ADDING A THIRD NORMAL TO CLUBB

by

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ABSTRACT

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The Cloud Layers Unified By Binormals (CLUBB) model uses the sum of two normal probability density function (pdf) components to represent subgrid variability within a single grid layer of an atmospheric model. This binormal approach, while computationally efficient, restricts the model's ability to capture the full spectrum of potential shapes encountered in real-world atmospheric data.

This thesis proposes to introduce a third normal pdf component strategically positioned between the existing two, significantly enhancing the model's representational flexibility. This trinormal representation allows for a wider range of grid-layer shapes while permitting analytic solutions for certain higher order moments.

The core of this work lies in deriving the necessary mathematical transformations for incorporating the third normal pdf seamlessly into the CLUBB framework. This thesis lists all formulas, inputs, and outputs associated with the extended model as well as gives an outline on how to check those equations. Additionally, it describes certain asymptotic behavior of the trinormal pdf under various parameter settings.

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LIST OF ACRONYMS

cas computer algebra system. 16, 45, 46

CLUBB Cloud Layers Unified By Binormals. ii, 1, 2, 4, 5, 11, 18, 26, 29, 30, 44–47

lhs left hand side. 11

pde partial differential equation. 1, 4, 5, 25

pdf probability density function. ii, 1, 6, 8, 10–14, 17, 18, 20, 23–25, 27–30, 40, 41, 44–46

rhs right hand side. 5, 11, 41

LIST OF SYMBOLS

- θ_l' Standardized liquid water potential temperature $(\theta_l'=\theta_l-\overline{\theta_l}).$ 15
- r_t' Standardized total water mixing ratio $(r_t' = r_t \overline{r_t})$. 15
- w' Standardized upward wind $(w'=w-\overline{w}).$ 15, 19

1 Introduction

The CLUBB model is a powerful tool used to simulate atmospheric behavior within climate models. This document explores an extension to the current CLUBB framework. Currently, CLUBB utilizes the sum of two normal pdfs to represent a single atmospheric grid layer. While effective, this approach limits the model's ability to capture the full spectrum of potential cloud layer shapes. This work proposes an innovative solution: incorporating a third normal pdf into the CLUBB framework. This addition aims to enhance the model's representational capabilities while maintaining computational efficiency and numerical stability. To achieve this, the document dives into the details of the proposed method.

We begin by outlining the core problem we aim to address (chapter 2) by starting with the motivation, proceeding with a short explanation on how to close turbulence partial differential equations (pdes) (section 2.2) and explaining how we derive the transformation from the formulas given by the paper "Using probability density functions to derive consistent closure relationships among higher-order moments" by Larson and Golaz (section 2.3). After that, we define the goal of this thesis (section 2.4), talk about the inputs and outputs (section 2.5) and provide steps for checking those formulas (section 2.6).

Following this motivational chapter, we establish a foundation with clear definitions of the relevant concepts, including normal distributions and the thermodynamic scalars crucial for atmospheric modeling (chapter 3).

Chapter 4 forms the heart of this work, presenting the actual formulas associated with the extended CLUBB model. This chapter details the introduction of the third normal pdf (section 4.1) and the derivation of key moments within the model (section 4.3 - section 4.4).

Additionally, section 4.6 proposes a diagnostic approach to account for the skewness of heat and moisture, while section 4.7 introduces analytic closure relations for higher-order moments based on the newly formed mixture of three normal distributions.

To handle the mathematical integrations required by the model, chapter 5 explores both exact parametric and numerical integration techniques of verifying the integrals, utilizing the SymPy library (section 5.1 & section 5.2).

Finally, chapter 6 investigates the asymptotic behavior of the extended model, providing valuable insights into its performance under various conditions.

Having talked about the trinormal representation within the CLUBB model, chapter 7 provides a concise recap of the key findings. This summary serves as a comprehensive overview of the essential concepts explored throughout this thesis.

The document concludes with an outlook in chapter 8, outlining potential future directions for research and exploration based on the findings presented here.

2 Problem

2.1 Motivation to add a third normal component

As is said in chapter 1, we try to describe more possible shapes by adding a third normal component. To illustrate that, we plot some of the shapes which are now possible with three normals but were not possible with only two. To be able to draw those plots, we are just using two variables, w, the upward wind, and θ_l , the liquid water potential temperature. To show how the binormal model handles strong winds, let us consider a scenario with a strong updraft at w_1 , as well as a strong downdraft at w_2 . The way the current binormal model would handle this could look like figure 2.1. However, this binormal distribution (figure 2.1)

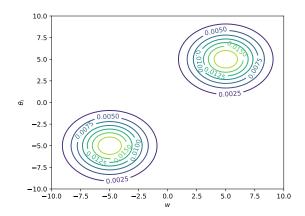


Figure 2.1: Binormal plot for two strong up-/downdrafts $w_1 = 5, w_2 = -5, \theta_{l1} = 5, \theta_{l2} = -5, \alpha = 0.5, \sigma_w = 2, \sigma_{\theta_{l1}} = 2, \sigma_{\theta_{l1}} = 2.$

does not accurately reflect reality. In nature, we would not expect such strong bi-modality between the strong up- and downdrafts at w_1 and w_2 . There would most likely be some weaker drafts present in-between. The current binormal model can attempt to capture this smoother transition by simply increasing the standard deviations of both wind, and liquid

water potential temperature distributions. This results in a broader distribution with a connection between the two peaks, as shown in figure 2.2. Seeing figure 2.2, the issue with



Figure 2.2: Binormal plot for two strong up-/downdrafts with increased standard deviations $w_1 = 5, w_2 = -5, \theta_{l1} = 5, \theta_{l2} = -5, \alpha = 0.5, \sigma_w = 5, \sigma_{\theta_{l1}} = 5, \sigma_{\theta_{l1}} = 5.$

having some values in the middle is mitigated but the general width of the normals was increased, too. Since CLUBB also has the simplification that there is no correlation between w and θ_l , and w and r_t – obviously – one cannot just increase it. Therefore, the idea is to add this third normal distribution, which actually has correlation between all three variables and especially in the bivariate case, between w and θ_l . Figure 2.2 would then change to figure 2.3. Now, one can easily model something like the described shape, as illustrated in figure 2.3. Also, some other (maybe weird) shapes are now possible, just like the one in figure 2.4.

2.2 Closing turbulence pdes by integration over a pdf

The CLUBB model relies on a set of pdes to represent atmospheric processes. These equations require closure, implying the expression of all terms solely in terms of known quantities. This closure process often involves integrals, and verifying their analytical solutions

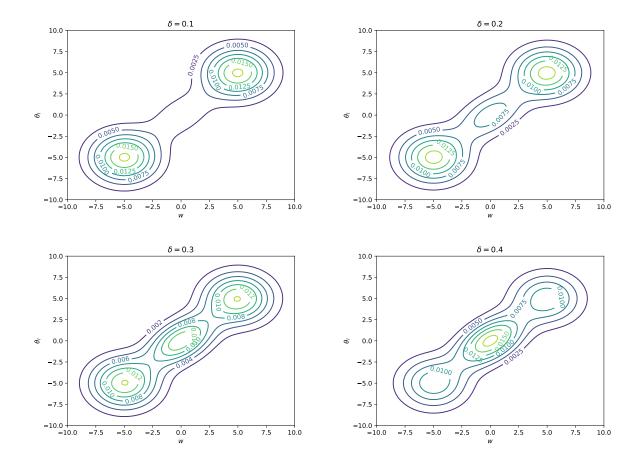


Figure 2.3: Trinormal plot for two strong up-/downdrafts with varying δ $w_1 = 5, \ w_2 = -5, \ \theta_{l1} = 5, \ \theta_{l2} = -5, \ \alpha = 0.5, \ \sigma_w = 2, \ \sigma_{\theta_{l1}} = 2, \ \sigma_{\theta_{l2}} = 2, \ \sigma_{w3} = 2, \ \sigma_{3\theta_{l}} = 2, \ \rho_{w\theta_{l}} = 0.5.$

ensures the model's mathematical integrity. For instance, consider the following prognostic pde [Lar22, p. 21]:

$$\frac{\partial \overline{w'\theta'_l}}{\partial t} = -\overline{w}\frac{\partial \overline{w'\theta'_l}}{\partial z} - \frac{1}{\rho_s}\frac{\partial \rho_s \overline{w'^2\theta'_l}}{\partial z} - \overline{w'^2}\frac{\partial \overline{\theta'_l}}{\partial z} - \overline{w'\theta'_l}\frac{\partial \overline{w}}{\partial z} + \dots$$

While the details of initial and boundary conditions are essential for formally closing the prognostic equations in CLUBB (omitted for brevity), this section emphasizes the importance of efficiently calculating moments on the right hand side (rhs) of these equations. That is because the model steps forward in time and therefore needs the repeated calculation of moments for each unclosed prognostic equation at every time step. Those already expensive computational steps need to use mathematically simpler moment representations



Figure 2.4: Trinormal plot for two strong up-/downdrafts with a third peak in the middle $w_1 = 5, w_2 = -5, \theta_{l1} = 5, \theta_{l2} = -5, \alpha = 0.5, \delta = 0.5, \sigma_w = 2, \sigma_{\theta_{l1}} = 2, \sigma_{\theta_{l2}} = 2, \sigma_{w3} = 2, \sigma_{\theta_{l3}} = 2, \rho_{w\theta_{l}} = 0.5.$

of e.g. $\overline{w'^2\theta'_l}$, even if they introduce slight limitations in capturing the full variability of the underlying atmospheric state.

2.3 Derivation of trinormal closures by transformation of binormal closures

Analytic closures between higher and lower order moments for the binormal case are available (see CLUBB-SILHS[Lar22]). We wish to derive similar analytic closures for the proposed trinormal pdf. Deriving an analytic closure for a general trinormal pdf is difficult. However, doing so is tractable in the special case that the third normal component is located at the mean of the binormal pdf. In fact, the trinormal closures can be derived by making a simple transformation of the binormal closures [LG05], e.g.

$$\overline{w'^2} = \alpha [(w_1 - \overline{w})^2 + \sigma_w^2] + (1 - \alpha)[(w_2 - \overline{w})^2 + \sigma_w^2]. \tag{2.3.1}$$

This section will demonstrate that the following transformations, denoted by the subscript "dGn" for the binormal case, successfully achieve this conversion.

$$\overline{w'^2} \frac{1 - \delta \lambda_w}{1 - \delta} = \overline{w'^2}_{dGn}, \tag{2.3.2}$$

$$\overline{w'^3} \frac{1}{1-\delta} = \overline{w'^3}_{dGn},\tag{2.3.3}$$

$$\frac{\overline{w'^3}}{\overline{w'^2}^{3/2}} \frac{(1-\delta)^{1/2}}{(1-\lambda_w \delta)^{3/2}} = \frac{\overline{w'^3}_{dGn}}{\overline{w'^2}_{dGn}^{3/2}},$$
(2.3.4)

$$\overline{\theta_l'^2} \frac{1 - \delta \lambda_\theta}{1 - \delta} = \overline{\theta_l'^2}_{dGn}, \tag{2.3.5}$$

$$\overline{w'\theta_l'} \frac{1 - \delta \lambda_{w\theta}}{1 - \delta} = \overline{w'\theta_{ldGn}'}, \tag{2.3.6}$$

$$\left(\overline{w'^4} - 3\delta\lambda_w^2 \left(\overline{w'^2}\right)^2\right) \frac{1}{1 - \delta} = \overline{w'^4}_{dGn}$$
(2.3.7)

$$\left(\frac{\overline{w'^4}}{(\overline{w'^2})^2} - 3\delta\lambda_w^2\right) \frac{1 - \delta}{(1 - \lambda_w \delta)^2} = \frac{\overline{w'^4}_{dGn}}{(\overline{w'^2}_{dGn})^2}$$
(2.3.8)

To get a sense of what those transformations mean and why they should work, we pick e.g. equation (2.3.2). If we substitute in the already defined formula for λ_w (equation (4.1.4)), we get

$$\overline{w'^2} \left(1 - \delta \frac{\sigma_{w3}^2}{\overline{w'^2}} \right) = (1 - \delta) \overline{w'^2}_{dGn}$$

$$\overline{w'^2} - \delta \sigma_{w3}^2 = (1 - \delta) \overline{w'^2}_{dGn}$$

$$\overline{w'^2} = \overline{w'^2}_{dGn} - \delta \overline{w'^2}_{dGn} + \delta \sigma_{w3}^2$$

$$\overline{w'^2} = \overline{w'^2}_{dGn} - \delta \left(\overline{w'^2}_{dGn} - \sigma_{w3}^2 \right). \tag{2.3.9}$$

Our analysis reveals a key relationship between the parameter δ and the overall variance (often referred to as "width") of the trinormal distribution. As the value of δ approaches 1

(but strictly remains less than 1), the standard deviation of the third normal distribution has a progressively stronger influence on the overall variance of the combined distribution. This intuitively makes sense because a larger weight assigned to the third normal distribution through δ will contribute more significantly to the spread of the combined pdf.

Also, if we look at equation (2.3.3), we see that there is no more λ_w present. It makes sense graphically, that as δ grows, which means that the normal pdf in the middle is growing, the overall skewness of all three normals has to change also, depending on the value of σ_{w3} . We can see this, as well as the relationship between the variance in table 2.1. Table 2.1 offers a visual representation of how the parameter δ influences the shape of the trinormal distribution. Each plot illustrates pdfs for different combinations of σ_{w3} (standard deviation of the third normal distribution) and δ . The row values in the table correspond to σ_{w3} , while the column values represent δ . We can observe two key trends within these plots:

- 1. Influence of σ_{w3} : As expected, varying σ_{w3} primarily affects the "width" or overall variance of the combined distribution. When σ_{w3} is larger than the width of the original binormal sum (orange/red line), choosing a larger δ allows the overall variance to increase significantly, as predicted by equation (2.3.2).
- 2. Decreasing skewness with increasing δ : The plots also reveal a distinct relationship between δ and the skewness of the resulting distribution. As δ increases, the skewness of the combined trinormal distribution (green line) progressively reduces. This phenomenon can be attributed to the placement of the third normal distribution. Placed directly between the two original normal distributions, the third normal distribution acts as a centralizing force. As the weight of the third normal distribution (controlled by δ) grows, its symmetric nature counteracts the potential skewness of the initial binormal sum. This effect is particularly strong in the bottom three plots, where a larger value of $\sigma_{w3} = 10$ is used. We observe a clear reduction in the skewness of the

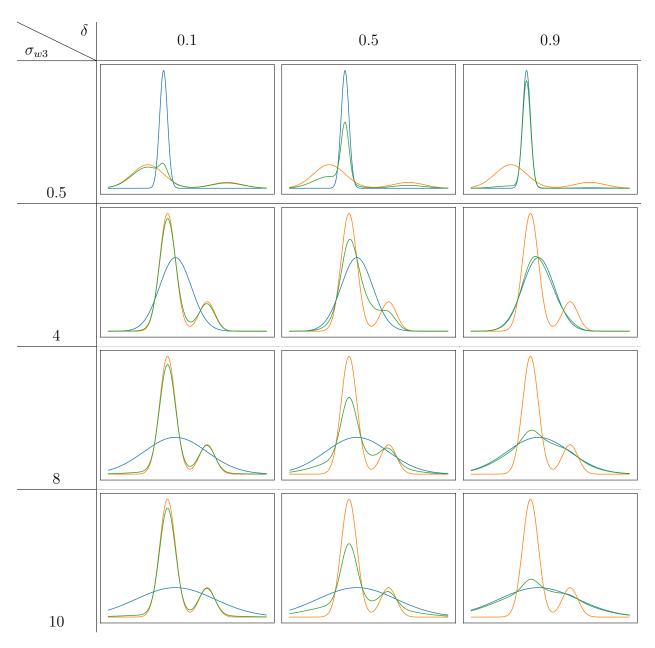


Table 2.1: 1D Plots for different δ and σ_{w3} $w_1=5, w_2=-5, \alpha=0.2, \sigma_w=2$. The blue plot represents the third normal, the orange/red one represents the binormal, and the green one represents the mixture. The x and y labels and ticks are omitted for clarity.

green plot (mixture) as δ approaches 1.

2.4 Goal of this thesis

The goal of this thesis is to verify closure for higher-order moments, such as the third order moment $\overline{w'^2\theta'_l}$ and others like it. This closure is achieved by expressing these higher-order moments – i.e. equation (4.7.3), equation (4.7.5), and equation (4.7.7) – analytically in terms of readily calculable lower-order moments. This analytic approach uses the relationships between moments within a normal distribution, enabling efficient model updates during the time-stepping process.

2.5 Inputs and outputs of the verification procedure

While defining inputs and outputs can seem challenging at first glance, it is a crucial step towards understanding a system.

2.5.1 Inputs and outputs of a forward run

When forecasting the weather ("forward run"), the code provides us with a set of moment terms: \overline{w} , $\overline{w'^2}$, $\overline{w'^3}$, $\overline{\theta_l}$, $\overline{w'\theta_l'}$, $\overline{r_t}$, $\overline{w'r_t'}$, $\overline{\theta_l'^2}$, $\overline{r_t'^2}$, $\overline{r_t'\theta_l'}$. These are the inputs. From these inputs, we want to determine certain parameters which describe the shape of the underlying pdf. Those pdf parameters are standardized and some also normalized. So we try to solve these pdf parameters (13), namely α , \widehat{w}_1 , \widehat{w}_2 , $\widetilde{\theta}_{l1}$, $\widetilde{\theta}_{l2}$, \widetilde{r}_{t1} , \widetilde{r}_{t2} , $\widetilde{\sigma}_w$, $\widetilde{\sigma}_{\theta_{l1}}$, $\widetilde{\sigma}_{\theta_{l2}}$, $\widetilde{\sigma}_{r_{t1}}$, $\widetilde{\sigma}_{r_{t2}}$, and $r_{r_t\theta_l}$. All the formulas are listed in chapter 4. Ultimately, the code needs to express even higher order moments such as $\overline{w'^2\theta_l'}$ in terms of the lower order moments. These higher order moments are the outputs in the "forward run".

2.5.2 Inputs and outputs of a backward run (verification direction)

Although a "forward run" models the higher order moments in terms of the lower order moments, we want to verify these formulas, namely equation (4.7.3), equation (4.7.5), and equation (4.7.7). To achieve this, we will take a more traditional approach, working in the "backward" direction. This means we will:

- 1. Specify the pdf parameters: Start by explicitly defining the parameters that characterize the underlying pdf.
- 2. Calculate the moments: Once the pdf is defined, we can then calculate the desired moments, such as \overline{w} , through integration.

This can be done, e.g. by calculating the integral:

$$\overline{w} = \int_{\mathbb{R}} \int_{\mathbb{R}} w \cdot P_{tmg} \, dw dr_t d\theta_l, \qquad (2.5.1)$$

where P_{tmg} (Trivariate Mixture of Gaussians) is the pdf of the sum of all three normal distributions. Since some integrals are challenging to verify symbolically with SymPy, we are using the quadrature method of SymPy to calculate the integrals and choose arbitrary values for the inputs. All of this can be seen in section 5.2.

2.6 Steps for checking the formulas

This section outlines a general approach for verifying all of those integral expressions employed within the CLUBB model. This approach ensures the accuracy of the computed moment relationships. Chapter 5 discusses some actual examples. We verify the expressions using the following method where the order is crucial. We always want to check if left hand side (lhs) equals rhs:

- 1. Choose dimensional parameters (parameters without any tilde or hat) that determine the pdf, i.e. choose dimensional pdf parameters, e.g. σ_{w3} . Then the pdf is known and any moments of it can be calculated by integration.
- 2. Calculate the means, e.g. $\overline{w} = \mathbb{E}[w]$ by integration over the pdf. The formula for \overline{w} (equation (4.3.1)) in terms of the pdf parameters can be checked.
- 3. Once the means are known, we calculate the central variances, e.g. $\overline{w'^2} = \overline{(w \overline{w})^2}$ by integration over the pdf. The formula for $\overline{w'^2}$ (equation (4.3.3)) in terms of the pdf parameters can be checked.
- 4. Once the variances, e.g. $\overline{w'^2}$, are known, then the non-dimensional pdf parameters such as λ_w (equation (4.1.4)) can be calculated by their definitions.
- 5. We can also calculate the covariances by 2D integration over a 2D pdf. Again, our formulas in terms of pdf parameters can be checked.
- 6. Finally, we can calculate the higher order moments, i.e. $\overline{w'^4}$ (equation (4.7.3)) or $\overline{w'^2\theta'_l}$ (equation (4.7.5)) or $\overline{w'\theta'_l^2}$ (equation (4.7.7)), by integration over the pdf.

3 Definitions

For better understanding of the topics covered in this thesis, it follows a brief introduction of all formulas and terms used.

3.1 Normal distribution

We say that a random variable X is distributed according to a normal distribution $(X \sim \mathcal{N}(\mu, \sigma^2))$ when it has the following pdf:

Definition 1 (pdf of a normal distribution)

$$f(x|\mu,\sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2} \left(\frac{x-\mu}{\sigma}\right)^2\right).$$
(3.1.1)

3.1.1 Multivariate normal distribution

We say that a random vector \boldsymbol{X} $(r \times r)$ is distributed according to a multivariate normal distribution when it has the following joint density function [Ize08, p. 59]:

Definition 2 (pdf of a multivariate normal distribution)

$$f(\boldsymbol{x}|\boldsymbol{\mu},\boldsymbol{\Sigma}) = (2\pi)^{-\frac{r}{2}} |\boldsymbol{\Sigma}|^{-\frac{1}{2}} \exp\left(-\frac{1}{2}(x-\boldsymbol{\mu})^{\top} \boldsymbol{\Sigma}^{-1}(x-\boldsymbol{\mu})\right), \boldsymbol{x} \in \mathbb{R}^{r},$$
(3.1.2)

where

$$\boldsymbol{\mu} = \begin{pmatrix} \mu_1 \\ \vdots \\ \mu_r \end{pmatrix} \in \mathbb{R}^r \tag{3.1.3}$$

is the mean vector, and

$$\Sigma = \begin{pmatrix} \sigma_1^2 & \rho_{12}\sigma_1\sigma_2 & \rho_{13}\sigma_1\sigma_3 & \dots & \rho_{1r}\sigma_1\sigma_r \\ \rho_{12}\sigma_1\sigma_2 & \sigma_2^2 & \rho_{23}\sigma_2\sigma_3 & \dots & \vdots \\ \rho_{13}\sigma_1\sigma_3 & \rho_{23}\sigma_2\sigma_3 & \sigma_3^2 & \dots & \vdots \\ \vdots & \dots & \dots & \ddots & \vdots \\ \rho_{1r}\sigma_1\sigma_r & \dots & \dots & \dots & \sigma_r^2 \end{pmatrix} \in \mathbb{R}^{r \times r}$$
(3.1.4)

is the (symmetric, positive definite) covariance matrix. This is also often expressed as $X \sim \mathcal{N}(\mu, \Sigma)$, meaning that X (r × r random vector) is distributed according to a multivariate normal distribution with the given parameters.

3.1.2 Moments

Especially for this thesis, we are interested in the moments of the given multivariate normal distribution. We can express the first order moment as the mean, denoted as $\overline{X} = \mathbb{E}[X]$, where X is a random variable. The second order moment is $\mathbb{E}[X^2]$, also denoted as the variance if it is a central moment. The standardized third and fourth order moments have special names, so-called skewness and kurtosis respectively. We denote this by the following:

$$\mathbb{E}[X^3] = \mathbb{E}\left[\left(\frac{X-\mu}{\sigma}\right)^3\right] = \frac{\mu_3}{\sigma^3} = \frac{\mathbb{E}[(X-\mu)^3]}{(\mathbb{E}[(X-\mu)^2])^{3/2}},\tag{3.1.5}$$

$$\mathbb{E}[X^4] = \mathbb{E}\left[\left(\frac{X-\mu}{\sigma}\right)^4\right] = \frac{\mathbb{E}[(X-\mu)^4]}{(\mathbb{E}[(X-\mu)^2])^2} = \frac{\mu_4}{\sigma^4}.$$
 (3.1.6)

3.2 Variates of the pdf

We denote the variates of the pdf by w, r_t , and θ_l , where w is the upward wind, r_t is the liquid water potential temperature and θ_l is the liquid water potential temperature [Lar22,

p. 10]. Variables denoted by w' are defined by $w - \overline{w}$ where \overline{w} is the mean of w over the whole pdf. We define r'_t and θ'_l in the same way.

4 Formulas that define the shape of the pdf and moments in terms of pdf parameters

This chapter lists all formulas which are derived from the binormal model to this model with an additional normal. All formulas listed are either tested by using a computer algebra system (cas) and calculating the integrals analytically with ranges $-\infty$ to ∞ or using the quadrature procedure with large enough ranges such that the error is (numerically) zero. Those two procedures are explained in chapter 5.

4.1 Definition of the trinormal distribution, P_{tmg}

We would like to add a third normal to the already existing two trivariate normals, which is placed right in the middle between those two. For our proposed mixture of normals we then have

$$P_{tmg}(w, \theta_l, r_t) = \alpha(1 - \delta)\mathcal{N}(\mu_1, \Sigma_1) + (1 - \alpha)(1 - \delta)\mathcal{N}(\mu_2, \Sigma_2) + \delta\mathcal{N}(\mu_3, \Sigma_3),$$
 (4.1.1)

where \mathcal{N} denotes the multivariate normal distribution, $\alpha \in (0,1)$ is the mixture fraction of the binormal, and $\delta \in [0,1)$ is the weight of the third normal. The mean vectors and the covariance matrices are defined in the following.

We define the mean vectors of the first and second normal distributions as $\mu_1 = (w_1, \theta_{l1}, r_{t1})^{\top}$, and $\mu_1 = (w_2, \theta_{l2}, r_{t2})^{\top}$, where $w_1 > w_2$ (due to a convention in the code) and the covariance

matrices as

$$\Sigma_{1} = \begin{pmatrix} \sigma_{w}^{2} & 0 & 0 \\ 0 & \sigma_{\theta_{l1}}^{2} & \rho_{\theta_{l}r_{t}}\sigma_{\theta_{l}3}\sigma_{r_{t}3} \\ 0 & \rho_{\theta_{l}r_{t}}\sigma_{\theta_{l}3}\sigma_{r_{t}3} & \sigma_{r_{t1}}^{2} \end{pmatrix}, \text{ and } \Sigma_{2} = \begin{pmatrix} \sigma_{w}^{2} & 0 & 0 \\ 0 & \sigma_{\theta_{l2}}^{2} & \rho_{\theta_{l}r_{t}}\sigma_{\theta_{l}3}\sigma_{r_{t}3} \\ 0 & \rho_{\theta_{l}r_{t}}\sigma_{\theta_{l}3}\sigma_{r_{t}3} & \sigma_{r_{t2}}^{2} \end{pmatrix}.$$

$$(4.1.2)$$

It might be of interest that there is no correlation between w and θ_l or w and r_t . That is to make the pdfs mathematically more tractable which also makes the pdf family less general. This is not the case for the third normal, though.

It has already been said, that we would like to place the third normal right at the mean, therefore μ_3 and Σ_3 are defined as

$$\mu_{3} = \begin{pmatrix} \overline{w} \\ \overline{\theta_{l}} \\ \overline{r_{t}} \end{pmatrix}, \text{ and } \Sigma_{3} = \begin{pmatrix} \sigma_{w3}^{2} & \rho_{w\theta_{l}3}\sigma_{w3}\sigma_{\theta_{l}3} & \rho_{wr_{t}3}\sigma_{w3}\sigma_{r_{t}3} \\ \rho_{w\theta_{l}3}\sigma_{w3}\sigma_{\theta_{l}3} & \sigma_{\theta_{l}3}^{2} & \rho_{\theta_{l}r_{t}3}\sigma_{\theta_{l}3}\sigma_{r_{t}3} \\ \rho_{wr_{t}3}\sigma_{w3}\sigma_{r_{t}3} & \rho_{\theta_{l}r_{t}3}\sigma_{\theta_{l}3}\sigma_{r_{t}3} & \sigma_{r_{t}3}^{2} \end{pmatrix}.$$

$$(4.1.3)$$

The advantage over just two normal pdfs is that we can now express a greater variety of shapes. We also define some additional relationships for this third normal distribution.

$$\lambda_w \equiv \frac{\sigma_{w3}^2}{\overline{w'^2}}, \quad \lambda_\theta \equiv \frac{\sigma_{\theta_l 3}^2}{\overline{\theta_l'^2}}, \quad \lambda_r \equiv \frac{\sigma_{r_t 3}^2}{\overline{r_t'^2}},$$
 (4.1.4)

$$\lambda_{\theta r} \equiv \frac{\rho_{\theta_l r_t} \sigma_{\theta_l 3} \sigma_{r_t 3}}{\overline{r_t' \theta_l'}}, \quad \lambda_{w \theta} \equiv \frac{\rho_{w \theta_l} \sigma_{w 3} \sigma_{\theta_l 3}}{\overline{w' \theta_l'}}, \quad \lambda_{w r} \equiv \frac{\rho_{w r_t} \sigma_{w 3} \sigma_{r_t 3}}{\overline{w' r_t'}}. \tag{4.1.5}$$

Hence, we can rewrite Σ_3 as

$$\Sigma_{3} = \begin{pmatrix} \sigma_{w3}^{2} & \overline{w'\theta_{l}'} \cdot \lambda_{w\theta} & \overline{w'r_{t}'} \cdot \lambda_{wr} \\ \overline{w'\theta_{l}'} \cdot \lambda_{w\theta} & \sigma_{\theta_{l}3}^{2} & \overline{r_{t}'\theta_{l}'} \cdot \lambda_{\theta r} \\ \overline{w'r_{t}'} \cdot \lambda_{wr} & \overline{r_{t}'\theta_{l}'} \cdot \lambda_{\theta r} & \sigma_{r_{t}3}^{2} \end{pmatrix}.$$

$$(4.1.6)$$

4.2 Normalized variables

Since CLUBB is mostly using "normalized variables", we are going to list those, which are given in standard form. We are also doing that for making the transformations easier.

$$\tilde{\theta}'_l \equiv \frac{\theta_l - \overline{\theta_l}}{\sqrt{\overline{\theta_l'^2}}} \frac{1}{\sqrt{\frac{1 - \delta \lambda_{\theta}}{1 - \delta}}},\tag{4.2.1}$$

$$\tilde{r}_t' \equiv \frac{r_t - \overline{r_t}}{\sqrt{\overline{r_t'^2}}} \frac{1}{\sqrt{\frac{1 - \delta \lambda_r}{1 - \delta}}},\tag{4.2.2}$$

where $\overline{\theta_l}$ and $\overline{r_t}$ are the means for the full summed up pdf and $\overline{\theta_l'^2}$ as well as $\overline{r_t'^2}$ are the variances for θ_l and r_t .

For the standard deviations, we define

$$\tilde{\sigma}_w \equiv \frac{\sigma_w}{\sqrt{\overline{w'^2}}} \frac{1}{\sqrt{\frac{1-\delta\lambda_w}{1-\delta}}},\tag{4.2.3}$$

where σ_w denotes the standard deviation of the w-component, $\overline{w'^2}$ is the variance for w,

$$\tilde{\sigma}_{\theta_l i} \equiv \frac{\sigma_{\theta_l i}}{\sqrt{\overline{\theta_l'^2}}} \frac{1}{\sqrt{\frac{1 - \delta \lambda_{\theta}}{1 - \delta}}},\tag{4.2.4}$$

where σ_{θ_l} denotes the standard deviation of the i^{th} θ_l -component, and

$$\tilde{\sigma}_{r_t i} \equiv \frac{\sigma_{r_t i}}{\sqrt{\overline{r_t'^2}}} \frac{1}{\sqrt{\frac{1 - \delta \lambda_r}{1 - \delta}}},\tag{4.2.5}$$

where $\sigma_{r_t i}$ denotes the standard deviation of the i^{th} σ_{r_t} -component.

4.3 A list of lower order moments expressed in terms of pdf parameters

We start by outlining the equations capturing lower-order moments, expressed in terms of pdf parameters. These equations can be presented in either dimensional or non-dimensional

form. While both representations are mathematically valid, the *non-dimensional* form offers a distinct advantage: it highlights the underlying connection to the bivariate case.

4.3.1 Moments for w

The relationship for \overline{w} is given as follows:

$$\overline{w} = (1 - \delta)\alpha w_1 + (1 - \delta)(1 - \alpha)w_2 + \delta w_3, \tag{4.3.1}$$

where $w_3 \equiv \alpha w_1 + (1 - \alpha)w_2$. Therefore the mean of w stays the same as in the bivariate case. The relationship for the *non-dimensional* form is:

$$0 = \alpha \widehat{w}_1 + (1 - \alpha)\widehat{w}_2 \tag{4.3.2}$$

For all other moments – except for the mean – we are using the standardized versions of the variables, written as w'.

The second order moment is given as:

$$\overline{w'^2} = (1 - \delta)\alpha[(w_1 - \overline{w})^2 + \sigma_w^2]$$

$$+ (1 - \delta)(1 - \alpha)[(w_2 - \overline{w})^2 + \sigma_w^2]$$

$$+ \delta\sigma_{w3}^2,$$
(4.3.3)

where σ_{w3} is defined as $\lambda_w \overline{w'^2}$. This moment is also the variance of w at the same time, since

$$\overline{w'^2} = \mathbb{E}[w'^2] = \mathbb{E}[(w - \overline{w})^2] = \mathbb{E}[(w - \mathbb{E}[w])^2] = \mathbb{E}[w^2 - 2w\mathbb{E}[w] + \mathbb{E}[w]^2]$$

$$= \mathbb{E}[w^2] - 2\mathbb{E}[w\mathbb{E}[w]] + \mathbb{E}[\mathbb{E}[w]^2] = \mathbb{E}[w^2] - 2\mathbb{E}[w]\mathbb{E}[w] + \mathbb{E}[w]^2$$

$$= \mathbb{E}[w^2] - \mathbb{E}[w]^2 = \text{Var}[w].$$

The non-dimensional relationship would then be:

$$\frac{1}{(1 - \tilde{\sigma}_w^2)} = \alpha \left(\hat{w}_1^2 + \frac{\tilde{\sigma}_w^2}{(1 - \tilde{\sigma}_w)^2} \right) + (1 - \alpha) \left(\hat{w}_2^2 + \frac{\tilde{\sigma}_w^2}{(1 - \tilde{\sigma}_w^2)} \right). \tag{4.3.4}$$

The third order moment is given as:

$$\overline{w'^3} = (1 - \delta)\alpha[(w_1 - \overline{w})^3 + 3\sigma_w^2(w_1 - \overline{w})]$$

$$+ (1 - \delta)(1 - \alpha)[(w_2 - \overline{w})^3 + 3\sigma_w^2(w_2 - \overline{w})]$$

$$(4.3.5)$$

Since we want to make use of the specific shape of the pdf, we also have a relationship for $\overline{w'^3}$, which is called \widehat{Sk}_w , meaning the skewness of the variable w:

$$\widehat{Sk}_w \equiv \frac{1}{(1 - \tilde{\sigma}_w^2)^{3/2}} \frac{\overline{w'^3}}{\left(\overline{w'^2}\right)^{3/2}} \frac{1}{\left(\frac{1 - \delta \lambda_w}{1 - \delta}\right)^{3/2}} \frac{1}{1 - \delta}$$

$$= \alpha \left(\widehat{w}_1^3 + 3\widehat{w}_1 \frac{\widetilde{\sigma}_w^2}{(1 - \widetilde{\sigma}_w^2)}\right) + (1 - \alpha) \left(\widehat{w}_2^3 + 3\widehat{w}_2 \frac{\widetilde{\sigma}_w^2}{(1 - \widetilde{\sigma}_w^2)}\right)$$
(4.3.6)

4.3.2 Moments for θ_l

For θ_l we have a similar non-dimensional relationship:

$$0 = \alpha \tilde{\theta}_{l1} + (1 - \alpha)\tilde{\theta}_{l2} \tag{4.3.7}$$

Similarly but with a different standard deviation, $\overline{\theta_l'^2}$ is given as:

$$\overline{\theta_l^{\prime 2}} = (1 - \delta)\alpha[(\theta_{l1} - \overline{\theta_l})^2 + \sigma_{\theta_{l1}}^2]
+ (1 - \delta)(1 - \alpha)[(\theta_{l2} - \overline{\theta_l})^2 + \sigma_{\theta_{l2}}^2]
+ \delta\sigma_{\theta_l 3}^2,$$
(4.3.8)

where $\sigma_{\theta_l 3}$ is defined as $\lambda_{\theta_l} \overline{\theta_l'^2}$. This can also be expressed as the variance following the same approach as the one for $\overline{w'^2}$.

The third order moment is given as:

$$\overline{\theta_l^{\prime 3}} = (1 - \delta)\alpha[(\theta_{l1} - \overline{\theta_l})^3 + 3\sigma_{\theta_{l1}}^2(\theta_{l1} - \overline{\theta_l})]
+ (1 - \delta)(1 - \alpha)[(\theta_{l2} - \overline{\theta_l})^3 + 3\sigma_{\theta_{l2}}^2(\theta_{l2} - \overline{\theta_l})]$$
(4.3.9)

Similarly to equation (4.3.6), we also list a moment which is more diagnosed than prognosed:

$$\widehat{Sk_{\theta_l}} \equiv \frac{\overline{\theta_l'^3}}{\left(\overline{\theta_l'^2}\right)^{3/2}} \left(\frac{1}{\frac{1-\delta\lambda_{\theta}}{1-\delta}}\right)^{3/2} \frac{1}{1-\delta}
= \alpha \left(\widetilde{\theta}_{l1}^3 + 3\widetilde{\theta}_{l1}\widetilde{\sigma}_{\theta_l1}^2\right) + (1-\alpha) \left(\widetilde{\theta}_{l2}^3 + 3\widetilde{\theta}_{l2}\widetilde{\sigma}_{\theta_l2}^2\right).$$
(4.3.10)

4.3.3 Moments for r_t

The relationships for r_t and $\overline{r_t'^2}$ are given as follows

$$0 = \alpha \tilde{r}_{t1} + (1 - \alpha)\tilde{r}_{t2}, \tag{4.3.11}$$

and

$$1 = \alpha \left(\tilde{r}_{t1}^2 + \tilde{\sigma}_{r_{t1}}^2 \right) + (1 - \alpha) \left(\tilde{r}_{t2}^2 + \tilde{\sigma}_{r_{t2}}^2 \right). \tag{4.3.12}$$

Since this relationship is similar to the relationships of θ_l and $\theta_l^{\prime 2}$, we are using nearly the same formulas:

$$\overline{r_t'^2} = (1 - \delta)\alpha[(r_{t1} - \overline{r_t})^2 + \sigma_{r_{t1}}^2]
+ (1 - \delta)(1 - \alpha)[(r_{t2} - \overline{r_t})^2 + \sigma_{\theta_{t2}}^2]
+ \delta\sigma_{r_t3}^2,$$
(4.3.13)

and

$$\overline{r_t'^3} = (1 - \delta)\alpha[(r_{t1} - \overline{r_t})^3 + 3\sigma_{r_{t1}}^2(r_{t1} - \overline{r_t})]$$

$$+ (1 - \delta)(1 - \alpha)[(r_{t2} - \overline{r_t})^3 + 3\sigma_{r_{t2}}^2(r_{t2} - \overline{r_t})].$$
(4.3.14)

4.3.4 Mixed moments

There are also equations for two or even three variables, which are listed in the following.

$$\overline{w'\theta_l'} = (1 - \delta)\alpha[(w_1 - \overline{w})(\theta_{l1} - \overline{\theta_l})]$$

$$+ (1 - \delta)(1 - \alpha)[(w_2 - \overline{w})(\theta_{l2} - \overline{\theta_l})]$$

$$+ \delta\lambda_{w\theta}\overline{w'\theta_l'},$$
(4.3.15)

$$\overline{w'r_t'} = (1 - \delta)\alpha[(w_1 - \overline{w})(r_{t1} - \overline{r_t})]$$

$$+ (1 - \delta)(1 - \alpha)[(w_2 - \overline{w})(r_{t2} - \overline{r_t})]$$

$$+ \delta\lambda_{wr}\overline{w'r_t'}, \qquad (4.3.16)$$

and

$$\overline{r_t'\theta_l'} = (1 - \delta)\alpha \left[(r_{t1} - \overline{r_t}) \left(\theta_{l1} - \overline{\theta_l} \right) + r_{r_t\theta_l}\sigma_{r_{t1}}\sigma_{\theta_{l1}} \right]
+ (1 - \delta)(1 - \alpha) \left[(r_{t2} - \overline{r_t}) \left(\theta_{l2} - \overline{\theta_l} \right) + r_{r_t\theta_l}\sigma_{r_{t2}}\sigma_{\theta_{l2}} \right]
+ \delta\lambda_{r\theta}\overline{r_t'\theta_l'}.$$
(4.3.17)

We have the non-dimensional relationship for those moments given as

$$\widehat{c}_{w\theta_{l}} \equiv \frac{1}{\left(1 - \widetilde{\sigma}_{w}^{2}\right)^{1/2}} \frac{\overline{w'\theta_{l}'}}{\sqrt{\overline{w'^{2}}} \sqrt{\overline{\theta_{l}'^{2}}}} \frac{1}{\sqrt{\frac{1 - \delta\lambda_{w}}{1 - \delta}}} \frac{1}{\sqrt{\frac{1 - \delta\lambda_{w}}{1 - \delta}}} \frac{1 - \delta\lambda_{w\theta}}{1 - \delta}$$

$$= \alpha \widehat{w}_{1} \widetilde{\theta}_{l1} + (1 - \alpha) \widehat{w}_{2} \widetilde{\theta}_{l2}, \tag{4.3.18}$$

$$\widehat{c}_{wr_t} \equiv \frac{1}{(1 - \widetilde{\sigma}_w^2)^{1/2}} \frac{\overline{w'r_t'}}{\sqrt{\overline{w'^2}}} \frac{1}{\sqrt{\frac{1 - \delta \lambda_w}{1 - \delta}}} \frac{1}{\sqrt{\frac{1 - \delta \lambda_w}{1 - \delta}}} \frac{1 - \delta \lambda_{wr}}{1 - \delta}$$

$$= \alpha \widehat{w}_1 \widetilde{r}_{t1} + (1 - \alpha) \widehat{w}_2 \widetilde{r}_{t2}, \tag{4.3.19}$$

and

$$\widehat{c}_{r_{t}\theta_{l}} \equiv \frac{\overline{r_{t}'\theta_{l}'}}{\sqrt{\overline{r_{t}'^{2}}}\sqrt{\overline{\theta_{l}'^{2}}}} \frac{1}{\sqrt{\frac{1-\delta\lambda_{q}}{1-\delta}}} \frac{1}{\sqrt{\frac{1-\delta\lambda_{\theta}}{1-\delta}}} \frac{1-\delta\lambda_{\theta r}}{1-\delta}
= \alpha \left(\widetilde{r}_{t1}\widetilde{\theta}_{l1} + r_{r_{t}\theta_{l}}\widetilde{\sigma}_{q_{t1}}\widetilde{\sigma}_{\theta_{l1}}\right) + (1-\alpha) \left(\widetilde{r}_{t2}\widetilde{\theta}_{l2} + r_{r_{t}\theta_{l}}\widetilde{\sigma}_{r_{t2}}\widetilde{\sigma}_{\theta_{l2}}\right), \tag{4.3.20}$$

where we can think about \hat{c} as the correlation.

We also list a trivariate moment $(\overline{w'r'_t\theta'_l})$, given by:

$$\overline{w'r_t'\theta_l'} = (1 - \delta)\alpha(w_1 - \overline{w}) \left[(r_{t1} - \overline{r_t}) \left(\theta_{l1} - \overline{\theta_l} \right) + r_{r_t\theta_l}\sigma_{r_{t1}}\sigma_{\theta_{l1}} \right]$$

$$+ (1 - \delta)(1 - \alpha)(w_2 - \overline{w}) \left[(r_{t2} - \overline{r_t}) \left(\theta_{l2} - \overline{\theta_l} \right) + r_{r_t\theta_l}\sigma_{r_{t2}}\sigma_{\theta_{l2}} \right].$$

$$(4.3.21)$$

4.4 Solving for pdf parameters by using the moment terms

Having established the prognosed moments for the desired pdf, we now try to retrieve the specific pdf that generates these moments. This process essentially involves inverting the relationship between the moments and the parameters that define the pdf.

In our case, we refer back to the normal mixture family of pdfs (equation (4.1.1)), which offers a representation for atmospheric grid layers. To select a particular member within this family that best aligns with the prognosed moments, we perform a parameter retrieval step.

This retrieval is achieved by inverting equations (4.3.2) to (4.3.20). These equations express the prognosed moments (mean, variance, covariances, etc.) as functions of the underlying pdf parameters (weights, means, and standard deviations). By inverting these relationships, we aim to find a set of pdf parameters that produces the distribution corresponding to the prognosed moments.

However, it is important to mention that this inversion is not a straightforward process. That is because the equations are non-linear with respect to the pdf parameters. Despite this non-linearity, the relatively simple structure of the normal mixture pdf (equation (4.1.1)) allows for an analytical solution to the inversion problem. This analytical solution enables

us to efficiently map the prognosed moments back to the corresponding pdf parameters.

The proposed solution procedure [LG05] is as follows.

1. Solve for α , \widehat{w}_1 , and \widehat{w}_2 from the equations for \overline{w} (equation (4.3.2)), $\overline{w'^2}$ (equation (4.3.4)), $\overline{w'^3}$ (equation (4.3.6)):

$$\alpha = \frac{1}{2} \left[1 - \widehat{Sk}_w \sqrt{\frac{1}{4 + \widehat{Sk}_w^2}} \right], \tag{4.4.1}$$

$$\widehat{w}_1 = \sqrt{\frac{1-\alpha}{\alpha}},\tag{4.4.2}$$

$$\widehat{w}_2 = -\sqrt{\frac{\alpha}{1-\alpha}}. (4.4.3)$$

Without loss of generality, it has been chosen to set $\widehat{w}_1 > \widehat{w}_2$.

2. Looking at equation equation (4.4.1), we see that \widehat{Sk}_w is determined only by α :

$$\widehat{Sk}_w = \frac{1 - 2\alpha}{\sqrt{\alpha(1 - \alpha)}}. (4.4.4)$$

3. $\tilde{\theta}_{l1}$ and $\tilde{\theta}_{l2}$ are taken from solving equation (4.3.7) for $\overline{\theta_l}$, and equation (4.3.18) for $\overline{w'\theta_l}$:

$$\tilde{\theta}_{l1} = -\frac{\widehat{c}_{w\theta_l}}{\widehat{w}_2},\tag{4.4.5}$$

$$\tilde{\theta}_{l2} = -\frac{\hat{c}_{w\theta_l}}{\hat{w}_1}.\tag{4.4.6}$$

4. We can get $\tilde{\sigma}_{\theta_l 1}$ and $\tilde{\sigma}_{\theta_l 2}$ by fulfilling equation (4.3.8) for $\overline{\theta_l'^2}$, and equation (4.3.9) for $\overline{\theta_l'^3}$:

$$\tilde{\sigma}_{\theta_l 1}^2 = \left(1 - \hat{c}_{w\theta_l}^2\right) + \left(\sqrt{\frac{1 - \alpha}{\alpha}}\right) \frac{1}{3\hat{c}_{w\theta_l}} \left(\widehat{Sk_{\theta_l}} - \hat{c}_{w\theta_l}^3 \widehat{Sk}_w\right), \tag{4.4.7}$$

$$\tilde{\sigma}_{\theta_l 2}^2 = \left(1 - \hat{c}_{w\theta_l}^2\right) - \left(\sqrt{\frac{\alpha}{1 - \alpha}}\right) \frac{1}{3\hat{c}_{w\theta_l}} \left(\widehat{Sk_{\theta_l}} - \hat{c}_{w\theta_l}^3 \widehat{Sk_w}\right). \tag{4.4.8}$$

 Sk_{θ_l} represents the skewness of θ_l , which has to be provided by an equation such as equation (4.3.10) below.

- 5. Finding formulas for \tilde{r}_{t1} , \tilde{r}_{t2} , $\tilde{\sigma}_{r_{t1}}^2$, and $\tilde{\sigma}_{r_{t2}}^2$ can be done by replacing θ_l by r_t everywhere in the equations (4.4.5), (4.4.6), (4.4.7), and (4.4.8).
- 6. The last step is to get a relationship between $r_{r_t\theta_l}$, the in-between normal correlation and $c_{r_t\theta_l}$, the total correlation. This can be done by using equation (4.3.17):

$$r_{r_t\theta_l} = \frac{\widehat{c}_{r_t\theta_l} - \widehat{c}_{wr_t}\widehat{c}_{w\theta_l}}{\alpha\widetilde{\sigma}_{r_t1}\widetilde{\sigma}_{\theta_l1} + (1 - \alpha)\widetilde{\sigma}_{r_t2}\widetilde{\sigma}_{\theta_l2}}.$$
(4.4.9)

4.5 Expressions for higher-order moments in terms of pdf parameters

Upon determining the pdf parameters, we gain the ability to compute all higher-order moments associated with the distribution. These moments play a crucial role for closing the already described pdes. The symbolic calculation of higher-order moments can be achieved through integration over the specified pdf. Formulas for calculating various higher-order moments within the context of a binormal pdf are readily available in the literature [LG05].

We state the transformed formulas needed for closure in the following.

$$\frac{1}{(1-\tilde{\sigma}_{w}^{2})^{2}} \frac{(1-\delta)}{(1-\delta\lambda_{w})^{2}} \frac{\overline{w'^{4}}}{\left(\overline{w'^{2}}\right)^{2}} = \alpha \left[\widehat{w}_{1}^{4} + 6\widehat{w}_{1}^{2} \frac{\tilde{\sigma}_{w}^{2}}{(1-\tilde{\sigma}_{w}^{2})} + 3 \frac{\tilde{\sigma}_{w}^{4}}{(1-\tilde{\sigma}_{w}^{2})^{2}} \right] + (1-\alpha) \left[\widehat{w}_{2}^{4} + 6\widehat{w}_{2}^{2} \frac{\tilde{\sigma}_{w}^{2}}{(1-\tilde{\sigma}_{w}^{2})} + 3 \frac{\tilde{\sigma}_{w}^{4}}{(1-\tilde{\sigma}_{w}^{2})^{2}} \right] + \frac{1}{(1-\tilde{\sigma}_{w}^{2})^{2}} \frac{(1-\delta)}{(1-\delta\lambda_{w})^{2}} \delta 3\lambda_{w}^{2}, \tag{4.5.1}$$

$$\frac{1}{(1-\tilde{\sigma}_{w}^{2})} \frac{(1-\delta)^{1/2}}{(1-\delta\lambda_{w})(1-\delta\lambda_{\theta})^{1/2}} \frac{\overline{w'^{2}\theta'_{l}}}{\overline{w'^{2}} \left(\overline{\theta'_{l}^{2}}\right)^{1/2}} = \alpha \left[\widehat{w}_{1}^{2} + \frac{\tilde{\sigma}_{w}^{2}}{(1-\tilde{\sigma}_{w}^{2})}\right] \tilde{\theta}_{l1} + (1-\alpha) \left[\widehat{w}_{2}^{2} + \frac{\tilde{\sigma}_{w}^{2}}{(1-\tilde{\sigma}_{w}^{2})}\right] \tilde{\theta}_{l2}, \tag{4.5.2}$$

$$\frac{1}{(1-\tilde{\sigma}_w^2)^{1/2}} \frac{(1-\delta)^{1/2}}{(1-\delta\lambda_w)^{1/2}(1-\delta\lambda_\theta)} \frac{\overline{w'\theta_l'^2}}{\left(\overline{w'^2}\right)^{1/2}} = \alpha \widehat{w}_1 \left(\tilde{\theta}_{l1}^2 + \tilde{\sigma}_{\theta_{l1}}^2\right) + (1-\alpha)\widehat{w}_2 \left(\tilde{\theta}_{l2}^2 + \tilde{\sigma}_{\theta_{l2}}^2\right), \tag{4.5.3}$$

$$\frac{1}{(1-\tilde{\sigma}_{w}^{2})^{1/2}} \frac{(1-\delta)^{1/2}}{(1-\delta\lambda_{w})^{1/2}(1-\delta\lambda_{\theta})^{1/2}(1-\delta\lambda_{q_{t}})^{1/2}} \frac{\overline{w'r'_{t}\theta'_{l}}}{\left(\overline{w'^{2}}\right)^{1/2}\left(\overline{r''_{t}^{2}}\right)^{1/2}\left(\overline{\theta''_{l}^{2}}\right)^{1/2}} \\
= \alpha\widehat{w}_{1}\left(\widetilde{r}_{t1}\widetilde{\theta}_{l1} + r_{r_{t}\theta_{l}}\widetilde{\sigma}_{r_{t1}}\widetilde{\sigma}_{\theta_{l1}}\right) + (1-\alpha)\widehat{w}_{2}\left(\widetilde{r}_{t2}\widetilde{\theta}_{l2} + r_{r_{t}\theta_{l}}\widetilde{\sigma}_{r_{t2}}\widetilde{\sigma}_{\theta_{l2}}\right) \tag{4.5.4}$$

Equations for $\overline{w'^2r'_t}$ and $\overline{w'r'^2_t}$ are similar to equation (4.5.2) and equation (4.5.3) by replacing θ_l with r_t everywhere.

4.6 Approximation of scalar skewnesses

Closing the system of prognostic equations within CLUBB needs the specification of the skewness terms Sk_{θ_l} and Sk_{r_t} . These skewness values appear in the solutions for $\tilde{\sigma}_{\theta_l 1}$ (equation (4.4.7)) and $\tilde{\sigma}_{\theta_l 2}$ (equation (4.4.8)), respectively. Traditionally, these skewness terms

could be treated as prognostic variables, requiring their own prognostic equations and adding to the overall intense computation.

Therefore, the paper "Using probability density functions to derive consistent closure relationships among higher-order moments" by Larson and Golaz which this work is based on, proposes an alternative approach that uses a diagnostic formula for skewness. The formula provides a reasonable estimate of the skewness terms based on the readily available prognostic moments, avoiding the need for dedicated prognostic equations for skewness. This strategy results in closure of the system of equations while maintaining a computationally tractable model. The proposed formula is the following:

$$\widehat{Sk}_{\theta_l} = \widehat{Sk}_w \widehat{c}_{w\theta_l} \left[\beta + (1 - \beta) \widehat{c}_{w\theta_l}^2 \right], \tag{4.6.1}$$

which is similar for \widehat{Sk}_{r_t} by again just replacing r_t with θ_l . They define a parameter β which is dimensionless. We also solve for β because we are going to need the equation later on to show that other equations are true.

$$\implies \beta = \frac{\widehat{Sk}_{\theta_l}}{\widehat{Sk}_w \widehat{c}_{w\theta_l}} - \widehat{c}_{w\theta_l}^2}{1 - \widehat{c}_{w\theta_l}^2} \tag{4.6.2}$$

Equation (4.6.1) presents a diagnostic formula for estimating the skewness of θ_l . This formula offers a physically intuitive relationship. It proposes a proportionality between Sk_{θ_l} and Sk_w . However, it's crucial to acknowledge the limitations in this diagnostic. The formula suggests that an increase in the parameter β leads to a larger magnitude of Sk_{θ_l} . This translates to a pdf with a more extended tail in the θ_l domain. Furthermore, the formula captures the behavior when w and θ_l are correlated. That is, positive skewness in w leads to positive skewness in θ_l (positive correlation), and vice versa (negative correlation). However, it is important to mention that real-world large eddy simulations may show deviations from this simplified relationship.

Another limitation appears when either Sk_w or the covariance between w and θ_l $(c_{w\theta_l})$

approaches zero. The formula predicts a vanishing Sk_{θ_l} in these scenarios, which may not always be true.

Finally, the diagnostic approach allows for the magnitude of $|Sk_{\theta_l}|$ to be either smaller or larger than $|Sk_w|$. This behavior depends on the interplay between the variance of w ($\tilde{\sigma}_w^2$), the covariance $(c_{w\theta_l})$, and the parameter β . This highlights the potential for an inconsistency between the estimated skewness and the other binormal moments, e.g. a single value of β may not correspond exactly to any trivariate normal distribution

To summarize, equation (4.6.1) offers a computationally efficient method for skewness estimation, but it comes with limitations. While it captures some key aspects of the relationship between the skewness in w and the skewness in θ_l , one should be aware of deviations from its predictions.

We proceed with using equation (4.3.10) for \widehat{Sk}_{θ_l} and find the following relationships [LG05] for $\tilde{\sigma}_{\theta_l 1}^2$ and $\tilde{\sigma}_{\theta_l 2}^2$:

$$\tilde{\sigma}_{\theta_l 1}^2 = \frac{\left(1 - \hat{c}_{w\theta_l}^2\right)}{\alpha} \left[\frac{1}{3} \beta + \alpha \left(1 - \frac{2}{3} \beta\right) \right], \tag{4.6.3}$$

and

$$\tilde{\sigma}_{\theta_l 2}^2 = \frac{\left(1 - \hat{c}_{w\theta_l}^2\right)}{1 - \alpha} \left\{ 1 - \left[\frac{1}{3}\beta + \alpha \left(1 - \frac{2}{3}\beta\right)\right] \right\}. \tag{4.6.4}$$

By using the previously stated expressions for the standard deviations (equations (4.6.3) and (4.6.4), with their r_t counterparts), we can substitute them into the formula for the correlation between r_t and θ_l (equation (4.4.9)). This substitution leads to a more concise representation.

$$r_{r_t \theta_l} = \frac{c_{r_t \theta_l} - \hat{c}_{w r_t} \hat{c}_{w \theta_l}}{\left(1 - \hat{c}_{w r_t}^2\right)^{1/2} \left(1 - \hat{c}_{w \theta_l}^2\right)^{1/2}},\tag{4.6.5}$$

where the correlation of r_t and θ_l within the individual normal distributions is $r_{r_t\theta_l}$, and $c_{r_t\theta_l}$ represents the total correlation across the entire trinormal pdf.

4.7 Formulating closure relationships for higher-order moments in terms of lower-order moments

This section delves into the derivation of closure relationships for crucial higher-order moments employed within the CLUBB parameterization.

Our focus here lies on achieving closure for the following terms:

- $\overline{w'^4}$: The fourth-order moment of up-/downdrafts,
- $\overline{w'^2\theta'_I}$: the so-called flux of flux,
- $\overline{w'\theta'^2_l}$: the flux of variance,
- $\overline{w'r'_t\theta'_l}$: and the flux of covariance.

Closure, in this context, refers to expressing these higher-order moments completely in terms of known quantities, typically lower-order moments that are directly prognosed by the model. The approach to derive those formulas is based on the previously established expressions for the pdf parameters (equations (4.4.1) to (4.4.9)). By substituting those derived pdf parameter expressions into the relevant equations for the higher-order moments (equations (4.5.1) to (4.5.4)), we find the desired closure relationships.

We first present the equation for the third moment of θ'_l , $\overline{\theta''_l}$ This expression is derived by dimensionalizing equation (4.6.1), which relates the skewness of θ_l to the skewness of w and other model parameters.

$$\overline{\theta_l'^3} = \frac{(1 - \delta \lambda_{w\theta})(1 - \delta \lambda_{\theta})}{(1 - \tilde{\sigma}_w^2)^2 (1 - \delta \lambda_w)^2} \frac{\overline{w'^3}}{\left(\overline{w'^2}\right)^2} \overline{\theta_l'^2} \, \overline{w'\theta_l'} \left(\beta + (1 - \beta) \frac{(1 - \delta \lambda_{w\theta})^2}{1 - \tilde{\sigma}_w^2 (1 - \delta \lambda_w)(1 - \delta \lambda_{\theta})} \frac{\left(\overline{w'\theta_l'}\right)^2}{\overline{w'^2} \, \overline{\theta_l'^2}} \right). \tag{4.7.1}$$

While the scalar third moments (e.g., $\overline{\theta_l'^3}$) may not directly participate in solving the prognostic equations within CLUBB, they hold an indirect yet crucial role in shaping cloud properties within atmospheric simulations. This influence is coming from the connection between the pdf and the cloud formation.

Cumulus cloud formation mostly occurs at the edges, or "tails" of the pdf for a specific variable. These tails represent regions where the probability of encountering extreme values of the variable is relatively higher. As the relative "width" of the normal distribution representing w increases $(\tilde{\sigma}_w)$, the magnitude of $\overline{\theta_l'^3}$ also grows (refer to equation (4.7.1) for details). In simpler terms, a larger value of $\overline{\theta_l'^3}$ corresponds to a broader pdf for the up-/downdraft variable. This broader pdf deviates more significantly from a double delta function, which is a construct with two spikes at zero.

Unlike the scalar third moment, $\overline{w'^4}$ does not depend on the thermodynamic scalar moments (such as $\overline{\theta_l'^3}$). Consequently, it is independent of the parameter β . To derive the explicit formula for $\overline{w'^4}$, we can substitute the previously stated expressions for $\widehat{w_1}$ (equation (4.4.2)) and $\widehat{w_2}$ (equation (4.4.3)) into equation (4.5.1).

$$\frac{1}{(1-\tilde{\sigma}_w^2)^2} \frac{(1-\delta)}{(1-\delta\lambda_w)^2} \frac{\overline{w'^4}}{\left(\overline{w'^2}\right)^2} = 3 \frac{\tilde{\sigma}_w^4}{(1-\tilde{\sigma}_w^2)^2} + 6 \frac{\tilde{\sigma}_w^2}{(1-\tilde{\sigma}_w^2)} + 1 + \widehat{Sk}_w^2 + \frac{1}{(1-\tilde{\sigma}_w^2)^2} \frac{(1-\delta)}{(1-\delta\lambda_w)^2} \delta 3\lambda_w^2, \tag{4.7.2}$$

leading to

$$\overline{w'^4} = \left(\overline{w'^2}\right)^2 \frac{(1 - \delta\lambda_w)^2}{(1 - \delta)} \left(3\tilde{\sigma}_w^4 + 6\left(1 - \tilde{\sigma}_w^2\right)\tilde{\sigma}_w^2 + \left(1 - \tilde{\sigma}_w^2\right)^2\right)
+ \frac{1}{(1 - \tilde{\sigma}_w^2)} \frac{1}{(1 - \delta\lambda_w)} \frac{\left(\overline{w'^3}\right)^2}{\overline{w'^2}}
+ \delta 3\lambda_w^2 \left(\overline{w'^2}\right)^2.$$
(4.7.3)

As observed with $\overline{w'^4}$, $\overline{w'^2\theta'_l}$ displays independence from the parameter β within the context of the chosen pdf.

To proceed, we can substitute the previously derived expressions for \widehat{w}_1 (equation (4.4.2)), \widehat{w}_2 (equation (4.4.3)), \widehat{Sk}_w (equation (4.3.6)), $\widetilde{\theta}_{l1}$ (equation (4.4.5)), and $\widetilde{\theta}_{l2}$ (equation (4.4.6)) into equation (4.5.2). This substitution process will yield an explicit formula for $\overline{w'^2\theta'_l}$ that solely relies on known quantities, such as the prognostic moments directly calculated by the model.

$$\frac{1}{(1-\tilde{\sigma}_w^2)} \frac{(1-\delta)^{1/2}}{(1-\delta\lambda_w)(1-\delta\lambda_\theta)^{1/2}} \frac{\overline{w'^2\theta_l'}}{\overline{w'^2} \left(\overline{\theta_l'^2}\right)^{1/2}} = \widehat{c}_{w\theta_l} \widehat{Sk}_w, \tag{4.7.4}$$

and

$$\overline{w'^2\theta'_l} = \frac{1}{(1 - \tilde{\sigma}_w^2)} \frac{1 - \delta \lambda_{w\theta}}{1 - \delta \lambda_w} \frac{\overline{w'^3}}{\overline{w'^2}} \overline{w'\theta'_l}.$$
(4.7.5)

 $\overline{w'\theta_l'^2}$ depends explicitly on Sk_{θ_l} . Substituting equation (4.4.2) - equation (4.4.8) into equation (4.5.4) yields

$$\frac{1}{(1-\tilde{\sigma}_w^2)^{1/2}} \frac{(1-\delta)^{1/2}}{(1-\delta\lambda_w)^{1/2}(1-\delta\lambda_\theta)} \frac{\overline{w'\theta_l'^2}}{\left(\overline{w'^2}\right)^{1/2}\overline{\theta_l'^2}} = \frac{2}{3} \widehat{c}_{w\theta_l}^2 \widehat{Sk}_w + \frac{1}{3} \frac{\widehat{Sk}_{\theta_l}}{\widehat{c}_{w\theta_l}}, \tag{4.7.6}$$

and

$$\overline{w'\theta_l'^2} = \frac{2}{3} \frac{(1 - \delta \lambda_{w\theta})^2}{(1 - \delta \lambda_w)^2} \frac{1}{(1 - \tilde{\sigma}_w^2)^2} \frac{\overline{w'^3}}{\left(\overline{w'^2}\right)^2} \left(\overline{w'\theta_l'}\right)^2 + \frac{1}{3} \frac{(1 - \delta \lambda_w)}{(1 - \delta \lambda_{w\theta})} \left(1 - \tilde{\sigma}_w^2\right) \frac{\overline{w'^2}}{\overline{w'\theta_l'}}.$$
(4.7.7)

5 Integration using SymPy

Throughout this thesis, symbolic manipulation plays a crucial role in verifying mathematical expressions, particularly integrals. To achieve this, we rely on SymPy [Meu+17] – a powerful Python library for symbolic mathematics. This chapter dives into the world of SymPy, showcasing its capabilities through a detailed example.

We begin by demonstrating the analytical approach to solving an integral. Next, we will explore the numerical side of integration. We are going to demonstrate how SymPy can be seamlessly integrated with numerical computing libraries to evaluate the integral for specific input values. This combined approach allows us to not only verify our analytical solution but also gain valuable insights into the integral's behavior for different scenarios. By following this step-by-step example, the reader will gain a solid understanding of how SymPy can be used, not only for this thesis.

5.1 Analytic integration

For simplicity and readability, we choose the check for the formula of $\overline{w'^2}$ (this is item 3 from section 2.6). One starts by importing and – obviously – installing the packages if they are not there yet. Importing the package display is useful for later on printing the equations. Thus, this results in the code in listing 5.1. In this listing, sympy was defined to be called sp and from sympy we directly imported some packages, too, which are needed later on.

Next, we define all symbols which are needed to calculate the given integral and therefore also to print the equations nicely. Since we are checking $\overline{w'^2}$, we need the (self-defined)

Listing 5.1: Import statements

```
import sympy as sp
from IPython.display import display
from sympy import abc, oo, Symbol, Integral
from sympy.stats import Normal, density
```

symbols listed in listing 5.2. Having defined the symbols, we can proceed with defining

Listing 5.2: Defining symbols

```
sigma_w = Symbol('\\sigma_w')
w_1 = Symbol('w_1')
w_2 = Symbol('w_2')
w_bar = Symbol('\\overline{w}')
sigma_w_3 = Symbol('\\sigma_{w3}')
w_prime_2_bar = Symbol('\\overline{w\'^2}')
```

the marginal distribution. Now, we are also using sympy.abc for displaying some standard symbols (listing 5.3). Having done that we can actually display the integral which we want

Listing 5.3: Defining the marginals

to compute (listing 5.4). Looking at figure 5.1, this is exactly the integral which we

Listing 5.4: Defining and displaying the needed integral

```
w_prime_2_bar_int = sp.Integral((sp.abc.w - w_bar) ** 2 * G_w, [sp.abc.w, -oo, oo])
display(sp.Eq(w_prime_2_bar, w_prime_2_bar_int))
```

want to compute. Using the command .doit(conds='none') in listing 5.5, we can actually

Figure 5.1: Output of listing 5.4

$$\overline{w'^{2}} = \int_{-\infty}^{\infty} (-\overline{w} + w)^{2} \left(\frac{\sqrt{2}\delta e^{-\frac{(-\overline{w} + w)^{2}}{2\sigma_{w}^{2}3}}}{2\sqrt{\pi}\sigma_{w3}} + \frac{\sqrt{2}\alpha (1 - \delta) e^{-\frac{(w - w_{1})^{2}}{2\sigma_{w}^{2}}}}{2\sqrt{\pi}\sigma_{w}} + \frac{\sqrt{2} \cdot (1 - \alpha) (1 - \delta) e^{-\frac{(w - w_{2})^{2}}{2\sigma_{w}^{2}}}}{2\sqrt{\pi}\sigma_{w}} \right) dw$$

calculate the given integral, where we assume that all given constants are real. We are also using .simplify() here to make the output more readable as well as more comparable to the actual function we want to check. We can now compare figure 5.2 to the given equation.

Listing 5.5: Calculating and printing the integral

```
w_prime_2_bar_int_val = w_prime_2_bar_int.doit(conds='none').simplify()
display(sp.Eq(w_prime_2_bar, w_prime_2_bar_int_val))
```

Figure 5.2: Output of listing 5.5

$$\overline{w'^2} = -\overline{w}^2\delta + \overline{w}^2 + 2\overline{w}\alpha\delta w_1 - 2\overline{w}\alpha\delta w_2 - 2\overline{w}\alpha w_1 + 2\overline{w}\alpha w_2 + 2\overline{w}\delta w_2 - 2\overline{w}w_2 - \sigma_w^2\delta + \sigma_w^2 + \sigma_{w3}^2\delta - \alpha\delta w_1^2 + \alpha\delta w_2^2 + \alpha w_1^2 - \alpha w_2^2 - \delta w_2^2 + w_2^2,$$

To do this, we first need to define the equation for equation (4.3.3) in listing 5.6. We can

Listing 5.6: Python function for the second order moment

print this equation using display again (listing 5.7). The last step is to check if those two

Listing 5.7: Printing the symbolic equation

display(sp.Eq(w_prime_2_bar, w_prime_2_bar_check()))

Figure 5.3: Output of listing 5.7

$$\overline{w'^{2}} = \sigma_{w3}^{2} \delta + \alpha (1 - \delta) \left(\sigma_{w}^{2} + (-\overline{w} + w_{1})^{2} \right) + (1 - \alpha) (1 - \delta) \left(\sigma_{w}^{2} + (-\overline{w} + w_{2})^{2} \right)$$

formulas are equivalent to each other. We can do this by using Eq(..) from the package SymPy. factor(..) tries to factor the given variables to make the comparison easier. All of this can be seen in listing 5.8. This code (listing 5.8) just displays True, which is exactly

Listing 5.8: Check if the integral and the given formula are the same

what we wanted to have.

5.2 Numeric integration

Again, for better readability, we choose to check the formula for $\overline{w'^2\theta'_l}$ (this is item 6 from section 2.6). As in section 5.1, there needs to be some packages imported. We are importing the same packages as in listing 5.1 together with some more (listing 5.9). Since we are going

Listing 5.9: Import statements

```
from itertools import product import pandas as pd import numpy as np
```

to need some more symbols, we also need to define those. We still use the symbols as in

listing 5.2, together with the ones in listing 5.10.

Listing 5.10: Defining symbols

```
theta_l_1 = Symbol('\\theta_{l2}')
theta_l_2 = Symbol('\\theta_{l2}')
theta_l_bar = Symbol('\\sigma_{\\theta_{l1}}')
sigma_theta_l_1 = Symbol('\\sigma_{\\theta_{l2}}')
sigma_theta_l_2 = Symbol('\\sigma_{\\theta_{l2}}')
sigma_theta_l_3 = Symbol('\\sigma_{\\theta_{l2}}')
rho_w_theta_l = Symbol('\\rho_{w\\theta_{l2}}')
w_prime_3_bar = Symbol('\\rho_{w\\theta_{l2}}')
w_prime_theta_l_prime_bar = Symbol('\\overline{w\'^3}')
w_prime_theta_l_prime_bar = Symbol('\\overline{w\'\\theta\'_l}')
sigma_tilde_w = Symbol('\\tilde{\\sigma}_w')
lambda_w_theta = Symbol('\\theta_{w\\theta}')
lambda_w = Symbol('\\lambda_w')
```

We start defining the integral by defining the marginals (listing 5.11).

Listing 5.11: Defining the marginals

```
G_1_w_theta = Normal(name='G_1_w_theta', mean=sp.Matrix([w_1, theta_1_1]),
    std=sp.Matrix([[sigma_w ** 2, 0], [0, sigma_theta_l_1 ** 2]]))
G_1_w_theta_density = density(G_1_w_theta)(sp.abc.w, sp.abc.theta)
G_2_w_theta = Normal(name='G_2_w_theta', mean=sp.Matrix([w_2, theta_1_2]),
    std=sp.Matrix([[sigma_w ** 2, 0], [0, sigma_theta_1_2 ** 2]]))
G_2_w_theta_density = density(G_2_w_theta)(sp.abc.w, sp.abc.theta)
G_3_w_theta = Normal(name='G_3_w_theta', mean=sp.Matrix([w_bar, theta_l_bar]),
    std=sp.Matrix([[sigma_w_3 ** 2,
        rho_w_theta_1 * sigma_w_3 * sigma_theta_1_3],
        [rho_w_theta_1 * sigma_w_3 * sigma_theta_1_3,
        sigma_theta_1_3 ** 2]]))
G_3_w_theta_density = sp.simplify(density(G_3_w_theta)(sp.abc.w, sp.abc.theta))
G_w_{theta} = (
(1 - sp.abc.delta) * sp.abc.alpha * density(G_1_w_theta)(sp.abc.w, sp.abc.theta)
+ (1 - sp.abc.delta) * (1 - sp.abc.alpha) * density(G_2_w_theta)(sp.abc.w, sp.abc.theta)
+ sp.abc.delta * G_3_w_theta_density)
```

The integral which needs to be computed is then defined as in listing 5.12.

Here (listing 5.12), the output is omitted for better readability. We do not yet compute the integral, because due to the complexity, unfortunately this is not working with SymPy.

Listing 5.12: Defining and displaying the needed integral

Since there is still the equation to check needed, we proceed by defining a function for that in listing 5.13. Looking at figure 5.4, there are some other equations needed like

Listing 5.13: Python function for $\overline{w'^2\theta_l}$

```
def w_prime_2_theta_l_prime_bar_check(sigma_tilde_w = sigma_tilde_w,
    delta = sp.abc.delta, lambda_w_theta = lambda_w_theta, lambda_w = lambda_w,
    w_prime_3_bar = w_prime_3_bar, w_prime_2_bar = w_prime_2_bar,
    w_prime_theta_l_prime_bar = w_prime_theta_l_prime_bar):
    return ((1 / (1 - sigma_tilde_w ** 2)) *
        ((1 - delta * lambda_w_theta) / (1 - delta * lambda_w)) *
        (w_prime_3_bar / w_prime_2_bar) *
        w_prime_theta_l_prime_bar)
display(sp.Eq(w_prime_2_theta_prime_l_bar, w_prime_2_theta_l_prime_bar_check()))
```

Figure 5.4: Output of listing 5.13

$$\overline{w'^{2}\theta'_{l}} = \frac{\overline{w'\theta'_{l}} \cdot \overline{w'^{3}} \left(-\lambda_{w\theta}\delta + 1\right)}{\overline{w'^{2}} \cdot \left(1 - \tilde{\sigma}_{w}^{2}\right) \left(-\lambda_{w}\delta + 1\right)}$$

equation (4.3.15), equation (4.3.5), equation (4.3.3), equation (4.2.3), and equation (4.1.4). We do not list the functions to those equations here, because they are defined the same way as the other equations are defined as functions.

Instead, since we cannot compute the integral analytically, we can create a dataframe using pandas[McK10]. The columns for this dataframe are going to be all the inputs we have. To get all permutations, this code (listing 5.14) is also using product(...) from the itertools package.

Listing 5.14: Create a dataframe and putting in arbitrary numbers

We append another column which is called "checkval" and lists the values for the given equation to check. This code also uses the function defined in listing 5.13, where all other

Listing 5.15: Attaching the "checkval" column to the dataframe

```
df['checkval'] = (df.apply(lambda x: w_prime_2_theta_l_prime_bar_check_val.subs({
        w_1: x[w_1], w_2: x[w_2], theta_l_1: x[theta_l_1], theta_l_2: x[theta_l_2],
        sigma_theta_l_1: x[sigma_theta_l_1], sigma_theta_l_2: x[sigma_theta_l_2],
        sigma_lambda_theta_l: x[sigma_lambda_theta_l], sigma_w: x[sigma_w],
        sigma_lambda_w: x[sigma_lambda_w], sp.abc.alpha: x[sp.abc.alpha],
        sp.abc.delta: x[sp.abc.delta], rho_w_theta_l: x[rho_w_theta_l]}), axis=1))
```

equations are substituted into. The function df.apply(..) is used to apply the function given in the parenthesis to all rows of the dataframe by specifying a lambda x, where x is corresponding to the given dataframe, df. Lastly, there is also the axis=1 parameter, which specifies the direction of applying the function.

Next, we are actually computing $\overline{w'^2\theta_l}$ numerically by using the quadrature method and applying the values of this integrals to a new column in the dataframe (listing 5.16). Here, we

Listing 5.16: Attaching the "numint" column to the dataframe

```
df['numint'] = (df.apply(lambda x: Rational(w_prime_2_theta_l_prime_bar.subs({
    w_1: x[w_1],w_2: x[w_2], theta_l_1: x[theta_l_1], theta_l_2: x[theta_l_2],
    sigma_theta_l_1: x[sigma_theta_l_1], sigma_theta_l_2: x[sigma_theta_l_2],
    sigma_lambda_theta_l: x[sigma_lambda_theta_l], sigma_w: x[sigma_w],
    sigma_lambda_w: x[sigma_lambda_w], sp.abc.alpha: x[sp.abc.alpha],
    sp.abc.delta: x[sp.abc.delta], rho_w_theta_l: x[rho_w_theta_l]
}).doit(conds='none', method='quad').evalf()), axis=1))
```

are using the integral which has been specified earlier and adding the parameter method='quad'

to the function .doit(...). After that, .evalf(...) just gives the numerical value. We try to prove that the integral value equals the function value, hence we are computing the error between those two columns (listing 5.17) and take the mean (numpy.mean(...) from the package NumPy [Har+20]) of these new columns (listing 5.18) to see if the error is actually numerically 0.

Listing 5.17: Attaching the "diffnum" column to the dataframe

```
df['diffnum'] = abs(df['checkval'].astype(float) - df['numint'].astype(float))
```

Listing 5.18: Calculating the mean difference

```
print('The mean error between the rhs and the lhs is:', np.mean(df['diffnum']))
```

Figure 5.5: Output of listing 5.18
The mean error between the rhs and the lhs is: 1.3753423344481015e-124

In figure 5.5, we see that the mean error is basically 0 which we wanted. It should be noted that based on the configuration of each individual computer, the solutions can slightly differ due to floating point arithmetic.

6 Asymptotics

Once we defined all functions, we see that we want certain behaviors for certain values as well as there is a need to restrict some parameter values.

We start with the "obvious" restrictions for the pdf parameters. The mixture fractions α and δ are meant to be $\alpha \in [0,1]$ and $\delta \in [0,1)$. But since the code tries to simplify a lot of things, the binormal representation also does not revert back to a single normal distribution. Therefore, we have $\alpha \in (0,1)$ due to the code. The restriction to δ makes sense in a way that we do not really want just the third normal to predict the whole shape. Also, most of the formulas, e.g. equation (4.3.6) have a $1 - \delta$ in the denominator.

In section 2.3, we saw, how the transformation between the sum of two normal distributions and the sum of three normal distributions are working. From those transformations, we see that we want

$$0 < \delta \lambda_w < 1, \qquad 0 < \delta \lambda_\theta < 1, \qquad 0 < \delta \lambda_r < 1,$$

$$\iff 0 < \delta \frac{\sigma_{w3}^2}{w'^2} < 1, \qquad 0 < \delta \frac{\sigma_{\theta_l 3}^2}{\theta_l'^2} < 1, \qquad 0 < \delta \frac{\sigma_{rt3}^2}{r_t'^2} < 1,$$

$$\iff 0 < \delta \sigma_{w3}^2 < \overline{w'^2}, \quad 0 < \delta \sigma_{\theta_l 3}^2 < \overline{\theta_l'^2}, \quad 0 < \delta \sigma_{rt3}^2 < \overline{r_t'^2}.$$

That is, for instance, that the variance of w over the whole pdf has to be strictly greater than δ times the squared standard deviation in w of the third normal distribution.

To make the resulting pdfs realizable, it turns out [Lar22], that we need to have $-1 < \hat{c}_{w\theta_l}, \hat{c}_{wr_t}, \hat{c}_{r_t\theta_l} < 1$. This is for instance:

$$c_{wr_t}^2 < \left(1 - \tilde{\sigma}_w^2\right) \left(\frac{(1 - \delta\lambda_w)(1 - \delta\lambda_r)}{(1 - \delta\lambda_{wr})^2}\right) \tag{6.0.1}$$

So it might be safer to set

$$\lambda_{w}, \lambda_{r} < \lambda_{wr} \iff \left(\frac{\sigma_{w3}^{2}}{\overline{w'^{2}}} < \frac{\rho_{wr_{t}}\sigma_{w3}\sigma_{r_{t}3}}{\overline{w'r'_{t}}}\right) \wedge \left(\frac{\sigma_{r_{t}3}^{2}}{\overline{r'_{t}^{2}}} < \frac{\rho_{wr_{t}}\sigma_{w3}\sigma_{r_{t}3}}{\overline{w'r'_{t}}}\right)$$

$$\iff \left(\sigma_{w3}\overline{w'r'_{t}} < \rho_{wr_{t}}\sigma_{r_{t}3}\overline{w'^{2}}\right) \wedge \left(\sigma_{r_{t}3}\overline{w'r'_{t}} < \rho_{wr_{t}}\sigma_{w3}\overline{r'_{t}^{2}}\right)$$

$$(6.0.2)$$

so that the rhs is greater and the bound is less restrictive. If we assume $\lambda_{\theta} = \lambda_r$ and $\lambda_{w\theta} = \lambda_{wr}$, then the model gains 5 new pdf parameters: δ , λ_w , λ_{θ} , $\lambda_{w\theta}$, $\lambda_{\theta r}$. If we want the pdf to revert to a single normal distribution in the limit of zero skewness, then we need

$$\delta, \lambda_w, \lambda_r, \lambda_\theta, \lambda_{wr}, \lambda_{w\theta}, \lambda_{\theta r} \to 1,$$
 (6.0.3)

as $Sk_w \to 0$. That being said, we can have a look at equation (4.3.6) and take the limit.

$$\lim_{\delta \to 1, \lambda_w \to 1} \left(\widehat{Sk}_w \right) = \lim_{\delta \to 1, \lambda_w \to 1} \frac{1}{\left(1 - \widetilde{\sigma}_w^2 \right)^{3/2}} \frac{\overline{w'^3}}{\left(\overline{w'^2} \right)^{3/2}} \frac{1}{\left(\frac{1 - \delta \lambda_w}{1 - \delta} \right)^{3/2}} \frac{1}{1 - \delta}$$

$$= \lim_{\delta \to 1, \lambda_w \to 1} \frac{1}{\left(1 - \widetilde{\sigma}_w^2 \right)^{3/2}} \frac{\overline{w'^3}}{\left(\overline{w'^2} \right)^{3/2}} \frac{(1 - \delta)^{3/2}}{(1 - \delta \lambda_w)^{3/2}} \frac{1}{1 - \delta}$$

$$= \lim_{\delta \to 1, \lambda_w \to 1} \frac{1}{\left(1 - \widetilde{\sigma}_w^2 \right)^{3/2}} \frac{\overline{w'^3}}{\left(\overline{w'^2} \right)^{3/2}} \frac{(1 - \delta)^{1/2}}{(1 - \delta \lambda_w)^{3/2}}$$

$$= 0 \tag{6.0.4}$$

Hence, if $\delta \to 1$ we get $Sk_w \to 0$. Of course, one needs to pay attention when computing those equations in the code, since we could run into a division by zero error, depending on which values are computed first.

Also, we want to see how the "main" equations behave in the limit of $\delta \to 1$ as well as any $\lambda \to 1$. For those limits, we assume all lower-order moments as constants because they are just given to us in the code.

6.1 Limits for $\delta \rightarrow 1$

We start with letting $\delta \to 1$.

6.1.1 Limit for $\overline{w'^4}$ as δ goes to 1

$$\lim_{\delta \to 1} \left(\overline{w'^4} \right) = \left(\overline{w'^2} \right)^2 \lim_{\delta \to 1} \left(\frac{(1 - \delta \lambda_w)^2}{(1 - \delta)} \right) + \frac{\left(\overline{w'^3} \right)^2}{\overline{w'^2}} \lim_{\delta \to 1} \left(\frac{1}{(1 - \delta \lambda_w)} \right) + 3\lambda_w^2 \left(\overline{w'^2} \right)^2 \quad (6.1.1)$$

Looking at this limit (for the calculation refer to appendix B.1), where we held the lowerorder moments fixed and not dependent on δ , unfortunately, we see that the kurtosis of w diverges.

6.1.2 Limit for $\overline{w'^2\theta'_l}$ as δ goes to 1

$$\lim_{\delta \to 1} \left(\overline{w'^2 \theta_l'} \right) = \frac{\overline{w'^3} \cdot \overline{w' \theta_l'}}{\overline{w'^2}} \lim_{\delta \to 1} \left(\frac{1 - \delta \lambda_{w\theta}}{1 - \delta \lambda_w} \right) \tag{6.1.2}$$

This limit (for the calculation refer to appendix B.2) is suggesting that if we want to have a limit as 0 as $\delta \to 1$ for $\overline{w'^2r'_t}$ we should set $\lambda_{w\theta} = 1$. Otherwise, if we set $\lambda_w = 0$, we get a limit that depends on the ratio between $\overline{w'^3} \cdot \overline{w'\theta'_l}$ and $\overline{w'^2}$.

6.1.3 Limit for $\overline{w'^2\theta'_l}$ as δ goes to 1

$$\lim_{\delta \to 1} \left(\overline{w'^2 \theta'_l} \right) = \frac{1}{3} \left(\frac{2\overline{w'^3} \left(\overline{w' \theta'_l} \right)^2}{\left(\overline{w'^2} \right)^2} \lim_{\delta \to 1} \left(\left(\frac{1 - \delta \lambda_{w\theta}}{1 - \delta \lambda_w} \right)^2 \right) + \frac{\overline{w'^2} \overline{\theta'_l^2}}{\overline{w' \theta'_l}} \lim_{\delta \to 1} \left(\frac{1 - \delta \lambda_w}{1 - \delta \lambda_{w\theta}} \right) \right)$$
(6.1.3)

This limit (for the calculation refer to appendix B.3)

6.1.4 Limit for $\overline{w'r'_t\theta'_l}$ as δ goes to 1

$$\lim_{\delta \to 1} \left(\overline{w' r_t' \theta_l'} \right) = \lim_{\delta \to 1} \left((1 - \delta) \alpha(w_1 - \overline{w}) \left[(r_{t1} - \overline{r_t}) \left(\theta_{l1} - \overline{\theta_l} \right) + r_{r_t \theta_l} \sigma_{r_{t1}} \sigma_{\theta_{l1}} \right] + (1 - \delta) (1 - \alpha) (w_2 - \overline{w}) \left[(r_{t2} - \overline{r_t}) \left(\theta_{l2} - \overline{\theta_l} \right) + r_{r_t \theta_l} \sigma_{r_{t2}} \sigma_{\theta_{l2}} \right] \right)$$

$$= 0 \tag{6.1.4}$$

7 Summary

This thesis explores the potential benefits of incorporating a third normal distribution into the CLUBB model, a framework used for parameterizing atmospheric processes. While the initial motivation for this exploration may not be immediately clear, section 2.1 delves into graphical illustrations that reveal distinct advantages associated with this trinormal representation for capturing specific atmospheric behaviors.

Following this initial groundwork, section 2.4 formally establishes the central objective of this research. That is, to demonstrate the continued validity of existing CLUBB model formulas within the context of the proposed trinormal distribution. Achieving this is based on using certain transformations, shown in section 2.3.

To validate the accuracy of the transformed formulas, a verification framework is established. This framework defines the inputs and outputs (section 2.5) associated with both the forward run (code used in the model) and the backward run (verification direction). This is followed by presenting a step-by-step verification procedure, ensuring that the transformed formulas are still valid.

The foundation for this investigation is laid out in chapter 3. This chapter provides a brief overview of pdfs, including both, the univariate and the multivariate normal distribution. Additionally, it explores the concepts of second, third, and fourth-order moments, which play a crucial role in characterizing certain statistical properties, but more importantly – at least for this work – the shapes of the distributions.

Building upon these definitions, section 4.1 introduces the newly proposed trinormal distribu-

tion, denoted as P_{tmg} . This distribution strategically positions the third normal component in-between the two existing components within the CLUBB model. Furthermore, the chapter establishes key properties associated with this new trinormal mixture pdf.

Chapter 4 details the transformation of the existing CLUBB formulas to work with the trinormal representation. This chapter serves as a comprehensive reference for the transformed equations employed throughout the thesis.

Following the establishment of the theoretical framework and the transformed formulas, chapter 5 delves into the actual calculation of the integrals. This chapter explores the application of a cas – specifically, SymPy – for tackling both, symbolic and numerical integration tasks.

The final chapter – chapter 6 – investigates the asymptotic behavior of the newly derived functions. This analysis shows on how the functions behave as their arguments approach specific values (e.g., one or zero). Additionally, the chapter identifies parameter value ranges or limitations that must be considered when working with these functions.

In essence, this thesis presents a comprehensive investigation into incorporating a trinormal distribution into the CLUBB model. The research demonstrates the compatibility of existing CLUBB model formulas with the proposed trinormal representation.

8 Outlook

For CLUBB there are new parameters, e.g. δ or λ_w , which can be chosen to "tweak" the representation of the underlying pdf for the prognosed moments. Ultimately one would like to fit this resulting pdf to real data, to get better relationships, as well as thresholds for some variables. To do this there are some approaches which unfortunately have not been discussed. A following thesis could e.g. incorporate some machine learning approach to learn optimal values for certain parameters.

The methodology established in chapter 5 extends far beyond the immediate application within the CLUBB model. This chapter serves as a blueprint for a generalizable approach to verifying and analyzing integral expressions. Its core strength lies in the utilization of SymPy, a powerful and well-supported cas. SymPy's community-driven nature provides continuous development and a vast library of mathematical capabilities. By leveraging this versatile tool, we can tackle a wide range of integral expressions, both analytically and numerically. This approach offers several advantages:

- Symbolic Verification: SymPy allows us to perform symbolic manipulations, enabling the derivation of exact solutions for integrals whenever possible.
- Numerical Approximation: For integrals that are analytically intractable, SymPy seamlessly integrates with numerical computing libraries. This allows us to efficiently approximate the integral's value for specific parameter choices. This combined approach ensures we can handle a broader range of integral expressions.
- Generalizability and Reusability: The framework outlined in chapter 5 is not specific to

the context of CLUBB. By focusing on the core functionalities of SymPy, this approach can be adapted to various scientific disciplines.

Overall, the methods we developed in this thesis using SymPy are not just useful for the CLUBB model. These methods can be applied to many other scientific problems because they can both solve integrals exactly (symbolically) and get close answers (numerically) for a wide range of equations. SymPy, being a powerful and widely-used tool, makes this possible.

Bibliography

- [Har+20] Charles R. Harris et al. "Array programming with NumPy". In: *Nature* 585.7825 (Sept. 2020), pp. 357–362. DOI: 10.1038/s41586-020-2649-2. URL: https://doi.org/10.1038/s41586-020-2649-2.
- [Ize08] Alan Julian Izenman. Modern multivariate statistical techniques: regression, classification, and manifold learning. Springer texts in statistics. OCLC: ocn225427579. New York; London: Springer, 2008. ISBN: 9780387781884.
- [Lar22] Vincent E. Larson. *CLUBB-SILHS: A parameterization of subgrid variability in the atmosphere*. 2022. arXiv: 1711.03675 [physics.ao-ph].
- [LG05] Vincent E Larson and Jean-Christophe Golaz. "Using probability density functions to derive consistent closure relationships among higher-order moments". In: Monthly Weather Review 133.4 (2005), pp. 1023–1042.
- [McK10] Wes McKinney. "Data Structures for Statistical Computing in Python". In: Proceedings of the 9th Python in Science Conference. Ed. by Stéfan van der Walt and Jarrod Millman. 2010, pp. 56–61. DOI: 10.25080/Majora-92bf1922-00a.
- [Meu+17] Aaron Meurer et al. "SymPy: symbolic computing in Python". In: *PeerJ Computer Science* 3 (Jan. 2017), e103. ISSN: 2376-5992. DOI: 10.7717/peerj-cs.103. URL: https://doi.org/10.7717/peerj-cs.103.

A Code

A.1 User Guide

A.1.1 Accessing the code

The code used for checking functions mentioned in the thesis is attached and can be accessed alongside this document.

A.1.2 Key files and their purposes

- checked_functions.py: This file hosts the definitions of all functions used for checking integrals.
- symbols.py: This file contains definitions of all symbols employed for computations with SymPy.

A.1.3 Working with functions

To obtain a function with symbols already incorporated, call it with an empty list of arguments (e.g., function_name()).

A.1.4 Displaying equations effectively

- 1. Import the display function from IPython.display.
- 2. Use display(...) to present statements or even equations visually.

A.1.5 Handling integrals

1. Displaying an integral: Use sympy.Integral(..) and put it into display(..) to visualize the integral.

- 2. Computing an integral symbolically: Apply .doit(..) to the integral object for symbolic computation.
- 3. Approximating an integral numerically: Add the option "method=quad" within the .doit(..) call to calculate the integral using the quadrature approximation method.

A.2 symbols.py

```
from sympy import Symbol, symbols
2
    # siqma
3
    sigma_w = Symbol('\\sigma_w')
4
5
    sigma_r_t_i, sigma_r_t_1, sigma_r_t_2 = (
6
7
        symbols('\sigma_{r_{ti}} \sigma_{r_{t1}} \sigma_{r_{t2}}'))
    sigma_theta_l_i, sigma_theta_l_1, sigma_theta_l_2 = (
9
        symbols('\sigma_{\theta_{11}} \sigma_{\theta_{12}}'))
10
11
    sigma_tilde_r_t_i, sigma_tilde_r_t_1, sigma_tilde_r_t_2 = (
12
        symbols('\\tilde{\\sigma}_{r_ti} \\tilde{\\sigma}_{r_t1} \\\tilde{\\sigma}_{r_t2}')
13
14
15
    sigma_tilde_theta_l_i, sigma_tilde_theta_l_1, sigma_tilde_theta_l_2 = (
16
        symbols(
17
18
             '\\tilde{\\sigma}_{\\theta_li} \\tilde{\\sigma}_{\\theta_l1}
             → \\tilde{\\sigma}_{\\theta_12}')
    )
19
20
    sigma_tilde_w_3 = Symbol('\\tilde{\\sigma}_{w3}')
21
    sigma_tilde_w = Symbol('\\tilde{\\sigma}_w')
22
    sigma_w_3 = Symbol('\\sigma_{w3}')
23
    sigma_theta_1_3 = Symbol('\\sigma_{\\theta_1 3}')
^{24}
    sigma_r_t_3 = Symbol('\sigma_{r_t_3}')
25
26
    # w
27
    w_bar = Symbol('\\overline{w}')
28
    w_prime = Symbol('w\'')
29
    w_i, w_1, w_2 = symbols('w_i w_1 w_2')
30
31
    w_hat_i, w_hat_1, w_hat_2, w_hat_3, w_hat_prime = (
32
        symbols('\hat{w}_i \hat{w}_1 \hat{w}_2 \hat{w}_3 \hat{w}'')
33
34
35
    w_prime_2_bar, w_prime_3_bar, w_prime_4_bar = symbols(
36
         \label{eq:condition} $$ \operatorname{w}^2  \wedge \operatorname{w}^3  \wedge \operatorname{w}^3  \\
37
38
39
    w_prime_r_t_prime_bar = Symbol('\\overline{w\'r\'_t}')
40
```

```
w_prime_2_theta_prime_l_bar = Symbol('\\overline{w\'^2\\theta\'_1}')
    w_prime_theta_prime_1_2_bar = Symbol('\\overline{w\'\\theta\'^2_1}')
42
    w_prime_theta_l_prime_bar = Symbol('\\overline{w\'\\theta\'_l}')
43
44
    w_prime_r_t_prime_theta_l_prime_bar = Symbol('\\overline{w\'{r_t}\'{\\theta_l}\'}')
45
46
47
    r_t = Symbol('r_t')
48
49
    r_t_bar, r_t_prime_2_bar, r_t_prime_3_bar = symbols(
50
        '\overline{r_t} \overline{r_t'^2} \overline{r_t'^3}'
51
52
53
    r_t_i, r_t_1, r_t_2 = symbols('r_{ti} r_{t1} r_{t2}')
54
55
    r_t_tilde_prime, r_t_i_tilde, r_t_1_tilde, r_t_2_tilde = symbols(
56
        57
58
59
    r_t_prime_theta_l_prime_bar = Symbol('\\overline{r_t\'\\theta_1\'}')
60
61
    # theta
62
    theta_l = Symbol('\\theta_l')
63
64
    theta_l_bar, theta_l_prime_2_bar, theta_l_prime_3_bar = symbols(
65
        '\\overline{\\theta_1\'^2} \\overline{\\theta_1\'^3}'
66
67
68
    theta_l_i, theta_l_1, theta_l_2 = symbols(
69
        '\\theta_{li} \\theta_{l1} \\theta_{l2}'
70
    )
71
72
    theta_tilde_prime_l = Symbol('\\tilde{\\theta}_l\'')
73
74
    theta_tilde_l_i, theta_tilde_l_1, theta_tilde_l_2 = symbols(
75
        \label{li} $$  \(\theta)_{1i} \tilde{\theta}_{11} \tilde{\theta}_{12}' 
76
    )
77
78
    # lambda
79
    lambda_theta = Symbol('\\lambda_\\theta')
80
    lambda_theta_r = Symbol('\\lambda_\\theta_r')
81
    lambda_r = Symbol('\\lambda_r')
82
    lambda_w = Symbol('\\lambda_w')
83
    lambda_w_theta = Symbol('\\lambda_{w\\theta}')
84
    lambda_w_r = Symbol('\\lambda_{wr}')
85
86
    r_r_t_theta_l = Symbol('r_{r_t\\theta_l}')
87
    triple_gaussian = Symbol('P_{tmg}(\\hat{\w\'}, \\tilde{\\theta\'_1}, \\tilde{\r\'_t})')
88
    sk_w_hat = Symbol('\\widehat{Sk}_w')
89
    sk_theta_l_hat = Symbol('\\widehat{Sk}_{\\theta_l}')
90
    c_w_theta_l_hat = Symbol('\\widehat{c}_{w\\theta_l}')
91
    sk_r_t_hat = Symbol('\\widehat{Sk}_{r_t}')
92
    c_w_r_t_hat = Symbol('\\widehat{c}_{wr_t}')
93
94
```

```
beta_theta_l = Symbol('\\beta_{\\theta_l}')
     beta_r_t = Symbol('\\beta_{r_t}')
96
     G_3 = Symbol('G_3')
98
     G_3_hat = Symbol('\hat{G_3}')
99
100
101
     G_w, G_1_w, G_2_w, G_3_w = symbols(
          'G_{w}(w) G_{1w}(w) G_{2w}(w) G_{3w}(w)'
102
103
104
     G_w_1_2 = Symbol('G_{w_{12}}')
105
106
     G_w_theta = Symbol('G_{w\\theta}(w,\\theta)')
107
     G_1_w_theta = Symbol('G_{1w\\theta}(w,\\theta)')
108
     G_2_w_theta = Symbol('G_{2w\\theta}(w,\\theta)')
109
     G_3_w_theta = Symbol('G_{3w\\theta}(w,\\theta)')
110
111
     G_theta_r = Symbol('G_{\\theta r}(\\theta, r)')
112
     G_1_{theta_r} = Symbol('G_{1 \setminus theta_r}((theta, r)'))
113
     G_2_{theta_r} = Symbol('G_{2} + r)(\theta, r)')
114
     G_3_{theta_r} = Symbol('G_{3}\backslash r)(\theta, r)')
115
     G_{w_theta_l_r_t} = Symbol('G_{w_{theta_l}(r_t)}(w, {\theta_l}, {r_t})')
117
     G_1_w_{theta_1_r_t} = Symbol('G_{1w{\cdot theta_1}(x_t)(w,{\cdot theta_1}, \{r_t\})')}
118
     G_2_w_{theta_l_r_t} = Symbol('G_{2w}(\theta_1)_{r_t})(w, (\theta_1), r_t))')
119
     G_3_w_theta_l_r_t = Symbol('G_{3w}(\theta_l)'(w,{\theta_l},{r_t})')
120
121
     G_theta, G_1_theta, G_2_theta, G_3_theta = symbols(
122
          G_{\theta}(\theta) G_{1\wedge (\theta) G_{2\wedge (\theta)}
123
          \hookrightarrow G_{3\\theta}(\\theta)'
     )
124
125
     rho_w_theta_1 = Symbol('\\rho_{w\\theta_1}')
126
     rho_w_r_t = Symbol('\\rho_{wr_t}')
127
     rho_theta_l_r_t = Symbol('\\rho_{\\theta_lr_t}')
128
```

Listing A.1: symbols.py

A.3 checked_functions.py

```
10
    def w_bar(alpha=sp.abc.alpha, delta=sp.abc.delta, w_1=sym.w_1, w_2=sym.w_2):
11
        return ((1 - delta) * alpha * w_1
12
                 + (1 - delta) * (1 - alpha) * w_2
13
                 + delta * (alpha * w_1 + (1 - alpha) * w_2))
14
15
16
    def w_prime_2_bar(alpha=sp.abc.alpha, delta=sp.abc.delta, w_1=sym.w_1, w_2=sym.w_2,
^{17}
                       w_bar=sym.w_bar, sigma_w=sym.sigma_w, sigma_w_3=sym.sigma_w_3):
18
        return (((1 - delta) * alpha * ((w_1 - w_bar) ** 2 + sigma_w ** 2)) +
19
                 ((1 - delta) * (1 - alpha) * ((w_2 - w_bar) ** 2 + sigma_w ** 2)) +
20
                 (delta * sigma_w_3 ** 2))
21
22
23
    def w_prime_3_bar(alpha=sp.abc.alpha, delta=sp.abc.delta, w_1=sym.w_1, w_2=sym.w_2,
24
                       w_bar=sym.w_bar, sigma_w=sym.sigma_w):
25
        return (((1 - delta) * alpha * ((w_1 - w_bar) ** 3 +
26
                                          3 * sigma_w ** 2 * (w_1 - w_bar))) +
27
                 ((1 - delta) * (1 - alpha) * ((w_2 - w_bar) ** 3 +
28
                                                 3 * sigma_w ** 2 * (w_2 - w_bar))))
29
30
31
    def w_prime_4_bar(w_prime_2_bar=sym.w_prime_2_bar,
32
                       w_prime_3_bar=sym.w_prime_3_bar,
33
                       delta=sp.abc.delta,
34
                       sigma_tilde_w=sym.sigma_tilde_w,
35
                       sigma_w_3=sym.sigma_w_3):
36
        return (w_prime_2_bar ** 2 *
37
                 ((1 - delta * (sigma_w_3 ** 2 / w_prime_2_bar)) ** 2 / (1 - delta)) *
38
                 (3 * sigma_tilde_w ** 4 +
39
                  6 * (1 - sigma_tilde_w ** 2) *
40
                  sigma_tilde_w ** 2 +
41
                  (1 - sigma_tilde_w ** 2) ** 2) +
42
                 ((1 / (1 - sigma_tilde_w ** 2)) *
43
                  (1 / (1 - delta * (sigma_w_3 ** 2 / w_prime_2_bar))) *
                  (w_prime_3_bar ** 2 / w_prime_2_bar)) +
45
                 (delta * 3 * sigma_w_3 ** 4))
46
47
48
49
50
    # theta_l equations
51
52
53
    def theta_l_bar(alpha=sp.abc.alpha, delta=sp.abc.delta,
54
                     theta_l_1=sym.theta_l_1, theta_l_2=sym.theta_l_2):
55
        return ((1 - delta) * alpha * theta_l_1
56
                 + (1 - delta) * (1 - alpha) * theta_1_2
57
                 + delta * (alpha * theta_l_1 + (1 - alpha) * theta_l_2))
58
59
60
    def theta_l_prime_2_bar(alpha=sp.abc.alpha,
61
                             delta=sp.abc.delta,
62
63
                             theta_l_1=sym.theta_l_1,
```

```
64
                              theta_1_2=sym.theta_1_2,
                              theta_l_bar=sym.theta_l_bar,
65
                               sigma_theta_l_1=sym.sigma_theta_l_1,
66
                               sigma_theta_1_2=sym.sigma_theta_1_2,
67
                               sigma_theta_1_3_1=sym.sigma_theta_1_3):
68
         return (((1 - delta) * alpha * ((theta_l_1 - theta_l_bar) ** 2 + sigma_theta_l_1 **
69

→ 2)) +

                  ((1 - delta) * (1 - alpha) *
70
                   ((theta_1_2 - theta_1_bar) ** 2 + sigma_theta_1_2 ** 2)) +
71
                  (delta * sigma_theta_1_3_1 ** 2))
72
73
74
     def theta_l_prime_3_bar(delta=sp.abc.delta,
75
                              alpha=sp.abc.alpha,
76
                              theta_l_1=sym.theta_l_1,
77
                              theta_1_2=sym.theta_1_2,
78
                              theta_l_bar=sym.theta_l_bar,
79
                               sigma_theta_l_1=sym.sigma_theta_l_1,
80
                              sigma_theta_1_2=sym.sigma_theta_1_2):
81
         return (((1 - delta) * alpha *
82
                   ((theta_l_1 - theta_l_bar) ** 3 +
83
                    3 * sigma_theta_l_1 ** 2 * (theta_l_1 - theta_l_bar))) +
84
                  ((1 - delta) * (1 - alpha) *
85
                   ((theta_l_2 - theta_l_bar) ** 3 +
86
                    3 * sigma_theta_l_2 ** 2 * (theta_l_2 - theta_l_bar))))
87
88
89
90
91
     \# r_t = equations
92
93
94
     def r_t_bar(alpha=sp.abc.alpha, delta=sp.abc.delta, r_t_1=sym.r_t_1, r_t_2=sym.r_t_2):
95
         return ((1 - delta) * alpha * r_t_1
96
                  + (1 - delta) * (1 - alpha) * r_t_2
97
                  + delta * (alpha * r_t_1 + (1 - alpha) * r_t_2))
98
99
100
     def r_t_prime_2_bar(delta=sp.abc.delta,
101
                          alpha=sp.abc.alpha,
102
                          r_t_1=sym.r_t_1,
103
                          r_t_2=sym.r_t_2,
104
                          r_t_bar=sym.r_t_bar,
105
                          sigma_r_t_1=sym.sigma_r_t_1,
106
                          sigma_r_t_2=sym.sigma_r_t_2,
107
                          sigma_r_t_3_t=sym.sigma_r_t_3):
108
         return (((1 - delta) * alpha * ((r_t_1 - r_t_bar) ** 2 + sigma_r_t_1 ** 2)) +
109
                  ((1 - delta) * (1 - alpha) * ((r_t_2 - r_t_bar) ** 2 + sigma_r_t_2 ** 2)) +
110
                  (delta * sigma_r_t_3_t ** 2))
111
112
113
     def r_t_prime_3_bar(alpha=sp.abc.alpha,
114
                          delta=sp.abc.delta,
115
116
                          r_t_1=sym.r_t_1,
```

```
117
                           r_t_2=sym.r_t_2,
                           r_t_{bar} = sym.r_t_{bar},
118
                           sigma_r_t_1=sym.sigma_r_t_1,
119
                           sigma_r_t_2=sym.sigma_r_t_2):
120
         return (((1 - delta) * alpha *
121
                   ((r_t_1 - r_t_bar) ** 3 +
122
                    3 * sigma_r_t_1 ** 2 * (r_t_1 - r_t_bar))) +
123
                  ((1 - delta) * (1 - alpha) *
124
                   ((r_t_2 - r_t_bar) ** 3 +
125
                    3 * sigma_r_t_2 ** 2 * (r_t_2 - r_t_bar))))
126
127
128
129
130
     # Mixed equations
131
132
133
     def w_prime_theta_l_prime_bar(delta=sp.abc.delta,
134
                                      alpha=sp.abc.alpha,
135
                                      w_1=sym.w_1,
136
                                      w_2=sym.w_2,
137
                                      w_bar=sym.w_bar,
138
                                      theta_l_1=sym.theta_l_1,
139
                                      theta_1_2=sym.theta_1_2,
140
                                      theta_l_bar=sym.theta_l_bar,
141
                                      cov_lambda_w_theta=sym.rho_w_theta_l * sym.sigma_w_3 *
142

    sym.sigma_theta_1_3):

         return (((1 - delta) * alpha * ((w_1 - w_bar) * (theta_l_1 - theta_l_bar))) +
143
                  ((1 - delta) * (1 - alpha) * ((w_2 - w_bar) * (theta_1_2 - theta_1_bar)))
                  + delta * cov_lambda_w_theta)
145
146
147
     def w_prime_r_t_prime_bar(alpha=sp.abc.alpha,
                                 delta=sp.abc.delta,
149
                                 w_1=sym.w_1,
150
                                 w_2=sym.w_2,
151
                                 w_bar=sym.w_bar,
152
                                 r_t_1=sym.r_t_1,
153
                                 r_t_2=sym.r_t_2,
154
                                 r_t_bar=sym.r_t_bar,
155
                                 cov_lambda_w_r=sym.rho_w_r_t * sym.sigma_w_3 *
156
                                  \rightarrow sym.sigma_r_t_3):
         return (((1 - delta) * alpha * ((w_1 - w_bar) * (r_t_1 - r_t_bar))) +
157
                  ((1 - delta) * (1 - alpha) * ((w_2 - w_bar) * (r_t_2 - r_t_bar)))
158
                  + delta * cov_lambda_w_r)
159
160
161
     def w_prime_2_theta_l_prime_bar(sigma_tilde_w=sym.sigma_tilde_w,
162
                                        delta=sp.abc.delta,
163
                                        lambda_w_theta=sym.lambda_w_theta,
164
                                        lambda_w=sym.lambda_w,
165
                                        w_prime_3_bar=sym.w_prime_3_bar,
166
                                        w_prime_2_bar=sym.w_prime_2_bar,
167
168
                                        w_prime_theta_l_prime=sym.w_prime_theta_l_prime_bar):
```

```
return ((1 / (1 - sigma_tilde_w ** 2)) *
169
                  ((1 - delta * lambda_w_theta) / (1 - delta * lambda_w)) *
170
                  (w_prime_3_bar / w_prime_2_bar) *
171
                  w_prime_theta_l_prime)
172
173
174
     def w_prime_theta_l_prime_2_bar(delta=sp.abc.delta,
175
                                       lambda_w_theta=sym.lambda_w_theta,
176
                                       lambda_w=sym.lambda_w,
177
                                       sigma_tilde_w=sym.sigma_tilde_w,
178
                                       w_prime_3_bar=sym.w_prime_3_bar,
179
                                       w_prime_2_bar=sym.w_prime_2_bar,
180
                                       w_prime_theta_l_prime_bar=sym.w_prime_theta_l_prime_bar,
181
                                       theta_l_prime_3_bar=sym.theta_l_prime_3_bar):
         return (Rational(2, 3) *
183
                  ((1 - delta * lambda_w_theta) ** 2 / (1 - delta * lambda_w) ** 2) *
                  (1 / (1 - sigma_tilde_w ** 2) ** 2) *
185
                  (w_prime_3_bar / w_prime_2_bar ** 2) *
                  w_prime_theta_l_prime_bar ** 2 +
187
                  Rational(1, 3) *
188
                  ((1 - delta * lambda_w) / (1 - delta * lambda_w_theta)) *
189
                  (1 - sigma_tilde_w ** 2) *
190
                  ((w_prime_2_bar * theta_1_prime_3_bar) / w_prime_theta_1_prime_bar))
191
192
193
     def w_prime_theta_l_prime_2_bar_beta(
194
             sigma_tilde_w=sym.sigma_tilde_w,
195
             delta=sp.abc.delta,
196
             lambda_theta=sym.lambda_theta,
197
             lambda_w=sym.lambda_w,
198
             w_prime_3_bar=sym.w_prime_3_bar,
199
             w_prime_2_bar=sym.w_prime_2_bar,
200
             beta=sp.abc.beta,
             theta_l_prime_2_bar=sym.theta_l_prime_2_bar,
202
             lambda_w_theta=sym.lambda_w_theta,
203
             w_prime_theta_l_prime_bar=sym.w_prime_theta_l_prime_bar):
204
         from sympy import Rational
205
         return (
206
                  (1 / (1 - sigma_tilde_w ** 2)) *
207
                  ((1 - delta * lambda_theta) / (1 - delta * lambda_w)) *
208
                  (w_prime_3_bar / w_prime_2_bar) *
209
                  (
210
                          Rational(1, 3) * beta * theta_l_prime_2_bar +
211
                          (
^{212}
                                   ((1 - Rational(1, 3) * beta) / (1 - sigma_tilde_w ** 2)) *
213
                                   ((1 - delta * lambda_w_theta) ** 2 /
214
                                    ((1 - delta * lambda_w) * (1 - delta * lambda_theta))) *
215
                                   (w_prime_theta_l_prime_bar ** 2 / w_prime_2_bar)
216
                          )
217
                  )
218
         )
219
220
221
     def w_prime_r_t_prime_theta_l_prime_bar(delta=sp.abc.delta,
```

```
223
                                                alpha=sp.abc.alpha,
                                                w_1=sym.w_1,
224
                                                w_2=sym.w_2,
225
                                                w_bar=sym.w_bar,
226
                                                r_t_1=sym.r_t_1,
227
228
                                                r_t_2=sym.r_t_2,
                                                r_t_bar=sym.r_t_bar,
229
                                                theta_l_1=sym.theta_l_1,
230
                                                theta_1_2=sym.theta_1_2,
231
                                                theta_l_bar=sym.theta_l_bar,
232
                                                r_r_t_theta_l=sym.r_r_t_theta_l,
233
                                                sigma_r_t_1=sym.sigma_r_t_1,
234
                                                sigma_r_t_2=sym.sigma_r_t_2,
235
                                                sigma_theta_l_1=sym.sigma_theta_l_1,
236
                                                sigma_theta_l_2=sym.sigma_theta_l_2):
237
         return (((1 - delta) * alpha * (w_1 - w_bar) *
238
                   (
239
                            (r_t_1 - r_t_bar) * (theta_l_1 - theta_l_bar) +
                           r_r_t_theta_l * sigma_r_t_1 * sigma_theta_l_1
241
                   )) +
242
                  ((1 - delta) * (1 - alpha) * (w_2 - w_bar) *
243
                            (r_t_2 - r_t_bar) * (theta_l_2 - theta_l_bar) +
245
                           r_r_t_theta_l * sigma_r_t_2 * sigma_theta_l_2
246
                   )))
247
248
249
     def w_prime_r_t_prime_theta_l_prime_bar_beta(
250
             beta=sp.abc.beta,
251
             sigma_tilde_w=sym.sigma_tilde_w,
252
             delta=sp.abc.delta,
253
             lambda_theta_r=sym.lambda_theta_r,
254
             lambda_w=sym.lambda_w,
             r_t_prime_theta_l_prime_bar=sym.r_t_prime_theta_l_prime_bar,
256
             w_prime_3_bar=sym.w_prime_3_bar,
257
             w_prime_2_bar=sym.w_prime_2_bar,
258
             lambda_w_r=sym.lambda_w_r,
259
             lambda_w_theta=sym.lambda_w_theta,
260
             w_prime_r_t_prime_bar=sym.w_prime_r_t_prime_bar,
261
             w_prime_theta_l_prime_bar=sym.w_prime_theta_l_prime_bar):
262
         from sympy import Rational
263
         return (
264
                  (
265
                           ((Rational(1, 3) * beta) / (1 - sigma_tilde_w ** 2)) *
266
                           ((1 - delta * lambda_theta_r) / (1 - delta * lambda_w)) *
267
                          r_t_prime_theta_l_prime_bar *
268
                           (w_prime_3_bar / w_prime_2_bar)
269
                  ) +
270
                  (
271
                           ((1 - Rational(1, 3) * beta) / (1 - sigma_tilde_w ** 2) ** 2) *
272
                           (((1 - delta * lambda_w_r) * (1 - delta * lambda_w_theta)) /
273
                            ((1 - delta * lambda_w) ** 2)) *
                          w_prime_r_t_prime_bar *
275
276
                          w_prime_theta_l_prime_bar *
```

```
277
                           (w_prime_3_bar / w_prime_2_bar ** 2)
                  )
278
         )
279
280
281
282
     def w_prime_r_t_prime_theta_l_prime_bar_E(
              E=sp.abc.E,
283
              sigma_tilde_w=sym.sigma_tilde_w,
284
              delta=sp.abc.delta,
285
              lambda_theta_r=sym.lambda_theta_r,
              lambda_w=sym.lambda_w,
287
              r_t_prime_theta_l_prime_bar=sym.r_t_prime_theta_l_prime_bar,
288
              w_prime_3_bar=sym.w_prime_3_bar,
289
              w_prime_2_bar=sym.w_prime_2_bar,
              lambda_w_r=sym.lambda_w_r,
291
              lambda_w_theta=sym.lambda_w_theta,
292
              w_prime_r_t_prime_bar=sym.w_prime_r_t_prime_bar,
293
              w_prime_theta_l_prime_bar=sym.w_prime_theta_l_prime_bar):
         from sympy import Rational
295
         return (
296
                  (
297
                           ((Rational(1, 2) * E) / (1 - sigma_tilde_w ** 2)) *
298
                           ((1 - delta * lambda_theta_r) / (1 - delta * lambda_w)) *
299
                          r_t_prime_theta_l_prime_bar *
300
                           (w_prime_3_bar / w_prime_2_bar)
301
                  ) +
302
                  (
303
                           ((1 - Rational(1, 2) * E) / (1 - sigma_tilde_w ** 2) ** 2) *
304
                           (((1 - delta * lambda_w_r) * (1 - delta * lambda_w_theta)) /
                            ((1 - delta * lambda_w) ** 2)) *
306
                          w_prime_r_t_prime_bar *
307
                          w_prime_theta_l_prime_bar *
308
                           (w_prime_3_bar / w_prime_2_bar ** 2)
                  )
310
         )
311
312
313
     def r_t_prime_theta_l_prime_bar(
314
              alpha=sp.abc.alpha, delta=sp.abc.delta,
315
              r_t_1=sym.r_t_1, r_t_2=sym.r_t_2, r_t_prime_bar=sym.r_t_bar,
316
              theta_l_1=sym.theta_l_1, theta_l_2=sym.theta_l_2,
317
              theta_l_bar=sym.theta_l_bar,
318
              r_r_t_theta_l=sym.r_r_t_theta_l,
319
              sigma\_r\_t\_1 = sym.sigma\_r\_t\_1, sigma\_r\_t\_2 = sym.sigma\_r\_t\_2,
320
              sigma_theta_l_1=sym.sigma_theta_l_1,
321
              sigma_theta_1_2=sym.sigma_theta_1_2,
322
              cov_lambda_r_theta=sym.rho_theta_l_r_t * sym.sigma_theta_l_3 * sym.sigma_r_t_3):
323
         return ((1 - delta) * alpha * (
324
                  (r_t_1 - r_t_prime_bar) * (theta_l_1 - theta_l_bar) +
325
                  r_r_t_theta_l * sigma_r_t_1 * sigma_theta_l_1) +
326
                  ((1 - delta) * (1 - alpha) * (
327
                           (r_t_2 - r_t_prime_bar) * (theta_l_2 - theta_l_bar) +
                          r_r_t_theta_1 * sigma_r_t_2 * sigma_theta_1_2)) +
329
330
                  delta * cov_lambda_r_theta)
```

```
331
332
333
334
     # Distributions
335
336
337
     G_1_theta_1 = Normal(name='G_1_theta_1', mean=sym.theta_1_1, std=sym.sigma_theta_1_1)
338
     G_1_theta_l_density = density(G_1_theta_l)(sym.theta_l)
339
340
     G_2_theta_1 = Normal(name='G_2_theta_1', mean=sym.theta_1_2, std=sym.sigma_theta_1_2)
341
     G_2_theta_1_density = density(G_2_theta_1)(sym.theta_1)
342
343
     G_3_theta_1 = Normal(name='G_3_theta_1', mean=sym.theta_1_bar, std=sym.sigma_theta_1_3)
344
     G_3_theta_l_density = density(G_3_theta_l)(sym.theta_l)
345
346
     G_theta = ((1 - sp.abc.delta) * sp.abc.alpha * G_1_theta_l_density +
347
                 (1 - sp.abc.delta) * (1 - sp.abc.alpha) * G_2_theta_l_density +
                 sp.abc.delta * G_3_theta_l_density)
349
350
351
352
     G_1_w = Normal(name='G_1_w', mean=sym.w_1, std=sym.sigma_w)
353
     G_1_w_{density} = density(G_1_w)(sp.abc.w)
354
355
     G_2_w = Normal(name='G_2_w', mean=sym.w_2, std=sym.sigma_w)
356
     G_2_w_density = density(G_2_w)(sp.abc.w)
357
358
     G_3_w = Normal(name='G_3_w', mean=sym.w_bar, std=sym.sigma_w_3)
359
     G_3_w_density = density(G_3_w)(sp.abc.w)
360
361
     G_w = ((1 - sp.abc.delta) * sp.abc.alpha * G_1_w_density +
362
            (1 - sp.abc.delta) * (1 - sp.abc.alpha) * G_2_w_density +
363
            sp.abc.delta * G_3_w_density)
364
365
366
367
     G_1_w_theta = Normal(name='G_1_w_theta', mean=sp.Matrix([sym.w_1, sym.theta_l_1]),
368
                           std=sp.Matrix([[sym.sigma_w ** 2, 0], [0, sym.sigma_theta_l_1 **
369

→ 211))

     G_1_w_theta_density = density(G_1_w_theta)(sp.abc.w, sp.abc.theta)
370
371
     G_2_w_theta = Normal(name='G_2_w_theta', mean=sp.Matrix([sym.w_2, sym.theta_1_2]),
372
                           std=sp.Matrix([[sym.sigma_w ** 2, 0], [0, sym.sigma_theta_1_2 **
373
                            \rightarrow 2]]))
     G_2_w_theta_density = density(G_2_w_theta)(sp.abc.w, sp.abc.theta)
374
375
     G_3_w_theta = Normal(name='G_3_w_theta', mean=sp.Matrix([sym.w_bar, sym.theta_l_bar]),
376
                           std=sp.Matrix([
377
                                [sym.sigma_w_3 ** 2,
378
                                sym.rho_w_theta_1 * sym.sigma_w_3 * sym.sigma_theta_1_3],
379
                                [sym.rho_w_theta_1 * sym.sigma_w_3 * sym.sigma_theta_1_3,
                                sym.sigma_theta_1_3 ** 2]
381
                           ]))
382
```

```
G_3_w_theta_density = sp.simplify(density(G_3_w_theta)(sp.abc.w, sp.abc.theta))
383
384
     G_w_theta = ((1 - sp.abc.delta) * sp.abc.alpha * G_1_w_theta_density +
385
                   (1 - sp.abc.delta) * (1 - sp.abc.alpha) * G_2_w_theta_density +
386
                   sp.abc.delta * G_3_w_theta_density)
387
388
389
390
     mu_1_theta_l_r_t = sp.Matrix([sym.theta_l_1, sym.r_t_1])
391
     Sigma_1_theta_l_r_t = sp.Matrix([[sym.sigma_theta_l_1 ** 2,
392
                                         sym.r_r_t_theta_l * sym.sigma_theta_l_1 *
393
                                          \rightarrow sym.sigma_r_t_1],
                                         [sym.r_r_t_theta_l * sym.sigma_theta_l_1 *
394
                                         \rightarrow sym.sigma_r_t_1,
                                         sym.sigma_r_t_1 ** 2]])
395
396
     G_1_theta_l_r_t = Normal(name='G_1_theta_l_r_t',
397
                                mean=mu_1_theta_l_r_t,
398
                                std=Sigma_1_theta_l_r_t)
399
400
     G_1_theta_l_r_t_density = density(G_1_theta_l_r_t)(sym.theta_l, sym.r_t)
401
402
     mu_2_theta_l_r_t = sp.Matrix([sym.theta_l_2, sym.r_t_2])
403
     Sigma_2_theta_l_r_t = sp.Matrix(
404
         [[sym.sigma_theta_1_2 ** 2,
405
           sym.r_r_t_theta_1 * sym.sigma_theta_1_2 * sym.sigma_r_t_2],
406
           [sym.r_r_t_theta_1 * sym.sigma_theta_1_2 * sym.sigma_r_t_2,
407
           sym.sigma_r_t_2 ** 2]])
408
409
     G_2_theta_l_r_t = Normal(name='G_2_theta_l_r_t',
410
                                mean=mu_2_theta_l_r_t,
411
                                std=Sigma_2_theta_l_r_t)
412
413
     G_2_theta_l_r_t_density = density(G_2_theta_l_r_t)(sym.theta_l, sym.r_t)
414
415
     mu_3_theta_l_r_t = sp.Matrix([sym.theta_l_bar, sym.r_t_bar])
416
     Sigma_3_theta_l_r_t = sp.Matrix(
417
         [[sym.sigma_theta_1_3 ** 2,
418
           sym.rho_theta_l_r_t * sym.sigma_theta_1_3 * sym.sigma_r_t_3],
419
           Γ
420
               sym.rho_theta_l_r_t * sym.sigma_theta_l_3 * sym.sigma_r_t_3,
421
               sym.sigma_r_t_3 ** 2]])
422
423
424
     G_3_theta_l_r_t = Normal(name='G_3_theta_l_r_t',
                                mean=mu_3_theta_1_r_t,
425
426
                                std=Sigma_3_theta_l_r_t)
427
     G_3_theta_l_r_t_density = density(G_3_theta_l_r_t)(sym.theta_l, sym.r_t)
428
429
     G_{theta_l_r_t} = ((1 - sp.abc.delta) * sp.abc.alpha * G_1_theta_l_r_t_density +
430
                       (1 - sp.abc.delta) * (1 - sp.abc.alpha) * G_2_theta_l_r_t_density +
431
                       sp.abc.delta * G_3_theta_l_r_t_density)
432
433
434
```

```
435
     mu_1_w_theta_l_r_t = sp.Matrix([sym.w_1, sym.theta_l_1, sym.r_t_1])
436
     Sigma_1_w_theta_l_r_t = sp.Matrix(
437
         [[sym.sigma_w ** 2,
438
            0.
439
            0],
440
           [0,
441
            sym.sigma_theta_l_1 ** 2,
442
            sym.r_r_t_theta_l * sym.sigma_theta_l_1 * sym.sigma_r_t_1],
443
444
            {\tt sym.r\_r\_t\_theta\_l~*~sym.sigma\_theta\_l\_1~*~sym.sigma\_r\_t\_1,}
445
            sym.sigma_r_t_1 ** 2]])
446
447
     G_1_w_theta_l_r_t = Normal(name='G_1_w_theta_l_r_t',
448
                                  mean=mu_1_w_theta_l_r_t,
449
                                  std=Sigma_1_w_theta_l_r_t)
450
451
     G_1_w_theta_l_r_t_density = density(G_1_w_theta_l_r_t)(sp.abc.w, sym.theta_l, sym.r_t)
452
453
     mu_2_w_theta_l_r_t = sp.Matrix([sym.w_2, sym.theta_l_2, sym.r_t_2])
454
     Sigma_2_w_theta_l_r_t = sp.Matrix([[sym.sigma_w ** 2,
455
456
                                            0,
                                            0],
457
                                           [0,
458
                                            sym.sigma_theta_1_2 ** 2,
459
                                            sym.r_r_t_theta_l * sym.sigma_theta_l_2 *
460
                                             \rightarrow sym.sigma_r_t_2],
                                           [0,
461
                                            sym.r_r_t_theta_l * sym.sigma_theta_l_2 *
462
                                             \rightarrow sym.sigma_r_t_2,
                                            sym.sigma_r_t_2 ** 2]])
463
464
     G_2_w_theta_l_r_t = Normal(name='G_2_w_theta_l_r_t',
465
                                  mean=mu_2_w_theta_l_r_t,
466
                                  std=Sigma_2_w_theta_l_r_t)
467
468
     G_2_w_theta_l_r_t_density = density(G_2_w_theta_l_r_t)(sp.abc.w, sym.theta_l, sym.r_t)
469
470
     mu_3_w_theta_l_r_t = sp.Matrix([sym.w_bar, sym.theta_l_bar, sym.r_t_bar])
471
     Sigma_3_w_theta_l_r_t = sp.Matrix(
472
         [[sym.sigma_w_3 ** 2,
473
            sym.rho_w_theta_1 * sym.sigma_w_3 * sym.sigma_theta_1_3,
474
            sym.rho_w_r_t * sym.sigma_theta_1_3 * sym.sigma_r_t_3],
475
           Γ
476
               sym.rho_w_theta_1 * sym.sigma_w_3 * sym.sigma_theta_1_3,
477
               sym.sigma_theta_1_3 ** 2,
478
               sym.rho_theta_l_r_t * sym.sigma_w_3 * sym.sigma_r_t_3],
479
           [sym.rho_w_r_t * sym.sigma_theta_1_3 * sym.sigma_r_t_3,
480
            sym.rho_theta_l_r_t * sym.sigma_w_3 * sym.sigma_r_t_3,
481
            sym.sigma_r_t_3 ** 2]])
482
483
     G_3_w_theta_l_r_t = Normal(name='G_3_w_theta_l_r_t',
484
                                  mean=mu_3_w_theta_l_r_t,
485
                                  std=Sigma_2_w_theta_l_r_t)
486
```

```
G_3_w_theta_l_r_t_density = density(G_3_w_theta_l_r_t)(sp.abc.w, sym.theta_l, sym.r_t)
487
488
     G_w_theta_l_r_t = ((1 - sp.abc.delta) * sp.abc.alpha * G_1_w_theta_l_r_t_density +
489
                         (1 - sp.abc.delta) * (1 - sp.abc.alpha) * G_2_w_theta_l_r_t_density +
490
                         sp.abc.delta * G_3_w_theta_l_r_t_density)
491
492
493
494
495
496
     # sigma equations
497
498
     def sigma_tilde_w(sigma_w=sym.sigma_w, w_prime_2_bar=sym.w_prime_2_bar,
499
                        delta=sp.abc.delta, lambda_w=sym.lambda_w):
500
         from sympy import sqrt
501
         return ((sigma_w / sqrt(w_prime_2_bar)) *
502
                  (1 / sqrt((1 - delta * lambda_w) / (1 - delta))))
503
504
505
     def sigma_tilde_r_t_1(sigma_r_t_1=sym.sigma_r_t_1, r_t_prime_2_bar=sym.r_t_prime_2_bar,
506
                            delta=sp.abc.delta, lambda_r=sym.lambda_r):
507
508
         from sympy import sqrt
         return ((sigma_r_t_1 / sqrt(r_t_prime_2_bar)) *
509
                  (1 / sqrt((1 - delta * lambda_r) / (1 - delta))))
510
511
512
     def sigma_tilde_r_t_2(sigma_r_t_2=sym.sigma_r_t_2, r_t_prime_2_bar=sym.r_t_prime_2_bar,
513
                            delta=sp.abc.delta, lambda_r=sym.lambda_r):
514
         from sympy import sqrt
515
         return ((sigma_r_t_2 / sqrt(r_t_prime_2_bar)) *
516
                  (1 / sqrt((1 - delta * lambda_r) / (1 - delta))))
517
518
     def sigma_tilde_theta_l_1(sigma_theta_l_1=sym.sigma_theta_l_1,
520
                                theta_l_prime_2_bar=sym.theta_l_prime_2_bar,
521
                                delta=sp.abc.delta, lambda_theta=sym.lambda_theta):
522
         from sympy import sqrt
523
         return ((sigma_theta_l_1 / sqrt(theta_l_prime_2_bar)) *
524
                  (1 / sqrt((1 - delta * lambda_theta) / (1 - delta))))
525
526
527
     def sigma_tilde_theta_1_2(sigma_theta_1_2=sym.sigma_theta_1_2,
528
                                theta_l_prime_2_bar=sym.theta_l_prime_2_bar,
529
                                 delta=sp.abc.delta, lambda_theta=sym.lambda_theta):
530
         from sympy import sqrt
531
         return ((sigma_theta_l_2 / sqrt(theta_l_prime_2_bar)) *
532
                  (1 / sqrt((1 - delta * lambda_theta) / (1 - delta))))
533
534
535
536
537
     # lambda equations
538
539
540
```

```
def lambda_w(sigma_w_3=sym.sigma_w_3, w_prime_2_bar=sym.w_prime_2_bar):
541
         return sigma_w_3 ** 2 / w_prime_2_bar
542
543
544
     def lambda_theta(sigma_theta_1_3=sym.sigma_theta_1_3,
545
                       theta_l_prime_2_bar=sym.theta_l_prime_2_bar):
546
         return sigma_theta_1_3 ** 2 / theta_1_prime_2_bar
547
548
549
     def lambda_r(sigma_r_t_3=sym.sigma_r_t_3,
550
                   r_t_prime_2_bar=sym.r_t_prime_2_bar):
551
         return sigma_r_t_3 ** 2 / r_t_prime_2_bar
552
553
554
     def lambda_w_theta(cov_lambda_w_theta=sym.rho_w_theta_1 * sym.sigma_w_3 *
555

    sym.sigma_theta_1_3,

                         w_prime_theta_l_prime_bar=sym.w_prime_theta_l_prime_bar):
556
         return cov_lambda_w_theta / w_prime_theta_l_prime_bar
558
559
     def lambda_w_r(cov_lambda_w_r=sym.rho_w_r_t * sym.sigma_w_3 * sym.sigma_r_t_3,
560
                     w_prime_r_t_prime_bar=sym.w_prime_r_t_prime_bar):
561
         return cov_lambda_w_r / w_prime_r_t_prime_bar
562
563
564
     def lambda_r_theta(cov_lambda_r_theta=sym.rho_theta_l_r_t * sym.sigma_r_t_3 *
565

→ sym.sigma_theta_1_3,

                         r_t_prime_theta_l_prime_bar=sym.r_t_prime_theta_l_prime_bar):
566
         return cov_lambda_r_theta / r_t_prime_theta_l_prime_bar
567
568
569
570
571
     # sk
572
573
574
     def sk_theta_l_hat_beta(sk_w_hat=sym.sk_w_hat, c_hat_w_theta_l=sym.c_w_theta_l_hat,
575
                              beta=sp.abc.beta):
576
         return sk_w_hat * c_hat_w_theta_1 * (beta + (1 - beta) * c_hat_w_theta_1 ** 2)
577
578
579
     def sk_theta_l_hat(theta_l_prime_3_bar=sym.theta_l_prime_3_bar,
580
                         theta_l_prime_2_bar=sym.theta_l_prime_2_bar,
581
                         delta=sp.abc.delta,
582
                         lambda_theta=sym.lambda_theta):
583
         from sympy import Rational
584
         return ((theta_1_prime_3_bar / theta_1_prime_2_bar ** Rational(3, 2)) *
585
                  (1 / ((1 - delta * lambda_theta) / (1 - delta)) ** Rational(3, 2)) *
586
                  (1 / (1 - delta)))
587
588
589
     def sk_r_t_hat(r_t_prime_3_bar=sym.r_t_prime_3_bar,
590
                     r_t_prime_2_bar=sym.r_t_prime_2_bar,
591
592
                     delta=sp.abc.delta,
```

```
593
                     lambda_r=sym.lambda_r):
         from sympy import Rational
594
         return ((r_t_prime_3_bar / r_t_prime_2_bar ** Rational(3, 2)) *
595
                  (1 / ((1 - delta * lambda_r) / (1 - delta)) ** Rational(3, 2)) *
596
                  (1 / (1 - delta)))
597
598
599
     def sk_w_hat(sigma_tilde_w=sym.sigma_tilde_w,
600
                   w_prime_3_bar=sym.w_prime_3_bar,
601
                   w_prime_2_bar=sym.w_prime_2_bar,
602
                   delta=sp.abc.delta,
603
                   lambda_w=sym.lambda_w):
604
         from sympy import Rational
605
         return ((1 / (1 - sigma_tilde_w ** 2) ** Rational(3, 2)) *
                  (w_prime_3_bar / (w_prime_2_bar ** Rational(3, 2))) *
607
                  (1 / ((1 - delta * lambda_w) / (1 - delta)) ** Rational(3, 2)) *
608
                  (1 / (1 - delta)))
609
610
611
612
613
     # c
614
615
     def c_w_theta_l_hat(sigma_w_tilde=sym.sigma_tilde_w,
616
                          w_prime_theta_l_prime_bar=sym.w_prime_theta_l_prime_bar,
617
                          w_prime_2_bar=sym.w_prime_2_bar,
618
                          theta_l_prime_2_bar=sym.theta_l_prime_2_bar,
619
                          delta=sp.abc.delta,
620
                          lambda_w=sym.lambda_w,
                          lambda_theta=sym.lambda_theta,
622
                          lambda_w_theta=sym.lambda_w_theta):
623
         from sympy import sqrt
624
         return ((1 / sqrt(1 - sigma_w_tilde ** 2)) *
625
                  (w_prime_theta_l_prime_bar / ((sqrt(w_prime_2_bar)) *
626

    sqrt(theta_l_prime_2_bar))) *
                  (1 / sqrt((1 - delta * lambda_w) / (1 - delta))) *
627
                  (1 / sqrt((1 - delta * lambda_theta) / (1 - delta))) *
628
                  ((1 - delta * lambda_w_theta) / (1 - delta)))
629
630
631
     def c_w_r_t_hat(sigma_w_tilde=sym.sigma_tilde_w,
632
                      w_prime_r_t_prime_bar=sym.w_prime_r_t_prime_bar,
633
                      w_prime_2_bar=sym.w_prime_2_bar,
634
                      r_t_prime_2_bar=sym.r_t_prime_2_bar,
635
                      delta=sp.abc.delta,
636
                      lambda_w=sym.lambda_w,
637
                      lambda_r=sym.lambda_r,
638
                      lambda_w_r=sym.lambda_w_r):
639
         from sympy import sqrt
640
         return ((1 / sqrt(1 - sigma_w_tilde ** 2)) *
641
                  (w_prime_r_t_prime_bar / ((sqrt(w_prime_2_bar)) * sqrt(r_t_prime_2_bar))) *
642
                  (1 / sqrt((1 - delta * lambda_w) / (1 - delta))) *
643
                  (1 / sqrt((1 - delta * lambda_r) / (1 - delta))) *
644
                  ((1 - delta * lambda_w_r) / (1 - delta)))
645
```

```
646
647
648
649
     # beta
650
651
652
     def beta_w_theta_l(c_w_theta_l_hat=sym.c_w_theta_l_hat,
653
                          sk_w_hat=sym.sk_w_hat,
654
                          sk_theta_l_hat=sym.sk_theta_l_hat):
655
         return (((c_w_theta_l_hat ** 3 * sk_w_hat) - sk_theta_l_hat) /
656
657
                  (c_w_{theta_l_hat * sk_w_hat * (c_w_{theta_l_hat ** 2 - 1))}
658
659
     def beta_w_r_t(c_w_r_t_hat=sym.c_w_r_t_hat,
660
                     sk_w_hat=sym.sk_w_hat,
661
                     sk_r_t_hat=sym.sk_r_t_hat):
662
         return (((c_w_r_t_hat ** 3 * sk_w_hat) - sk_r_t_hat) /
663
                  (c_w_r_t_hat * sk_w_hat * (c_w_r_t_hat ** 2 - 1)))
664
665
666
667
668
669
670
671
     def E(alpha=sp.abc.alpha, xi=sp.abc.xi):
672
         from sympy import Rational
673
         return ((1 - Rational(1, 2) * ((2 * alpha) / (1 - 2 * alpha)) * xi) /
674
                  (1 + Rational(1, 2) * xi))
675
676
677
678
679
680
     \# xi
681
682
683
     def xi(alpha=sp.abc.alpha, sigma_tilde_r_t_1=sym.sigma_tilde_r_t_1,
684
             sigma_tilde_r_t_2=sym.sigma_tilde_r_t_2,
685

    sigma_tilde_theta_l_1=sym.sigma_tilde_theta_l_1,
             sigma_tilde_theta_l_2=sym.sigma_tilde_theta_l_2):
686
         return (((1 - alpha) / alpha) *
687
                  (sigma_tilde_r_t_1 / sigma_tilde_r_t_2) *
688
                  (sigma_tilde_theta_l_1 / sigma_tilde_theta_l_2) - 1)
689
690
691
```

Listing A.2: checked_functions.py

A.4 w_prime_4_bar.py

```
#!/usr/bin/env python
2
    # coding: utf-8
3
    # In[1]:
4
5
6
    import sympy as sp
    from IPython.display import display
8
    from sympy import abc, oo, init_printing
9
10
    import checked_functions as c_f
11
    import symbols as sym
12
    init_printing()
13
14
15
    # # This document aims to analytically check f\overline{w'^4}f
16
17
    # ## Define the marginal distributions with those parameters.
18
19
    # In[2]:
20
21
22
    display(sp.Eq(sym.G_1_w, c_f.G_1_theta_l_density))
23
^{24}
25
    # In[3]:
26
27
28
    display(sp.Eq(sym.G_2_w, c_f.G_2_theta_l_density))
29
30
31
    # In[4]:
32
33
34
    display(sp.Eq(sym.G_3_w, c_f.G_3_theta_l_density))
35
36
37
    # In[5]:
38
39
40
    display(sp.Eq(sym.G_w, c_f.G_w))
41
42
43
44
    # Calculate the moment analytically:
45
    # In[6]:
46
47
48
    w_prime_4_bar_int = sp.Integral((sp.abc.w - sym.w_bar) ** 4 * c_f.G_w, [sp.abc.w, -oo,
49
    → oo])
```

```
display(sp.Eq(sym.w_prime_4_bar, w_prime_4_bar_int))
50
51
52
     # In[7]:
53
54
55
     w_prime_4_bar_int_val = w_prime_4_bar_int.doit(conds='none').simplify()
56
     display(sp.Eq(sym.w_prime_4_bar, w_prime_4_bar_int_val))
57
58
59
     # The equation in the document is:
60
61
62
     # In[8]:
63
64
     display(sp.Eq(sym.w_prime_4_bar, c_f.w_prime_4_bar()))
65
66
67
     # where
68
69
     # In[9]:
70
71
72
73
     display(sp.Eq(sym.sigma_tilde_w, c_f.sigma_tilde_w()))
74
75
     # and
76
77
     # In[10]:
78
79
80
     display(sp.Eq(sym.w_prime_2_bar, c_f.w_prime_2_bar()))
81
82
83
     # and
84
85
     # In[11]:
86
87
88
     display(sp.Eq(sym.w_prime_3_bar, c_f.w_prime_2_bar()))
89
90
91
     # So,
92
93
     # In[12]:
94
95
96
     lambda_w_val = c_f.lambda_w().subs({
97
         sym.w_prime_2_bar: c_f.w_prime_2_bar()
98
99
     display(sp.Eq(sym.lambda_w, lambda_w_val))
100
101
102
     # In[13]:
103
```

```
104
105
     w_prime_4_bar_check_val = c_f.w_prime_4_bar().subs({
106
         sym.w_prime_2_bar: c_f.w_prime_2_bar(),
107
         sym.w_prime_3_bar: c_f.w_prime_3_bar(),
108
         sym.sigma_tilde_w: c_f.sigma_tilde_w().subs({
109
              sym.w_prime_2_bar: c_f.w_prime_2_bar(),
110
              sym.lambda_w: c_f.lambda_w()
111
         })
112
     })
113
114
     display(sp.Eq(sym.w_prime_4_bar, w_prime_4_bar_check_val))
115
116
117
     # In[14]:
118
119
120
121
     display(sp.Eq(w_prime_4_bar_int_val, w_prime_4_bar_check_val, evaluate=True)
              .subs({sym.w_bar: c_f.w_bar()}).simplify())
122
123
```

Listing A.3: w_prime_4_bar.py

A.5 w_prime_2_theta_l_prime_bar.py

```
#!/usr/bin/env python
1
    # coding: utf-8
2
3
    # In[1]:
4
5
6
    from itertools import product
7
    import pandas as pd
9
10
    pd.set_option('display.max_columns', None)
11
    pd.set_option('display.max_rows', None)
12
13
    import sympy as sp
14
    from IPython.display import display
15
    from sympy import abc, oo, Rational
16
17
    import checked_functions as c_f
18
    import symbols as sym
19
20
^{21}
    # # This document aims to numerically check f\overline{w'^2\theta_l'}f
22
23
    # ## Define the marginal distributions.
24
```

```
25
    # In[2]:
26
27
28
    display(sp.Eq(sym.G_1_w_theta, c_f.G_1_w_theta_density))
29
30
31
    # In[3]:
32
33
34
    display(sp.Eq(sym.G_2_w_theta, c_f.G_2_w_theta_density))
35
36
37
    # In[4]:
38
39
40
    display(sp.Eq(sym.G_3_w_theta, c_f.G_3_w_theta_density))
41
42
43
    # In[5]:
44
45
46
    display(sp.Eq(sym.G_w_theta, c_f.G_w_theta, evaluate=False))
47
48
49
    # In[6]:
50
51
52
53
    w_prime_2_theta_l_prime_bar = sp.Integral(
         (sp.abc.w - sym.w_bar) ** 2 * (sp.abc.theta - sym.theta_l_bar) * c_f.G_w_theta,
54
         [sp.abc.w, -oo, oo],
55
         [sp.abc.theta, -oo, oo])
56
57
    display(sp.Eq(sym.w_prime_2_theta_prime_l_bar, w_prime_2_theta_l_prime_bar))
58
59
    # In[7]:
60
61
62
63
    w_prime_2_theta_l_prime_bar = (
         w_prime_2_theta_l_prime_bar.subs({
64
             sym.w_bar: c_f.w_bar(),
65
             sym.theta_l_bar: c_f.theta_l_bar()
66
         }))
67
68
    display(sp.Eq(sym.w_prime_2_theta_prime_1_bar,
69
70
                   w_prime_2_theta_l_prime_bar))
71
72
    # The equation in the document is:
73
74
    # In [8]:
75
76
77
    display(sp.Eq(sym.w_prime_2_theta_prime_l_bar, c_f.w_prime_2_theta_l_prime_bar()))
```

```
79
80
     # For this we still need f \in \{sigma_w\}_{f}:
81
82
     # In[9]:
83
84
85
     display(sp.Eq(sym.sigma_tilde_w, c_f.sigma_tilde_w()))
86
87
88
     # And £\overline{w'^{2}}£:
89
90
91
     # In[10]:
92
93
     display(sp.Eq(sym.w_prime_2_bar, c_f.w_prime_2_bar()))
94
95
96
     # And f \in \{w'^{3}\}:
97
98
     # In[11]:
99
100
101
102
     display(sp.Eq(sym.w_prime_3_bar, c_f.w_prime_3_bar()))
103
104
     # And £ \setminus lambda_w£:
105
106
     # In[12]:
107
108
109
     display(sp.Eq(sym.lambda_w, c_f.lambda_w()))
110
111
112
     # And f \leq f(w) # And f \leq f(w)
113
114
     # In[13]:
115
116
117
     display(sp.Eq(sym.lambda_w_theta, c_f.lambda_w_theta()))
118
119
120
     # And f \in \{w' \mid theta_l'\} £:
121
122
     # In[14]:
123
124
125
     display(sp.Eq(sym.w_prime_theta_l_prime_bar, c_f.w_prime_theta_l_prime_bar()))
126
127
128
     # Putting those all together yields:
129
130
     # In[15]:
131
132
```

```
133
     w_prime_2_theta_l_prime_bar_check_val = (
134
         c_f.w_prime_2_theta_l_prime_bar().subs({
135
             sym.sigma_tilde_w: c_f.sigma_tilde_w(),
136
              sym.lambda_w: c_f.lambda_w(),
137
             sym.w_prime_2_bar: c_f.w_prime_2_bar(),
138
              sym.w_prime_3_bar: c_f.w_prime_3_bar(),
139
             sym.lambda_w_theta: c_f.lambda_w_theta(),
140
              sym.w_prime_theta_l_prime_bar: c_f.w_prime_theta_l_prime_bar()
141
         }))
142
143
     w_prime_2_theta_l_prime_bar_check_val = (
144
         w_prime_2_theta_l_prime_bar_check_val.subs({
145
             sym.w_prime_2_bar: c_f.w_prime_2_bar(),
146
             sym.w_bar: c_f.w_bar(),
147
             sym.theta_l_bar: c_f.theta_l_bar()
148
         }))
149
     display(sp.Eq(sym.w_prime_2_theta_prime_1_bar,
151
                    w_prime_2_theta_l_prime_bar_check_val))
152
153
154
     # Since the integral is too difficult to be calculated analytically, at least with
155
        sympy, we try to put in some arbitrary numbers for the pdf parameters, to simplify
         the equations.
156
     # We create a dataframe to get all possible permutations and therefore also all possible
157
        evaluations of the integrals.
158
     # In[16]:
159
160
161
     df = pd.DataFrame(
162
         product([0, 1],
163
                  [-2, 2],
164
                  [-1, 2],
165
                  [0, 3],
166
                  [Rational(1, 10)],
167
                  [Rational(3, 10)],
168
                  [Rational(4, 10)],
169
                  [Rational(7, 10)],
170
                  [Rational(6, 10)],
171
                  [Rational(5, 10)],
172
                  [Rational(1, 10), Rational(5, 10)],
173
                  [Rational(5, 10)]),
174
         columns=[sym.w_1,
175
                   sym.w_2,
176
                   sym.theta_l_1,
177
                   sym.theta_1_2,
178
                   sym.sigma_theta_l_1,
179
                   sym.sigma_theta_1_2,
180
                   sym.sigma_lambda_theta_l,
                   sym.sigma_w,
182
                   sym.sigma_lambda_w,
183
```

```
sp.abc.alpha,
184
                   sp.abc.delta,
185
                   sym.rho_w_theta_l])
186
187
188
     # In[17]:
189
190
191
     df['check_val'] = (
192
         df.apply(lambda x:
193
                   w_prime_2_theta_l_prime_bar_check_val.subs({
194
                       sym.w_1: x[sym.w_1],
195
                        sym.w_2: x[sym.w_2],
196
                        sym.theta_l_1: x[sym.theta_l_1],
197
                       sym.theta_1_2: x[sym.theta_1_2],
198
                       sym.sigma_theta_l_1: x[sym.sigma_theta_l_1],
199
                       sym.sigma_theta_1_2: x[sym.sigma_theta_1_2],
200
                       sym.sigma_lambda_theta_l: x[sym.sigma_lambda_theta_l],
                       sym.sigma_w: x[sym.sigma_w],
202
                       sym.sigma_lambda_w: x[sym.sigma_lambda_w],
203
                       sp.abc.alpha: x[sp.abc.alpha],
204
                       sp.abc.delta: x[sp.abc.delta],
205
                       sym.rho_w_theta_1: x[sym.rho_w_theta_1]
206
                   }), axis=1))
207
208
209
     # Calculate the moment analytically:
210
211
     # In[18]:
212
213
214
     df['num_int'] = (
215
         df.apply(lambda x: Rational(w_prime_2_theta_l_prime_bar.subs({
216
              sym.w_1: x[sym.w_1],
217
              sym.w_2: x[sym.w_2],
218
              sym.theta_l_1: x[sym.theta_l_1],
219
              sym.theta_1_2: x[sym.theta_1_2],
              sym.sigma_theta_l_1: x[sym.sigma_theta_l_1],
221
              sym.sigma_theta_1_2: x[sym.sigma_theta_1_2],
222
              sym.sigma_lambda_theta_l: x[sym.sigma_lambda_theta_l],
223
              sym.sigma_w: x[sym.sigma_w],
224
              sym.sigma_lambda_w: x[sym.sigma_lambda_w],
225
              sp.abc.alpha: x[sp.abc.alpha],
226
              sp.abc.delta: x[sp.abc.delta],
227
              sym.rho_w_theta_1: x[sym.rho_w_theta_1]
228
         }).doit(conds='none', method='quad').evalf()), axis=1))
229
230
231
     # In[19]:
232
233
234
     df['diff'] = abs(df['check_val'] - df['num_int'])
235
236
237
```

```
# In[20]:
238
239
     df['diff_num'] = abs(df['check_val'].astype(float) - df['num_int'].astype(float))
241
242
243
     # In[21]:
244
245
246
     display(df)
247
248
249
250
     # In[22]:
251
252
     import numpy as np
253
254
     print('The mean error between the rhs and the lhs is:', np.mean(df['diff_num']))
255
256
```

Listing A.4: w_prime_2_theta_l_prime_bar.py

A.6 w_prime_theta_l_prime_2_bar.py

```
#!/usr/bin/env python
2
    # coding: utf-8
3
    # In[1]:
4
5
6
    from itertools import product
7
    import pandas as pd
9
10
    pd.set_option('display.max_columns', None)
11
    pd.set_option('display.max_rows', None)
12
13
    import sympy as sp
14
    from IPython.display import display
15
    from sympy import abc, oo, Rational, init_printing
16
17
    import checked_functions as c_f
18
    import symbols as sym
19
    init_printing()
20
21
22
    # # This document aims to numerically check f\overline{w'\theta_l'^2}f
23
24
    # ## Define the marginal distributions.
25
```

```
26
    # In[2]:
27
28
29
    display(sp.Eq(sym.G_1_w_theta, c_f.G_1_w_theta_density))
30
31
32
    # In[3]:
33
34
35
    display(sp.Eq(sym.G_2_w_theta, c_f.G_2_w_theta_density))
36
37
38
    # In[4]:
39
40
41
    display(sp.Eq(sym.G_3_w_theta, c_f.G_3_w_theta_density))
42
43
44
    # In[5]:
45
46
47
    display(sp.Eq(sym.G_w_theta, c_f.G_w_theta, evaluate=False))
48
49
50
    # In[6]:
51
52
53
    w_prime_theta_l_2_prime_bar = sp.Integral(
54
         (sp.abc.w - sym.w_bar) * (sp.abc.theta - sym.theta_1_bar) ** 2 * c_f.G_w_theta,
55
         [sp.abc.w, -oo, oo],
56
         [sp.abc.theta, -oo, oo])
57
58
    display(sp.Eq(sym.w_prime_theta_prime_l_2_bar, w_prime_theta_l_2_prime_bar))
59
60
61
    # In[7]:
62
63
64
    w_prime_theta_1_2_prime_bar = w_prime_theta_1_2_prime_bar.subs({
65
         sym.w_bar: c_f.w_bar(),
66
         sym.theta_l_bar: c_f.theta_l_bar()
67
    })
68
69
    display(sp.Eq(sym.w_prime_theta_prime_l_2_bar, w_prime_theta_l_2_prime_bar))
70
71
72
    # The equation in the document is:
73
74
    # In[8]:
75
76
77
    display(sp.Eq(sym.w_prime_theta_prime_l_2_bar, c_f.w_prime_theta_l_prime_2_bar()))
78
79
```

```
80
     # For this we still need f\tilde{\sigma_w}f:
81
82
     # In[9]:
83
84
85
     display(sp.Eq(sym.sigma_tilde_w, c_f.sigma_tilde_w()))
86
87
88
     # And f\overline{w'^{2}}f:
89
90
     # In[10]:
91
92
93
     display(sp.Eq(sym.w_prime_2_bar, c_f.w_prime_2_bar()))
94
95
96
     # And f \in \{w'^{3}\}:
97
98
     # In[11]:
99
100
101
     display(sp.Eq(sym.w_prime_3_bar, c_f.w_prime_3_bar()))
102
103
104
     # And £\overline{w'\theta'_l}£:
105
106
     # In[12]:
107
108
109
     display(sp.Eq(sym.w_prime_theta_l_prime_bar, c_f.w_prime_theta_l_prime_bar()))
110
111
112
113
     # And £ \setminus lambda_w£:
114
     # In[13]:
115
116
117
     display(sp.Eq(sym.lambda_w, c_f.lambda_w()))
118
119
120
     # And \pounds \setminus lambda_{w} \in \mathcal{L}:
121
122
     # In[14]:
123
124
125
     display(sp.Eq(sym.lambda_w_theta, c_f.lambda_w_theta()))
126
127
128
     # And £\overline{\theta_l'^3}£:
129
130
     # In[15]:
131
132
133
```

```
display(sp.Eq(sym.theta_l_prime_3_bar, c_f.theta_l_prime_3_bar()))
134
135
136
     # Putting those all together yields:
137
138
     # In[16]:
139
140
141
     w_prime_theta_l_prime_2_bar_check_val = c_f.w_prime_theta_l_prime_2_bar().subs({
142
         sym.theta_l_prime_3_bar: c_f.theta_l_prime_3_bar(),
143
         sym.sigma_tilde_w: c_f.sigma_tilde_w(),
144
145
         sym.lambda_w: c_f.lambda_w(),
146
         sym.w_prime_2_bar: c_f.w_prime_2_bar(),
         sym.w_prime_3_bar: c_f.w_prime_3_bar(),
147
         sym.lambda_w_theta: c_f.lambda_w_theta(),
148
         sym.w_prime_theta_l_prime_bar: c_f.w_prime_theta_l_prime_bar()
149
     })
150
151
     w_prime_theta_l_prime_2_bar_check_val = w_prime_theta_l_prime_2_bar_check_val.subs({
152
         sym.w_prime_2_bar: c_f.w_prime_2_bar(),
153
         sym.lambda_w: c_f.lambda_w(),
154
         sym.w_bar: c_f.w_bar(),
         sym.theta_l_bar: c_f.theta_l_bar()
156
     })
157
158
     display(sp.Eq(sym.w_prime_theta_prime_1_2_bar, w_prime_theta_1_prime_2_bar_check_val))
159
160
161
     # Since the integral is too difficult to be calculated analytically, at least with
162
      → sympy, we try to put in some arbitrary numbers for the pdf parameters, to simplify
        the equations.
163
     # We create a dataframe to get all possible permutations and therefore also all possible
164
      \rightarrow evaluations of the integrals.
165
     # In [17]:
166
167
168
     df = pd.DataFrame(
169
         product([0, 1],
170
                  [-2, 2],
171
                  [-1, 2],
172
                  [0, 3],
173
                  [Rational(1, 10)],
174
                  [Rational(3, 10)],
175
                  [Rational(4, 10)],
176
                  [Rational(7, 10)],
177
                  [Rational(6, 10)],
178
                  [Rational(5, 10)],
179
                  [Rational(1, 10), Rational(5, 10)],
180
                  [Rational(5, 10)]),
181
         columns=[sym.w_1,
182
                   sym.w_2,
183
                   sym.theta_l_1,
184
```

```
185
                   sym.theta_1_2,
                   sym.sigma_theta_l_1,
186
                   sym.sigma_theta_1_2,
187
                   sym.sigma_theta_1_3,
188
                   sym.sigma_w,
189
                   sym.sigma_w_3,
190
                   sp.abc.alpha,
191
                   sp.abc.delta,
192
                   sym.rho_w_theta_l])
193
194
195
     # In[18]:
196
197
198
     df['check_val'] = (
199
         df.apply(lambda x:
200
201
                   w_prime_theta_l_prime_2_bar_check_val.subs({
                        sym.w_1: x[sym.w_1],
                        sym.w_2: x[sym.w_2],
203
                        sym.theta_l_1: x[sym.theta_l_1],
204
                        sym.theta_1_2: x[sym.theta_1_2],
205
                        sym.sigma_theta_l_1: x[sym.sigma_theta_l_1],
206
                        sym.sigma_theta_1_2: x[sym.sigma_theta_1_2],
207
                        sym.sigma_theta_1_3: x[sym.sigma_theta_1_3],
208
                        sym.sigma_w: x[sym.sigma_w],
209
                        sym.sigma_w_3: x[sym.sigma_w_3],
210
                        sp.abc.alpha: x[sp.abc.alpha],
211
                        sp.abc.delta: x[sp.abc.delta],
212
                        sym.rho_w_theta_1: x[sym.rho_w_theta_1]
213
                   }).evalf(), axis=1))
214
215
216
217
     # Calculate the moment analytically:
218
     # In[19]:
219
220
221
     df['num_int'] = (
222
         df.apply(lambda x: w_prime_theta_l_2_prime_bar.subs({
223
              sym.w_1: x[sym.w_1],
224
              sym.w_2: x[sym.w_2],
225
              sym.theta_l_1: x[sym.theta_l_1],
226
              sym.theta_1_2: x[sym.theta_1_2],
227
              sym.sigma_theta_l_1: x[sym.sigma_theta_l_1],
228
              sym.sigma_theta_1_2: x[sym.sigma_theta_1_2],
229
              sym.sigma_theta_1_3: x[sym.sigma_theta_1_3],
230
              sym.sigma_w: x[sym.sigma_w],
231
              sym.sigma_w_3: x[sym.sigma_w_3],
232
              sp.abc.alpha: x[sp.abc.alpha],
233
              sp.abc.delta: x[sp.abc.delta],
234
              sym.rho_w_theta_l: x[sym.rho_w_theta_l]
235
         }).doit(conds='none', method='quad').evalf(), axis=1))
237
238
```

```
# In[20]:
239
240
     df['diff'] = abs(df['check_val'] - df['num_int'])
242
243
244
     # In[21]:
245
246
247
     df['diff_num'] = abs(df['check_val'].astype(float) - df['num_int'].astype(float))
^{248}
249
250
251
     # In[22]:
252
253
     display(df)
254
255
256
     # In[23]:
257
258
259
     import numpy as np
260
261
     print('The mean error between the rhs and the lhs is:', np.mean(df['diff_num']))
262
263
```

Listing A.5: w_prime_theta_l_prime_2_bar.py

A.7 w_prime_r_t_prime_theta_l_prime_bar.py

```
#!/usr/bin/env python
    # coding: utf-8
2
3
    # In[2]:
4
5
6
    from itertools import product
7
8
    import pandas as pd
9
10
    pd.set_option('display.max_columns', None)
11
    pd.set_option('display.max_rows', None)
12
13
    import sympy as sp
14
    from IPython.display import display
15
    from sympy import abc, oo, Rational, init_printing
16
17
    import checked_functions as c_f
    import symbols as sym
19
```

```
20
    init_printing()
21
22
23
    # # This document aims to numerically check f\overline{w'r_t'\theta_l'}f
24
25
26
    # ## Define the normal distributions.
27
    # In[3]:
28
29
30
    display(sp.Eq(sp.symbols('\\mu_1'), c_f.mu_1_w_theta_l_r_t, evaluate=False))
31
32
    display(sp.Eq(sp.symbols('\\Sigma_1'), c_f.Sigma_1_w_theta_l_r_t, evaluate=False))
    \#display(sp.Eq(sym.G_1_w_theta_l_r_t, c_f.G_1_w_theta_l_r_t_density))
33
34
35
    # In[4]:
36
38
    display(sp.Eq(sp.symbols('\\mu_2'), c_f.mu_2_w_theta_l_r_t, evaluate=False))
39
    display(sp.Eq(sp.symbols('\\Sigma_2'), c_f.Sigma_2_w_theta_l_r_t, evaluate=False))
40
    \#display(sp.Eq(sym.G_2\_w\_theta\_l\_r\_t, c\_f.G_2\_w\_theta\_l\_r\_t\_density))
41
42
43
    # In[5]:
44
45
46
    display(sp.Eq(sp.symbols('\mu_3'), c_f.mu_3_w_theta_l_r_t, evaluate=False))
47
    display(sp.Eq(sp.symbols('\\Sigma_3'), c_f.Sigma_3_w_theta_l_r_t, evaluate=False))
48
    \#display(sp.Eq(sym.G_3\_w\_theta\_l\_r\_t, c\_f.G_3\_w\_theta\_l\_r\_t\_density))
49
50
51
    # In[6]:
52
53
54
    display(sp.Eq(sym.G_w_theta_l_r_t, c_f.G_w_theta_l_r_t))
55
56
57
    # In[7]:
58
59
60
    w_prime_r_t_prime_theta_l_prime_bar = sp.Integral(
61
         (sp.abc.w - sym.w_bar) * (sym.r_t - sym.r_t_bar) * (sp.abc.theta - sym.theta_l_bar)
62
         \rightarrow * c_f.G_w_theta_l_r_t,
         [sp.abc.w, -oo, oo],
63
         [sym.theta_1, -oo, oo],
64
         [sym.r_t, -oo, oo])
65
    display(sp.Eq(sym.w_prime_r_t_prime_theta_l_prime_bar,
66
       w_prime_r_t_prime_theta_l_prime_bar))
67
68
    # In [87:
69
70
71
```

```
w_prime_r_t_prime_theta_l_prime_bar = (
72
         w_prime_r_t_prime_theta_l_prime_bar.subs({
73
             sym.w_bar: c_f.w_bar(),
74
             sym.r_t_bar: c_f.r_t_bar(),
75
             sym.theta_l_bar: c_f.theta_l_bar()
76
         }))
77
78
     display(sp.Eq(sym.w_prime_r_t_prime_theta_l_prime_bar,
     → w_prime_r_t_prime_theta_l_prime_bar))
79
80
     # The equation in the document is:
81
82
83
     # In[9]:
84
85
     display(sp.Eq(sym.w_prime_r_t_prime_theta_l_prime_bar,
86
     87
88
     # Since the integral is too difficult to be calculated analytically, at least with
89
     → sympy, we try to put in some arbitrary numbers for the pdf parameters, to simplify
        the equations.
90
     # We also use the method `nquad(..)` from `sympy` to get a numerical evaluation of the
91
     \rightarrow 3d integral.
92
     # We create a dataframe to get all possible permutations and therefore also all possible
93
     \rightarrow evaluations of the integrals.
94
     # In[10]:
95
96
97
     df = pd.DataFrame(
98
         product([3, 1],
99
                  [-2],
100
                  [-1, 3],
101
                  [2],
102
                  [1, 4],
103
                  [2],
104
                  [1.1],
105
                  [1.3],
106
                  [1.4],
107
                  [1.7],
108
                  [1.2],
109
                  [1.5],
110
                  [1.9],
111
112
                  [1.6],
                  [.55],
113
                  [.8],
114
                  [.65],
115
                  [.45],
116
                  [.35],
117
                  [.5]),
118
         columns=[sym.w_1,
```

```
sym.w_2,
120
                   sym.theta_l_1,
121
                   sym.theta_1_2,
122
                   sym.r_t_1,
123
                   sym.r_t_2,
124
                   sym.sigma_theta_l_1,
125
                   sym.sigma_theta_1_2,
126
                   sym.sigma_theta_1_3,
127
                   sym.sigma_w,
128
                   sym.sigma_r_t_1,
129
                   sym.sigma_r_t_2,
130
                   sym.sigma_r_t_3,
131
                   sym.sigma_w_3,
132
                   sp.abc.alpha,
133
                   sp.abc.delta,
134
                   sym.rho_w_theta_l,
135
                   sym.rho_w_r_t,
136
                   sym.rho_theta_l_r_t,
137
                   sym.r_r_t_theta_l])
138
139
140
     # In[11]:
141
142
143
     w_prime_r_t_prime_theta_l_prime_bar_check_sym_val = (
144
          c_f.w_prime_r_t_prime_theta_l_prime_bar().subs({
145
              sym.w_bar: c_f.w_bar(),
146
              sym.r_t_bar: c_f.r_t_bar(),
147
              sym.theta_l_bar: c_f.theta_l_bar()
          }))
149
150
151
     # In[12]:
152
153
154
     df['check_val'] = (
155
          df.apply(lambda x: Rational(c_f.w_prime_r_t_prime_theta_l_prime_bar().subs({
156
              sym.w_bar: c_f.w_bar(),
157
              sym.theta_l_bar: c_f.theta_l_bar(),
158
              sym.r_t_bar: c_f.r_t_bar(),
159
              sym.w_1: x[sym.w_1],
160
              sym.w_2: x[sym.w_2],
161
              sym.theta_l_1: x[sym.theta_l_1],
162
              sym.theta_1_2: x[sym.theta_1_2],
163
              sym.r_t_1: x[sym.r_t_1],
164
              sym.r_t_2: x[sym.r_t_2],
165
              sym.sigma_theta_l_1: x[sym.sigma_theta_l_1],
166
              sym.sigma_theta_1_2: x[sym.sigma_theta_1_2],
167
              sym.sigma_r_t_1: x[sym.sigma_r_t_1],
168
              sym.sigma_r_t_2: x[sym.sigma_r_t_2],
169
              sp.abc.alpha: x[sp.abc.alpha],
170
              sp.abc.delta: x[sp.abc.delta],
              sym.r_r_t_theta_1: x[sym.r_r_t_theta_1]
172
          }).evalf()), axis=1))
173
```

```
174
175
     # Calculate the moment numerically:
176
177
     # In[13]:
178
179
180
     import scipy
181
182
     df['num_int'] = df.apply(lambda x: scipy.integrate.nquad(
183
         sp.lambdify(
184
185
              [sp.abc.w, sym.r_t, sym.theta_1],
              (((sp.abc.w - c_f.w_bar()) *
186
                (sym.r_t - c_f.r_t_bar()) *
                (sym.theta_l - c_f.theta_l_bar()) *
188
                c_f.G_w_theta_l_r_t))
189
              .subs({
190
                  sym.w_bar: c_f.w_bar(),
191
                  sym.r_t_bar: c_f.r_t_bar(),
192
                  sym.theta_l_bar: c_f.theta_l_bar(),
193
                  sym.w_1: x[sym.w_1],
194
                  sym.w_2: x[sym.w_2],
195
                  sym.theta_l_1: x[sym.theta_l_1],
196
                  sym theta_1_2: x[sym theta_1_2],
197
                  sym.r_t_1: x[sym.r_t_1],
198
                  sym.r_t_2: x[sym.r_t_2],
199
                  sym.sigma_w: x[sym.sigma_w],
200
                  sym.sigma_w_3: x[sym.sigma_w_3],
201
                  sym.sigma_theta_l_1: x[sym.sigma_theta_l_1],
202
                  sym.sigma_theta_1_2: x[sym.sigma_theta_1_2],
203
                  sym.sigma_theta_1_3: x[sym.sigma_theta_1_3],
204
                  sym.sigma_r_t_1: x[sym.sigma_r_t_1],
205
                  sym.sigma_r_t_2: x[sym.sigma_r_t_2],
206
                  sym.sigma_r_t_3: x[sym.sigma_r_t_3],
207
                  sp.abc.alpha: x[sp.abc.alpha],
208
                  sp.abc.delta: x[sp.abc.delta],
209
                  sym.rho_w_theta_l: x[sym.rho_w_theta_l],
210
                  sym.rho_w_r_t: x[sym.rho_w_r_t],
211
                  sym.rho_theta_l_r_t: x[sym.rho_theta_l_r_t],
212
                  sym.r_r_t_theta_l: x[sym.r_r_t_theta_l]
213
              })),
214
         ranges=[[-30, 30], [-30, 30], [-30, 30]])[0],
215
                                axis=1)
216
217
218
     # In[14]:
219
220
221
     df['diff'] = abs(df['check_val'] - df['num_int'])
222
223
224
     # In[15]:
225
226
227
```

```
df['diff_num'] = abs(df['check_val'].astype(float) - df['num_int'])
228
229
230
     # In[16]:
^{231}
232
233
     display(df)
234
235
236
     # In[17]:
^{237}
238
239
240
     import numpy as np
241
     print('The mean error between the rhs and the lhs is:', np.mean(df['diff_num']))
242
^{243}
```

Listing A.6: w_prime_r_t_prime_theta_l_prime_bar.py

B Calculation of limits

For the calculation, it has been used, that (based on equation (4.2.3))

$$\tilde{\sigma}_w^2 = \frac{\sigma_w^2 (1 - \delta)}{\overline{w'^2} (1 - \delta \lambda_w)},\tag{B.0.1}$$

and

$$\tilde{\sigma}_w^4 = \frac{\sigma_w^4 (1 - \delta)^2}{\left(\overline{w'^2}\right)^2 (1 - \delta \lambda_w)^2}.$$
(B.0.2)

We also treat the lower-order moments as fixed, as well as all the λ 's because those are inputs in the code. To make the calculation even more readable, we calculate two limits here.

$$\lim_{\delta \to 1} \left(\tilde{\sigma}_w^2 \right) = \lim_{\delta \to 1} \left(\frac{\sigma_w^2 (1 - \delta)^{\bullet 0}}{\overline{w'^2} (1 - \delta \lambda_w)} \right) = 0, \tag{B.0.3}$$

and

$$\lim_{\delta \to 1} \left(\tilde{\sigma}_w^4 \right) = \lim_{\delta \to 1} \left(\frac{\sigma_w^4 \left(1 - \delta \right)^{\frac{2}{2}}^0}{\left(\overline{w'^2} \right)^2 \left(1 - \delta \lambda_w \right)^2} \right) = 0.$$
 (B.0.4)

B.1 Calculation for the limit for $\overline{w'^4}$ as δ goes to 1

$$\lim_{\delta \to 1} \left(\overline{w'^4} \right) = \lim_{\delta \to 1} \left(\left(\overline{w'^2} \right)^2 \frac{(1 - \delta \lambda_w)^2}{(1 - \delta)} \left(3\tilde{\sigma}_w^4 + 6 \left(1 - \tilde{\sigma}_w^2 \right) \tilde{\sigma}_w^2 + \left(1 - \tilde{\sigma}_w^2 \right)^2 \right)$$

$$+ \frac{1}{(1 - \tilde{\sigma}_w^2)} \frac{1}{(1 - \delta \lambda_w)} \frac{\left(\overline{w'^3} \right)^2}{\overline{w'^2}} + \delta 3\lambda_w^2 \left(\overline{w'^2} \right)^2 \right)$$

$$= \lim_{\delta \to 1} \left(\frac{\left(\overline{w'^2} \right)^2 (1 - \delta \lambda_w)^2 (4\tilde{\sigma}_w^2 - 2\tilde{\sigma}_w^2 + 1)}{(1 - \delta)} \right)$$

$$+ \frac{\left(\overline{w'^3} \right)^2 + \delta 3\lambda_w^2 \left(\overline{w'^2} \right)^3 (1 - \tilde{\sigma}_w^2) (1 - \delta \lambda_w)}{(1 - \delta \lambda_w) \overline{w'^2}}$$

$$(B.1.2)$$

$$= \lim_{\delta \to 1} \left(\frac{\left(\overline{w'^2}\right)^2 (1 - \delta \lambda_w)^2}{(1 - \delta)} + \frac{\left(\overline{w'^3}\right)^2 + \delta 3 \lambda_w^2 \left(\overline{w'^2}\right)^3 (1 - \delta \lambda_w)}{(1 - \delta \lambda_w) \overline{w'^2}} \right)$$

$$= \lim_{\delta \to 1} \left(\frac{\left(\overline{w'^2}\right)^2 (1 - \delta \lambda_w)^2}{(1 - \delta)} \right) + \lim_{\delta \to 1} \left(\frac{\left(\overline{w'^3}\right)^2}{(1 - \delta \lambda_w) \overline{w'^2}} \right) + \lim_{\delta \to 1} \left(\delta 3 \lambda_w^2 \left(\overline{w'^2}\right)^2 \right)$$
(B.1.4)

$$= \left(\overline{w'^2}\right)^2 \lim_{\delta \to 1} \left(\frac{(1 - \delta \lambda_w)^2}{(1 - \delta)}\right) + \frac{\left(\overline{w'^3}\right)^2}{\overline{w'^2}} \lim_{\delta \to 1} \left(\frac{1}{(1 - \delta \lambda_w)}\right) + 3\lambda_w^2 \left(\overline{w'^2}\right)^2 \quad (B.1.5)$$

B.2 Calculation for the limit for $\overline{w'^2\theta'_l}$ as δ goes to 1

$$\lim_{\delta \to 1} \left(\overline{w'^2 \theta_l'} \right) = \lim_{\delta \to 1} \left(\frac{1}{\left(1 - \tilde{\sigma}_w^2 \right)^{-1}} \frac{1 - \delta \lambda_{w\theta}}{1 - \delta \lambda_w} \frac{\overline{w'^3}}{\overline{w'^2}} \overline{w' \theta_l'} \right)$$
(B.2.1)

$$= \lim_{\delta \to 1} \left(\frac{(1 - \delta \lambda_{w\theta}) \cdot \overline{w'^3} \cdot \overline{w'\theta'_l}}{(1 - \delta \lambda_w) \overline{w'^2}} \right)$$
 (B.2.2)

$$= \frac{\overline{w'^3} \cdot \overline{w'\theta'_l}}{\overline{w'^2}} \lim_{\delta \to 1} \left(\frac{1 - \delta \lambda_{w\theta}}{1 - \delta \lambda_w} \right)$$
 (B.2.3)

B.3 Calculation for the limit for $\overline{w'\theta_l'^2}$ as δ goes to 1

$$\lim_{\delta \to 1} \left(\overline{w'\theta_l'^2} \right) = \lim_{\delta \to 1} \left(\frac{2(1 - \delta \lambda_{w\theta})^2 \overline{w'^3} \left(\overline{w'\theta_l'} \right)^2}{3(1 - \delta \lambda_w)^2 \left(1 - \tilde{\sigma}_w^2 \right)^2 \left(\overline{w'^2} \right)^2} + \frac{(1 - \delta \lambda_w) \left(1 - \tilde{\sigma}_w^2 \right) \overline{w'^2} \overline{\theta_l'^2}}{3(1 - \delta \lambda_{w\theta}) \overline{w'\theta_l'}} \right)$$
(B.3.1)

$$= \frac{2}{3} \lim_{\delta \to 1} \left(\frac{(1 - \delta \lambda_{w\theta})^2 \overline{w'^3} \left(\overline{w'\theta_l'} \right)^2}{(1 - \delta \lambda_w)^2 \left(\overline{w'^2} \right)^2} \right) + \lim_{\delta \to 1} \left(\frac{(1 - \delta \lambda_w) \overline{w'^2} \overline{\theta_l'^2}}{3(1 - \delta \lambda_{w\theta}) \overline{w'\theta_l'}} \right)$$
(B.3.2)

$$= \frac{1}{3} \left(\frac{2\overline{w'^3} \left(\overline{w'\theta_l'}\right)^2}{\left(\overline{w'^2}\right)^2} \lim_{\delta \to 1} \left(\left(\frac{1 - \delta \lambda_{w\theta}}{1 - \delta \lambda_w} \right)^2 \right) + \frac{\overline{w'^2} \overline{\theta_l'^2}}{\overline{w'\theta_l'}} \lim_{\delta \to 1} \left(\frac{1 - \delta \lambda_w}{1 - \delta \lambda_{w\theta}} \right) \right)$$
(B.3.3)