

# ADDING A THIRD GAUSSIAN TO CLUBB

by

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# ABSTRACT

## ADDING A THIRD GAUSSIAN TO CLUBB

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The Cloud Layers Unified By Binormals (CLUBB) model plays a crucial role in simulating atmospheric phenomena. It uses the sum of two probability density functions (pdfs) to represent a single grid layer. This 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 an innovative extension to the CLUBB model. We introduce a third normal CLUBB 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 maintaining computational tractability.

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. Additionally, it tries to describe certain asymptotic behavior of the trinormal pdf under various parameter settings.

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# List of Acronyms

**cas** computer algebra system. 13, 42

**CLUBB** Cloud Layers Unified By Binormals. ii, 1, 7–9, 14, 27, 42, 43

**lhs** left hand side. 11

**pde** partial differential equation. 8

**pdf** probability density function. ii, 1, 3, 6, 10, 11, 13–18, 20, 23, 25–29, 40, 42

**rhs** right hand side. 9, 11, 12

# List of Symbols

$\theta'_l$  Standardized liquid water potential temperature ( $\theta'_l = \theta_l - \overline{\theta_l}$ ). 5

$r'_t$  Standardized total water mixing ratio ( $r'_t = r_t - \overline{r_t}$ ). 5

$w'$  Standardized upward wind ( $w' = w - \overline{w}$ ). 5, 19

# Acknowledgments

Type acknowledgments here.

# 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 delves into the details of the proposed method. We begin by establishing a foundation with clear definitions of the relevant concepts, including normal distributions and the thermodynamic scalars crucial for atmospheric modeling (chapter 2).

Following this foundation, chapter 3 outlines the core problem we aim to address. Details regarding the model's inputs, outputs, and a step-by-step approach for verifying the formulas are provided.

Chapter 4 forms the heart of this work, presenting the actual formulas associated with the extended CLUBB model. This section details the introduction of the third normal pdf (section 2.1), the transformation of existing equations (section 4.3), and the derivation of key moments within the model (section 4.4 - section 4.5). Additionally, section 4.7 proposes a diagnostic approach to account for the skewness of heat and moisture, while section 4.8 introduces 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 analytic and numerical integration techniques, potentially 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.

The document concludes with an outlook in chapter 7, outlining potential future directions for research and exploration based on the findings presented here.

## 2 Definitions

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

### 2.1 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)**

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

### 2.2 Multivariate Normal distribution

We say that a random vector  $\mathbf{X}$  ( $r \times r$ ) is distributed according to a multivariate normal when it has the following joint density function:<sup>1</sup>

**Definition 2 (pdf of a multivariate normal distribution)**

$$f(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = (2\pi)^{-\frac{r}{2}} |\boldsymbol{\Sigma}|^{-\frac{1}{2}} \exp\left(-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\mathbf{x} - \boldsymbol{\mu})\right), \mathbf{x} \in \mathbb{R}^r, \quad (2.2.1)$$

---

<sup>1</sup>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, p. 59.

where

$$\boldsymbol{\mu} = \begin{pmatrix} \mu_1 \\ \vdots \\ \mu_r \end{pmatrix} \in \mathbb{R}^r \quad (2.2.2)$$

is the mean vector, and

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

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

## 2.2.1 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  $\bar{X} = \mathbb{E}[X]$ , 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:

$$\mathbb{E}[X^3] = \mathbb{E}\left[\left(\frac{X - \mu}{\sigma}\right)^3\right] = \frac{\mu_3}{\sigma^3} = \frac{\mathbb{E}[(X - \mu)^3]}{(\mathbb{E}[(X - \mu)^2])^{3/2}} = \frac{\kappa_3}{\kappa_2^{3/2}}, \quad (2.2.3)$$

$$\mathbb{E}[X^4] = \mathbb{E}\left[\left(\frac{X - \mu}{\sigma}\right)^4\right] = \frac{\mathbb{E}[(X - \mu)^4]}{(\mathbb{E}[(X - \mu)^2])^2} = \frac{\mu_4}{\sigma^4}. \quad (2.2.4)$$

## 2.3 Thermodynamic Scalars

We denote the thermodynamic scalars by  $w$ ,  $r_t$ , and  $\theta_l$ , where  $w$  is the upward wind,  $r_t$  is the liquid water potential temperature and  $\theta_l$  is the liquid water potential temperature.<sup>2</sup> Variables denoted by  $w'$  are defined by  $w - \bar{w}$  where  $\bar{w}$  is the mean of  $w$  over the whole pdf. We define  $r'_t$  and  $\theta'_l$  in the same way.

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<sup>2</sup>Vincent E. Larson. *CLUBB-SILHS: A parameterization of subgrid variability in the atmosphere*. 2022. arXiv: 1711.03675 [physics.ao-ph], p. 10.



# 3 Problem

## 3.1 Motivation

As being said in the chapter 1, we try to describe more possible shapes with adding a third pdf. To illustrate that, we plotted some of the shapes which are now possible but were not possible before. To be able to draw those plots, we are just using two variables,  $w$ , the upward wind, and  $\theta_l$ , the liquid water potential temperature. To illustrate how the binormal model handles strong winds, let us consider a scenario with strong upward winds at two locations  $w_1$ , as well as at  $w_2$ . The way the current binormal model would model this could look like figure 3.1.

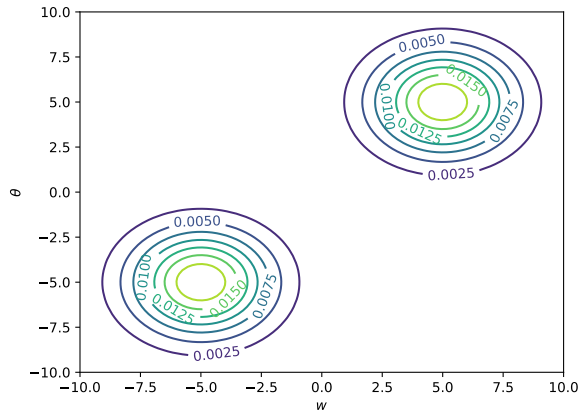


Figure 3.1: Binormal plot for two strong upward winds

With fixed variables:  $w_1 = 5$ ,  $w_2 = -5$ ,  $\theta_{l1} = 5$ ,  $\theta_{l2} = -5$ ,  $\alpha = 0.5$ ,  $\sigma_w = 2$ ,  $\sigma_{\theta_{l1}} = 2$ ,  $\sigma_{\theta_{l2}} = 2$ .

However, this bimodal distribution (figure 3.1) doesn't accurately reflect reality. In nature, we would not expect such a sharp jump between the strong upward winds at  $w_1$  and  $w_2$ . There would likely be some weaker upward winds 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 3.2.

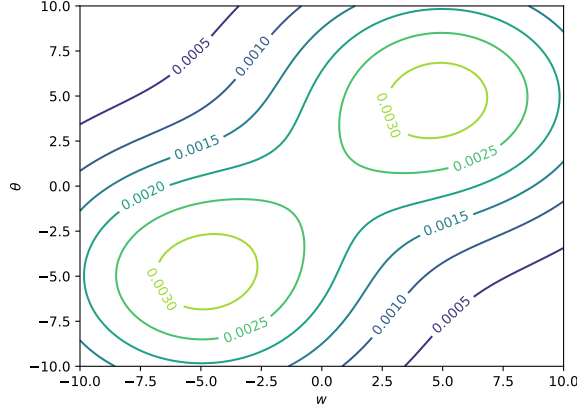


Figure 3.2: Binormal plot for two strong upward winds with increased standard deviations  
 With fixed variables:  $w_1 = 5$ ,  $w_2 = -5$ ,  $\theta_{l1} = 5$ ,  $\theta_{l2} = -5$ ,  $\alpha = 0.5$ ,  $\sigma_w = 5$ ,  $\sigma_{\theta_{l1}} = 5$ ,  
 $\sigma_{\theta_{l1}} = 5$ .

Seeing figure 3.2, the issue with having some values in the middle is slightly fixed but the general width of the normals was increased, too. Since CLUBB also has the simplification that there is no correlation between  $w$  and  $\theta_l$ , and  $w$  and  $r_t$ , obviously one cannot just increase it. Therefore, the idea is to add this third normal, which actually has correlation between all three variables and especially in the bivariate case, between  $w$  and  $\theta_l$ . Figure 3.2 would then change to figure 3.3.

Now, one can easily model something like the described shape, as illustrated in figure 3.3. Also, some other (maybe weird) shapes are now possible, just like the one in figure 3.4.

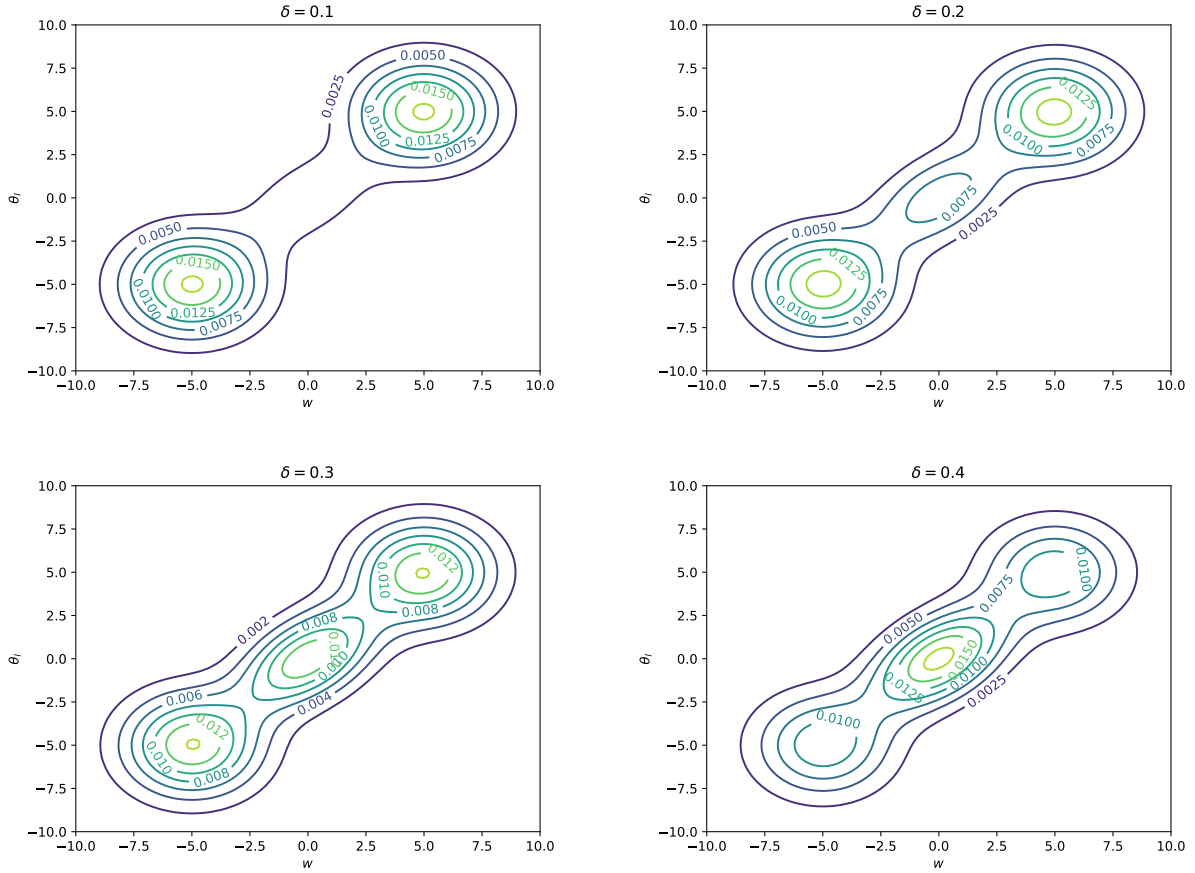


Figure 3.3: Trinormal plot for two strong upward winds with varying  $\delta$   
 With fixed variables:  $w_1 = 5$ ,  $w_2 = -5$ ,  $\theta_{l1} = 5$ ,  $\theta_{l2} = -5$ ,  $\alpha = 0.5$ ,  $\sigma_w = 2$ ,  $\sigma_{\theta_{l1}} = 2$ ,  
 $\sigma_{\theta_{l2}} = 2$ ,  $\sigma_{3w} = 2$ ,  $\sigma_{3\theta_l} = 2$ ,  $\rho_{w\theta_l} = 0.5$ .

## 3.2 Closing PDEs

The CLUBB model relies on a set of partial differential equations (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 ensures the model's mathematical integrity.

For instance, consider the following prognostic pde:<sup>1</sup>

<sup>1</sup>Larson, *CLUBB-SILHS: A parameterization of subgrid variability in the atmosphere*, p. 21.

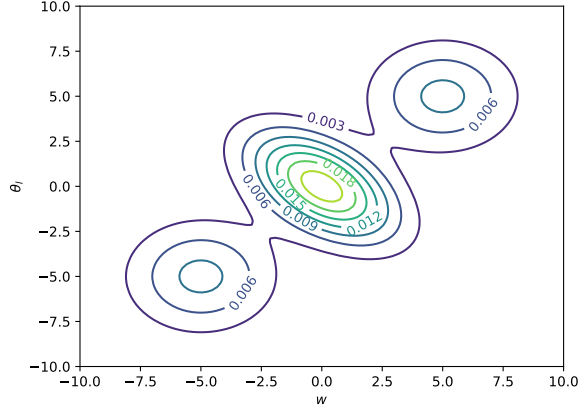


Figure 3.4: Trinormal plot for two strong upward winds with a third peak in the middle

With fixed variables:  $w_1 = 5$ ,  $w_2 = -5$ ,  $\theta_{l1} = 5$ ,  $\theta_{l2} = -5$ ,  $\alpha = 0.5$ ,  $\delta = 0.5$ ,  $\sigma_w = 2$ ,  
 $\sigma_{\theta_{l1}} = 2$ ,  $\sigma_{\theta_{l2}} = 2$ ,  $\sigma_{3w} = 2$ ,  $\sigma_{3\theta_l} = 2$ ,  $\rho_{w\theta_l} = 0.5$ .

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

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, even if they introduce slight limitations in capturing the full variability of the underlying atmospheric state.

Our focus here is on achieving closure for higher-order moments, such as the fourth moment of the vertical wind ( $\overline{w'^4}$ ). This closure is achieved by expressing these higher-order moments in terms of readily calculable lower-order moments. This approach uses the relationships between moments within a probability distribution, enabling efficient model updates during

the time-stepping process.

### 3.3 Inputs and Outputs

While defining inputs and outputs can seem challenging at first glance, it's a crucial step towards understanding a system. In this context, the code provides us with a set of moment terms:  $\overline{w}$ ,  $\overline{w'^2}$ ,  $\overline{w'^3}$ ,  $\overline{\theta_l}$ ,  $\overline{w'\theta'_l}$ ,  $\overline{r_t}$ ,  $\overline{w'r'_t}$ ,  $\overline{\theta_l'^2}$ ,  $\overline{r_t'^2}$ ,  $\overline{r_t'\theta'_l}$ . From these, we want to determine certain parameters which are describing the shape of the underlying pdf. Those parameters are standardized and some also normalized. So we try to solve for 13 unknowns, namely  $\alpha$ ,  $\widehat{w}_1$ ,  $\widehat{w}_2$ ,  $\tilde{\theta}_{l1}$ ,  $\tilde{\theta}_{l2}$ ,  $\tilde{r}_{t1}$ ,  $\tilde{r}_{t2}$ ,  $\tilde{\sigma}_w$ ,  $\tilde{\sigma}_{\theta_{l1}}$ ,  $\tilde{\sigma}_{\theta_{l2}}$ ,  $\tilde{\sigma}_{r_{t1}}$ ,  $\tilde{\sigma}_{r_{t2}}$ , and  $r_{r_t\theta_l}$ . All the formulas are listed in chapter 4.

While the code seems to derive the desired moments from a set of parameters, we want to establish a formal mathematical foundation for these relationships. To achieve this, we will take a more traditional approach, working in the “forward” direction. This means we will:

1. *Define 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:

$$\overline{w} = \int_{\mathbb{R}} \int_{\mathbb{R}} \int_{\mathbb{R}} w \cdot P_{tmg} dw dr_t d\theta_l, \quad (3.3.1)$$

where  $P_{tmg}^2$  is the pdf of the sum of all three normal distributions. Since some integrals are challenging to solve analytically, even with the help of SymPy, we are using the quadrature

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<sup>2</sup>Trivariate Mixture of Gaussians

method to calculate the integrals and choose arbitrary values for the inputs. All of this can be seen in section 5.2.

### 3.4 Steps for checking the formulas

We want to state a general approach for checking all those formulas and try to reference to the following steps in chapter 5 where there are actual examples stated. One way, or at least the way, which is used in this document is the following, where 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.  $\sigma_{w3}$ . Then the pdf is known, and any moments of it can be calculated by integration.
2. Calculate the means, e.g.  $\bar{w} = \mathbb{E}[w]$  by integration over the pdf. Our formula for  $\bar{w}$  (equation (4.4.1)) in terms of the pdf parameters can be checked.
3. Once the means are known, calculate the central variances, e.g.  $\overline{w'^2} = \overline{(w - \bar{w})^2}$  by integration over the pdf. Our formula for  $\overline{w'^2}$  (equation (4.4.3)) in terms of the pdf parameters can be checked.
4. Once the variances, e.g.  $\overline{w'^2}$ , are known, then *non-dimensional* pdf parameters such as  $\lambda_w$  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, e.g.  $\overline{w'^4}$  or  $\overline{w'^2 \theta'_l}$ , by integration over the pdf. Again, we can check if lhs = rhs.

7. The integral  $\overline{w'\theta_l'^2}$  is complicated. If it is written in terms of  $\overline{\theta_l'^3}$  (equation (4.8.7)), then  $\overline{\theta_l'^3}$  can be integrated (equation (4.4.9)) and substituted into the rhs of equation (4.8.7). If  $\overline{w'\theta_l'^2}$  is written in terms of  $\beta$  (equation (4.8.9)), then we need to integrate to find  $\overline{\theta_l'^3}$ , back out  $\beta$  from equation (4.8.1), and finally substitute  $\beta$  into equation (4.8.7).
8. To verify equation (4.8.19) for  $\overline{w'r_t'\theta_l'}$ , use equation (4.4.21).

## 4 Formulas

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  $\infty$  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 Third Normal

We would like to define a third normal to the already existing two trivariate normals, which is right in the middle between those two. Using the following formula for a multivariate normal, we can just define the sum of our three normals by using a vector for the mean, as well as the covariance matrix. For the purpose of readability, we define the mean vectors of the first and second normal distributions as  $\mu_1 = (w_1, \theta_{l1}, r_{t1})^\top$ , and  $\mu_2 = (w_2, \theta_{l2}, r_{t2})^\top$ , where  $w_1 > w_2$  (due to a restriction in the code) and the covariance matrices as

$$\Sigma_1 = \begin{pmatrix} \sigma_w^2 & 0 & 0 \\ 0 & \sigma_{\theta_{l1}}^2 & \rho_{\theta_l r_t} \sigma_{\theta_{l3}} \sigma_{r_{t3}} \\ 0 & \rho_{\theta_l r_t} \sigma_{\theta_{l3}} \sigma_{r_{t3}} & \sigma_{r_{t1}}^2 \end{pmatrix}, \text{ and } \Sigma_2 = \begin{pmatrix} \sigma_w^2 & 0 & 0 \\ 0 & \sigma_{\theta_{l2}}^2 & \rho_{\theta_l r_t} \sigma_{\theta_{l3}} \sigma_{r_{t3}} \\ 0 & \rho_{\theta_l r_t} \sigma_{\theta_{l3}} \sigma_{r_{t3}} & \sigma_{r_{t2}}^2 \end{pmatrix}$$

It might be of interest that there is no correlation between  $w$  and  $\theta_l$  or  $w$  and  $r_t$ . That is to make the pdfs mathematically more tractable by therefore also taking away some variability. 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  $\mu_3$  and  $\Sigma_3$  are defined as

$$\mu_3 = \begin{pmatrix} \overline{w} \\ \overline{\theta_l} \\ \overline{r_t} \end{pmatrix}, \text{ and } \Sigma_3 = \begin{pmatrix} \sigma_{w3}^2 & \rho_{w\theta_l3}\sigma_{w3}\sigma_{\theta_l3} & \rho_{wr_t3}\sigma_{w3}\sigma_{r_t3} \\ \rho_{w\theta_l3}\sigma_{w3}\sigma_{\theta_l3} & \sigma_{\theta_l3}^2 & \rho_{\theta_lr_t3}\sigma_{\theta_l3}\sigma_{r_t3} \\ \rho_{wr_t3}\sigma_{w3}\sigma_{r_t3} & \rho_{\theta_lr_t3}\sigma_{\theta_l3}\sigma_{r_t3} & \sigma_{r_t3}^2 \end{pmatrix}.$$

For our proposed mix of normals we then have

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

where  $\mathcal{N}$  denotes the multivariate normal distribution. The advantage over just two normal pdfs is that we can now express more shapes of functions. We also define some additional relationships for this third normal distribution.

$$\lambda_w = \frac{\sigma_{w3}}{w'^2}, \quad \lambda_\theta = \frac{\sigma_{\theta_l3}}{\theta_l'^2}, \quad \lambda_r = \frac{\sigma_{r_t3}}{r_t'^2}, \quad (4.1.2)$$

$$\lambda_{\theta r} = \frac{\rho_{\theta_lr_t}\sigma_{\theta_l3}\sigma_{r_t3}}{r_t'\theta_l'}, \quad \lambda_{w\theta} = \frac{\rho_{w\theta_l}\sigma_{w3}\sigma_{\theta_l3}}{w'\theta_l'}, \quad \lambda_{wr} = \frac{\rho_{wr_t}\sigma_{w3}\sigma_{r_t3}}{w'r_t'}. \quad (4.1.3)$$

Hence, we can rewrite  $\Sigma_3$  as

$$\Sigma_3 = \begin{pmatrix} \sigma_{w3}^2 & \overline{w'\theta_l'} \cdot \lambda_{wr} & \overline{w'r_t'} \cdot \lambda_{wr} \\ \overline{w'\theta_l'} \cdot \lambda_{wr} & \sigma_{\theta_l3}^2 & \overline{r_t'\theta_l'} \cdot \lambda_{\theta r} \\ \overline{w'r_t'} \cdot \lambda_{wr} & \overline{r_t'\theta_l'} \cdot \lambda_{\theta r} & \sigma_{r_t3}^2 \end{pmatrix}. \quad (4.1.4)$$

## 4.2 Normalized Variables

Since CLUBB is mostly using “normalized variables”, we are going to list those, which are given in standard form.

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

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

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

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

$$\tilde{\sigma}_{\theta_{li}} \equiv \frac{\sigma_{\theta_{li}}}{\sqrt{\overline{\theta'^2_l}}} \frac{1}{\sqrt{\frac{1-\delta\lambda_\theta}{1-\delta}}}, \quad (4.2.4)$$

$$\tilde{\sigma}_{r_{ti}} \equiv \frac{\sigma_{r_{ti}}}{\sqrt{\overline{r'^2_t}}} \frac{1}{\sqrt{\frac{1-\delta\lambda_r}{1-\delta}}}. \quad (4.2.5)$$

## 4.3 Transformation of the equations

Having established the definition of the sum of normal distributions in section 4.1 to enhance mathematical tractability, we now delve into the transformation of equations from the existing binormal representation used in CLUBB-SILHS<sup>1</sup> to a trinormal one. While the formulas for the binormal case are well-defined (see CLUBB-SILHS<sup>2</sup>), the simplicity of the means and standard deviations employed in the trinormal representation suggests the existence of a specific transformation that holds true. This chapter will demonstrate that the following transformations, denoted by the subscript “dGn” for the binormal case, successfully achieve this conversion.

$$\overline{w'^2} \frac{1 - \delta\lambda_w}{1 - \delta} = \overline{w'^2}_{dGn}, \quad (4.3.1)$$

$$\overline{w'^3} \frac{1}{1 - \delta} = \overline{w'^3}_{dGn}, \quad (4.3.2)$$

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<sup>1</sup>Larson, *CLUBB-SILHS: A parameterization of subgrid variability in the atmosphere*.

<sup>2</sup>Ibid.

$$\frac{\overline{w'^3}}{w'^{2^{3/2}}} \frac{(1-\delta)^{1/2}}{(1-\lambda_w\delta)^{3/2}} = \frac{\overline{w'^3}_{dGn}}{w'^{2^{3/2}}_{dGn}}, \quad (4.3.3)$$

$$\frac{\overline{\theta_l'^2}}{\theta_l'^2} \frac{1-\delta\lambda_\theta}{1-\delta} = \overline{\theta_l'^2}_{dGn}, \quad (4.3.4)$$

$$\frac{\overline{w'\theta_l'}}{w'\theta_l'} \frac{1-\delta\lambda_{w\theta}}{1-\delta} = \overline{w'\theta_l'}_{dGn}, \quad (4.3.5)$$

$$\left( \frac{\overline{w'^4}}{w'^4} - 3\delta\lambda_w^2 \left( \frac{\overline{w'^2}}{w'^2} \right)^2 \right) \frac{1}{1-\delta} = \overline{w'^4}_{dGn} \quad (4.3.6)$$

$$\left( \frac{\overline{w'^4}}{(\overline{w'^2})^2} - 3\delta\lambda_w^2 \right) \frac{1-\delta}{(1-\lambda_w\delta)^2} = \frac{\overline{w'^4}_{dGn}}{(\overline{w'^2}_{dGn})^2} \quad (4.3.7)$$

To get a sense of what those transformations mean and why they should work, we pick e.g. equation (4.3.1). If we substitute in the already defined formula for  $\lambda_w$  (equation (4.1.2)), we get

$$\begin{aligned} \frac{\overline{w'^2}}{w'^2} \frac{1-\delta\lambda_w}{1-\delta} &= \overline{w'^2}_{dGn} \\ \overline{w'^2} (1 - \delta \frac{\sigma_{w3}}{w'^2}) &= (1-\delta) \overline{w'^2}_{dGn} \\ \overline{w'^2} - \delta\sigma_{w3} &= (1-\delta) \overline{w'^2}_{dGn} \\ \overline{w'^2} &= \overline{w'^2}_{dGn} - \delta \overline{w'^2}_{dGn} + \delta\sigma_{w3} \\ \overline{w'^2} &= \overline{w'^2}_{dGn} - \delta \left( \overline{w'^2}_{dGn} - \sigma_{w3} \right) \end{aligned}$$

Our analysis reveals a key relationship between the parameter  $\delta$  and the overall variance (often referred to as “width”) of the trinormal distribution. As the value of  $\delta$  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  $\delta$  will contribute more significantly to the spread of the combined pdf.

Also, if we look at equation (4.3.2), we see that there is no more  $\lambda_w$  present.

$$\overline{w'^3} = (1-\delta) \overline{w'^3}_{dGn}$$

It makes sense graphically, that as delta 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  $\sigma_{w3}$ . We can see this, as well as the relationship between the variance in table 4.1. Table 4.1 offers a visual representation of how the parameter  $\delta$  influences the

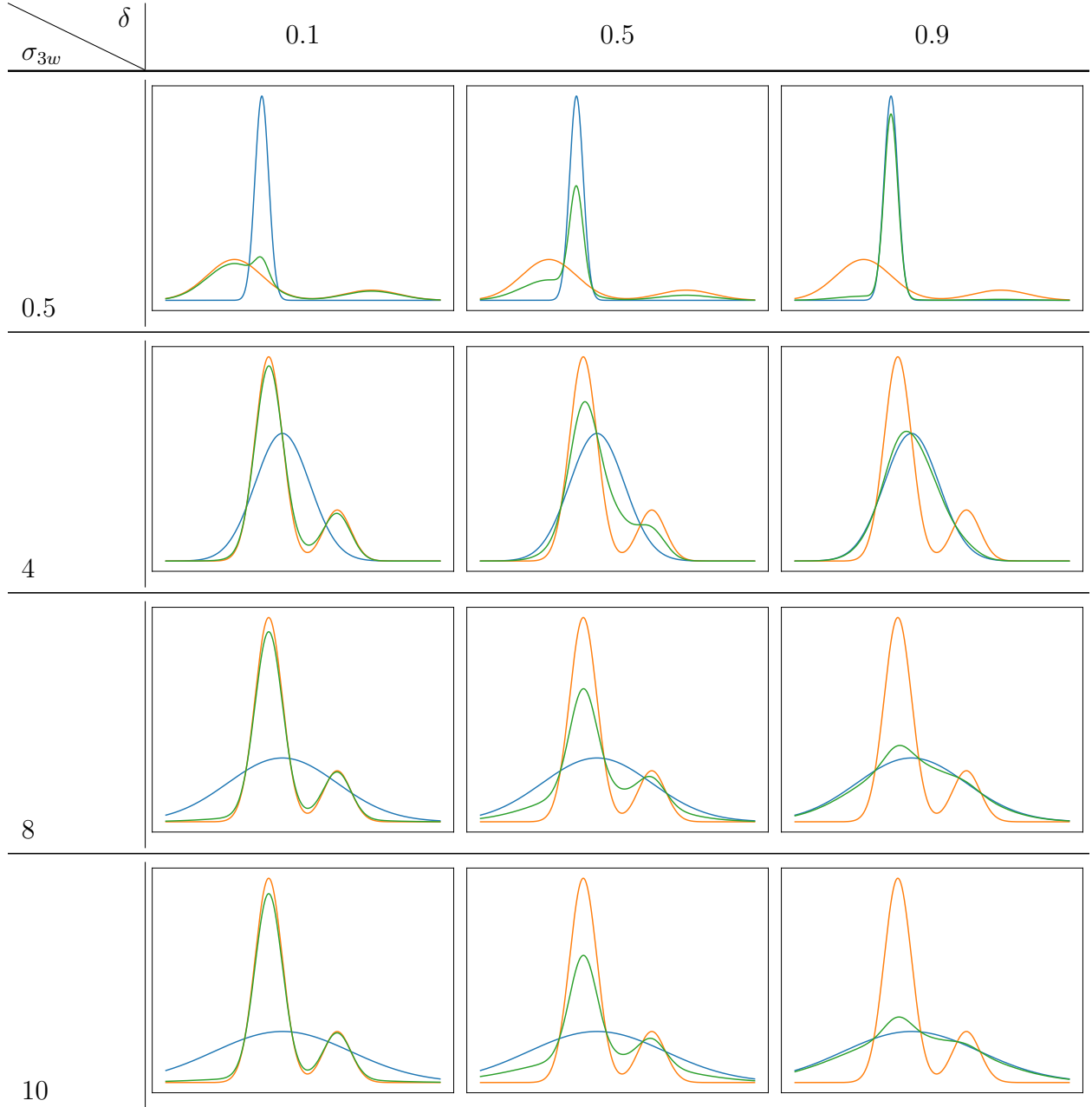


Table 4.1: 1D Plots for different  $\delta$  and  $\sigma_{w3}$

With fixed variables:  $w_1 = 5$ ,  $w_2 = -5$ ,  $\alpha = 0.2$ ,  $\sigma_w = 2$ .

The blue plot represents the third normal, the orange/red one represents the binormal, and the blue one represents the mixture. The x and y labels and ticks are omitted for clarity.

shape of the trinormal distribution. Each plot illustrates pdfs for different combinations of  $\sigma_{w3}$  (standard deviation of the third normal distribution) and  $\delta$ . The row values in the table correspond to  $\sigma_{w3}$ , while the column values represent  $\delta$ .

We can observe two key trends within these plots:

1. *Influence of  $\sigma_{w3}$* : As expected, varying  $\sigma_{w3}$  primarily affects the “width” or overall variance of the combined distribution. When  $\sigma_{w3}$  is larger than the width of the original binormal sum (orange/red line), choosing a larger  $\delta$  allows the overall variance to increase significantly, as predicted by equation (4.3.1).
2. *Decreasing Skewness with Increasing  $\delta$* : The plots also reveal a distinct relationship between  $\delta$  and the skewness of the resulting distribution. As  $\delta$  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  $\delta$ ) grows, its symmetric nature counteracts the potential skewness of the initial binormal sum. This effect is particularly evident 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 green plot (mixture) as  $\delta$  approaches 1.

## 4.4 Deduced Moments

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.

## 4.4.1 Lower Order Moments

### 4.4.1.1 Moments for $w$

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

$$\bar{w} = (1 - \delta)\alpha w_1 + (1 - \delta)(1 - \alpha)w_2 + \delta w_3, \quad (4.4.1)$$

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:

$$0 = \alpha \hat{w}_1 + (1 - \alpha) \hat{w}_2 \quad (4.4.2)$$

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:

$$\begin{aligned} \overline{w'^2} &= (1 - \delta)\alpha[(w_1 - \bar{w})^2 + \sigma_w^2] \\ &\quad + (1 - \delta)(1 - \alpha)[(w_2 - \bar{w})^2 + \sigma_w^2] \\ &\quad + \delta\sigma_{w3}^2, \end{aligned} \quad (4.4.3)$$

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

$$\begin{aligned} \overline{w'^2} &= \mathbb{E}[w'^2] = \mathbb{E}[(w - \bar{w})^2] = \mathbb{E}[(w - \mathbb{E}[w])^2] = \mathbb{E}[w^2 - 2w\mathbb{E}[w] + \mathbb{E}[w]^2] \\ &= \mathbb{E}[w^2] - 2\mathbb{E}[w\mathbb{E}[w]] + \mathbb{E}[\mathbb{E}[w]^2] = \mathbb{E}[w^2] - 2\mathbb{E}[w]\mathbb{E}[w] + \mathbb{E}[w]^2 \\ &= \mathbb{E}[w^2] - \mathbb{E}[w]^2 = \text{Var}[w]. \end{aligned}$$

The *non-dimensional* relationship would then be:

$$\frac{1}{(1 - \tilde{\sigma}_w^2)} = \alpha \left( \hat{w}_1^2 + \frac{\tilde{\sigma}_w^2}{(1 - \tilde{\sigma}_w^2)} \right) + (1 - \alpha) \left( \hat{w}_2^2 + \frac{\tilde{\sigma}_w^2}{(1 - \tilde{\sigma}_w^2)} \right). \quad (4.4.4)$$

The third order moment is given as:

$$\begin{aligned} \overline{w'^3} &= (1 - \delta)\alpha[(w_1 - \bar{w})^3 + 3\sigma_w^2(w_1 - \bar{w})] \\ &\quad + (1 - \delta)(1 - \alpha)[(w_2 - \bar{w})^3 + 3\sigma_w^2(w_2 - \bar{w})] \end{aligned} \quad (4.4.5)$$

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

$$\begin{aligned} \widehat{Sk}_w &\equiv \frac{1}{(1 - \tilde{\sigma}_w^2)^{3/2}} \frac{\overline{w'^3}}{\left(\overline{w'^2}\right)^{3/2}} \frac{1}{\left(\frac{1 - \delta\lambda_w}{1 - \delta}\right)^{3/2}} \frac{1}{1 - \delta} \\ &= \alpha \left( \hat{w}_1^3 + 3\hat{w}_1 \frac{\tilde{\sigma}_w^2}{(1 - \tilde{\sigma}_w^2)} \right) + (1 - \alpha) \left( \hat{w}_2^3 + 3\hat{w}_2 \frac{\tilde{\sigma}_w^2}{(1 - \tilde{\sigma}_w^2)} \right) \end{aligned} \quad (4.4.6)$$

#### 4.4.1.2 Moments for $\theta_l$

For  $\theta_l$  we have a similar *non-dimensional* relationship:

$$0 = \alpha\tilde{\theta}_{l1} + (1 - \alpha)\tilde{\theta}_{l2} \quad (4.4.7)$$

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

$$\begin{aligned} \overline{\theta_l'^2} &= (1 - \delta)\alpha[(\theta_{l1} - \bar{\theta}_l)^2 + \sigma_{\theta_{l1}}^2] \\ &\quad + (1 - \delta)(1 - \alpha)[(\theta_{l2} - \bar{\theta}_l)^2 + \sigma_{\theta_{l2}}^2] \\ &\quad + \delta\sigma_{\theta_{l3}}^2, \end{aligned} \quad (4.4.8)$$

where  $\sigma_{\theta_{l3}}$  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:

$$\begin{aligned}\overline{\theta_l'^3} &= (1 - \delta)\alpha[(\theta_{l1} - \overline{\theta_l})^3 + 3\sigma_{\theta_{l1}}^2(\theta_{l1} - \overline{\theta_l})] \\ &\quad + (1 - \delta)(1 - \alpha)[(\theta_{l2} - \overline{\theta_l})^3 + 3\sigma_{\theta_{l2}}^2(\theta_{l2} - \overline{\theta_l})]\end{aligned}\quad (4.4.9)$$

Similarly to equation (4.4.6), we also list a moment which is more diagnosed than prognosed:

$$\begin{aligned}\widehat{Sk_{\theta_l}} &\equiv \frac{\overline{\theta_l'^3}}{(\overline{\theta_l'^2})^{3/2}} \left( \frac{1}{\frac{1-\delta\lambda_\theta}{1-\delta}} \right)^{3/2} \frac{1}{1-\delta} \\ &= \alpha \left( \tilde{\theta}_{l1}^3 + 3\tilde{\theta}_{l1}\tilde{\sigma}_{\theta_{l1}}^2 \right) + (1 - \alpha) \left( \tilde{\theta}_{l2}^3 + 3\tilde{\theta}_{l2}\tilde{\sigma}_{\theta_{l2}}^2 \right).\end{aligned}\quad (4.4.10)$$

#### 4.4.1.3 Moments for $r_t$

The relationships for  $r_t$  and  $r_t'^2$  are given as follows

$$0 = \alpha\tilde{r}_{t1} + (1 - \alpha)\tilde{r}_{t2}, \quad (4.4.11)$$

and

$$1 = \alpha \left( \tilde{r}_{t1}^2 + \tilde{\sigma}_{r_{t1}}^2 \right) + (1 - \alpha) \left( \tilde{r}_{t2}^2 + \tilde{\sigma}_{r_{t2}}^2 \right). \quad (4.4.12)$$

Since this relationship is similar to the relationships of  $\theta_l$  and  $\theta_l'^2$ , we are using kind of the same formulas:

$$\begin{aligned}\overline{r_t'^2} &= (1 - \delta)\alpha[(r_{t1} - \overline{r_t})^2 + \sigma_{r_{t1}}^2] \\ &\quad + (1 - \delta)(1 - \alpha)[(r_{t2} - \overline{r_t})^2 + \sigma_{r_{t2}}^2] \\ &\quad + \delta\sigma_{r_{t3}}^2,\end{aligned}\quad (4.4.13)$$

and

$$\begin{aligned}\overline{r_t'^3} &= (1 - \delta)\alpha[(r_{t1} - \overline{r_t})^3 + 3\sigma_{r_{t1}}^2(r_{t1} - \overline{r_t})] \\ &\quad + (1 - \delta)(1 - \alpha)[(r_{t2} - \overline{r_t})^3 + 3\sigma_{r_{t2}}^2(r_{t2} - \overline{r_t})]\end{aligned}\quad (4.4.14)$$



#### 4.4.1.4 Mixed Moments

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

$$\begin{aligned}\overline{w'\theta'_l} &= (1 - \delta)\alpha[(w_1 - \bar{w})(\theta_{l1} - \bar{\theta}_l)] \\ &\quad + (1 - \delta)(1 - \alpha)[(w_2 - \bar{w})(\theta_{l2} - \bar{\theta}_l)] \\ &\quad + \delta\lambda_{w\theta}\overline{w'\theta'_l},\end{aligned}\tag{4.4.15}$$

$$\begin{aligned}\overline{w'r'_t} &= (1 - \delta)\alpha[(w_1 - \bar{w})(r_{t1} - \bar{r}_t)] \\ &\quad + (1 - \delta)(1 - \alpha)[(w_2 - \bar{w})(r_{t2} - \bar{r}_t)] \\ &\quad + \delta\lambda_{wr}\overline{w'r'_t},\end{aligned}\tag{4.4.16}$$

and

$$\begin{aligned}\overline{r'_t\theta'_l} &= (1 - \delta)\alpha[(r_{t1} - \bar{r}_t)(\theta_{l1} - \bar{\theta}_l) + r_{r_t\theta_l}\sigma_{r_{t1}}\sigma_{\theta_{l1}}] \\ &\quad + (1 - \delta)(1 - \alpha)[(r_{t2} - \bar{r}_t)(\theta_{l2} - \bar{\theta}_l) + r_{r_t\theta_l}\sigma_{r_{t2}}\sigma_{\theta_{l2}}] \\ &\quad + \delta\lambda_{r\theta}\overline{r'_t\theta'_l}.\end{aligned}\tag{4.4.17}$$

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

$$\begin{aligned}\hat{c}_{w\theta_l} &\equiv \frac{1}{(1 - \tilde{\sigma}_w^2)^{1/2}} \frac{\overline{w'\theta'_l}}{\sqrt{w'^2}\sqrt{\theta_l'^2}} \frac{1}{\sqrt{\frac{1-\delta\lambda_w}{1-\delta}}} \frac{1}{\sqrt{\frac{1-\delta\lambda_\theta}{1-\delta}}} \frac{1 - \delta\lambda_{w\theta}}{1 - \delta} \\ &= \alpha\hat{w}_1\tilde{\theta}_{l1} + (1 - \alpha)\hat{w}_2\tilde{\theta}_{l2},\end{aligned}\tag{4.4.18}$$

$$\begin{aligned}\hat{c}_{wr_t} &\equiv \frac{1}{(1 - \tilde{\sigma}_w^2)^{1/2}} \frac{\overline{w'r'_t}}{\sqrt{w'^2}\sqrt{r_t'^2}} \frac{1}{\sqrt{\frac{1-\delta\lambda_w}{1-\delta}}} \frac{1}{\sqrt{\frac{1-\delta\lambda_r}{1-\delta}}} \frac{1 - \delta\lambda_{wr}}{1 - \delta} \\ &= \alpha\hat{w}_1\tilde{r}_{t1} + (1 - \alpha)\hat{w}_2\tilde{r}_{t2},\end{aligned}\tag{4.4.19}$$

and

$$\begin{aligned}\hat{c}_{r_t\theta_l} &\equiv \frac{\overline{r'_t\theta'_l}}{\sqrt{r_t'^2}\sqrt{\theta_l'^2}} \frac{1}{\sqrt{\frac{1-\delta\lambda_r}{1-\delta}}} \frac{1}{\sqrt{\frac{1-\delta\lambda_\theta}{1-\delta}}} \frac{1 - \delta\lambda_{r\theta}}{1 - \delta} \\ &= \alpha\left(\tilde{r}_{t1}\tilde{\theta}_{l1} + r_{r_t\theta_l}\tilde{\sigma}_{r_{t1}}\tilde{\sigma}_{\theta_{l1}}\right) + (1 - \alpha)\left(\tilde{r}_{t2}\tilde{\theta}_{l2} + r_{r_t\theta_l}\tilde{\sigma}_{r_{t2}}\tilde{\sigma}_{\theta_{l2}}\right),\end{aligned}\tag{4.4.20}$$

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

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

$$\begin{aligned}\overline{w'r'_t\theta'_l} &= (1 - \delta)\alpha(w_1 - \overline{w})[(r_{t1} - \overline{r}_t)(\theta_{l1} - \overline{\theta}_l) + r_{r_t\theta_l}\sigma_{r_{t1}}\sigma_{\theta_{l1}}] \\ &\quad + (1 - \delta)(1 - \alpha)(w_2 - \overline{w})[(r_{t2} - \overline{r}_t)(\theta_{l2} - \overline{\theta}_l) + r_{r_t\theta_l}\sigma_{r_{t2}}\sigma_{\theta_{l2}}]\end{aligned}\quad (4.4.21)$$

## 4.5 Finding pdf parameters in terms of moments

We now select a particular member of the normal mixture family by mapping the prognosed moments to the pdf parameters. In other words, we invert equation (4.4.2) - equation (4.4.20) in order to find the set of pdf parameters that guarantees that the resulting pdf has moments that correspond to the prognosed ones. The inversion is non-trivial because the equations are non-linear in the pdf parameters. However, the pdf (equation (4.1.1)) is simple enough to permit an analytic solution.

The solution procedure is as follows.

1. Solve for the pdf parameters  $\alpha$ ,  $\widehat{w}_1$ , and  $\widehat{w}_2$  from the moment equations for  $\overline{w}$  (equation (4.4.2)),  $\overline{w'^2}$  (equation (4.4.4)),  $\overline{w'^3}$  (equation (4.4.6)):

$$\alpha = \frac{1}{2} \left[ 1 - \widehat{S}k_w \sqrt{\frac{1}{4 + \widehat{S}k_w^2}} \right], \quad (4.5.1)$$

$$\widehat{w}_1 = \sqrt{\frac{1 - \alpha}{\alpha}}, \quad (4.5.2)$$

$$\widehat{w}_2 = -\sqrt{\frac{\alpha}{1 - \alpha}}. \quad (4.5.3)$$

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

2. Equation (4.5.1) implies that  $\widehat{Sk}_w$  is determined solely by  $\alpha$ :

$$\widehat{Sk}_w = \frac{1 - 2\alpha}{\sqrt{\alpha(1 - \alpha)}}. \quad (4.5.4)$$

3. We can obtain  $\tilde{\theta}_{l1}$  and  $\tilde{\theta}_{l2}$  from equation (4.4.7) for  $\overline{\theta}_l$ , and equation (4.4.18) for  $\overline{w'\theta'_l}$ :

$$\tilde{\theta}_{l1} = -\frac{\widehat{c}_{w\theta_l}}{\widehat{w}_2}, \quad (4.5.5)$$

$$\tilde{\theta}_{l2} = -\frac{\widehat{c}_{w\theta_l}}{\widehat{w}_1}. \quad (4.5.6)$$

4. The widths of the Normals,  $\tilde{\sigma}_{\theta_{l1}}$  and  $\tilde{\sigma}_{\theta_{l2}}$ , are determined by satisfying equation (4.4.8) for  $\overline{\theta'_l{}^2}$ , and equation (4.4.9) for  $\overline{\theta'_l{}^3}$ :

$$\tilde{\sigma}_{\theta_{l1}}^2 = (1 - \widehat{c}_{w\theta_l}^2) + \left( \sqrt{\frac{1 - \alpha}{\alpha}} \right) \frac{1}{3\widehat{c}_{w\theta_l}} \left( \widehat{Sk}_{\theta_l} - \widehat{c}_{w\theta_l}^3 \widehat{Sk}_w \right), \quad (4.5.7)$$

$$\tilde{\sigma}_{\theta_{l2}}^2 = (1 - \widehat{c}_{w\theta_l}^2) - \left( \sqrt{\frac{\alpha}{1 - \alpha}} \right) \frac{1}{3\widehat{c}_{w\theta_l}} \left( \widehat{Sk}_{\theta_l} - \widehat{c}_{w\theta_l}^3 \widehat{Sk}_w \right). \quad (4.5.8)$$

Here  $Sk_{\theta_l}$  is the skewness of  $\theta_l$ . It must be provided either by a prognostic equation or by a diagnostic equation such as equation (4.4.10) below.

5. Equations for  $\tilde{r}_{t1}$ ,  $\tilde{r}_{t2}$ ,  $\tilde{\sigma}_{r_{t1}}^2$ , and  $\tilde{\sigma}_{r_{t2}}^2$  are found by expressions identical to equation (4.5.5), equation (4.5.6), equation (4.5.7), and equation (4.5.8), except that  $\theta_l$  is replaced everywhere by  $r_t$ .

6. Finally, from equation (4.4.17) for  $\overline{r'_t\theta'_l}$  we find

$$r_{r_t\theta_l} = \frac{\widehat{c}_{r_t\theta_l} - \widehat{c}_{wr_t}\widehat{c}_{w\theta_l}}{\alpha\tilde{\sigma}_{r_{t1}}\tilde{\sigma}_{\theta_{l1}} + (1 - \alpha)\tilde{\sigma}_{r_{t2}}\tilde{\sigma}_{\theta_{l2}}}. \quad (4.5.9)$$

Here  $r_{r_t\theta_l}$  is the in-between normal correlation and  $c_{r_t\theta_l}$  is the total correlation.

## 4.6 Higher-order moments in terms of pdf parameters

Once the pdf parameters have been specified, all higher-order moments can be calculated by integration over the pdf. The needed formulas are:

$$\begin{aligned} \frac{1}{(1 - \tilde{\sigma}_w^2)^2} \frac{(1 - \delta)}{(1 - \delta\lambda_w)^2} \frac{\overline{w'^4}}{(\overline{w'^2})^2} &= \alpha \left[ \hat{w}_1^4 + 6\hat{w}_1^2 \frac{\tilde{\sigma}_w^2}{(1 - \tilde{\sigma}_w^2)} + 3 \frac{\tilde{\sigma}_w^4}{(1 - \tilde{\sigma}_w^2)^2} \right] \\ &+ (1 - \alpha) \left[ \hat{w}_2^4 + 6\hat{w}_2^2 \frac{\tilde{\sigma}_w^2}{(1 - \tilde{\sigma}_w^2)} + 3 \frac{\tilde{\sigma}_w^4}{(1 - \tilde{\sigma}_w^2)^2} \right] \\ &+ \frac{1}{(1 - \tilde{\sigma}_w^2)^2} \frac{(1 - \delta)}{(1 - \delta\lambda_w)^2} \delta 3\lambda_w^2, \end{aligned} \quad (4.6.1)$$

$$\begin{aligned} \frac{1}{(1 - \tilde{\sigma}_w^2)} \frac{(1 - \delta)^{1/2}}{(1 - \delta\lambda_w)(1 - \delta\lambda_\theta)^{1/2}} \frac{\overline{w'^2\theta'_l}}{w'^2 (\overline{\theta'^2})^{1/2}} &= \alpha \left[ \hat{w}_1^2 + \frac{\tilde{\sigma}_w^2}{(1 - \tilde{\sigma}_w^2)} \right] \tilde{\theta}_{l1} \\ &+ (1 - \alpha) \left[ \hat{w}_2^2 + \frac{\tilde{\sigma}_w^2}{(1 - \tilde{\sigma}_w^2)} \right] \tilde{\theta}_{l2}, \end{aligned} \quad (4.6.2)$$

$$\frac{1}{(1 - \tilde{\sigma}_w^2)^{1/2}} \frac{(1 - \delta)^{1/2}}{(1 - \delta\lambda_w)^{1/2}(1 - \delta\lambda_\theta)} \frac{\overline{w'\theta'_l{}^2}}{(\overline{w'^2})^{1/2} \overline{\theta'^2}} = \alpha \hat{w}_1 \left( \tilde{\theta}_{l1}^2 + \tilde{\sigma}_{\theta_{l1}}^2 \right) + (1 - \alpha) \hat{w}_2 \left( \tilde{\theta}_{l2}^2 + \tilde{\sigma}_{\theta_{l2}}^2 \right), \quad (4.6.3)$$

$$\begin{aligned} \frac{1}{(1 - \tilde{\sigma}_w^2)^{1/2}} \frac{(1 - \delta)^{1/2}}{(1 - \delta\lambda_w)^{1/2}(1 - \delta\lambda_\theta)^{1/2}(1 - \delta\lambda_{qt})^{1/2}} \frac{\overline{w'r'_t\theta'_l}}{(\overline{w'^2})^{1/2} (\overline{r'^2})^{1/2} (\overline{\theta'^2})^{1/2}} \\ = \alpha \hat{w}_1 \left( \tilde{r}_{t1} \tilde{\theta}_{l1} + r_{r_t\theta_l} \tilde{\sigma}_{r_{t1}} \tilde{\sigma}_{\theta_{l1}} \right) + (1 - \alpha) \hat{w}_2 \left( \tilde{r}_{t2} \tilde{\theta}_{l2} + r_{r_t\theta_l} \tilde{\sigma}_{r_{t2}} \tilde{\sigma}_{\theta_{l2}} \right) \end{aligned} \quad (4.6.4)$$

The equations for  $\overline{w'^2 r'_t}$  and  $\overline{w' r'^2}$  are analogous to equation (4.6.3) and equation (4.6.4).

## 4.7 A diagnostic ansatz for the skewness of heat and moisture

We cannot close the system of equations until we specify the skewness of  $\theta_l$ ,  $Sk_{\theta_l}$ , that appears in equation (4.5.7) for  $\tilde{\sigma}_{\theta_l 1}$ , and equation (4.5.8) for  $\tilde{\sigma}_{\theta_l 2}$ . Likewise, we need to specify  $Sk_{r_t}$ . We could prognose these scalar skewnesses, but this would involve additional computational expense, storage, and complexity. In some cases, the extra complexity may be worthwhile. However, here we instead propose the following diagnostic formula

$$\widehat{Sk}_{\theta_l} = \widehat{Sk}_w \widehat{c}_{w\theta_l} [\beta + (1 - \beta) \widehat{c}_{w\theta_l}^2], \quad (4.7.1)$$

and a similar formula for  $\widehat{Sk}_{r_t}$ . The parameter  $\beta$  is dimensionless. We also solve for  $\beta$  because we are going to need the equation later on to show that other equations are true.

$$\implies \beta = \frac{\frac{\widehat{Sk}_{\theta_l}}{\widehat{Sk}_w \widehat{c}_{w\theta_l}} - \widehat{c}_{w\theta_l}^2}{1 - \widehat{c}_{w\theta_l}^2} \quad (4.7.2)$$

Equation (4.7.1) is physically plausible but limited at the same time. The formula states that  $Sk_{\theta_l}$  is proportional to  $Sk_w$ , the skewness of  $w$ . An increase in  $\beta$  leads to an increase in  $|Sk_{\theta_l}|$ , which, in turn, leads to a pdf with a longer  $\theta_l$ -tail.  $Sk_{\theta_l}$  and  $Sk_w$  have the same sign when  $w$  and  $\theta_l$  are positively correlated;  $Sk_{\theta_l}$  and  $Sk_w$  have opposite sign when  $w$  and  $\theta_l$  are negatively correlated. In those large eddy simulations, this is usually but not always true.  $Sk_{\theta_l}$  vanishes when either  $Sk_w$  or  $c_{w\theta_l}$  vanishes; clearly this need not be true in nature.  $|Sk_{\theta_l}|$  can be either smaller or larger than  $|Sk_w|$ , depending on the values of  $\tilde{\sigma}_w^2$ ,  $c_{w\theta_l}$ , and  $\beta$ .

If we assume our ansatz (equation (4.4.10)) for  $\widehat{Sk}_{\theta_l}$ , then the  $\theta_l$ -widths of the first (equation (4.5.7)) and secondnormal(equation (4.5.7)) reduce to

$$\tilde{\sigma}_{\theta_l 1}^2 = \frac{(1 - \widehat{c}_{w\theta_l}^2)}{\alpha} \left[ \frac{1}{3} \beta + \alpha \left( 1 - \frac{2}{3} \beta \right) \right], \quad (4.7.3)$$

and

$$\tilde{\sigma}_{\theta_l 2}^2 = \frac{(1 - \hat{c}_{w\theta_l}^2)}{1 - \alpha} \left\{ 1 - \left[ \frac{1}{3}\beta + \alpha \left( 1 - \frac{2}{3}\beta \right) \right] \right\}. \quad (4.7.4)$$

Substituting equation (4.7.3), equation (4.7.4), and their  $r_t$  counterparts into the expression for  $r_{r_t\theta_l}$  equation (4.5.9) yields the simplified form:

$$r_{r_t\theta_l} = \frac{c_{r_t\theta_l} - \hat{c}_{wr_t}\hat{c}_{w\theta_l}}{(1 - \hat{c}_{wr_t}^2)^{1/2} (1 - \hat{c}_{w\theta_l}^2)^{1/2}}. \quad (4.7.5)$$

Here,  $r_{r_t\theta_l}$  is the correlation of  $r_t$  and  $\theta_l$  in-between the Normals and  $c_{r_t\theta_l}$  is the total correlation.

CLUBB chose a specific formula for the  $w$ -“width” of the individual Gaussians, which is the following:

$$\tilde{\sigma}_w^2 = \gamma [1 - \max(c_{w\theta_l}^2, c_{wr_t}^2)]. \quad (4.7.6)$$

This makes  $\tilde{\sigma}_w^2$  depend on  $c_{wr_t}^2$  and  $c_{w\theta_l}^2$ . Here  $0 \leq \gamma < 1$  is a dimensionless constant. This formula helps ensure that when  $c_{wr_t}$  or  $c_{w\theta_l}$  becomes large in magnitude,  $0 \leq \hat{c}_{w\theta_l}^2, \hat{c}_{wr_t}^2 < 1$  and hence  $\tilde{\sigma}_{r_t 1,2}^2$ ,  $\tilde{\sigma}_{\theta_l 1,2}^2$ , and  $r_{r_t\theta_l}$  remain realistic.

## 4.8 Proposed closures for third- and fourth-order moments based on the mixture of trivariate normals

This section lists formulas for the higher-order moments that are needed for closure in the parameterization of:  $\overline{w'^4}$ ,  $\overline{w'^2\theta'_l}$ ,  $\overline{w'\theta'_l{}^2}$ , and  $\overline{w'r'_t\theta'_l}$ . These are obtained by substituting the expressions for the pdf parameters (equation (4.5.1) - equation (4.5.9)) into the equations for the higher-order moments (equation (4.6.1) - equation (4.6.4)). Formulas for  $\overline{w'^2r'_t}$  and

$\overline{w'r_t'^2}$ , which are also needed, are identical to those for  $\overline{w'^2\theta_l'}$  and  $\overline{w'\theta_l'^2}$  except that  $r_t$  replaces  $\theta_l$  everywhere.

First, we list the equation for  $\theta_l'^3$ , which is obtained by dimensionalizing equation (4.7.1):

$$\overline{\theta_l'^3} = \frac{(1 - \delta\lambda_{w\theta})(1 - \delta\lambda_\theta)}{(1 - \tilde{\sigma}_w^2)^2 (1 - \delta\lambda_w)^2} \frac{\overline{w'^3}}{(\overline{w'^2})^2} \overline{\theta_l'^2} \overline{w'\theta_l'} \left( \beta + (1 - \beta) \frac{(1 - \delta\lambda_{w\theta})^2}{1 - \tilde{\sigma}_w^2 (1 - \delta\lambda_w)(1 - \delta\lambda_\theta)} \frac{(\overline{w'\theta_l'})^2}{\overline{w'^2} \overline{\theta_l'^2}} \right). \quad (4.8.1)$$

While the scalar third moments are not essential for solving the prognostic equations directly, they still play a role in shaping cloud properties. This is because cumulus clouds tend to form at the edges, or “tails”, of the pdf for a specific variable. Typically, as the relative “width” of the normal distribution in  $w$  (represented by  $\tilde{\sigma}_w^2 = \sigma_w^2/\overline{w'^2}$ ) increases, the value of  $\overline{\theta_l'^3}$  also grows (see equation (4.8.1)) for details). In simpler terms, a larger  $\overline{\theta_l'^3}$  corresponds to a broader  $w$ -marginal pdf, which deviates further from a double delta function (a function with two spikes at zero).

$\overline{w'^4}$  does not depend on the thermodynamic scalar moments; therefore, it does not depend on  $\beta$ . Substituting equation (4.5.2) and equation (4.5.2) into equation (4.6.1) and using equation (4.4.6), we find

$$\begin{aligned} \frac{1}{(1 - \tilde{\sigma}_w^2)^2} \frac{(1 - \delta)}{(1 - \delta\lambda_w)^2} \frac{\overline{w'^4}}{(\overline{w'^2})^2} &= 3 \frac{\tilde{\sigma}_w^4}{(1 - \tilde{\sigma}_w^2)^2} + 6 \frac{\tilde{\sigma}_w^2}{(1 - \tilde{\sigma}_w^2)} + 1 \\ &+ \widehat{Sk}_w^2 + \frac{1}{(1 - \tilde{\sigma}_w^2)^2} \frac{(1 - \delta)}{(1 - \delta\lambda_w)^2} \delta 3\lambda_w^2, \end{aligned} \quad (4.8.2)$$

and also

$$\begin{aligned} \overline{w'^4} &= (\overline{w'^2})^2 \frac{(1 - \delta\lambda_w)^2}{(1 - \delta)} \left( 3\tilde{\sigma}_w^4 + 6(1 - \tilde{\sigma}_w^2) \tilde{\sigma}_w^2 + (1 - \tilde{\sigma}_w^2)^2 \right) \\ &+ \frac{1}{(1 - \tilde{\sigma}_w^2)} \frac{1}{(1 - \delta\lambda_w)} \frac{(\overline{w'^3})^2}{\overline{w'^2}} \\ &+ \delta 3\lambda_w^2 (\overline{w'^2})^2. \end{aligned} \quad (4.8.3)$$

Similar to  $\overline{w'^4}$ ,  $\overline{w'^2\theta'_l}$  does not depend on  $\beta$  for our particular pdf family. Substituting equation (4.5.2) - equation (4.5.6) into equation (4.6.2), we find

$$\frac{1}{(1 - \tilde{\sigma}_w^2)} \frac{(1 - \delta)^{1/2}}{(1 - \delta\lambda_w)(1 - \delta\lambda_\theta)^{1/2}} \frac{\overline{w'^2\theta'_l}}{w'^2 \left(\overline{\theta'^2_l}\right)^{1/2}} = \widehat{c}_{w\theta_l} \widehat{Sk}_w, \quad (4.8.4)$$

and

$$\overline{w'^2\theta'_l} = \frac{1}{(1 - \tilde{\sigma}_w^2)} \frac{1 - \delta\lambda_{w\theta}}{1 - \delta\lambda_w} \frac{\overline{w'^3}}{w'^2} \overline{w'\theta'_l}. \quad (4.8.5)$$

$\overline{w'\theta'^2_l}$  depends explicitly on  $Sk_{\theta_l}$ . Substituting equation (4.5.2) - equation (4.5.8) into equation (4.6.4) yields

$$\frac{1}{(1 - \tilde{\sigma}_w^2)^{1/2}} \frac{(1 - \delta)^{1/2}}{(1 - \delta\lambda_w)^{1/2}(1 - \delta\lambda_\theta)} \frac{\overline{w'\theta'^2_l}}{\left(\overline{w'^2}\right)^{1/2} \overline{\theta'^2_l}} = \frac{2}{3} \widehat{c}_{w\theta_l}^2 \widehat{Sk}_w + \frac{1}{3} \frac{\widehat{Sk}_{\theta_l}}{\widehat{c}_{w\theta_l}}, \quad (4.8.6)$$

and

$$\begin{aligned} \overline{w'\theta'^2_l} &= \frac{2}{3} \frac{(1 - \delta\lambda_{w\theta})^2}{(1 - \delta\lambda_w)^2} \frac{1}{(1 - \tilde{\sigma}_w^2)^2} \frac{\overline{w'^3}}{\left(\overline{w'^2}\right)^2} \left(\overline{w'\theta'_l}\right)^2 \\ &\quad + \frac{1}{3} \frac{(1 - \delta\lambda_w)}{(1 - \delta\lambda_{w\theta})} (1 - \tilde{\sigma}_w^2) \frac{\overline{w'^2} \overline{\theta'^3_l}}{\overline{w'\theta'_l}}. \end{aligned} \quad (4.8.7)$$

The formula has a problem because  $\overline{w'\theta'_l}$  is in the denominator. As  $\overline{w'\theta'_l}$  gets closer to zero, the formula becomes infinitely large, which is called a singularity. This can cause issues if we use the formula directly with real-world measurements of  $\overline{\theta'^3_l}$  and  $\overline{w'\theta'_l}$ . The resulting diagnosis of  $\overline{w'\theta'^2_l}$  would be very sensitive to small changes in the measurements and might not be reliable (noisy). We can fix this singularity by either

- substitute in the ansatz for  $Sk_{\theta_l}$  (equation (4.4.10)) into the original formula (equation (4.6.3)),
- or, equivalently, substitute equation (4.8.1) for  $\overline{\theta'^3_l}$ . This is possible because equation (4.8.1) shows that  $\overline{\theta'^3_l}$  is proportional to  $\overline{w'\theta'_l}$ .



Both approaches effectively remove the singularity from the formula. Therefore, we find:

$$\frac{1}{(1 - \tilde{\sigma}_w^2)^{1/2}} \frac{(1 - \delta)^{1/2}}{(1 - \delta\lambda_w)^{1/2}(1 - \delta\lambda_\theta)} \frac{\overline{w'\theta_l'^2}}{\left(\overline{w'^2}\right)^{1/2} \overline{\theta_l'^2}} = \widehat{S}k_w \left[ \frac{1}{3}\beta + \left(1 - \frac{1}{3}\beta\right) \widehat{c}_{w\theta_l}^2 \right], \quad (4.8.8)$$

and

$$\overline{w'\theta_l'^2} = \frac{1}{(1 - \tilde{\sigma}_w^2)} \frac{(1 - \delta\lambda_\theta)}{(1 - \delta\lambda_w)} \frac{\overline{w'^3}}{\overline{w'^2}} \left[ \frac{1}{3}\beta \overline{\theta_l'^2} + \frac{(1 - \frac{1}{3}\beta)}{(1 - \tilde{\sigma}_w^2)} \frac{(1 - \delta\lambda_{w\theta})^2}{(1 - \delta\lambda_w)(1 - \delta\lambda_\theta)} \frac{(\overline{w'\theta_l'})^2}{\overline{w'^2}} \right]. \quad (4.8.9)$$

Finally, substituting equation (4.5.2) - equation (4.5.9) into equation (4.6.4) yields the following formula for the turbulent flux of  $\overline{r_t'\theta_l'}$ ,  $\overline{w'r_t'\theta_l'}$ :

$$\begin{aligned} & \frac{(1 - \delta)^{1/2}}{(1 - \delta\lambda_w)^{1/2}(1 - \delta\lambda_\theta)^{1/2}(1 - \delta\lambda_{r_t})^{1/2}} \frac{\overline{w'r_t'\theta_l'}}{(1 - \tilde{\sigma}_w^2)^{1/2} \left(\overline{w'^2}\right)^{1/2} \left(\overline{r_t'^2}\right)^{1/2} \left(\overline{\theta_l'^2}\right)^{1/2}} \\ &= \widehat{c}_{wr_t} \widehat{c}_{w\theta_l} \widehat{S}k_w + E(w, q_t, \theta_l) \frac{1}{2} \widehat{S}k_w (c_{q_t\theta_l} - \widehat{c}_{wr_t} \widehat{c}_{w\theta_l}), \end{aligned} \quad (4.8.10)$$

and

$$\begin{aligned} \overline{w'r_t'\theta_l'} &= \frac{\frac{1}{2}E}{(1 - \tilde{\sigma}_w^2)} \frac{(1 - \delta\lambda_{\theta q})}{(1 - \delta\lambda_w)} \frac{\overline{w'^3}}{\overline{w'^2}} \overline{r_t'\theta_l'} \\ &+ \frac{1 - \frac{1}{2}E}{(1 - \tilde{\sigma}_w^2)^2} \frac{(1 - \delta\lambda_{wq})(1 - \delta\lambda_{w\theta})}{(1 - \delta\lambda_w)^2} \overline{w'r_t'} \overline{w'\theta_l'} \frac{\overline{w'^3}}{\left(\overline{w'^2}\right)^2}. \end{aligned} \quad (4.8.11)$$

The function  $E(w, r_t, \theta_l)$  is

$$E = \frac{1 - \frac{1}{2} \frac{2\alpha}{1-2\alpha} \xi}{1 + \frac{1}{2} \xi}, \quad (4.8.12)$$

where

$$1 + \xi = \frac{1 - \alpha}{\alpha} \frac{\tilde{\sigma}_{r_{t2}}}{\tilde{\sigma}_{r_{t1}}} \frac{\tilde{\sigma}_{\theta_{l2}}}{\tilde{\sigma}_{\theta_{l1}}} = \left( \frac{A_{r_t} - B_{r_t}}{-A_{r_t} - B_{r_t}} \right)^{1/2} \left( \frac{A_{\theta_l} - B_{\theta_l}}{-A_{\theta_l} - B_{\theta_l}} \right)^{1/2}, \quad (4.8.13)$$

and

$$A_{\theta_l} = S k_{\theta_l} - \frac{3}{2} \widehat{c}_{w\theta_l} \widehat{S}k_w + \frac{1}{2} \widehat{c}_{w\theta_l}^3 \widehat{S}k_w, \quad (4.8.14)$$

$$B_{\theta_l} = \frac{3}{2} \left( 4 + \widehat{Sk}_w^2 \right)^{1/2} \widehat{c}_{w\theta_l} (1 - \widehat{c}_{w\theta_l}^2), \quad (4.8.15)$$

and  $A_{r_t}$  and  $B_{r_t}$  are analogous. We now list two cases in which the expression for  $E$  simplifies.

First, if

$$\frac{\tilde{\sigma}_{r_{t2}}}{\tilde{\sigma}_{r_{t1}}} \frac{\tilde{\sigma}_{\theta_{l2}}}{\tilde{\sigma}_{\theta_{l1}}} = 1$$

then  $E = 0$ . This would occur, for instance, if the “widths” of the first and second normal were equal to each other for both  $r_t$  and  $\theta_l$ , that is, if  $\tilde{\sigma}_{r_{t2}} = \tilde{\sigma}_{r_{t1}}$  and  $\tilde{\sigma}_{\theta_{l2}} = \tilde{\sigma}_{\theta_{l1}}$ . Second, if we use the diagnostic ansatz (equation (4.4.10)) for the scalar skewnesses, then

$$\xi = \frac{1 - 2\zeta}{\zeta}, \quad (4.8.16)$$

where

$$\zeta = \alpha + \frac{1}{3}\beta(1 - 2\alpha). \quad (4.8.17)$$

Then we find

$$E = \frac{2}{3}\beta, \quad (4.8.18)$$

and finally

$$\begin{aligned} \overline{w'r'_t\theta'_l} &= \frac{\frac{1}{3}\beta}{(1 - \tilde{\sigma}_w^2)} \frac{(1 - \delta\lambda_{\theta r})}{(1 - \delta\lambda_w)} \overline{r'_t\theta'_l} \frac{\overline{w'^3}}{\overline{w'^2}} \\ &+ \frac{1 - \frac{1}{3}\beta}{(1 - \tilde{\sigma}_w^2)^2} \frac{(1 - \delta\lambda_{wr})(1 - \delta\lambda_{w\theta})}{(1 - \delta\lambda_w)^2} \overline{w'r'_t} \overline{w'\theta'_l} \frac{\overline{w'^3}}{(\overline{w'^2})^2}. \end{aligned} \quad (4.8.19)$$

## 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,<sup>1</sup> a powerful Python library for symbolic mathematics. This chapter delves into the world of SymPy,<sup>2</sup> 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<sup>3</sup> 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<sup>4</sup> can be used, not only for this thesis.

### 5.1 Analytic integration

For simplicity and readability, we choose the check for the formula of  $\overline{w'^2}$ . One starts by importing and – obviously – installing the packages if they are not there yet. Importing the

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<sup>1</sup>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>.

<sup>2</sup>Ibid.

<sup>3</sup>Ibid.

<sup>4</sup>Ibid.

package `display` is useful for later on printing the equations. Thus, there is the following code: In this listing, `sympy` was defined to be called `sp` and from `sympy` we directly imported

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
```

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 following (self-defined) symbols: Having defined the symbols, we can proceed with defining the marginal

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_lambda_w = Symbol('\sigma_{\lambda w}')
w_prime_2_bar = Symbol('\overline{w^2}')
```

distribution. Now, we are also using `sympy.abc` for displaying some standard symbols. Having done that, we can actually display the integral, which we want to compute. Looking

Listing 5.3: Defining the marginals

```
G_1_w = Normal(name='G_1_w', mean=w_1, std=sigma_w)
G_1_w_density = density(G_1_w)(sp.abc.w)
G_2_w = Normal(name='G_2_w', mean=w_2, std=sigma_w)
G_2_w_density = density(G_2_w)(sp.abc.w)
G_3_w = Normal(name='G_3_w', mean=w_bar, std=sigma_lambda_w)
G_3_w_density = density(G_3_w)(sp.abc.w)
G_w = ((1 - sp.abc.delta) * sp.abc.alpha * G_1_w_density +
        (1 - sp.abc.delta) * (1 - sp.abc.alpha) * G_2_w_density +
        sp.abc.delta * G_3_w_density)
```

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))
```

Figure 5.1: Output of listing 5.4

$$\overline{w'^2} = \int_{-\infty}^{\infty} (-\overline{w} + w)^2 \left( \frac{\sqrt{2}\delta e^{-\frac{(-\overline{w}+w)^2}{2\sigma_{\lambda w}^2}}}{2\sqrt{\pi}\sigma_{\lambda w}} + \frac{\sqrt{2}\alpha(1-\delta)e^{-\frac{(w-w_1)^2}{2\sigma_w^2}}}{2\sqrt{\pi}\sigma_w} + \frac{\sqrt{2} \cdot (1-\alpha)(1-\delta)e^{-\frac{(w-w_2)^2}{2\sigma_w^2}}}{2\sqrt{\pi}\sigma_w} \right) dw$$

at figure 5.1, this is exactly the integral, which we want to compute. Using the command `.doit(conds='none')`, we can actually 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

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

$$\begin{aligned} \overline{w'^2} = & -\overline{w}^2\delta + \overline{w}^2 + 2\overline{w}\alpha\delta w_1 - 2\overline{w}\alpha\delta w_2 - 2\overline{w}\alpha w_1 + 2\overline{w}\alpha w_2 + 2\overline{w}\delta w_2 - 2\overline{w}w_2 \\ & -\sigma_w^2\delta + \sigma_w^2 + \sigma_{\lambda w}^2\delta - \alpha\delta w_1^2 + \alpha\delta w_2^2 + \alpha w_1^2 - \alpha w_2^2 - \delta w_2^2 + w_2^2, \end{aligned}$$

compare figure 5.2 to the given equation. To do this, we first need to define the equation for equation (4.4.3). We can print this equation, using `display` again. The last step is to check if those two formulas are equivalent to each other. We can do this by just using `Eq(...)` from the package `SymPy`. `factor(...)` just tries to factor the given variables to make

Listing 5.6: Python function for the second order moment

```
def w_prime_2_bar_check(delta=sp.abc.delta, alpha=sp.abc.alpha, w_1=w_1, w_2=w_2,
w_bar=w_bar, sigma_w=sigma_w, sigma_lambda_w=sigma_lambda_w):
    return (((1 - delta) * alpha * ((w_1 - w_bar) ** 2 + sigma_w ** 2))
            + ((1 - delta) * (1 - alpha) * ((w_2 - w_bar) ** 2 + sigma_w ** 2))
            + (delta * sigma_lambda_w ** 2))
```

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

$$\overline{w'^2} = \sigma_{\lambda w}^2 \delta + \alpha (1 - \delta) (\sigma_w^2 + (-\overline{w} + w_1)^2) + (1 - \alpha) (1 - \delta) (\sigma_w^2 + (-\overline{w} + w_2)^2)$$

the comparison easier. This code just displays **True**, which is exactly what we wanted to

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

```
display(sp.factor(sp.Eq(w_prime_2_bar_int_val, w_prime_2_bar_check()),
sp.abc.alpha, sp.abc.delta))
```

have.

## 5.2 Numeric integration

Again, for better readability, we choose to check the formula for  $\overline{w'^2 \theta'_l}$ . As above, there needs to be some packages imported. We are importing the same packages as in listing 5.1 together with some more. Since we are going to need some more symbols, we also need to define those. We still use the symbols as in listing 5.2, together with the following:

We start defining the integral by defining the marginals.

Listing 5.9: Import statements

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

Listing 5.10: Defining symbols

```
sigma_lambda_theta_1 = Symbol('\sigma_{\lambda\theta_1}')
theta_1_1 = Symbol('\theta_{11}')
theta_1_2 = Symbol('\theta_{12}')
theta_1_bar = Symbol('\overline{\theta_1}')
sigma_theta_1_1 = Symbol('\sigma_{\theta_{11}}')
sigma_theta_1_2 = Symbol('\sigma_{\theta_{12}}')
rho_w_theta_1 = Symbol('\rho_{w\theta_1}')
w_prime_3_bar = Symbol('\overline{w^3}')
w_prime_theta_1_prime_bar = Symbol('\overline{w'\theta_1}')
w_prime_2_theta_prime_1_bar = Symbol('\overline{w'^2\theta_1}')
sigma_tilde_w = Symbol('\Tilde{\sigma}_w')
lambda_w_theta = Symbol('\lambda_{w\theta}')
lambda_w = Symbol('\lambda_w')
```

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_1_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_1_bar]),
    std=sp.Matrix([[sigma_lambda_w ** 2,
        rho_w_theta_1 * sigma_lambda_w * sigma_lambda_theta_1,
        rho_w_theta_1 * sigma_lambda_w * sigma_lambda_theta_1,
        sigma_lambda_theta_1 ** 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, the output is omitted for better readability. We do not yet compute the integral, because due to the complexity, this is not working with SymPy unfortunately.

Listing 5.12: Defining and displaying the needed integral

```
w_prime_2_theta_l_prime_bar = sp.Integral((sp.abc.w - w_bar) ** 2 *
    (sp.abc.theta - theta_l_bar) * G_w_theta,
    [sp.abc.w, -oo, oo], [sp.abc.theta, -oo, oo])
display(sp.Eq(w_prime_2_theta_prime_l_bar, w_prime_2_theta_l_prime_bar))
```

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

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

equation (4.4.15), equation (4.4.5), equation (4.4.3), equation (4.2.3), and equation (4.1.2). We do not list the functions to those equations here, because they are defined the same way like the other equations are defined as functions.

Instead, since we cannot compute the integral analytically, we can create a **dataframe** using **pandas**.<sup>5</sup> The columns for this dataframe are going to be all the inputs we have. To get all permutations, this code is also using **product(...)** from the **itertools** package.

<sup>5</sup>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.



Listing 5.14: Create a dataframe and putting in arbitrary numbers

```
df = pd.DataFrame(product([0, 1], [-2, 2], [-1, 2], [0, 3], [Rational(1, 10)],
    [Rational(3, 10)], [Rational(4, 10)], [Rational(7, 10)], [Rational(6, 10)],
    [Rational(5, 10)], [Rational(1, 10)], [Rational(5, 10)], [Rational(5, 10)]),
    columns=[w_1, w_2, theta_l_1, theta_l_2, sigma_theta_l_1, sigma_theta_l_2,
    sigma_lambda_theta_l, sigma_w, sigma_lambda_w, sp.abc.alpha, sp.abc.delta,
    rho_w_theta_l])
```

We append another column which is called “checkval” and lists the values for the given equation to check.

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))
```

This code also uses the function defined in listing 5.13, where all other 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.

Here, we 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 and take the mean of this new column to see if the error is actually numerically 0.

Listing 5.16: Attaching the “numint” column to the dataframe

```
df['numint'] = (df.apply(lambda x: Rational(w_prime_2_theta_1_prime_bar.subs({
    w_1: x[w_1], w_2: x[w_2], theta_1_1: x[theta_1_1], theta_1_2: x[theta_1_2],
    sigma_theta_1_1: x[sigma_theta_1_1], sigma_theta_1_2: x[sigma_theta_1_2],
    sigma_lambda_theta_1: x[sigma_lambda_theta_1], 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_1: x[rho_w_theta_1]
})).doit(conds='none', method='quad').evalf()), axis=1))
```

Listing 5.17: Attaching the “diffnum” column to the dataframe

```
df['diffnum'] = abs(df['check_val'].astype(float) - df['ana_int'].astype(float))
```

Listing 5.18: Calculating the mean difference

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

Figure 5.5: Output of listing 5.18

The mean error between the rhs and the lhs is: 1.3753423344481015e-124

We see that the mean error is basically 0. 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  $\alpha$  and  $\delta$  are meant to be  $\alpha \in [0, 1]$  and  $\delta \in [0, 1)$ . The restriction to  $\delta$  vs the one to  $\alpha$  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 (4.4.6) have a  $1 - \delta$  in the denominator.
- In section 4.3, 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 That is, for instance, that the variance of  $w$  over the

$$\begin{aligned}
 & 0 < \delta\lambda_w < 1, & 0 < \delta\lambda_\theta < 1, & 0 < \delta\lambda_r < 1, \\
 \iff & 0 < \delta\frac{\sigma_{w3}}{w'^2} < 1, & 0 < \delta\frac{\sigma_{\theta_l3}}{\theta_l'^2} < 1, & 0 < \delta\frac{\sigma_{r_t3}}{r_t'^2} < 1, \\
 \iff & 0 < \delta\sigma_{w3} < \overline{w'^2}, & 0 < \delta\sigma_{\theta_l3} < \overline{\theta_l'^2}, & 0 < \delta\sigma_{r_t3} < \overline{r_t'^2}.
 \end{aligned}$$

whole pdf has to be strictly greater than  $\delta$  times the standard deviation in  $w$  of the third normal distribution.

For realizability, it turns out that we want  $-1 < \hat{c}_{w\theta_l}, \hat{c}_{wr_t}, \hat{c}_{r_t\theta_l} < 1$ . This is for instance:

$$\begin{aligned}
& -1 < \hat{c}_{w\theta_l} < 1 \iff (\hat{c}_{w\theta_l})^2 < 1 \\
& \iff \left( \frac{1}{(1 - \tilde{\sigma}_w^2)^{1/2}} \frac{\overline{w'r'_t}}{\sqrt{w'^2} \sqrt{r_t'^2}} \frac{1}{\sqrt{\frac{1-\delta\lambda_w}{1-\delta}}} \frac{1}{\sqrt{\frac{1-\delta\lambda_r}{1-\delta}}} \frac{1-\delta\lambda_{wr}}{1-\delta} \right)^2 < 1 \\
& \iff \frac{1}{(1 - \tilde{\sigma}_w^2)} \frac{(\overline{w'r'_t})^2}{\overline{w'^2 r_t'^2}} \frac{1-\delta}{1-\delta\lambda_w} \frac{1-\delta}{1-\delta\lambda_r} \frac{(1-\delta\lambda_{wr})^2}{(1-\delta)^2} < 1 \\
& \iff \frac{(1-\delta\lambda_{wr})^2 (\overline{w'r'_t})^2}{(1-\delta\lambda_w)(1-\delta\lambda_r) \overline{w'^2 r_t'^2}} < (1 - \tilde{\sigma}_w^2) \\
& \iff \frac{(1-\delta\lambda_{wr})^2 (\overline{w'r'_t})^2}{(1-\delta\lambda_w)(1-\delta\lambda_r) \overline{w'^2 r_t'^2}} < 1 - \left( \frac{\sigma_w^2(1-\delta)}{\overline{w'^2}(1-\delta\lambda_w)} \right) \\
& \iff \frac{(1-\delta\lambda_{wr})^2 (\overline{w'r'_t})^2}{(1-\delta\lambda_w)(1-\delta\lambda_r) \overline{w'^2 r_t'^2}} + \frac{\sigma_w^2(1-\delta)}{\overline{w'^2}(1-\delta\lambda_w)} < 1 \\
& \iff \frac{(1-\delta\lambda_{wr})^2 (\overline{w'r'_t})^2 + \sigma_w^2(1-\delta)(1-\delta\lambda_r) \overline{r_t'^2}}{(1-\delta\lambda_w)(1-\delta\lambda_r) \overline{w'^2 r_t'^2}} < 1
\end{aligned}$$

## 7 Outlook

We have seen that adding a third normal distribution right in the middle of the two defined (simplified) normal distributions does not change the “closed” formulas too much, neither it makes it too complicated. So for CLUBB there are new parameters, e.g.  $\delta$  or  $\lambda_w$ , 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

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# 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 houses the definitions of all functions used for checking integrals.
- `symbols.py`: This file contains definitions of all symbols employed for computations with SymPy, a powerful library for symbolic mathematics.

### 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 visualie 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

```

1  from sympy import Symbol, symbols
2
3  # sigma
4  sigma_w = Symbol('\sigma_w')
5
6  sigma_r_t_i, sigma_r_t_1, sigma_r_t_2 = (
7      symbols('\sigma_{r_{ti}} \sigma_{r_{t1}} \sigma_{r_{t2}}'))
8
9  sigma_theta_l_i, sigma_theta_l_1, sigma_theta_l_2 = (
10     symbols('\sigma_{\theta_{li}} \sigma_{\theta_{l1}} \sigma_{\theta_{l2}}'))
11
12  sigma_tilde_r_t_i, sigma_tilde_r_t_1, sigma_tilde_r_t_2 = (
13     symbols('\tilde{\sigma}_{r_{ti}} \tilde{\sigma}_{r_{t1}} \tilde{\sigma}_{r_{t2}}'))
14  )
15
16  sigma_tilde_theta_l_i, sigma_tilde_theta_l_1, sigma_tilde_theta_l_2 = (
17     symbols(
18         '\tilde{\sigma}_{\theta_{li}} \tilde{\sigma}_{\theta_{l1}}
19         \rightarrow \tilde{\sigma}_{\theta_{l2}}')
20  )
21
22  sigma_tilde_lambda_w = Symbol('\tilde{\sigma}_{\lambda_w}')
23  sigma_tilde_w = Symbol('\tilde{\sigma}_w')
24  sigma_lambda_w = Symbol('\sigma_{\lambda_w}')
25  sigma_lambda_theta_l = Symbol('\sigma_{\lambda\theta_l}')
26  sigma_lambda_r_t = Symbol('\sigma_{\{\lambda\}r_t}')
27
28  # w
29  w_bar = Symbol('\overline{w}')
30  w_prime = Symbol('w\prime')
31  w_i, w_1, w_2 = symbols('w_i w_1 w_2')
32
33  w_hat_i, w_hat_1, w_hat_2, w_hat_3, w_hat_prime = (
34     symbols('\hat{w}_i \hat{w}_1 \hat{w}_2 \hat{w}_3 \hat{w}\prime')
35  )
36
37  w_prime_2_bar, w_prime_3_bar, w_prime_4_bar = symbols(
38     '\overline{w\prime^2} \overline{w\prime^3} \overline{w\prime^4}')
39  )
40  w_prime_r_t_prime_bar = Symbol('\overline{w\prime_r\prime_t}')

```

```

41 w_prime_2_theta_prime_1_bar = Symbol('\overline{w}^{\prime 2} \theta \prime_1')
42 w_prime_theta_prime_1_2_bar = Symbol('\overline{w} \theta \prime^2_1')
43 w_prime_theta_1_prime_bar = Symbol('\overline{w} \theta \prime_1')
44
45 w_prime_r_t_prime_theta_1_prime_bar = Symbol('\overline{w} \{r_t\} \{ \theta_1 \} \prime')
46
47 # r
48 r_t = Symbol('r_t')
49
50 r_t_bar, r_t_prime_2_bar = symbols(
51     '\overline{r_t} \overline{r_t}^{\prime 2}'
52 )
53
54 r_t_i, r_t_1, r_t_2 = symbols('r_{ti} r_{t1} r_{t2}')
55
56 r_t_tilde_prime, r_t_i_tilde, r_t_1_tilde, r_t_2_tilde = symbols(
57     '\tilde{r_t} \tilde{r_{ti}} \tilde{r_{t1}} \tilde{r_{t2}}'
58 )
59
60 # theta
61 theta_1 = Symbol('\theta_1')
62
63 theta_1_bar, theta_1_prime_2_bar, theta_1_prime_3_bar = symbols(
64     '\overline{\theta_1} \overline{\theta_1}^{\prime 2} \overline{\theta_1}^{\prime 3}'
65 )
66
67 theta_1_prime_r_t_prime_bar = Symbol('\overline{\theta_1} r_t \prime')
68
69 theta_1_i, theta_1_1, theta_1_2 = symbols(
70     '\theta_{1i} \theta_{11} \theta_{12}'
71 )
72
73 theta_tilde_prime_1 = Symbol('\tilde{\theta}_1 \prime')
74
75 theta_tilde_1_i, theta_tilde_1_1, theta_tilde_1_2 = symbols(
76     '\tilde{\theta}_{1i} \tilde{\theta}_{11} \tilde{\theta}_{12}'
77 )
78
79 # lambda
80 lambda_theta = Symbol('\lambda \theta')
81 lambda_theta_r = Symbol('\lambda \theta_r')
82 lambda_r = Symbol('\lambda_r')
83 lambda_w = Symbol('\lambda_w')
84 lambda_w_theta = Symbol('\lambda_{w \theta}')
85 lambda_w_r = Symbol('\lambda_{wr}')
86
87 r_r_t_theta_1 = Symbol('r_{r_t \theta_1}')
88 triple_gaussian = Symbol('P_{tmg}(\hat{w}, \tilde{\theta}_1, \tilde{r}_{\prime t})')
89 sk_hat_w = Symbol('\widehat{Sk}_w')
90 sk_theta_1_hat = Symbol('\widehat{Sk}_{\theta_1}')
91 c_w_theta_1_hat = Symbol('\hat{c}_{w \theta_1}')
92 G_3 = Symbol('G_3')
93 G_3_hat = Symbol('\hat{G}_3')
94

```

```

95 G_w, G_1_w, G_2_w, G_3_w = symbols(
96     'G_{w}(w) G_{1w}(w) G_{2w}(w) G_{3w}(w)'
97 )
98
99 G_w_1_2 = Symbol('G_{w_{12}}')
100
101 G_w_theta = Symbol('G_{w\\theta}(w,\\theta)')
102 G_1_w_theta = Symbol('G_{1w\\theta}(w,\\theta)')
103 G_2_w_theta = Symbol('G_{2w\\theta}(w,\\theta)')
104 G_3_w_theta = Symbol('G_{3w\\theta}(w,\\theta)')
105
106 G_theta_r = Symbol('G_{\\theta r}(\\theta, r)')
107 G_1_theta_r = Symbol('G_{1\\theta r}(\\theta, r)')
108 G_2_theta_r = Symbol('G_{2\\theta r}(\\theta, r)')
109 G_3_theta_r = Symbol('G_{3\\theta r}(\\theta, r)')
110
111 G_w_theta_l_r_t = Symbol('G_{w\\theta_l}{r_t}(w,\\theta_l,{r_t})')
112 G_1_w_theta_l_r_t = Symbol('G_{1w\\theta_l}{r_t}(w,\\theta_l,{r_t})')
113 G_2_w_theta_l_r_t = Symbol('G_{2w\\theta_l}{r_t}(w,\\theta_l,{r_t})')
114 G_3_w_theta_l_r_t = Symbol('G_{3w\\theta_l}{r_t}(w,\\theta_l,{r_t})')
115
116 G_theta, G_1_theta, G_2_theta, G_3_theta = symbols(
117     'G_{\\theta}(\\theta) G_{1\\theta}(\\theta) G_{2\\theta}(\\theta)
118     ↦ G_{3\\theta}(\\theta)'
119 )
120
121 rho_w_theta_l = Symbol('\\rho_{w\\theta_l}')
122 rho_w_r_t = Symbol('\\rho_{wr_t}')
123 rho_theta_l_r_t = Symbol('\\rho_{\\theta_lr_t}')

```

Listing A.1: symbols.py

## A.3 checked\_functions.py

```

1  import sympy as sp
2  from sympy import Rational
3  from sympy.stats import Normal, density
4
5  import symbols as sym
6
7
8  # w equations
9  # -----
10
11 def w_bar(alpha=sp.abc.alpha, delta=sp.abc.delta, w_1=sym.w_1, w_2=sym.w_2):
12     return ((1 - delta) * alpha * w_1
13             + (1 - delta) * (1 - alpha) * w_2
14             + delta * (alpha * w_1 + (1 - alpha) * w_2))
15

```

```

16
17 def w_prime_2_bar(delta=sp.abc.delta, alpha=sp.abc.alpha, w_1=sym.w_1, w_2=sym.w_2,
18                 w_bar=sym.w_bar, sigma_w=sym.sigma_w,
19                 ↪ sigma_lambda_w=sym.sigma_lambda_w):
19     return (((1 - delta) * alpha * ((w_1 - w_bar) ** 2 + sigma_w ** 2)) +
20            ((1 - delta) * (1 - alpha) * ((w_2 - w_bar) ** 2 + sigma_w ** 2)) +
21            (delta * sigma_lambda_w ** 2))
22
23
24 def w_prime_3_bar(delta=sp.abc.delta, alpha=sp.abc.alpha, w_1=sym.w_1, w_2=sym.w_2,
25                 w_bar=sym.w_bar, sigma_w=sym.sigma_w):
26     return (((1 - delta) * alpha * ((w_1 - w_bar) ** 3 +
27                                     3 * sigma_w ** 2 * (w_1 - w_bar))) +
28            ((1 - delta) * (1 - alpha) * ((w_2 - w_bar) ** 3 +
29                                     3 * sigma_w ** 2 * (w_2 - w_bar))))
30
31
32 def w_prime_4_bar(w_prime_2_bar=sym.w_prime_2_bar,
33                 w_prime_3_bar=sym.w_prime_3_bar,
34                 delta=sp.abc.delta,
35                 sigma_tilde_w=sym.sigma_tilde_w,
36                 sigma_lambda_w=sym.sigma_lambda_w):
37     return (w_prime_2_bar ** 2 *
38            ((1 - delta * (sigma_lambda_w ** 2 / w_prime_2_bar)) ** 2 / (1 - delta)) *
39            (3 * sigma_tilde_w ** 4 +
40             6 * (1 - sigma_tilde_w ** 2) *
41             sigma_tilde_w ** 2 +
42             (1 - sigma_tilde_w ** 2) ** 2) +
43            ((1 / (1 - sigma_tilde_w ** 2)) *
44             (1 / (1 - delta * (sigma_lambda_w ** 2 / w_prime_2_bar)))) *
45            (w_prime_3_bar ** 2 / w_prime_2_bar)) +
46            (delta * 3 * sigma_lambda_w ** 4))
47
48
49 # -----
50
51 # theta_l equations
52 # -----
53
54 def theta_l_bar(alpha=sp.abc.alpha, delta=sp.abc.delta,
55                theta_l_1=sym.theta_l_1, theta_l_2=sym.theta_l_2):
56     return ((1 - delta) * alpha * theta_l_1
57            + (1 - delta) * (1 - alpha) * theta_l_2
58            + delta * (alpha * theta_l_1 + (1 - alpha) * theta_l_2))
59
60
61 def theta_l_prime_2_bar(delta=sp.abc.delta,
62                        alpha=sp.abc.alpha,
63                        theta_l_1=sym.theta_l_1,
64                        theta_l_2=sym.theta_l_2,
65                        theta_l_bar=sym.theta_l_bar,
66                        sigma_theta_l_1=sym.sigma_theta_l_1,
67                        sigma_theta_l_2=sym.sigma_theta_l_2,
68                        sigma_lambda_theta_l=sym.sigma_lambda_theta_l):

```

```

69     return (((1 - delta) * alpha * ((theta_l_1 - theta_l_bar) ** 2 + sigma_theta_l_1 **
70         ↪ 2)) +
71         ((1 - delta) * (1 - alpha) *
72         ((theta_l_2 - theta_l_bar) ** 2 + sigma_theta_l_2 ** 2)) +
73         (delta * sigma_lambda_theta_l ** 2))
74
75 def theta_l_prime_3_bar(delta=sp.abc.delta,
76     alpha=sp.abc.alpha,
77     theta_l_1=sym.theta_l_1,
78     theta_l_2=sym.theta_l_2,
79     theta_l_bar=sym.theta_l_bar,
80     sigma_theta_l_1=sym.sigma_theta_l_1,
81     sigma_theta_l_2=sym.sigma_theta_l_2):
82     return (((1 - delta) * alpha *
83         ((theta_l_1 - theta_l_bar) ** 3 +
84         3 * sigma_theta_l_1 ** 2 * (theta_l_1 - theta_l_bar))) +
85         ((1 - delta) * (1 - alpha) *
86         ((theta_l_2 - theta_l_bar) ** 3 +
87         3 * sigma_theta_l_2 ** 2 * (theta_l_2 - theta_l_bar))))
88
89
90 # -----
91
92 # r_t equations
93 # -----
94
95 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):
96     return ((1 - delta) * alpha * r_t_1
97         + (1 - delta) * (1 - alpha) * r_t_2
98         + delta * (alpha * r_t_1 + (1 - alpha) * r_t_2))
99
100
101 def r_t_prime_2_bar(delta=sp.abc.delta,
102     alpha=sp.abc.alpha,
103     r_t_1=sym.r_t_1,
104     r_t_2=sym.r_t_2,
105     r_t_bar=sym.r_t_bar,
106     sigma_r_t_1=sym.sigma_r_t_1,
107     sigma_r_t_2=sym.sigma_r_t_2,
108     sigma_lambda_r_t=sym.sigma_lambda_r_t):
109     return (((1 - delta) * alpha * ((r_t_1 - r_t_bar) ** 2 + sigma_r_t_1 ** 2)) +
110         ((1 - delta) * (1 - alpha) * ((r_t_2 - r_t_bar) ** 2 + sigma_r_t_2 ** 2)) +
111         (delta * sigma_lambda_r_t ** 2))
112
113
114 # -----
115
116 # Mixed equations
117 # -----
118
119 def w_prime_theta_l_prime_bar(delta=sp.abc.delta,
120     alpha=sp.abc.alpha,
121     w_1=sym.w_1,

```

```

122         w_2=sym.w_2,
123         w_bar=sym.w_bar,
124         theta_l_1=sym.theta_l_1,
125         theta_l_2=sym.theta_l_2,
126         theta_l_bar=sym.theta_l_bar,
127         cov_lambda_w_theta=sym.rho_w_theta_1 * sym.sigma_lambda_w
            ↪ *
            sym.sigma_lambda_theta_1):
128
129     return (((1 - delta) * alpha * ((w_1 - w_bar) * (theta_l_1 - theta_l_bar))) +
130            ((1 - delta) * (1 - alpha) * ((w_2 - w_bar) * (theta_l_2 - theta_l_bar)))
131            + delta * cov_lambda_w_theta)
132
133
134 def w_prime_r_t_prime_bar(delta=sp.abc.delta,
135                            alpha=sp.abc.alpha,
136                            w_1=sym.w_1,
137                            w_2=sym.w_2,
138                            w_bar=sym.w_bar,
139                            r_t_1=sym.r_t_1,
140                            r_t_2=sym.r_t_2,
141                            r_t_bar=sym.r_t_bar,
142                            cov_lambda_w_r=sym.rho_w_r_t * sym.sigma_lambda_w *
143                            sym.sigma_lambda_r_t):
144     return (((1 - delta) * alpha * ((w_1 - w_bar) * (r_t_1 - r_t_bar))) +
145            ((1 - delta) * (1 - alpha) * ((w_2 - w_bar) * (r_t_2 - r_t_bar)))
146            + delta * cov_lambda_w_r)
147
148
149 def w_prime_2_theta_l_prime_bar(sigma_tilde_w=sym.sigma_tilde_w,
150                                 delta=sp.abc.delta,
151                                 lambda_w_theta=sym.lambda_w_theta,
152                                 lambda_w=sym.lambda_w,
153                                 w_prime_3_bar=sym.w_prime_3_bar,
154                                 w_prime_2_bar=sym.w_prime_2_bar,
155                                 w_prime_theta_l_prime=sym.w_prime_theta_l_prime_bar):
156     return ((1 / (1 - sigma_tilde_w ** 2)) *
157            ((1 - delta * lambda_w_theta) / (1 - delta * lambda_w)) *
158            (w_prime_3_bar / w_prime_2_bar) *
159            w_prime_theta_l_prime)
160
161
162 def w_prime_theta_l_prime_2_bar(delta=sp.abc.delta,
163                                 lambda_w_theta=sym.lambda_w_theta,
164                                 lambda_w=sym.lambda_w,
165                                 sigma_tilde_w=sym.sigma_tilde_w,
166                                 w_prime_3_bar=sym.w_prime_3_bar,
167                                 w_prime_2_bar=sym.w_prime_2_bar,
168                                 w_prime_theta_l_prime_bar=sym.w_prime_theta_l_prime_bar,
169                                 theta_l_prime_3_bar=sym.theta_l_prime_3_bar):
170     return (Rational(2, 3) *
171            ((1 - delta * lambda_w_theta) ** 2 / (1 - delta * lambda_w) ** 2) *
172            (1 / (1 - sigma_tilde_w ** 2) ** 2) *
173            (w_prime_3_bar / w_prime_2_bar ** 2) *
174            w_prime_theta_l_prime_bar ** 2 +

```

```

175         Rational(1, 3) *
176         ((1 - delta * lambda_w) / (1 - delta * lambda_w_theta)) *
177         (1 - sigma_tilde_w ** 2) *
178         ((w_prime_2_bar * theta_l_prime_3_bar) / w_prime_theta_l_prime_bar))
179
180
181 def w_prime_theta_l_prime_2_bar_beta(
182     sigma_tilde_w=sym.sigma_tilde_w,
183     delta=sp.abc.delta,
184     lambda_theta=sym.lambda_theta,
185     lambda_w=sym.lambda_w,
186     w_prime_3_bar=sym.w_prime_3_bar,
187     w_prime_2_bar=sym.w_prime_2_bar,
188     beta=sp.abc.beta,
189     theta_l_prime_2_bar=sym.theta_l_prime_2_bar,
190     lambda_w_theta=sym.lambda_w_theta,
191     w_prime_theta_l_prime_bar=sym.w_prime_theta_l_prime_bar):
192     from sympy import Rational
193     return (
194         (1 / (1 - sigma_tilde_w ** 2)) *
195         ((1 - delta * lambda_theta) / (1 - delta * lambda_w)) *
196         (w_prime_3_bar / w_prime_2_bar) *
197         (
198             Rational(1, 3) * beta * theta_l_prime_2_bar +
199             (
200                 ((1 - Rational(1, 3) * beta) / (1 - sigma_tilde_w ** 2)) *
201                 ((1 - delta * lambda_w_theta) ** 2 /
202                  ((1 - delta * lambda_w) * (1 - delta * lambda_theta))) *
203                 (w_prime_theta_l_prime_bar ** 2 / w_prime_2_bar)
204             )
205         )
206     )
207
208
209 def w_prime_r_t_prime_theta_l_prime_bar(delta=sp.abc.delta,
210     alpha=sp.abc.alpha,
211     w_1=sym.w_1,
212     w_2=sym.w_2,
213     w_bar=sym.w_bar,
214     r_t_1=sym.r_t_1,
215     r_t_2=sym.r_t_2,
216     r_t_bar=sym.r_t_bar,
217     theta_l_1=sym.theta_l_1,
218     theta_l_2=sym.theta_l_2,
219     theta_l_bar=sym.theta_l_bar,
220     r_r_t_theta_l=sym.r_r_t_theta_l,
221     sigma_r_t_1=sym.sigma_r_t_1,
222     sigma_r_t_2=sym.sigma_r_t_2,
223     sigma_theta_l_1=sym.sigma_theta_l_1,
224     sigma_theta_l_2=sym.sigma_theta_l_2):
225     return (((1 - delta) * alpha * (w_1 - w_bar) *
226         (
227             (r_t_1 - r_t_bar) * (theta_l_1 - theta_l_bar) +
228             r_r_t_theta_l * sigma_r_t_1 * sigma_theta_l_1

```

```

229         )) +
230         ((1 - delta) * (1 - alpha) * (w_2 - w_bar) *
231         (
232             (r_t_2 - r_t_bar) * (theta_l_2 - theta_l_bar) +
233             r_r_t_theta_l * sigma_r_t_2 * sigma_theta_l_2
234         )))
235
236
237 def w_prime_r_t_prime_theta_l_prime_bar_beta(
238     beta=sp.abc.beta,
239     sigma_tilde_w=sym.sigma_tilde_w,
240     delta=sp.abc.delta,
241     lambda_theta_r=sym.lambda_theta_r,
242     lambda_w=sym.lambda_w,
243     theta_l_prime_r_t_prime_bar=sym.theta_l_prime_r_t_prime_bar,
244     w_prime_3_bar=sym.w_prime_3_bar,
245     w_prime_2_bar=sym.w_prime_2_bar,
246     lambda_w_r=sym.lambda_w_r,
247     lambda_w_theta=sym.lambda_w_theta,
248     w_prime_r_t_prime_bar=sym.w_prime_r_t_prime_bar,
249     w_prime_theta_l_prime_bar=sym.w_prime_theta_l_prime_bar):
250     from sympy import Rational
251     return (
252         (
253             ((Rational(1, 3) * beta) / (1 - sigma_tilde_w ** 2)) *
254             ((1 - delta * lambda_theta_r) / (1 - delta * lambda_w)) *
255             theta_l_prime_r_t_prime_bar *
256             (w_prime_3_bar / w_prime_2_bar)
257         ) +
258         (
259             ((1 - Rational(1, 3) * beta) / (1 - sigma_tilde_w ** 2) ** 2) *
260             (((1 - delta * lambda_w_r) * (1 - delta * lambda_w_theta)) /
261              ((1 - delta * lambda_w) ** 2)) *
262             w_prime_r_t_prime_bar *
263             w_prime_theta_l_prime_bar *
264             (w_prime_3_bar / w_prime_2_bar ** 2)
265         )
266     )
267
268
269 def r_t_prime_theta_l_prime_bar(alpha=sp.abc.alpha, delta=sp.abc.delta,
270     r_t_1=sym.r_t_1, r_t_2=sym.r_t_2,
271     ↪ r_t_prime_bar=sym.r_t_bar,
272     theta_l_1=sym.theta_l_1, theta_l_2=sym.theta_l_2,
273     theta_l_bar=sym.theta_l_bar,
274     r_r_t_theta_l=sym.r_r_t_theta_l,
275     sigma_r_t_1=sym.sigma_r_t_1,
276     ↪ sigma_r_t_2=sym.sigma_r_t_2,
277     sigma_theta_l_1=sym.sigma_theta_l_1,
278     sigma_theta_l_2=sym.sigma_theta_l_2,
279     cov_lambda_r_theta=sym.rho_theta_l_r_t *
280         sym.sigma_lambda_theta_l *
281         sym.sigma_lambda_r_t):
282     return ((1 - delta) * alpha * (

```



```

281         (r_t_1 - r_t_prime_bar) * (theta_l_1 - theta_l_bar) +
282         r_r_t_theta_l * sigma_r_t_1 * sigma_theta_l_1) +
283         ((1 - delta) * (1 - alpha) * (
284             (r_t_2 - r_t_prime_bar) * (theta_l_2 - theta_l_bar) +
285             r_r_t_theta_l * sigma_r_t_2 * sigma_theta_l_2)) +
286         delta * cov_lambda_r_theta)
287
288
289 # ---
290
291 # Distributions
292 # ---
293
294 G_1_theta_l = Normal(name='G_1_theta_l', mean=sym.theta_l_1, std=sym.sigma_theta_l_1)
295 G_1_theta_l_density = density(G_1_theta_l)(sym.theta_l)
296
297 G_2_theta_l = Normal(name='G_2_theta_l', mean=sym.theta_l_2, std=sym.sigma_theta_l_2)
298 G_2_theta_l_density = density(G_2_theta_l)(sym.theta_l)
299
300 G_3_theta_l = Normal(name='G_3_theta_l', mean=sym.theta_l_bar,
301     ↪ std=sym.sigma_lambda_theta_l)
302 G_3_theta_l_density = density(G_3_theta_l)(sym.theta_l)
303
304 G_theta = ((1 - sp.abc.delta) * sp.abc.alpha * G_1_theta_l_density +
305             (1 - sp.abc.delta) * (1 - sp.abc.alpha) * G_2_theta_l_density +
306             sp.abc.delta * G_3_theta_l_density)
307
308 # ---
309
310 G_1_w = Normal(name='G_1_w', mean=sym.w_1, std=sym.sigma_w)
311 G_1_w_density = density(G_1_w)(sp.abc.w)
312
313 G_2_w = Normal(name='G_2_w', mean=sym.w_2, std=sym.sigma_w)
314 G_2_w_density = density(G_2_w)(sp.abc.w)
315
316 G_3_w = Normal(name='G_3_w', mean=sym.w_bar, std=sym.sigma_lambda_w)
317 G_3_w_density = density(G_3_w)(sp.abc.w)
318
319 G_w = ((1 - sp.abc.delta) * sp.abc.alpha * G_1_w_density +
320         (1 - sp.abc.delta) * (1 - sp.abc.alpha) * G_2_w_density +
321         sp.abc.delta * G_3_w_density)
322
323 # ---
324
325 G_1_w_theta = Normal(name='G_1_w_theta', mean=sp.Matrix([sym.w_1, sym.theta_l_1]),
326     ↪ std=sp.Matrix([[sym.sigma_w ** 2, 0], [0, sym.sigma_theta_l_1 **
327     ↪ 2]]))
328 G_1_w_theta_density = density(G_1_w_theta)(sp.abc.w, sp.abc.theta)
329
330 G_2_w_theta = Normal(name='G_2_w_theta', mean=sp.Matrix([sym.w_2, sym.theta_l_2]),
331     ↪ std=sp.Matrix([[sym.sigma_w ** 2, 0], [0, sym.sigma_theta_l_2 **
332     ↪ 2]]))
333 G_2_w_theta_density = density(G_2_w_theta)(sp.abc.w, sp.abc.theta)

```

```

332 G_3_w_theta = Normal(name='G_3_w_theta', mean=sp.Matrix([sym.w_bar, sym.theta_l_bar]),
333                      std=sp.Matrix([
334                          [sym.sigma_lambda_w ** 2,
335                           sym.rho_w_theta_l * sym.sigma_lambda_w *
336                             ↪ sym.sigma_lambda_theta_l],
337                          [sym.rho_w_theta_l * sym.sigma_lambda_w *
338                             ↪ sym.sigma_lambda_theta_l,
339                           sym.sigma_lambda_theta_l ** 2]
340                      ]))
341 G_3_w_theta_density = sp.simplify(density(G_3_w_theta)(sp.abc.w, sp.abc.theta))
342
343 G_w_theta = ((1 - sp.abc.delta) * sp.abc.alpha * G_1_w_theta_density +
344              (1 - sp.abc.delta) * (1 - sp.abc.alpha) * G_2_w_theta_density +
345              sp.abc.delta * G_3_w_theta_density)
346
347 # -----
348 mu_1_theta_l_r_t = sp.Matrix([sym.theta_l_1, sym.r_t_1])
349 Sigma_1_theta_l_r_t = sp.Matrix([[sym.sigma_theta_l_1 ** 2,
350                                   sym.r_r_t_theta_l * sym.sigma_theta_l_1 *
351                                     ↪ sym.sigma_r_t_1],
352                                   [sym.r_r_t_theta_l * sym.sigma_theta_l_1 *
353                                     ↪ sym.sigma_r_t_1,
354                                   sym.sigma_r_t_1 ** 2]])
355
356 G_1_theta_l_r_t = Normal(name='G_1_theta_l_r_t',
357                           mean=mu_1_theta_l_r_t,
358                           std=Sigma_1_theta_l_r_t)
359
360 G_1_theta_l_r_t_density = density(G_1_theta_l_r_t)(sym.theta_l, sym.r_t)
361
362 mu_2_theta_l_r_t = sp.Matrix([sym.theta_l_2, sym.r_t_2])
363 Sigma_2_theta_l_r_t = sp.Matrix([
364     [sym.sigma_theta_l_2 ** 2,
365      sym.r_r_t_theta_l * sym.sigma_theta_l_2 * sym.sigma_r_t_2],
366     [sym.r_r_t_theta_l * sym.sigma_theta_l_2 * sym.sigma_r_t_2,
367      sym.sigma_r_t_2 ** 2]])
368
369 G_2_theta_l_r_t = Normal(name='G_2_theta_l_r_t',
370                           mean=mu_2_theta_l_r_t,
371                           std=Sigma_2_theta_l_r_t)
372
373 G_2_theta_l_r_t_density = density(G_2_theta_l_r_t)(sym.theta_l, sym.r_t)
374
375 mu_3_theta_l_r_t = sp.Matrix([sym.theta_l_bar, sym.r_t_bar])
376 Sigma_3_theta_l_r_t = sp.Matrix([
377     [sym.sigma_lambda_theta_l ** 2,
378      sym.rho_theta_l_r_t * sym.sigma_lambda_theta_l * sym.sigma_lambda_r_t],
379     [
380         sym.rho_theta_l_r_t * sym.sigma_lambda_theta_l * sym.sigma_lambda_r_t,
381         sym.sigma_lambda_r_t ** 2]])
382
383 G_3_theta_l_r_t = Normal(name='G_3_theta_l_r_t',
384                           mean=mu_3_theta_l_r_t,

```

```

382         std=Sigma_2_theta_l_r_t)
383 G_3_theta_l_r_t_density = density(G_3_theta_l_r_t)(sym.theta_l, sym.r_t)
384
385 G_theta_l_r_t = ((1 - sp.abc.delta) * sp.abc.alpha * G_1_theta_l_r_t_density +
386                 (1 - sp.abc.delta) * (1 - sp.abc.alpha) * G_2_theta_l_r_t_density +
387                 sp.abc.delta * G_3_theta_l_r_t_density)
388
389 # ---
390
391 mu_1_w_theta_l_r_t = sp.Matrix([sym.w_1, sym.theta_l_1, sym.r_t_1])
392 Sigma_1_w_theta_l_r_t = sp.Matrix(
393     [[sym.sigma_w ** 2,
394      0,
395      0],
396     [0,
397      sym.sigma_theta_l_1 ** 2,
398      sym.r_r_t_theta_l * sym.sigma_theta_l_1 * sym.sigma_r_t_1],
399     [0,
400      sym.r_r_t_theta_l * sym.sigma_theta_l_1 * sym.sigma_r_t_1,
401      sym.sigma_r_t_1 ** 2]])
402
403 G_1_w_theta_l_r_t = Normal(name='G_1_w_theta_l_r_t',
404                             mean=mu_1_w_theta_l_r_t,
405                             std=Sigma_1_w_theta_l_r_t)
406
407 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)
408
409 mu_2_w_theta_l_r_t = sp.Matrix([sym.w_2, sym.theta_l_2, sym.r_t_2])
410 Sigma_2_w_theta_l_r_t = sp.Matrix([[sym.sigma_w ** 2,
411                                     0,
412                                     0],
413                                     [0,
414                                     sym.sigma_theta_l_2 ** 2,
415                                     sym.r_r_t_theta_l * sym.sigma_theta_l_2 *
416                                     ↪ sym.sigma_r_t_2],
417                                     [0,
418                                     sym.r_r_t_theta_l * sym.sigma_theta_l_2 *
419                                     ↪ sym.sigma_r_t_2,
420                                     sym.sigma_r_t_2 ** 2]])
421
422 G_2_w_theta_l_r_t = Normal(name='G_2_w_theta_l_r_t',
423                             mean=mu_2_w_theta_l_r_t,
424                             std=Sigma_2_w_theta_l_r_t)
425
426 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)
427
428 mu_3_w_theta_l_r_t = sp.Matrix([sym.w_bar, sym.theta_l_bar, sym.r_t_bar])
429 Sigma_3_w_theta_l_r_t = sp.Matrix(
430     [[sym.sigma_lambda_w ** 2,
431      sym.rho_w_theta_l * sym.sigma_lambda_w * sym.sigma_lambda_theta_l,
432      sym.rho_w_r_t * sym.sigma_lambda_theta_l * sym.sigma_lambda_r_t],
433     [
434         sym.rho_w_theta_l * sym.sigma_lambda_w * sym.sigma_lambda_theta_l,
435         sym.sigma_lambda_theta_l ** 2,

```

```

434         sym.rho_theta_l_r_t * sym.sigma_lambda_w * sym.sigma_lambda_r_t],
435         [sym.rho_w_r_t * sym.sigma_lambda_theta_l * sym.sigma_lambda_r_t,
436         sym.rho_theta_l_r_t * sym.sigma_lambda_w * sym.sigma_lambda_r_t,
437         sym.sigma_lambda_r_t ** 2]])
438
439 G_3_w_theta_l_r_t = Normal(name='G_3_w_theta_l_r_t',
440                             mean=mu_3_w_theta_l_r_t,
441                             std=Sigma_2_w_theta_l_r_t)
442 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)
443
444 G_w_theta_l_r_t = ((1 - sp.abc.delta) * sp.abc.alpha * G_1_w_theta_l_r_t_density +
445                    (1 - sp.abc.delta) * (1 - sp.abc.alpha) * G_2_w_theta_l_r_t_density +
446                    sp.abc.delta * G_3_w_theta_l_r_t_density)
447
448
449 # -----
450
451 # sigma equations
452 # -----
453
454 def sigma_tilde_w(sigma_w=sym.sigma_w, w_prime_2_bar=sym.w_prime_2_bar,
455                  delta=sp.abc.delta, lambda_w=sym.lambda_w):
456     from sympy import sqrt
457     return ((sigma_w / sqrt(w_prime_2_bar)) *
458            (1 / sqrt((1 - delta * lambda_w) / (1 - delta))))
459
460
461 # -----
462
463 # lambda equations
464 # -----
465
466 def lambda_w(sigma_lambda_w=sym.sigma_lambda_w, w_prime_2_bar=sym.w_prime_2_bar):
467     return sigma_lambda_w ** 2 / w_prime_2_bar
468
469
470 def lambda_theta(sigma_lambda_theta=sym.sigma_lambda_theta_l,
471                 theta_l_prime_2_bar=sym.theta_l_prime_2_bar):
472     return sigma_lambda_theta ** 2 / theta_l_prime_2_bar
473
474
475 def lambda_r(sigma_lambda_r=sym.sigma_lambda_r_t,
476              r_t_prime_2_bar=sym.r_t_prime_2_bar):
477     return sigma_lambda_r ** 2 / r_t_prime_2_bar
478
479
480 def lambda_w_theta(cov_lambda_w_theta=
481                   sym.rho_w_theta_l * sym.sigma_lambda_w * sym.sigma_lambda_theta_l,
482                   w_prime_theta_l_prime_bar=sym.w_prime_theta_l_prime_bar):
483     return cov_lambda_w_theta / w_prime_theta_l_prime_bar
484
485
486 def lambda_w_r(cov_lambda_w_r=
487               sym.rho_w_r_t * sym.sigma_lambda_w * sym.sigma_lambda_r_t,

```

```

488         w_prime_r_t_prime_bar=sym.w_prime_r_t_prime_bar):
489     return cov_lambda_w_r / w_prime_r_t_prime_bar
490
491
492 def lambda_r_theta(cov_lambda_r_theta=
493     sym.rho_theta_l_r_t * sym.sigma_lambda_r_t *
494     ↪ sym.sigma_lambda_theta_l,
495     r_t_prime_theta_l_prime_bar=sym.theta_l_prime_r_t_prime_bar):
496     return cov_lambda_r_theta / r_t_prime_theta_l_prime_bar
497
498 # ---
499
500 # sk
501 # ---
502
503 def sk_theta_l_hat_beta(sk_hat_w=sym.sk_hat_w, c_hat_w_theta_l=sym.c_w_theta_l_hat,
504     beta=sp.abc.beta):
505     return sk_hat_w * c_hat_w_theta_l * (beta + (1 - beta) * c_hat_w_theta_l ** 2)
506
507
508 def sk_theta_l_hat(theta_l_prime_3_bar=sym.theta_l_prime_3_bar,
509     theta_l_prime_2_bar=sym.theta_l_prime_2_bar,
510     delta=sp.abc.delta,
511     lambda_theta=sym.lambda_theta):
512     from sympy import Rational
513     return ((theta_l_prime_3_bar / theta_l_prime_2_bar ** Rational(3, 2)) *
514         (1 / ((1 - delta * lambda_theta) / (1 - delta)) ** Rational(3, 2)) *
515         (1 / (1 - delta)))
516
517
518 def sk_w_hat(sigma_tilde_w=sym.sigma_tilde_w,
519     w_prime_3_bar=sym.w_prime_3_bar,
520     w_prime_2_bar=sym.w_prime_2_bar,
521     delta=sp.abc.delta,
522     lambda_w=sym.lambda_w):
523     from sympy import Rational
524     return ((1 / (1 - sigma_tilde_w ** 2) ** Rational(3, 2)) *
525         (w_prime_3_bar / (w_prime_2_bar ** Rational(3, 2))) *
526         (1 / ((1 - delta * lambda_w) / (1 - delta)) ** Rational(3, 2)) *
527         (1 / (1 - delta)))
528
529
530 def c_w_theta_l_hat(sigma_w_tilde=sym.sigma_tilde_w,
531     w_prime_theta_l_prime_bar=sym.w_prime_theta_l_prime_bar,
532     w_prime_2_bar=sym.w_prime_2_bar,
533     theta_l_prime_2_bar=sym.theta_l_prime_2_bar,
534     delta=sp.abc.delta,
535     lambda_w=sym.lambda_w,
536     lambda_theta=sym.lambda_theta,
537     lambda_w_theta=sym.lambda_w_theta):
538     from sympy import sqrt
539     return ((1 / sqrt(1 - sigma_w_tilde ** 2)) *

```

```

540         (w_prime_theta_l_prime_bar / ((sqrt(w_prime_2_bar)) *
541         ↪ sqrt(theta_l_prime_2_bar))) *
542         (1 / sqrt((1 - delta * lambda_w) / (1 - delta))) *
543         (1 / sqrt((1 - delta * lambda_theta) / (1 - delta))) *
544         ((1 - delta * lambda_w_theta) / (1 - delta)))
545
546 # -- -- -- -- --
547
548 # sk
549 # -- -- -- -- --
550
551 def beta(c_w_theta_l_hat=sym.c_w_theta_l_hat,
552         sk_w_hat=sym.sk_hat_w,
553         sk_theta_l_hat=sym.sk_theta_l_hat):
554     return (((c_w_theta_l_hat ** 3 * sk_w_hat) - sk_theta_l_hat) /
555             (c_w_theta_l_hat * sk_w_hat * (c_w_theta_l_hat ** 2 - 1)))
556
557 # -- -- -- -- --

```

Listing A.2: checked\_functions.py

## A.4 w\_prime\_4\_bar.py

```

1  #!/usr/bin/env python
2  # coding: utf-8
3
4  # In[2]:
5
6
7  import sympy as sp
8  from IPython.display import display
9  from sympy import oo
10
11 import checked_functions as c_f
12 import symbols as sym
13
14 # # This document aims to analytically check  $\overline{w'^4}f$ 
15
16 # ## Define the marginal distributions with those parameters.
17
18 # In[2]:
19
20
21 display(sp.Eq(sym.G_1_w, c_f.G_1_theta_l_density))
22
23 # In[3]:
24
25

```

```

26 display(sp.Eq(sym.G_2_w, c_f.G_2_theta_1_density))
27
28 # In[4]:
29
30
31 display(sp.Eq(sym.G_3_w, c_f.G_3_theta_1_density))
32
33 # In[5]:
34
35
36 display(sp.Eq(sym.G_w, c_f.G_w))
37
38 # Calculate the moment analytically:
39
40 # In[6]:
41
42
43 w_prime_4_bar_int = sp.Integral((sp.abc.w - sym.w_bar) ** 4 * c_f.G_w, [sp.abc.w, -oo,
44 ↪ oo])
45 display(sp.Eq(sym.w_prime_4_bar, w_prime_4_bar_int))
46
47 # In[7]:
48
49
50 w_prime_4_bar_int_val = w_prime_4_bar_int.doit(conds='none').simplify()
51 display(sp.Eq(sym.w_prime_4_bar, w_prime_4_bar_int_val))
52
53 # The equation in the document is:
54
55 # In[8]:
56
57
58 display(sp.Eq(sym.w_prime_4_bar, c_f.w_prime_4_bar()))
59
60 # where
61
62 # In[9]:
63
64
65 display(sp.Eq(sym.sigma_tilde_w, c_f.sigma_tilde_w()))
66
67 # and
68
69 # In[10]:
70
71
72 display(sp.Eq(sym.w_prime_2_bar, c_f.w_prime_2_bar()))
73
74 # and
75
76 # In[11]:
77
78
79 display(sp.Eq(sym.w_prime_3_bar, c_f.w_prime_2_bar()))

```

```

79
80 # So,
81
82 # In[12]:
83
84
85 lambda_w_val = c_f.lambda_w().subs({
86     sym.w_prime_2_bar: c_f.w_prime_2_bar()
87 })
88 display(sp.Eq(sym.lambda_w, lambda_w_val))
89
90 # In[13]:
91
92
93 w_prime_4_bar_check_val = c_f.w_prime_4_bar().subs({
94     sym.w_prime_2_bar: c_f.w_prime_2_bar(),
95     sym.w_prime_3_bar: c_f.w_prime_3_bar(),
96     sym.sigma_tilde_w: c_f.sigma_tilde_w().subs({
97         sym.w_prime_2_bar: c_f.w_prime_2_bar(),
98         sym.lambda_w: c_f.lambda_w()
99     })
100 })
101
102 display(sp.Eq(sym.w_prime_4_bar, w_prime_4_bar_check_val))
103
104 # In[14]:
105
106
107 display(sp.Eq(w_prime_4_bar_int_val, w_prime_4_bar_check_val, evaluate=True)
108     .subs({sym.w_bar: c_f.w_bar()}).simplify())

```

Listing A.3: w\_prime\_4\_bar.py