to the vertical profile of reflectivity and to the conditions of radar operation. An inverse solution method is used to identify the vertical profile of reflectivity corresponding to the observed ratio of reflectivities. The advantages and limitations of the proposed method are discussed.

1. Introduction

The hydrological use of weather radar is subject to many sources of errors, described at length in the literature (see, for example, the summaries of Wilson and Brandes 1979; Doviak 1983; Austin 1987; and Joss and Waldvogel 1990). Zawadski (1984) proposed a classification of discrepancies between radar measurements and rainfall rates. Reducing these uncertainties can be addressed by three different approaches:

1) Early efforts in quantitative radar hydrology were focused on the relation between radar reflectivity factor and rainfall intensity; many \( Z-R \) relations have been proposed in this way (Battan 1973) since the initial work of Marshall et al. (1947). Much more recently, improved estimates of rainfall intensities have been expected from advances in the radar system. Going beyond the use of a conventional reflectivity factor, additional parameters are measured to provide information about the type and size of hydrometeors (Atlas et al. 1984), such as differential reflectivity (Messaoud and Pointin 1990).

2) Taking rain gauge data into account is the second approach to improving precipitation measurement by radar. Rain gauge data serve first to correct the systematic bias that is often found in radar measurements. This correction originally took the form of a mean calibration factor applied to the radar image; spatial and temporal variations of this factor were later introduced (Wilson and Brandes 1979; Brandes 1975). Recent improvements in the principle of systematic bias correction include the work of Smith and Krajewski (1991). The adjustment of the radar data by pluviographic data has also been used to correct local errors (Collier et al. 1983). More sophisticated techniques based on a geostatistical approach for combining radar and ground-based data have, furthermore, shown their utility (Creutin et al. 1988; Seo et al. 1989). The disadvantage of these approaches is that they operate too homogeneously in space to effectively take account of the distance-dependent errors caused by the influence of the vertical variability of precipitation with altitude on the radar measurement (Koistinen and Puhakka 1986).

3) The third approach to the correction of radar observations takes the vertical variability of precipitation into account by introducing the vertical profile of reflectivity (VPR). It consists of converting a radar measurement made from a given altitude into an equivalent measurement at a reference level—chosen, for example, at ground level according to the influence of this VPR. In spite of early interest in the VPR,
garded as a major component of the radar observation [see, for example, the pioneering work of Austin and Bemis (1950) on the bright band], the first attempts to incorporate the VPR in a radar measurement correction procedure were made about 20 years later (Joss and Waldvogel 1970). According to Smith (1990), very different techniques can now be grouped under this name. They include, on the one hand, the distance-dependent corrections that treat the consequences of the vertical heterogeneity of the radar measurement without determining the VPR and, on the other, methods of identifying the vertical profile of reflectivity.

The method described below belongs to this second category. The objective is to provide, automatically, the VPR associated with a rain field from the data of a conventional radar operating with at least two different elevations. The main reasons for this choice are 1) to propose a method that uses only the radar measurements, simplifying its operational use; 2) to be able to apply this VPR determination to data concerning short time steps, avoiding the tricky problem of defining types of weather required for establishing mean VPRs (the application described concerns hourly data, but a shorter time step could be considered); and 3) to automate the determination procedure while using a reasonable calculation time.

This first paper is devoted to the formulation and use of the method. Section 2 discusses the influence of the VPR on the radar measurement on the basis of the physics of the radar measurement and introduces the notion of apparent VPR. The influences of several parameters on this error are also described. Section 3 presents briefly the main types of approaches used to determine the VPR. In this part, it is also shown that an effective correction of this source of error involves the determination of the true VPR. The method of identification of the VPR is described in section 4. This method is based on the evolution of the ratio of reflectivities (or intensities) measured at different elevation angles versus distance. This function will be called, hereafter, the “function of reflectivity ratios.” The existence of a close link between reflectivity ratios and vertical profile is established. The identification procedure consists of determining the VPR consistent with a given function of reflectivity ratios. This problem is solved using an inverse method. The formulation of this method is accompanied by a discussion of the various assumptions made. Section 5 deals with the practical use of the method. Further remarks on the feasibility of the procedure and conclusions are given in the last section. A companion paper (Andrieu et al. 1995) deals with a sensitivity analysis of the identification of VPR and a test of its efficiency through a case study.

2. Influence of the vertical profile of reflectivity on the measurement of precipitation by radar

An analytical expression between rainfall rate at the reference level, characteristics of radar beam, and VPR is established. This makes it possible to quantify errors due to VPR and to study their sensitivity to different parameters: beamwidth, elevation angle, and VPR shape.

a. Introduction of the apparent vertical profile of reflectivity

The radar equation assumes that reflectivity is uniform in the radar beam. This assumption ceases to be valid if the reflectivity depends on the altitude. It is, however, possible to simply introduce the VPR into the radar equation. The radar reflectivity \(Z(u, h)\) depends on the geographical location \(u = (x, y)\) of the point in question and on its altitude \(h\). In what follows, it will be assumed that this function \(Z\) can be broken down into two independent functions in the following form:

\[
Z(u, h) = Z_0(u)z(h),
\]

where \(Z_0(u)\) represents the radar reflectivity at reference altitude \(h_0\); \(Z_0(u) = Z(u, h = h_0)\), which will most often be ground level. For its part, \(z(h)\) is a function that represents only the vertical variability of reflectivity with respect to the reference level. The function \(z(h)\) is called the vertical profile of reflectivity. It is assumed that the VPR is the same at any point \(u\) of the zone studied. Furthermore, the VPR is independent of the horizontal variability of rainfall intensities. These assumptions will be discussed in a later paragraph. To simplify notations, the direction of the radar beam will be taken as the axis \(Ox\), assuming that the horizontal variability of the rain field is described only by the horizontal component \(x\) of the distance from the radar to the target. It then follows that

\[
Z(x, h) = Z_0(x)z(h).
\]

Applying the simplified radar equation to an elementary target of area \(d^2\) located in the beam, the power \(d^2p_s\) backscattered by the latter is expressed, in the conventional notation,

\[
d^2p_s(x, A, \theta, \alpha) = \frac{P_sG^2\lambda^2}{(4\pi)^3} f^2(\theta) \frac{d^2\sigma_s(x, A, \theta, \alpha)}{(x^2 + h^2)^2},
\]

where \(P_s\) is the radiated power, \(G\) the antenna gain, \(\lambda\) the wavelength, \(A\) the elevation angle of the radar beam, and \(d^2\sigma_s\) the backscattering cross section. The position of \(d^2\) in the beam is defined by angles \(\theta, \alpha\), and altitude \(h\) (Fig. 1). The radar pulse width is neglected in the following derivations. The distribution of the power \(f(\theta)\) in the beam is assumed to be Gaussian (Bogush 1989). It is given by

\[
f(\theta) = \exp \left[ -\ln 2 \left( \frac{\theta}{\theta_s} \right)^2 \right],
\]
where $2\theta_3$ is the 3-dB beamwidth [defined by the relation $f(\theta_3) = 1/2$]. The effective backscattering cross section $d^2\sigma_s$ of this element is written

$$d^2\sigma_s(x, A, \theta, \alpha) = \frac{\pi^5}{\lambda^4} |K|^2 Z(x, h) d^2s(x, A, \theta, \alpha),$$

with $|K|^2 = 0.93$, the dielectric constant of water.

Assuming the ground surface to be horizontal and the diameter of the beam small with respect to the distance from the radar, $h$ and $d^2s$ are given by

$$h = h_B + x\theta \cos \alpha$$
$$d^2s = (x^2 + h^2)\theta d\theta d\alpha.$$  

The altitude of the beam axis is $h_B$ such that

$$h_B = x \tan A + \frac{3x^2}{8\rho_E},$$

where $\rho_E$ is the radius of the earth.

The expression of $h$ takes into account the inclination of the target due to the elevation angle. Finally, the power $d^2p_s$ backscattered by $d^2s$ is

$$d^2p_s(x, A, \theta, \alpha) = \frac{C}{(x^2 + h^2)} Z_0(x) f^2(\theta)$$
$$\times z(h_B + x\theta \cos \alpha) \theta d\theta d\alpha.$$  

All constant terms in this expression are represented by $C$. To facilitate the integration, it is assumed that all points of the beam are at the same distance from the radar, written $x_B$, such that $x_B^2 = x^2 + h_B^2$; therefore, $x_B^2 \approx x^2 + h^2$. The total power backscattered $p$ is

$$p(x, A) = \int_0^{\theta_6} \int_0^{2\pi} d^2p_s(x, A, \theta, \alpha).$$

The beamwidth used to determine $p$ is to be considered carefully. On one hand, a significant part of the radar sensitivity (25%) is outside the 3-dB beam. The influence of the side lobes can be significant in the presence of a bright band causing strong vertical variations of the reflectivity. On the other hand, for commonly used low-elevation angles, a part of the side lobes reaches the ground very close to the radar. In the following, the adopted compromise consists of using the 6-dB beamwidth, noted $2\theta_6$. It is related to the 3-dB beam by $\theta_6 = \sqrt{2}\theta_3$ and includes 93.75% of the radar sensitivity. But for the sake of convenience, we will still refer to the aperture of the main beam. The integration of Eq. (9) to the beam of width $2\theta_6$ then gives

$$p(x, A) = \frac{C}{x_B^2} Z_0(x) z_a(x, A).$$

The function $z_a$ for its part is written

$$z_a(x, A)$$
$$= \int_0^{\theta_6} \int_0^{2\pi} f^2(\theta) z(h_B + x_B \theta \cos \alpha) \theta d\theta d\alpha.$$

Hereinafter, $z_a$ will be called the “apparent vertical profile of reflectivity.” It is comparable to the notion of vertical rain-rate profile introduced by Hill et al. (1981) to reduce brightband effects (appendix A of this paper). It amounts to the VPR as modified by the characteristics of the radar beam. It is an implicit func-
tion of $A$ by $h_B$. This function is very important, in particular because it is used to quantify the errors of measurement of precipitation caused by the VPR. The mean reflectivity measured by the radar is

$$\bar{Z}(x) = Z_0(x)z_u(x, A).$$

(12)

It is possible to illustrate the smoothing effect introduced by the radar beam by an example. For that, let us consider two fictitious but realistic VPRs. One, VPR1, decreases regularly from the value 1.0 at the level of the radar to 0.0 at an altitude of 4 km, representing the case of warm clouds of moderate vertical extent, often observed in Mediterranean regions. The other, VPR2, has a similar shape, but has a reflectivity peak 1.8 km above the radar. It is an example of a cold cloud having a marked bright band caused by the melting of ice particles, and its variations versus altitude are much more marked than those of VPR1. For the sake of simplicity, each of these VPRs is represented by five linear segments (Fig. 2a). To make the diagram clearer (Fig. 2b), the VPR scale ($X$ axis) is in decibels and the linearity does not appear. The beamwidth is $2\theta_B = 1.5^\circ$, the elevation angle ranges from $\theta_3$ to the vertical, and the distance from the radar is from 0 to 100 km. The role played by the radar beam is illustrated by calculating the apparent VPR defined by Eq. (11)

Fig. 2. (a) Principle of representation of a VPR by five linear segments. (b) Shape of the two example VPR: the $X$ axis is expressed in decibels.

versus distance and altitude. The results are given in Fig. 3. This figure represents the apparent VPR observed by the radar at a given distance and beam axis altitude. The lowest part is shielded because of the earth curvature. Near the radar, both apparent VPRs differ very little from the true VPR of Fig. 2. When the distance from the radar increases, the bottom of the profile is less and less correctly perceived, and this profile appears considerably smoothed. This finding is true especially in the case of VPR2, for which it becomes nearly impossible to extract the characteristic signature of the bright band beyond 70 km.

b. Influence of the VPR on measurement of precipitation

The rainfall intensity at the reference level, the ground, and distance $x$, written $R_0(x)$, is given by

Fig. 3. Influence of the distance and of the beam-axis height on the apparent VPR in the case of VPR1 and VPR2. Isolines represent the apparent VPR (in decibels of reflectivity). The beam axis cannot reach the shaded area because of the earth’s curvature.
\begin{equation}
R_0(x) = \left[ \frac{Z_0(x)}{a} \right]^{1/b},
\end{equation}

where \( a \) and \( b \) are the parameters of the \( Z-R \) relationship. Furthermore, the corresponding mean reflectivity in the beam \( \bar{Z}(x) \) yields an erroneous estimate of the rainfall intensity at ground level \( R_e \):

\begin{equation}
R_e(x) = \left[ \frac{\bar{Z}(x)}{a} \right]^{1/b},
\end{equation}

which can also be written

\begin{equation}
R_e(x) = \left[ \frac{Z_0(x)z_a(x, A)}{a} \right]^{1/b}.
\end{equation}

Combining Eqs. (13) and (15), it is possible to determine the relative error \( \text{Er} \) of estimate of rainfall intensities due to the influence of the VPR. It can be expressed

\begin{equation}
\text{Er}(x, A) = \frac{R_e}{R} - 1
\end{equation}

\begin{equation}
\text{Er}(x, A) = z_a(x, A)^{1/b} - 1.
\end{equation}

This error, therefore, depends only on the VPR shape and the characteristics of the beam. As an illustration, its magnitude can be evaluated in the particular cases of VPR1 and VPR2, mentioned previously. Figure 4 represents the evolution of this error versus distance for a beamwidth \( 2\theta_3 = 1.5^\circ \) and an elevation angle \( A = 1.5^\circ \). An increasing underestimate is observed for VPR1, whereas VPR2 produces a large overestimate of the intensities that persists until a distance of 80 km. Figure 5 shows the sensitivity of the relative error to the radar elevation angle. The beamwidth is also 1.5\(^\circ\) and the elevation ranges from 1.0\(^\circ\) to 2.0\(^\circ\). It thus appears that for VPR1 and VPR2, the error of estimate of precipitation depends significantly on this parameter. Finally, the measurement error is also influenced by the beamwidth. Figure 6 shows the evolution of the error of estimate caused by VPR2 versus distance for various beamwidth values, the elevation angle being 1.5\(^\circ\): the smaller the beamwidth, the larger the maximum error. It should, however, be noted that the influence of the beamwidth is negligible in the case of VPR1, of which the variations with altitude are more regular.

In summary, the VPR can cause significant errors in the rainfall estimations at ground level when the distance to the radar is over 40 km. The spatial distribution of these errors depends on the shape of the VPR and the characteristics of the radar beam. Moreover, it is not possible to base the correction of these errors on observed VPR obtained with volume scans or RHI (range–height indicator; vertical scan of the atmosphere at a constant azimuth). This difficulty arises due to the inability to deduce the true reflectivity at the reference level \( Z_0(x) \) from the apparent reflectivity measured by the radar \( Z_0(x)z(x, A) \).

3. Direct methods of identifying the vertical profile of reflectivity

In order to improve the accuracy of rainfall radar estimates, several authors have proposed methods for determining representative VPR (Joss and Waldvogel 1990; Koistinen 1991 for instance). These VPR are used mainly for three types of corrections:

1) The extrapolation at the ground level of radar echoes recorded at a high altitude. These data are used when corresponding low-altitude radar data are contaminated by ground clutters or beam blockage.
2) The suppression of brightband effect.
3) The correction of partial beam filling.

The term “representative” means that the VPR is assumed to be spatially homogeneous [see Eq. (1)] and that a VPR observed in a noncontaminated area remains valid in a domain where it cannot be determined.

The identification of VPR is almost never based on a vertically pointed antenna that is as yet the only way to observe this function. Vertical pointing is not a task that operational radars perform routinely. Another reason is that it often does not rain at the radar site. The proposed methods use radar images at different elevation angles or better, volume scans that give a more refined description of the vertical structure of radar reflectivity. Another approach focuses on developing physically based models in order to relate vertical changes of reflectivity to physical processes affecting water particles in the atmosphere. The main types of method are described in the remaining part of this section.
(It is an arc in this particular case.) The radar reflectivities measured at altitude $h$ for this elevation angle can be characterized by their mean value $\bar{Z}_A(h)$ expressed

$$\bar{Z}_A(h) = \frac{1}{D_{A,h}} \int_{D_{A,h}} Z_A(u, h) du,$$

(17)

where $Z_A(u, h)$ is the reflectivity at location $u$ and altitude $h$ when the elevation angle is $A$. Alternative parameters, for instance, the maximum reflectivity in the domain (Joss and Waldvogel 1990), can be adopted. Under a factorization similar to that of Eq. (1), the previous expression becomes

$$z(h) = \frac{\bar{Z}_A(h)}{\bar{Z}_0(h)},$$

with

$$\bar{Z}_0(h) = \frac{1}{D_{A,h}} \int_{D_{A,h}} Z_0(u) du,$$

(18)

where $\bar{Z}_0(h)$ is the mean reflectivity at the level of reference in subdomain $D_{A,h}$. Since $\bar{Z}_0(h)$ is not sampled by the beam, its value is not known, and the VPR $z(h)$ cannot be determined. Let us suppose that several PPI images at different elevation angles are available. For the same maximum distance, the range of explored altitudes is more important. The altitude $h$ is reached by different beams. The domain $D_h$ grouping all the points where the radar measures the reflectivity at altitude $h$ is larger and the statistics are more robust. The VPR becomes

$$\bar{Z}(h) = z(h) \bar{Z}_0[D_h] \quad \text{and} \quad D_h = \sum_A D_{A,h}.$$

(19)

\textbf{Fig. 5.} Sensitivity of the relative error in the rain rate to the beam elevation angle for VPR1 and VPR2.

\textit{a. Methods using mean}

The most popular approach consists of determining a mean VPR reliable in both space and time. The region used to calculate this mean VPR must be close to the radar so that beam smoothing effect can be neglected. A maximum distance not exceeding 40–50 km is generally chosen. Figure 3 indicates that this distance is reasonable, the apparent reflectivity being similar to the true one. To describe these methods, one imagines an ideal and hypothetical beamwidth small enough to suppose that the radar delivers quasi-punctual measurements. Moreover, the reflectivity can be factorized in accordance with Eq. (1).

For each PPI (plan position indicator) image with an elevation angle $A$, it can be defined a subdomain $D_{A,h}$ grouping all the points of the beam at altitude $h$.

\textbf{Fig. 6.} Sensitivity of the relative error in the rain rate to the beamwidth in the case of VPR2 for different beamwidths: $\theta_3 = 1.0^\circ$ (solid line), $\theta_3 = 1.5^\circ$ (dotted line), and $\theta_3 = 2.0^\circ$ (dashed line).
The VPR still depends on the horizontal distribution of the radar reflectivity at the level of reference \( \bar{Z}_0(D_0) \). To resolve this difficulty, a set of observations must be grouped (a day, a month, or a type of weather). It is assumed that the grouped observations have similar VPR and that the reflectivity field at the reference level \( Z_0 \) is stationary, implying that \( E[Z_0(u)] = m_0 \) is constant and does not depend on \( u \). Calculating the mathematical expectation of Eq. (19) gives the expression of the VPR \( z(h) \):

\[
E[\bar{Z}(h)] = z(h)E[\bar{Z}_0(D_0)]
\]

or

\[
z(h) = \frac{E[\bar{Z}(h)]}{m_0}.
\] (20)

Then, the VPR is obtained by dividing the expected reflectivity at altitude \( h \) by the expected reflectivity at the reference level. [See results of Koistinen (1991) for a set of daily data.]

b. Methods using ratios

It is obvious that the main limit of methods using mean is due to the strong assumption concerning the uniformity of the horizontal structure of the reflectivity field, the goal being to filter this variability. A second approach was proposed initially by Harrold and Kitchingham (1975) to detect the presence of a bright band. Smith (1986) used a close principle to develop a brightband identification method. It consists of calculating the ratio of radar reflectivity factors observed at two elevation angles \( A_1 \) and \( A_2 \) \((A_1 < A_2)\) versus horizontal distance from the radar:

\[
q_z(x, A_1, A_2) = \frac{Z(x, h_{A_2})}{Z(x, h_{A_1})},
\] (21)

with \( q_z \) being the ratio of the reflectivities and \( h_{A_1} \) and \( h_{A_2} \) the altitudes of the axis of the beam at the distance \( x \) for elevations \( A_2 \) and \( A_1 \). Taking into account the invariance of the VPR and the breakdown of the reflectivity of Eq. (2) gives

\[
q_z(x, A_1, A_2) = \frac{z(h_{A_2})}{z(h_{A_1})} = \frac{z(x \tan A_2 + h_E)}{z(x \tan A_1 + h_E)},
\] (22)

where \( h_E \) is the component due to the curvature of the earth. The reflectivity ratio function filters out the horizontal variability of the reflectivity and depends only on the VPR. To illustrate the link between the ratio function and VPR, let us consider the case where the low elevation is horizontal \((A_1 \approx 0.0)\). If the beamwidth is assumed to be very small, it can be admitted that \( h_{A_1} \approx 0.0 \) and \( h_E \approx 0.0 \) as long as the distance from the radar is not too large, and, therefore, \( z(h_{A_1}) = 1.0 \). The ratio of reflectivities then becomes

\[
q_z(x, A_1, A_2) \approx z(x \tan A_2).
\] (23)

The ratios function, therefore, represents exactly the VPR. The interest of this finding lies in three elements: 1) it does not need any reflectivity assessment at the reference level; 2) the filtering out of the horizontal variability of reflectivities makes this possible; and 3) it is easy to calculate the ratios of reflectivities experimentally in the domain in question when at least two PPIs are available. The spirit of this method is close to the approach based on the ratio of the radar data and rain gauges data proposed by Collier (1986a). Let us assume that rain gauges measurements \( R(x) \) can be transformed into equivalent reflectivities \( Z_0(x, A_1 = 0) \). If radar data are accurate, it happens \( Z_0(x, 0) \approx Z_0(x) \) and Eq. (22) can be written

\[
q_z(x, A_1 = 0, A_2) = \frac{Z_0(x)z(h_{A_2})}{Z_0(x)} \approx z(h_{A_2}).
\] (24)

The assessment factor introduced to correct radar data is comparable to the function of ratios introduced in this section. But this approach uses an external source of information that is beyond the scope of this paper.

c. Microphysical models of bright band

Solving the problem of bright band is one of the main objectives of VPR identification. This peak of reflectivity can cause important errors; it is accompanied by very strong gradients that make it difficult to correct. Bright band is associated mostly with the melting layer and is due to the change of the dielectric constant of melting particles and to the increase of their fall velocities. Willis and Heymsfield (1989) provide a detailed description of microphysical processes occurring in the proximity of the melting layer. Theoretical models are proposed to represent these processes. They simulate the melting rate of iced water particles and couple it with the transfer of heat between water particles and the ambient air (Hardaker et al. 1991). More sophisticated models take into account collisions between particles and changes in the drop size distribution (Willis and Heymsfield 1989; Klaassen 1988). It is then possible to generate values of reflectivity and to study the sensitivity of bright band to different parameters. For instance, a link might exist between width of bright band and reflectivity after melting (Klaassen 1988), but this result remains to be confirmed (Hardaker et al. 1991).

d. Limitations of these methods

Microphysical models could be very helpful in the future to improve the identification of VPR. But this approach is not yet compatible with constraints of real-time applications. The direct methods described previously in this section are subject to two main difficulties. The first lies in the fact that the different events of the set of observations are assumed to have the same VPR and primarily concern methods using mean. A
correct use of this first method supposes that the set of observations is large enough to satisfy the hypothesis of stationarity in $Z_0$ but remains small enough to group events having the same VPR. This equilibrium is not easy to find. The second limitation is due to the beam integration that is related to distance from the radar and concerns both methods. The radar does not measure the reflectivity at a given altitude as we have previously assumed. It delivers the mean value of the reflectivity in a vertical part of the atmosphere whose thickness increases with distance from the radar.

This second limitation can be illustrated using the example of VPR1 and VPR2 described in the previous section with a beamwidth of $2\theta_3 = 1.5^\circ$. The radar performs a volume scanning and the different elevation angles $A_i$ that ensure continuity of the sampling are defined by

$$A_i = \theta_3 + 2(i - 1)\theta_3.$$  \hspace{1cm} (25)

It is thus possible to represent the apparent VPR as it is seen by radar for different distances (Fig. 7). The figure shows that at distances greater than 60 km, only the three lowest levels are useful. Furthermore, it confirms that the influence of the discretization causes a considerable loss of information when there are strong vertical gradients in the VPR (VPR2). This example proves clearly that volume scanning is therefore not sufficient to determine the VPR at medium distances (approximately 60–90 km) that are in the hydrological range of the radar.

Two solutions have been proposed to solve this difficulty. The first is to reduce the range used to determine the VPR in order to limit the smoothing effect of the radar beam. However, this solution is at fault when rainy areas are located at medium distances outside the domain where the VPR is well observed. Another solution is to weight the vertical profiles as an inverse function of the distance [see Koistinen (1991) and Joss and Waldvogel (1990)]. This type of weighting can be introduced explicitly, for instance, by changing the distance exponent in the radar equation ($r^{2.8}$ instead $r^2$). This procedure is equivalent to defining a climatological correction of the VPR influence with a factor that increases with distance.

To avoid problems attached to the direct identification of the vertical profile of reflectivity, an indirect method is proposed in the next section. The term "indirect" means that it identifies the most probable VPR attached to the radar observations of a rain field and is consistent with the radar equation and the influence of the beam [Eqs. (10) and (11)]. The approach uses the radar reflectivity (or intensity) ratio function and requires radar images at two, or more, elevation angles. It can be applied to a single observation or a set of observations and gives information (variance of estimate) on the reliability of the identified VPR.

**4. Method of identification of the vertical profile of reflectivity**

The expression of reflectivity ratio introduced previously confirms [(Eq. 22)] that this quantity is independent of the reflectivity at reference level and depends only on VPR. The inverse method used to perform the identification of the discretized VPR is described in detail.

**a. Ratio of reflectivities**

According to the expression for the apparent VPR [Eq. (11)],

$$q_2(x, A_1, A_2) = \frac{\int_0^3 \int_0^{2\pi} f^2(\theta) z(h_{A_2} + x\theta \cos \alpha) d\theta d\alpha}{\int_0^3 \int_0^{2\pi} f^2(\theta) z(h_{A_1} + x\theta \cos \alpha) d\theta d\alpha}, \hspace{1cm} (26)$$
where \( q_z \) is the ratio of the reflectivity measured at elevation \( A_2 \) by the one measured at elevation \( A_1 \); \( h_{A_1} \) and \( h_{A_2} \) are the altitudes of the axis of the beam at horizontal distance \( x \) for elevation angles \( A_1 \) and \( A_2 \), and \( 2\theta_0 \) is the 6-dB beamwidth.

This relation shows that the reflectivity ratio function depends only on the characteristics of the radar beam and the true VPR. However, there is no simple analytical relation for Eq. (26), except in the special case used in the preceding section to introduce this function. In fact, the function \( q_z \) gives an image of the VPR modified by the geometry of the beam and the use of a ratio to eliminate the influence of the horizontal variability. [See the sensitivity study presented in the second part of Andrieu et al. (1995).] This approach is justified, however, by the ease of calculating the experimental values of these ratios. Therefore, the objective pursued is to determine the VPR that best serves to reconstitute the reflectivity ratio observations with the theoretical model defined by Eq. (26). The described method uses only radar data at two elevations; it is therefore applied to a relatively difficult case. However, the example of Fig. 7 shows that when the distance increases, only the first two or three elevations are informative, and the chosen situation becomes representative of realistic conditions. In addition, it can easily be extended to the case where several elevations are available, with the addition of data leading to greater effectiveness. Finally, it is simpler to describe it with only two elevations.

b. Discretization of the problem

In the absence of a simple analytical relation between the ratios function and the VPR, Eq. (26) must be simplified to evaluate a numerical solution. For this purpose, a linear breakdown of the VPR is performed. It consists of representing the VPR by a piecewise constant function

\[
z(h) = \sum_{i=1}^{i=n_z} z_i e_i(h),
\]

where \( \{e_i, i = 1, n_z\} \) is a base of functions defined, for instance, by

\[
e_i(h) = \begin{cases} 1, & \text{if } h_i^- = (i - 1) \Delta h \leq h \leq h_i^+ = i \Delta h \\ 0, & \text{otherwise}. \end{cases}
\]

The number of vertical discretizations is \( n_z \) and \( \Delta h \) is the height of the discretization.

The apparent VPR can then be expressed in a linear manner with respect to the components of the VPR by

\[
z_a(x, A) = \sum_{i=1}^{i=n_z} \beta_i(x, A) z_i
\]

in which the beamwidth is an implicit parameter. The calculation of \( \beta_i \) and the expression of this coefficient are described in appendix A. In the end, the reflectivity ratios function is related to the VPR by the following formula:

\[
q_z(x, A_1, A_2) = \frac{\sum_{i=1}^{i=n_z} \beta_i(x, A_2) z_i}{\sum_{i=1}^{i=n_z} \beta_i(x, A_1) z_i}.
\]

It often happens that radar data are available in rainfall intensities—for example, when hydrological totals are studied during a time interval. Since intensities are obtained generally with a relation \( Z = aR^b \), the ratio of reflectivities can be transformed into a ratio of intensities (written \( q_i \)) given by

\[
q_i(x, A_1, A_2) = q_z(x, A_1, A_2)^{1/b}.
\]

c. Identification of the VPR from the reflectivities ratio function

To describe the proposed approach, it is practical to consider a space \( E^{n_z+n_p} \) of dimension \( n_z + n_p \) in which each point having coordinates \((z, q)\) represents the state of the physical system studied. (See Fig. 8, where the subspaces \( E^{n_z} \) and \( E^{n_p} \) describing the VPR and the

![Fig. 8. Joint probability distribution for measured ratio and a priori VPR (dashed lines). The proposed solution \( z', q' \) fits the theoretical model (black triangle on the solid line), and it is bounded by extreme possibilities where \( z_0 \) (black circle) or \( q_0 \) (black square) are retained as such.](image)
ratios function, respectively, are taken as the $x$ and $y$ axes in a plane representing $E^{n_x,n_y}$. Out of the infinity of possible states of the system, only subset $S$ is allowed by the model described in the previous section and summed up by the equation $q = m(z)$. This subset is represented by the curve (solid line) of Fig. 8. For an observed ratios function (vector $q$), the determination of the VPR consists of finding the VPR (vector $z$) that agrees with the theoretical model describing the physical phenomenon ($m$). The approach used to determine this VPR calls for several remarks:

- The inverse problem to be solved is nonlinear to the extent that the reflectivity ratios are stated in a nonlinear way versus without there being any simple analytical statement of the model $m^{-1}$. This problem is also explicit and discrete because of the nature of Eq. (28) and the available data.

- The problem is not clearly under- or overdetermined. In effect, the characteristics of the radar beam (elevation angles, distance from the radar, etc.), together with the desired level of discretization of the VPR, may lead either to the existence of more than one solution (underdetermination) or no exact solution (overdetermination).

- The experimental values of the ratios $q$ are affected by measurement errors. Moreover, the assumption of invariance of the VPR in the geographical zone in question is an approximate reality. One must therefore accept that the result is a simplified representation of reality. In the end, various sources of uncertainties must be taken into account.

- It may happen that a priori information on the VPR is available. For example, the VPR always has the value of zero beyond a certain altitude (the echotop level); the finding of a bright band contributes information about the shape of the VPR.

The method chosen to solve this inverse problem, including accounting for all of these remarks and constraints, belongs to discrete inverse theory, which constitutes an extension of probability theory to the identification of parameters and functions. General descriptions of discrete inverse theory are given by Menke (1989) and Tarantola (1987). The algorithm used in this work is that proposed by Tarantola and Valette (1982a,b).

Let us assume that the ratios $q$ and the VPR $z$ are realizations of two random vectors called $Q$ and $Z$ of which the statistical distribution follows a Gaussian law. The a priori knowledge about the state of the system consists of the observed ratio vector, designated as $q_0$, and possible information about the VPR described by the vector $z_0$. The statistical distribution of this a priori information is therefore

$$F_a(z) = \exp \left\{ -\frac{1}{2} (z - z_0)^T C_z^{-1} (z - z_0) \right\}$$

$$F_a(q) = \exp \left\{ -\frac{1}{2} (q - q_0)^T C_q^{-1} (q - q_0) \right\},$$

where $F_a$ is a Gaussian probability density, $C_z$ is the matrix of covariance of the various components of the VPR, $C_q$ is that of the observed ratios, and $T$ signifies transpose. The joint probability density $F_a(z, q)$ is also Gaussian. Assuming that the distribution of the observed data is independent of the a priori information available about the parameters, this entails (Menke 1989)

$$F_a(z, q) = F_a(z) F_a(q). \quad (33)$$

In Fig. 8, this joint probability density is illustrated by the ellipses shown in dotted lines. The solution is in the form of the maximum likelihood for a pair of vectors $(z', q')$ such that the relation $q' = m(z')$ is verified and the joint probability density $F_a(z', q')$ is maximum. In geometrical terms, the method selects from subset $S$ (the solid curve of Fig. 8) the point (black triangle of the same figure) at which the probability density (isolines) is greatest. The technique of Lagrange multipliers is the appropriate method to solve the problem:

$$\Phi(z, q) = (z - z_0)^T C_z^{-1} (z - z_0) + (q - q_0)^T$$

$$\times C_q^{-1} (q - q_0) \text{ maximum}$$

$$q = m(z), \quad (34)$$

where $\Phi$ is the likelihood function to maximize. The solution vector $z'$ satisfies the following relation (see appendix B for details of the mathematical derivations):

$$z' = z_0 + C_z M^T (M C_z M^T + C_q)^{-1}$$

$$\times [q_0 - m(z') + M(z' - z_0)], \quad (35)$$

where $M = (\partial m_i / \partial z_j)$ is the partial derivatives of the model $m$. Equation (35) is solved using an iterative fixed point method when the elements of $M$ can be regarded as continuous functions (in other words, when the nonlinearity remains small). Starting from an arbitrary initial point $z_1$, one generally uses $z_0 = z_1$, the following iterative formula is used:

$$z_{k+1} = z_0 + C_z M_k (M_k^T C_z M_k + C_q)^{-1}$$

$$\times [q_0 - m(z_k) + M_k(z_k - z_0)], \quad (36)$$

in which $z_k$ constitutes the result of the $k$th iteration and $M_k$ the matrix of partial derivatives at point $z_k$. Further information about the stability, convergence, and uniqueness of the solution of such nonlinear problems can be found in chapter 9 of Menke (1989) and in Tarantola and Valette (1982a,b). It should merely be noted that if the problem is overdetermined, the solution is independent of the starting point of the iterative process, but in the case of underdetermination, the solution is no longer independent of this starting point, and the greater the underdetermination the larger its influence. In addition to the estimate of the VPR, the algorithm gives the vector of the reflectivity
ratios $q_j$ corresponding to the solution found, providing information about the quality of the obtained result. Finally, it is also possible to calculate the a posteriori matrix of covariance associated with the solution of the problem (Tarantola and Valette 1982a,b).

The method presented above appears to be capable of taking into account the important aspects issues for the identification of the VPR: nonlinearity and inverse conditioning, under- and overdetermination, errors in the data and parameters, and integration of available a priori information. The next section deals with the implementation of this method.

5. Use of the method of identification of the VPR

The statistical inference of data and parameters (i.e., the adjustment of statistical tools to the available data) constitutes the first aspect to be considered in applying the proposed method of VPR identification. On the one hand, the vector of the observations $q_i$ (or $q_k$) and that of the parameters $z$ are assumed to be random vectors. These observations are not perfect and the distribution of the observation errors can be described by a normal law. By the same way, it is accepted that the error between the a priori VPR and the true one is distributed according to a normal law. The solution of system of Eq. (34) therefore involves checking the hypothesis of normality and determining both first moments: mean and covariance. On the other hand, the available data are the observed values of the ratios $q_i(x_i, A_1, A_2)$ measured in the domain in question, completed by the a priori information about the vector of parameters to be identified: for example, an approximate altitude for the top of the echoes or of the bright band deduced from the meteorological context. When the objective is to determine VPRs at very short time steps, as is the case in this paper, it could be preferable to define the statistical properties (mean, covariance) for each rainfall event rather than to apply a climatological analysis.

As for the vector of the ratios of reflectivities or of intensities $q_i$ or $q_k$, each of the $n_z$ components $q_{iz}$ can be regarded as a random variable of which the value is estimated using all observations located at the same distance $x_i$ from the radar. In other words, at this distance, $n_z$ distinct azimuths have been explored at both elevations $A_1$ and $A_2$. It is thus possible to check the initial hypothesis of Gaussian distribution and to determine the mean and the covariance of the ratios:

$$\overline{q}_{ik} = \frac{1}{n_k} \sum_{m=1}^{m=n_k} q_i(x_i^m, A_1, A_2)$$

$$\text{cov}(q_{ik}, q_{ik}) = \frac{1}{n_k - 1} \sum_{m=1}^{m=n_k} [q_i(x_i^m, A_1, A_2) - \overline{q}_{ik}] \times [q_i(x_i^m, A_1, A_2) - \overline{q}_{ik}], \quad (37)$$

where $x_i^m$ represents the points located at distance $x_i$ and $q_{ik}(x_i^m, A_1, A_2)$ the corresponding observed ratios.

Because of the physical link between the VPR and the ratios, there naturally exists a high correlation between nearby ratios of reflectivities; but it is also likely that the errors on these ratios are correlated. To improve the robustness of the statistical inference, theoretical relations are introduced to model the mean error and the covariance:

$$\sigma_{q_j} = \alpha \bar{q}_j + \gamma$$

$$\text{cov}(q_j, q_k) = \sigma_{q_j} \sigma_{q_k} \exp \left[ - \frac{(x_j - x_k)^2}{D_q^2} \right]. \quad (38)$$

In these equations, the standard deviation of the measurement error $\sigma_{q_j}$ on a ratio is a linear function of this same ratio, therefore, introducing two parameters: $\alpha$ and $\gamma$. The last parameter $\gamma$ is mainly to keep $\sigma_q$ positive when the ratio is zero. Then $\alpha$ is equivalent to the coefficient of variation of the statistical distribution of the ratio error; it is assumed to be independent of the distance. For its part, $D_q$ is the decorrelation distance of the error on the ratios. The second relation is consistent with the hypothesis of normal distribution at ratio error, even though it is not really possible to check it. Finally, it must be borne in mind that only the spatial variability of the ratios is taken into account, and the temporal variability does not necessarily have the same characteristics.

Let us now consider the case of the VPR $z$; only the a priori information can assist the inference. It is impossible to verify the Gaussian hypothesis. The VPR $z_0$ can be initialized by different approaches. The crudest is to use a very simple shape, equal to 1.0 from the reference level up to the altitude corresponding to half that of the echo-top altitude (noted htop) above which it linearly falls off to zero. A more elaborate approach could be to use a climatological VPR (Joss and Pittini 1991) or to make use of meteorological information—for example, statistics of the 0°C isotherm altitude (Collier 1976). When the VPR identification is made regularly, every hour for example, an alternative approach could be to initialize the algorithm with the VPR determined at the previous time step. The choice of covariance matrix $C_z$ is undoubtedly the most difficult part of the statistical inference. In effect, there is no objective element to assist this choice, but its impact on the identification procedure is substantial. If the covariance of $z$ is very low, the algorithm assumes that the initial value given to the VPR a priori are reliable and the end result will remain very close to this. Conversely, if $\sigma_z$ is very large with respect to $\sigma_q$, it means that very little importance should be attached to $z_0$, the value of which is regarded as not very reliable. For the sake of simplicity, the standard deviation of the error on the components of the VPR is assumed constant at all altitudes, and an exponential model, consistent with the Gaussian hypothesis, is selected for the covariance function:
\[ \sigma_{z_i} = \sigma_z \]

\[ \text{cov}(z_i, z_j) = \sigma_z^2 \exp\left[-\left(\frac{h_i - h_j}{D_z}\right)^2\right], \quad (39) \]

where \( h_i \) and \( h_j \) are the respective altitudes of components \( z_i \) and \( z_j \) of the VPR and \( D_z \) is the decorrelation distance. This last parameter \( D_z \) is also very important because it is the one that allows the components close to the VPR to vary more or less with respect to one another.

The last point to be taken into account in using the VPR determination procedure concerns the model \( m \) that acts in Eq. (35) through the matrix of partial derivatives \( \mathbf{M} \). There is no difficulty in deriving Eq. (30) or its equivalent in terms of intensity ratios. We find for example \( \mathbf{M} = (m_{z_0}) \) in the case of the reflectivity ratios:

\[ m_{z_0} = \frac{\partial q_z(x_i, A_1, A_2)}{\partial z_j} \sum_{k=1}^{k=n_z} z_k [\beta_j(x_i, A_2)\beta_k(x_i, A_1) - \beta_j(x_i, A_1)\beta_k(x_i, A_2)] \]

\[ m_{z_0} = \frac{1}{\sum_{k=1}^{k=n_z} z_k \beta_k(x_i, A_2)} \sum_{k=1}^{k=n_z} z_k \beta_k(x_i, A_2) \]

and for the intensity ratios \( \mathbf{M} = (m_{q_0}) \); taking Eq. (31) into account:

\[ m_{q_0} = \frac{1}{b} \left[ q_r(x_i, A_1, A_2) \right]^{1/b} m_{z_0}, \quad (41) \]

where \( b \) is the exponent of the \( Z-R \) relationship.

6. Further remarks and conclusions

In the application of this method of VPR identification, a few simple ideas must be borne in mind concerning the assumptions and the encountered limitations.

First, the proposed method is based on the existence of a mean VPR representative of the vertical structure of reflectivity in the domain investigated. This assumption can of course be challenged, and it is sometimes in default. Collier (1976) studying the climatology of the 0°C isotherm, illustrates its spatial heterogeneity and Harrold et al. (1968) show examples of rapid changes of the melting layer level. However, there is a lack of objective information to specify how well the mean VPR represents the true VPR. The statistical analysis of voluminal radar data or information provided by a vertically pointing radar could be the path to consider to better define the conditions of validity of the VPR homogeneity assumption. In each case, it is appropriate to select time- and space scales that make this assumption plausible given the dynamics of the atmospheric phenomena of the meteorological situation in question.

A second important issue concerns the over- or underdetermination of the problem to be solved. To cover a rather large geographical area, the radar beam elevation angles must remain low. Because of this, the lower part of the VPR is over sampled by a beam having a very good resolution (close to the radar), while the upper part of the VPR is undersampled since the diameter of the beam increases with the distance. The problem of the determination of the VPR is therefore heterogeneously determined. In any case, the results obtained are more reliable in the lower part of the VPR where the fluctuations of reflectivities remain small. The results are probably less reliable in the upper part of the VPR where the determination of the characteristics of the VPR is of more interest. In other words, the a priori information introduced by the VPR \( z_0 \) has a larger influence in the upper part of the VPR. By taking into account images at several elevations, it could be possible to deal with this problem. But it remains a very partial solution, since the number of useful measurements on a given vertical decreases with increasing distance (see Fig. 7).

The third remark concerns checking the obtained VPR. There is no direct way of checking the validity of the result except during experiments where data from a radar aimed vertically provide this possibility. Indirect checking is therefore the only approach that can be considered. One procedure consists of checking whether the measured ratios \( q_0 \) agree with the calculated ratios \( q' \). The effectiveness of the method can be judged by checking that \( q' \) is closer to \( q_0 \) than are the ratios associated with the a priori VPR [\( m(z_0) \)]. When rain gauge data are available, the results can be checked by statistically comparing differences between ground and radar measurements to the theoretical differences due to the influence of the VPR. [This approach is illustrated in Joss and Pittini (1991).]

It should be noted that this procedure can be simplified or extended as the intended application requires. For example, the formulation and the inference can be simplified considerably by assuming that all the covariance matrices are diagonal and that the variances \( \sigma_q \) are constant. On the other hand, significant improvements can be considered. The description covers the case where only two elevations are available, that is, where the vertical information available is limited at short to medium distances (Fig. 7). This formulation can be extended without difficulty to the case where a larger number of elevations exist. It is then possible to determine several ratio functions and to enrich the number of observations, that is, the number of components of the vector \( q \). This development opens the way to two types of improvements: more reliable results and the prospect of identifying local VPRs rather than just a single mean VPR. But the extension of this
method to multielevation angles radar data is to investigate.

In conclusion, the proposed method has two main advantages. First, it takes the physical principles of the radar measurement, in particular the integration performed by the radar beam, explicitly into account. Unlike purely statistical methods, it can be adjusted to the operating protocol and characteristics of the radar. Additionally, based on a simple optimality criteria, it opens the way to an automatic procedure for identification of the VPR for very short time steps.

APPENDIX A

Calculation of the Apparent VPR

The apparent VPR is expressed by Eq. (11), recalled below:

\[
\begin{align*}
  z_a(x, A) &= \int_{0}^{\theta_0} \int_{0}^{2\pi} f^2(\theta) z(h_B + x\theta \cos A) \theta d\theta d\alpha, \\
  (A1)
\end{align*}
\]

where \(x\) is the horizontal distance from the radar, \(A\) is the elevation angle, and \(h_B\) is the beam axis altitude. The value of the beamwidth \(2\theta_0\) is discussed below.

Let us suppose that the VPR can be represented by the following discretized function [Eq. (26)]:

\[
  z(h) = \sum_{i=1}^{n_e} z_{i,e}(h), \\
  (A2)
\]

with \(e_{i}(h) = 1\) if \(h\) belongs to the interval \([h_i^-, h_i^+] = h_i^- + \Delta h\), \(e_{i}(h) = 0\) outside this interval, and \(h_i^- = (i - 1)\Delta h\). The increment of the vertical discretization is \(\Delta h\) and \(n_e\) the number of increments.

The position of each elementary part of the VPR in the radar beam is defined by two angles \(\alpha_i^-\) and \(\alpha_i^+\) (Fig. A1):

\[
  \cos \alpha_i^- = \frac{h_B - h_i^-}{R_B} \frac{1}{\cos A},
\]

and

\[
  \cos \alpha_i^+ = \frac{h_B - h_i^+}{R_B} \frac{1}{\cos A}. \quad (A3)
\]

In the previous expressions, \(A\) is the beam elevation angle, \(h_B\) the altitude of the beam axis given by the Eq. 7, and \(R_B\) its radius such \(R_B = x\theta_0/\cos A\), \(\theta_0\) being the half-beamwidth. Finally, \(\alpha_i^-\) and \(\alpha_i^+\) take the following form:

\[
  \alpha_i^- = \cos^{-1}\left(\frac{h_B - h_i^-}{x\theta_0}\right),
\]

and

\[
  \alpha_i^+ = \cos^{-1}\left(\frac{h_B - h_i^+}{x\theta_0}\right),
\]

with

\[
  \alpha_i^\pm = \begin{cases} 
  0, & h_i^\pm \leq h_B - x\theta_0, \\
  \pi, & h_i^\pm > h_B + x\theta_0.
\end{cases} \quad (A4)
\]

Introducing this linear decomposition of the VPR leads to a new expression of the apparent VPR:

\[
  z_a(x, A, \theta_0, z) = \sum_{i=1}^{n_e} z_i\beta_i, \quad (A5)
\]

\[
  \beta_i = \int_{D_i} f^2(\theta) \theta d\theta d\alpha, \quad (A6)
\]

**Fig. A1.** Principle of calculation of the apparent VPR.
where $D_i$ is the part of the beam section delimited by the two angles $\alpha_i^+$ and $\alpha_i^-$, and $f(\theta)$ is the power distribution in the radar beam. Each coefficient $\beta_i$ represents the contribution of the elementary component number $i$ to the mean value measured by the radar. The calculation of the coefficients $\beta_i$ can be done with a numerical integration of Eq. (A6). According to Eq. (11) of section 2, $2\theta_0$ is the 6-dB beamwidth. A more simple analytical expression can be derived if the power distribution in the beam is assumed to be uniform. The beamwidth to consider is the 3-dB beam. In this particular case, $\beta_i$ is the proportion of the beam section occupied by the component number $i$ of the discretized VPR. It can be expressed

$$\beta_i = \frac{1}{\pi} \left[ (\alpha_i^+ - \alpha_i^-) - (\sin \alpha_i^+ \cos \alpha_i^+ - \sin \alpha_i^- \cos \alpha_i^-) \right]. \quad (A7)$$

### APPENDIX B

#### Lagrange Minimization

The problem consists of minimizing the quantity $\Phi(z, q)$ under the constraint $q = m(z)$, which can be written as $\sum_{j=1}^{n_q} B_j = q_j - m_j(z) = 0$. According to Lagrange, the solution sought $(z', q')$ is such that

$$\Phi(z, q) + \sum_{j=1}^{n_q} \mu_j B_j \text{ minimum} \quad (B1)$$

and $B_j = 0$ for every $j$ from 1 to $n_q$, where $\mu_j$ are $n_q$ additional parameters called Lagrange multipliers. The method of Lagrange multipliers provides a way to minimize the quantity $\Phi$ in introducing a set of constraints ($B_j = 0$). This method is detailed in the book by Menke (1989) (appendix A). Differentiating Eq. (B1) and setting to zero gives

$$d\Phi + \sum_{j=1}^{n_q} \mu_j dB_j = 0, \quad (B2)$$

which is equivalent to the system

$$\frac{\partial \Phi(z, q)}{\partial z_i} - \sum_{j=1}^{n_q} \mu_j \frac{\partial m_j(z)}{\partial z_i} = 0 \quad (B3)$$

for every $i$ from 1 to $n_z$, followed by

$$\frac{\partial \Phi(z, q)}{\partial q_j} + 2\mu_j = 0 \quad (B4)$$

for every $j$ from 1 to $n_q$.

In a matrix form, Eqs. (B3) and (B4) can be written

$$(z - z_0)^T C_z^{-1} - \mu^T M = 0,$$

$$(q - q_0)^T C_q^{-1} + \mu^T I = 0, \quad (B5)$$

where $M = (\partial m_j/\partial z_i)$ is the $(n_z, n_q)$ matrix of the partial derivatives of $m$, $I$ denotes the $(n_q, n_q)$ identity matrix, $C_z$ and $C_q$ the covariance matrix of $z$ and $q$, and $\mu$ is the vector of Lagrange multipliers. Linearizing the system Eq. (B5) leads to

$$\mu^T M C_z M^T - (z - z_0)^T M^T = 0,$$

$$\mu^T C_q + (q - q_0)^T = 0. \quad (B6)$$

At the solution $(z', q')$, the vector $\mu$ must check:

$$\mu^T = [(z' - z_0)^T M^T - (q' - q_0)^T] \times (M C_z M^T + C_q)^{-1}. \quad (B7)$$

Bringing this value of $\mu$ in Eq. (B5), one obtains the following equivalent system:

$$(z' - z_0)^T = [(z' - z_0)^T M^T - (q' - q_0)^T] \times (M C_z M^T + C_q)^{-1} M C_z,$$

$$(q' - q_0)^T = [(z' - z_0)^T M^T - (q' - q_0)^T] \times (M C_z M^T + C_q)^{-1} C_q. \quad (B8)$$

Let us introduce the constraint $q = m(z)$ in the previous system in replacing $q'$ by $m(z')$. In effect, if the previous equality is right, the system Eq. (B8) becomes

$$z' = z_0 + C_z M (M C_z M^T + C_q)^{-1}$$

$$q' = q_0 + C_q (M C_z M^T + C_q)^{-1} m(z') \quad (B9)$$

Conversely, if Eq. (B9) is satisfied, premultiplying its first equation by $M$ and adding member to member to the second equation leads directly to $q' = m(z')$. Equation (B9) defines the solution of the initial Lagrange system. The first equation of (B9) gives the estimated VPR $z'$; the second equation gives the smoothed function of ratios $q'$.

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