

ADDING A THIRD NORMAL TO CLUBB

by

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ABSTRACT

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

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

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

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TABLE OF CONTENTS

LIST OF FIGURES	vi
LIST OF TABLES	vii
LIST OF LISTINGS	viii
LIST OF ACRONYMS	x
LIST OF SYMBOLS	xi
1 Introduction	1
2 Problem	3
2.1 Motivation to add a third normal component	3
2.2 Closing turbulence pdes by integration over a pdf	4
2.3 Derivation of trinormal closures by transformation of binormal closures . . .	6
2.4 Goal of this thesis	10
2.5 Inputs and outputs of the verification procedure	10
2.5.1 Inputs and outputs of a forward run	10
2.5.2 Inputs and outputs of a backward run (verification direction)	11
2.6 Steps for checking the formulas	11
3 Definitions	13
3.1 Normal distribution	13
3.1.1 Multivariate normal distribution	13
3.1.2 Moments	14
3.2 Variates of the pdf	14
4 Formulas that define the shape of the pdf and moments in terms of pdf parameters	16
4.1 Definition of the trinormal distribution, P_{tmg}	16
4.2 Normalized variables	18
4.3 A list of lower order moments expressed in terms of pdf parameters	18
4.3.1 Moments for w	19
4.3.2 Moments for θ_l	20
4.3.3 Moments for r_t	21
4.3.4 Mixed moments	22
4.4 Solving for pdf parameters by using the moment terms	23
4.5 Expressions for higher-order moments in terms of pdf parameters	25
4.6 Approximation of scalar skewnesses	26

4.7	Formulating closure relationships for higher-order moments in terms of lower-order moments	29
5	Integration using SymPy	32
5.1	Analytic integration	32
5.2	Numeric integration	35
6	Asymptotics	40
6.1	Limits for $\delta \rightarrow 1$	44
6.1.1	Limit for $\overline{w'^4}$ as δ goes to 1	44
6.1.2	Limit for $\overline{w'^2\theta'_l}$ as δ goes to 1	45
6.1.3	Limit for $\overline{w'^2\theta'_l}$ as δ goes to 1	45
6.1.4	Limit for $\overline{w'r'_l\theta'_l}$ as δ goes to 1	45
7	Summary	46
8	Outlook	48
	Bibliography	50
A	Calculation of limits	51
A.1	Calculation for the limit for $\overline{w'^4}$ as δ goes to 1	51
A.2	Calculation for the limit for $\overline{w'^2\theta'_l}$ as δ goes to 1	52
A.3	Calculation for the limit for $\overline{w'\theta_l'^2}$ as δ goes to 1	52
B	Code	53
B.1	User Guide	53
B.1.1	Accessing the code	53
B.1.2	Key files and their purposes	53
B.1.3	Working with functions	53
B.1.4	Displaying equations effectively	53
B.1.5	Handling integrals	53
B.2	symbols.py	54
B.3	checked_functions.py	56
B.4	w_prime_4_bar.py	70
B.5	w_prime_2_theta_l_prime_bar.py	72
B.6	w_prime_theta_l_prime_2_bar.py	77
B.7	w_prime_r_t_prime_theta_l_prime_bar.py	82

LIST OF FIGURES

2.1	Binormal plot for two strong up-/downdrafts	3
2.2	Binormal plot for two strong up-/downdrafts with increased standard deviations	4
2.3	Trinormal plot for two strong up-/downdrafts with varying δ	5
2.4	Trinormal plot for two strong up-/downdrafts with a third peak in the middle	6
5.1	Output of listing 5.4	34
5.2	Output of listing 5.5	34
5.3	Output of listing 5.7	35
5.4	Output of listing 5.13	37
5.5	Output of listing 5.18	39

LIST OF TABLES

2.1 1D Plots for different δ and σ_{w3} 9

LIST OF LISTINGS

5.1	Import statements	33
5.2	Defining symbols	33
5.3	Defining the marginals	33
5.4	Defining and displaying the needed integral	33
5.5	Calculating and printing the integral	34
5.6	Python function for the second order moment	34
5.7	Printing the symbolic equation	35
5.8	Check if the integral and the given formula are the same	35
5.9	Import statements	35
5.10	Defining symbols	36
5.11	Defining the marginals	36
5.12	Defining and displaying the needed integral	37
5.13	Python function for $\overline{w'^2\theta_l}$	37
5.14	Create a dataframe and putting in arbitrary numbers	38
5.15	Attaching the “checkval” column to the dataframe	38
5.16	Attaching the “numint” column to the dataframe	38
5.17	Attaching the “diffnum” column to the dataframe	39
5.18	Calculating the mean difference	39
B.1	symbols.py	56
B.2	checked_functions.py	69
B.3	w_prime_4_bar.py	72
B.4	w_prime_2_theta_1_prime_bar.py	77

B.5	w_prime_theta_l_prime_2_bar.py	82
B.6	w_prime_r_t_prime_theta_l_prime_bar.py	87

LIST OF ACRONYMS

cas computer algebra system. 16, 47, 48

CLUBB Cloud Layers Unified By Binormals. ii, 1, 2, 4, 5, 11, 18, 26, 29, 30, 46–49

lhs left hand side. 11

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

pdf probability density function. ii, 1, 6, 8, 10–14, 17, 18, 20, 23–25, 27–30, 40, 41, 46–48

rhs right hand side. 5, 11, 41

LIST OF SYMBOLS

θ'_l Standardized liquid water potential temperature ($\theta'_l = \theta_l - \overline{\theta_l}$). 15

r'_t Standardized total water mixing ratio ($r'_t = r_t - \overline{r_t}$). 15

w' Standardized upward wind ($w' = w - \overline{w}$). 15, 19

1 Introduction

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

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

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

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

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

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

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

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

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

2 Problem

2.1 Motivation to add a third normal component

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



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

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

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

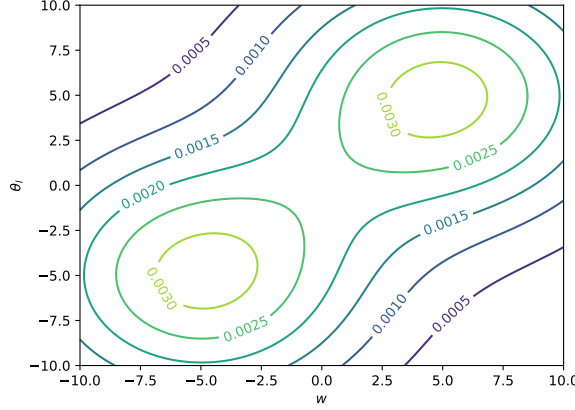


Figure 2.2: Binormal plot for two strong up-/downdrafts with increased standard deviations $w_1 = 5$, $w_2 = -5$, $\theta_{l1} = 5$, $\theta_{l2} = -5$, $\alpha = 0.5$, $\sigma_w = 5$, $\sigma_{\theta_{l1}} = 5$, $\sigma_{\theta_{l1}} = 5$.

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

2.2 Closing turbulence pdes by integration over a pdf

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

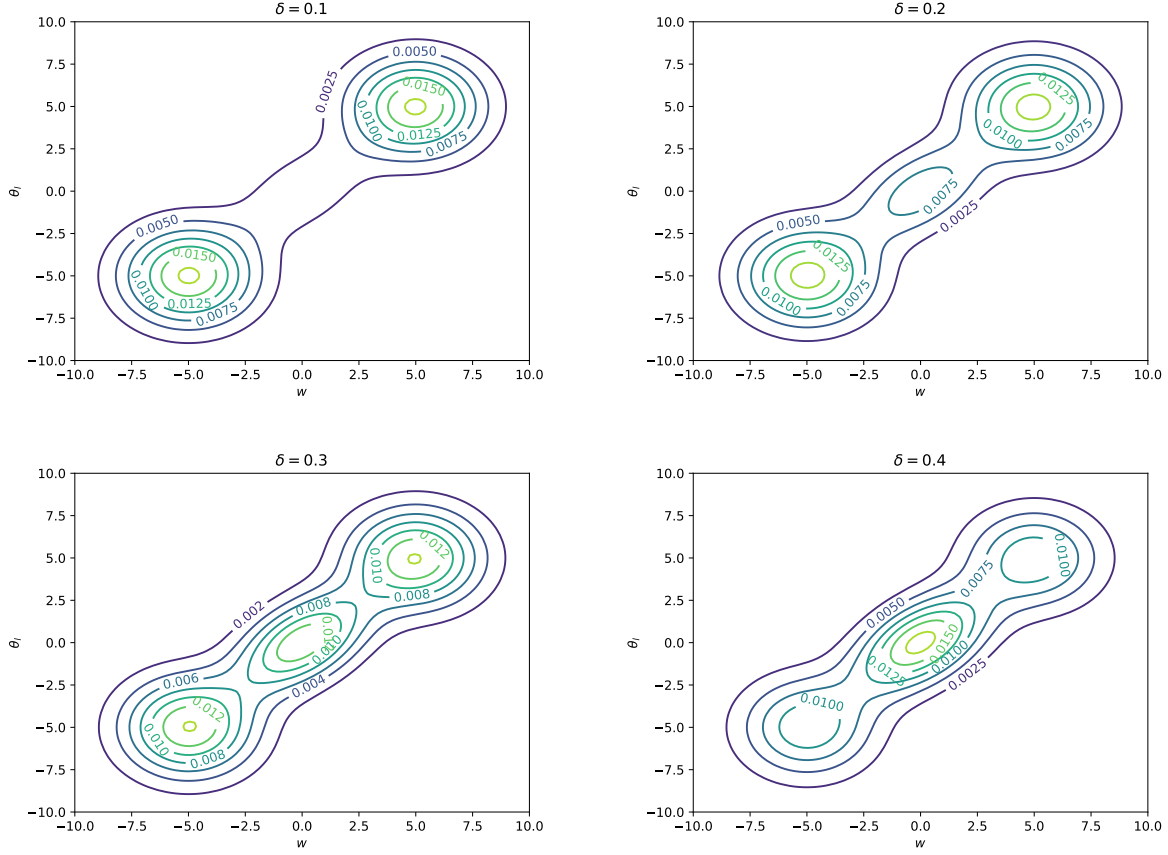


Figure 2.3: Trinormal plot for two strong up-/downdrafts with varying δ
 $w_1 = 5$, $w_2 = -5$, $\theta_{l1} = 5$, $\theta_{l2} = -5$, $\alpha = 0.5$, $\sigma_w = 2$, $\sigma_{\theta_{l1}} = 2$, $\sigma_{\theta_{l2}} = 2$, $\sigma_{w3} = 2$, $\sigma_{3\theta_l} = 2$,
 $\rho_{w\theta_l} = 0.5$.

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

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

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



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

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

2.3 Derivation of trinormal closures by transformation of binormal closures

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

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

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

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

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

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

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

$$\overline{w' \theta_l'} \frac{1 - \delta \lambda_{w\theta}}{1 - \delta} = \overline{w' \theta_l'}_{dGn}, \quad (2.3.6)$$

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

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

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

$$\begin{aligned} \overline{w'^2} \left(1 - \delta \frac{\sigma_{w3}^2}{\overline{w'^2}} \right) &= (1 - \delta) \overline{w'^2}_{dGn} \\ \overline{w'^2} - \delta \sigma_{w3}^2 &= (1 - \delta) \overline{w'^2}_{dGn} \\ \overline{w'^2} &= \overline{w'^2}_{dGn} - \delta \overline{w'^2}_{dGn} + \delta \sigma_{w3}^2 \\ \overline{w'^2} &= \overline{w'^2}_{dGn} - \delta \left(\overline{w'^2}_{dGn} - \sigma_{w3}^2 \right). \end{aligned} \quad (2.3.9)$$

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

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

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

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

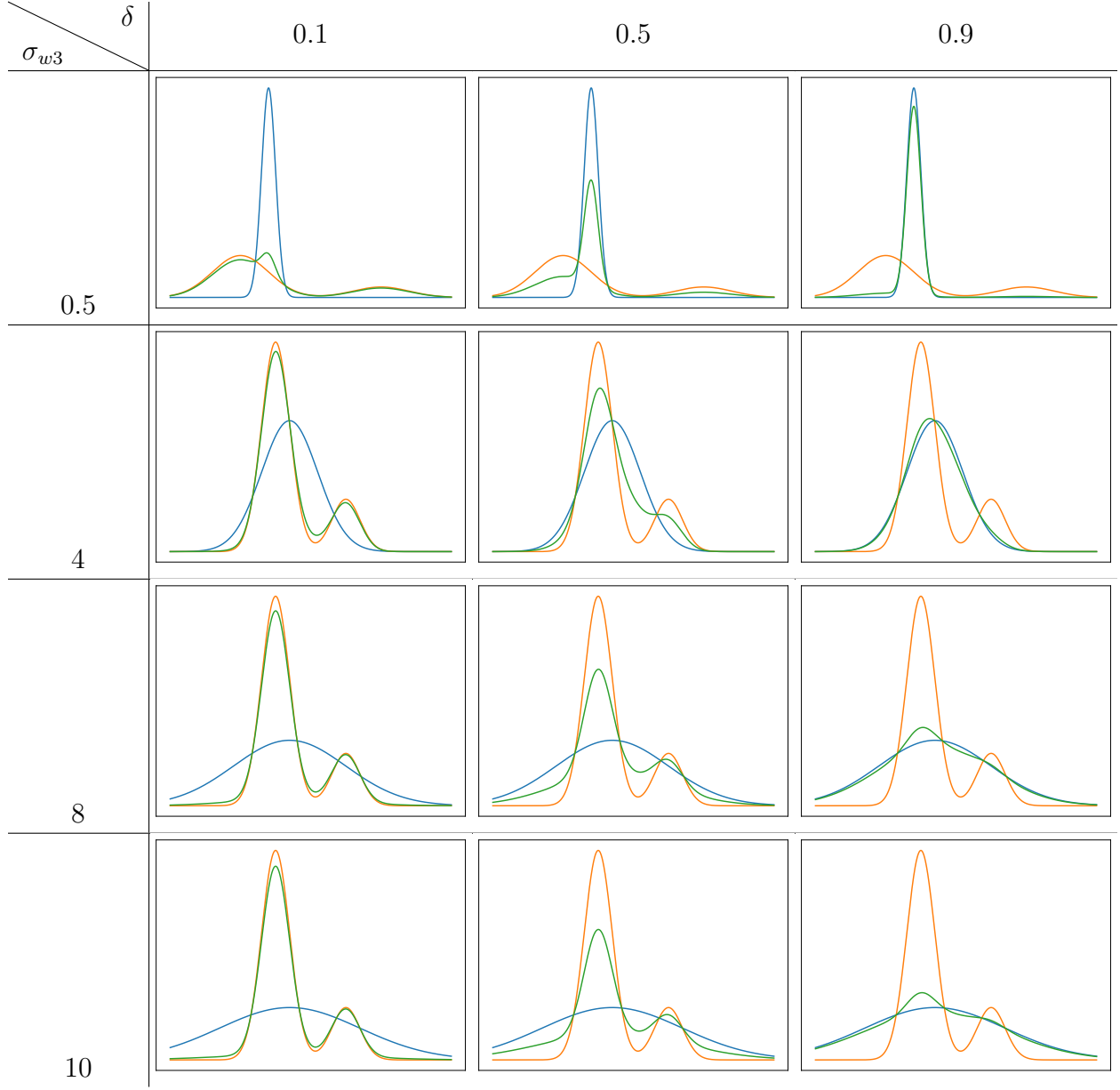


Table 2.1: 1D Plots for different δ and σ_{w3}
 $w_1 = 5$, $w_2 = -5$, $\alpha = 0.2$, $\sigma_w = 2$. The blue plot represents the third normal, the orange/red one represents the binormal, and the green one represents the mixture. The x and y labels and ticks are omitted for clarity.

green plot (mixture) as δ approaches 1.

2.4 Goal of this thesis

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

2.5 Inputs and outputs of the verification procedure

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

2.5.1 Inputs and outputs of a forward run

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

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

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

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

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

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

where P_{tmg} (**T**ri-variate **M**ixture of **G**aussians) is the pdf of the sum of all three normal distributions. Since some integrals are challenging to verify symbolically with SymPy, we are using the quadrature method of SymPy to calculate the integrals and choose arbitrary values for the inputs. All of this can be seen in section 5.2.

2.6 Steps for checking the formulas

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

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

3 Definitions

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

3.1 Normal distribution

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

Definition 1 (pdf of a normal distribution)

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

3.1.1 Multivariate normal distribution

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

Definition 2 (pdf of a multivariate normal distribution)

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

where

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

is the mean vector, and

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

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

3.1.2 Moments

Especially for this thesis, we are interested in the moments of the given multivariate normal distribution. We can express the first order moment as the mean, denoted as $\bar{X} = \mathbb{E}[X]$, 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:

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

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

3.2 Variates of the pdf

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

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

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

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

4.1 Definition of the trinormal distribution, P_{tmg}

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

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

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

We define the mean vectors of the first and second normal distributions as $\mu_1 = (w_1, \theta_{l1}, r_{t1})^\top$, and $\mu_2 = (w_2, \theta_{l2}, r_{t2})^\top$, where $w_1 > w_2$ (due to a convention in the code) and the covariance

matrices as

$$\Sigma_1 = \begin{pmatrix} \sigma_w^2 & 0 & 0 \\ 0 & \sigma_{\theta_{l1}}^2 & \rho_{\theta_l r_t} \sigma_{\theta_{l3}} \sigma_{r_{t3}} \\ 0 & \rho_{\theta_l r_t} \sigma_{\theta_{l3}} \sigma_{r_{t3}} & \sigma_{r_{t1}}^2 \end{pmatrix}, \text{ and } \Sigma_2 = \begin{pmatrix} \sigma_w^2 & 0 & 0 \\ 0 & \sigma_{\theta_{l2}}^2 & \rho_{\theta_l r_t} \sigma_{\theta_{l3}} \sigma_{r_{t3}} \\ 0 & \rho_{\theta_l r_t} \sigma_{\theta_{l3}} \sigma_{r_{t3}} & \sigma_{r_{t2}}^2 \end{pmatrix}. \quad (4.1.2)$$

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

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

$$\mu_3 = \begin{pmatrix} \overline{w} \\ \overline{\theta_l} \\ \overline{r_t} \end{pmatrix}, \text{ and } \Sigma_3 = \begin{pmatrix} \sigma_{w3}^2 & \rho_{w\theta_{l3}} \sigma_{w3} \sigma_{\theta_{l3}} & \rho_{wr_{t3}} \sigma_{w3} \sigma_{r_{t3}} \\ \rho_{w\theta_{l3}} \sigma_{w3} \sigma_{\theta_{l3}} & \sigma_{\theta_{l3}}^2 & \rho_{\theta_l r_{t3}} \sigma_{\theta_{l3}} \sigma_{r_{t3}} \\ \rho_{wr_{t3}} \sigma_{w3} \sigma_{r_{t3}} & \rho_{\theta_l r_{t3}} \sigma_{\theta_{l3}} \sigma_{r_{t3}} & \sigma_{r_{t3}}^2 \end{pmatrix}. \quad (4.1.3)$$

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

$$\lambda_w \equiv \frac{\sigma_{w3}^2}{w'^2}, \quad \lambda_\theta \equiv \frac{\sigma_{\theta_{l3}}^2}{\theta_l'^2}, \quad \lambda_r \equiv \frac{\sigma_{r_{t3}}^2}{r_t'^2}, \quad (4.1.4)$$

$$\lambda_{\theta r} \equiv \frac{\rho_{\theta_l r_t} \sigma_{\theta_{l3}} \sigma_{r_{t3}}}{r_t' \theta_l'}, \quad \lambda_{w\theta} \equiv \frac{\rho_{w\theta_l} \sigma_{w3} \sigma_{\theta_{l3}}}{w' \theta_l'}, \quad \lambda_{wr} \equiv \frac{\rho_{wr_t} \sigma_{w3} \sigma_{r_{t3}}}{w' r_t'}. \quad (4.1.5)$$

Hence, we can rewrite Σ_3 as

$$\Sigma_3 = \begin{pmatrix} \sigma_{w3}^2 & \overline{w' \theta_l'} \cdot \lambda_{w\theta} & \overline{w' r_t'} \cdot \lambda_{wr} \\ \overline{w' \theta_l'} \cdot \lambda_{w\theta} & \sigma_{\theta_{l3}}^2 & \overline{r_t' \theta_l'} \cdot \lambda_{\theta r} \\ \overline{w' r_t'} \cdot \lambda_{wr} & \overline{r_t' \theta_l'} \cdot \lambda_{\theta r} & \sigma_{r_{t3}}^2 \end{pmatrix}. \quad (4.1.6)$$

4.2 Normalized variables

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

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

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

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

For the standard deviations, we define

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

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

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

where $\sigma_{\theta_{li}}$ denotes the standard deviation of the i^{th} θ_l -component, and

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

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

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

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

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

4.3.1 Moments for w

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

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

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

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

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

The second order moment is given as:

$$\begin{aligned} \overline{w'^2} &= (1 - \delta)\alpha[(w_1 - \bar{w})^2 + \sigma_w^2] \\ &\quad + (1 - \delta)(1 - \alpha)[(w_2 - \bar{w})^2 + \sigma_w^2] \\ &\quad + \delta\sigma_{w3}^2, \end{aligned} \quad (4.3.3)$$

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

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

The *non-dimensional* relationship would then be:

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

The third order moment is given as:

$$\begin{aligned}\overline{w'^3} &= (1 - \delta)\alpha[(w_1 - \bar{w})^3 + 3\sigma_w^2(w_1 - \bar{w})] \\ &\quad + (1 - \delta)(1 - \alpha)[(w_2 - \bar{w})^3 + 3\sigma_w^2(w_2 - \bar{w})]\end{aligned}\quad (4.3.5)$$

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

$$\begin{aligned}\widehat{Sk}_w &\equiv \frac{1}{(1 - \tilde{\sigma}_w^2)^{3/2}} \frac{\overline{w'^3}}{\left(\overline{w'^2}\right)^{3/2}} \frac{1}{\left(\frac{1 - \delta\lambda_w}{1 - \delta}\right)^{3/2}} \frac{1}{1 - \delta} \\ &= \alpha \left(\widehat{w}_1^3 + 3\widehat{w}_1 \frac{\tilde{\sigma}_w^2}{(1 - \tilde{\sigma}_w^2)} \right) + (1 - \alpha) \left(\widehat{w}_2^3 + 3\widehat{w}_2 \frac{\tilde{\sigma}_w^2}{(1 - \tilde{\sigma}_w^2)} \right)\end{aligned}\quad (4.3.6)$$

4.3.2 Moments for θ_l

For θ_l we have a similar *non-dimensional* relationship:

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

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

$$\begin{aligned}\overline{\theta_l'^2} &= (1 - \delta)\alpha[(\theta_{l1} - \bar{\theta}_l)^2 + \sigma_{\theta_{l1}}^2] \\ &\quad + (1 - \delta)(1 - \alpha)[(\theta_{l2} - \bar{\theta}_l)^2 + \sigma_{\theta_{l2}}^2] \\ &\quad + \delta\sigma_{\theta_{l3}}^2,\end{aligned}\quad (4.3.8)$$

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:

$$\begin{aligned}\overline{\theta_l'^3} &= (1 - \delta)\alpha[(\theta_{l1} - \bar{\theta}_l)^3 + 3\sigma_{\theta_{l1}}^2(\theta_{l1} - \bar{\theta}_l)] \\ &\quad + (1 - \delta)(1 - \alpha)[(\theta_{l2} - \bar{\theta}_l)^3 + 3\sigma_{\theta_{l2}}^2(\theta_{l2} - \bar{\theta}_l)]\end{aligned}\quad (4.3.9)$$

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

$$\begin{aligned}\widehat{Sk_{\theta_l}} &\equiv \frac{\overline{\theta_l'^3}}{\left(\overline{\theta_l'^2}\right)^{3/2}} \left(\frac{1}{\frac{1-\delta\lambda_\theta}{1-\delta}}\right)^{3/2} \frac{1}{1-\delta} \\ &= \alpha \left(\tilde{\theta}_{l1}^3 + 3\tilde{\theta}_{l1}\tilde{\sigma}_{\theta_{l1}}^2\right) + (1-\alpha) \left(\tilde{\theta}_{l2}^3 + 3\tilde{\theta}_{l2}\tilde{\sigma}_{\theta_{l2}}^2\right).\end{aligned}\quad (4.3.10)$$

4.3.3 Moments for r_t

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

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

and

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

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

$$\begin{aligned}\overline{r_t'^2} &= (1-\delta)\alpha[(r_{t1} - \overline{r_t})^2 + \sigma_{r_{t1}}^2] \\ &\quad + (1-\delta)(1-\alpha)[(r_{t2} - \overline{r_t})^2 + \sigma_{\theta_{l2}}^2] \\ &\quad + \delta\sigma_{r_{t3}}^2,\end{aligned}\quad (4.3.13)$$

and

$$\begin{aligned}\overline{r_t'^3} &= (1-\delta)\alpha[(r_{t1} - \overline{r_t})^3 + 3\sigma_{r_{t1}}^2(r_{t1} - \overline{r_t})] \\ &\quad + (1-\delta)(1-\alpha)[(r_{t2} - \overline{r_t})^3 + 3\sigma_{r_{t2}}^2(r_{t2} - \overline{r_t})].\end{aligned}\quad (4.3.14)$$

4.3.4 Mixed moments

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

$$\begin{aligned}\overline{w'\theta'_l} &= (1 - \delta)\alpha[(w_1 - \bar{w})(\theta_{l1} - \bar{\theta}_l)] \\ &\quad + (1 - \delta)(1 - \alpha)[(w_2 - \bar{w})(\theta_{l2} - \bar{\theta}_l)] \\ &\quad + \delta\lambda_{w\theta}\overline{w'\theta'_l},\end{aligned}\tag{4.3.15}$$

$$\begin{aligned}\overline{w'r'_t} &= (1 - \delta)\alpha[(w_1 - \bar{w})(r_{t1} - \bar{r}_t)] \\ &\quad + (1 - \delta)(1 - \alpha)[(w_2 - \bar{w})(r_{t2} - \bar{r}_t)] \\ &\quad + \delta\lambda_{wr}\overline{w'r'_t},\end{aligned}\tag{4.3.16}$$

and

$$\begin{aligned}\overline{r'_t\theta'_l} &= (1 - \delta)\alpha[(r_{t1} - \bar{r}_t)(\theta_{l1} - \bar{\theta}_l) + r_{r_t\theta_l}\sigma_{r_{t1}}\sigma_{\theta_{l1}}] \\ &\quad + (1 - \delta)(1 - \alpha)[(r_{t2} - \bar{r}_t)(\theta_{l2} - \bar{\theta}_l) + r_{r_t\theta_l}\sigma_{r_{t2}}\sigma_{\theta_{l2}}] \\ &\quad + \delta\lambda_{r\theta}\overline{r'_t\theta'_l}.\end{aligned}\tag{4.3.17}$$

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

$$\begin{aligned}\hat{c}_{w\theta_l} &\equiv \frac{1}{(1 - \tilde{\sigma}_w^2)^{1/2}} \frac{\overline{w'\theta'_l}}{\sqrt{w'^2}\sqrt{\theta_l'^2}} \frac{1}{\sqrt{\frac{1-\delta\lambda_w}{1-\delta}}} \frac{1}{\sqrt{\frac{1-\delta\lambda_\theta}{1-\delta}}} \frac{1 - \delta\lambda_{w\theta}}{1 - \delta} \\ &= \alpha\hat{w}_1\tilde{\theta}_{l1} + (1 - \alpha)\hat{w}_2\tilde{\theta}_{l2},\end{aligned}\tag{4.3.18}$$

$$\begin{aligned}\hat{c}_{wr_t} &\equiv \frac{1}{(1 - \tilde{\sigma}_w^2)^{1/2}} \frac{\overline{w'r'_t}}{\sqrt{w'^2}\sqrt{r_t'^2}} \frac{1}{\sqrt{\frac{1-\delta\lambda_w}{1-\delta}}} \frac{1}{\sqrt{\frac{1-\delta\lambda_r}{1-\delta}}} \frac{1 - \delta\lambda_{wr}}{1 - \delta} \\ &= \alpha\hat{w}_1\tilde{r}_{t1} + (1 - \alpha)\hat{w}_2\tilde{r}_{t2},\end{aligned}\tag{4.3.19}$$

and

$$\begin{aligned}\hat{c}_{r_t\theta_l} &\equiv \frac{\overline{r'_t\theta'_l}}{\sqrt{r_t'^2}\sqrt{\theta_l'^2}} \frac{1}{\sqrt{\frac{1-\delta\lambda_r}{1-\delta}}} \frac{1}{\sqrt{\frac{1-\delta\lambda_\theta}{1-\delta}}} \frac{1 - \delta\lambda_{r\theta}}{1 - \delta} \\ &= \alpha\left(\tilde{r}_{t1}\tilde{\theta}_{l1} + r_{r_t\theta_l}\tilde{\sigma}_{r_{t1}}\tilde{\sigma}_{\theta_{l1}}\right) + (1 - \alpha)\left(\tilde{r}_{t2}\tilde{\theta}_{l2} + r_{r_t\theta_l}\tilde{\sigma}_{r_{t2}}\tilde{\sigma}_{\theta_{l2}}\right),\end{aligned}\tag{4.3.20}$$

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

We also list a trivariate moment $(\overline{w'r_t'\theta_l'})$, given by:

$$\begin{aligned}\overline{w'r_t'\theta_l'} &= (1 - \delta)\alpha(w_1 - \overline{w}) \left[(r_{t1} - \overline{r_t}) (\theta_{l1} - \overline{\theta_l}) + r_{r_t\theta_l} \sigma_{r_{t1}} \sigma_{\theta_{l1}} \right] \\ &\quad + (1 - \delta)(1 - \alpha)(w_2 - \overline{w}) \left[(r_{t2} - \overline{r_t}) (\theta_{l2} - \overline{\theta_l}) + r_{r_t\theta_l} \sigma_{r_{t2}} \sigma_{\theta_{l2}} \right].\end{aligned}\tag{4.3.21}$$

4.4 Solving for pdf parameters by using the moment terms

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

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

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

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

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

The proposed solution procedure [LG05] is as follows.

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

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

$$\widehat{w}_1 = \sqrt{\frac{1 - \alpha}{\alpha}}, \quad (4.4.2)$$

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

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

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

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

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

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

$$\tilde{\theta}_{l2} = -\frac{\widehat{c}_{w\theta_l}}{\widehat{w}_1}. \quad (4.4.6)$$

4. We can get $\tilde{\sigma}_{\theta_{l1}}$ and $\tilde{\sigma}_{\theta_{l2}}$ by fulfilling equation (4.3.8) for $\overline{\theta_l'^2}$, and equation (4.3.9) for $\overline{\theta_l'^3}$:

$$\tilde{\sigma}_{\theta_{l1}}^2 = (1 - \widehat{c}_{w\theta_l}^2) + \left(\sqrt{\frac{1 - \alpha}{\alpha}} \right) \frac{1}{3\widehat{c}_{w\theta_l}} \left(\widehat{Sk}_{\theta_l} - \widehat{c}_{w\theta_l}^3 \widehat{Sk}_w \right), \quad (4.4.7)$$

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

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

5. Finding formulas for \tilde{r}_{t1} , \tilde{r}_{t2} , $\tilde{\sigma}_{r_t 1}^2$, and $\tilde{\sigma}_{r_t 2}^2$ can be done by replacing θ_l by r_t everywhere in the equations (4.4.5), (4.4.6), (4.4.7), and (4.4.8).
6. The last step is to get a relationship between $r_{r_t \theta_l}$, the in-between normal correlation and $c_{r_t \theta_l}$, the total correlation. This can be done by using equation (4.3.17):

$$r_{r_t \theta_l} = \frac{\hat{c}_{r_t \theta_l} - \hat{c}_{wr_t} \hat{c}_{w\theta_l}}{\alpha \tilde{\sigma}_{r_t 1} \tilde{\sigma}_{\theta_l 1} + (1 - \alpha) \tilde{\sigma}_{r_t 2} \tilde{\sigma}_{\theta_l 2}}. \quad (4.4.9)$$

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

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

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

$$\begin{aligned}
\frac{1}{(1 - \tilde{\sigma}_w^2)^2} \frac{(1 - \delta)}{(1 - \delta\lambda_w)^2} \frac{\overline{w'^4}}{(\overline{w'^2})^2} &= \alpha \left[\widehat{w}_1^4 + 6\widehat{w}_1^2 \frac{\tilde{\sigma}_w^2}{(1 - \tilde{\sigma}_w^2)} + 3 \frac{\tilde{\sigma}_w^4}{(1 - \tilde{\sigma}_w^2)^2} \right] \\
&+ (1 - \alpha) \left[\widehat{w}_2^4 + 6\widehat{w}_2^2 \frac{\tilde{\sigma}_w^2}{(1 - \tilde{\sigma}_w^2)} + 3 \frac{\tilde{\sigma}_w^4}{(1 - \tilde{\sigma}_w^2)^2} \right] \\
&+ \frac{1}{(1 - \tilde{\sigma}_w^2)^2} \frac{(1 - \delta)}{(1 - \delta\lambda_w)^2} \delta 3\lambda_w^2, \tag{4.5.1}
\end{aligned}$$

$$\begin{aligned}
\frac{1}{(1 - \tilde{\sigma}_w^2)} \frac{(1 - \delta)^{1/2}}{(1 - \delta\lambda_w)(1 - \delta\lambda_\theta)^{1/2}} \frac{\overline{w'^2\theta'_l}}{w'^2 (\overline{\theta'^2})^{1/2}} &= \alpha \left[\widehat{w}_1^2 + \frac{\tilde{\sigma}_w^2}{(1 - \tilde{\sigma}_w^2)} \right] \tilde{\theta}_{l1} \\
&+ (1 - \alpha) \left[\widehat{w}_2^2 + \frac{\tilde{\sigma}_w^2}{(1 - \tilde{\sigma}_w^2)} \right] \tilde{\theta}_{l2}, \tag{4.5.2}
\end{aligned}$$

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

$$\begin{aligned}
\frac{1}{(1 - \tilde{\sigma}_w^2)^{1/2}} \frac{(1 - \delta)^{1/2}}{(1 - \delta\lambda_w)^{1/2}(1 - \delta\lambda_\theta)^{1/2}(1 - \delta\lambda_{q_t})^{1/2}} \frac{\overline{w'r'_t\theta'_l}}{(\overline{w'^2})^{1/2} (\overline{r'^2_t})^{1/2} (\overline{\theta'^2_l})^{1/2}} \\
= \alpha \widehat{w}_1 \left(\tilde{r}_{t1} \tilde{\theta}_{l1} + r_{rt\theta_l} \tilde{\sigma}_{r_{t1}} \tilde{\sigma}_{\theta_{l1}} \right) + (1 - \alpha) \widehat{w}_2 \left(\tilde{r}_{t2} \tilde{\theta}_{l2} + r_{rt\theta_l} \tilde{\sigma}_{r_{t2}} \tilde{\sigma}_{\theta_{l2}} \right) \tag{4.5.4}
\end{aligned}$$

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

4.6 Approximation of scalar skewnesses

Closing the system of prognostic equations within CLUBB needs the specification of the skewness terms Sk_{θ_l} and Sk_{r_t} . These skewness values appear in the solutions for $\tilde{\sigma}_{\theta_{l1}}$ (equation (4.4.7)) and $\tilde{\sigma}_{\theta_{l2}}$ (equation (4.4.8)), respectively. Traditionally, these skewness terms

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

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

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

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

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

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

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

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

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

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

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

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

and

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

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

$$r_{r_t \theta_l} = \frac{c_{r_t \theta_l} - \widehat{c}_{wr_t} \widehat{c}_{w\theta_l}}{(1 - \widehat{c}_{wr_t}^2)^{1/2} (1 - \widehat{c}_{w\theta_l}^2)^{1/2}}, \quad (4.6.5)$$

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

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

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

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

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

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

We first present the equation for the third moment of θ'_l , $\overline{\theta'^3_l}$. This expression is derived by dimensionalizing equation (4.6.1), which relates the skewness of θ_l to the skewness of w and other model parameters.

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

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

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

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

$$\begin{aligned} \frac{1}{(1 - \tilde{\sigma}_w^2)^2} \frac{(1 - \delta)}{(1 - \delta\lambda_w)^2} \frac{\overline{w'^4}}{(\overline{w'^2})^2} &= 3 \frac{\tilde{\sigma}_w^4}{(1 - \tilde{\sigma}_w^2)^2} + 6 \frac{\tilde{\sigma}_w^2}{(1 - \tilde{\sigma}_w^2)} + 1 \\ &+ \widehat{Sk}_w^2 + \frac{1}{(1 - \tilde{\sigma}_w^2)^2} \frac{(1 - \delta)}{(1 - \delta\lambda_w)^2} \delta 3\lambda_w^2, \end{aligned} \quad (4.7.2)$$

leading to

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

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

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

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

and

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

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

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

and

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

5 Integration using SymPy

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

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

5.1 Analytic integration

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

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

Listing 5.1: Import statements

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

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

Listing 5.2: Defining symbols

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

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

Listing 5.3: Defining the marginals

```
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_w_3)
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)
```

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

Listing 5.4: Defining and displaying the needed integral

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

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

Figure 5.1: Output of listing 5.4

$$\overline{w'^2} = \int_{-\infty}^{\infty} (-\overline{w} + w)^2 \left(\frac{\sqrt{2}\delta e^{-\frac{(-\overline{w}+w)^2}{2\sigma_{w3}^2}}}{2\sqrt{\pi}\sigma_{w3}} + \frac{\sqrt{2}\alpha(1-\delta) e^{-\frac{(w-w_1)^2}{2\sigma_w^2}}}{2\sqrt{\pi}\sigma_w} + \frac{\sqrt{2} \cdot (1-\alpha)(1-\delta) e^{-\frac{(w-w_2)^2}{2\sigma_w^2}}}{2\sqrt{\pi}\sigma_w} \right) dw$$

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

Listing 5.5: Calculating and printing the integral

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

Figure 5.2: Output of listing 5.5

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

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

Listing 5.6: Python function for the second order moment

```
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_w_3=sigma_w_3):
    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_w_3 ** 2))
```

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

Listing 5.7: Printing the symbolic equation

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

Figure 5.3: Output of listing 5.7

$$\overline{w'^2} = \sigma_{w3}^2 \delta + \alpha (1 - \delta) (\sigma_w^2 + (-\overline{w} + w_1)^2) + (1 - \alpha) (1 - \delta) (\sigma_w^2 + (-\overline{w} + w_2)^2)$$

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

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

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

what we wanted to have.

5.2 Numeric integration

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

Listing 5.9: Import statements

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

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

listing 5.2, together with the ones in listing 5.10.

Listing 5.10: Defining symbols

```
theta_l_1 = Symbol('\theta_{l1}')
theta_l_2 = Symbol('\theta_{l2}')
theta_l_bar = Symbol('\overline{\theta_l}')
sigma_theta_l_1 = Symbol('\sigma_{\theta_{l1}}')
sigma_theta_l_2 = Symbol('\sigma_{\theta_{l2}}')
sigma_theta_l_3 = Symbol('\sigma_{\theta_l_3}')
rho_w_theta_l = Symbol('\rho_{w\theta_l}')
w_prime_3_bar = Symbol('\overline{w}^3')
w_prime_theta_l_prime_bar = Symbol('\overline{w}^{\theta_l}_{\prime}')
w_prime_2_theta_prime_l_bar = Symbol('\overline{w}^2_{\theta_{\prime l}}')
sigma_tilde_w = Symbol('\tilde{\sigma}_w')
lambda_w_theta = Symbol('\lambda_{w\theta}')
lambda_w = Symbol('\lambda_w')
```

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

Listing 5.11: Defining the marginals

```
G_1_w_theta = Normal(name='G_1_w_theta', mean=sp.Matrix([w_1, theta_l_1]),
    std=sp.Matrix([[sigma_w ** 2, 0], [0, sigma_theta_l_1 ** 2]]))
G_1_w_theta_density = density(G_1_w_theta)(sp.abc.w, sp.abc.theta)
G_2_w_theta = Normal(name='G_2_w_theta', mean=sp.Matrix([w_2, theta_l_2]),
    std=sp.Matrix([[sigma_w ** 2, 0], [0, sigma_theta_l_2 ** 2]]))
G_2_w_theta_density = density(G_2_w_theta)(sp.abc.w, sp.abc.theta)
G_3_w_theta = Normal(name='G_3_w_theta', mean=sp.Matrix([w_bar, theta_l_bar]),
    std=sp.Matrix([[sigma_w_3 ** 2,
        rho_w_theta_l * sigma_w_3 * sigma_theta_l_3],
        [rho_w_theta_l * sigma_w_3 * sigma_theta_l_3,
        sigma_theta_l_3 ** 2]]))
G_3_w_theta_density = sp.simplify(density(G_3_w_theta)(sp.abc.w, sp.abc.theta))
G_w_theta = (
    (1 - sp.abc.delta) * sp.abc.alpha * density(G_1_w_theta)(sp.abc.w, sp.abc.theta)
    + (1 - sp.abc.delta) * (1 - sp.abc.alpha) * density(G_2_w_theta)(sp.abc.w, sp.abc.theta)
    + sp.abc.delta * G_3_w_theta_density)
```

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

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

Listing 5.12: Defining and displaying the needed integral

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

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

Listing 5.14: Create a dataframe and putting in arbitrary numbers

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

Listing 5.15: Attaching the “checkval” column to the dataframe

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

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

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

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

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

we are using the integral which has been specified earlier and specify the numerical integration

method by adding the parameter `method='quad'`¹ to the function `.doit(..)`. After that, `.evalf(..)` just gives the numerical value. We try to prove that the integral value equals the function value, hence we are computing the error between those two columns (listing 5.17) and take the mean (`numpy.mean(..)` from the package NumPy [Har+20]) of these new columns (listing 5.18) to see if the error is actually numerically 0.

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

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

Listing 5.18: Calculating the mean difference

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

Figure 5.5: Output of listing 5.18

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

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

¹This parameter is telling SymPy to use the quadrature method to compute the given integral numerically. For further explanation on how this method is working, we refer to the SymPy documentation which can be found here: <https://docs.sympy.org/latest/modules/integrals/integrals.html>, as well as the SciPy documentation on integration, which can be found here: <https://docs.scipy.org/doc/scipy/reference/generated/scipy.integrate.quad.html>. Some SciPy [Vir+20] functions are called by the SymPy library. Therefore, this reference shows up here.

6 Asymptotics

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

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

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

$$\begin{aligned} & 0 < \delta\lambda_w < 1, \quad 0 < \delta\lambda_\theta < 1, \quad 0 < \delta\lambda_r < 1, \\ \iff & 0 < \delta\frac{\sigma_{w3}^2}{w'^2} < 1, \quad 0 < \delta\frac{\sigma_{\theta l 3}^2}{\theta_l'^2} < 1, \quad 0 < \delta\frac{\sigma_{r_t 3}^2}{r_t'^2} < 1, \\ \iff & 0 < \delta\sigma_{w3}^2 < \overline{w'^2}, \quad 0 < \delta\sigma_{\theta l 3}^2 < \overline{\theta_l'^2}, \quad 0 < \delta\sigma_{r_t 3}^2 < \overline{r_t'^2}. \end{aligned}$$

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

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

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

So it might be safer to set

$$\begin{aligned}
\lambda_w, \lambda_r < \lambda_{wr} &\iff \left(\frac{\sigma_{w3}^2}{w'^2} < \frac{\rho_{wr_t} \sigma_{w3} \sigma_{r_t3}}{w' r'_t} \right) \wedge \left(\frac{\sigma_{r_t3}^2}{r'^2_t} < \frac{\rho_{wr_t} \sigma_{w3} \sigma_{r_t3}}{w' r'_t} \right) \\
&\iff \left(\sigma_{w3} \overline{w' r'_t} < \rho_{wr_t} \sigma_{r_t3} \overline{w'^2} \right) \wedge \left(\sigma_{r_t3} \overline{w' r'_t} < \rho_{wr_t} \sigma_{w3} \overline{r'^2_t} \right)
\end{aligned} \tag{6.0.2}$$

so that the rhs is greater and the bound is less restrictive. If we assume $\lambda_\theta = \lambda_r$ and $\lambda_{w\theta} = \lambda_{wr}$, then the model gains 5 new pdf parameters: δ , λ_w , λ_θ , $\lambda_{w\theta}$, $\lambda_{\theta r}$. Considering that the skewness goes to zero ($Sk_w \rightarrow 0$), we want the pdf to revert to a single normal distribution. Therefore, we need

$$\delta, \lambda_w, \lambda_r, \lambda_\theta, \lambda_{wr}, \lambda_{w\theta}, \lambda_{\theta r} \rightarrow 1. \tag{6.0.3}$$

In this limit, there are no third-order moments anymore, so they have to go to 0 as well. Also, we want to have that the kurtosis is approaching 3 (value of the kurtosis of a standard normal distribution). To ensure those points, as well as no division by zero in the code, we can define the following properties:

$$\lim_{\delta \rightarrow 1} (1 - \delta) \propto |Sk_w|, \tag{6.0.4}$$

which means that in the limit as $\delta \rightarrow 1$, $(1 - \delta)$ should “behave as” the absolute value of the skewness of w ,

$$0 < \lim_{\delta \rightarrow 1} \left(\frac{1 - \delta \lambda_x}{1 - \delta} \right) < \infty, \tag{6.0.5}$$

where x means any of w , r_t , or θ_l ,

$$0 < \lim_{\delta \rightarrow 1} \left(\frac{1 - \delta \lambda_x}{1 - \delta \lambda_y} \right) < \infty \tag{6.0.6}$$

where x is the same as above and y means any of w , r_t , or θ_l , $x \neq y$,

$$0 < \lim_{\delta \rightarrow 1} (\tilde{\sigma}_w)^2 = \lim_{\delta \rightarrow 1} \left(\frac{\sigma_w^2}{w'^2} \frac{1 - \delta}{1 - \delta \lambda_w} \right) < 1. \tag{6.0.7}$$

To ensure equation (6.0.4), we can use a linear “fit”, which looks like

$$\lambda_w = \lambda_\theta = \lambda_q = (1 - c_1)\delta + c_1 + \epsilon(1 - c_1), \quad (6.0.8)$$

where c_1 is some constant and ϵ is a very small number to avoid a division by zero in any of the equations. The fit for the other λ 's is

$$\lambda_{w\theta} = \lambda_{q\theta} = \lambda_{wq} = (1 - c_2)\delta + c_2 - \epsilon(1 - c_2), \quad (6.0.9)$$

where again c_2 is some constant and ϵ is the same as above. If we now look at the limit with the proposed fit (equation (6.0.8)), where we treat ϵ as zero, we get:

$$\lim_{\delta \rightarrow 1} \left(\frac{1 - \delta\lambda_w}{1 - \delta} \right) = \lim_{\delta \rightarrow 1} \left(\frac{1 - \delta((1 - c_1)\delta + c_1)}{1 - \delta} \right) = \lim_{\delta \rightarrow 1} \left(\frac{1 - ((1 - c_1)\delta^2 + c_1\delta)}{1 - \delta} \right) \quad (6.0.10)$$

$$= \lim_{\delta \rightarrow 1} \left(\frac{1 - \delta^2 + c_1\delta^2 - c_1\delta}{1 - \delta} \right) = \lim_{\delta \rightarrow 1} \left(\frac{1 - \delta^2 + c_1\delta(\delta - 1)}{1 - \delta} \right) \quad (6.0.11)$$

$$= \lim_{\delta \rightarrow 1} \left(\frac{1 - \delta^2}{1 - \delta} \right) - \lim_{\delta \rightarrow 1} \left(\frac{c_1\delta(1 - \delta)}{1 - \delta} \right) \quad (6.0.12)$$

$$(\text{L'Hôpital}) \stackrel{[\frac{0}{0}]}{=} \lim_{\delta \rightarrow 1} \left(\frac{-2\delta}{-1} \right) - \lim_{\delta \rightarrow 1} (c_1\delta) \quad (6.0.13)$$

$$= 2 - c_1. \quad (6.0.14)$$

Then we can also define the range of c_1 which should be $(0, 2)$ because we want to have $0 < \delta\lambda_w < 1$. For the reciprocal, we then have

$$\lim_{\delta \rightarrow 1} \left(\frac{1 - \delta}{1 - \delta\lambda_w} \right) = \lim_{\delta \rightarrow 1} \left(\frac{1 - \delta}{1 - \delta^2 + c_1\delta^2 - c_1\delta} \right) \stackrel{[\frac{0}{0}]}{=} \lim_{\delta \rightarrow 1} \left(\frac{-1}{-2\delta + 2c_1\delta - c_1} \right) \quad (6.0.15)$$

$$= \frac{-1}{-2 + c_1} = \frac{1}{2 - c_1}. \quad (6.0.16)$$

We now proceed and calculate all the other limits. First, we use (based on equation (4.2.3))

$$\tilde{\sigma}_w^2 = \frac{\sigma_w^2(1 - \delta)}{w'^2(1 - \delta\lambda_w)}, \quad (6.0.17)$$

and

$$\tilde{\sigma}_w^4 = \frac{\sigma_w^4(1 - \delta)^2}{\left(\overline{w'^2}\right)^2(1 - \delta\lambda_w)^2}. \quad (6.0.18)$$

We also treat the lower-order moments as fixed. To make the calculation even more readable, we calculate two limits here.

$$\lim_{\delta, \lambda_w \rightarrow 1} (\tilde{\sigma}_w^2) = \lim_{\delta, \lambda_w \rightarrow 1} \left(\frac{\sigma_w^2(1-\delta)}{\overline{w'^2}(1-\delta\lambda_w)} \right) = c \cdot \frac{\sigma_w^2}{\overline{w'^2}}, \quad (6.0.19)$$

and

$$\lim_{\delta, \lambda_w \rightarrow 1} (\tilde{\sigma}_w^4) = \lim_{\delta, \lambda_w \rightarrow 1} \left(\frac{\sigma_w^4(1-\delta)^2}{\left(\overline{w'^2}\right)^2 (1-\delta\lambda_w)^2} \right) = c \cdot \left(\frac{\sigma_w^2}{\overline{w'^2}} \right)^2. \quad (6.0.20)$$

That being said, we can have a look at equation (4.3.6) and take the limit.

$$\begin{aligned} \lim_{\delta \rightarrow 1} (\widehat{Sk}_w) &= \lim_{\delta \rightarrow 1} \left(\frac{1}{(1-\tilde{\sigma}_w^2)^{3/2}} \frac{\overline{w'^3}}{\left(\overline{w'^2}\right)^{3/2}} \frac{1}{\left(\frac{1-\delta\lambda_w}{1-\delta}\right)^{3/2}} \frac{1}{1-\delta} \right) \\ &= \lim_{\delta \rightarrow 1} \left(\frac{1}{(1-\tilde{\sigma}_w^2)^{3/2}} \frac{\overline{w'^3}}{\left(\overline{w'^2}\right)^{3/2}} \frac{(1-\delta)^{3/2}}{(1-\delta\lambda_w)^{3/2}} \frac{1}{1-\delta} \right) \\ &= \lim_{\delta \rightarrow 1} \left(\frac{1}{(1-\tilde{\sigma}_w^2)^{3/2}} \frac{\overline{w'^3}}{\left(\overline{w'^2}\right)^{3/2}} \frac{\cancel{(1-\delta)^{1/2}}^0}{(1-\delta\lambda_w)^{3/2}} \right) \\ &= 0 \end{aligned} \quad (6.0.21)$$

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

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

6.1 Limits for $\delta \rightarrow 1$

We start with letting $\delta \rightarrow 1$. Also, we are evaluating the following proposed fit for λ_w :

$$\lambda_w = \frac{1 - \sqrt[3]{1 - \delta}}{\delta}, \quad (6.1.1)$$

where we treat λ_w as a constant until the final step.

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

$$\lim_{\delta \rightarrow 1} (\overline{w'^4}) = (\overline{w'^2})^2 \lim_{\delta \rightarrow 1} \left(\frac{(1 - \delta \lambda_w)^2}{1 - \delta} \right) + \frac{(\overline{w'^3})^2}{\overline{w'^2}} \lim_{\delta \rightarrow 1} \left(\frac{1}{1 - \delta \lambda_w} \right) + \lim_{\delta \rightarrow 1} \left(\delta 3 \lambda_w^2 (\overline{w'^2})^2 \right) \quad (6.1.2)$$

Looking at this limit (for the calculation refer to appendix A.1), where we held the lower-order moments fixed and not depending on δ , unfortunately, we see that the fourth-order moment of w diverges. We try the proposed fit for λ_w :

$$\lim_{\delta \rightarrow 1} (\overline{w'^4}) = (\overline{w'^2})^2 \lim_{\delta \rightarrow 1} \left(\frac{(1 - (1 - \sqrt[3]{1 - \delta})^0)^2}{1 - \delta} \right) \quad (6.1.3)$$

$$+ \frac{(\overline{w'^3})^2}{\overline{w'^2}} \lim_{\delta \rightarrow 1} \left(\frac{1}{1 - (1 - (1 - \sqrt[3]{1 - \delta})^0)} \right) \quad (6.1.4)$$

$$+ 3 \lim_{\delta \rightarrow 1} \left(\left(1 - (1 - \sqrt[3]{1 - \delta})^0 \right)^2 (\overline{w'^2})^2 \right) \quad (6.1.5)$$

$$= \frac{(\overline{w'^3})^2}{\overline{w'^2}} \quad (6.1.6)$$

At least, we have a convergence to a ratio between the squared skewness and the variance now.

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

$$\lim_{\delta \rightarrow 1} \left(\overline{w'^2\theta'_l} \right) = \frac{\overline{w'^3} \cdot \overline{w'\theta'_l}}{\overline{w'^2}} \lim_{\delta \rightarrow 1} \left(\frac{1 - \delta\lambda_{w\theta}}{1 - \delta\lambda_w} \right) \quad (6.1.7)$$

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

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

$$\lim_{\delta \rightarrow 1} \left(\overline{w'^2\theta'_l} \right) = \frac{1}{3} \left(\frac{2\overline{w'^3} (\overline{w'\theta'_l})^2}{(\overline{w'^2})^2} \lim_{\delta \rightarrow 1} \left(\left(\frac{1 - \delta\lambda_{w\theta}}{1 - \delta\lambda_w} \right)^2 \right) + \frac{\overline{w'^2} \overline{\theta'^2_l}}{\overline{w'\theta'_l}} \lim_{\delta \rightarrow 1} \left(\frac{1 - \delta\lambda_w}{1 - \delta\lambda_{w\theta}} \right) \right) \quad (6.1.8)$$

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

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

$$\begin{aligned} \lim_{\delta \rightarrow 1} \left(\overline{w'r'_t\theta'_l} \right) &= \lim_{\delta \rightarrow 1} \left((1 - \delta)\alpha(w_1 - \overline{w}) \left[(r_{t1} - \overline{r_t}) (\theta_{l1} - \overline{\theta_l}) + r_{r_t\theta_l} \sigma_{r_{t1}} \sigma_{\theta_{l1}} \right] \right. \\ &\quad \left. + (1 - \delta)(1 - \alpha)(w_2 - \overline{w}) \left[(r_{t2} - \overline{r_t}) (\theta_{l2} - \overline{\theta_l}) + r_{r_t\theta_l} \sigma_{r_{t2}} \sigma_{\theta_{l2}} \right] \right) \\ &= 0 \end{aligned} \quad (6.1.9)$$

7 Summary

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

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

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

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

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

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

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

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

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

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

8 Outlook

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

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

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

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

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

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A Calculation of limits

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

$$\begin{aligned} \lim_{\delta \rightarrow 1} (\overline{w'^4}) &= \lim_{\delta \rightarrow 1} \left(\left(\overline{w'^2} \right)^2 \frac{(1 - \delta \lambda_w)^2}{(1 - \delta)} \left(3\tilde{\sigma}_w^4 + 6(1 - \tilde{\sigma}_w^2) \tilde{\sigma}_w^2 + (1 - \tilde{\sigma}_w^2)^2 \right) \right. \\ &\quad \left. + \frac{1}{(1 - \tilde{\sigma}_w^2)} \frac{1}{(1 - \delta \lambda_w)} \frac{\left(\overline{w'^3} \right)^2}{\overline{w'^2}} + \delta 3\lambda_w^2 \left(\overline{w'^2} \right)^2 \right) \end{aligned} \quad (\text{A.1.1})$$

$$\begin{aligned} &= \lim_{\delta \rightarrow 1} \left(\frac{\left(\overline{w'^2} \right)^2 (1 - \delta \lambda_w)^2 (4\tilde{\sigma}_w^2 - 2\tilde{\sigma}_w^4 + 1)}{(1 - \delta)} \right. \\ &\quad \left. + \frac{\left(\overline{w'^3} \right)^2 + \delta 3\lambda_w^2 \left(\overline{w'^2} \right)^3 (1 - \delta \lambda_w)}{(1 - \tilde{\sigma}_w^2)(1 - \delta \lambda_w)\overline{w'^2}} \right) \end{aligned} \quad (\text{A.1.2})$$

$$= \lim_{\delta \rightarrow 1} \left(\frac{\left(\overline{w'^2} \right)^2 (1 - \delta \lambda_w)^2}{(1 - \delta)} + \frac{\left(\overline{w'^3} \right)^2 + \delta 3\lambda_w^2 \left(\overline{w'^2} \right)^3 (1 - \delta \lambda_w)}{(1 - \delta \lambda_w)\overline{w'^2}} \right) \quad (\text{A.1.3})$$

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

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

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

$$\lim_{\delta \rightarrow 1} (\overline{w'^2\theta'_l}) = \lim_{\delta \rightarrow 1} \left(\frac{1}{(1 - \tilde{\sigma}_w^2)^2} \frac{1 - \delta\lambda_{w\theta} \overline{w'^3}}{1 - \delta\lambda_w \overline{w'^2}} \overline{w'\theta'_l} \right) \quad (\text{A.2.1})$$

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

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

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

$$\lim_{\delta \rightarrow 1} (\overline{w'\theta'^2_l}) = \lim_{\delta \rightarrow 1} \left(\frac{2(1 - \delta\lambda_{w\theta})^2 \overline{w'^3} (\overline{w'\theta'_l})^2}{3(1 - \delta\lambda_w)^2 (1 - \tilde{\sigma}_w^2)^2 (\overline{w'^2})^2} + \frac{(1 - \delta\lambda_w) (1 - \tilde{\sigma}_w^2)^{\frac{1}{2}} \overline{w'^2} \overline{\theta'^2_l}}{3(1 - \delta\lambda_{w\theta}) \overline{w'\theta'_l}} \right) \quad (\text{A.3.1})$$

$$= \frac{2}{3} \lim_{\delta \rightarrow 1} \left(\frac{(1 - \delta\lambda_{w\theta})^2 \overline{w'^3} (\overline{w'\theta'_l})^2}{(1 - \delta\lambda_w)^2 (\overline{w'^2})^2} \right) + \lim_{\delta \rightarrow 1} \left(\frac{(1 - \delta\lambda_w) \overline{w'^2} \overline{\theta'^2_l}}{3(1 - \delta\lambda_{w\theta}) \overline{w'\theta'_l}} \right) \quad (\text{A.3.2})$$

$$= \frac{1}{3} \left(\frac{2\overline{w'^3} (\overline{w'\theta'_l})^2}{(\overline{w'^2})^2} \lim_{\delta \rightarrow 1} \left(\left(\frac{1 - \delta\lambda_{w\theta}}{1 - \delta\lambda_w} \right)^2 \right) + \frac{\overline{w'^2} \overline{\theta'^2_l}}{\overline{w'\theta'_l}} \lim_{\delta \rightarrow 1} \left(\frac{1 - \delta\lambda_w}{1 - \delta\lambda_{w\theta}} \right) \right) \quad (\text{A.3.3})$$

B Code

B.1 User Guide

B.1.1 Accessing the code

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

B.1.2 Key files and their purposes

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

B.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()`).

B.1.4 Displaying equations effectively

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

B.1.5 Handling integrals

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

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

B.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_w_3 = Symbol('\tilde{\sigma}_{w3}')
23  sigma_tilde_w = Symbol('\tilde{\sigma}_w')
24  sigma_w_3 = Symbol('\sigma_{w3}')
25  sigma_theta_l_3 = Symbol('\sigma_{\theta_l 3}')
26  sigma_r_t_3 = Symbol('\sigma_{r_t 3}')
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_l_bar = Symbol('\overline{w}^2\theta\_l')
42 w_prime_theta_prime_l_2_bar = Symbol('\overline{w}\theta^2\_l')
43 w_prime_theta_l_prime_bar = Symbol('\overline{w}\theta\_l')
44
45 w_prime_r_t_prime_theta_l_prime_bar = Symbol('\overline{w}\{r_t\}\{\theta_l\}')
46
47 # r
48 r_t = Symbol('r_t')
49
50 r_t_bar, r_t_prime_2_bar, r_t_prime_3_bar = symbols(
51     '\overline{r_t} \overline{r_t}^2 \overline{r_t}^3'
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 r_t_prime_theta_l_prime_bar = Symbol('\overline{r_t}\theta\_l')
61
62 # theta
63 theta_l = Symbol('\theta_l')
64
65 theta_l_bar, theta_l_prime_2_bar, theta_l_prime_3_bar = symbols(
66     '\overline{\theta_l} \overline{\theta_l}^2 \overline{\theta_l}^3'
67 )
68
69 theta_l_i, theta_l_1, theta_l_2 = symbols(
70     '\theta_{li} \theta_{l1} \theta_{l2}'
71 )
72
73 theta_tilde_prime_l = Symbol('\tilde{\theta}_l')
74
75 theta_tilde_l_i, theta_tilde_l_1, theta_tilde_l_2 = symbols(
76     '\tilde{\theta}_{li} \tilde{\theta}_{l1} \tilde{\theta}_{l2}'
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_l = Symbol('r_{r_t}\theta_l')
88 triple_gaussian = Symbol('P_{tmg}(\hat{w}, \tilde{\theta}_l, \tilde{r\_t})')
89 sk_w_hat = Symbol('\widehat{Sk}_w')
90 sk_theta_l_hat = Symbol('\widehat{Sk}_{\theta_l}')
91 c_w_theta_l_hat = Symbol('\widehat{c}_{w\theta_l}')
92 sk_r_t_hat = Symbol('\widehat{Sk}_{r_t}')
93 c_w_r_t_hat = Symbol('\widehat{c}_{wr_t}')
94

```

```

95 | beta_theta_1 = Symbol('\\beta_{\\theta_1}')
96 | beta_r_t = Symbol('\\beta_{r_t}')
97 |
98 | G_3 = Symbol('G_3')
99 | G_3_hat = Symbol('\\hat{G_3}')
100 |
101 | G_w, G_1_w, G_2_w, G_3_w = symbols(
102 |     'G_{w}(w) G_{1w}(w) G_{2w}(w) G_{3w}(w)'
103 | )
104 |
105 | G_w_1_2 = Symbol('G_{w_{12}}')
106 |
107 | G_w_theta = Symbol('G_{w\\theta}(w,\\theta)')
108 | G_1_w_theta = Symbol('G_{1w\\theta}(w,\\theta)')
109 | G_2_w_theta = Symbol('G_{2w\\theta}(w,\\theta)')
110 | G_3_w_theta = Symbol('G_{3w\\theta}(w,\\theta)')
111 |
112 | G_theta_r = Symbol('G_{\\theta r}(\\theta, r)')
113 | G_1_theta_r = Symbol('G_{1\\theta r}(\\theta, r)')
114 | G_2_theta_r = Symbol('G_{2\\theta r}(\\theta, r)')
115 | G_3_theta_r = Symbol('G_{3\\theta r}(\\theta, r)')
116 |
117 | G_w_theta_1_r_t = Symbol('G_{w{\\theta_1}{r_t}}(w,{\\theta_1},{r_t})')
118 | G_1_w_theta_1_r_t = Symbol('G_{1w{\\theta_1}{r_t}}(w,{\\theta_1},{r_t})')
119 | G_2_w_theta_1_r_t = Symbol('G_{2w{\\theta_1}{r_t}}(w,{\\theta_1},{r_t})')
120 | G_3_w_theta_1_r_t = Symbol('G_{3w{\\theta_1}{r_t}}(w,{\\theta_1},{r_t})')
121 |
122 | G_theta, G_1_theta, G_2_theta, G_3_theta = symbols(
123 |     'G_{\\theta}(\\theta) G_{1\\theta}(\\theta) G_{2\\theta}(\\theta)
124 |     ↪ G_{3\\theta}(\\theta)'
125 | )
126 | rho_w_theta_1 = Symbol('\\rho_{w\\theta_1}')
127 | rho_w_r_t = Symbol('\\rho_{wr_t}')
128 | rho_theta_1_r_t = Symbol('\\rho_{\\theta_1r_t}')

```

Listing B.1: symbols.py

B.3 checked_functions.py

```

1 | import sympy as sp
2 | from sympy import abc, 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(alpha=sp.abc.alpha, delta=sp.abc.delta, w_1=sym.w_1, w_2=sym.w_2,
18                  w_bar=sym.w_bar, sigma_w=sym.sigma_w, sigma_w_3=sym.sigma_w_3):
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_w_3 ** 2))
22
23
24 def w_prime_3_bar(alpha=sp.abc.alpha, delta=sp.abc.delta, 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_w_3=sym.sigma_w_3):
37     return (w_prime_2_bar ** 2 *
38            ((1 - delta * (sigma_w_3 ** 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_w_3 ** 2 / w_prime_2_bar))) *
45             (w_prime_3_bar ** 2 / w_prime_2_bar)) +
46            (delta * 3 * sigma_w_3 ** 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(alpha=sp.abc.alpha,
62                        delta=sp.abc.delta,
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_theta_l_3_1=sym.sigma_theta_l_3):
69     return (((1 - delta) * alpha * ((theta_l_1 - theta_l_bar) ** 2 + sigma_theta_l_1 **
    ↪ 2)) +
70            ((1 - delta) * (1 - alpha) *
71             ((theta_l_2 - theta_l_bar) ** 2 + sigma_theta_l_2 ** 2)) +
72            (delta * sigma_theta_l_3_1 ** 2))
73
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_r_t_3_t=sym.sigma_r_t_3):
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_r_t_3_t ** 2))
112
113
114 def r_t_prime_3_bar(alpha=sp.abc.alpha,
115                   delta=sp.abc.delta,
116                   r_t_1=sym.r_t_1,

```

```

117         r_t_2=sym.r_t_2,
118         r_t_bar=sym.r_t_bar,
119         sigma_r_t_1=sym.sigma_r_t_1,
120         sigma_r_t_2=sym.sigma_r_t_2):
121     return (((1 - delta) * alpha *
122             ((r_t_1 - r_t_bar) ** 3 +
123              3 * sigma_r_t_1 ** 2 * (r_t_1 - r_t_bar))) +
124            ((1 - delta) * (1 - alpha) *
125             ((r_t_2 - r_t_bar) ** 3 +
126              3 * sigma_r_t_2 ** 2 * (r_t_2 - r_t_bar))))
127
128
129 # -----
130
131 # Mixed equations
132 # -----
133
134 def w_prime_theta_l_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                               theta_l_1=sym.theta_l_1,
140                               theta_l_2=sym.theta_l_2,
141                               theta_l_bar=sym.theta_l_bar,
142                               cov_lambda_w_theta=sym.rho_w_theta_l * sym.sigma_w_3 *
143                               ↪ sym.sigma_theta_l_3):
144     return (((1 - delta) * alpha * ((w_1 - w_bar) * (theta_l_1 - theta_l_bar))) +
145            ((1 - delta) * (1 - alpha) * ((w_2 - w_bar) * (theta_l_2 - theta_l_bar)))
146            + delta * cov_lambda_w_theta)
147
148 def w_prime_r_t_prime_bar(alpha=sp.abc.alpha,
149                            delta=sp.abc.delta,
150                            w_1=sym.w_1,
151                            w_2=sym.w_2,
152                            w_bar=sym.w_bar,
153                            r_t_1=sym.r_t_1,
154                            r_t_2=sym.r_t_2,
155                            r_t_bar=sym.r_t_bar,
156                            cov_lambda_w_r=sym.rho_w_r_t * sym.sigma_w_3 *
157                            ↪ sym.sigma_r_t_3):
158     return (((1 - delta) * alpha * ((w_1 - w_bar) * (r_t_1 - r_t_bar))) +
159            ((1 - delta) * (1 - alpha) * ((w_2 - w_bar) * (r_t_2 - r_t_bar)))
160            + delta * cov_lambda_w_r)
161
162 def w_prime_2_theta_l_prime_bar(sigma_tilde_w=sym.sigma_tilde_w,
163                                  delta=sp.abc.delta,
164                                  lambda_w_theta=sym.lambda_w_theta,
165                                  lambda_w=sym.lambda_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=sym.w_prime_theta_l_prime_bar):

```

```

169     return ((1 / (1 - sigma_tilde_w ** 2)) *
170            ((1 - delta * lambda_w_theta) / (1 - delta * lambda_w)) *
171            (w_prime_3_bar / w_prime_2_bar) *
172            w_prime_theta_l_prime)
173
174
175 def w_prime_theta_l_prime_2_bar(delta=sp.abc.delta,
176                                lambda_w_theta=sym.lambda_w_theta,
177                                lambda_w=sym.lambda_w,
178                                sigma_tilde_w=sym.sigma_tilde_w,
179                                w_prime_3_bar=sym.w_prime_3_bar,
180                                w_prime_2_bar=sym.w_prime_2_bar,
181                                w_prime_theta_l_prime_bar=sym.w_prime_theta_l_prime_bar,
182                                theta_l_prime_3_bar=sym.theta_l_prime_3_bar):
183     return (Rational(2, 3) *
184            ((1 - delta * lambda_w_theta) ** 2 / (1 - delta * lambda_w) ** 2) *
185            (1 / (1 - sigma_tilde_w ** 2) ** 2) *
186            (w_prime_3_bar / w_prime_2_bar ** 2) *
187            w_prime_theta_l_prime_bar ** 2 +
188            Rational(1, 3) *
189            ((1 - delta * lambda_w) / (1 - delta * lambda_w_theta)) *
190            (1 - sigma_tilde_w ** 2) *
191            ((w_prime_2_bar * theta_l_prime_3_bar) / w_prime_theta_l_prime_bar))
192
193
194 def w_prime_theta_l_prime_2_bar_beta(
195     sigma_tilde_w=sym.sigma_tilde_w,
196     delta=sp.abc.delta,
197     lambda_theta=sym.lambda_theta,
198     lambda_w=sym.lambda_w,
199     w_prime_3_bar=sym.w_prime_3_bar,
200     w_prime_2_bar=sym.w_prime_2_bar,
201     beta=sp.abc.beta,
202     theta_l_prime_2_bar=sym.theta_l_prime_2_bar,
203     lambda_w_theta=sym.lambda_w_theta,
204     w_prime_theta_l_prime_bar=sym.w_prime_theta_l_prime_bar):
205     from sympy import Rational
206     return (
207         (1 / (1 - sigma_tilde_w ** 2)) *
208         ((1 - delta * lambda_theta) / (1 - delta * lambda_w)) *
209         (w_prime_3_bar / w_prime_2_bar) *
210         (
211             Rational(1, 3) * beta * theta_l_prime_2_bar +
212             (
213                 ((1 - Rational(1, 3) * beta) / (1 - sigma_tilde_w ** 2)) *
214                 ((1 - delta * lambda_w_theta) ** 2 /
215                  ((1 - delta * lambda_w) * (1 - delta * lambda_theta))) *
216                 (w_prime_theta_l_prime_bar ** 2 / w_prime_2_bar)
217             )
218         )
219     )
220
221
222 def w_prime_r_t_prime_theta_l_prime_bar(delta=sp.abc.delta,

```

```

223         alpha=sp.abc.alpha,
224         w_1=sym.w_1,
225         w_2=sym.w_2,
226         w_bar=sym.w_bar,
227         r_t_1=sym.r_t_1,
228         r_t_2=sym.r_t_2,
229         r_t_bar=sym.r_t_bar,
230         theta_l_1=sym.theta_l_1,
231         theta_l_2=sym.theta_l_2,
232         theta_l_bar=sym.theta_l_bar,
233         r_r_t_theta_l=sym.r_r_t_theta_l,
234         sigma_r_t_1=sym.sigma_r_t_1,
235         sigma_r_t_2=sym.sigma_r_t_2,
236         sigma_theta_l_1=sym.sigma_theta_l_1,
237         sigma_theta_l_2=sym.sigma_theta_l_2):
238     return (((1 - delta) * alpha * (w_1 - w_bar) *
239             (
240                 (r_t_1 - r_t_bar) * (theta_l_1 - theta_l_bar) +
241                 r_r_t_theta_l * sigma_r_t_1 * sigma_theta_l_1
242             )) +
243             ((1 - delta) * (1 - alpha) * (w_2 - w_bar) *
244             (
245                 (r_t_2 - r_t_bar) * (theta_l_2 - theta_l_bar) +
246                 r_r_t_theta_l * sigma_r_t_2 * sigma_theta_l_2
247             )))
248
249
250 def w_prime_r_t_prime_theta_l_prime_bar_beta(
251     beta=sp.abc.beta,
252     sigma_tilde_w=sym.sigma_tilde_w,
253     delta=sp.abc.delta,
254     lambda_theta_r=sym.lambda_theta_r,
255     lambda_w=sym.lambda_w,
256     r_t_prime_theta_l_prime_bar=sym.r_t_prime_theta_l_prime_bar,
257     w_prime_3_bar=sym.w_prime_3_bar,
258     w_prime_2_bar=sym.w_prime_2_bar,
259     lambda_w_r=sym.lambda_w_r,
260     lambda_w_theta=sym.lambda_w_theta,
261     w_prime_r_t_prime_bar=sym.w_prime_r_t_prime_bar,
262     w_prime_theta_l_prime_bar=sym.w_prime_theta_l_prime_bar):
263     from sympy import Rational
264     return (
265         (
266             ((Rational(1, 3) * beta) / (1 - sigma_tilde_w ** 2)) *
267             ((1 - delta * lambda_theta_r) / (1 - delta * lambda_w)) *
268             r_t_prime_theta_l_prime_bar *
269             (w_prime_3_bar / w_prime_2_bar)
270         ) +
271         (
272             ((1 - Rational(1, 3) * beta) / (1 - sigma_tilde_w ** 2) ** 2) *
273             (((1 - delta * lambda_w_r) * (1 - delta * lambda_w_theta)) /
274              ((1 - delta * lambda_w) ** 2)) *
275             w_prime_r_t_prime_bar *
276             w_prime_theta_l_prime_bar *

```



```

277         (w_prime_3_bar / w_prime_2_bar ** 2)
278     )
279 )
280
281
282 def w_prime_r_t_prime_theta_l_prime_bar_E(
283     E=sp.abc.E,
284     sigma_tilde_w=sym.sigma_tilde_w,
285     delta=sp.abc.delta,
286     lambda_theta_r=sym.lambda_theta_r,
287     lambda_w=sym.lambda_w,
288     r_t_prime_theta_l_prime_bar=sym.r_t_prime_theta_l_prime_bar,
289     w_prime_3_bar=sym.w_prime_3_bar,
290     w_prime_2_bar=sym.w_prime_2_bar,
291     lambda_w_r=sym.lambda_w_r,
292     lambda_w_theta=sym.lambda_w_theta,
293     w_prime_r_t_prime_bar=sym.w_prime_r_t_prime_bar,
294     w_prime_theta_l_prime_bar=sym.w_prime_theta_l_prime_bar):
295     from sympy import Rational
296     return (
297         (
298             ((Rational(1, 2) * E) / (1 - sigma_tilde_w ** 2)) *
299             ((1 - delta * lambda_theta_r) / (1 - delta * lambda_w)) *
300             r_t_prime_theta_l_prime_bar *
301             (w_prime_3_bar / w_prime_2_bar)
302         ) +
303         (
304             ((1 - Rational(1, 2) * E) / (1 - sigma_tilde_w ** 2) ** 2) *
305             (((1 - delta * lambda_w_r) * (1 - delta * lambda_w_theta)) /
306              ((1 - delta * lambda_w) ** 2)) *
307             w_prime_r_t_prime_bar *
308             w_prime_theta_l_prime_bar *
309             (w_prime_3_bar / w_prime_2_bar ** 2)
310         )
311     )
312
313
314 def r_t_prime_theta_l_prime_bar(
315     alpha=sp.abc.alpha, delta=sp.abc.delta,
316     r_t_1=sym.r_t_1, r_t_2=sym.r_t_2, r_t_prime_bar=sym.r_t_bar,
317     theta_l_1=sym.theta_l_1, theta_l_2=sym.theta_l_2,
318     theta_l_bar=sym.theta_l_bar,
319     r_r_t_theta_l=sym.r_r_t_theta_l,
320     sigma_r_t_1=sym.sigma_r_t_1, sigma_r_t_2=sym.sigma_r_t_2,
321     sigma_theta_l_1=sym.sigma_theta_l_1,
322     sigma_theta_l_2=sym.sigma_theta_l_2,
323     cov_lambda_r_theta=sym.rho_theta_l_r_t * sym.sigma_theta_l_3 * sym.sigma_r_t_3):
324     return ((1 - delta) * alpha * (
325         (r_t_1 - r_t_prime_bar) * (theta_l_1 - theta_l_bar) +
326         r_r_t_theta_l * sigma_r_t_1 * sigma_theta_l_1) +
327         ((1 - delta) * (1 - alpha) * (
328             (r_t_2 - r_t_prime_bar) * (theta_l_2 - theta_l_bar) +
329             r_r_t_theta_l * sigma_r_t_2 * sigma_theta_l_2)) +
330         delta * cov_lambda_r_theta)

```

```

331
332
333 # ---
334
335 # Distributions
336 # ---
337
338 G_1_theta_1 = Normal(name='G_1_theta_1', mean=sym.theta_1_1, std=sym.sigma_theta_1_1)
339 G_1_theta_1_density = density(G_1_theta_1)(sym.theta_1)
340
341 G_2_theta_1 = Normal(name='G_2_theta_1', mean=sym.theta_1_2, std=sym.sigma_theta_1_2)
342 G_2_theta_1_density = density(G_2_theta_1)(sym.theta_1)
343
344 G_3_theta_1 = Normal(name='G_3_theta_1', mean=sym.theta_1_bar, std=sym.sigma_theta_1_3)
345 G_3_theta_1_density = density(G_3_theta_1)(sym.theta_1)
346
347 G_theta = ((1 - sp.abc.delta) * sp.abc.alpha * G_1_theta_1_density +
348            (1 - sp.abc.delta) * (1 - sp.abc.alpha) * G_2_theta_1_density +
349            sp.abc.delta * G_3_theta_1_density)
350
351 # ---
352
353 G_1_w = Normal(name='G_1_w', mean=sym.w_1, std=sym.sigma_w)
354 G_1_w_density = density(G_1_w)(sp.abc.w)
355
356 G_2_w = Normal(name='G_2_w', mean=sym.w_2, std=sym.sigma_w)
357 G_2_w_density = density(G_2_w)(sp.abc.w)
358
359 G_3_w = Normal(name='G_3_w', mean=sym.w_bar, std=sym.sigma_w_3)
360 G_3_w_density = density(G_3_w)(sp.abc.w)
361
362 G_w = ((1 - sp.abc.delta) * sp.abc.alpha * G_1_w_density +
363        (1 - sp.abc.delta) * (1 - sp.abc.alpha) * G_2_w_density +
364        sp.abc.delta * G_3_w_density)
365
366 # ---
367
368 G_1_w_theta = Normal(name='G_1_w_theta', mean=sp.Matrix([sym.w_1, sym.theta_1_1]),
369                    std=sp.Matrix([[sym.sigma_w ** 2, 0], [0, sym.sigma_theta_1_1 **
370                    ↪ 2]]))
371 G_1_w_theta_density = density(G_1_w_theta)(sp.abc.w, sp.abc.theta)
372
373 G_2_w_theta = Normal(name='G_2_w_theta', mean=sp.Matrix([sym.w_2, sym.theta_1_2]),
374                    std=sp.Matrix([[sym.sigma_w ** 2, 0], [0, sym.sigma_theta_1_2 **
375                    ↪ 2]]))
376 G_2_w_theta_density = density(G_2_w_theta)(sp.abc.w, sp.abc.theta)
377
378 G_3_w_theta = Normal(name='G_3_w_theta', mean=sp.Matrix([sym.w_bar, sym.theta_1_bar]),
379                    std=sp.Matrix([
380                    sym.sigma_w_3 ** 2,
381                    sym.rho_w_theta_1 * sym.sigma_w_3 * sym.sigma_theta_1_3],
382                    [sym.rho_w_theta_1 * sym.sigma_w_3 * sym.sigma_theta_1_3,
383                    sym.sigma_theta_1_3 ** 2]
384                    ]))

```

```

383 G_3_w_theta_density = sp.simplify(density(G_3_w_theta)(sp.abc.w, sp.abc.theta))
384
385 G_w_theta = ((1 - sp.abc.delta) * sp.abc.alpha * G_1_w_theta_density +
386              (1 - sp.abc.delta) * (1 - sp.abc.alpha) * G_2_w_theta_density +
387              sp.abc.delta * G_3_w_theta_density)
388
389 # -----
390
391 mu_1_theta_l_r_t = sp.Matrix([sym.theta_l_1, sym.r_t_1])
392 Sigma_1_theta_l_r_t = sp.Matrix([[sym.sigma_theta_l_1 ** 2,
393                                  sym.r_r_t_theta_l * sym.sigma_theta_l_1 *
394                                  ↪ sym.sigma_r_t_1],
395                                  [sym.r_r_t_theta_l * sym.sigma_theta_l_1 *
396                                  ↪ sym.sigma_r_t_1,
397                                  sym.sigma_r_t_1 ** 2]])
398
399 G_1_theta_l_r_t = Normal(name='G_1_theta_l_r_t',
400                           mean=mu_1_theta_l_r_t,
401                           std=Sigma_1_theta_l_r_t)
402
403 G_1_theta_l_r_t_density = density(G_1_theta_l_r_t)(sym.theta_l, sym.r_t)
404
405 mu_2_theta_l_r_t = sp.Matrix([sym.theta_l_2, sym.r_t_2])
406 Sigma_2_theta_l_r_t = sp.Matrix(
407     [[sym.sigma_theta_l_2 ** 2,
408       sym.r_r_t_theta_l * sym.sigma_theta_l_2 * sym.sigma_r_t_2],
409     [sym.r_r_t_theta_l * sym.sigma_theta_l_2 * sym.sigma_r_t_2,
410       sym.sigma_r_t_2 ** 2]])
411
412 G_2_theta_l_r_t = Normal(name='G_2_theta_l_r_t',
413                           mean=mu_2_theta_l_r_t,
414                           std=Sigma_2_theta_l_r_t)
415
416 G_2_theta_l_r_t_density = density(G_2_theta_l_r_t)(sym.theta_l, sym.r_t)
417
418 mu_3_theta_l_r_t = sp.Matrix([sym.theta_l_bar, sym.r_t_bar])
419 Sigma_3_theta_l_r_t = sp.Matrix(
420     [[sym.sigma_theta_l_3 ** 2,
421       sym.rho_theta_l_r_t * sym.sigma_theta_l_3 * sym.sigma_r_t_3],
422     [sym.rho_theta_l_r_t * sym.sigma_theta_l_3 * sym.sigma_r_t_3,
423       sym.sigma_r_t_3 ** 2]])
424
425 G_3_theta_l_r_t = Normal(name='G_3_theta_l_r_t',
426                           mean=mu_3_theta_l_r_t,
427                           std=Sigma_3_theta_l_r_t)
428
429 G_3_theta_l_r_t_density = density(G_3_theta_l_r_t)(sym.theta_l, sym.r_t)
430
431 G_theta_l_r_t = ((1 - sp.abc.delta) * sp.abc.alpha * G_1_theta_l_r_t_density +
432                  (1 - sp.abc.delta) * (1 - sp.abc.alpha) * G_2_theta_l_r_t_density +
433                  sp.abc.delta * G_3_theta_l_r_t_density)
434
435 # -----

```

```

435
436 mu_1_w_theta_l_r_t = sp.Matrix([sym.w_1, sym.theta_l_1, sym.r_t_1])
437 Sigma_1_w_theta_l_r_t = sp.Matrix(
438     [[sym.sigma_w ** 2,
439      0,
440      0],
441     [0,
442      sym.sigma_theta_l_1 ** 2,
443      sym.r_r_t_theta_l * sym.sigma_theta_l_1 * sym.sigma_r_t_1],
444     [0,
445      sym.r_r_t_theta_l * sym.sigma_theta_l_1 * sym.sigma_r_t_1,
446      sym.sigma_r_t_1 ** 2]])
447
448 G_1_w_theta_l_r_t = Normal(name='G_1_w_theta_l_r_t',
449                             mean=mu_1_w_theta_l_r_t,
450                             std=Sigma_1_w_theta_l_r_t)
451
452 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)
453
454 mu_2_w_theta_l_r_t = sp.Matrix([sym.w_2, sym.theta_l_2, sym.r_t_2])
455 Sigma_2_w_theta_l_r_t = sp.Matrix([[sym.sigma_w ** 2,
456                                     0,
457                                     0],
458                                    [0,
459                                     sym.sigma_theta_l_2 ** 2,
460                                     sym.r_r_t_theta_l * sym.sigma_theta_l_2 *
461                                     ↪ sym.sigma_r_t_2],
462                                    [0,
463                                     sym.r_r_t_theta_l * sym.sigma_theta_l_2 *
464                                     ↪ sym.sigma_r_t_2,
465                                     sym.sigma_r_t_2 ** 2]])
466
467 G_2_w_theta_l_r_t = Normal(name='G_2_w_theta_l_r_t',
468                             mean=mu_2_w_theta_l_r_t,
469                             std=Sigma_2_w_theta_l_r_t)
470
471 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)
472
473 mu_3_w_theta_l_r_t = sp.Matrix([sym.w_bar, sym.theta_l_bar, sym.r_t_bar])
474 Sigma_3_w_theta_l_r_t = sp.Matrix(
475     [[sym.sigma_w_3 ** 2,
476      sym.rho_w_theta_l * sym.sigma_w_3 * sym.sigma_theta_l_3,
477      sym.rho_w_r_t * sym.sigma_theta_l_3 * sym.sigma_r_t_3],
478     [
479      sym.rho_w_theta_l * sym.sigma_w_3 * sym.sigma_theta_l_3,
480      sym.sigma_theta_l_3 ** 2,
481      sym.rho_theta_l_r_t * sym.sigma_w_3 * sym.sigma_r_t_3],
482     [sym.rho_w_r_t * sym.sigma_theta_l_3 * sym.sigma_r_t_3,
483      sym.rho_theta_l_r_t * sym.sigma_w_3 * sym.sigma_r_t_3,
484      sym.sigma_r_t_3 ** 2]])
485
486 G_3_w_theta_l_r_t = Normal(name='G_3_w_theta_l_r_t',
487                             mean=mu_3_w_theta_l_r_t,
488                             std=Sigma_2_w_theta_l_r_t)

```

```

487 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)
488
489 G_w_theta_l_r_t = ((1 - sp.abc.delta) * sp.abc.alpha * G_1_w_theta_l_r_t_density +
490                    (1 - sp.abc.delta) * (1 - sp.abc.alpha) * G_2_w_theta_l_r_t_density +
491                    sp.abc.delta * G_3_w_theta_l_r_t_density)
492
493
494 # -----
495
496 # sigma equations
497 # -----
498
499 def sigma_tilde_w(sigma_w=sym.sigma_w, w_prime_2_bar=sym.w_prime_2_bar,
500                  delta=sp.abc.delta, lambda_w=sym.lambda_w):
501     from sympy import sqrt
502     return ((sigma_w / sqrt(w_prime_2_bar)) *
503            (1 / sqrt((1 - delta * lambda_w) / (1 - delta))))
504
505
506 def sigma_tilde_r_t_1(sigma_r_t_1=sym.sigma_r_t_1, r_t_prime_2_bar=sym.r_t_prime_2_bar,
507                      delta=sp.abc.delta, lambda_r=sym.lambda_r):
508     from sympy import sqrt
509     return ((sigma_r_t_1 / sqrt(r_t_prime_2_bar)) *
510            (1 / sqrt((1 - delta * lambda_r) / (1 - delta))))
511
512
513 def sigma_tilde_r_t_2(sigma_r_t_2=sym.sigma_r_t_2, r_t_prime_2_bar=sym.r_t_prime_2_bar,
514                      delta=sp.abc.delta, lambda_r=sym.lambda_r):
515     from sympy import sqrt
516     return ((sigma_r_t_2 / sqrt(r_t_prime_2_bar)) *
517            (1 / sqrt((1 - delta * lambda_r) / (1 - delta))))
518
519
520 def sigma_tilde_theta_l_1(sigma_theta_l_1=sym.sigma_theta_l_1,
521                          theta_l_prime_2_bar=sym.theta_l_prime_2_bar,
522                          delta=sp.abc.delta, lambda_theta=sym.lambda_theta):
523     from sympy import sqrt
524     return ((sigma_theta_l_1 / sqrt(theta_l_prime_2_bar)) *
525            (1 / sqrt((1 - delta * lambda_theta) / (1 - delta))))
526
527
528 def sigma_tilde_theta_l_2(sigma_theta_l_2=sym.sigma_theta_l_2,
529                          theta_l_prime_2_bar=sym.theta_l_prime_2_bar,
530                          delta=sp.abc.delta, lambda_theta=sym.lambda_theta):
531     from sympy import sqrt
532     return ((sigma_theta_l_2 / sqrt(theta_l_prime_2_bar)) *
533            (1 / sqrt((1 - delta * lambda_theta) / (1 - delta))))
534
535
536 # -----
537
538 # lambda equations
539 # -----
540

```

```

541 def lambda_w(sigma_w_3=sym.sigma_w_3, w_prime_2_bar=sym.w_prime_2_bar):
542     return sigma_w_3 ** 2 / w_prime_2_bar
543
544
545 def lambda_theta(sigma_theta_l_3=sym.sigma_theta_l_3,
546                 theta_l_prime_2_bar=sym.theta_l_prime_2_bar):
547     return sigma_theta_l_3 ** 2 / theta_l_prime_2_bar
548
549
550 def lambda_r(sigma_r_t_3=sym.sigma_r_t_3,
551             r_t_prime_2_bar=sym.r_t_prime_2_bar):
552     return sigma_r_t_3 ** 2 / r_t_prime_2_bar
553
554
555 def lambda_w_theta(cov_lambda_w_theta=sym.rho_w_theta_l * sym.sigma_w_3 *
556                  ↪ sym.sigma_theta_l_3,
557                  w_prime_theta_l_prime_bar=sym.w_prime_theta_l_prime_bar):
558     return cov_lambda_w_theta / w_prime_theta_l_prime_bar
559
560 def lambda_w_r(cov_lambda_w_r=sym.rho_w_r_t * sym.sigma_w_3 * sym.sigma_r_t_3,
561              w_prime_r_t_prime_bar=sym.w_prime_r_t_prime_bar):
562     return cov_lambda_w_r / w_prime_r_t_prime_bar
563
564
565 def lambda_r_theta(cov_lambda_r_theta=sym.rho_theta_l_r_t * sym.sigma_r_t_3 *
566                  ↪ sym.sigma_theta_l_3,
567                  r_t_prime_theta_l_prime_bar=sym.r_t_prime_theta_l_prime_bar):
568     return cov_lambda_r_theta / r_t_prime_theta_l_prime_bar
569
570 # ---
571
572 # sk
573 # ---
574
575 def sk_theta_l_hat_beta(sk_w_hat=sym.sk_w_hat, c_hat_w_theta_l=sym.c_w_theta_l_hat,
576                       beta=sp.abc.beta):
577     return sk_w_hat * c_hat_w_theta_l * (beta + (1 - beta) * c_hat_w_theta_l ** 2)
578
579
580 def sk_theta_l_hat(theta_l_prime_3_bar=sym.theta_l_prime_3_bar,
581                  theta_l_prime_2_bar=sym.theta_l_prime_2_bar,
582                  delta=sp.abc.delta,
583                  lambda_theta=sym.lambda_theta):
584     from sympy import Rational
585     return ((theta_l_prime_3_bar / theta_l_prime_2_bar ** Rational(3, 2)) *
586            (1 / ((1 - delta * lambda_theta) / (1 - delta)) ** Rational(3, 2)) *
587            (1 / (1 - delta)))
588
589
590 def sk_r_t_hat(r_t_prime_3_bar=sym.r_t_prime_3_bar,
591              r_t_prime_2_bar=sym.r_t_prime_2_bar,
592              delta=sp.abc.delta,

```

```

593         lambda_r=sym.lambda_r):
594     from sympy import Rational
595     return ((r_t_prime_3_bar / r_t_prime_2_bar ** Rational(3, 2)) *
596             (1 / ((1 - delta * lambda_r) / (1 - delta)) ** Rational(3, 2)) *
597             (1 / (1 - delta)))
598
599
600 def sk_w_hat(sigma_tilde_w=sym.sigma_tilde_w,
601             w_prime_3_bar=sym.w_prime_3_bar,
602             w_prime_2_bar=sym.w_prime_2_bar,
603             delta=sp.abc.delta,
604             lambda_w=sym.lambda_w):
605     from sympy import Rational
606     return ((1 / (1 - sigma_tilde_w ** 2) ** Rational(3, 2)) *
607             (w_prime_3_bar / (w_prime_2_bar ** Rational(3, 2))) *
608             (1 / ((1 - delta * lambda_w) / (1 - delta)) ** Rational(3, 2)) *
609             (1 / (1 - delta)))
610
611
612 # -----
613
614 # c
615
616 def c_w_theta_l_hat(sigma_w_tilde=sym.sigma_tilde_w,
617                    w_prime_theta_l_prime_bar=sym.w_prime_theta_l_prime_bar,
618                    w_prime_2_bar=sym.w_prime_2_bar,
619                    theta_l_prime_2_bar=sym.theta_l_prime_2_bar,
620                    delta=sp.abc.delta,
621                    lambda_w=sym.lambda_w,
622                    lambda_theta=sym.lambda_theta,
623                    lambda_w_theta=sym.lambda_w_theta):
624     from sympy import sqrt
625     return ((1 / sqrt(1 - sigma_w_tilde ** 2)) *
626             (w_prime_theta_l_prime_bar / ((sqrt(w_prime_2_bar)) *
627             ↪ sqrt(theta_l_prime_2_bar))) *
628             (1 / sqrt((1 - delta * lambda_w) / (1 - delta))) *
629             (1 / sqrt((1 - delta * lambda_theta) / (1 - delta))) *
630             ((1 - delta * lambda_w_theta) / (1 - delta)))
631
632
633 def c_w_r_t_hat(sigma_w_tilde=sym.sigma_tilde_w,
634                w_prime_r_t_prime_bar=sym.w_prime_r_t_prime_bar,
635                w_prime_2_bar=sym.w_prime_2_bar,
636                r_t_prime_2_bar=sym.r_t_prime_2_bar,
637                delta=sp.abc.delta,
638                lambda_w=sym.lambda_w,
639                lambda_r=sym.lambda_r,
640                lambda_w_r=sym.lambda_w_r):
641     from sympy import sqrt
642     return ((1 / sqrt(1 - sigma_w_tilde ** 2)) *
643             (w_prime_r_t_prime_bar / ((sqrt(w_prime_2_bar)) * sqrt(r_t_prime_2_bar))) *
644             (1 / sqrt((1 - delta * lambda_w) / (1 - delta))) *
645             (1 / sqrt((1 - delta * lambda_r) / (1 - delta))) *
646             ((1 - delta * lambda_w_r) / (1 - delta)))

```

```

646
647
648 # ---
649
650 # beta
651 # ---
652
653 def beta_w_theta_l(c_w_theta_l_hat=sym.c_w_theta_l_hat,
654                   sk_w_hat=sym.sk_w_hat,
655                   sk_theta_l_hat=sym.sk_theta_l_hat):
656     return (((c_w_theta_l_hat ** 3 * sk_w_hat) - sk_theta_l_hat) /
657            (c_w_theta_l_hat * sk_w_hat * (c_w_theta_l_hat ** 2 - 1)))
658
659
660 def beta_w_r_t(c_w_r_t_hat=sym.c_w_r_t_hat,
661               sk_w_hat=sym.sk_w_hat,
662               sk_r_t_hat=sym.sk_r_t_hat):
663     return (((c_w_r_t_hat ** 3 * sk_w_hat) - sk_r_t_hat) /
664            (c_w_r_t_hat * sk_w_hat * (c_w_r_t_hat ** 2 - 1)))
665
666
667 # ---
668
669 # E
670 # ---
671
672 def E(alpha=sp.abc.alpha, xi=sp.abc.xi):
673     from sympy import Rational
674     return ((1 - Rational(1, 2) * ((2 * alpha) / (1 - 2 * alpha)) * xi) /
675            (1 + Rational(1, 2) * xi))
676
677
678 # ---
679
680
681 # xi
682 # ---
683
684 def xi(alpha=sp.abc.alpha, sigma_tilde_r_t_1=sym.sigma_tilde_r_t_1,
685        sigma_tilde_r_t_2=sym.sigma_tilde_r_t_2,
686        sigma_tilde_theta_l_1=sym.sigma_tilde_theta_l_1,
687        sigma_tilde_theta_l_2=sym.sigma_tilde_theta_l_2):
688     return (((1 - alpha) / alpha) *
689            (sigma_tilde_r_t_1 / sigma_tilde_r_t_2) *
690            (sigma_tilde_theta_l_1 / sigma_tilde_theta_l_2) - 1)
691
692 # ---

```

Listing B.2: checked_functions.py

B.4 w_prime_4_bar.py

```
1  #!/usr/bin/env python
2  # coding: utf-8
3
4  # In[1]:
5
6
7  import sympy as sp
8  from IPython.display import display
9  from sympy import abc, oo, init_printing
10
11  import checked_functions as c_f
12  import symbols as sym
13  init_printing()
14
15
16  # # This document aims to analytically check  $\overline{w^4}$ 
17
18  # ## Define the marginal distributions with those parameters.
19
20  # In[2]:
21
22
23  display(sp.Eq(sym.G_1_w, c_f.G_1_theta_1_density))
24
25
26  # In[3]:
27
28
29  display(sp.Eq(sym.G_2_w, c_f.G_2_theta_1_density))
30
31
32  # In[4]:
33
34
35  display(sp.Eq(sym.G_3_w, c_f.G_3_theta_1_density))
36
37
38  # In[5]:
39
40
41  display(sp.Eq(sym.G_w, c_f.G_w))
42
43
44  # Calculate the moment analytically:
45
46  # In[6]:
47
48
49  w_prime_4_bar_int = sp.Integral((sp.abc.w - sym.w_bar) ** 4 * c_f.G_w, [sp.abc.w, -oo,
↪  oo])
```

```

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

```

```

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

```

Listing B.3: w_prime_4_bar.py

B.5 w_prime_2_theta_l_prime_bar.py

```

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

```

```

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

```

```

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

```

```

133
134 w_prime_2_theta_l_prime_bar_check_val = (
135     c_f.w_prime_2_theta_l_prime_bar().subs({
136         sym.sigma_tilde_w: c_f.sigma_tilde_w(),
137         sym.lambda_w: c_f.lambda_w(),
138         sym.w_prime_2_bar: c_f.w_prime_2_bar(),
139         sym.w_prime_3_bar: c_f.w_prime_3_bar(),
140         sym.lambda_w_theta: c_f.lambda_w_theta(),
141         sym.w_prime_theta_l_prime_bar: c_f.w_prime_theta_l_prime_bar()
142     }))
143
144 w_prime_2_theta_l_prime_bar_check_val = (
145     w_prime_2_theta_l_prime_bar_check_val.subs({
146         sym.w_prime_2_bar: c_f.w_prime_2_bar(),
147         sym.w_bar: c_f.w_bar(),
148         sym.theta_l_bar: c_f.theta_l_bar()
149     }))
150
151 display(sp.Eq(sym.w_prime_2_theta_prime_l_bar,
152               w_prime_2_theta_l_prime_bar_check_val))
153
154
155 # Since the integral is too difficult to be calculated analytically, at least with
156 ↪ sympy, we try to put in some arbitrary numbers for the pdf parameters, to simplify
157 ↪ the equations.
158
159 # We create a dataframe to get all possible permutations and therefore also all possible
160 ↪ evaluations of the integrals.
161
162 # In[16]:
163
164 df = pd.DataFrame(
165     product([0, 1],
166            [-2, 2],
167            [-1, 2],
168            [0, 3],
169            [Rational(1, 10)],
170            [Rational(3, 10)],
171            [Rational(4, 10)],
172            [Rational(7, 10)],
173            [Rational(6, 10)],
174            [Rational(5, 10)],
175            [Rational(1, 10), Rational(5, 10)],
176            [Rational(5, 10)]),
177     columns=[sym.w_1,
178             sym.w_2,
179             sym.theta_l_1,
180             sym.theta_l_2,
181             sym.sigma_theta_l_1,
182             sym.sigma_theta_l_2,
183             sym.sigma_lambda_theta_l,
184             sym.sigma_w,
185             sym.sigma_lambda_w,

```

```

184         sp.abc.alpha,
185         sp.abc.delta,
186         sym.rho_w_theta_l])
187
188
189 # In[17]:
190
191
192 df['check_val'] = (
193     df.apply(lambda x:
194         w_prime_2_theta_l_prime_bar_check_val.subs({
195             sym.w_1: x[sym.w_1],
196             sym.w_2: x[sym.w_2],
197             sym.theta_l_1: x[sym.theta_l_1],
198             sym.theta_l_2: x[sym.theta_l_2],
199             sym.sigma_theta_l_1: x[sym.sigma_theta_l_1],
200             sym.sigma_theta_l_2: x[sym.sigma_theta_l_2],
201             sym.sigma_lambda_theta_l: x[sym.sigma_lambda_theta_l],
202             sym.sigma_w: x[sym.sigma_w],
203             sym.sigma_lambda_w: x[sym.sigma_lambda_w],
204             sp.abc.alpha: x[sp.abc.alpha],
205             sp.abc.delta: x[sp.abc.delta],
206             sym.rho_w_theta_l: x[sym.rho_w_theta_l]
207         })), axis=1))
208
209
210 # Calculate the moment analytically:
211
212 # In[18]:
213
214
215 df['num_int'] = (
216     df.apply(lambda x: Rational(w_prime_2_theta_l_prime_bar.subs({
217         sym.w_1: x[sym.w_1],
218         sym.w_2: x[sym.w_2],
219         sym.theta_l_1: x[sym.theta_l_1],
220         sym.theta_l_2: x[sym.theta_l_2],
221         sym.sigma_theta_l_1: x[sym.sigma_theta_l_1],
222         sym.sigma_theta_l_2: x[sym.sigma_theta_l_2],
223         sym.sigma_lambda_theta_l: x[sym.sigma_lambda_theta_l],
224         sym.sigma_w: x[sym.sigma_w],
225         sym.sigma_lambda_w: x[sym.sigma_lambda_w],
226         sp.abc.alpha: x[sp.abc.alpha],
227         sp.abc.delta: x[sp.abc.delta],
228         sym.rho_w_theta_l: x[sym.rho_w_theta_l]
229     })).doit(conds='none', method='quad').evalf()), axis=1))
230
231
232 # In[19]:
233
234
235 df['diff'] = abs(df['check_val'] - df['num_int'])
236
237

```

```

238 # In[20]:
239
240
241 df['diff_num'] = abs(df['check_val'].astype(float) - df['num_int'].astype(float))
242
243
244 # In[21]:
245
246
247 display(df)
248
249
250 # In[22]:
251
252
253 import numpy as np
254
255 print('The mean error between the rhs and the lhs is:', np.mean(df['diff_num']))
256

```

Listing B.4: w_prime_2_theta_l_prime_bar.py

B.6 w_prime_theta_l_prime_2_bar.py

```

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

```



```

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

```

```

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

```

```

134 display(sp.Eq(sym.theta_l_prime_3_bar, c_f.theta_l_prime_3_bar()))
135
136
137 # Putting those all together yields:
138
139 # In[16]:
140
141
142 w_prime_theta_l_prime_2_bar_check_val = c_f.w_prime_theta_l_prime_2_bar().subs({
143     sym.theta_l_prime_3_bar: c_f.theta_l_prime_3_bar(),
144     sym.sigma_tilde_w: c_f.sigma_tilde_w(),
145     sym.lambda_w: c_f.lambda_w(),
146     sym.w_prime_2_bar: c_f.w_prime_2_bar(),
147     sym.w_prime_3_bar: c_f.w_prime_3_bar(),
148     sym.lambda_w_theta: c_f.lambda_w_theta(),
149     sym.w_prime_theta_l_prime_bar: c_f.w_prime_theta_l_prime_bar()
150 })
151
152 w_prime_theta_l_prime_2_bar_check_val = w_prime_theta_l_prime_2_bar_check_val.subs({
153     sym.w_prime_2_bar: c_f.w_prime_2_bar(),
154     sym.lambda_w: c_f.lambda_w(),
155     sym.w_bar: c_f.w_bar(),
156     sym.theta_l_bar: c_f.theta_l_bar()
157 })
158
159 display(sp.Eq(sym.w_prime_theta_prime_l_2_bar, w_prime_theta_l_prime_2_bar_check_val))
160
161
162 # Since the integral is too difficult to be calculated analytically, at least with
163 → sympy, we try to put in some arbitrary numbers for the pdf parameters, to simplify
164 → the equations.
165
166 # We create a dataframe to get all possible permutations and therefore also all possible
167 → evaluations of the integrals.
168
169 # In[17]:
170
171 df = pd.DataFrame(
172     product([0, 1],
173             [-2, 2],
174             [-1, 2],
175             [0, 3],
176             [Rational(1, 10)],
177             [Rational(3, 10)],
178             [Rational(4, 10)],
179             [Rational(7, 10)],
180             [Rational(6, 10)],
181             [Rational(5, 10)],
182             [Rational(1, 10), Rational(5, 10)],
183             [Rational(5, 10)]),
184     columns=[sym.w_1,
185             sym.w_2,
186             sym.theta_l_1,

```

```

185         sym.theta_l_2,
186         sym.sigma_theta_l_1,
187         sym.sigma_theta_l_2,
188         sym.sigma_theta_l_3,
189         sym.sigma_w,
190         sym.sigma_w_3,
191         sp.abc.alpha,
192         sp.abc.delta,
193         sym.rho_w_theta_l])
194
195
196 # In[18]:
197
198
199 df['check_val'] = (
200     df.apply(lambda x:
201         w_prime_theta_l_prime_2_bar_check_val.subs({
202             sym.w_1: x[sym.w_1],
203             sym.w_2: x[sym.w_2],
204             sym.theta_l_1: x[sym.theta_l_1],
205             sym.theta_l_2: x[sym.theta_l_2],
206             sym.sigma_theta_l_1: x[sym.sigma_theta_l_1],
207             sym.sigma_theta_l_2: x[sym.sigma_theta_l_2],
208             sym.sigma_theta_l_3: x[sym.sigma_theta_l_3],
209             sym.sigma_w: x[sym.sigma_w],
210             sym.sigma_w_3: x[sym.sigma_w_3],
211             sp.abc.alpha: x[sp.abc.alpha],
212             sp.abc.delta: x[sp.abc.delta],
213             sym.rho_w_theta_l: x[sym.rho_w_theta_l]
214         })).evalf(), axis=1))
215
216
217 # Calculate the moment analytically:
218
219 # In[19]:
220
221
222 df['num_int'] = (
223     df.apply(lambda x: w_prime_theta_l_2_prime_bar.subs({
224         sym.w_1: x[sym.w_1],
225         sym.w_2: x[sym.w_2],
226         sym.theta_l_1: x[sym.theta_l_1],
227         sym.theta_l_2: x[sym.theta_l_2],
228         sym.sigma_theta_l_1: x[sym.sigma_theta_l_1],
229         sym.sigma_theta_l_2: x[sym.sigma_theta_l_2],
230         sym.sigma_theta_l_3: x[sym.sigma_theta_l_3],
231         sym.sigma_w: x[sym.sigma_w],
232         sym.sigma_w_3: x[sym.sigma_w_3],
233         sp.abc.alpha: x[sp.abc.alpha],
234         sp.abc.delta: x[sp.abc.delta],
235         sym.rho_w_theta_l: x[sym.rho_w_theta_l]
236     })).doit(conds='none', method='quad').evalf(), axis=1))
237
238

```

```

239 # In[20]:
240
241
242 df['diff'] = abs(df['check_val'] - df['num_int'])
243
244
245 # In[21]:
246
247
248 df['diff_num'] = abs(df['check_val'].astype(float) - df['num_int'].astype(float))
249
250
251 # In[22]:
252
253
254 display(df)
255
256
257 # In[23]:
258
259
260 import numpy as np
261
262 print('The mean error between the rhs and the lhs is:', np.mean(df['diff_num']))
263

```

Listing B.5: w_prime_theta_l_prime_2_bar.py

B.7 w_prime_r_t_prime_theta_l_prime_bar.py

```

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

```

```

20
21 init_printing()
22
23
24 # # This document aims to numerically check  $\int \overline{w(r_t|\theta_l)} \mathcal{L}$ 
25
26 # ## Define the normal distributions.
27
28 # In[3]:
29
30
31 display(sp.Eq(sp.symbols('\mu_1'), c_f.mu_1_w_theta_l_r_t, evaluate=False))
32 display(sp.Eq(sp.symbols('\Sigma_1'), c_f.Sigma_1_w_theta_l_r_t, evaluate=False))
33 #display(sp.Eq(sym.G_1_w_theta_l_r_t, c_f.G_1_w_theta_l_r_t_density))
34
35
36 # In[4]:
37
38
39 display(sp.Eq(sp.symbols('\mu_2'), c_f.mu_2_w_theta_l_r_t, evaluate=False))
40 display(sp.Eq(sp.symbols('\Sigma_2'), c_f.Sigma_2_w_theta_l_r_t, evaluate=False))
41 #display(sp.Eq(sym.G_2_w_theta_l_r_t, c_f.G_2_w_theta_l_r_t_density))
42
43
44 # In[5]:
45
46
47 display(sp.Eq(sp.symbols('\mu_3'), c_f.mu_3_w_theta_l_r_t, evaluate=False))
48 display(sp.Eq(sp.symbols('\Sigma_3'), c_f.Sigma_3_w_theta_l_r_t, evaluate=False))
49 #display(sp.Eq(sym.G_3_w_theta_l_r_t, c_f.G_3_w_theta_l_r_t_density))
50
51
52 # In[6]:
53
54
55 display(sp.Eq(sym.G_w_theta_l_r_t, c_f.G_w_theta_l_r_t))
56
57
58 # In[7]:
59
60
61 w_prime_r_t_prime_theta_l_prime_bar = sp.Integral(
62     (sp.abc.w - sym.w_bar) * (sym.r_t - sym.r_t_bar) * (sp.abc.theta - sym.theta_l_bar)
63     ↪ * c_f.G_w_theta_l_r_t,
64     [sp.abc.w, -oo, oo],
65     [sym.theta_l, -oo, oo],
66     [sym.r_t, -oo, oo])
67 display(sp.Eq(sym.w_prime_r_t_prime_theta_l_prime_bar,
68     ↪ w_prime_r_t_prime_theta_l_prime_bar))
69
70
71 # In[8]:

```

```

72 w_prime_r_t_prime_theta_l_prime_bar = (
73     w_prime_r_t_prime_theta_l_prime_bar.subs({
74         sym.w_bar: c_f.w_bar(),
75         sym.r_t_bar: c_f.r_t_bar(),
76         sym.theta_l_bar: c_f.theta_l_bar()
77     }))
78 display(sp.Eq(sym.w_prime_r_t_prime_theta_l_prime_bar,
79     ↪ w_prime_r_t_prime_theta_l_prime_bar))
80
81 # The equation in the document is:
82
83 # In[9]:
84
85
86 display(sp.Eq(sym.w_prime_r_t_prime_theta_l_prime_bar,
87     ↪ c_f.w_prime_r_t_prime_theta_l_prime_bar()))
88
89 # Since the integral is too difficult to be calculated analytically, at least with
90 ↪ sympy, we try to put in some arbitrary numbers for the pdf parameters, to simplify
91 ↪ the equations.
92
93 # We also use the method `nquad(..)` from `sympy` to get a numerical evaluation of the
94 ↪ 3d integral.
95
96 # We create a dataframe to get all possible permutations and therefore also all possible
97 ↪ evaluations of the integrals.
98
99 # In[10]:
100
101 df = pd.DataFrame(
102     product([3, 1],
103         [-2],
104         [-1, 3],
105         [2],
106         [1, 4],
107         [2],
108         [1.1],
109         [1.3],
110         [1.4],
111         [1.7],
112         [1.2],
113         [1.5],
114         [1.9],
115         [1.6],
116         [.55],
117         [.8],
118         [.65],
119         [.45],
120         [.35],
121         [.5]),
122     columns=[sym.w_1,

```

```

120         sym.w_2,
121         sym.theta_l_1,
122         sym.theta_l_2,
123         sym.r_t_1,
124         sym.r_t_2,
125         sym.sigma_theta_l_1,
126         sym.sigma_theta_l_2,
127         sym.sigma_theta_l_3,
128         sym.sigma_w,
129         sym.sigma_r_t_1,
130         sym.sigma_r_t_2,
131         sym.sigma_r_t_3,
132         sym.sigma_w_3,
133         sp.abc.alpha,
134         sp.abc.delta,
135         sym.rho_w_theta_l,
136         sym.rho_w_r_t,
137         sym.rho_theta_l_r_t,
138         sym.r_r_t_theta_l])
139
140
141 # In[11]:
142
143
144 w_prime_r_t_prime_theta_l_prime_bar_check_sym_val = (
145     c_f.w_prime_r_t_prime_theta_l_prime_bar().subs({
146         sym.w_bar: c_f.w_bar(),
147         sym.r_t_bar: c_f.r_t_bar(),
148         sym.theta_l_bar: c_f.theta_l_bar()
149     }))
150
151
152 # In[12]:
153
154
155 df['check_val'] = (
156     df.apply(lambda x: Rational(c_f.w_prime_r_t_prime_theta_l_prime_bar().subs({
157         sym.w_bar: c_f.w_bar(),
158         sym.theta_l_bar: c_f.theta_l_bar(),
159         sym.r_t_bar: c_f.r_t_bar(),
160         sym.w_1: x[sym.w_1],
161         sym.w_2: x[sym.w_2],
162         sym.theta_l_1: x[sym.theta_l_1],
163         sym.theta_l_2: x[sym.theta_l_2],
164         sym.r_t_1: x[sym.r_t_1],
165         sym.r_t_2: x[sym.r_t_2],
166         sym.sigma_theta_l_1: x[sym.sigma_theta_l_1],
167         sym.sigma_theta_l_2: x[sym.sigma_theta_l_2],
168         sym.sigma_r_t_1: x[sym.sigma_r_t_1],
169         sym.sigma_r_t_2: x[sym.sigma_r_t_2],
170         sp.abc.alpha: x[sp.abc.alpha],
171         sp.abc.delta: x[sp.abc.delta],
172         sym.r_r_t_theta_l: x[sym.r_r_t_theta_l]
173     })).evalf(), axis=1))

```



```

174
175
176 # Calculate the moment numerically:
177
178 # In[13]:
179
180
181 import scipy
182
183 df['num_int'] = df.apply(lambda x: scipy.integrate.nquad(
184     sp.lambdify(
185         [sp.abc.w, sym.r_t, sym.theta_l],
186         (((sp.abc.w - c_f.w_bar()) *
187            (sym.r_t - c_f.r_t_bar()) *
188            (sym.theta_l - c_f.theta_l_bar()) *
189            c_f.G_w_theta_l_r_t))
190         .subs({
191             sym.w_bar: c_f.w_bar(),
192             sym.r_t_bar: c_f.r_t_bar(),
193             sym.theta_l_bar: c_f.theta_l_bar(),
194             sym.w_1: x[sym.w_1],
195             sym.w_2: x[sym.w_2],
196             sym.theta_l_1: x[sym.theta_l_1],
197             sym.theta_l_2: x[sym.theta_l_2],
198             sym.r_t_1: x[sym.r_t_1],
199             sym.r_t_2: x[sym.r_t_2],
200             sym.sigma_w: x[sym.sigma_w],
201             sym.sigma_w_3: x[sym.sigma_w_3],
202             sym.sigma_theta_l_1: x[sym.sigma_theta_l_1],
203             sym.sigma_theta_l_2: x[sym.sigma_theta_l_2],
204             sym.sigma_theta_l_3: x[sym.sigma_theta_l_3],
205             sym.sigma_r_t_1: x[sym.sigma_r_t_1],
206             sym.sigma_r_t_2: x[sym.sigma_r_t_2],
207             sym.sigma_r_t_3: x[sym.sigma_r_t_3],
208             sp.abc.alpha: x[sp.abc.alpha],
209             sp.abc.delta: x[sp.abc.delta],
210             sym.rho_w_theta_l: x[sym.rho_w_theta_l],
211             sym.rho_w_r_t: x[sym.rho_w_r_t],
212             sym.rho_theta_l_r_t: x[sym.rho_theta_l_r_t],
213             sym.r_r_t_theta_l: x[sym.r_r_t_theta_l]
214         })),
215     ranges=[[-30, 30], [-30, 30], [-30, 30]][0],
216     axis=1)
217
218
219 # In[14]:
220
221
222 df['diff'] = abs(df['check_val'] - df['num_int'])
223
224
225 # In[15]:
226
227

```

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

Listing B.6: w_prime_r_t_prime_theta_l_prime_bar.py