Adding a third normal to CLUBB

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Cloud **L**ayers **U**nified **B**y **B**inormals . . .

. . . is an atmospheric model that tries to predict the weather based on modeling a grid box with a sum of two normal distributions.

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Nature does not look like this, this is too binormal.
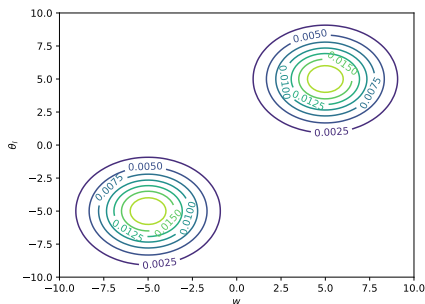
Figure: Binormal plot for two strong up-/downdrafts

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

To reduce the bimodality we can increase the widths.

Figure: Binormal plot for two strong up-/downdrafts with increased standard deviations

$$w_1 = 5, \ w_2 = -5, \ \theta_{l1} = 5, \ \theta_{l2} = -5, \ \alpha = 0.5, \ \sigma_w = 5, \ \sigma_{\theta_{l1}} = 5, \ \sigma_{\theta_{l1}} = 5.$$

Adding a third normal is more realistic.
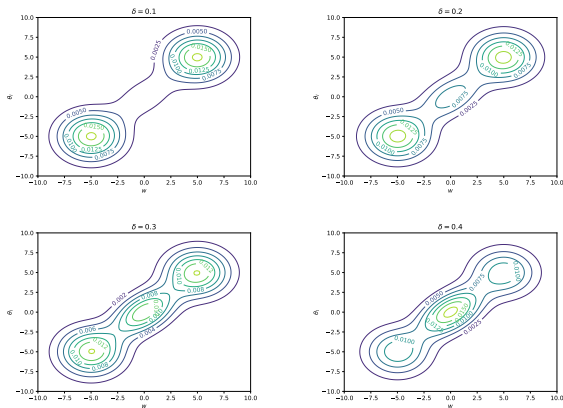
Figure: Trinormal plot for two strong up-/downdrafts with varying δ

$$w_1 = 5,\ w_2 = -5,\ \theta_{l1} = 5,\ \theta_{l2} = -5,\ \alpha = 0.5,\ \sigma_w = 2,\ \sigma_{\theta_{l1}} = 2,\ \sigma_{\theta_{l2}} = 2,$$
$$\sigma_{w3} = 2,\ \sigma_{3\theta_l} = 2,\ \rho_{w\theta_l} = 0.5.$$
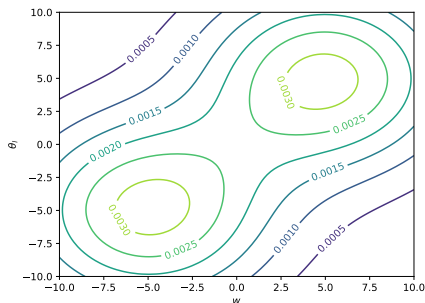
A third normal even allows "weird" shapes.
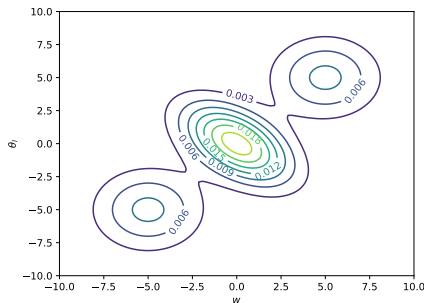
Figure: Trinormal plot for two strong up-/downdrafts with a third peak in the middle

$$w_1 = 5,\ w_2 = -5,\ \theta_{l1} = 5,\ \theta_{l2} = -5,\ \alpha = 0.5,\ \delta = 0.5,\ \sigma_w = 2,\ \sigma_{\theta_{l1}} = 2,$$
$$\sigma_{\theta_{l2}} = 2,\ \sigma_{w3} = 2,\ \sigma_{\theta_{l3}} = 2,\ \rho_{w\theta_l} = 0.5.$$

Consider the following prognostic pde [Lar22, p. 21]:

$$\frac{\partial \overline{w'\theta_l'}}{\partial t} = -\overline{w}\frac{\partial \overline{w'\theta_l'}}{\partial z} - \frac{1}{\rho_s}\frac{\partial \rho_s \overline{w'^2\theta_l'}}{\partial z} - \overline{w'^2}\frac{\partial \overline{\theta_l'}}{\partial z} - \overline{w'\theta_l'}\frac{\partial \overline{w}}{\partial z} + \ldots$$

We need to close the third order moment ($\overline{w'^2\theta_l'}$) by integration over the pdf.

There already exist closures that assume a binormal pdf [LG05], e.g.

$$\overline{w'^2} = \alpha[(w_1 - \overline{w})^2 + \sigma_w^2] + (1 - \alpha)[(w_2 - \overline{w})^2 + \sigma_w^2]. \qquad (2.1)$$

We can transform to a trinormal pdf using the following formulas:

$$\overline{w'^2}\frac{1-\delta\lambda_w}{1-\delta} = \overline{w'^2}_{dGn} \tag{2.2}$$

$$\overline{w'^3}\frac{1}{1-\delta} = \overline{w'^3}_{dGn} \tag{2.3}$$

$$\frac{\overline{w'^3}}{\overline{w'^2}^{3/2}}\frac{(1-\delta)^{1/2}}{(1-\lambda_w\delta)^{3/2}} = \frac{\overline{w'^3}_{dGn}}{\overline{w'^2}_{dGn}^{3/2}} \tag{2.4}$$

$$\overline{\theta_l'^2}\frac{1-\delta\lambda_\theta}{1-\delta} = \overline{\theta_l'^2}_{dGn} \tag{2.5}$$

$$\overline{w'\theta_l'}\frac{1-\delta\lambda_{w\theta}}{1-\delta} = \overline{w'\theta_l'}_{dGn} \tag{2.6}$$

If we substitute in a formula for λ_w (4.6), which will be explained later on, we get

$$\overline{w'^2}\left(1 - \delta\frac{\sigma_{w3}^2}{\overline{w'^2}}\right) = (1-\delta)\overline{w'^2}_{dGn} \tag{2.7}$$

$$\iff \overline{w'^2} = \overline{w'^2}_{dGn} - \delta\left(\overline{w'^2}_{dGn} - \sigma_{w3}^2\right) \tag{2.8}$$
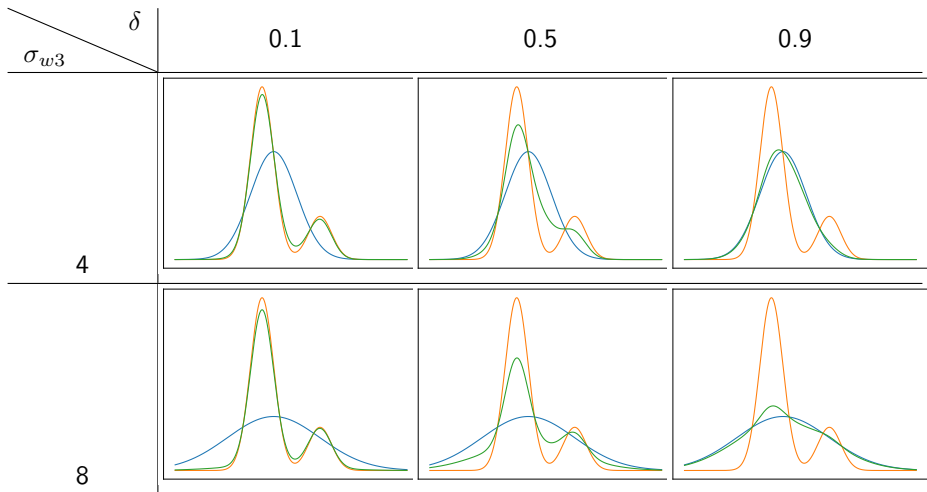
Table: 1D Plots for different δ and σ_{w3}

$w_1 = 5$, $w_2 = -5$, $\alpha = 0.2$, $\sigma_w = 2$. The blue plot represents the third normal, the orange/red one represents the binormal, and the green one represents the mixture. The x and y labels and ticks are omitted for clarity.

The goal of this thesis is to verify that all the transformations work out well.

Forward run (weather forecast)

- Given: $\overline{w}$, $\overline{w'^2}$, $\overline{w'^3}$, $\overline{\theta_l}$, $\overline{w'\theta_l'}$, $\overline{r_t}$, $\overline{w'r_t'}$, $\overline{\theta_l'^2}$, $\overline{r_t'^2}$, $\overline{r_t'\theta_l'}$.

Forward run (weather forecast)

- Given: $\overline{w}$, $\overline{w'^2}$, $\overline{w'^3}$, $\overline{\theta_l}$, $\overline{w'\theta_l'}$, $\overline{r_t}$, $\overline{w'r_t'}$, $\overline{\theta_l'^2}$, $\overline{r_t'^2}$, $\overline{r_t'\theta_l'}$.
- Find: Parameters, which describe the shape of the underlying pdf, for ultimately describing higher-order moments, e.g. $\overline{w'^2\theta_l'}$ in terms of lower-order moments.

Backward run (verification direction)

- Given: pdf parameters, e.g. mean, standard deviation

Backward run (verification direction)

- Given: pdf parameters, e.g. mean, standard deviation
- Find: lower- and higher-order moments

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Multivariate

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

> **Definition (pdf of a multivariate normal distribution)**
>
> $$f(\boldsymbol{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = (2\pi)^{-\frac{r}{2}} \, |\boldsymbol{\Sigma}|^{-\frac{1}{2}} \exp\left(-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^{\top}\boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu})\right), \boldsymbol{x} \in \mathbb{R}^r, \quad (3.1)$$
>
> where
>
> $$\boldsymbol{\mu} = \begin{pmatrix} \mu_1 \\ \vdots \\ \mu_r \end{pmatrix} \in \mathbb{R}^r, \text{ and } \boldsymbol{\Sigma} = \begin{pmatrix} \sigma_1^2 & \rho_{12}\sigma_1\sigma_2 & \dots & \rho_{1r}\sigma_1\sigma_r \\ \rho_{12}\sigma_1\sigma_2 & \sigma_2^2 & \dots & \vdots \\ \vdots & \dots & \ddots & \vdots \\ \rho_{1r}\sigma_1\sigma_r & \dots & \dots & \sigma_r^2 \end{pmatrix} \in \mathbb{R}^{r \times r}$$
>
> $$(3.2)$$

Moments

We denote the skewness and kurtosis by the following:

$$\mathbb{E}[X^3] = \mathbb{E}\left[\left(\frac{X-\mu}{\sigma}\right)^3\right] = \frac{\mathbb{E}[(X-\mu)^3]}{(\mathbb{E}[(X-\mu)^2])^{3/2}} = \frac{\mu_3}{\sigma^3} \tag{3.3}$$

$$\mathbb{E}[X^4] = \mathbb{E}\left[\left(\frac{X-\mu}{\sigma}\right)^4\right] = \frac{\mathbb{E}[(X-\mu)^4]}{(\mathbb{E}[(X-\mu)^2])^2} = \frac{\mu_4}{\sigma^4} \tag{3.4}$$

- w - upward wind (or up-/downdraft)
- r_t - total water mixing ratio
- θ_l - liquid water potential temperature

The variables mostly appear in centered form, e.g. $w' = w - \overline{w}$.
For example $\overline{w'^2}$ is the centered variance.

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Normal Mixture

$$\begin{aligned}
P_{tmg}(w, \theta_l, r_t) = {} & \alpha(1-\delta)\mathcal{N}(\mu_1, \Sigma_1) \\
& + (1-\alpha)(1-\delta)\mathcal{N}(\mu_2, \Sigma_2) \\
& + \delta\mathcal{N}(\mu_3, \Sigma_3),
\end{aligned} \tag{4.1}$$

where $\mathcal{N}$ denotes the multivariate normal distribution, $\alpha \in (0, 1)$ is the mixture fraction of the binormal, and $\delta \in [0, 1)$ is the weight of the third normal.

Mean of first and second component

$$\mu_1 = \begin{pmatrix} w_1 \\ \theta_{l1} \\ r_{t1} \end{pmatrix}, \mu_2 = \begin{pmatrix} w_2 \\ \theta_{l2} \\ r_{t2} \end{pmatrix} \tag{4.2}$$

Covariance matrices of first and second component

$$\Sigma_1 = \begin{pmatrix} \sigma_w^2 & 0 & 0 \\ 0 & \sigma_{\theta l 1}^2 & \rho_{\theta_l r_t} \sigma_{\theta_l 3} \sigma_{r_t 3} \\ 0 & \rho_{\theta_l r_t} \sigma_{\theta_l 3} \sigma_{r_t 3} & \sigma_{r_{t1}}^2 \end{pmatrix} \tag{4.3}$$

$$\Sigma_2 = \begin{pmatrix} \sigma_w^2 & 0 & 0 \\ 0 & \sigma_{\theta l 2}^2 & \rho_{\theta_l r_t} \sigma_{\theta_l 3} \sigma_{r_t 3} \\ 0 & \rho_{\theta_l r_t} \sigma_{\theta_l 3} \sigma_{r_t 3} & \sigma_{r_{t2}}^2 \end{pmatrix} \tag{4.4}$$

Placing of the third component

We place the third normal component at the mean in order to simplify the math.

$$\mu_3 = \begin{pmatrix} \overline{w} \\ \overline{\theta_l} \\ \overline{r_t} \end{pmatrix}, \text{ and } \Sigma_3 = \begin{pmatrix} \sigma_{w3}^2 & \rho_{w\theta_l3}\sigma_{w3}\sigma_{\theta_l3} & \rho_{wr_t3}\sigma_{w3}\sigma_{r_t3} \\ \rho_{w\theta_l3}\sigma_{w3}\sigma_{\theta_l3} & \sigma_{\theta_l3}^2 & \rho_{\theta_lr_t3}\sigma_{\theta_l3}\sigma_{r_t3} \\ \rho_{wr_t3}\sigma_{w3}\sigma_{r_t3} & \rho_{\theta_lr_t3}\sigma_{\theta_l3}\sigma_{r_t3} & \sigma_{r_t3}^2 \end{pmatrix} \quad (4.5)$$

Additional definitions

$$\lambda_w \equiv \frac{\sigma_{w3}^2}{\overline{w'^2}}, \quad \lambda_\theta \equiv \frac{\sigma_{\theta_l 3}^2}{\overline{\theta_l'^2}}, \quad \lambda_r \equiv \frac{\sigma_{r_t 3}^2}{\overline{r_t'^2}}, \tag{4.6}$$

$$\lambda_{\theta r} \equiv \frac{\rho_{\theta_l r_t} \sigma_{\theta_l 3} \sigma_{r_t 3}}{\overline{r_t' \theta_l'}}, \quad \lambda_{w\theta} \equiv \frac{\rho_{w\theta_l} \sigma_{w3} \sigma_{\theta_l 3}}{\overline{w'\theta_l'}}, \quad \lambda_{wr} \equiv \frac{\rho_{wr_t} \sigma_{w3} \sigma_{r_t 3}}{\overline{w'r_t'}} \tag{4.7}$$

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

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

$$+ \delta 3\lambda_w^2 \left(\overline{w'^2}\right)^2 \tag{5.1}$$

$$\overline{w'^2\theta_l'} = \frac{1}{(1-\tilde{\sigma}_w^2)} \frac{1-\delta\lambda_{w\theta}}{1-\delta\lambda_w} \frac{\overline{w'^3}}{\overline{w'^2}} \overline{w'\theta_l'} \tag{5.2}$$

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

$$+ \frac{1}{3} \frac{(1 - \delta\lambda_w)}{(1 - \delta\lambda_{w\theta})} \left(1 - \tilde{\sigma}_w^2\right) \frac{\overline{w'^2} \; \overline{\theta_l'^3}}{\overline{w'\theta_l'}} \tag{5.3}$$

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

As skewness goes to zero we want the pdf to revert to a single normal ($\delta \to 1$).

$$\lim_{\delta \to 1} \left(\overline{w'^4} \right) = \left(\frac{\left(\overline{w'^3} \right)^2}{(1 - \delta \lambda_w) \left(\overline{w'^2} - \frac{\sigma_w^2}{2 - c_1} \right)} \right) + 3 \left(\overline{w'^2} \right)^2 \qquad (6.1)$$

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

As skewness goes to zero we want the pdf to revert to a single normal ($\delta \to 1$).

$$\lim_{\delta \to 1} \left(\overline{w'^2\theta_l'} \right) = \frac{(c_1 - 2)^2 \overline{w'\theta_l'} \cdot \overline{w'^3}}{(c_2 - 2)\left((c_1 - 2)\overline{w'^2} + \sigma_w^2 \right)} \tag{6.2}$$

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

As skewness goes to zero we want the pdf to revert to a single normal ($\delta \to 1$).

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

$$\left. + \frac{1}{3} \frac{(1 - \delta\lambda_w)}{(1 - \delta\lambda_{w\theta})} \left(1 - \tilde{\sigma}_w^2\right) \frac{\overline{w'^2}}{\overline{w'\theta_l'}} \frac{\overline{\theta_l'^3}}{\overline{w'\theta_l'}} \right) \qquad (6.3)$$

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We have checked the higher-order moment formulas using SymPy.

DEMONSTRATION
(Analytic integration using SymPy [Meu+17])

Code to follow along the demonstration I

Listing: Import statements

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

Listing: Defining symbols

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

Code to follow along the demonstration II

Listing: Defining the marginals

```
G_1_w = Normal(name='G_1_w', mean=w_1, std=sigma_w)
G_1_w_density = density(G_1_w)(sp.abc.w)
G_2_w = Normal(name='G_2_w', mean=w_2, std=sigma_w)
G_2_w_density = density(G_2_w)(sp.abc.w)
G_3_w = Normal(name='G_3_w', mean=w_bar, std=sigma_w_3)
G_3_w_density = density(G_3_w)(sp.abc.w)
G_w = ((1 - sp.abc.delta) * sp.abc.alpha * G_1_w_density +
    (1 - sp.abc.delta) * (1 - sp.abc.alpha) * G_2_w_density +
    sp.abc.delta * G_3_w_density)
```

Listing: 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))
```

Code to follow along the demonstration III

Listing: 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))
```

Listing: Python function for the second order moment

```
def w_prime_2_bar_check(delta=sp.abc.delta, alpha=sp.abc.alpha, w_1=w_1,
↪ w_2=w_2, w_bar=w_bar, sigma_w=sigma_w, sigma_w_3=sigma_w_3):
return (((1 - delta) * alpha * ((w_1 - w_bar) ** 2 + sigma_w ** 2))
    + ((1 - delta) * (1 - alpha) * ((w_2 - w_bar) ** 2 + sigma_w ** 2))
    + (delta * sigma_w_3 ** 2))
```

Listing: Printing the symbolic equation

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

Code to follow along the demonstration IV

Listing: 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))
```

References

[Ize08]   Alan Julian Izenman. *Modern multivariate statistical techniques: regression, classification, and manifold learning*. Springer texts in statistics. OCLC: ocn225427579. New York ; London: Springer, 2008. ISBN: 9780387781884.

[Lar22]   Vincent E. Larson. *CLUBB-SILHS: A parameterization of subgrid variability in the atmosphere*. 2022. arXiv: 1711.03675 [physics.ao-ph].

[LG05]   Vincent E Larson and Jean-Christophe Golaz. "Using probability density functions to derive consistent closure relationships among higher-order moments". In: *Monthly Weather Review* 133.4 (2005), pp. 1023–1042.

[Meu+17]   Aaron Meurer et al. "SymPy: symbolic computing in Python". In: *PeerJ Computer Science* 3 (Jan. 2017), e103. ISSN: 2376-5992. DOI: 10.7717/peerj-cs.103. URL: https://doi.org/10.7717/peerj-cs.103.

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 (pdf of a normal distribution)

$$f(x|\mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2\right) \tag{8.1}$$

Considering that the skewness goes to zero ($Sk_w \to 0$), we want the pdf to revert to a single normal distribution. Therefore, we need

$$\delta, \lambda_w, \lambda_r, \lambda_\theta, \lambda_{wr}, \lambda_{w\theta}, \lambda_{\theta r} \to 1. \tag{8.2}$$

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

$$\lim_{\delta \to 1}(1 - \delta) \propto |Sk_w|, \tag{8.3}$$

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

$$0 < \lim_{\delta \to 1}\left(\frac{1 - \delta\lambda_x}{1 - \delta}\right) < \infty, \tag{8.4}$$

where x means any of w, r_t, or θ_l,

$$0 < \lim_{\delta \to 1} \left(\frac{1 - \delta \lambda_x}{1 - \delta \lambda_y} \right) < \infty \tag{8.5}$$

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

$$0 < \lim_{\delta \to 1} \left(\tilde{\sigma}_w \right)^2 = \lim_{\delta \to 1} \left(\frac{\sigma_w^2}{w'^2} \frac{1 - \delta}{1 - \delta \lambda_w} \right) < 1. \tag{8.6}$$

To ensure (8.3), we can use a linear "fit", which looks like

$$\lambda_w = \lambda_\theta = \lambda_q = (1 - c_1)\delta + c_1, \tag{8.7}$$

where c_1 is some constant. The fit for the other λ's is

$$\lambda_{w\theta} = \lambda_{q\theta} = \lambda_{wq} = (1 - c_2)\delta + c_2, \tag{8.8}$$

where again c_2 is some constant. Note, that we already have a definition for the λ's ((4.6)). This definition is just for the backward run though, because we actually have to choose λ in the forward direction.

If we now look at the limit with the proposed fit ((8.7)), where x is one of the three variates, we get:

$$\lim_{\delta \to 1} \left(\frac{1 - \delta \lambda_x}{1 - \delta} \right) = \lim_{\delta \to 1} \left(\frac{1 - \delta((1 - c_1)\delta + c_1)}{1 - \delta} \right) = \lim_{\delta \to 1} \left(\frac{1 - ((1 - c_1)\delta^2 + c_1\delta)}{1 - \delta} \right) \tag{8.9}$$

$$= \lim_{\delta \to 1} \left(\frac{1 - \delta^2 + c_1\delta^2 - c_1\delta}{1 - \delta} \right) = \lim_{\delta \to 1} \left(\frac{1 - \delta^2 + c_1\delta(\delta - 1)}{1 - \delta} \right) \tag{8.10}$$

$$= \lim_{\delta \to 1} \left(\frac{1 - \delta^2}{1 - \delta} \right) - \lim_{\delta \to 1} \left(\frac{c_1\delta(1 - \delta)}{1 - \delta} \right) \tag{8.11}$$

$$\text{(L'Hôpital)} \overset{\left[\frac{0}{0}\right]}{=} \lim_{\delta \to 1} \left(\frac{-2\delta}{-1} \right) - \lim_{\delta \to 1} (c_1\delta) \tag{8.12}$$

$$= 2 - c_1. \tag{8.13}$$

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

$$\lim_{\delta \to 1} \left(\frac{1-\delta}{1-\delta\lambda_x} \right) = \lim_{\delta \to 1} \left(\frac{1-\delta}{1-\delta^2 + c_1\delta^2 - c_1\delta} \right) \overset{\left[\frac{0}{0}\right]}{=} \lim_{\delta \to 1} \left(\frac{-1}{-2\delta + 2c_1\delta - c_1} \right) \tag{8.14}$$

$$= \frac{-1}{-2 + c_1} = \frac{1}{2 - c_1}. \tag{8.15}$$