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MAXIMUM ENTROPY PDFS UNDER NEAR-EQUILIBRIUM CONDITIONS

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Abstract. *Since its inception, the maximum entropy method has been perceived as a potential tool for investigating the near-equilibrium region in kinetic theory of gases, thus providing an alternative to the more traditional small disturbance expansions, such as Chapman-Enskog and Grad's method. However, it became clear early on that one would have to overcome some major mathematical difficulties, before that goal could be achieved. Chief among these difficulties is the so-called moment problem, which consists of solving for the probability density function (pdf) parameters in terms of its moments. Although it can be solved by means of numerical methods, the application outlined above requires an analytical solution. This work presents a method for obtaining an analytic solution to the moment problem associated with maximum entropy pdfs. This method allows one to express pdf parameters in terms of constrained moments, alone. The results thus obtained hold for pdfs that represent small perturbations from a known pdf within this class. Since the Maxwellian is itself a maximum entropy pdf, the method effectively opens up the possibility of using this class of pdfs to investigate the near-equilibrium region.*

Keywords: *moment problem, pdf methods, maximum entropy, small disturbance expansion*

1. Introduction

According to kinetic theory, the thermodynamic state of a gas is characterized by the distribution of thermal velocities of its molecules and its number density (Vincenti and Kruger, 1986). Owing to the stochastic nature of molecular interactions, this distribution represents a probability density function (pdf). Moments of thermal velocities, in turn, represent macroscopic physical quantities, such as temperature, viscous stresses and heat flux, which are the usual variables of interest in the description of thermodynamic processes.

Hence, to specify the thermodynamic state of a gas in terms of the usual macroscopic quantities, one must establish a relation between them and a thermal velocity distribution. Since the latter is a pdf, while the former are statistical moments, the whole problem boils down to specifying a pdf that satisfies a set of conditions imposed on its moments. On assuming that one can find a suitable analytic representation for this pdf, then its specification hinges on one's ability to evaluate the parameters that characterize that representation in terms of its moments. This is the so-called moment problem (Lawrence et al., 1984).

Perhaps the most widely recognized example of the moment problem is that associated with a monatomic perfect gas in thermodynamic equilibrium. Its thermal velocity distribution is Maxwellian (Vincenti and Kruger, 1986), and it is fully specified by the absolute temperature of the gas. It is a well-known fact that the Maxwellian represents a Gaussian pdf with zero mean. This pdf is specified by a single parameter, which is a function of the second order moment of thermal velocities, that is, a function of the absolute temperature of the gas.

The correspondence between the Maxwellian distribution and thermodynamic equilibrium is certainly one of the most important theoretical results of kinetic theory of gases, and it has far reaching consequences throughout the whole of thermodynamics. However, most flows in nature involve non-equilibrium phenomena, and their modeling requires other pdf representations. Over the years, a variety of methods were proposed to that end. Most of them attempt to capture the physics of the near-equilibrium regime, that is, when departure from equilibrium is small. This is partly because a large portion of problems of interest falls into that group, and partly owed to conceptual difficulties associated with the very characterization of a thermodynamic state, when departure from equilibrium is extreme.

A systematic review of those methods is presented in (Volpe, 2001). In addition to the well-known Chapman-Enskog expansion and Grad's method, some alternative pdf representations are also considered. Among them, the one proposed by Koopman, 1969, stands out as specially attractive.

Koopman proposed a pdf representation that is based on the maximum entropy method (mem). The main reasons for its attractiveness lie in the conceptual foundations of the method and in certain properties of these pdfs. As it is shown in detail in (Volpe, 2001), these pdfs do not exhibit negative excursions and the closure relations they yield allow for interdependence between even and odd order moments.

In essence, the mem is an inference tool that allows one to associate a pdf to a given set of moments with minimum bias (Papoulis, 1991). It defines a functional that measures statistical entropy. Then, the pdfs are gotten on maximizing this functional subject to constraints, which represent conditions that are imposed on a set of moments.

In this work, we are primarily interested in a subgroup of maximum entropy pdfs that includes the representation proposed by Koopman, 1969. These are pdfs for which one constrains moments of products of the variables of interest. Given a generic random variable x, on prescribing the moments ($\langle 1\rangle$, $\langle x_i\rangle$, $\langle x_ix_j\rangle$, $\langle x_ix_jx_k\rangle$, $\langle x_ix_jx_kx_l\rangle$...), one would get a pdf $f(x)$ of the form:

$$\begin{cases} f(\mathbf{x}) \quad = \exp[-\psi(\mathbf{x};\underline{\lambda})] \\ \psi(\mathbf{x};\underline{\lambda}) = \lambda_0 + \lambda_i x_i + \lambda_{ij}x_ix_j + \lambda_{ijk}x_ix_jx_k + \lambda_{ijkl}x_ix_jx_kx_l + ... \end{cases} \tag{1}$$

where the parameters $(\lambda_0, \lambda_i, \lambda_{ij}, \lambda_{ijk}, ...)$ are Lagrange multipliers that correspond to the constrained moments listed above. It is worth noting that the Gaussian pdf belongs in this group, as can be seen by setting to zero all parameters of order higher than two ($\lambda_{ijk} = \lambda_{ijkl} = ... = 0$).

In effect, the λ are the parameters that fully specify pdfs in this class. Thus, the moment problem for them implies solving for the λ in terms of constrained moments. However, the strong nonlinearity of eq. (1) poses extraordinary difficulties to finding the functional dependence between parameters and constrained moments. Except for the simplest cases, such as the jointly Gaussian, this dependence is unknown. Obviously, one could use numerical methods to tackle the problem. But numerical solutions do not provide much insight into this functional dependence. Therefore, one cannot rely solely on them for the application considered here.

A small disturbance method was developed by Volpe, 2001, to overcome this difficulty. It allows one to obtain an analytic solution to the moment problem, which is approximate in the sense of small disturbances. Effectively, it expresses pdf parameters in terms of constrained moments, and the results hold for pdfs that represent small perturbations from a known pdf within this class. A prospective application for this method would be to explore the near-equilibrium region. In principle, one can develop a small disturbance expansion about the Maxwellian, and follow the steps proposed by Koopman to represent non-equilibrium effects such as heat fluxes and viscous stresses.

The purpose of this paper is to present the small disturbance method and discuss its applications. Since the subject involves the concept of moment problem and touches the subject closure relations, it is convenient to start the discussion by proposing appropriate definitions for them. Then the relevant properties of these pdfs are discussed and the method is presented. For the sake of simplicity, the 1-D case is presented first, followed by the extension to multidimensional pdfs.

2. Formal Definitions of the Moment Problem and Closure Relations

As presented by Baganoff, 1996, let us assume that a suitable analytic representation is chosen for a pdf. This representation must be characterized by a set of parameters a_k. If it is a convergent representation, then one may assume as an approximation that $a_k = 0$ for $(k > N)$. Additionally, if one can carry out the integration to obtain analytic expressions for the moments $\langle x^k\rangle = m_k$, then one would be able to express them as functions of the parameters alone, $m_k = m_k(a_1, a_2, ...a_N)$.

At least in principle, if the first N of these relations could be inverted, then one would be able to write the pdf parameters in terms of the first N moments $a_k = a_k(m_1, m_2, ...m_N)$. These expressions represent the solution to the moment problem. If such solution is feasible, then one can substitute the $a_k = a_k(m_1, m_2, ...m_N)$ into the expressions for moments of order higher than N, $m_{N+1} = m_{N+1}(a_1, a_2, ...a_N)$. On doing so, one obtains expressions of the form $m_{N+1} = m_{N+1}(m_1, m_2, ...m_N)$, which are the closure relations.

3. Properties of the Maximum Entropy PDFs

A central concept in this study is the partition function, which is defined as the normalization integral of the pdf. For further clarity in introducing this and related concepts, it is convenient to change the definition of $\psi(x;\underline{\lambda}) = \psi(x)$ and treat the normalization parameter separately

$$\begin{cases} f(x) = A\exp[-\psi(x)] \\ \psi(x) = \lambda_1 x + \lambda_2 x^2 + ... + \lambda_N x^N \end{cases} \tag{2}$$

where the constrained moments correspond to the set $\{\langle 1\rangle, \langle x\rangle, \langle x^2\rangle, ..., \langle x^N\rangle\}$. Realizability implies that $\psi(x)$ is an even order polynomial ($N = 2M$), as discussed in (Volpe, 2001), and A stands for the normalization parameter: $A = e^{-\lambda_0}$. The partition function Z is just the inverse of the normalization parameter A (Papoulis, 1991),

$$Z = \frac{1}{A} = e^{+\lambda_0} = \int_{-\infty}^{\infty} e^{-\psi(x)}\, dx \tag{3}$$

Clearly, the quantities Z, A and λ_0 depend only on pdf parameters λ_i, that is: $Z = Z(\lambda_1, ..., \lambda_N)$, $A = A(\lambda_1, ..., \lambda_N)$ and $\lambda_0 = \lambda_0(\lambda_1, ..., \lambda_N)$. Moreover, under the conditions $\lambda_i \in \Re$ and $\lambda_N > 0$, where N is even, the integral in eq.(3) is convergent (Volpe, 2001).

As mentioned above, the Gaussian corresponds to reducing $\psi(x)$ to a second order polynomial: $f_G(x) = A \exp\left[-\left(\lambda_1 x + \lambda_2 x^2\right)\right]$. In fact, the Gaussian partition function is one of the few that is known in closed form:

$$Z_G(\lambda_1, \lambda_2) = \sqrt{\frac{\pi}{\lambda_2}} \exp\left(\frac{\lambda_1^2}{4\lambda_2}\right) \tag{4}$$

Partition functions for other pdfs in this class are derived in (Volpe, 2001). However, they involve very complicated series representations, which are not useful to our purposes.

The partition functions associated with these pdfs have very useful properties, which are discussed in detail in (Volpe, 2001). Here, we shall focus on those that are relevant to our purposes. These are the moment theorem, the equivalence relations and moment differentiation formulas, which are presented below.

3.1. Moment Theorem and Equivalence Relations

It is a well-known result that one can relate constrained moments to derivatives of the partition function (Papoulis, 1991):

$$\frac{1}{Z}\frac{\partial Z}{\partial \lambda_k} = -m_k \tag{5}$$

where the notation $m_k = \langle x^k \rangle$ was introduced to simplify the presentation. This result can be easily extended to compute higher order moments, by successive differentiation of the partition function (Volpe, 2001).

$$\frac{1}{Z}\frac{\partial^{l+r+s} Z}{\partial \lambda_i^l \partial \lambda_j^r \partial \lambda_k^s} = (-1)^{(l+r+s)} m_{(li+rj+sk)} \tag{6}$$

Equation (6) represents the moment theorem associated with the partition function Z, and eq. (5) can be seen as a particular case of the theorem.

If an expression for $Z(\underline{\lambda})$ is known explicitly, then one can use the moment theorem to compute any moments of the corresponding pdf. However, eq. (6) implies and even more important result: it can be used to show that partial derivatives of $Z(\underline{\lambda})$ satisfy an infinite set of equivalence relations (Volpe, 2001), which are given by.

$$\frac{\partial^{l+r+s} Z}{\partial \lambda_i^l \partial \lambda_j^r \partial \lambda_k^s} = (-1)^{(l+r+s-p-q)} \frac{\partial^{p+q} Z}{\partial \lambda_m^p \partial \lambda_n^q} \tag{7}$$

provided that: $li + rj + sk = pm + qn$ and $1 \leq i, j, k, m, n \leq N$. That is, any partial derivatives of Z that correspond to a given moment m_k are related to each other by (7).

3.2. The Jacobian Matrix

Equation (5) establishes a relationship between constrained moments and the parameters $\underline{\lambda}$ through the partition function Z, and this is its most important property. On the flip side, it also shows how the normalization integral changes by changing pdf parameters $\underline{\lambda}$. By the same logic, one can evaluate how moments change by changing pdf parameters. On taking the integral of a generic moment $\langle x^p \rangle$, where $(p = 1, 2...)$, differentiating it with respect to λ_k $(1 \leq k \leq N)$ and making use of eq. (5), one gets:

$$\frac{\partial m_p}{\partial \lambda_k} = m_p m_k - m_{(p+k)} \tag{8}$$

which holds for $1 \leq k \leq N$, and $p = 1, 2, ...$ If the constrained moments are known as explicit functions of pdf parameters $m_k(\underline{\lambda})$, then one can use (8) to express higher order moments in terms of the same parameters $m_{(k+p)}(\underline{\lambda})$. Unfortunately, the $m_k(\underline{\lambda})$ are not available in most cases and, thus, eq.(8) cannot be used for that purpose.

On the other hand, one can use eq. (8) to evaluate changes in constrained moments that are caused by small perturbations in the $\underline{\lambda}$. To that end, one can define the Jacobian matrix (Volpe, 2001)

$$\frac{\partial(\underline{m})}{\partial(\underline{\lambda})} \equiv \frac{\partial(m_1, m_2, ..., m_N)}{\partial(\lambda_1, \lambda_2, ..., \lambda_N)} = \begin{pmatrix} \frac{\partial m_1}{\partial \lambda_1} & \frac{\partial m_1}{\partial \lambda_2} & \cdots & \frac{\partial m_1}{\partial \lambda_N} \\ \frac{\partial m_2}{\partial \lambda_1} & \frac{\partial m_2}{\partial \lambda_2} & \cdots & \frac{\partial m_2}{\partial \lambda_N} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial m_N}{\partial \lambda_1} & \frac{\partial m_N}{\partial \lambda_2} & \cdots & \frac{\partial m_N}{\partial \lambda_N} \end{pmatrix} \tag{9}$$

The mem assumes that constrained moments are independent of each other (Papoulis, 1991). Then, one should expect $m_k(\underline{\lambda})$ to be functionally independent, and the matrix (9) should be invertible. If this is the case, then one can write

$$\frac{\partial m_i}{\partial m_j} = \frac{\partial m_i}{\partial \lambda_p}\frac{\partial \lambda_p}{\partial m_j} = \delta_{ij} \tag{10}$$

for $1 \leq i, j, p \leq N$. On the flip side, higher order moments should depend on the constrained moments. After all, this is the primary reason why one can derive closure relations (Baganoff, 1996). Hence, on computing the derivatives of unconstrained moments, represented by $\langle x^{(N+p)} \rangle = m_{(N+p)}$, one has

$$\frac{\partial m_{(N+p)}}{\partial m_j} = \frac{\partial m_{(N+p)}}{\partial \lambda_k}\frac{\partial \lambda_k}{\partial m_j} = \sum_{k=0}^{N}\left[m_{(N+p)}m_k - m_{(N+p+k)}\right]\frac{\partial \lambda_k}{\partial m_j} \tag{11}$$

where $1 \leq j, k \leq N$.

On using the Jacobian matrix (9), one can write the total differential of the constrained moments with respect to pdf parameters $\underline{\lambda}$

$$dm_k = \frac{\partial m_k}{\partial \lambda_p}\, d\lambda_p \tag{12}$$

where the summation rule applies. This relation, in turn, can be approximated in the sense of small disturbances, by

$$\delta m_k \approx \frac{\partial m_k}{\partial \lambda_p}\delta\lambda_p \tag{13}$$

and, on assuming that the Jacobian is invertible, one gets

$$\delta\lambda_p \approx \frac{\partial \lambda_p}{\partial m_k}\delta m_k \tag{14}$$

Equation (14) is the core of the small disturbance method. Along with the differentiation formulas (8) and (11), it allows one to obtain approximate solutions to the moment problem in the neighborhood of a known maximum entropy pdf, as will be shown next.

As a side note, the Jacobian matrix is real and symmetric. Therefore, it has a complete eigensystem and can be diagonalized by a similarity transformation. Although we have not fully explored this possibility, it strongly suggests that some very interesting results may follow from it.

4. Small Disturbance Expansions

The primary goal of this work is to investigate the possibility of using maximum entropy pdfs to represent the near-equilibrium region. Since the equilibrium condition is associated with the pure Gaussian pdf, it is convenient to present the method by developing a small disturbance expansion about a 1-D pure Gaussian:

$$f_{G_0}(x) = A\exp\left(-\lambda_{2G}x^2\right) \tag{15}$$

Some important non-equilibrium effects are associated with the asymmetry of the underlying pdf. In the 1-D case, some asymmetry can be introduced by specifying a non-zero third order moment, while keeping the zero mean condition. As discussed above, realizability then requires a fourth order moment to be specified as well. Hence, the perturbed pdf shall exhibit the form

$$f(x) = A\exp\left[-\left(\lambda_1 x + \lambda_2 x^2 + \lambda_3 x^3 + \lambda_4 x^4\right)\right] \tag{16}$$

which is termed full quartic pdf. This expansion involves computing a Jacobian matrix (9) at the point where that pdf reduces to the pure Gaussian, that is, where λ_1, λ_3 and λ_4 all go to zero.

$$\left.\frac{\partial(\underline{m})}{\partial(\underline{\lambda})}\right|_{G_0} = \left.\frac{\partial(m_1, m_2, m_3, m_4)}{\partial(\lambda_1, \lambda_2, \lambda_3, \lambda_4)}\right|_{\lambda_1, \lambda_3, \lambda_4 = 0} \tag{17}$$

In principle, one could evaluate all derivatives in (17) by differentiating the full quartic partition function with respect to its parameters. However, $Z(\lambda_1, \lambda_2, \lambda_3, \lambda_4)$ is not known. The Gaussian partition function cannot be used to that end either, since it corresponds to a particular case $Z_G = Z(\lambda_1, \lambda_2, 0, 0)$, which is independent of λ_3 and λ_4 (Volpe, 2001).

That is where the differentiation formula (8) comes in handy. It expresses the derivatives in terms of moments, alone. On using it to compute (17), it yields

$$\left.\frac{\partial(\underline{m})}{\partial(\underline{\lambda})}\right|_{G_0} = \begin{pmatrix} m_1^2 & m_1 m_2 & m_1 m_3 & m_1 m_4 \\ m_2 m_1 & m_2^2 & m_2 m_3 & m_2 m_4 \\ m_3 m_1 & m_3 m_2 & m_3^2 & m_3 m_4 \\ m_4 m_1 & m_4 m_2 & m_4 m_3 & m_4^2 \end{pmatrix}_{G_0} - \begin{pmatrix} m_2 & m_3 & m_4 & m_5 \\ m_3 & m_4 & m_5 & m_6 \\ m_4 & m_5 & m_6 & m_7 \\ m_5 & m_6 & m_7 & m_8 \end{pmatrix}_{G_0} \tag{18}$$

This expression actually enables one to compute the Jacobian matrix at the point where the full quartic pdf reduces to a Gaussian. For, at that point, the moments of both pdfs are precisely the same, and one knows how to compute any Gaussian moment analytically, from its partition function Z_G.

To be more specific, we are interested in perturbing the pure Gaussian. All odd-order moments of this pdf are identically zero. Thus, on computing the even order moments from eq. (4), at $\lambda_1 = 0$, and substituting them into (18), one obtains an invertible matrix (Volpe, 2001). Then, on computing its inverse, it results

$$\left.\frac{\partial(\underline{\lambda})}{\partial(\underline{m})}\right|_{G_0} = \begin{pmatrix} -5\lambda_{2G} & 0 & 2\lambda_{2G}^2 & 0 \\ 0 & -8\lambda_{2G}^2 & 0 & 2\lambda_{2G}^3 \\ 2\lambda_{2G}^2 & 0 & \frac{-4\lambda_{2G}^3}{3} & 0 \\ 0 & 2\lambda_{2G}^3 & 0 & \frac{-2\lambda_{2G}^4}{3} \end{pmatrix} \tag{19}$$

This matrix, in turn, can be introduced in (14) to obtain a small disturbance expansion about pure Gaussian. Hence, one would expect that the $\underline{\lambda}$ of the perturbed pdf be given by

$$\underline{\lambda} = \begin{pmatrix} 0 \\ \lambda_{2G} \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} \delta\lambda_1 \\ \delta\lambda_2 \\ \delta\lambda_3 \\ \delta\lambda_4 \end{pmatrix} \tag{20}$$

and the values of the constrained moments are assumed to be close to those of the pure Gaussian. That is, the perturbations are assumed small $|\delta\underline{m}| \ll 1$

$$\underline{m} = \begin{pmatrix} 0 \\ m_{2G} \\ 0 \\ m_{4G} \end{pmatrix} + \begin{pmatrix} 0 \\ \delta m_2 \\ \delta m_3 \\ \delta m_4 \end{pmatrix} \tag{21}$$

where $\delta m_1 = 0$, so that the perturbed pdf will also have zero mean.

On combining equations (19) - (21), one gets

$$\begin{cases} \lambda_1 \approx 2\lambda_{2G}^2 \delta m_3 \\ \lambda_2 \approx \lambda_{2G} - 8\lambda_{2G}^2 \delta m_2 + 2\lambda_{2G}^3 \delta m_4 \\ \lambda_3 \approx -\frac{4}{3}\lambda_{2G}^3 \delta m_3 \\ \lambda_4 \approx 2\lambda_{2G}^3 \delta m_2 - \frac{2}{3}\lambda_{2G}^4 \delta m_4 \end{cases} \tag{22}$$

These results represent an approximate solution to the moment problem in the near-equilibrium region. Moreover, the same reasoning can clearly be applied to other pdfs in the class defined by (2). Therefore, it actually constitutes a method for obtaining approximate solutions to the moment problem in that region.

Given the strong nonlinearity of these pdfs, even crude first order estimates like (22) can be extremely valuable. However, what is most important about them is that they provide a means to assess the physical meaning of those pdf parameters. To that end, it is useful to cast them in a cleaner dimensionless form. On taking λ_{2G} as a scale factor and defining the following dimensionless quantities

$$x = x\sqrt{\lambda_{2G}} \qquad \eta_k = \lambda_k \lambda_{2G}^{-k/2} \qquad \tilde{m}_p = m_p \lambda_{2G}^{p/2} \tag{23}$$

On substituting these definitions into (16) and (22), one can write them as

$$f(\tilde{x}) = \tilde{A}\exp\left[-\left(\eta_1\tilde{x} + \eta_2\tilde{x}^2 + \eta_3\tilde{x}^3 + \eta_4\tilde{x}^4\right)\right] \qquad \begin{cases} \eta_1 \approx 2\delta\tilde{m}_3 \\ \eta_2 \approx 1 - 8\delta\tilde{m}_2 + 2\delta\tilde{m}_4 \\ \eta_3 \approx -\frac{4}{3}\delta\tilde{m}_3 \\ \eta_4 \approx 2\delta\tilde{m}_2 - \frac{2}{3}\delta\tilde{m}_4 \end{cases} \tag{24}$$

where $\tilde{A} = A/\sqrt{\lambda_{2G}}$ and the dimensionless perturbed moments are given by

$$\underline{\tilde{m}} = \begin{pmatrix} 0 \\ \frac{1}{2} \\ 0 \\ \frac{3}{4} \end{pmatrix} + \begin{pmatrix} 0 \\ \delta\tilde{m}_2 \\ \delta\tilde{m}_3 \\ \delta\tilde{m}_4 \end{pmatrix} \tag{25}$$

The first thing to be noticed in (24) is that even parameters η_2 and η_4 depend only on even moments and, conversely, odd parameters η_1 and η_3 depend only on odd moments. To some extent, the split between even and odd moments should be expected in a linear approximation. When $\eta_1 = \eta_3 = 0$ the pdf is even and all odd moments are zero. Hence, on changing only $\tilde{m}_2$ and $\tilde{m}_4$ and keeping $\tilde{m}_1 = \tilde{m}_3 = 0$ one should expect that η_1 and η_3 remain 0, otherwise the resulting pdf would loose its symmetry and the odd moments would no longer be zero.

On the other hand, (24) also show limitations of a first order approximation. In principle, one should be able to perturb only $\tilde{m}_3$ and keep the other constrained moments equal to their corresponding Gaussian counterparts: $\underline{\tilde{m}} = \{0, 1/2, \delta\tilde{m}_3, 3/4\}$. However, on substituting $\delta\tilde{m}_2 = \delta\tilde{m}_4 = 0$ and $\delta\tilde{m}_3 \neq 0$ into (24), one gets $\eta_3 \neq 0$, but $\eta_4 = 0$, which breaks down the realizability of the pdf. Another instance when realizability is affected is when $\tilde{m}_2$ and $\tilde{m}_4$ are perturbed in such a way that $\delta\tilde{m}_2 < \delta\tilde{m}_4/3$, since this leads to $\eta_4 < 0$.

4.1. Higher Order Expansions

A means of improving matters on these limitations would be to extend the expansion to second order

$$\lambda_p = \lambda_p\Big|_{G_0} + \frac{\partial\lambda_p}{\partial m_k}\Big|_{G_0}\delta m_k + \frac{1}{2}\frac{\partial^2\lambda_p}{\partial m_k\partial m_j}\Big|_{G_0}\delta m_k\delta m_j + \mathcal{O}(|\delta\underline{m}|^3) \tag{26}$$

This requires that one evaluates the third order tensor $\partial^2\lambda_p/\partial m_k\partial m_j$ for the Gaussian. In order to do so, one must invert the Jacobian matrix in its generic form (18). This can be easily accomplished by using a software package for symbolic manipulation. The final form of this matrix is quite complicated, algebraically, and will not be reproduced here. It suffices to note that it is a collection of nonlinear functions of moments up to order $2N$: $\partial\lambda_p/\partial m_k = f_{pk}\left(m_1, ..., m_N, m_{N+1}, ..., m_{2N}\right)$. Therefore, it can be differentiated analytically, by simply using the differentiation formulas (10) and (11)

Similarly, these operations can be performed by using symbolic manipulation software. When these expressions are computed for the Gaussian, accounting for the nullity of odd order moments and substituting appropriate expressions for even moments ($\lambda_{1G} = 0$), the results are strikingly simple. Then, on substituting these results in (26), computing the second order approximation and introducing the definitions (23) one gets

$$\begin{cases} \eta_1 \approx \left(2 + 20\delta\tilde{m}_2 - \frac{28}{3}\delta\tilde{m}_4\right)\delta\tilde{m}_3 \\ \eta_2 \approx 1 - 8\delta\tilde{m}_2 + 2\delta\tilde{m}_4 - 50\delta\tilde{m}_2^2 - 8\delta\tilde{m}_3^2 + 44\delta\tilde{m}_2\delta\tilde{m}_4 - \frac{28}{3}\delta\tilde{m}_4^2 \\ \eta_3 \approx \left(-\frac{4}{3} - 16\delta\tilde{m}_2 + 8\delta\tilde{m}_4\right)\delta\tilde{m}_3 \\ \eta_4 \approx 2\delta\tilde{m}_2 - \frac{2}{3}\delta\tilde{m}_4 + 22\delta\tilde{m}_2^2 + 4\delta\tilde{m}_3^2 - \frac{56}{3}\delta\tilde{m}_2\delta\tilde{m}_4 + 4\delta\tilde{m}_4^2 \end{cases} \tag{27}$$

The first thing one notices on comparing (27) to (24) is that these results exhibit full interdependence between moments and parameters. This interdependence reveals features of the pdf that cannot be captured by linear expressions. For instance, the dependence of η_1 and η_3 on $\delta\tilde{m}_2$ and $\delta\tilde{m}_4$ is such that these parameters will change in response to perturbations in the even moments if, and only if, $\delta\tilde{m}_3 \neq 0$, thus keeping the symmetry of the pdf whenever $\delta\tilde{m}_3 = 0$. Moreover, η_2 and η_4 depend on $\delta\tilde{m}_3^2$, so that their change in response to the introduction of "skewness" is independent of the sign of $\delta\tilde{m}_3$. It is also worth noting that even on perturbing only $\tilde{m}_2$ from its Gaussian value leads to $\eta_4 \neq 0$, that is, a quartic pdf. On the flip side, the absence of $\delta\tilde{m}_3^2$ in the expressions for η_1 and η_3 seems to indicate that these parameters depend strongly on the sign of $\delta\tilde{m}_3$.

These trends are amply verified by numerical computations (Volpe, 2001). Therefore, the second order expansion indeed improves our understanding of these parameters. However, (27) is still a truncated series and, hence, realizability problems cannot be completely ruled out.

In principle, one could compute still higher order terms of the series expansion (26), and this could be done by the same procedure used above. However, the number of terms grows geometrically with the order of differentiation, and the computations become too cumbersome to tackle.

On the other hand, with so few terms available in (27) there is no means of finding out whether the series is convergent. Hence, one must ask the question as to whether these expressions can provide reasonable estimates of the parameters in the neighborhood of the Gaussian. That can only be ascertained by comparing their predictions to known results.

5. Approximate versus Exact Results

The following procedure is proposed to test small disturbance estimates: 1) A range is defined for the parameters $(\eta_1, \eta_2, \eta_3, \eta_4)$ in the neighborhood of the Gaussian point $(0, 1, 0, 0)$. 2) The pdfs that correspond to values of η_k in this range have the moments $(\tilde{m}_1, \tilde{m}_2, \tilde{m}_3, \tilde{m}_4)$ computed, and their departure from Gaussianity $(\delta\underline{\tilde{m}})$ is evaluated by means of eq. (25). 3) On introducing $(\delta\underline{\tilde{m}})$ into eqs. (24) and (27), one gets small disturbance estimates of the parameters $(\eta_1, \eta_2, \eta_3, \eta_4)$. 4) These estimates can, in turn, be compared to the original values that were assigned to the parameters.

Since the moments and parameters considered here make up an eight-dimensional space, one must test perturbations separately. The first test that was carried out focused on the even order moments $\tilde{m}_2$ and $\tilde{m}_4$, only. The parameters η_1 and η_3 were kept constant at $\eta_1 = \eta_3 = 0$, which corresponds to constant values for the odd order moments $\tilde{m}_1 = \tilde{m}_3 = 0$. Hence, the perturbed pdf should be symmetric and have the form $f(\tilde{x}) = A \exp\left[-\left(\eta_2 \tilde{x}^2 + \eta_4 \tilde{x}^4\right)\right]$. This is the symmetric quartic pdf and it is actually one of the few pdfs in this class for which the partition function is known in closed form (Volpe, 2001). Hence, one can compute its moments exactly, by means of the moment theorem (5).

The results of this test are shown in Figure (1). The parameters η_2 and η_4 cover the ranges $0.9 \leq \eta_2 \leq 1.1$ and $0 \leq \eta_4 \leq 0.5$, respectively. First order estimates are plotted in (1.a) and (1.b). Whereas, second order estimates are plotted in (1.c) and (1.d). In all plots, the mesh represents analytical results, the dots represent small disturbance predictions and the Gaussian point is marked by a circle.

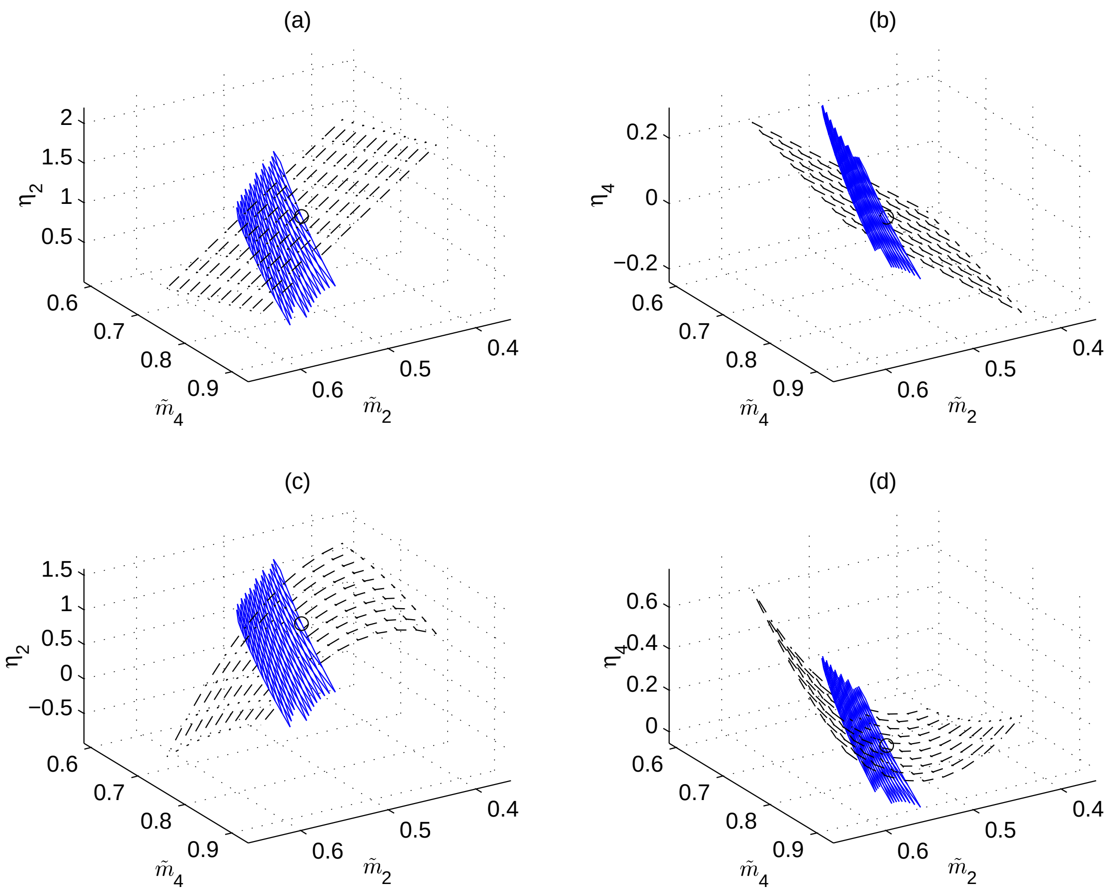

Figure 1: Test of small disturbance approximations: (a) 1st order $\eta_2(\tilde{m}_2, \tilde{m}_4)$. (b) 1st order $\eta_4(\tilde{m}_2, \tilde{m}_4)$. (c) 2nd order $\eta_2(\tilde{m}_2, \tilde{m}_4)$. (d) 2nd order $\eta_4(\tilde{m}_2, \tilde{m}_4)$. Mesh, exact solution; dash-dot lines, small disturbance; circle, Gaussian.

The small disturbance predictions seem to agree reasonably well with the actual values of the parameters η_2 and η_4 over a small region in the neighborhood of the Gaussian point. Although the second order approximation does not seem to be markedly superior.

5.1. Test of Small Disturbance Estimates for $\tilde{m}_3 \neq 0$

Differently from the symmetric quartic, a full quartic pdf does not necessarily have zero mean. However, the small disturbance estimates satisfy this condition and, thus, it must be enforced on the pdf for the comparison. This is accomplished by shifting the pdf to the position where $\tilde{m}_1 = 0$.

In addition to that, the second order estimates (27) exhibit full interdependence between moments and parameters. This implies that $\tilde{m}_2$, $\tilde{m}_3$ and $\tilde{m}_4$ must all be perturbed, while keeping $\tilde{m}_1 = 0$. As for the moments, one could either compute them numerically or by using the full quartic partition function, which was derived in (Volpe, 2001). Unfortunately, that partition function is given by a series with relatively slow convergence rate. Therefore, the numerical quadrature is preferred.

On accounting for these changes, the test procedure used in this case becomes: 1) The parameters are assigned intervals about the Gaussian point ($-0.3 \leq \eta_1 \leq 0.3$, $\eta_2 = 1$, $-0.3 \leq \eta_3 \leq 0.3$, $0 \leq \eta_4 \leq 0.3$). 2) The corresponding pdfs have their mean evaluated numerically. 3) Then, they are shifted to zero mean and the η_i of the shifted pdfs are computed Volpe, 2001. 4) The moments $\tilde{m}_2$, $\tilde{m}_3$ and $\tilde{m}_4$ of the shifted pdfs are computed numerically, and their departure from Gaussianity is evaluated by (25). 5) On substituting $(\delta\underline{\tilde{m}})$ into the small disturbance formulas (24) and (27), one gets estimates for the η_i. 6) These estimates should be compared to the shifted values of those parameters, which were gotten in step 2.

Since all parameters and moments change in the test, there are many different ways of presenting results. On the other hand, perturbations of $\tilde{m}_2$ and $\tilde{m}_4$ have already been discussed above. Hence, it is useful to focus on perturbations $\delta\tilde{m}_3$, and consider their effects. Figure (2) shows a representative example of this test. Small perturbations $\delta\tilde{m}_3 = \tilde{m}_3$, $|\tilde{m}_3| \ll 1$, are introduced in a symmetric quartic pdf, which is in the neighborhood of the pure Gaussian ($\eta_2 = 0.99$, $\eta_4 = 1.6 \times 10^{-2}$). Since the first order approximations of η_2 and η_4 are independent of $\tilde{m}_3$, only their second order estimates are plotted.

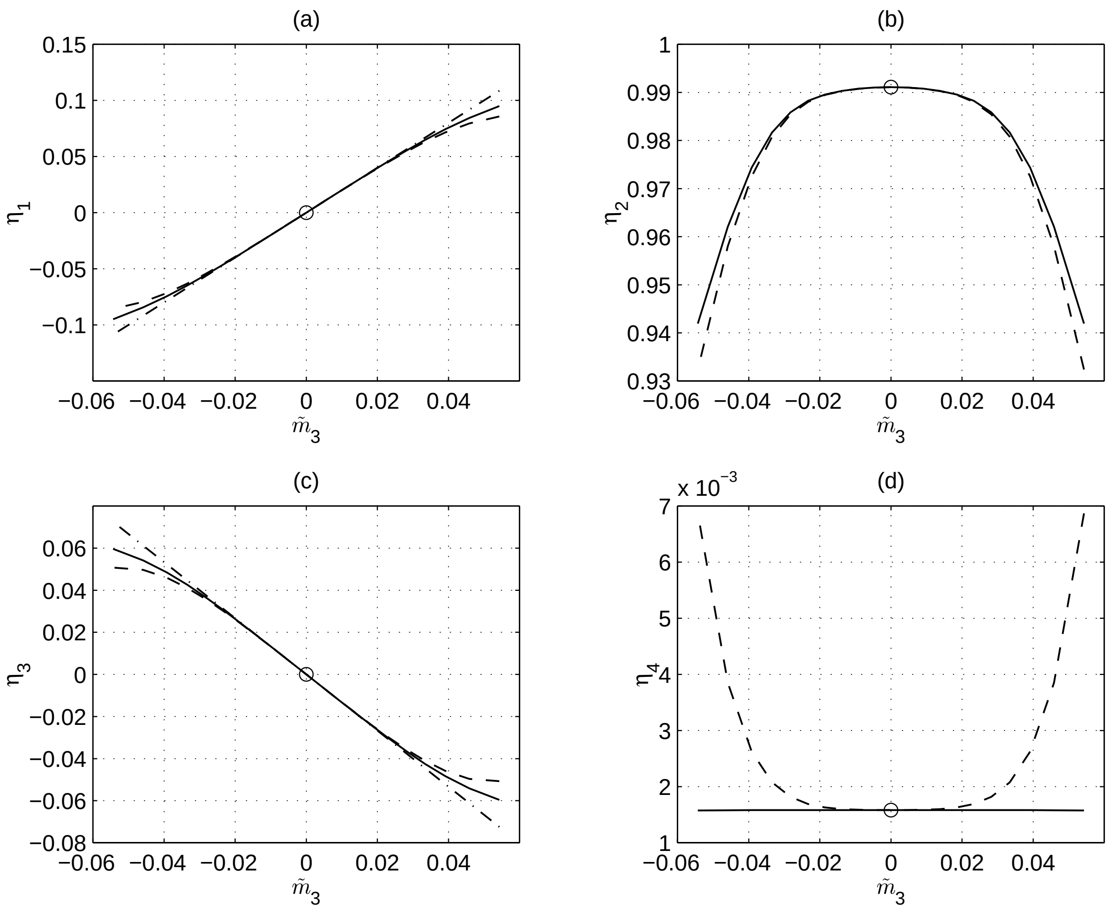

Figure 2: Test of small disturbance estimates: (a) $\eta_1(\tilde{m}_3)$, (b) $\eta_2(\tilde{m}_3)$, (c) $\eta_3(\tilde{m}_3)$, (d) $\eta_2(\tilde{m}_3)$, Solid line, numeric evaluation; dash-dot line 1st order s. d. for η_1 and η_3; dashed line, 2nd order s. d.; circle, symmetric quartic.

As can be seen, the small disturbance estimates for η_1 and η_3 predict the correct slope of the curves $\eta_1(\tilde{m}_3)$

and $\eta_3(\tilde{m}_3)$ at the symmetric quartic ($\tilde{m}_3 = 0$). It is worth noting that the linear estimate is indeed a good approximation for those curves in the neighborhood of $\tilde{m}_3 = 0$. A considerable departure from linearity can be seen in the extremities of those curves. In part, it can be attributed to higher order terms, such as $\mathcal{O}(\delta\tilde{m}_3^3)$. However, in part it is a result of the perturbations $\delta\tilde{m}_2$ and $\delta\tilde{m}_4$ coupled with $\delta\tilde{m}_3$, as can be seen in (27). The second order estimate of $\eta_2(\tilde{m}_3)$ shows a good fit over the whole range of $\tilde{m}_3$. In contrast, the estimate of $\eta_4(\tilde{m}_3)$ shows considerably less accuracy over the same range.

An important result of this analysis is that for full quartic pdfs the zero mean condition ($\tilde{m}_1 = 0$) imposes a relation between the parameters η_3 and η_1. This relation can be verified by simply plotting one against the other, as presented in Figure (3). This Figure also shows estimates of such relation that are gotten from the first and second order small disturbance approximations. These results clearly indicate that a constant

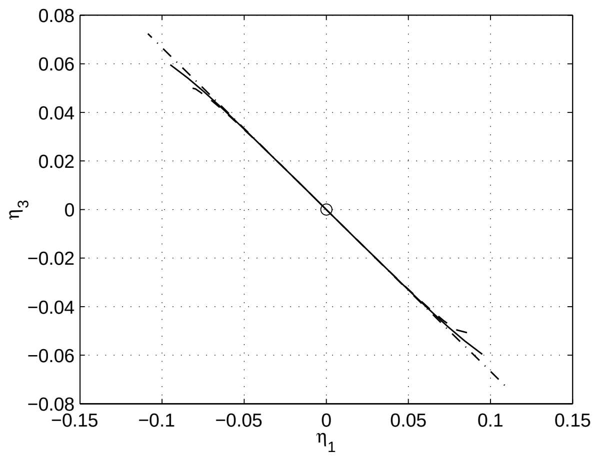

Figure 3: Functional relation $\eta_3(\eta_1)$ for $\tilde{m}_1 = 0$. Solid line, numeric evaluation; dash-dot line 1st order s. d.; dashed line, 2nd order s. d.; circle, symmetric quartic.

ratio, $\eta_3/\eta_1 = -2/3$, is a good approximation for the relation between η_3 and η_1 that leads to $\tilde{m}_1 = 0$, in the neighborhood of the Gaussian.

6. Extension to Multidimensional PDFs

In order to extend the method to multidimensional pdfs $f(\mathbf{x})$, one must first generalize the differentiation formulas. To that end, it is useful to start from a more general definition of a maximum entropy pdf

$$\begin{cases} f(\mathbf{x}) = A\exp[-\psi(\mathbf{x})] \\ \psi(\mathbf{x}) = \lambda_i g_i(\mathbf{x}) \end{cases} \tag{28}$$

where A is the normalization parameter, the constrained moments are $\langle g_i(\mathbf{x})\rangle$, $1 \le i \le N$, and the summation convention applies. Clearly, the pdf defined in (1) is a particular case of this definition, for which $\langle g_i(\mathbf{x})\rangle = \langle x_i x_j x_k\rangle$. Here again, on differentiating both sides of the normalization integral with respect to λ_k, $1 \le k \le N$, one gets Volpe, 2001

$$\frac{\partial \ln(A)}{\partial \lambda_k} = -\frac{\partial \ln(Z)}{\partial \lambda_k} = \langle g_k(\mathbf{x})\rangle = \langle g_k\rangle \tag{29}$$

which is entirely similar to its 1-D counterpart (5). Then, on differentiating the integral of a given moment $\langle h(\mathbf{x})\rangle$ with respect to λ_k ($1 \le k \le N$) and using (29), one gets

$$\frac{\partial\langle h\rangle}{\partial \lambda_k} = \langle h\rangle\langle g_k\rangle - \langle h g_k\rangle \tag{30}$$

A particular case of (30) that is of special interest to us is when $h(\mathbf{x}) = g_p(\mathbf{x})$, for $1 \le p \le N$,

$$\frac{\partial\langle g_p\rangle}{\partial \lambda_k} = \langle g_p\rangle\langle g_k\rangle - \langle g_p g_k\rangle \tag{31}$$

which holds for $1 \leq k, p \leq N$. Again, the result is similar to the 1-D (8), which is actually a particular case of (31). On the basis of this result, one can define a Jacobian matrix analogous with (9)

$$\frac{\partial(\langle \underline{g} \rangle)}{\partial(\underline{\lambda})} \equiv \frac{\partial(\langle g_1 \rangle, \langle g_2 \rangle, ..., \langle g_N \rangle)}{\partial(\lambda_1, \lambda_2, ..., \lambda_N)} = \begin{pmatrix} \frac{\partial \langle g_1 \rangle}{\partial \lambda_1} & \frac{\partial \langle g_1 \rangle}{\partial \lambda_2} & \cdots & \frac{\partial \langle g_1 \rangle}{\partial \lambda_N} \\ \frac{\partial \langle g_2 \rangle}{\partial \lambda_1} & \frac{\partial \langle g_2 \rangle}{\partial \lambda_2} & \cdots & \frac{\partial \langle g_2 \rangle}{\partial \lambda_N} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial \langle g_N \rangle}{\partial \lambda_1} & \frac{\partial \langle g_N \rangle}{\partial \lambda_2} & \cdots & \frac{\partial \langle g_N \rangle}{\partial \lambda_N} \end{pmatrix} \tag{32}$$

and (31) implies that this is a symmetric matrix. If the determinant of (32) is nonzero, then the constrained moments are functionally independent, and this allows one to write

$$\frac{\partial \langle g_i \rangle}{\partial \langle g_j \rangle} = \frac{\partial \langle g_i \rangle}{\partial \lambda_p} \frac{\partial \lambda_p}{\partial \langle g_j \rangle} = \delta_{ij} \tag{33}$$

for $1 \leq i, j, p \leq N$. This result is analogous with (10). On the other hand, derivatives of unconstrained moments $\langle h(\mathbf{x}) \rangle$ with respect to constrained moments are given by Volpe, 2001

$$\frac{\partial \langle h \rangle}{\partial \langle g_j \rangle} = \sum_{k=0}^{N} [\langle h \rangle \langle g_k \rangle - \langle h g_k \rangle] \frac{\partial \lambda_k}{\partial \langle g_j \rangle} \tag{34}$$

where $1 \leq j, k \leq N$. Here again, the result is analogous with its 1-D version (11).

The Jacobian matrix (32) enables one to compute the total differential of the constrained moments with respect to pdf parameters λ_k

$$d\langle g_k \rangle = \frac{\partial \langle g_k \rangle}{\partial \lambda_p} d\lambda_p \tag{35}$$

where the summation rule applies. On approximating this relation in the sense of small disturbances, $|\delta\underline{\lambda}| \ll 1$, one gets

$$\delta \langle g_k \rangle \approx \frac{\partial \langle g_k \rangle}{\partial \lambda_p} \delta \lambda_p \tag{36}$$

and, on assuming that the Jacobian matrix is invertible, this equation leads to

$$\delta \lambda_p \approx \frac{\partial \lambda_p}{\partial \langle g_k \rangle} \delta \langle g_k \rangle \tag{37}$$

where it is assumed that $|\delta\langle g_k \rangle| \ll 1$. Equation (37) represents a small disturbance first order approximation to the moment problem solution, provided that the Jacobian determinant is nonzero. That is, provided that the constrained moments are independent functions of the pdf parameters. Furthermore, on making an analogy with the 1-D case, one could use eqs. (33) and (34) to compute higher order estimates of that solution.

In what follows, a small disturbance first order approximation is developed for the Koopman pdf (Koopman, 1969). For simplicity, the example is limited to the case of two r.vs.

6.1. Koopman pdf

The pdf representation proposed by Koopman, 1969 constrains third order moments that represent non-equilibrium effects $\langle x_i x^2 \rangle$. Then, realizability requires that a fourth order moment be constrained as well (Volpe, 2001). In its general form, it reads

$$f_k(\mathbf{x}) = A \exp\left\{ -\left[\underbrace{\lambda_i x_i + \lambda_{ij} x_i x_j}_{\text{Gaussian}} + \gamma_i x_i x_k x_k + \Lambda (x_p x_p)^2 \right] \right\} \tag{38}$$

Differently from (2), this pdf does not constrain all elements of the third order moment $\langle x_i x_j x_k \rangle$, but only a particular contraction of it $\langle x_i x_k x_k \rangle$. Similarly, not all elements of $\langle x_i x_j x_k x_p \rangle$ are constrained. Instead, it only constrains $\langle (x_p x_p)^2 \rangle$, which is enough to ensure realizability. This represents a rather important simplification, since it reduces significantly the number of pdf parameters and constrained moments in the model. As a result, the remaining third and fourth order moments, which were not constrained, should be given by closure relations (Volpe, 2001). In particular, for two r.vs. this pdf is given by

$$f_k(x, y) = A \exp\left\{ -\left[\lambda_x x + \lambda_y y + \lambda_{xx} x^2 + \lambda_{yy} y^2 + \gamma_x x (x^2 + y^2) + \gamma_y y (x^2 + y^2) + \Lambda (x^2 + y^2)^2 \right] \right\} \tag{39}$$

and the constrained moments are

$$\begin{array}{lllll} \langle g_x\rangle = \langle x\rangle \; ; & \langle g_{xx}\rangle = \langle x^2\rangle \; ; & \langle g_{qx}\rangle = \langle x^3\rangle + \langle xy^2\rangle \equiv q_x \; ; & \langle g_4\rangle = \langle (x^2+y^2)^2\rangle \equiv M_4 \; ; \\ \langle g_y\rangle = \langle y\rangle \; ; & \langle g_{yy}\rangle = \langle y^2\rangle \; ; & \langle g_{qy}\rangle = \langle x^2 y\rangle + \langle y^3\rangle \equiv q_y & \end{array} \tag{40}$$

It is worth noting that one can always write the pdf (39) in the main coordinate system of $\langle x_i x_j\rangle$, where this tensor is diagonal. Furthermore, we are interested in developing a small disturbance expansion about the Maxwellian, which is a symmetric Gaussian with zero mean, $f_M(x,y) = A_M \exp\left[-\lambda_{2M}\left(x^2+y^2\right)\right]$. This brings further simplifications in the model: Symmetry implies that $\langle x_i x_j\rangle$ is a hydrostatic tensor, which reduces the number parameters to only one, λ_{2M}. The zero mean condition, in turn, implies that all moments that involve an odd power of either x or y are identically zero (Volpe, 2001), and this simplifies computations enormously.

The small disturbance expansion in this case follows eq. (37). The Jacobian matrix is defined in (32) and the moment differentiation formula is given by (31). The moments, in turn, can be evaluated by successive differentiation of the 2-D Gaussian partition function. Hence, on following the same reasoning as in the 1-D case, one can develop a first order small disturbance expansion about the Maxwellian, in the form of a Koopman pdf $f_k(x,y)$. Such an expansion was developed by Volpe, 2001, and the results are presented below. For simplicity, parameters and moments are put in dimensionless form, by using λ_{2M} as a scale.

$$\begin{array}{llllll} \tilde{A} = A\lambda_{2M}^{-1/2} \; ; & \eta_x = \lambda_x\lambda_{2M}^{-1/2} \; ; & \eta_{xx} = \lambda_{xx}\lambda_{2M}^{-1} \; ; & \nu_x = \gamma_x\lambda_{2M}^{-3/2} \; ; & \Xi = \Lambda\lambda_{2M}^{-2} \\ \tilde{x} = x\lambda_{2M}^{1/2} \; ; & \langle\tilde{x}\rangle = \langle x\rangle\lambda_{2M}^{1/2} \; ; & \langle\tilde{x}^2\rangle = \langle x^2\rangle\lambda_{2M} \; ; & \tilde{q}_x = q_x\lambda_{2M}^{3/2} \; ; & \tilde{M}_4 = M_4\lambda_{2M}^2 \end{array} \tag{41}$$

Similar definitions apply to moments of the variable y and corresponding parameters. On casting the results in terms of these quantities, they read

$$\begin{aligned} f_k(\tilde{x},\tilde{y}) = {} & \tilde{A}_K \exp\{-[\eta_x\tilde{x} + \eta_y\tilde{y} + \eta_{xx}\tilde{x}^2 + \\ & + \eta_{yy}\tilde{y}^2 + \nu_x\tilde{x}(\tilde{x}^2+\tilde{y}^2) + \\ & + \nu_y\tilde{y}(\tilde{x}^2+\tilde{y}^2) + \Xi(\tilde{x}^2+\tilde{y}^2)^2]\} \end{aligned} \qquad \left\{ \begin{array}{ll} \eta_x & \approx 2\delta\tilde{q}_x \\ \eta_y & \approx 2\delta\tilde{q}_y \\ \eta_{xx} & \approx 1 + (\delta\tilde{M}_4 - 6\delta\langle\tilde{x}^2\rangle - 4\delta\langle\tilde{y}^2\rangle) \\ \eta_{yy} & \approx 1 + (\delta\tilde{M}_4 - 4\delta\langle\tilde{x}^2\rangle - 6\delta\langle\tilde{y}^2\rangle) \\ \nu_x & \approx -\delta\tilde{q}_x \\ \nu_y & \approx -\delta\tilde{q}_y \\ \Xi & \approx (\delta\langle\tilde{x}^2\rangle + \delta\langle\tilde{y}^2\rangle) + \frac{\delta\tilde{M}_4}{4} \end{array} \right. \tag{42}$$

where the first order moments are not perturbed, so as to keep the zero mean condition. An example of small disturbance expansion about the Maxwellian, in the form of a Koopman pdf, is presented in Figure (4), where the former is represented by dashed lines and the latter is represented by a mesh. The Maxwellian moments are perturbed and the perturbations are substituted in (42) to estimate Koopman pdf parameters. Then the moments of the resulting Koopman pdf are computed and compared to the values that were assigned to the perturbed moments. Table 1 shows results of the comparison. As can be seen, the perturbed pdf exhibits

Table 1: Constrained Moments of a 2-D Koopman pdf

pdf	$\langle\tilde{x}\rangle$	$\langle\tilde{y}\rangle$	$\langle\tilde{x}^2\rangle$	$\langle\tilde{y}^2\rangle$	$\tilde{q}_x$	$\tilde{q}_y$	$\tilde{M}_4$
Maxwellian	0	0	0.5	0.5	0	0	2
s.d. input	0	0	0.51	0.52	0.02	0.03	2.05
Koopman	-8.8×10^{-5}	1.5×10^{-4}	0.5110	0.5218	0.0184	0.0292	2.0702

some asymmetry, in the form of nonzero third order moments (q_x, q_y). As a result of such asymmetry and the normalization condition, its peak is displaced downwards from the Maxwellian peak. On the flip side, Table (1) shows that the differences between input values and actual moments are not larger than the perturbations introduced. In particular, it satisfies the zero mean condition within an error of order 10^{-4}.

7. Conclusions

In effect, the method discussed above allows one to develop small disturbance expansions about the Gaussian, in terms of a class of pdfs generated by the maximum entropy method. Although its solutions are approximate, it does circumvent the mathematical difficulties that are associated with the moment problem for these pdfs.

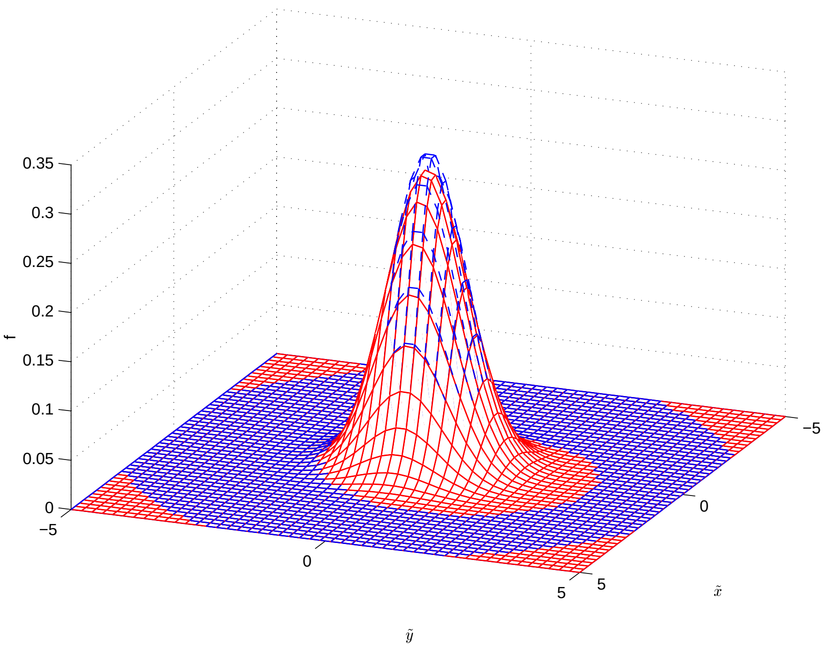

Figure 4: Example of a 2-D Koopman pdf gotten by s.d.t. expansion about a 2-D Maxwellian. Koopman, mesh; Maxwellian, dashed lines.

It is certainly convenient that the Gaussian pdf belongs in this class, and that it can be used as the starting point for small disturbance expansions. However, it must be noted that the same method can be applied to virtually any pdf in this class, and this can be used to extend the range of small disturbance approximations in certain applications (Volpe, 2001).

The test results presented above show that the small disturbance expansions are only accurate over small intervals about the Gaussian, and that can be seen as a liability. On the other hand, they effectively enable one to access the physical meaning of pdf parameters in that region. That is a crucial step if one is to use these pdfs to explore the near-equilibrium region, as proposed by Koopman, 1969.

The examples above have shown that, in order to constrain third order moments, one must include a fourth order moment to ensure realizability. This situation is bound to happen whenever the relevant moments do not imply a realizable pdf by themselves. This is certainly a liability of the method, since one may be lead to constrain moments that do not represent meaningful quantities. However, as the Koopman pdf shows, there is a good deal of flexibility as to which higher order moments need be included to ensure realizability. That is clearly an attractive feature of these pdfs.

8. Acknowledgements

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