ADDING A THIRD GAUSSIAN TO CLUBB

by

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ABSTRACT

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The Cloud Layers Unified By Binormals (CLUBB) model plays a crucial role in simulating atmospheric phenomena. It uses the sum of two probability density functions (pdfs) to represent a single grid layer. This approach, while computationally efficient, restricts the model's ability to capture the full spectrum of potential shapes encountered in real-world atmospheric data.

This thesis proposes an innovative extension to the CLUBB model. We introduce a third normal pdf strategically positioned between the existing two, significantly enhancing the model's representational flexibility. This trinormal representation allows for a wider range of grid-layer shapes while maintaining computational tractability.

The core of this work lies in deriving the necessary mathematical transformations for incorporating the third normal pdf seamlessly into the CLUBB framework. This thesis lists all formulas, inputs, and outputs associated with the extended model. Additionally, it tries to describe certain asymptotic behavior of the trinormal pdf under various parameter settings.

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List of Acronyms

cas computer algebra system. 13, 43

CLUBB Cloud Layers Unified By Binormals. ii, 1, 2, 4–6, 14, 27, 43, 44

lhs left hand side. 8

pde partial differential equation. 5

pdf probability density function. ii, 1, 3, 7, 8, 10, 13–17, 19, 20, 23–26, 28, 29, 40, 43

rhs right hand side. 6, 8, 9

List of Symbols

 θ_l' Standardized liquid water potential temperature $(\theta_l'=\theta_l-\overline{\theta_l}).$ 12

 r_t' Standardized total water mixing ratio $(r_t' = r_t - \overline{r_t})$. 12

w' Standardized upward wind $(w'=w-\overline{w}).$ 12, 19

Acknowledgments

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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). The motivation, details regarding the model's inputs and outputs, and a step-by-step approach for verifying the formulas are provided.

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 section details the introduction of the third normal pdf (section 3.1), the transformation of existing equations (section 4.3), and the derivation of key moments within the model (section 4.4 - section 4.5). Additionally, section 4.7 proposes a diagnostic approach to account for the skewness of heat and moisture, while section 4.8 introduces closure relations for higher-order moments based on the newly formed mixture of three normal distributions.

To handle the mathematical integrations required by the model, chapter 5 explores both analytic and numerical integration techniques, potentially utilizing the SymPy library (section 5.1 & section 5.2).

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

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

As being said in the chapter 1, we try to describe more possible shapes with adding a third pdf. To illustrate that, we plotted some of the shapes which are now possible but were not possible before. To be able to draw those plots, we are just using two variables, w, the upward wind, and θ_l , the liquid water potential temperature. To illustrate 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 model this could look like figure 2.1.

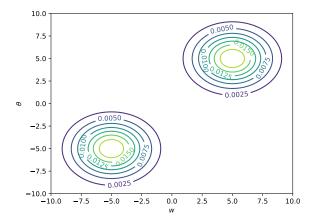


Figure 2.1: Binormal plot for two strong upward winds With fixed variables: $w_1 = 5$, $w_2 = -5$, $\theta_{l1} = 5$, $\theta_{l2} = -5$, $\alpha = 0.5$, $\sigma_w = 2$, $\sigma_{\theta_{l1}} = 2$, $\sigma_{\theta_{l1}} = 2$.

However, this bimodal distribution (figure 2.1) doesn't accurately reflect reality. In nature, we would not expect such a sharp jump between the strong upward winds at w_1 and w_2 . There would likely be some weaker upward winds present in between. The current binormal

model can attempt to capture this smoother transition by simply increasing the standard deviations of both wind and liquid water potential temperature distributions. This results in a broader distribution with a connection between the two peaks, as shown in figure 2.2.

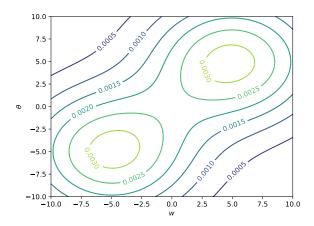


Figure 2.2: Binormal plot for two strong upward winds with increased standard deviations With fixed variables: $w_1 = 5$, $w_2 = -5$, $\theta_{l1} = 5$, $\theta_{l2} = -5$, $\alpha = 0.5$, $\sigma_w = 5$, $\sigma_{\theta_{l1}} = 5$, $\sigma_{\theta_{l1}} = 5$.

Seeing figure 2.2, the issue with having some values in the middle is slightly fixed but the general width of the normals was increased, too. Since CLUBB also has the simplification that there is no correlation between w and θ_l , and w and r_t , obviously one cannot just increase it. Therefore, the idea is to add this third normal, which actually has correlation between all three variables and especially in the bivariate case, between w and 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.

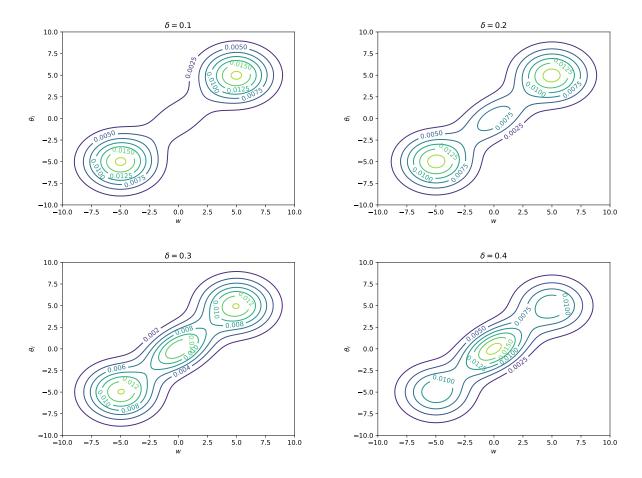


Figure 2.3: Trinormal plot for two strong upward winds with varying δ With fixed variables: $w_1=5, \ w_2=-5, \ \theta_{l1}=5, \ \theta_{l2}=-5, \ \alpha=0.5, \ \sigma_w=2, \ \sigma_{\theta_{l1}}=2, \ \sigma_{\theta_{l2}}=2, \ \sigma_{w\theta_{l}}=2, \ \rho_{w\theta_{l}}=0.5.$

2.2 Closing PDEs

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

For instance, consider the following prognostic pde:¹

Vincent E. Larson. *CLUBB-SILHS: A parameterization of subgrid variability in the atmosphere*. 2022. arXiv: 1711.03675 [physics.ao-ph], p. 21.

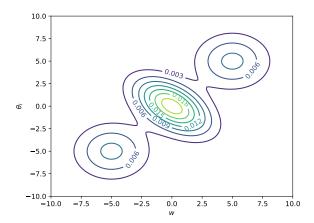


Figure 2.4: Trinormal plot for two strong upward winds with a third peak in the middle With fixed variables: $w_1 = 5$, $w_2 = -5$, $\theta_{l1} = 5$, $\theta_{l2} = -5$, $\alpha = 0.5$, $\delta = 0.5$, $\sigma_w = 2$, $\sigma_{\theta_{l1}} = 2$, $\sigma_{\theta_{l2}} = 2$, $\sigma_{w3} = 2$, $\sigma_{\theta_{l3}}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

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

While the details of initial and boundary conditions are essential for formally closing the prognostic equations in CLUBB (omitted for brevity), this section emphasizes the importance of efficiently calculating moments on the right hand side (rhs) of these equations.

That is because the model steps forward in time and therefore needs the repeated calculation of moments for each unclosed prognostic equation at every time step. Those already expensive computational steps need to use mathematically simpler moment representations, even if they introduce slight limitations in capturing the full variability of the underlying atmospheric state.

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

the time-stepping process.

2.3 Inputs and Outputs

While defining inputs and outputs can seem challenging at first glance, it's a crucial step towards understanding a system. In this context, the code provides us with a set of moment terms: \overline{w} , $\overline{w'^2}$, $\overline{w'^3}$, $\overline{\theta_l}$, $\overline{w'\theta_l'}$, $\overline{r_t}$, $\overline{w'r_t'}$, $\overline{\theta_l'^2}$, $\overline{r_t'^2}$, $\overline{r_t'\theta_l'}$. From these, we want to determine certain parameters which are describing the shape of the underlying pdf. Those parameters are standardized and some also normalized. So we try to solve for 13 unknowns, namely α , \widehat{w}_1 , \widehat{w}_2 , $\widetilde{\theta}_{l1}$, $\widetilde{\theta}_{l2}$, \widetilde{r}_{t1} , \widetilde{r}_{t2} , $\widetilde{\sigma}_w$, $\widetilde{\sigma}_{\theta_{l1}}$, $\widetilde{\sigma}_{\theta_{l2}}$, $\widetilde{\sigma}_{r_{t1}}$, $\widetilde{\sigma}_{r_{t2}}$, and $r_{r_{t}\theta_{l}}$. All the formulas are listed in chapter 4.

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

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

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

$$\overline{w} = \int_{\mathbb{R}} \int_{\mathbb{R}} \int_{\mathbb{R}} w \cdot P_{tmg} \, dw dr_t d\theta_t, \qquad (2.3.1)$$

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

²Trivariate Mixture of Gaussians

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

2.4 Steps for checking the formulas

We want to state a general approach for checking all those formulas and try to reference to the following steps in chapter 5 where there are actual examples stated. One way, or at least the way, which is used in this document is the following, where we always want to check if left hand side (lhs) equals rhs:

- 1. Choose dimensional parameters (parameters without any tilde or hat) that determine the pdf. I.e., choose dimensional PDF parameters, e.g. σ_{w3} . Then the pdf is known, and any moments of it can be calculated by integration.
- 2. Calculate the means, e.g. $\overline{w} = \mathbb{E}[w]$ by integration over the pdf. Our formula for \overline{w} (equation (4.4.1)) in terms of the pdf parameters can be checked.
- 3. Once the means are known, calculate the central variances, e.g. $\overline{w'^2} = \overline{(w-\overline{w})^2}$ by integration over the pdf. Our formula for $\overline{w'^2}$ (equation (4.4.3)) in terms of the pdf parameters can be checked.
- 4. Once the variances, e.g. $\overline{w'^2}$, are known, then non-dimensional pdf parameters such as λ_w can be calculated by their definitions.
- 5. We can also calculate the covariances by 2D integration over a 2D pdf. Again, our formulas in terms of pdf parameters can be checked.
- 6. Finally, we can calculate the higher order moments, e.g. $\overline{w'^4}$ or $\overline{w'^2\theta'_l}$, by integration over the pdf. Again, we can check if lhs = rhs.

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

3 Definitions

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

3.1 Normal distribution

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

Definition 1 (pdf of a normal distribution)

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

3.2 Multivariate Normal distribution

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

Definition 2 (pdf of a multivariate normal distribution)

$$f(\boldsymbol{x}|\boldsymbol{\mu},\boldsymbol{\Sigma}) = (2\pi)^{-\frac{r}{2}} |\boldsymbol{\Sigma}|^{-\frac{1}{2}} \exp\left(-\frac{1}{2}(x-\boldsymbol{\mu})^{\top} \boldsymbol{\Sigma}^{-1}(x-\boldsymbol{\mu})\right), \boldsymbol{x} \in \mathbb{R}^{r},$$
(3.2.1)

¹Alan Julian Izenman. *Modern multivariate statistical techniques: regression, classification, and manifold learning*. Springer texts in statistics. OCLC: ocn225427579. New York; London: Springer, 2008. ISBN: 9780387781884, p. 59.

where

$$\boldsymbol{\mu} = \begin{pmatrix} \mu_1 \\ \vdots \\ \mu_r \end{pmatrix} \in \mathbb{R}^r \tag{3.2.2}$$

is the mean vector, and

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

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

3.2.1 Moments

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

$$\mathbb{E}[X^3] = \mathbb{E}\left[\left(\frac{X-\mu}{\sigma}\right)^3\right] = \frac{\mu_3}{\sigma^3} = \frac{\mathbb{E}[(X-\mu)^3]}{(\mathbb{E}[(X-\mu)^2])^{3/2}} = \frac{\kappa_3}{\kappa_2^{3/2}},\tag{3.2.3}$$

$$\mathbb{E}[X^4] = \mathbb{E}\left[\left(\frac{X-\mu}{\sigma}\right)^4\right] = \frac{\mathbb{E}[(X-\mu)^4]}{(\mathbb{E}[(X-\mu)^2])^2} = \frac{\mu_4}{\sigma^4}.$$
 (3.2.4)

3.3 Thermodynamic Scalars

We denote the thermodynamic scalars 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.² Variables denoted by w' are defined by $w - \overline{w}$ where \overline{w} is the mean of w over the whole pdf. We define r'_t and θ'_l in the same way.

²Larson, CLUBB-SILHS: A parameterization of subgrid variability in the atmosphere, p. 10.

4 Formulas

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

4.1 Third Normal

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

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

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 by therefore also taking away some variability. This is not the case for the third normal, though. It has already been said, that we would

like to place the third normal right at the mean, therefore μ_3 and Σ_3 are defined as

$$\mu_3 = \begin{pmatrix} \overline{w} \\ \overline{\theta_l} \\ \overline{r_t} \end{pmatrix}, \text{ and } \Sigma_3 = \begin{pmatrix} \sigma_{w3}^2 & \rho_{w\theta_l 3} \sigma_{w3} \sigma_{\theta_l 3} & \rho_{wr_t 3} \sigma_{w3} \sigma_{r_t 3} \\ \rho_{w\theta_l 3} \sigma_{w3} \sigma_{\theta_l 3} & \sigma_{\theta_l 3}^2 & \rho_{\theta_l r_t 3} \sigma_{\theta_l 3} \sigma_{r_t 3} \\ \rho_{wr_t 3} \sigma_{w3} \sigma_{r_t 3} & \rho_{\theta_l r_t 3} \sigma_{\theta_l 3} \sigma_{r_t 3} & \sigma_{r_t 3}^2 \end{pmatrix}.$$

For our proposed mix of normals we then have

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

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

$$\lambda_w = \frac{\sigma_{w3}^2}{\overline{w'^2}}, \quad \lambda_\theta = \frac{\sigma_{\theta_l 3}^2}{\overline{\theta_l'^2}}, \quad \lambda_r = \frac{\sigma_{r_t 3}^2}{\overline{r_t'^2}}, \tag{4.1.2}$$

$$\lambda_{\theta r} = \frac{\rho_{\theta l r_t} \sigma_{\theta l 3} \sigma_{r_t 3}}{\overline{r_t' \theta_l'}}, \quad \lambda_{w \theta} = \frac{\rho_{w \theta_l} \sigma_{w 3} \sigma_{\theta_l 3}}{\overline{w' \theta_l'}}, \quad \lambda_{w r} = \frac{\rho_{w r_t} \sigma_{w 3} \sigma_{r_t 3}}{\overline{w' r_t'}}. \tag{4.1.3}$$

Hence, we can rewrite Σ_3 as

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

$$(4.1.4)$$

4.2 Normalized Variables

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

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

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

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

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

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

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

4.3 Transformation of the equations

Having established the definition of the sum of normal distributions in section 4.1 to enhance mathematical tractability, we now delve into the transformation of equations from the existing binormal representation used in CLUBB-SILHS¹ to a trinormal one. While the formulas for the binormal case are well-defined (see CLUBB-SILHS²), the simplicity of the means and standard deviations employed in the trinormal representation suggests the existence of a specific transformation that holds true. This chapter will demonstrate that the following transformations, denoted by the subscript "dGn" for the binormal case, successfully achieve this conversion.

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

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

¹Larson, CLUBB-SILHS: A parameterization of subgrid variability in the atmosphere.

²Ibid.

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

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

$$\overline{w'\theta_l'} \frac{1 - \delta \lambda_{w\theta}}{1 - \delta} = \overline{w'\theta_{ldGn}'},\tag{4.3.5}$$

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

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

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

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

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

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

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

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

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 (4.3.2), we see that there is no more λ_w present.

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

It makes sense graphically, that as delta grows, which means that the normal pdf in the middle is growing, the overall skewness of all three normals has to change also, depending on the value of σ_{w3} . We can see this, as well as the relationship between the variance in table 4.1. Table 4.1 offers a visual representation of how the parameter 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 (4.3.1).
- 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 evident in the bottom three plots, where a larger value of $\sigma_{w3} = 10$ is used. We observe a clear reduction in the skewness of the green plot (mixture) as δ approaches 1.

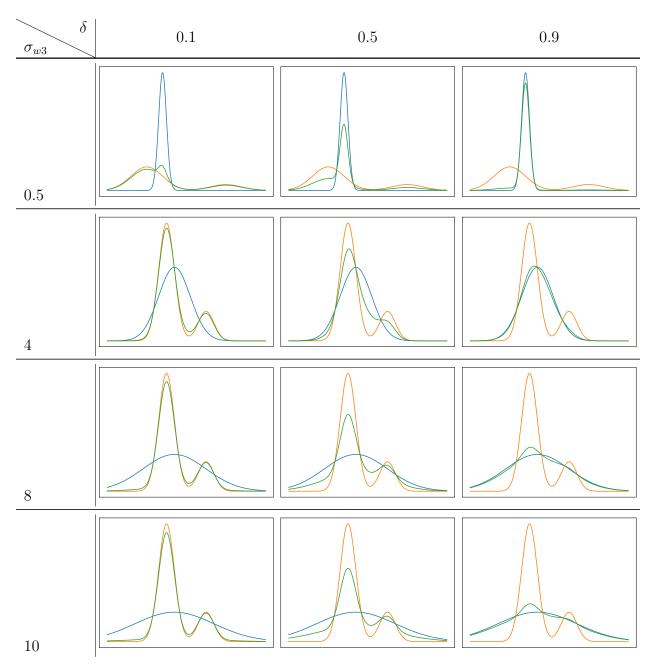


Table 4.1: 1D Plots for different δ and σ_{w3} With fixed variables: $w_1 = 5, w_2 = -5, \alpha = 0.2, \sigma_w = 2.$

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

4.4 Deduced Moments

We start by outlining the equations capturing lower-order moments, expressed in terms of pdf parameters. These equations can be presented in either dimensional or non-dimensional form. While both representations are mathematically valid, the non-dimensional form offers a distinct advantage: it highlights the underlying connection to the bivariate case.

4.4.1 Lower Order Moments

4.4.1.1 Moments for w

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

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

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

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

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

The second order moment is given as:

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

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

$$+ \delta\sigma_{w3}^2,$$
(4.4.3)

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

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

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

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

The non-dimensional relationship would then be:

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

The third order moment is given as:

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

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

$$(4.4.5)$$

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

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

$$= \alpha \left(\widehat{w}_{1}^{3} + 3\widehat{w}_{1} \frac{\tilde{\sigma}_{w}^{2}}{(1 - \tilde{\sigma}_{w}^{2})}\right) + (1 - \alpha) \left(\widehat{w}_{2}^{3} + 3\widehat{w}_{2} \frac{\tilde{\sigma}_{w}^{2}}{(1 - \tilde{\sigma}_{w}^{2})}\right)$$
(4.4.6)

4.4.1.2 Moments for θ_l

For θ_l we have a similar non-dimensional relationship:

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

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

$$\overline{\theta_l'^2} = (1 - \delta)\alpha[(\theta_{l1} - \overline{\theta_l})^2 + \sigma_{\theta_{l1}}^2]
+ (1 - \delta)(1 - \alpha)[(\theta_{l2} - \overline{\theta_l})^2 + \sigma_{\theta_{l2}}^2]
+ \delta\sigma_{\theta_l3}^2,$$
(4.4.8)

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

The third order moment is given as:

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

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

$$\widehat{Sk_{\theta_l}} \equiv \frac{\overline{\theta_l'^3}}{\left(\overline{\theta_l'^2}\right)^{3/2}} \left(\frac{1}{\frac{1-\delta\lambda_{\theta}}{1-\delta}}\right)^{3/2} \frac{1}{1-\delta}$$

$$= \alpha \left(\widetilde{\theta}_{l1}^3 + 3\widetilde{\theta}_{l1}\widetilde{\sigma}_{\theta_l1}^2\right) + (1-\alpha) \left(\widetilde{\theta}_{l2}^3 + 3\widetilde{\theta}_{l2}\widetilde{\sigma}_{\theta_l2}^2\right). \tag{4.4.10}$$

4.4.1.3 Moments for r_t

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

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

and

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

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

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

and

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

$$+ (1 - \delta)(1 - \alpha)[(r_{t2} - \overline{r_t})^3 + 3\sigma_{r_{t2}}^2(r_{t2} - \overline{r_t})]$$
(4.4.14)

4.4.1.4 Mixed Moments

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

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

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

$$+ \delta\lambda_{w\theta}\overline{w'\theta'_l},$$

$$(4.4.15)$$

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

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

$$+ \delta\lambda_{wr}\overline{w'r_t'},$$

$$(4.4.16)$$

and

$$\overline{r_t'\theta_l'} = (1 - \delta)\alpha[(r_{t1} - \overline{r_t})(\theta_{l1} - \overline{\theta_l}) + r_{r_t\theta_l}\sigma_{r_{t1}}\sigma_{\theta_{l1}}]
+ (1 - \delta)(1 - \alpha)[(r_{t2} - \overline{r_t})(\theta_{l2} - \overline{\theta_l}) + r_{r_t\theta_l}\sigma_{r_{t2}}\sigma_{\theta_{l2}}]
+ \delta\lambda_{r\theta}\overline{r_t'\theta_l'}.$$
(4.4.17)

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

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

$$= \alpha \widehat{w}_{1} \widetilde{\theta}_{l1} + (1 - \alpha) \widehat{w}_{2} \widetilde{\theta}_{l2}, \tag{4.4.18}$$

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

$$= \alpha \widehat{w}_1 \widetilde{r}_{t1} + (1 - \alpha) \widehat{w}_2 \widetilde{r}_{t2}, \tag{4.4.19}$$

and

$$\widehat{c}_{r_{t}\theta_{l}} \equiv \frac{\overline{r_{t}'\theta_{l}'}}{\sqrt{\overline{r_{t}'^{2}}}\sqrt{\overline{\theta_{l}'^{2}}}} \frac{1}{\sqrt{\frac{1-\delta\lambda_{q}}{1-\delta}}} \frac{1}{\sqrt{\frac{1-\delta\lambda_{q}}{1-\delta}}} \frac{1-\delta\lambda_{\theta r}}{1-\delta}
= \alpha \left(\widetilde{r}_{t1}\widetilde{\theta}_{l1} + r_{r_{t}\theta_{l}}\widetilde{\sigma}_{q_{t1}}\widetilde{\sigma}_{\theta_{l1}}\right) + (1-\alpha) \left(\widetilde{r}_{t2}\widetilde{\theta}_{l2} + r_{r_{t}\theta_{l}}\widetilde{\sigma}_{r_{t2}}\widetilde{\sigma}_{\theta_{l2}}\right), \tag{4.4.20}$$

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

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

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

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

$$(4.4.21)$$

4.5 Finding pdf parameters in terms of moments

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

The solution procedure is as follows.

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

$$\alpha = \frac{1}{2} \left[1 - \widehat{Sk}_w \sqrt{\frac{1}{4 + \widehat{Sk}_w^2}} \right], \tag{4.5.1}$$

$$\widehat{w}_1 = \sqrt{\frac{1-\alpha}{\alpha}},\tag{4.5.2}$$

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

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

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

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

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

$$\tilde{\theta}_{l1} = -\frac{\hat{c}_{w\theta_l}}{\hat{w}_2},\tag{4.5.5}$$

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

4. The widths of the Normals, $\tilde{\sigma}_{\theta_l 1}$ and $\tilde{\sigma}_{\theta_l 2}$, are determined by satisfying equation (4.4.8) for $\overline{\theta_l'^2}$, and equation (4.4.9) for $\overline{\theta_l'^3}$:

$$\tilde{\sigma}_{\theta_l 1}^2 = \left(1 - \hat{c}_{w\theta_l}^2\right) + \left(\sqrt{\frac{1 - \alpha}{\alpha}}\right) \frac{1}{3\hat{c}_{w\theta_l}} \left(\widehat{Sk_{\theta_l}} - \hat{c}_{w\theta_l}^3 \widehat{Sk_w}\right), \tag{4.5.7}$$

$$\tilde{\sigma}_{\theta_l 2}^2 = \left(1 - \hat{c}_{w\theta_l}^2\right) - \left(\sqrt{\frac{\alpha}{1 - \alpha}}\right) \frac{1}{3\hat{c}_{w\theta_l}} \left(\widehat{Sk_{\theta_l}} - \hat{c}_{w\theta_l}^3 \widehat{Sk_w}\right). \tag{4.5.8}$$

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

- 5. Equations for \tilde{r}_{t1} , \tilde{r}_{t2} , $\tilde{\sigma}_{r_{t1}}^{2}$, and $\tilde{\sigma}_{r_{t2}}^{2}$ are found by expressions identical to equation (4.5.5), equation (4.5.6), equation (4.5.7), and equation (4.5.8), except that θ_{l} is replaced everywhere by r_{t} .
- 6. Finally, from equation (4.4.17) for $\overline{r_t'\theta_l'}$ we find

$$r_{r_t\theta_l} = \frac{\widehat{c}_{r_t\theta_l} - \widehat{c}_{wr_t}\widehat{c}_{w\theta_l}}{\alpha\widetilde{\sigma}_{r_t1}\widetilde{\sigma}_{\theta_l1} + (1 - \alpha)\widetilde{\sigma}_{r_t2}\widetilde{\sigma}_{\theta_l2}}.$$
(4.5.9)

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

4.6 Higher-order moments in terms of pdf parameters

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

$$\frac{1}{(1-\tilde{\sigma}_{w}^{2})^{2}} \frac{(1-\delta)}{(1-\delta\lambda_{w})^{2}} \frac{\overline{w'^{4}}}{\left(\overline{w'^{2}}\right)^{2}} = \alpha \left[\widehat{w}_{1}^{4} + 6\widehat{w}_{1}^{2} \frac{\tilde{\sigma}_{w}^{2}}{(1-\tilde{\sigma}_{w}^{2})} + 3 \frac{\tilde{\sigma}_{w}^{4}}{(1-\tilde{\sigma}_{w}^{2})^{2}} \right] + (1-\alpha) \left[\widehat{w}_{2}^{4} + 6\widehat{w}_{2}^{2} \frac{\tilde{\sigma}_{w}^{2}}{(1-\tilde{\sigma}_{w}^{2})} + 3 \frac{\tilde{\sigma}_{w}^{4}}{(1-\tilde{\sigma}_{w}^{2})^{2}} \right] + \frac{1}{(1-\tilde{\sigma}_{w}^{2})^{2}} \frac{(1-\delta)}{(1-\delta\lambda_{w})^{2}} \delta 3\lambda_{w}^{2}, \tag{4.6.1}$$

$$\frac{1}{(1-\tilde{\sigma}_{w}^{2})} \frac{(1-\delta)^{1/2}}{(1-\delta\lambda_{w})(1-\delta\lambda_{\theta})^{1/2}} \frac{\overline{w'^{2}\theta'_{l}}}{\overline{w'^{2}} \left(\overline{\theta'_{l}^{2}}\right)^{1/2}} = \alpha \left[\widehat{w}_{1}^{2} + \frac{\tilde{\sigma}_{w}^{2}}{(1-\tilde{\sigma}_{w}^{2})}\right] \tilde{\theta}_{l1} + (1-\alpha) \left[\widehat{w}_{2}^{2} + \frac{\tilde{\sigma}_{w}^{2}}{(1-\tilde{\sigma}_{w}^{2})}\right] \tilde{\theta}_{l2}, \tag{4.6.2}$$

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

$$\frac{1}{(1 - \tilde{\sigma}_{w}^{2})^{1/2}} \frac{(1 - \delta)^{1/2}}{(1 - \delta \lambda_{w})^{1/2} (1 - \delta \lambda_{\theta})^{1/2} (1 - \delta \lambda_{q_{t}})^{1/2}} \frac{\overline{w' r'_{t} \theta'_{l}}}{\left(\overline{w'^{2}}\right)^{1/2} \left(\overline{r'^{2}_{t}}\right)^{1/2} \left(\overline{\theta'^{2}_{l}}\right)^{1/2}}$$

$$= \alpha \widehat{w}_{1} \left(\widetilde{r}_{t1} \widetilde{\theta}_{l1} + r_{r_{t}\theta_{l}} \widetilde{\sigma}_{r_{t1}} \widetilde{\sigma}_{\theta_{l1}}\right) + (1 - \alpha) \widehat{w}_{2} \left(\widetilde{r}_{t2} \widetilde{\theta}_{l2} + r_{r_{t}\theta_{l}} \widetilde{\sigma}_{r_{t2}} \widetilde{\sigma}_{\theta_{l2}}\right) \tag{4.6.4}$$

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

4.7 A diagnostic ansatz for the skewness of heat and moisture

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

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

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

$$\implies \beta = \frac{\frac{\widehat{S}k_{\theta_l}}{\widehat{S}k_w\widehat{c}_{w\theta_l}} - \widehat{c}_{w\theta_l}^2}{1 - \widehat{c}_{w\theta_l}^2}$$

$$(4.7.2)$$

Equation (4.7.1) is physically plausible but limited at the same time. The formula states that Sk_{θ_l} is proportional to Sk_w , the skewness of w. An increase in β leads to an increase in $|Sk_{\theta_l}|$, which, in turn, leads to a pdf with a longer θ_l -tail. Sk_{θ_l} and Sk_w have the same sign when w and θ_l are positively correlated; Sk_{θ_l} and Sk_w have opposite sign when w and θ_l are negatively correlated. In those large eddy simulations, this is usually but not always

true. Sk_{θ_l} vanishes when either Sk_w or $c_{w\theta_l}$ vanishes; clearly this need not be true in nature. $|Sk_{\theta_l}|$ can be either smaller or larger than $|Sk_w|$, depending on the values of $\tilde{\sigma}_w^2$, $c_{w\theta_l}$, and β .

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

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

and

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

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

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

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

CLUBB chose a specific formula for the w-"width" of the individual normals, which is the following:

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

This makes $\tilde{\sigma}_w^2$ depend on $c_{wr_t}^2$ and $c_{w\theta_l}^2$. Here $0 \leq \gamma < 1$ is a dimensionless constant. This formula helps ensure that when c_{wr_t} or $c_{w\theta_l}$ becomes large in magnitude, $0 \leq \hat{c}_{w\theta_l}^2$, $\hat{c}_{wr_t}^2 < 1$ and hence $\tilde{\sigma}_{r_t1,2}^2$, $\tilde{\sigma}_{\theta_l1,2}^2$, and $r_{r_t\theta_l}$ remain realistic.

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

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

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

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

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

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

equation (4.4.6), we find

$$\frac{1}{(1-\tilde{\sigma}_w^2)^2} \frac{(1-\delta)}{(1-\delta\lambda_w)^2} \frac{\overline{w'^4}}{\left(\overline{w'^2}\right)^2} = 3 \frac{\tilde{\sigma}_w^4}{(1-\tilde{\sigma}_w^2)^2} + 6 \frac{\tilde{\sigma}_w^2}{(1-\tilde{\sigma}_w^2)} + 1 + \widehat{Sk}_w^2 + \frac{1}{(1-\tilde{\sigma}_w^2)^2} \frac{(1-\delta)}{(1-\delta\lambda_w)^2} \delta 3\lambda_w^2, \tag{4.8.2}$$

and also

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

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

$$+ \delta 3\lambda_w^2 \left(\overline{w'^2}\right)^2. \tag{4.8.3}$$

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

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

and

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

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

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

and

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

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

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

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

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

and

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

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

$$\frac{(1-\delta)^{1/2}}{(1-\delta\lambda_{w})^{1/2}(1-\delta\lambda_{\theta})^{1/2}(1-\delta\lambda_{r_{t}})^{1/2}} \frac{\overline{w'r'_{t}\theta'_{l}}}{(1-\tilde{\sigma}_{w}^{2})^{1/2}\left(\overline{w'^{2}}\right)^{1/2}\left(\overline{r'_{t}^{2}}\right)^{1/2}\left(\overline{\theta'_{l}^{2}}\right)^{1/2}}$$

$$= \widehat{c}_{wr_{t}}\widehat{c}_{w\theta_{l}}\widehat{Sk}_{w} + E(w, q_{t}, \theta_{l})\frac{1}{2}\widehat{Sk}_{w}\left(c_{q_{t}\theta_{l}} - \widehat{c}_{wr_{t}}\widehat{c}_{w\theta_{l}}\right), \qquad (4.8.10)$$

and

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

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

$$E = \frac{1 - \frac{1}{2} \frac{2\alpha}{1 - 2\alpha} \xi}{1 + \frac{1}{2} \xi},\tag{4.8.12}$$

where

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

and

$$A_{\theta_l} = Sk_{\theta_l} - \frac{3}{2}\widehat{c}_{w\theta_l}\widehat{Sk}_w + \frac{1}{2}\widehat{c}_{w\theta_l}^3\widehat{Sk}_w, \tag{4.8.14}$$

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

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

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

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

$$\xi = \frac{1 - 2\zeta}{\zeta},\tag{4.8.16}$$

where

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

Then we find

$$E = \frac{2}{3}\beta,\tag{4.8.18}$$

and finally

$$\overline{w'r_t'\theta_l'} = \frac{\frac{1}{3}\beta}{(1-\tilde{\sigma}_w^2)} \frac{(1-\delta\lambda_{\theta r})}{(1-\delta\lambda_w)} \overline{r_t'\theta_l'} \frac{\overline{w'^3}}{\overline{w'^2}} + \frac{1-\frac{1}{3}\beta}{(1-\tilde{\sigma}_w^2)^2} \frac{(1-\delta\lambda_{wr})(1-\delta\lambda_{w\theta})}{(1-\delta\lambda_w)^2} \overline{w'r_t'} \, \overline{w'\theta_l'} \frac{\overline{w'^3}}{\left(\overline{w'^2}\right)^2}.$$
(4.8.19)

5 Integration using SymPy

Throughout this thesis, symbolic manipulation plays a crucial role in verifying mathematical expressions, particularly integrals. To achieve this, we rely on SymPy, ¹ a powerful Python library for symbolic mathematics. This chapter delves 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 $\overline{w'^2}$. 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, there is the following code: In this listing, sympy was defined to be called sp and from sympy we directly imported

¹Aaron Meurer et al. "SymPy: symbolic computing in Python". In: *PeerJ Computer Science* 3 (Jan. 2017), e103. ISSN: 2376-5992. DOI: 10.7717/peerj-cs.103. URL: https://doi.org/10.7717/peerj-cs.103.

Listing 5.1: Import statements

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

some packages, too, which are needed later on.

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

Listing 5.2: Defining symbols

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

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

Listing 5.3: Defining the marginals

at figure 5.1, this is exactly the integral, which we want to compute. Using the command .doit(conds='none'), we can actually calculate the given integral, where we assume, that all given constants are real. We are also using .simplify() here to make the output more

Listing 5.4: Defining and displaying the needed integral

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

Figure 5.1: Output of listing 5.4

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

readable as well as more comparable to the actual function we want to check. We can now

Listing 5.5: Calculating and printing the integral

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

Figure 5.2: Output of listing 5.5

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

compare figure 5.2 to the given equation. To do this, we first need to define the equation for equation (4.4.3). We can print this equation, using display again. The last step is

Figure 5.3: Output of listing 5.7

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

to check if those two formulas are equivalent to each other. We can do this by just using

Listing 5.6: Python function for the second order moment

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

Listing 5.7: Printing the symbolic equation

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

Eq(..) from the package SymPy. factor(..) just tries to factor the given variables to make the comparison easier. This code just displays True, which is exactly what we wanted to

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

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

have.

5.2 Numeric integration

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

Listing 5.9: Import statements

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

define those. We still use the symbols as in listing 5.2, together with the following:

Listing 5.10: Defining symbols

```
sigma_lambda_theta_1 = Symbol('\sigma_{\lambda\\theta_1}')
theta_1_1 = Symbol('\\theta_{11}')
theta_1_2 = Symbol('\\theta_{12}')
theta_1_bar = Symbol('\overline{\\theta_1}')
sigma_theta_1_1 = Symbol('\\sigma_{\\theta_{11}}')
sigma_theta_1_2 = Symbol('\\sigma_{\\theta_{12}}')
rho_w_theta_1 = Symbol('\\rho_{w\\theta_1}')
w_prime_3_bar = Symbol('\overline{w\'^3}')
w_prime_theta_1_prime_bar = Symbol('\overline{w\'\\theta\'_1}')
w_prime_2_theta_prime_1_bar = Symbol('\overline{w\'\2\\theta\'_1}')
sigma_tilde_w = Symbol('\Tilde{\\sigma}_w')
lambda_w_theta = Symbol('\lambda_{w\\theta}')
lambda_w = Symbol('\lambda_w')
```

We start defining the integral by defining the marginals.

Listing 5.11: Defining the marginals

```
G_1_w_theta = Normal(name='G_1_w_theta', mean=sp.Matrix([w_1, theta_1_1]),
    std=sp.Matrix([[sigma_w ** 2, 0], [0, sigma_theta_l_1 ** 2]]))
G_1_w_theta_density = density(G_1_w_theta)(sp.abc.w, sp.abc.theta)
G_2_w_theta = Normal(name='G_2_w_theta', mean=sp.Matrix([w_2, theta_1_2]),
    std=sp.Matrix([[sigma_w ** 2, 0], [0, sigma_theta_1_2 ** 2]]))
G_2_w_theta_density = density(G_2_w_theta)(sp.abc.w, sp.abc.theta)
G_3_w_theta = Normal(name='G_3_w_theta', mean=sp.Matrix([w_bar, theta_l_bar]),
    std=sp.Matrix([[sigma_lambda_w ** 2,
        rho_w_theta_l * sigma_lambda_w * sigma_lambda_theta_l],
        [rho_w_theta_l * sigma_lambda_w * sigma_lambda_theta_l,
        sigma_lambda_theta_1 ** 2]]))
G_3_w_theta_density = sp.simplify(density(G_3_w_theta)(sp.abc.w, sp.abc.theta))
G_w_{theta} = (
(1 - sp.abc.delta) * sp.abc.alpha * density(G_1_w_theta)(sp.abc.w, sp.abc.theta)
+ (1 - sp.abc.delta) * (1 - sp.abc.alpha) * density(G_2_w_theta)(sp.abc.w, sp.abc.theta)
+ sp.abc.delta * G_3_w_theta_density)
```

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

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))
```

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

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

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

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

Figure 5.4: Output of listing 5.13

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

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

Instead, since we cannot compute the integral analytically, we can create a dataframe using pandas.² The columns for this dataframe are going to be all the inputs we have. To get all permutations, this code is also using product(..) from the itertools package.

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

²Wes McKinney. "Data Structures for Statistical Computing in Python". In: *Proceedings of the 9th*

Listing 5.14: Create a dataframe and putting in arbitrary numbers

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

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

This code also uses the function defined in listing 5.13, where all other equations are substituted into. The function df.apply(..) is used to apply the function given in the parenthesis to all rows of the dataframe by specifying a lambda x, where x is corresponding to the given dataframe, df. Lastly, there is also the axis=1 parameter, which specifies the direction of applying the function.

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

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))
```

Python in Science Conference. Ed. by Stéfan van der Walt and Jarrod Millman. 2010, pp. 56–61. DOI: 10.25080/Majora-92bf1922-00a.

Here, we are using the integral which has been specified earlier and adding the parameter method='quad' to the function .doit(..). After that, .evalf(..) just gives the numerical value. We try to prove that the integral value equals the function value, hence we are computing the error between those two columns and take the mean of this new column to see if the error is actually numerically 0.

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

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

Listing 5.18: Calculating the mean difference

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

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

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

6 Asymptotics

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

We start with the "obvious" restrictions for the pdf parameters.

- The mixture fractions α and δ are meant to be $\alpha \in [0,1]$ and $\delta \in [0,1)$. The restriction to δ vs the one to α makes sense in a way that we do not really want just the third normal to predict the whole shape. Also, most of the formulas, e.g. equation (4.4.6) have a 1δ in the denominator.
- In section 4.3, we saw, how the transformation between the sum of two normal distributions and the sum of three normal distributions are working. From those transformations, we see that we want

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

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

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

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

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

$$\begin{aligned}
&-1 < \widehat{c}_{w\theta_{l}} < 1 \iff (\widehat{c}_{w\theta_{l}})^{2} < 1 \\
\iff \left(\frac{1}{(1-\widetilde{\sigma}_{w}^{2})^{1/2}} \frac{\overline{w'r'_{l}}}{\sqrt{\overline{w'^{2}}} \sqrt{\overline{r_{t}'^{2}}}} \frac{1}{\sqrt{\frac{1-\delta\lambda_{w}}{1-\delta}}} \frac{1}{\sqrt{\frac{1-\delta\lambda_{w}}{1-\delta}}} \frac{1-\delta\lambda_{wr}}{1-\delta} \right)^{2} < 1 \\
\iff \frac{1}{(1-\widetilde{\sigma}_{w}^{2})} \frac{(\overline{w'r'_{l}})^{2}}{\overline{w'^{2}r'^{2}}} \frac{1-\delta}{1-\delta\lambda_{w}} \frac{1-\delta}{1-\delta\lambda_{r}} \frac{(1-\delta\lambda_{wr})^{2}}{(1-\delta\lambda_{r})^{2}} < 1 \\
\iff \frac{(1-\delta\lambda_{wr})^{2} (\overline{w'r'_{l}})^{2}}{(1-\delta\lambda_{w})(1-\delta\lambda_{r})\overline{w'^{2}r'^{2}}} < (1-\widetilde{\sigma}_{w}^{2}) \\
\iff \frac{(1-\delta\lambda_{wr})^{2} (\overline{w'r'_{l}})^{2}}{(1-\delta\lambda_{w})(1-\delta\lambda_{r})\overline{w'^{2}r'^{2}}} < 1 - \left(\frac{\sigma_{w}^{2}(1-\delta)}{\overline{w'^{2}}(1-\delta\lambda_{w})}\right) \\
\iff \frac{(1-\delta\lambda_{wr})^{2} (\overline{w'r'_{l}})^{2}}{(1-\delta\lambda_{w})(1-\delta\lambda_{r})\overline{w'^{2}r'^{2}}} + \frac{\sigma_{w}^{2}(1-\delta)}{\overline{w'^{2}}(1-\delta\lambda_{w})} < 1 \\
\iff \frac{(1-\delta\lambda_{wr})^{2} (\overline{w'r'_{l}})^{2} + \sigma_{w}^{2}(1-\delta)(1-\delta\lambda_{r})\overline{r'^{2}}}{(1-\delta\lambda_{w})(1-\delta\lambda_{r})\overline{r'^{2}}} < 1
\end{aligned}$$

7 Summary

8 Outlook

We have seen that adding a third normal distribution right in the middle of the two defined (simplified) normal distributions does not change the "closed" formulas too much, neither it makes it too complicated. So for CLUBB there are new parameters, e.g. δ or λ_w , which can be chosen to "tweak" the representation of the underlying pdf for the prognosed moments. Ultimately one would like to fit this resulting pdf to real data, to get better relationships, as well as thresholds for some variables. To do this there are some approaches which unfortunately have not been discussed. A following thesis could e.g. incorporate some machine learning approach to learn optimal values for certain parameters.

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

- Symbolic Verification: SymPy allows us to perform symbolic manipulations, enabling the derivation of exact solutions for integrals whenever possible.
- Numerical Approximation: For integrals that are analytically intractable, SymPy seamlessly integrates with numerical computing libraries. This allows us to efficiently approximate the integral's value for specific parameter choices. This combined approach ensures we can handle a broader range of integral expressions.

• Generalizability and Reusability: The framework outlined in chapter 5 is not specific to the context of CLUBB. By focusing on the core functionalities of SymPy, this approach can be adapted to various scientific disciplines.

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

Bibliography

- Izenman, Alan Julian. Modern multivariate statistical techniques: regression, classification, and manifold learning. Springer texts in statistics. OCLC: ocn225427579. New York; London: Springer, 2008. ISBN: 9780387781884.
- Larson, Vincent E. *CLUBB-SILHS: A parameterization of subgrid variability in the atmosphere*. 2022. arXiv: 1711.03675 [physics.ao-ph].
- McKinney, Wes. "Data Structures for Statistical Computing in Python". In: *Proceedings of the 9th Python in Science Conference*. Ed. by Stéfan van der Walt and Jarrod Millman. 2010, pp. 56–61. DOI: 10.25080/Majora-92bf1922-00a.
- Meurer, Aaron et al. "SymPy: symbolic computing in Python". In: *PeerJ Computer Science* 3 (Jan. 2017), e103. ISSN: 2376-5992. DOI: 10.7717/peerj-cs.103. URL: https://doi.org/10.7717/peerj-cs.103.

A Code

A.1 User Guide

A.1.1 Accessing the code

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

A.1.2 Key files and their purposes

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

A.1.3 Working with functions

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

A.1.4 Displaying equations effectively

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

A.1.5 Handling integrals

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

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

A.2 symbols.py

```
from sympy import Symbol, symbols
2
    # siqma
3
    sigma_w = Symbol('\sigma_w')
4
5
    sigma_r_t_i, sigma_r_t_1, sigma_r_t_2 = (
6
7
         symbols('\sigma_{r_{ti}} \sigma_{r_{t1}} \sigma_{r_{t2}}'))
    sigma_theta_l_i, sigma_theta_l_1, sigma_theta_l_2 = (
9
         symbols('\sigma_{\theta_{11}} \sigma_{\theta_{12}}'))
10
11
    sigma_tilde_r_t_i, sigma_tilde_r_t_1, sigma_tilde_r_t_2 = (
12
         symbols('\\tilde{\\sigma}_{r_ti} \\tilde{\\sigma}_{r_t1} \\\tilde{\\sigma}_{r_t2}')
13
14
15
    sigma_tilde_theta_l_i, sigma_tilde_theta_l_1, sigma_tilde_theta_l_2 = (
16
         symbols(
17
18
             '\\tilde{\\sigma}_{\\theta_li} \\tilde{\\sigma}_{\\theta_l1}
              → \\tilde{\\sigma}_{\\theta_12}')
    )
19
20
    sigma_tilde_lambda_w = Symbol('\\tilde{\sigma}_{\lambda_w}')
21
    sigma_tilde_w = Symbol('\\tilde{\sigma}_w')
22
    sigma_lambda_w = Symbol('\sigma_{\lambda_w}')
23
    sigma_lambda_theta_1 = Symbol('\sigma_{\lambda\\theta_1}')
24
    sigma_lambda_r_t = Symbol('\sigma_{{\lambda}r_t}')
25
26
    # w
27
    w_bar = Symbol('\overline{w}')
28
    w_prime = Symbol('w\'')
29
    w_i, w_1, w_2 = symbols('w_i w_1 w_2')
30
31
    w_hat_i, w_hat_1, w_hat_2, w_hat_3, w_hat_prime = (
32
         symbols('\hat{$\mathbb{W}_i  \hat{$\mathbb{W}_1  \hat{$\mathbb{W}_2  \hat{$\mathbb{W}_3  \hat{$\mathbb{W}$''}}}}
33
34
35
    w_prime_2_bar, w_prime_3_bar, w_prime_4_bar = symbols(
36
         \label{lower-line} $$ \operatorname{w}^2 \operatorname{w}^3 \operatorname{w}^3$ \operatorname{w}^4$'
37
38
39
    w_prime_r_t_prime_bar = Symbol('\overline{w\'r\'_t}')
40
```

```
w_prime_2_theta_prime_1_bar = Symbol('\overline{w\'^2\\theta\'_1}')
    w_prime_theta_prime_l_2_bar = Symbol('\overline{w\'\\theta\'^2_l}')
42
    w_prime_theta_l_prime_bar = Symbol('\overline{w\'\\theta\'_1}')
43
44
    w_prime_r_t_prime_theta_l_prime_bar = Symbol('\overline\{w\'\{r_t\}\'\{\\theta_l\}\'\}')
45
46
47
    r_t = Symbol('r_t')
48
49
    r_t_bar, r_t_prime_2_bar = symbols(
50
        '\overline{r_t} \overline{r_t\'^2}'
51
52
53
    r_t_i, r_t_1, r_t_2 = symbols('r_{ti} r_{t1} r_{t2}')
54
55
    r_t_tilde_prime, r_t_i_tilde, r_t_1_tilde, r_t_2_tilde = symbols(
56
        57
58
59
    # theta
60
    theta_1 = Symbol('\\theta_1')
61
62
    theta_l_bar, theta_l_prime_2_bar, theta_l_prime_3_bar = symbols(
63
        '\overline{\\theta_1\'^2} \overline{\\theta_1\'^3}'
64
    )
65
66
    theta_l_prime_r_t_prime_bar = Symbol('\overline{\\theta_l\'r_t\'}')
67
68
    theta_l_i, theta_l_1, theta_l_2 = symbols(
69
        '\\theta_{li} \\theta_{l1} \\theta_{l2}'
70
    )
71
72
    theta_tilde_prime_l = Symbol('\\tilde{\\theta}_l\'')
73
74
    theta_tilde_l_i, theta_tilde_l_1, theta_tilde_l_2 = symbols(
75
        \label{li} $$  \(\theta)_{1i} \tilde{\theta}_{11} \tilde{\theta}_{12}' 
76
    )
77
78
    # lambda
79
    lambda_theta = Symbol('\lambda_\\theta')
80
    lambda_theta_r = Symbol('\lambda_\\theta_r')
81
    lambda_r = Symbol('\lambda_r')
82
    lambda_w = Symbol('\lambda_w')
83
    lambda_w_theta = Symbol('\lambda_{w\\theta}')
84
    lambda_w_r = Symbol('\lambda_{wr}')
85
86
    r_r_t_t = Symbol('r_{r_t})
87
    triple_gaussian = Symbol('P_{tmg}(\hat{w\'}, \\tilde{\\theta\'_l}, \\tilde{r\'_t})')
88
    sk_hat_w = Symbol('\widehat{Sk}_w')
89
    sk_theta_l_hat = Symbol('\widehat{Sk}_{\\theta_l}')
90
    c_w_theta_l_hat = Symbol('\hat{c}_{w\\theta_l}')
91
    G_3 = Symbol('G_3')
92
    G_3_hat = Symbol('\hat{G_3}')
93
94
```

```
G_w, G_1_w, G_2_w, G_3_w = symbols(
         'G_{w}(w) G_{1w}(w) G_{2w}(w) G_{3w}(w)'
96
97
98
     G_w_1_2 = Symbol('G_{w_{12}}')
99
100
101
     G_w_theta = Symbol('G_{w\\theta}(w,\\theta)')
     G_1_w_theta = Symbol('G_{1w\\theta}(w,\\theta)')
102
     G_2_w_theta = Symbol('G_{2w}\wedge theta)(w, \wedge theta)')
103
     G_3_w_theta = Symbol('G_{3w\\theta}(w,\\theta)')
104
105
     G_{theta_r} = Symbol('G_{(\theta_r)(\theta, r)'})
106
     G_1_{theta_r} = Symbol('G_{1} + r)(\theta, r)')
107
     G_2_{theta_r} = Symbol('G_{2} + r)(\theta, r)')
108
     G_3_{theta_r} = Symbol('G_{3}\backslash r)(\backslash r)'
109
110
     G_w_theta_l_r_t = Symbol('G_{w_{\cdot}}(r_t))')
111
     G_1_w_{theta_1_r_t} = Symbol('G_{1w{\cdot theta_1}{r_t}}(w,{\cdot theta_1},{r_t})')
      G_2_w_{theta_l_r_t} = Symbol('G_{2w}(\theta_1)_{r_t})(w, (\theta_1), \{r_t\})') 
113
     G_3_w_theta_1_r_t = Symbol('G_{3w}(\theta_1)_{r_t})(w,{\theta_1},{r_t})')
114
115
     G_theta, G_1_theta, G_2_theta, G_3_theta = symbols(
116
          G_{\theta}(\theta) G_{1\wedge (\theta) G_{2\wedge (\theta)}
117
          \hookrightarrow G_{3\\theta}(\\theta)'
     )
118
119
     rho_w_theta_1 = Symbol('\\rho_{w\\theta_1}')
120
     rho_w_r_t = Symbol('\\rho_{\wr_t}')
121
     rho_theta_l_r_t = Symbol('\\rho_{\\theta_lr_t}')
122
```

Listing A.1: symbols.py

A.3 checked_functions.py

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

```
16
    def w_prime_2_bar(delta=sp.abc.delta, alpha=sp.abc.alpha, w_1=sym.w_1, w_2=sym.w_2,
17
                       w_bar=sym.w_bar, sigma_w=sym.sigma_w,
18

    sigma_lambda_w=sym.sigma_lambda_w):

        return (((1 - delta) * alpha * ((w_1 - w_bar) ** 2 + sigma_w ** 2)) +
19
                 ((1 - delta) * (1 - alpha) * ((w_2 - w_bar) ** 2 + sigma_w ** 2)) +
20
                 (delta * sigma_lambda_w ** 2))
21
22
23
    def w_prime_3_bar(delta=sp.abc.delta, alpha=sp.abc.alpha, w_1=sym.w_1, w_2=sym.w_2,
24
                       w_bar=sym.w_bar, sigma_w=sym.sigma_w):
25
        return (((1 - delta) * alpha * ((w_1 - w_bar) ** 3 +
26
                                          3 * sigma_w ** 2 * (w_1 - w_bar))) +
27
                 ((1 - delta) * (1 - alpha) * ((w_2 - w_bar) ** 3 +
28
                                                 3 * sigma_w ** 2 * (w_2 - w_bar))))
29
30
31
    def w_prime_4_bar(w_prime_2_bar=sym.w_prime_2_bar,
32
                       w_prime_3_bar=sym.w_prime_3_bar,
33
                       delta=sp.abc.delta,
34
                       sigma_tilde_w=sym.sigma_tilde_w,
35
36
                       sigma_lambda_w=sym.sigma_lambda_w):
        return (w_prime_2_bar ** 2 *
37
                 ((1 - delta * (sigma_lambda_w ** 2 / w_prime_2_bar)) ** 2 / (1 - delta)) *
38
                 (3 * sigma_tilde_w ** 4 +
39
                  6 * (1 - sigma_tilde_w ** 2) *
40
                  sigma_tilde_w ** 2 +
41
                  (1 - sigma_tilde_w ** 2) ** 2) +
42
                 ((1 / (1 - sigma_tilde_w ** 2)) *
43
                  (1 / (1 - delta * (sigma_lambda_w ** 2 / w_prime_2_bar))) *
44
                  (w_prime_3_bar ** 2 / w_prime_2_bar)) +
45
                 (delta * 3 * sigma_lambda_w ** 4))
46
47
48
49
50
    # theta_l equations
51
52
53
    def theta_l_bar(alpha=sp.abc.alpha, delta=sp.abc.delta,
54
                     theta_l_1=sym.theta_l_1, theta_l_2=sym.theta_l_2):
55
        return ((1 - delta) * alpha * theta_l_1
56
                 + (1 - delta) * (1 - alpha) * theta_1_2
57
                 + delta * (alpha * theta_l_1 + (1 - alpha) * theta_l_2))
58
59
60
    def theta_l_prime_2_bar(delta=sp.abc.delta,
61
                              alpha=sp.abc.alpha,
62
                              theta_1_1=sym.theta_1_1,
63
                             theta_1_2=sym.theta_1_2,
64
                             theta_l_bar=sym.theta_l_bar,
65
                              sigma_theta_l_1=sym.sigma_theta_l_1,
66
                              sigma_theta_1_2=sym.sigma_theta_1_2,
67
68
                              sigma_lambda_theta_l=sym.sigma_lambda_theta_l):
```

```
return (((1 - delta) * alpha * ((theta_l_1 - theta_l_bar) ** 2 + sigma_theta_l_1 **
69

→ 2)) +

                  ((1 - delta) * (1 - alpha) *
70
                   ((theta_1_2 - theta_1_bar) ** 2 + sigma_theta_1_2 ** 2)) +
71
                  (delta * sigma_lambda_theta_l ** 2))
72
73
74
     def theta_l_prime_3_bar(delta=sp.abc.delta,
75
                              alpha=sp.abc.alpha,
76
                              theta_l_1=sym.theta_l_1,
77
                              theta_1_2=sym.theta_1_2,
78
79
                              theta_l_bar=sym.theta_l_bar,
                               sigma_theta_l_1=sym.sigma_theta_l_1,
80
                               sigma_theta_1_2=sym.sigma_theta_1_2):
81
         return (((1 - delta) * alpha *
82
                   ((theta_l_1 - theta_l_bar) ** 3 +
83
                    3 * sigma_theta_l_1 ** 2 * (theta_l_1 - theta_l_bar))) +
84
                  ((1 - delta) * (1 - alpha) *
85
                   ((theta_l_2 - theta_l_bar) ** 3 +
86
                    3 * sigma_theta_1_2 ** 2 * (theta_1_2 - theta_1_bar))))
87
88
89
90
91
     \# r_t = equations
92
93
94
     def r_t_bar(alpha=sp.abc.alpha, delta=sp.abc.delta, r_t_1=sym.r_t_1, r_t_2=sym.r_t_2):
95
         return ((1 - delta) * alpha * r_t_1
96
                  + (1 - delta) * (1 - alpha) * r_t_2
97
                  + delta * (alpha * r_t_1 + (1 - alpha) * r_t_2))
98
99
     def r_t_prime_2_bar(delta=sp.abc.delta,
101
                          alpha=sp.abc.alpha,
102
                          r_t_1=sym.r_t_1,
103
                          r_t_2=sym.r_t_2,
104
                          r_t_bar=sym.r_t_bar,
105
                          sigma_r_t_1=sym.sigma_r_t_1,
106
                          sigma_r_t_2=sym.sigma_r_t_2,
107
                          sigma_lambda_r_t=sym.sigma_lambda_r_t):
108
         return (((1 - delta) * alpha * ((r_t_1 - r_t_bar) ** 2 + sigma_r_t_1 ** 2)) +
109
                  ((1 - delta) * (1 - alpha) * ((r_t_2 - r_t_bar) ** 2 + sigma_r_t_2 ** 2)) +
110
                  (delta * sigma_lambda_r_t ** 2))
111
112
113
114
115
     # Mixed equations
116
117
118
     def w_prime_theta_l_prime_bar(delta=sp.abc.delta,
119
                                     alpha=sp.abc.alpha,
120
121
                                     w_1=sym.w_1,
```

```
122
                                     w_2=sym.w_2,
                                     w_bar=sym.w_bar,
123
                                     theta_l_1=sym.theta_l_1,
124
                                     theta_1_2=sym.theta_1_2,
125
                                     theta_l_bar=sym.theta_l_bar,
126
                                     cov_lambda_w_theta=sym.rho_w_theta_l * sym.sigma_lambda_w
127
                                                         sym.sigma_lambda_theta_l):
128
         return (((1 - delta) * alpha * ((w_1 - w_bar) * (theta_l_1 - theta_l_bar))) +
129
                  ((1 - delta) * (1 - alpha) * ((w_2 - w_bar) * (theta_l_2 - theta_l_bar)))
130
                  + delta * cov_lambda_w_theta)
131
132
133
     def w_prime_r_t_prime_bar(delta=sp.abc.delta,
134
                                 alpha=sp.abc.alpha,
135
                                w_1=sym.w_1,
136
                                 w_2 = sym.w_2,
137
                                 w_bar=sym.w_bar,
138
                                r_t_1=sym.r_t_1,
139
                                r_t_2=sym.r_t_2,
140
                                r_t_bar=sym.r_t_bar,
141
142
                                 cov_lambda_w_r=sym.rho_w_r_t * sym.sigma_lambda_w *
                                                sym.sigma_lambda_r_t):
143
         return (((1 - delta) * alpha * ((w_1 - w_bar) * (r_t_1 - r_t_bar))) +
144
                  ((1 - delta) * (1 - alpha) * ((w_2 - w_bar) * (r_t_2 - r_t_bar)))
145
                  + delta * cov_lambda_w_r)
146
147
148
     def w_prime_2_theta_l_prime_bar(sigma_tilde_w=sym.sigma_tilde_w,
149
                                       delta=sp.abc.delta,
150
                                       lambda_w_theta=sym.lambda_w_theta,
151
                                       lambda_w=sym.lambda_w,
152
                                       w_prime_3_bar=sym.w_prime_3_bar,
                                       w_prime_2_bar=sym.w_prime_2_bar,
154
                                       w_prime_theta_l_prime=sym.w_prime_theta_l_prime_bar):
155
         return ((1 / (1 - sigma_tilde_w ** 2)) *
156
                  ((1 - delta * lambda_w_theta) / (1 - delta * lambda_w)) *
157
                  (w_prime_3_bar / w_prime_2_bar) *
158
                  w_prime_theta_l_prime)
159
160
161
     def w_prime_theta_l_prime_2_bar(delta=sp.abc.delta,
162
                                       lambda_w_theta=sym.lambda_w_theta,
163
                                       lambda_w=sym.lambda_w,
164
                                       sigma_tilde_w=sym.sigma_tilde_w,
165
                                       w_prime_3_bar=sym.w_prime_3_bar,
166
                                       w_prime_2_bar=sym.w_prime_2_bar,
167
                                       w_prime_theta_l_prime_bar=sym.w_prime_theta_l_prime_bar,
                                       theta_l_prime_3_bar=sym.theta_l_prime_3_bar):
169
         return (Rational(2, 3) *
170
                  ((1 - delta * lambda_w_theta) ** 2 / (1 - delta * lambda_w) ** 2) *
171
                  (1 / (1 - sigma_tilde_w ** 2) ** 2) *
                  (w_prime_3_bar / w_prime_2_bar ** 2) *
173
174
                  w_prime_theta_l_prime_bar ** 2 +
```

```
175
                  Rational(1, 3) *
                  ((1 - delta * lambda_w) / (1 - delta * lambda_w_theta)) *
176
                  (1 - sigma_tilde_w ** 2) *
177
                  ((w_prime_2_bar * theta_l_prime_3_bar) / w_prime_theta_l_prime_bar))
178
179
180
     def w_prime_theta_l_prime_2_bar_beta(
181
             sigma_tilde_w=sym.sigma_tilde_w,
182
             delta=sp.abc.delta,
183
             lambda_theta=sym.lambda_theta,
             lambda_w=sym.lambda_w,
185
             w_prime_3_bar=sym.w_prime_3_bar,
             w_prime_2_bar=sym.w_prime_2_bar,
187
             beta=sp.abc.beta,
             theta_l_prime_2_bar=sym.theta_l_prime_2_bar,
189
             lambda_w_theta=sym.lambda_w_theta,
             w_prime_theta_l_prime_bar=sym.w_prime_theta_l_prime_bar):
191
         from sympy import Rational
192
         return (
193
                  (1 / (1 - sigma_tilde_w ** 2)) *
194
                  ((1 - delta * lambda_theta) / (1 - delta * lambda_w)) *
195
                  (w_prime_3_bar / w_prime_2_bar) *
196
                  (
197
                          Rational(1, 3) * beta * theta_l_prime_2_bar +
198
199
                                   ((1 - Rational(1, 3) * beta) / (1 - sigma_tilde_w ** 2)) *
200
                                   ((1 - delta * lambda_w_theta) ** 2 /
201
                                    ((1 - delta * lambda_w) * (1 - delta * lambda_theta))) *
202
                                   (w_prime_theta_l_prime_bar ** 2 / w_prime_2_bar)
                          )
204
                  )
205
206
208
     def w_prime_r_t_prime_theta_l_prime_bar(delta=sp.abc.delta,
209
                                                alpha=sp.abc.alpha,
210
                                                w_1=sym.w_1,
211
                                                w_2=sym.w_2,
212
                                                w_bar=sym.w_bar,
213
                                                r_t_1=sym.r_t_1,
214
                                                r_t_2=sym.r_t_2,
215
                                                r_t_bar=sym.r_t_bar,
216
217
                                                theta_l_1=sym.theta_l_1,
                                                theta_1_2=sym.theta_1_2,
^{218}
                                                theta_l_bar=sym.theta_l_bar,
219
                                                r_r_t_theta_l=sym.r_r_t_theta_l,
220
                                                sigma_r_t_1=sym.sigma_r_t_1,
221
                                                sigma_r_t_2=sym.sigma_r_t_2,
222
                                                sigma_theta_l_1=sym.sigma_theta_l_1,
223
                                                sigma_theta_1_2=sym.sigma_theta_1_2):
224
         return (((1 - delta) * alpha * (w_1 - w_bar) *
225
                            (r_t_1 - r_t_bar) * (theta_l_1 - theta_l_bar) +
227
228
                           r_r_t_theta_l * sigma_r_t_1 * sigma_theta_l_1
```

```
)) +
229
                  ((1 - delta) * (1 - alpha) * (w_2 - w_bar) *
230
231
                            (r_t_2 - r_t_bar) * (theta_l_2 - theta_l_bar) +
232
                            r_r_t_theta_1 * sigma_r_t_2 * sigma_theta_1_2
233
                   )))
234
235
236
     def w_prime_r_t_prime_theta_l_prime_bar_beta(
237
              beta=sp.abc.beta,
238
              sigma_tilde_w=sym.sigma_tilde_w,
239
              delta=sp.abc.delta,
240
              lambda_theta_r=sym.lambda_theta_r,
241
              lambda_w=sym.lambda_w,
242
              theta_l_prime_r_t_prime_bar=sym.theta_l_prime_r_t_prime_bar,
243
              w_prime_3_bar=sym.w_prime_3_bar,
244
              w_prime_2_bar=sym.w_prime_2_bar,
245
              lambda_w_r=sym.lambda_w_r,
              lambda_w_theta=sym.lambda_w_theta,
247
              w_prime_r_t_prime_bar=sym.w_prime_r_t_prime_bar,
248
              w_prime_theta_l_prime_bar=sym.w_prime_theta_l_prime_bar):
249
250
         from sympy import Rational
         return (
251
252
                           ((Rational(1, 3) * beta) / (1 - sigma_tilde_w ** 2)) *
253
                           ((1 - delta * lambda_theta_r) / (1 - delta * lambda_w)) *
254
                           theta_l_prime_r_t_prime_bar *
255
                           (w_prime_3_bar / w_prime_2_bar)
256
                  ) +
257
258
                           ((1 - Rational(1, 3) * beta) / (1 - sigma_tilde_w ** 2) ** 2) *
259
                           (((1 - delta * lambda_w_r) * (1 - delta * lambda_w_theta)) /
260
                            ((1 - delta * lambda_w) ** 2)) *
                           w_prime_r_t_prime_bar *
262
                           w_prime_theta_l_prime_bar *
263
                           (w_prime_3_bar / w_prime_2_bar ** 2)
264
                  )
265
266
267
268
     def r_t_prime_theta_l_prime_bar(alpha=sp.abc.alpha, delta=sp.abc.delta,
269
                                       r_t_1=sym.r_t_1, r_t_2=sym.r_t_2,
270
                                        \hookrightarrow r_t_prime_bar=sym.r_t_bar,
                                        theta_l_1=sym.theta_l_1, theta_l_2=sym.theta_l_2,
271
                                        theta_l_bar=sym.theta_l_bar,
272
                                        r_r_t_theta_l=sym.r_r_t_theta_l,
273
                                        sigma_r_t_1=sym.sigma_r_t_1,
274
                                        \rightarrow sigma_r_t_2=sym.sigma_r_t_2,
                                        sigma_theta_l_1=sym.sigma_theta_l_1,
275
                                        sigma_theta_1_2=sym.sigma_theta_1_2,
276
                                        cov_lambda_r_theta=sym.rho_theta_l_r_t *
277
                                                            sym.sigma_lambda_theta_l *
                                                            sym.sigma_lambda_r_t):
279
280
         return ((1 - delta) * alpha * (
```

```
281
                  (r_t_1 - r_t_prime_bar) * (theta_l_1 - theta_l_bar) +
                 r_r_t_theta_l * sigma_r_t_1 * sigma_theta_l_1) +
282
                  ((1 - delta) * (1 - alpha) * (
283
                          (r_t_2 - r_t_prime_bar) * (theta_l_2 - theta_l_bar) +
284
                          r_r_t_theta_1 * sigma_r_t_2 * sigma_theta_1_2)) +
285
                  delta * cov_lambda_r_theta)
286
287
288
289
290
291
     # Distributions
292
293
     G_1_theta_1 = Normal(name='G_1_theta_1', mean=sym.theta_1_1, std=sym.sigma_theta_1_1)
294
     G_1_theta_l_density = density(G_1_theta_l)(sym.theta_l)
295
296
     G_2_theta_1 = Normal(name='G_2_theta_1', mean=sym.theta_1_2, std=sym.sigma_theta_1_2)
297
     G_2_theta_l_density = density(G_2_theta_1)(sym.theta_1)
298
299
     G_3_theta_1 = Normal(name='G_3_theta_1', mean=sym.theta_1_bar,
300

    std=sym.sigma_lambda_theta_l)

     G_3_theta_l_density = density(G_3_theta_1)(sym.theta_1)
301
302
     G_theta = ((1 - sp.abc.delta) * sp.abc.alpha * G_1_theta_l_density +
303
                (1 - sp.abc.delta) * (1 - sp.abc.alpha) * G_2_theta_l_density +
304
                sp.abc.delta * G_3_theta_l_density)
305
306
307
308
     G_1_w = Normal(name='G_1_w', mean=sym.w_1, std=sym.sigma_w)
309
     G_1_w_density = density(G_1_w)(sp.abc.w)
310
311
     G_2_w = Normal(name='G_2_w', mean=sym.w_2, std=sym.sigma_w)
312
     G_2_w_density = density(G_2_w)(sp.abc.w)
313
314
     G_3_w = Normal(name='G_3_w', mean=sym.w_bar, std=sym.sigma_lambda_w)
315
     G_3_w_density = density(G_3_w)(sp.abc.w)
316
317
     G_w = ((1 - sp.abc.delta) * sp.abc.alpha * G_1_w_density +
318
            (1 - sp.abc.delta) * (1 - sp.abc.alpha) * G_2_w_density +
319
            sp.abc.delta * G_3_w_density)
320
321
322
323
     G_1_w_theta = Normal(name='G_1_w_theta', mean=sp.Matrix([sym.w_1, sym.theta_l_1]),
324
                           std=sp.Matrix([[sym.sigma_w ** 2, 0], [0, sym.sigma_theta_l_1 **
325
     G_1_w_theta_density = density(G_1_w_theta)(sp.abc.w, sp.abc.theta)
326
327
     G_2_w_theta = Normal(name='G_2_w_theta', mean=sp.Matrix([sym.w_2, sym.theta_1_2]),
328
                           std=sp.Matrix([[sym.sigma_w ** 2, 0], [0, sym.sigma_theta_1_2 **
329

→ 2]]))
     G_2_w_theta_density = density(G_2_w_theta)(sp.abc.w, sp.abc.theta)
330
331
```

```
G_3_w_theta = Normal(name='G_3_w_theta', mean=sp.Matrix([sym.w_bar, sym.theta_l_bar]),
332
                           std=sp.Matrix([
333
                               [sym.sigma_lambda_w ** 2,
334
                                sym.rho_w_theta_l * sym.sigma_lambda_w *
335
                                 [sym.rho_w_theta_l * sym.sigma_lambda_w *
336

→ sym.sigma_lambda_theta_l,

                                sym.sigma_lambda_theta_l ** 2]
337
                           ]))
338
     G_3_w_theta_density = sp.simplify(density(G_3_w_theta)(sp.abc.w, sp.abc.theta))
339
340
     G_w_theta = ((1 - sp.abc.delta) * sp.abc.alpha * G_1_w_theta_density +
341
                   (1 - sp.abc.delta) * (1 - sp.abc.alpha) * G_2_w_theta_density +
342
                   sp.abc.delta * G_3_w_theta_density)
343
344
345
346
     mu_1_theta_l_r_t = sp.Matrix([sym.theta_l_1, sym.r_t_1])
     Sigma_1_theta_l_r_t = sp.Matrix([[sym.sigma_theta_l_1 ** 2,
348
                                         sym.r_r_t_theta_l * sym.sigma_theta_l_1 *
349
                                         \rightarrow sym.sigma_r_t_1],
                                        [sym.r_r_t_theta_l * sym.sigma_theta_l_1 *
350
                                        \rightarrow sym.sigma_r_t_1,
                                         sym.sigma_r_t_1 ** 2]])
351
352
     G_1_theta_l_r_t = Normal(name='G_1_theta_l_r_t',
353
                               mean=mu_1_theta_l_r_t,
354
                               std=Sigma_1_theta_l_r_t)
355
356
     G_1_theta_l_r_t_density = density(G_1_theta_l_r_t)(sym.theta_l, sym.r_t)
357
358
     mu_2_theta_l_r_t = sp.Matrix([sym.theta_l_2, sym.r_t_2])
359
     Sigma_2_theta_l_r_t = sp.Matrix(
360
         [[sym.sigma_theta_1_2 ** 2,
361
           sym.r_r_t_theta_1 * sym.sigma_theta_1_2 * sym.sigma_r_t_2],
362
          [sym.r_r_t_theta_1 * sym.sigma_theta_1_2 * sym.sigma_r_t_2,
363
           sym.sigma_r_t_2 ** 2]])
364
365
     G_2_theta_l_r_t = Normal(name='G_2_theta_l_r_t',
366
                               mean=mu_2_theta_l_r_t,
367
                               std=Sigma_2_theta_l_r_t)
368
369
     G_2_theta_l_r_t_density = density(G_2_theta_l_r_t)(sym.theta_l, sym.r_t)
370
371
     mu_3_theta_l_r_t = sp.Matrix([sym.theta_l_bar, sym.r_t_bar])
372
     Sigma_3_theta_l_r_t = sp.Matrix(
373
         [[sym.sigma_lambda_theta_1 ** 2,
374
           sym.rho_theta_l_r_t * sym.sigma_lambda_theta_l * sym.sigma_lambda_r_t],
375
          Γ
376
              sym.rho_theta_l_r_t * sym.sigma_lambda_theta_l * sym.sigma_lambda_r_t,
377
              sym.sigma_lambda_r_t ** 2]])
378
379
     G_3_theta_l_r_t = Normal(name='G_3_theta_l_r_t',
380
381
                               mean=mu_3_theta_l_r_t,
```

```
std=Sigma_2_theta_l_r_t)
382
     G_3_theta_l_r_t_density = density(G_3_theta_l_r_t)(sym.theta_l, sym.r_t)
383
384
     G_theta_l_r_t = ((1 - sp.abc.delta) * sp.abc.alpha * G_1_theta_l_r_t_density +
385
                       (1 - sp.abc.delta) * (1 - sp.abc.alpha) * G_2_theta_l_r_t_density +
386
                       sp.abc.delta * G_3_theta_l_r_t_density)
387
388
389
390
     mu_1_w_theta_l_r_t = sp.Matrix([sym.w_1, sym.theta_l_1, sym.r_t_1])
391
     Sigma_1_w_theta_l_r_t = sp.Matrix(
392
          [[sym.sigma_w ** 2,
393
           0,
394
           0],
395
           [0,
396
           sym.sigma_theta_l_1 ** 2,
397
           sym.r_r_t_theta_l * sym.sigma_theta_l_1 * sym.sigma_r_t_1],
398
           sym.r_r_t_theta_l * sym.sigma_theta_l_1 * sym.sigma_r_t_1,
400
           sym.sigma_r_t_1 ** 2]])
401
402
     G_1_w_theta_l_r_t = Normal(name='G_1_w_theta_l_r_t',
403
                                  mean=mu_1_w_theta_l_r_t,
404
                                  std=Sigma_1_w_theta_l_r_t)
405
406
     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)
407
408
     mu_2_w_theta_l_r_t = sp.Matrix([sym.w_2, sym.theta_l_2, sym.r_t_2])
409
     Sigma_2_w_theta_l_r_t = sp.Matrix([[sym.sigma_w ** 2,
410
411
                                            0],
412
                                           [0,
413
                                            sym.sigma_theta_1_2 ** 2,
414
                                            sym.r_r_t_theta_l * sym.sigma_theta_l_2 *
415
                                            \rightarrow sym.sigma_r_t_2],
                                           [0.
416
                                            sym.r_r_t_theta_l * sym.sigma_theta_l_2 *
417
                                            \rightarrow sym.sigma_r_t_2,
                                            sym.sigma_r_t_2 ** 2]])
418
419
     G_2_w_theta_l_r_t = Normal(name='G_2_w_theta_l_r_t',
420
                                  mean=mu_2_w_theta_l_r_t,
421
                                  std=Sigma_2_w_theta_l_r_t)
422
423
     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)
424
425
     mu_3_w_theta_l_r_t = sp.Matrix([sym.w_bar, sym.theta_l_bar, sym.r_t_bar])
426
     Sigma_3_w_theta_l_r_t = sp.Matrix(
427
          [[sym.sigma_lambda_w ** 2,
428
           sym.rho_w_theta_1 * sym.sigma_lambda_w * sym.sigma_lambda_theta_1,
429
           sym.rho_w_r_t * sym.sigma_lambda_theta_l * sym.sigma_lambda_r_t],
430
               sym.rho_w_theta_l * sym.sigma_lambda_w * sym.sigma_lambda_theta_l,
432
433
               sym.sigma_lambda_theta_l ** 2,
```

```
434
               sym.rho_theta_l_r_t * sym.sigma_lambda_w * sym.sigma_lambda_r_t],
          [sym.rho_w_r_t * sym.sigma_lambda_theta_l * sym.sigma_lambda_r_t,
435
           sym.rho_theta_l_r_t * sym.sigma_lambda_w * sym.sigma_lambda_r_t,
436
           sym.sigma_lambda_r_t ** 2]])
437
438
     G_3_w_theta_l_r_t = Normal(name='G_3_w_theta_l_r_t',
439
                                 mean=mu_3_w_theta_l_r_t,
440
                                 std=Sigma_2_w_theta_l_r_t)
441
     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)
442
443
     G_w_theta_l_r_t = ((1 - sp.abc.delta) * sp.abc.alpha * G_1_w_theta_l_r_t_density +
444
                         (1 - sp.abc.delta) * (1 - sp.abc.alpha) * G_2_w_theta_l_r_t_density +
445
                         sp.abc.delta * G_3_w_theta_l_r_t_density)
446
447
448
449
450
     # sigma equations
451
452
453
     def sigma_tilde_w(sigma_w=sym.sigma_w, w_prime_2_bar=sym.w_prime_2_bar,
454
                        delta=sp.abc.delta, lambda_w=sym.lambda_w):
455
         from sympy import sqrt
456
         return ((sigma_w / sqrt(w_prime_2_bar)) *
457
                  (1 / sqrt((1 - delta * lambda_w) / (1 - delta))))
458
459
460
461
     # lambda equations
463
464
465
     def lambda_w(sigma_lambda_w=sym.sigma_lambda_w, w_prime_2_bar=sym.w_prime_2_bar):
466
         return sigma_lambda_w ** 2 / w_prime_2_bar
467
468
469
     def lambda_theta(sigma_lambda_theta=sym.sigma_lambda_theta_l,
470
                       theta_l_prime_2_bar=sym.theta_l_prime_2_bar):
471
         return sigma_lambda_theta ** 2 / theta_l_prime_2_bar
472
473
474
     def lambda_r(sigma_lambda_r=sym.sigma_lambda_r_t,
475
                   r_t_prime_2_bar=sym.r_t_prime_2_bar):
476
         return sigma_lambda_r ** 2 / r_t_prime_2_bar
477
478
479
     def lambda_w_theta(cov_lambda_w_theta=
480
                         sym.rho_w_theta_1 * sym.sigma_lambda_w * sym.sigma_lambda_theta_1,
481
                         w_prime_theta_l_prime_bar=sym.w_prime_theta_l_prime_bar):
482
         return cov_lambda_w_theta / w_prime_theta_l_prime_bar
483
484
485
     def lambda_w_r(cov_lambda_w_r=
486
487
                     sym.rho_w_r_t * sym.sigma_lambda_w * sym.sigma_lambda_r_t,
```

```
488
                     w_prime_r_t_prime_bar=sym.w_prime_r_t_prime_bar):
         return cov_lambda_w_r / w_prime_r_t_prime_bar
489
490
491
     def lambda_r_theta(cov_lambda_r_theta=
492
                         sym.rho_theta_l_r_t * sym.sigma_lambda_r_t *
493
                         r_t_prime_theta_l_prime_bar=sym.theta_l_prime_r_t_prime_bar):
494
         return cov_lambda_r_theta / r_t_prime_theta_l_prime_bar
495
496
497
498
499
     # sk
500
501
502
     def sk_theta_l_hat_beta(sk_hat_w=sym.sk_hat_w, c_hat_w_theta_l=sym.c_w_theta_l_hat,
503
                              beta=sp.abc.beta):
504
         return sk_hat_w * c_hat_w_theta_l * (beta + (1 - beta) * c_hat_w_theta_l ** 2)
505
506
507
     def sk_theta_l_hat(theta_l_prime_3_bar=sym.theta_l_prime_3_bar,
508
                         theta_l_prime_2_bar=sym.theta_l_prime_2_bar,
509
                         delta=sp.abc.delta,
510
                         lambda_theta=sym.lambda_theta):
511
         from sympy import Rational
512
         return ((theta_1_prime_3_bar / theta_1_prime_2_bar ** Rational(3, 2)) *
513
                  (1 / ((1 - delta * lambda_theta) / (1 - delta)) ** Rational(3, 2)) *
514
                  (1 / (1 - delta)))
516
517
     def sk_w_hat(sigma_tilde_w=sym.sigma_tilde_w,
518
                  w_prime_3_bar=sym.w_prime_3_bar,
                  w_prime_2_bar=sym.w_prime_2_bar,
520
                  delta=sp.abc.delta,
521
                  lambda_w=sym.lambda_w):
522
         from sympy import Rational
523
         return ((1 / (1 - sigma_tilde_w ** 2) ** Rational(3, 2)) *
524
                  (w_prime_3_bar / (w_prime_2_bar ** Rational(3, 2))) *
525
                  (1 / ((1 - delta * lambda_w) / (1 - delta)) ** Rational(3, 2)) *
526
                  (1 / (1 - delta)))
527
528
529
     def c_w_theta_l_hat(sigma_w_tilde=sym.sigma_tilde_w,
530
                          w_prime_theta_l_prime_bar=sym.w_prime_theta_l_prime_bar,
531
                          w_prime_2_bar=sym.w_prime_2_bar,
532
                          theta_l_prime_2_bar=sym.theta_l_prime_2_bar,
533
                          delta=sp.abc.delta,
534
                          lambda_w=sym.lambda_w,
535
                          lambda_theta=sym.lambda_theta,
536
                          lambda_w_theta=sym.lambda_w_theta):
537
         from sympy import sqrt
538
         return ((1 / sqrt(1 - sigma_w_tilde ** 2)) *
539
```

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

Listing A.2: checked_functions.py

A.4 w_prime_4_bar.py

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

```
display(sp.Eq(sym.G_2_w, c_f.G_2_theta_l_density))
26
27
    # In[4]:
28
29
30
    display(sp.Eq(sym.G_3_w, c_f.G_3_theta_l_density))
31
32
    # In[5]:
33
34
35
    display(sp.Eq(sym.G_w, c_f.G_w))
36
37
38
    # Calculate the moment analytically:
39
    # In[6]:
40
41
42
43
    w_prime_4_bar_int = sp.Integral((sp.abc.w - sym.w_bar) ** 4 * c_f.G_w, [sp.abc.w, -oo,
     → oo])
    display(sp.Eq(sym.w_prime_4_bar, w_prime_4_bar_int))
44
45
    # In[7]:
46
47
48
    w_prime_4_bar_int_val = w_prime_4_bar_int.doit(conds='none').simplify()
49
    display(sp.Eq(sym.w_prime_4_bar, w_prime_4_bar_int_val))
50
51
    # The equation in the document is:
52
53
    # In[8]:
54
55
56
    display(sp.Eq(sym.w_prime_4_bar, c_f.w_prime_4_bar()))
57
58
    # where
59
60
    # In[9]:
61
62
63
    display(sp.Eq(sym.sigma_tilde_w, c_f.sigma_tilde_w()))
64
65
    # and
66
67
    # In[10]:
68
69
70
71
    display(sp.Eq(sym.w_prime_2_bar, c_f.w_prime_2_bar()))
72
    # and
73
74
    # In [117:
75
76
77
    display(sp.Eq(sym.w_prime_3_bar, c_f.w_prime_2_bar()))
```

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

Listing A.3: w_prime_4_bar.py

A.5 w_prime_2_theta_l_prime_bar.py

```
#!/usr/bin/env python
    # coding: utf-8
2
3
    # In[2]:
4
5
6
    import sympy as sp
7
    from IPython.display import display
8
    from sympy import abc, oo
9
10
    import checked_functions as c_f
11
    import symbols as sym
12
13
    # # This document aims to analytically check f\overline{w'^4}f
14
```

```
15
    # ## Define the marginal distributions with those parameters.
16
17
    # In[2]:
18
19
20
    display(sp.Eq(sym.G_1_w, c_f.G_1_theta_l_density))
21
^{22}
    # In[3]:
23
24
25
    display(sp.Eq(sym.G_2_w, c_f.G_2_theta_l_density))
26
27
    # In[4]:
28
29
30
    display(sp.Eq(sym.G_3_w, c_f.G_3_theta_l_density))
31
32
    # In [5]:
33
34
35
    display(sp.Eq(sym.G_w, c_f.G_w))
36
37
    # Calculate the moment analytically:
38
39
    # In[6]:
40
41
42
    w_prime_4_bar_int = sp.Integral((sp.abc.w - sym.w_bar) ** 4 * c_f.G_w, [sp.abc.w, -oo,
43
     \rightarrow oo])
    display(sp.Eq(sym.w_prime_4_bar, w_prime_4_bar_int))
44
45
    # In[7]:
46
47
48
    w_prime_4_bar_int_val = w_prime_4_bar_int.doit(conds='none').simplify()
49
    display(sp.Eq(sym.w_prime_4_bar, w_prime_4_bar_int_val))
50
51
    # The equation in the document is:
52
53
    # In[8]:
54
55
56
    display(sp.Eq(sym.w_prime_4_bar, c_f.w_prime_4_bar()))
57
58
    # where
59
60
    # In[9]:
61
62
63
    display(sp.Eq(sym.sigma_tilde_w, c_f.sigma_tilde_w()))
64
65
    # and
66
67
```

```
# In[10]:
68
69
70
     display(sp.Eq(sym.w_prime_2_bar, c_f.w_prime_2_bar()))
71
72
     # and
73
74
     # In[11]:
75
76
77
     display(sp.Eq(sym.w_prime_3_bar, c_f.w_prime_2_bar()))
78
79
     # So,
80
81
     # In[12]:
82
83
84
     lambda_w_val = c_f.lambda_w().subs({
85
         sym.w_prime_2_bar: c_f.w_prime_2_bar()
86
87
     display(sp.Eq(sym.lambda_w, lambda_w_val))
88
89
     # In[13]:
90
91
92
     w_prime_4_bar_check_val = c_f.w_prime_4_bar().subs({
93
         sym.w_prime_2_bar: c_f.w_prime_2_bar(),
94
         sym.w_prime_3_bar: c_f.w_prime_3_bar(),
95
         sym.sigma_tilde_w: c_f.sigma_tilde_w().subs({
96
              sym.w_prime_2_bar: c_f.w_prime_2_bar(),
97
              sym.lambda_w: c_f.lambda_w()
98
         })
99
     })
100
101
     display(sp.Eq(sym.w_prime_4_bar, w_prime_4_bar_check_val))
102
103
     # In[14]:
104
105
106
     display(sp.Eq(w_prime_4_bar_int_val, w_prime_4_bar_check_val, evaluate=True)
107
              .subs({sym.w_bar: c_f.w_bar()}).simplify())
108
```

Listing A.4: w_prime_2_theta_l_prime_bar.py

A.6 w_prime_theta_l_prime_2_bar.py

```
#!/usr/bin/env python
coding: utf-8
```

```
# In[1]:
4
5
6
    from itertools import product
7
8
    import pandas as pd
9
10
    pd.set_option('display.max_columns', None)
11
    pd.set_option('display.max_rows', None)
12
13
    import sympy as sp
14
15
    from IPython.display import display
    from sympy import abc, oo, Rational
16
17
    import checked_functions as c_f
18
    import symbols as sym
19
20
21
    # # This document aims to numerically check f\overline{w'\theta_l'^2}f
22
    # ## Define the marginal distributions.
23
24
    # In[2]:
25
26
27
    display(sp.Eq(sym.G_1_w_theta, c_f.G_1_w_theta_density))
28
29
    # In[3]:
30
31
32
    display(sp.Eq(sym.G_2_w_theta, c_f.G_2_w_theta_density))
33
34
    # In[4]:
35
36
37
    display(sp.Eq(sym.G_3_w_theta, c_f.G_3_w_theta_density))
38
39
    # In[5]:
40
41
42
    display(sp.Eq(sym.G_w_theta, c_f.G_w_theta, evaluate=False))
43
44
    # In[6]:
45
46
47
    w_prime_theta_l_2_prime_bar = sp.Integral(
48
         (sp.abc.w - sym.w_bar) * (sp.abc.theta - sym.theta_l_bar) ** 2 * c_f.G_w_theta,
49
         [sp.abc.w, -oo, oo],
50
         [sp.abc.theta, -oo, oo])
51
52
    display(sp.Eq(sym.w_prime_theta_prime_l_2_bar, w_prime_theta_l_2_prime_bar))
53
54
    # In[7]:
55
56
57
```

```
w_prime_theta_1_2_prime_bar = w_prime_theta_1_2_prime_bar.subs({
          sym.w_bar: c_f.w_bar(),
59
          sym.theta_l_bar: c_f.theta_l_bar()
60
     })
61
62
     display(sp.Eq(sym.w_prime_theta_prime_l_2_bar, w_prime_theta_l_2_prime_bar))
63
64
     # The equation in the document is:
65
66
     # In[8]:
67
68
69
70
     display(sp.Eq(sym.w_prime_theta_prime_l_2_bar, c_f.w_prime_theta_l_prime_2_bar()))
71
     # For this we still need f\tilde{\sigma_w}f:
72
73
     # In [9]:
74
75
76
     display(sp.Eq(sym.sigma_tilde_w, c_f.sigma_tilde_w()))
77
78
     # And £\overline{w'^{2}}£:
79
80
     # In[10]:
81
82
83
     display(sp.Eq(sym.w_prime_2_bar, c_f.w_prime_2_bar()))
84
85
     # And £\overline{w'^{3}}£:
86
87
     # In[11]:
88
89
90
     display(sp.Eq(sym.w_prime_3_bar, c_f.w_prime_3_bar()))
91
92
     # And f\overline{w'\theta'_l}f:
93
94
     # In[12]:
95
96
97
     display(sp.Eq(sym.w_prime_theta_l_prime_bar, c_f.w_prime_theta_l_prime_bar()))
98
99
     # And £ \setminus lambda_w£:
100
101
     # In[13]:
102
103
104
     display(sp.Eq(sym.lambda_w, c_f.lambda_w()))
105
106
     # And \mathcal{L} \subset \mathcal{L}_{w \in \mathcal{L}_{\varepsilon}}
107
108
     # In[14]:
109
110
111
```

```
display(sp.Eq(sym.lambda_w_theta, c_f.lambda_w_theta()))
112
113
     # And f\overline{\theta_l'^3}f:
114
115
     # In[15]:
116
117
118
     display(sp.Eq(sym.theta_l_prime_3_bar, c_f.theta_l_prime_3_bar()))
119
120
     # Putting those all together yields:
121
122
123
     # In[16]:
124
125
     w_prime_theta_l_prime_2_bar_check_val = c_f.w_prime_theta_l_prime_2_bar().subs({
126
         sym.theta_l_prime_3_bar: c_f.theta_l_prime_3_bar(),
127
         sym.sigma_tilde_w: c_f.sigma_tilde_w(),
128
         sym.lambda_w: c_f.lambda_w(),
129
         sym.w_prime_2_bar: c_f.w_prime_2_bar(),
130
         sym.w_prime_3_bar: c_f.w_prime_3_bar(),
131
         sym.lambda_w_theta: c_f.lambda_w_theta(),
132
         sym.w_prime_theta_l_prime_bar: c_f.w_prime_theta_l_prime_bar()
133
     })
134
135
     w_prime_theta_l_prime_2_bar_check_val = w_prime_theta_l_prime_2_bar_check_val.subs({
136
         sym.w_prime_2_bar: c_f.w_prime_2_bar(),
137
         sym.lambda_w: c_f.lambda_w(),
138
         sym.w_bar: c_f.w_bar(),
139
         sym.theta_l_bar: c_f.theta_l_bar()
140
     })
141
142
     display(sp.Eq(sym.w_prime_theta_prime_l_2_bar, w_prime_theta_l_prime_2_bar_check_val))
143
144
     # Since the integral is too difficult to be calculated analytically, at least with
145
     → sympy, we try to put in some arbitrary numbers for the pdf parameters, to simplify
        the equations.
146
     # We create a dataframe to get all possible permutations and therefore also all possible
147
     → evaluations of the integrals.
148
     # In[17]:
149
150
151
     df = pd.DataFrame(
152
         product([0, 1],
153
                  [-2, 2],
154
                  [-1, 2],
155
                  [0, 3],
156
                  [Rational(1, 10)],
157
                  [Rational(3, 10)],
                  [Rational(4, 10)],
159
                  [Rational(7, 10)],
160
                  [Rational(6, 10)],
161
                  [Rational(5, 10)],
162
```

```
[Rational(1, 10), Rational(5, 10)],
163
                  [Rational(5, 10)]),
164
         columns=[sym.w_1,
165
                   sym.w_2,
166
                   sym.theta_l_1,
167
168
                   sym.theta_1_2,
                   sym.sigma_theta_l_1,
169
                   sym.sigma_theta_1_2,
170
                   sym.sigma_lambda_theta_l,
171
                   sym.sigma_w,
172
                   sym.sigma_lambda_w,
173
                   sp.abc.alpha,
174
                   sp.abc.delta,
175
                   sym.rho_w_theta_1])
176
177
     # In[18]:
178
179
180
     df['check_val'] = (
181
         df.apply(lambda x:
182
                   w_prime_theta_l_prime_2_bar_check_val.subs({
183
                        sym.w_1: x[sym.w_1],
184
                        sym.w_2: x[sym.w_2],
185
                        sym.theta_l_1: x[sym.theta_l_1],
186
                        sym.theta_1_2: x[sym.theta_1_2],
                        sym.sigma_theta_l_1: x[sym.sigma_theta_l_1],
188
                        sym.sigma_theta_1_2: x[sym.sigma_theta_1_2],
189
                        sym.sigma_lambda_theta_l: x[sym.sigma_lambda_theta_l],
190
                        sym.sigma_w: x[sym.sigma_w],
                        sym.sigma_lambda_w: x[sym.sigma_lambda_w],
192
                        sp.abc.alpha: x[sp.abc.alpha],
193
                        sp.abc.delta: x[sp.abc.delta],
194
                        sym.rho_w_theta_l: x[sym.rho_w_theta_l]
195
                   }).evalf(), axis=1))
196
197
     # Calculate the moment analytically:
198
199
     # In[19]:
200
201
202
     df['num_int'] = (
203
         df.apply(lambda x: w_prime_theta_1_2_prime_bar.subs({
204
              sym.w_1: x[sym.w_1],
205
              sym.w_2: x[sym.w_2],
206
              sym.theta_l_1: x[sym.theta_l_1],
207
              sym.theta_1_2: x[sym.theta_1_2],
208
              sym.sigma_theta_l_1: x[sym.sigma_theta_l_1],
209
              sym.sigma_theta_1_2: x[sym.sigma_theta_1_2],
210
              sym.sigma_lambda_theta_l: x[sym.sigma_lambda_theta_l],
211
              sym.sigma_w: x[sym.sigma_w],
212
              sym.sigma_lambda_w: x[sym.sigma_lambda_w],
213
              sp.abc.alpha: x[sp.abc.alpha],
214
              sp.abc.delta: x[sp.abc.delta],
215
              sym.rho_w_theta_1: x[sym.rho_w_theta_1]
216
```

```
}).doit(conds='none', method='quad').evalf(), axis=1))
217
218
     # In[20]:
219
220
221
     df['diff'] = abs(df['check_val'] - df['num_int'])
222
223
     # In[21]:
224
225
^{226}
     df['diff_num'] = abs(df['check_val'].astype(float) - df['num_int'].astype(float))
227
228
229
     # In[22]:
230
231
     display(df)
232
233
     # In[23]:
234
235
236
     import numpy as np
237
238
     print('The mean error between the rhs and the lhs is:', np.mean(df['diff_num']))
239
```

Listing A.5: w_prime_theta_l_prime_2_bar.py

A.7 w_prime_r_t_prime_theta_l_prime_bar.py

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

```
22
    # ## Define the normal distributions.
23
24
    # In[2]:
25
26
27
    display(sp.Eq(sp.symbols('\mu_1'), c_f.mu_1_w_theta_l_r_t, evaluate=False))
28
    display(sp.Eq(sp.symbols('\Sigma_1'), c_f.Sigma_1_w_theta_l_r_t, evaluate=False))
29
    \# display(sp.Eq(sym.G_1\_w\_theta\_l\_r\_t, c\_f.G_1\_w\_theta\_l\_r\_t\_density))
30
31
32
    # In[3]:
33
34
35
    display(sp.Eq(sp.symbols('\mu_2'), c_f.mu_2_w_theta_l_r_t, evaluate=False))
36
    display(sp.Eq(sp.symbols('\Sigma_2'), c_f.Sigma_2_w_theta_l_r_t, evaluate=False))
37
    \# display(sp.Eq(sym.G_2\_w\_theta\_l\_r\_t, c\_f.G_2\_w\_theta\_l\_r\_t\_density))
38
40
    # In[4]:
41
42
43
    display(sp.Eq(sp.symbols('\mu_3'), c_f.mu_3_w_theta_l_r_t, evaluate=False))
44
    display(sp.Eq(sp.symbols('\Sigma_3'), c_f.Sigma_3_w_theta_l_r_t, evaluate=False))
45
    \# display(sp.Eq(sym.G_3_w_theta_l_r_t, c_f.G_3_w_theta_l_r_t_density))
46
47
48
    # In[5]:
49
50
51
    display(sp.Eq(sym.G_w_theta_l_r_t, c_f.G_w_theta_l_r_t))
52
53
    # In[6]:
54
55
56
    w_prime_r_t_prime_theta_l_prime_bar = sp.Integral(
57
         (sp.abc.w - sym.w_bar) * (sym.r_t - sym.r_t_bar) * (
58
                      sp.abc.theta - sym.theta_l_bar) * c_f.G_w_theta_l_r_t,
59
         [sp.abc.w, -oo, oo],
60
         [sym.theta_1, -oo, oo],
61
         [sym.r_t, -oo, oo])
62
    display(sp.Eq(sym.w_prime_r_t_prime_theta_l_prime_bar,
63
       w_prime_r_t_prime_theta_l_prime_bar))
64
    # In[7]:
65
66
67
    w_prime_r_t_prime_theta_l_prime_bar = (
68
         w_prime_r_t_prime_theta_l_prime_bar.subs({
69
             sym.w_bar: c_f.w_bar(),
70
             sym.r_t_bar: c_f.r_t_bar(),
71
             sym.theta_l_bar: c_f.theta_l_bar()
72
         }))
73
```

```
display(sp.Eq(sym.w_prime_r_t_prime_theta_l_prime_bar,
74

    w_prime_r_t_prime_theta_l_prime_bar))

75
     # The equation in the document is:
76
77
     # In[8]:
78
79
80
     display(sp.Eq(sym.w_prime_r_t_prime_theta_l_prime_bar,
81
        c_f.w_prime_r_t_prime_theta_l_prime_bar()))
82
     # Since the integral is too difficult to be calculated analytically, at least with
83
      → sympy, we try to put in some arbitrary numbers for the pdf parameters, to simplify
        the equations.
84
     # We also use a the method `nquad(..)` from `sympy` to get a numerical evaluation of the
85
     \rightarrow 3d integral.
86
     # We create a dataframe to get all possible permutations and therefore also all possible
87
      → evaluations of the integrals.
88
     # In[9]:
89
90
91
     df = pd.DataFrame(
92
          product([3, 1],
93
                  [-2],
94
                   [-1, 3],
95
                  [2],
96
                   [1, 4],
97
                  [2],
98
                   [1.1],
99
                  [1.3],
100
                  [1.4],
101
102
                  [1.7],
                  [1.2],
103
                  [1.5],
104
                  [1.9],
105
                  [1.6],
106
                  [.55],
107
                  [.8],
108
                  [.65],
109
                  [.45],
110
                  [.35],
111
                  [.5]),
112
          columns=[sym.w_1,
113
                   sym.w_2,
114
                   sym.theta_l_1,
115
                   sym.theta_1_2,
116
                   sym.r_t_1,
117
                   sym.r_t_2,
118
                   sym.sigma_theta_l_1,
119
                   sym.sigma_theta_1_2,
120
                   sym.sigma_lambda_theta_l,
121
```

```
122
                   sym.sigma_w,
                   sym.sigma_r_t_1,
123
                   sym.sigma_r_t_2,
124
                   sym.sigma_lambda_r_t,
125
                   sym.sigma_lambda_w,
126
                   sp.abc.alpha,
127
                   sp.abc.delta,
128
                   sym.rho_w_theta_l,
129
                   sym.rho_w_r_t,
130
                   sym.rho_theta_l_r_t,
131
                   sym.r_r_t_theta_l])
132
133
     # In[10]:
134
135
136
     w_prime_r_t_prime_theta_l_prime_bar_check_sym_val = (
137
          c_f.w_prime_r_t_prime_theta_l_prime_bar().subs({
138
              sym.w_bar: c_f.w_bar(),
139
              sym.r_t_bar: c_f.r_t_bar(),
140
              sym.theta_l_bar: c_f.theta_l_bar()
141
         }))
142
     # In[11]:
144
145
146
     df['check_val'] = (
147
          df.apply(lambda x: Rational(c_f.w_prime_r_t_prime_theta_l_prime_bar().subs({
148
              sym.w_bar: c_f.w_bar(),
149
              sym.theta_l_bar: c_f.theta_l_bar(),
150
              sym.r_t_bar: c_f.r_t_bar(),
151
              sym.w_1: x[sym.w_1],
152
              sym.w_2: x[sym.w_2],
153
              sym.theta_l_1: x[sym.theta_l_1],
              sym.theta_1_2: x[sym.theta_1_2],
155
              sym.r_t_1: x[sym.r_t_1],
156
              sym.r_t_2: x[sym.r_t_2],
157
              sym.sigma_theta_l_1: x[sym.sigma_theta_l_1],
158
              sym.sigma_theta_1_2: x[sym.sigma_theta_1_2],
159
              sym.sigma_r_t_1: x[sym.sigma_r_t_1],
160
              sym.sigma_r_t_2: x[sym.sigma_r_t_2],
161
              sp.abc.alpha: x[sp.abc.alpha],
162
              sp.abc.delta: x[sp.abc.delta],
163
              sym.r_r_t_theta_l: x[sym.r_r_t_theta_l]
164
          }).evalf()), axis=1))
165
166
     # Calculate the moment numerically:
167
168
     # In[12]:
169
170
171
     import scipy
172
173
     df['num_int'] = df.apply(lambda x: scipy.integrate.nquad(
174
175
          sp.lambdify(
```

```
[sp.abc.w, sym.r_t, sym.theta_1],
176
              (((sp.abc.w - c_f.w_bar()) *
177
                (sym.r_t - c_f.r_t_bar()) *
178
                (sym.theta_l - c_f.theta_l_bar()) *
179
                c_f.G_w_theta_l_r_t))
180
              .subs({
181
                  sym.w_bar: c_f.w_bar(),
182
                  sym.r_t_bar: c_f.r_t_bar(),
183
                  sym.theta_l_bar: c_f.theta_l_bar(),
184
                  sym.w_1: x[sym.w_1],
185
                  sym.w_2: x[sym.w_2],
186
187
                  sym.theta_l_1: x[sym.theta_l_1],
                  sym.theta_1_2: x[sym.theta_1_2],
188
                  sym.r_t_1: x[sym.r_t_1],
                  sym.r_t_2: x[sym.r_t_2],
190
                  sym.sigma_w: x[sym.sigma_w],
191
                  sym.sigma_theta_l_1: x[sym.sigma_theta_l_1],
192
                  sym.sigma_theta_1_2: x[sym.sigma_theta_1_2],
193
                  sym.sigma_lambda_theta_l: x[sym.sigma_lambda_theta_l],
194
                  sym.sigma_lambda_w: x[sym.sigma_lambda_w],
195
                  sym.sigma_lambda_r_t: x[sym.sigma_lambda_r_t],
196
                  sym.sigma_r_t_1: x[sym.sigma_r_t_1],
197
                  sym.sigma_r_t_2: x[sym.sigma_r_t_2],
198
                  sp.abc.alpha: x[sp.abc.alpha],
199
                  sp.abc.delta: x[sp.abc.delta],
200
                  sym.rho_w_theta_l: x[sym.rho_w_theta_l],
201
                  sym.rho_w_r_t: x[sym.rho_w_r_t],
202
                  sym.rho_theta_l_r_t: x[sym.rho_theta_l_r_t],
203
                  sym.r_r_t_theta_l: x[sym.r_r_t_theta_l]
204
              })),
205
          ranges=[[-30, 30], [-30, 30], [-30, 30]])[0],
206
                                axis=1)
207
208
     # In [13]:
209
210
211
     df['diff'] = abs(df['check_val'] - df['num_int'])
212
213
     # In[14]:
214
215
216
     df['diff_num'] = abs(df['check_val'].astype(float) - df['num_int'])
217
218
     # In[15]:
^{219}
220
221
222
     display(df)
223
     # In[16]:
224
225
226
227
     import numpy as np
228
```

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

Listing A.6: w_prime_r_t_prime_theta_l_prime_bar.py