Asymptotic behavior of solutions to the linear Becker-Döring equations

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Gradient flows face-to-face

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UNIVERSIDAD DE GRANADA



Introduction

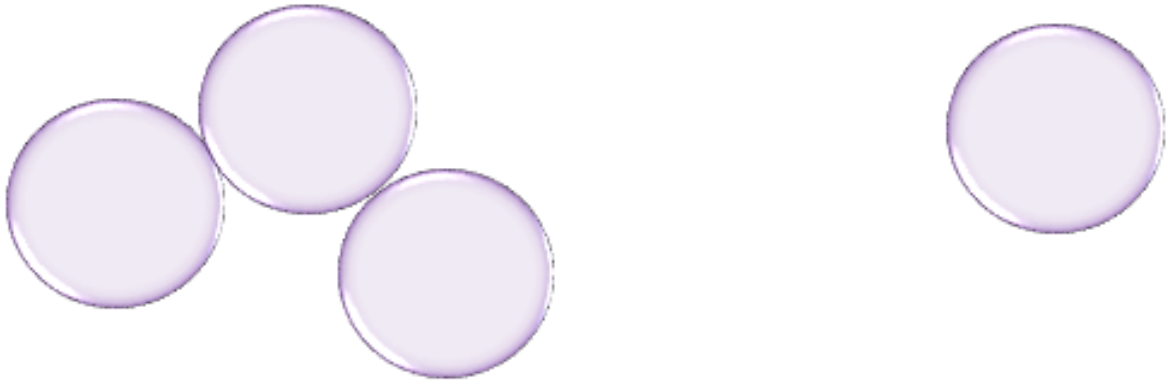
- The Becker-Döring equations describe the process of nucleation and growth in phase transitions.
- They were introduced in 1935 to model the kinetics of particle aggregation.

Mathematical Model (Becker and Döring [1935])

$$\frac{dc_i}{dt} = W_{i-1} - W_i, \ i \geq 2$$

$$W_i := a_i c_1 c_i - b_{i+1} c_{i+1}, \ i \geq 1$$

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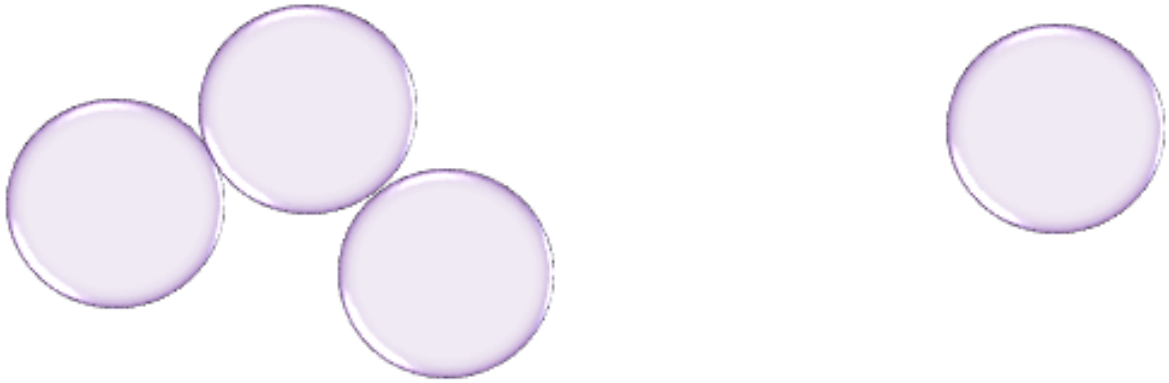


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Question: If we want mass of the solution to be conserved, which equation must c_1 satisfy?

Becker-Döring Equations

$$\frac{d}{dt}\sum_{i=1}^{\infty} ic_i(t) = 0$$

$$\frac{d}{dt}\sum_{i=1}^{\infty} ic_i(t) = \frac{d}{dt}c_1(t) + W_1(t) + \sum_{i=1}^{\infty} W_i(t)$$

Becker-Döring Equations

$$\frac{d}{dt}\sum_{i=1}^{\infty} i c_i(t) = 0$$

$$\frac{d}{dt}\sum_{i=1}^{\infty} i c_i(t) = \frac{d}{dt}c_1(t) + W_1(t) + \sum_{i=1}^{\infty} W_i(t)$$

Mathematical Model

$$\begin{cases} \dfrac{dc_i}{dt} = W_{i-1} - W_i, \ i \geq 2 \\ \\ \dfrac{dc_1}{dt} = -W_1 - \displaystyle\sum_{i=1}^{\infty} W_i \end{cases}$$

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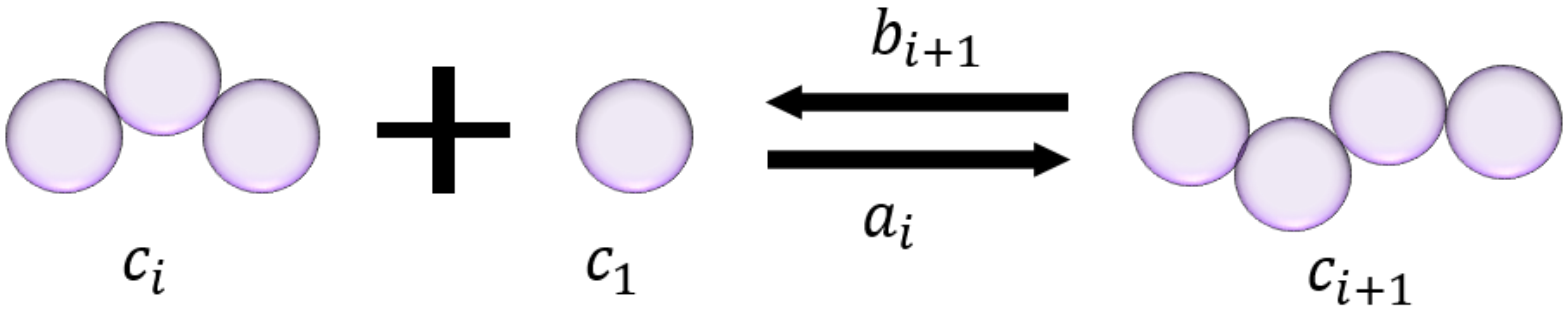
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Applications:

- Phase transitions in physics and chemistry
- Modeling aerosol formation
- Regulation by accessory proteins

What if we take c_1 constant?



$$\begin{cases} \dfrac{dc_i}{dt} & = W_{i-1} - W_i, \ i \geq 2 \\ c_1 & = z \text{ (const.)} \end{cases}$$

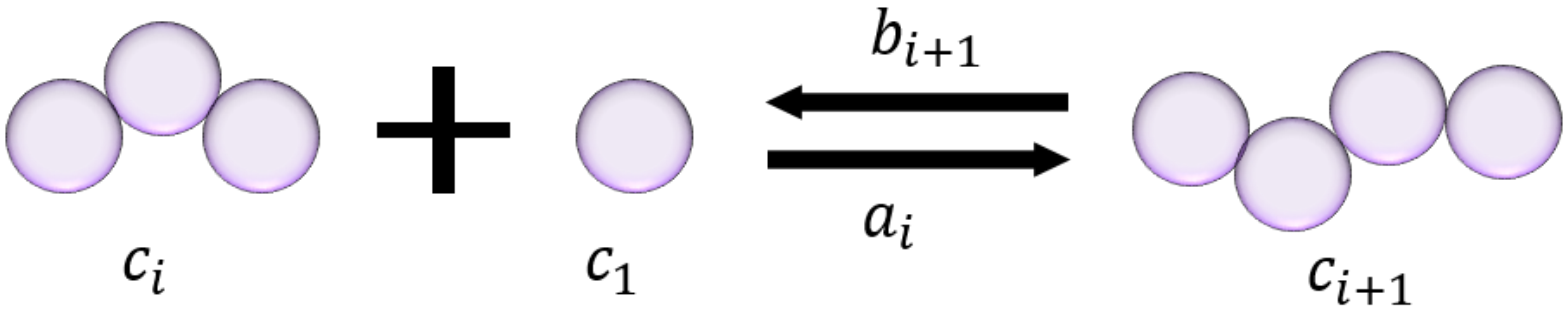
$c_i \equiv$ number density of clusters of size i

$a_i \equiv$ coagulation coefficient

$b_i \equiv$ fragmentation coefficient

$$W_i := a_i z c_i - b_{i+1} c_{i+1}, \ i \geq 1$$

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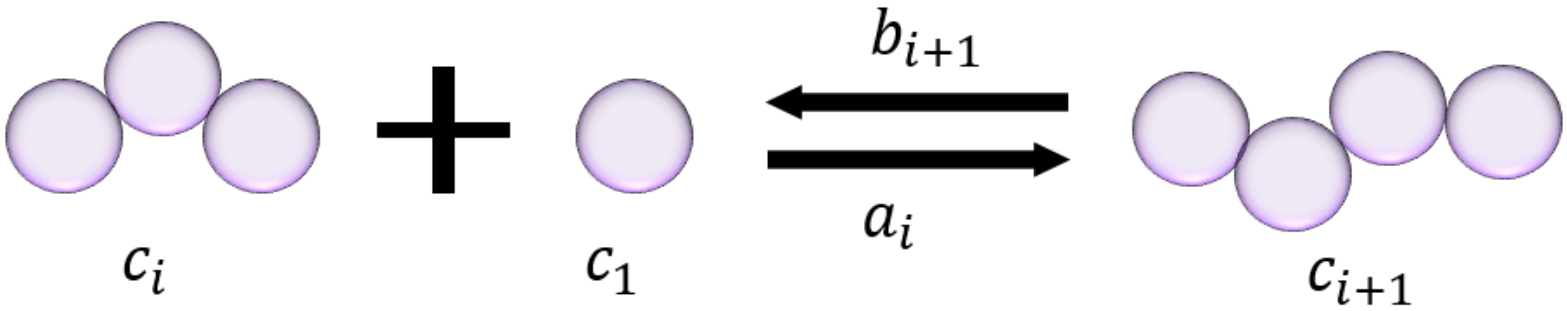
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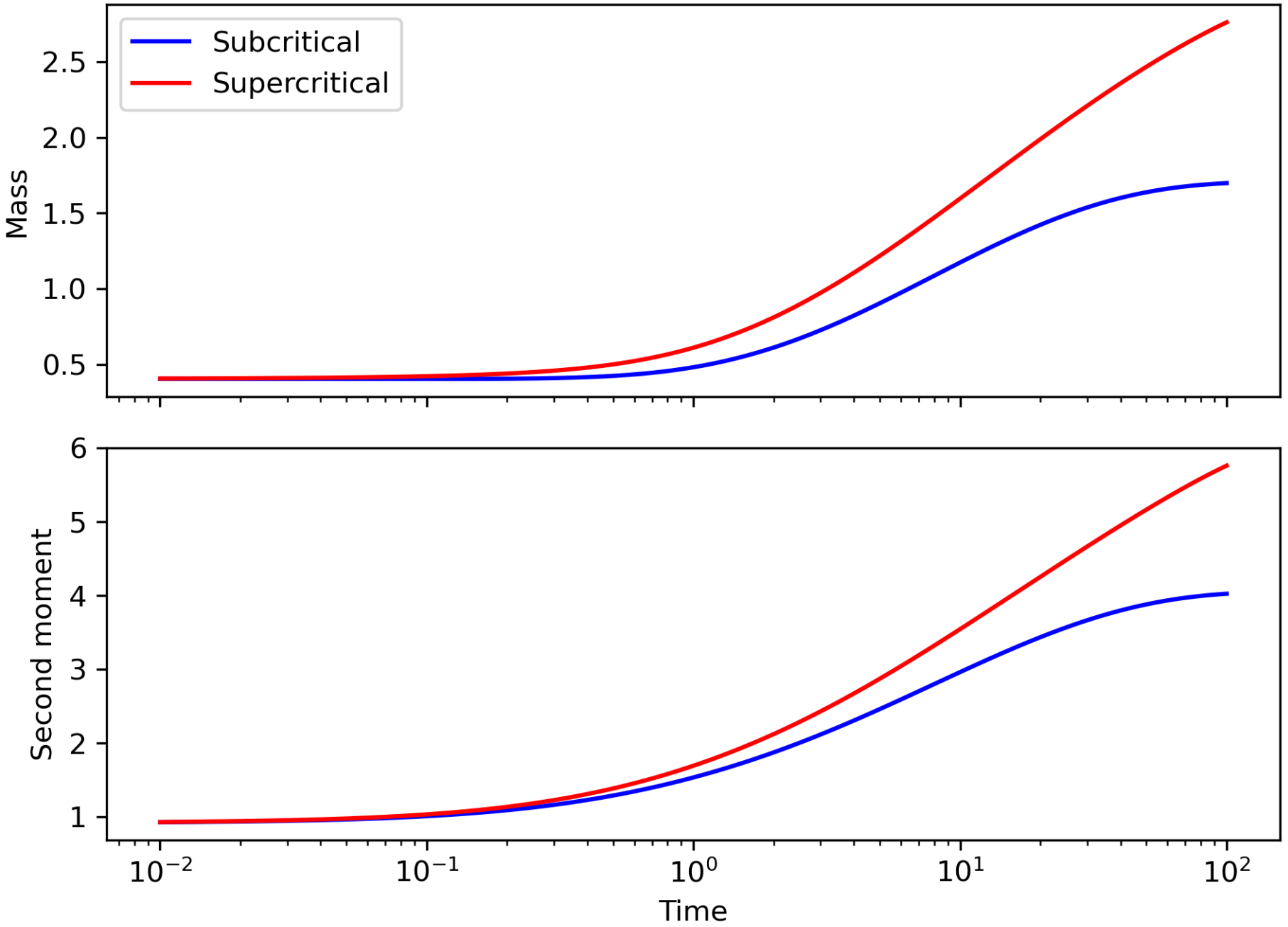
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- Mass of the solution is not conserved.
- Weak formulation of the solutions

$$\frac{d}{dt} \sum_{i=1}^{\infty} \varphi_i c_i(t) = \varphi_2 W_1(t) + \sum_{i=2}^{\infty} (\varphi_{i+1} - \varphi_i) W_i(t)$$


Subcritical
Supercritical
Mass
2.5
2.0
1.5
1.0
0.5
Second moment
6
5
4
3
2
1
10^{-2}
10^{-1}
10^{0}
10^{1}
10^{2}
Time

Equilibria

If $W_i = 0$ for all $i \geq 1$ (Simplest equilibrium solution):

$$T_i = Q_i z^i.$$

Where $\{Q_i\}_{i \geq 1}$ is the sequence defined by

$$Q_1 = 1 \quad \text{and} \quad Q_i = \frac{a_{i-1}}{b_i} Q_{i-1} \text{ for } i \geq 2$$

Equilibria

If $W_i = 0$ for all $i \geq 1$ (Simplest equilibrium solution):

$$T_i = Q_i z^i.$$

If $W_i = J$ for all $i \geq 1$ (General equilibrium solution):

$$T_i = Q_i z^i \left(1 - J \sum_{j=1}^{i-1} \frac{1}{a_i z^{i+1} Q_i}\right).$$

Where $\{Q_i\}_{i \geq 1}$ is the sequence defined by

$$Q_1 = 1 \quad \text{and} \quad Q_i = \frac{a_{i-1}}{b_i} Q_{i-1} \text{ for } i \geq 2$$

and

$$J = \left(\sum_{i=1}^{\infty} \frac{1}{a_i Q_i z^{i+1}}\right)^{-1}.$$

Commonly used coefficients

Commonly, in physics and chemistry, the most used coefficients are

$$a_i = i^\tau, \quad 0 \leq \tau < 1,$$
$$Q_i = e^{-(i-1)^\mu}, \quad 0 < \mu < 1,$$
$$b_i = (i-1)^\alpha e^{(i-1)^\mu - (i-2)^\mu}.$$

These coefficients appear, for example, in Cañizo and Lods [2013].

Entropy method I

Firstly, we need a free energy (Lyapunov function). For our purposes, we work with the entropy given by Keer [1993]:

$$H(v) = \sum_{i=1}^{\infty} v_i^2 Q_i z^i,$$

with $v_i = \dfrac{c_i - T_i}{Q_i z^i}$.

We calculate the dissipation of the entropy, which is the function $D(v) \geq 0$ such that

$$\frac{d}{dt} H(v) = -D(v)$$

In this case,

$$D(v) = 2 \sum_{i=1}^{\infty} \left(v_{i+1} - v_i\right)^2 Q_i a_i z^{i+1}.$$

Entropy method II

Lemma (Left-sided Hardy's inequality)

For any two positive weights $\{\mu_i\}_{i\geq 1}$ *and* $\{\nu_i\}_{i\geq 1}$, *there exists* $A > 0$ *such that*

$$\sum_{i=2}^{\infty} \mu_i f_i^2 \leq A \sum_{i=2}^{\infty} \nu_i (f_i - f_{i-1})^2,$$

for all vectors $f = (f_1, \dots, f_i, \dots)$ *such that* $f_1 = 0$, *if and only if*

$$B = \sup_{k\geq 2} \left(\sum_{i=k}^{\infty} \mu_i \right) \left(\sum_{i=2}^{k} \frac{1}{\nu_i} \right) < \infty.$$

Moreover, if these conditions hold true, then $B \leq A \leq 4B$.

Entropy method III

Lemma (Right-sided Hardy's inequality)

For any two positive weights $\mu = \{\mu_i\}_{i\geq 1}$ *and* $\nu = \{\nu_i\}_{i\geq 1}$, *there exists* $A > 0$ *such that*

$$\sum_{i=1}^{\infty} \mu_i f_i^2 \leq A \sum_{i=1}^{\infty} \nu_i (f_{i+1} - f_i)^2,$$

for all vectors $f = (f_1, \dots, f_i, \dots)$ *such that* $\lim_{i\to\infty} f_i = 0$, *if and only if*

$$B = \sup_{k\geq 1} \left(\sum_{i=1}^{k} \mu_i \right) \left(\sum_{i=k}^{\infty} \frac{1}{\nu_i} \right) < \infty.$$

Moreover, if these conditions hold true, then $B \leq A \leq 4B$.

Entropy method IV

Theorem (P. Barik, I.B., J.A. Cañizo)

Suppose the coefficients a_i and b_i satisfy (A1)–(A3). Consider the solution $c := (c_i)_{i\geq 1}$ with initial data $c_0 \in \ell^1$. Let $T = (T_i)$ be a sequence of equilibrium solution. Then

$$H(v(t)) \leq H(v_0)e^{-\lambda t},$$

where $v_i = \dfrac{c_i - T_i}{Q_i z^i}$ and the positive λ is estimated using the Hardy inequality for both subcritical $(z < z_s)$ and supercritical $(z > z_s)$ cases.

Asymptotic behavior of the spectral gap

Corollary (P. Barik, I.B., J.A. Cañizo)

Let the coefficients a_i, b_i, Q_i be given with $0 \leq \alpha < 1$, $0 < \mu < 1$, and consider $z > z_s$.
Then, there exist constants $C_1, C_2 > 0$ and $\beta > 0$, depending on α, μ, such that the spectral gap λ satisfies the bounds

$$C_1(z - z_s)^\beta \leq \lambda \leq C_2(z - z_s)^\beta.$$

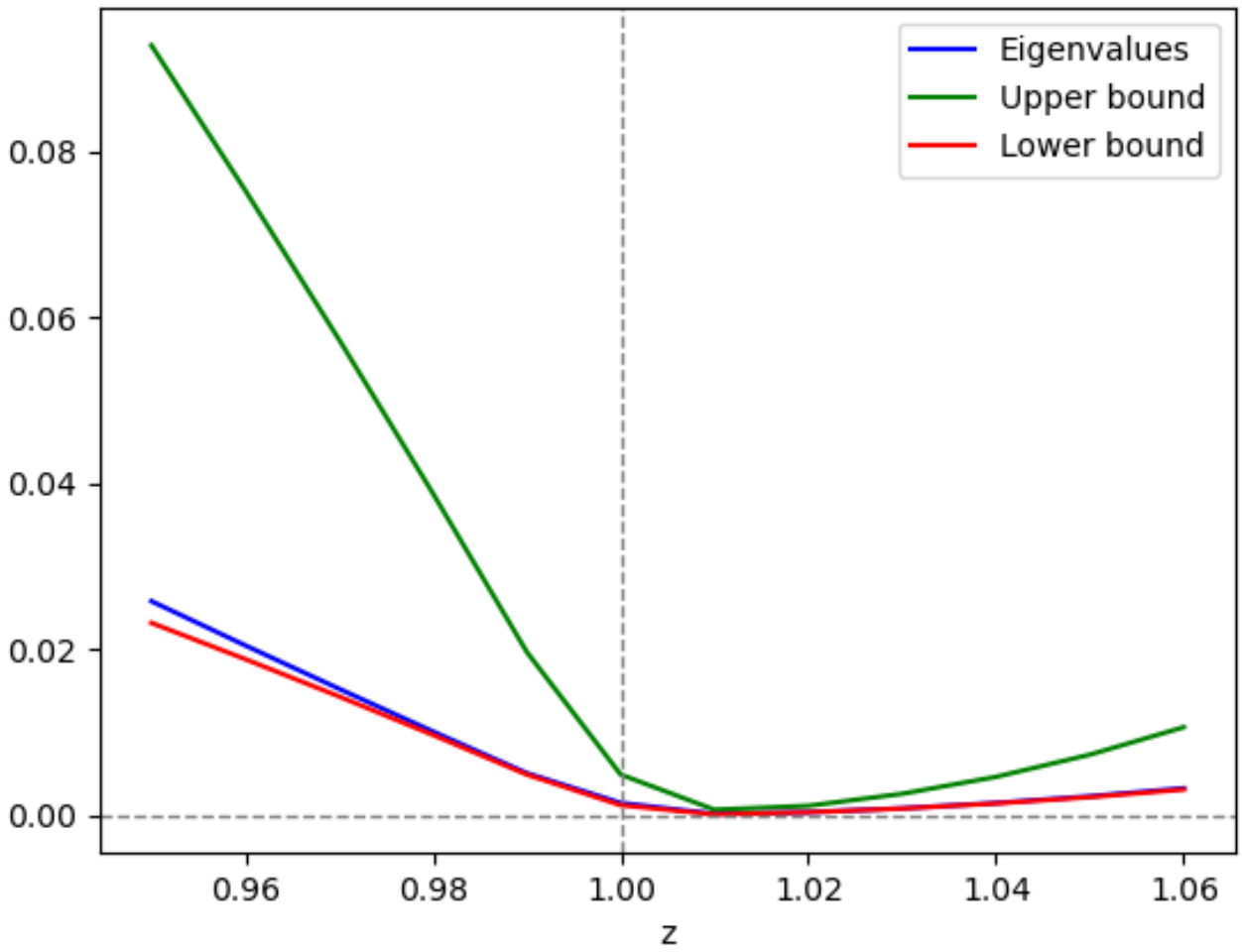


Figure: Truncated matrix for n = 3000.

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