GAMM Workshop on
Applied and Numerical Linear Algebra
with Special Emphasis on Model Reduction
September 22nd and 23rd, 2011

A Goal Oriented Low Rank Dual ADI Iteration for Balanced Truncation

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joint work with
Peter Benner and Patrick Kürschner

Max Planck Institute for Dynamics of Complex Technical Systems
Computational Methods in Systems and Control Theory

Outline

Balanced Truncation in a Nutshell

Basic Idea

Idea:

- The system Σ, in realization (A, B, C), is called balanced, if the solutions P, Q of the Lyapunov equations

$$AP + PA^T + BB^T = 0, \qquad A^TQ + QA + C^TC = 0,$$

satisfy: $P = Q = \mathrm{diag}(\sigma_1, \ldots, \sigma_n)$ where $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_n > 0$.

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- $\{\sigma_1, \ldots, \sigma_n\}$ are the Hankel singular values (HSVs) of Σ.
- A balanced realization is computed via state space transformation

$$\begin{aligned}\mathcal{T} : (A, B, C) &\mapsto (TAT^{-1}, TB, CT^{-1}) \\ &= \left(\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}, \begin{bmatrix} B_1 \\ B_2 \end{bmatrix}, \begin{bmatrix} C_1 & C_2 \end{bmatrix} \right).\end{aligned}$$

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- Truncation $\rightsquigarrow$ reduced order model: $(\hat{A}, \hat{B}, \hat{C}) = (A_{11}, B_1, C_1)$.

Balanced Truncation in a Nutshell

Implementation

The SR Method

1. Compute (Cholesky)factors of the solutions to the Lyapunov equation,

$$P = S^T S, \quad Q = R^T R.$$

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3. Define
$$W := R^T V_1 \Sigma_1^{-1/2}, \qquad V := S^T U_1 \Sigma_1^{-1/2}.$$
4. Then the reduced order model is $(W^T AV, W^T B, CV)$.

Solving Large Lyapunov Equations

LRCF-ADI

Lyapunov equation

Consider

$$FX + XF^T = -GG^T$$

with $F \in \mathbb{R}^{n\times n}$ Hurwitz, $G \in \mathbb{R}^{n\times m}$, $m \ll n$.

Observation in practice:

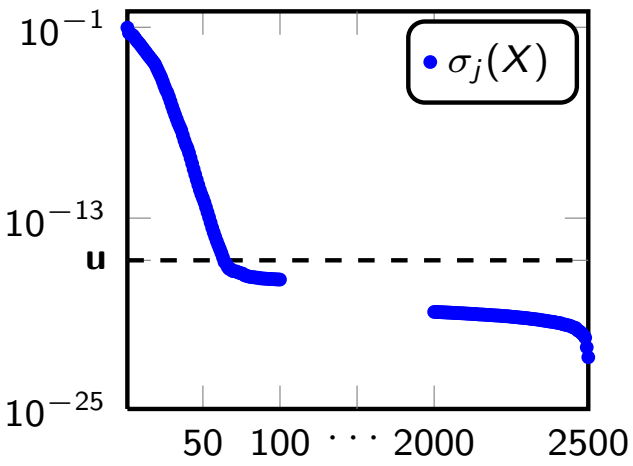
[Penzl '99, Ant./Sor./Zhou '02, Grasedyck '04]

$$\operatorname{rank}(X, \tau) = r \ll n$$

$\Rightarrow$ Compute *low-rank solution factor* $\tilde{Z} \in \mathbb{R}^{n\times r}$, $r \ll n$.

$$X \approx \tilde{Z}\tilde{Z}^T.$$

singular values for $n = 2\,500$ example



Solving Large Lyapunov Equations

LRCF-ADI

e.g.,[Benner/Li/Penzl '08]

Consider $FX + XF^T = -GG^T$ $F \in \mathbb{R}^{n\times n}, G \in \mathbb{R}^{n\times p}$

Task Find $Z \in \mathbb{C}^{n,nz}$, such that $nz \ll n$ and $X \approx ZZ^H$

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Algorithm

$$V_1 = \sqrt{-2\operatorname{Re} p_1}(F + p_1 I)^{-1} G, \qquad Z_1 = V_1$$

$$V_i = \frac{\sqrt{\operatorname{Re} p_i}}{\sqrt{\operatorname{Re} p_{i-1}}}\left[I - (p_i + \overline{p_{i-1}})(F + p_i I)^{-1}\right] V_{i-1} \qquad Z_i = [Z_{i-1} V_i]$$

For certain shift parameters $\{p_1, ..., p_J\} \subset \mathbb{C}_{<0}$.

Stop if

- $\|V_i V_i^H\|$ is small, or
- $\|FZ_iZ_i^H + Z_iZ_i^H F^T + GG^T\|$ is small.

Solving Large Lyapunov Equations

G-LRCF-ADI (E invertible)

e.g.,[S. '09]

Consider $FXE^T + EXF^T = -GG^T \qquad E, F \in \mathbb{R}^{n\times n}, G \in \mathbb{R}^{n\times p}$

Task Find $Z \in \mathbb{C}^{n,nz}$, such that $nz \ll n$ and $X \approx ZZ^H$

Algorithm

$$V_1 = \sqrt{-2\operatorname{Re} p_1}(F + p_1 E)^{-1} G, \qquad Z_1 = V_1$$

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Solving Large Lyapunov Equations

S-LRCF-ADI **((E, F) index 1)** **e.g.,**[Rommes/Freitas/Martins '08]

Consider $\tilde{F} X E_{11}^T + E_{11} X \tilde{F}^T = -\tilde{G}\tilde{G}^T \qquad E_{11}, \tilde{F} \in \mathbb{R}^{n\times n}, \tilde{G} \in \mathbb{R}^{n\times p}$

Task Find $Z \in \mathbb{C}^{n,nz}$, such that $nz \ll n$ and $X \approx ZZ^H$

Algorithm

$$\begin{bmatrix} V_1 \\ * \end{bmatrix} = \sqrt{-2\operatorname{Re} p_1} \begin{bmatrix} F_{11} + p_1 E_{11} & F_{12} \\ F_{21} & F_{22} \end{bmatrix}^{-1} \begin{bmatrix} B_1 \\ B_2 \end{bmatrix}, \qquad Z_1 = V_1$$

$$\begin{bmatrix} V_i \\ * \end{bmatrix} = \frac{\sqrt{\operatorname{Re} p_i}}{\sqrt{\operatorname{Re} p_{i-1}}} \left[I - (p_i + \overline{p_{i-1}}) \begin{bmatrix} F_{11} + p_i E_{11} & F_{12} \\ F_{21} & F_{22} \end{bmatrix}^{-1} \right] \begin{bmatrix} E_{11} V_{i-1} \\ 0 \end{bmatrix} \qquad Z_i = [Z_{i-1} V_i]$$

For certain shift parameters $\{p_1, ..., p_J\} \subset \mathbb{C}_{<0}$.

Stop if

- $\|V_i V_i^H\|$ is small, or
- $\|\tilde{F} Z_i Z_i^H E_{11}^T + E_{11} Z_i Z_i^H \tilde{F}^T + \tilde{G}\tilde{G}^T\|$ is small.

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e.g.,[Rommes/Freitas/Martins '08]

Consider $\tilde{F}XE_{11}^T + E_{11}X\tilde{F}^T = -\tilde{G}\tilde{G}^T \qquad E_{11}, \tilde{F} \in \mathbb{R}^{n\times n}, \tilde{G} \in \mathbb{R}^{n\times p}$

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Can ensure $Z \in \mathbb{R}^{n,nz}$ even if $\{p_1, ..., p_J\} \not\subset \mathbb{R}$

see next talk by Patrick Kürschner

Solving Large Lyapunov Equations

Drawbacks of LR-ADI Based BT

- Performing LR-ADI based BT is computationally expensive compared to simple Krylov based approaches.
- Main effort is solving the dual Lyapunov equations.

Central Question

Can we reduce the time for computing the balancing transformations?

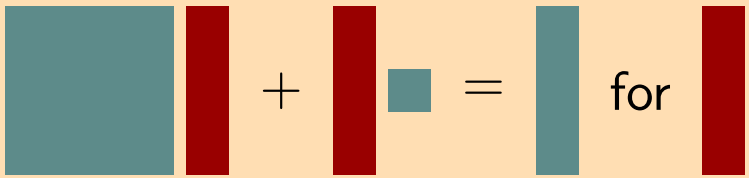
Existing Approaches "Simultaneously" Treating the Dual Lyapunov Equations

Cross Gramian based Methods **e.g.** [Fernando/Nicholson '83; Sorensen/Antoulas '02]

Idea

- Solve $AX + XA = -BC$ for the cross gramian X,
- Proceed with knowledge $X^2 = PQ$, i.e., for the HSV $\sigma_i = |\lambda_j(X)|$.

e.g., repeatedly solve projected equations of the form



- Requires symmetric system or symmetrizer Ψ, such that

$$A\Psi = \Psi A^*, \qquad B = \Psi C^*,$$

- Ψ may be expensive to compute
- number of inputs and outputs must coincide.

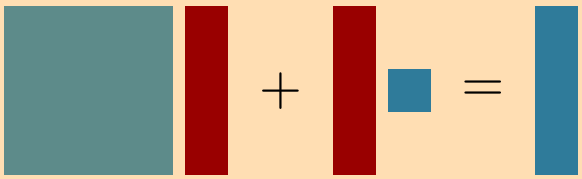
Existing Approaches "Simultaneously" Treating the Dual Lyapunov Equations

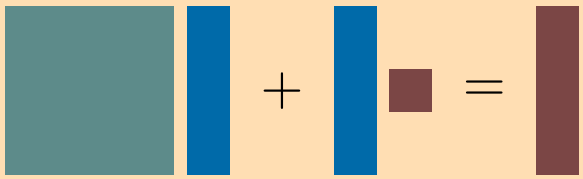
Approximate Implicit Subspace Iteration with Alternating Directions (AISIAD)
[Zhou/Sorensen '08]

Idea

- Solve $AP + PA^T = -BB^T$ and $A^TQ + QA = -C^TC$ simultaneously.
- Alternate the projection spaces.

alternatingly solve 2 equations of the form





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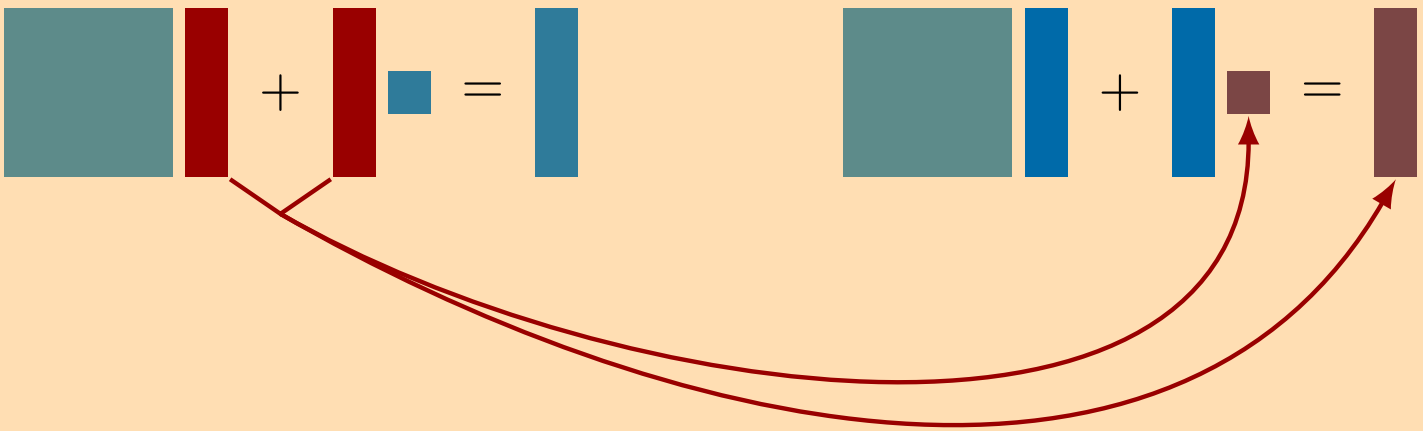

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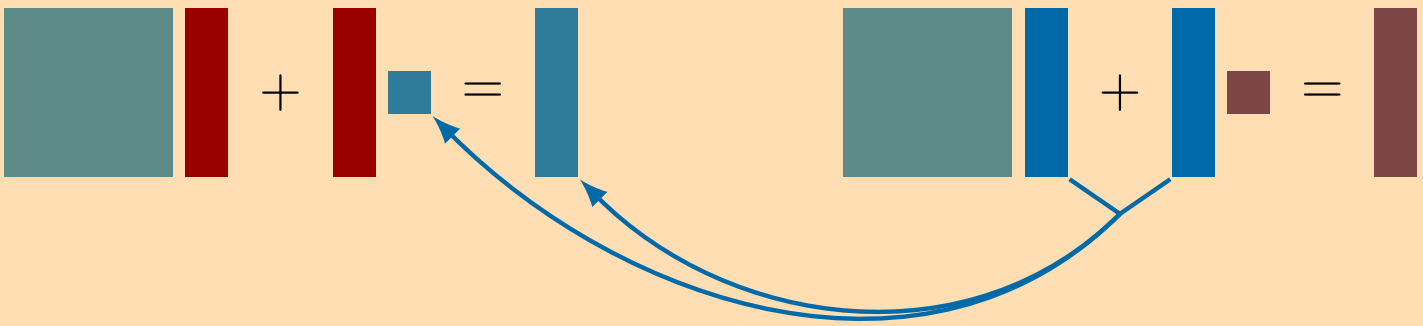

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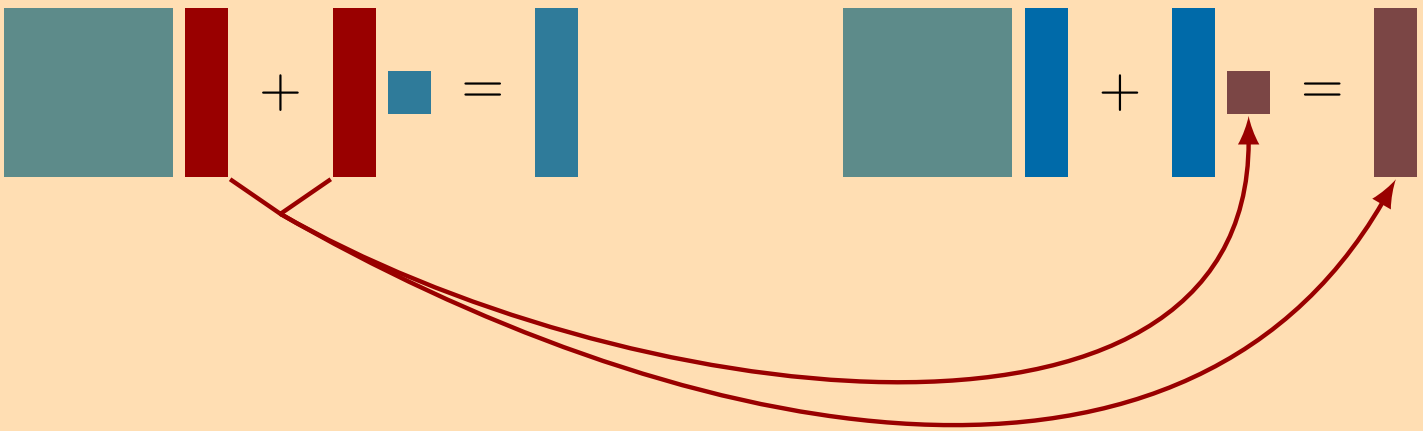

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After convergence use  and  to compute balancing transformations.

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- Solve $AP + PA^T = -BB^T$ and $A^TQ + QA = -C^TC$ simultaneously.
- Alternate the projection spaces.

- Initial projection basis required.
- 2 growingly expensive linear equations per step.
- Reuse of solvers for the step equations?

Dual LR-BT-ADI

Simultaneous Solution of the Dual Lyapunov Equations

Key Target

Reuse LU-factorizations in a sparse direct solver framework.

$$V_i = \frac{\sqrt{\operatorname{Re} p_i}}{\sqrt{\operatorname{Re} p_{i-1}}} \left[I - (p_i + \overline{p_{i-1}})(F + p_i E)^{-1} \right] E V_{i-1},$$

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$$LU := (F + p_i E) \quad \Rightarrow \quad U^H L^H = (F^T + \overline{p_i} E^T)$$

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- complex shifts come in conjugate pair,
- they are used one after another,

$\rightsquigarrow$ reverse order of complex conjugate shifts for the second equation.

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$$W_i = \frac{\sqrt{\operatorname{Re} p_i}}{\sqrt{\operatorname{Re} p_{i-1}}} \left[I - (\overline{p_i} + p_{i-1}) L^{-H} U^{-H} \right] E^T W_{i-1}.$$

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Stopping the Iteration

Problem

- Number of columns in LRCFs limits ROM dimension.
- Lyapunov residuals usually totally unrelated to ROM quality.

Idea

Use goal oriented stopping criteria.

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In Balanced Truncation MOR:

Assume we are interested in an order k ROM.

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In Balanced Truncation MOR:

Assume we are interested in an order k ROM.

- Monitor the relative change of k leading HSVs.
- Stop when leading HSVs do no longer change.

Numerical Results

Test Examples and Hardware

Rail Model [Benner/S. '03-'05]

- Oberwolfach Collection Rail Cooling[a]
- $n = 1357$
- inputs 7, outputs 6

[a] http://portal.uni-freiburg.de/imteksimulation/downloads/benchmark/Steel\Profiles\(38881)

BIPS07 [Freitas/Rommes/Martins '08]

- index 1 descriptor model of a power network[b]
- $n = 13\,275$, $n_{E_{11}} = 1693$
- inputs 4, outputs 4
- $\mathrm{condest}(A_{22}) = 8.275 \cdot 10^{26}$

[b] http://sites.google.com/site/rommes/software/bips07_1693.mat

Numerical Results

Test Examples and Hardware

Hardware

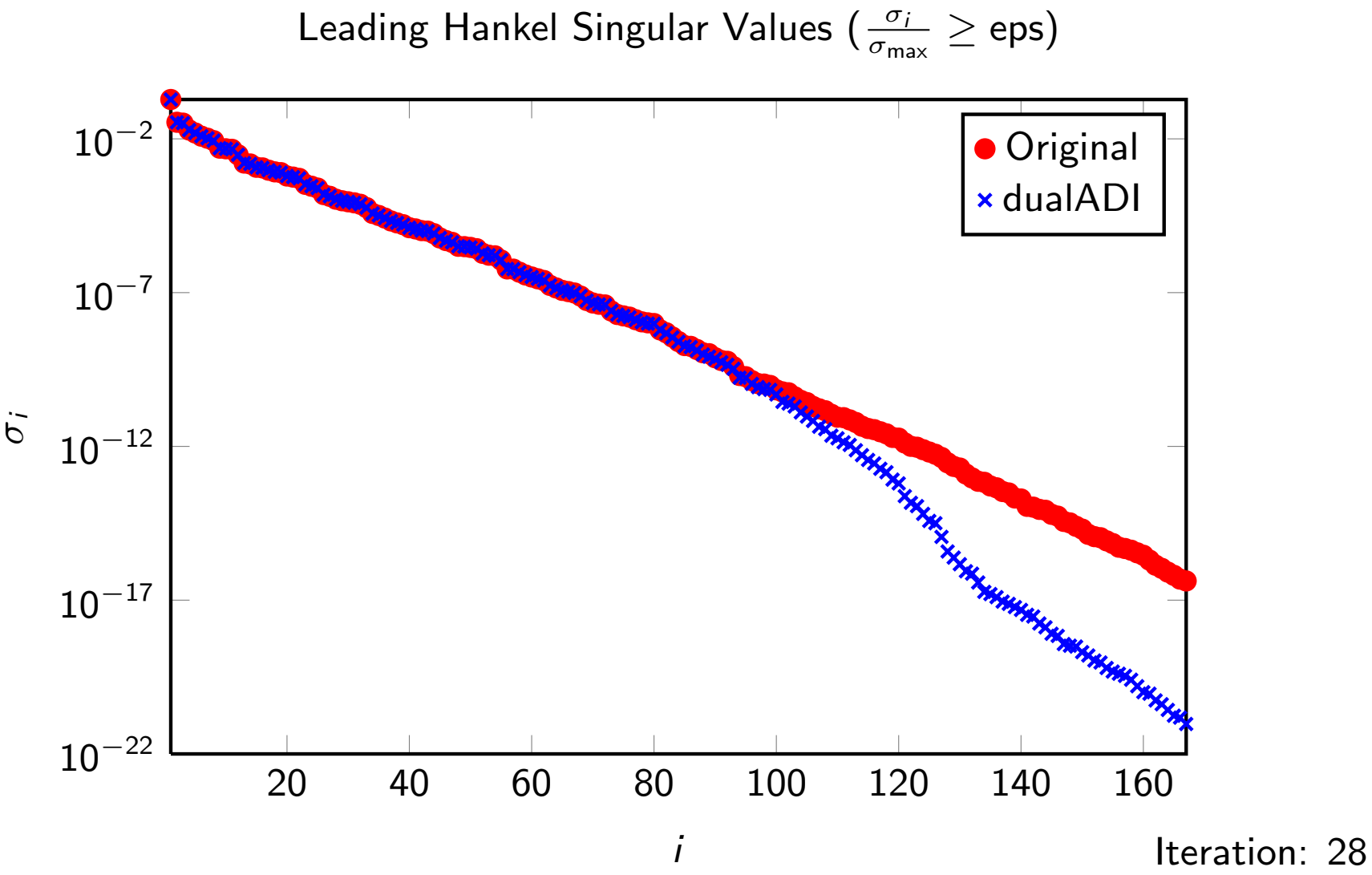
- dual Intel®Xeon®W3503 @ 2.40GHz
- Cache Size: 4MB
- RAM: 6GB

Sofware

- OS: Ubuntu Linux 10.04LTS
- 32bit kernel 2.6.32-25-generic-pae
- MATLAB® 7.11.0 (R2010b)

Numerical Results

Rail Model



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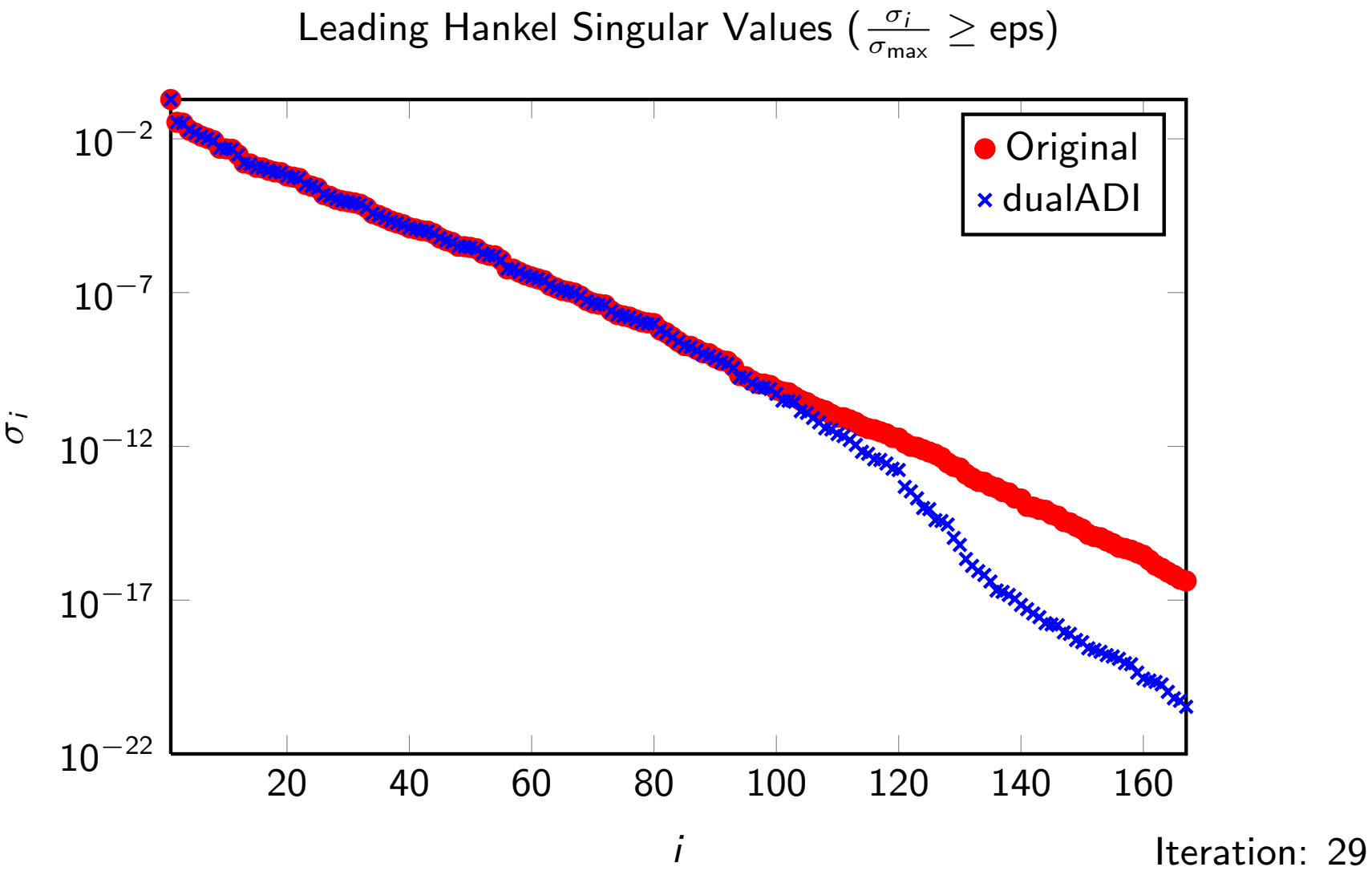

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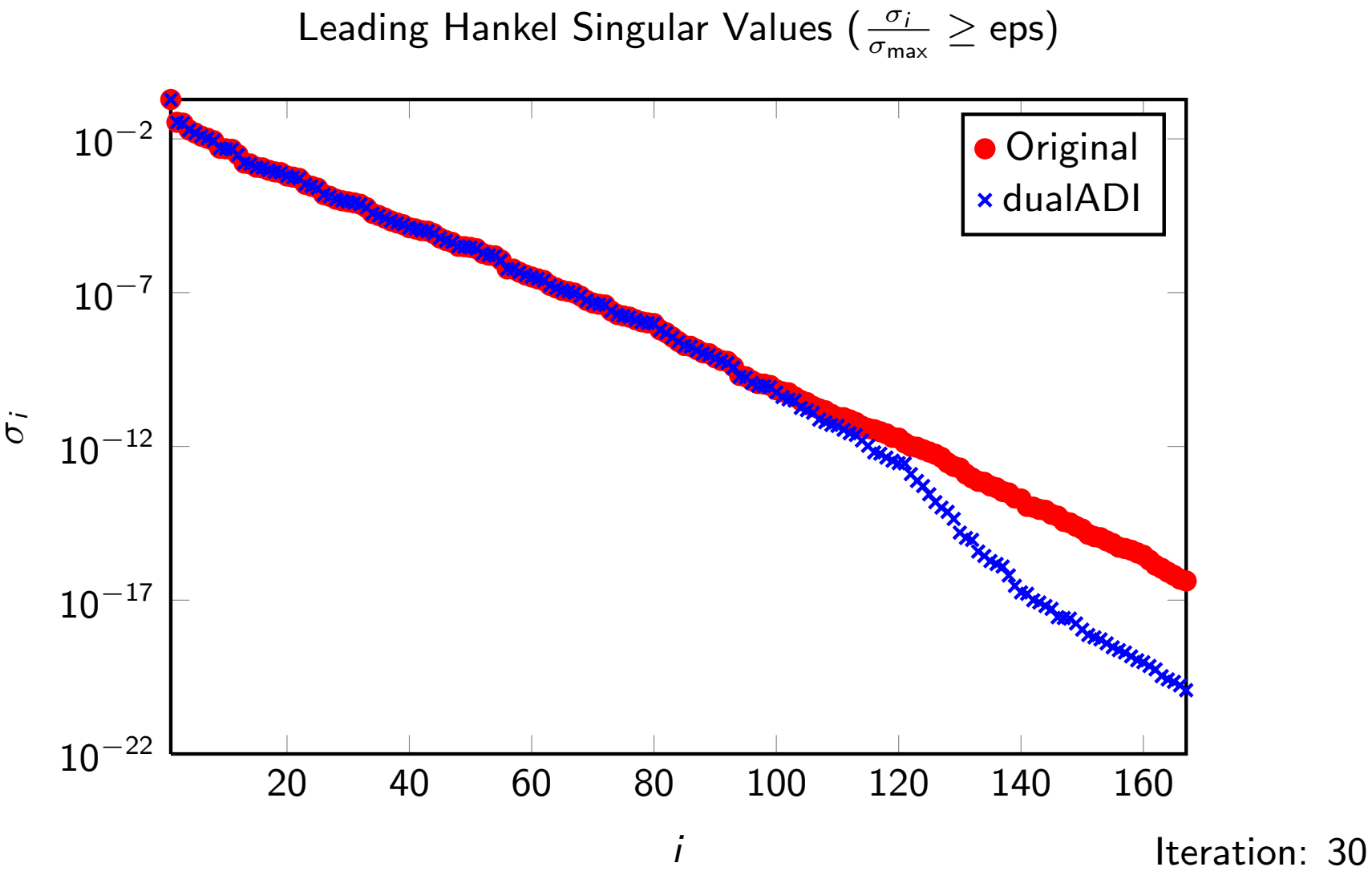

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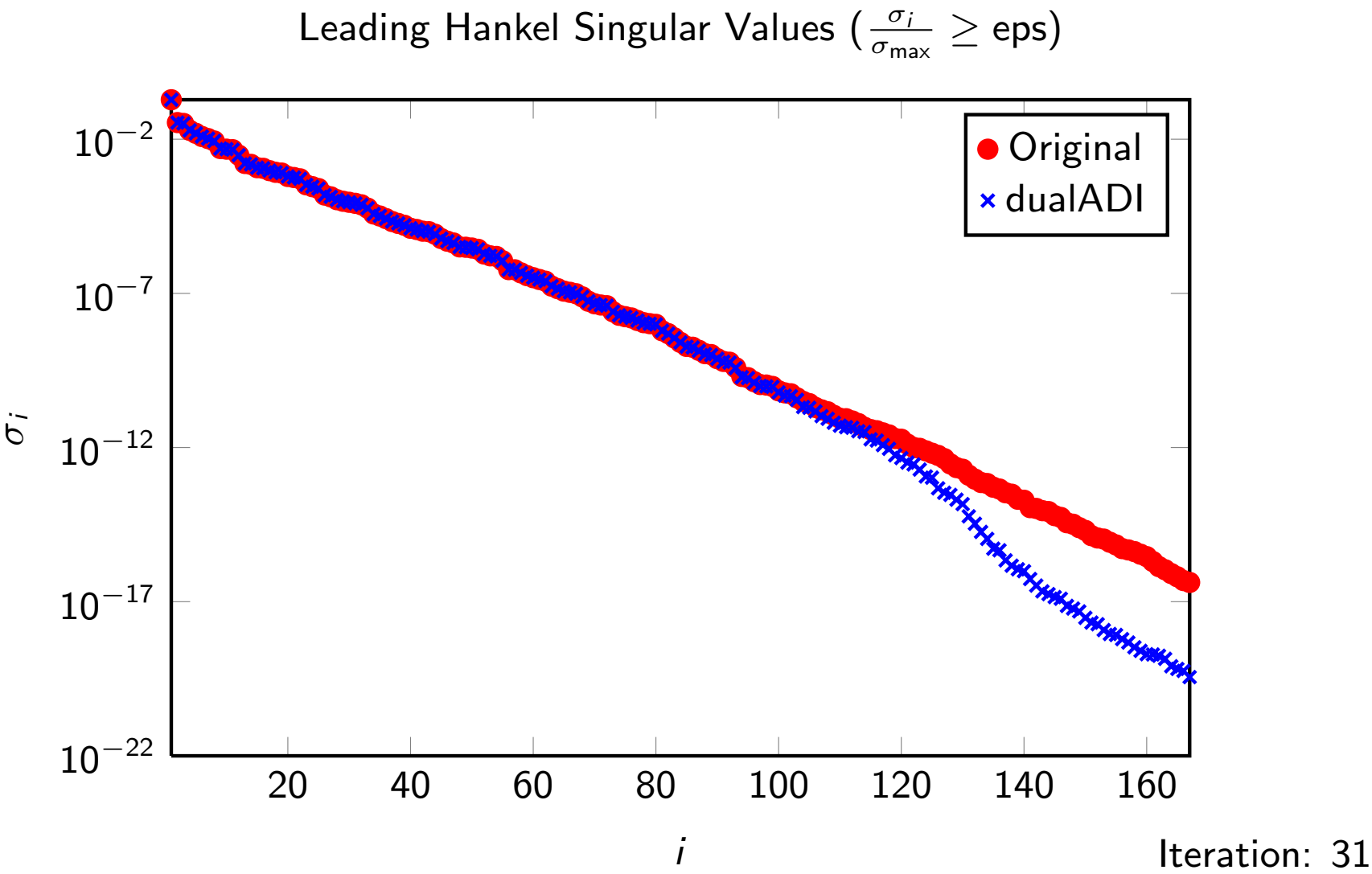

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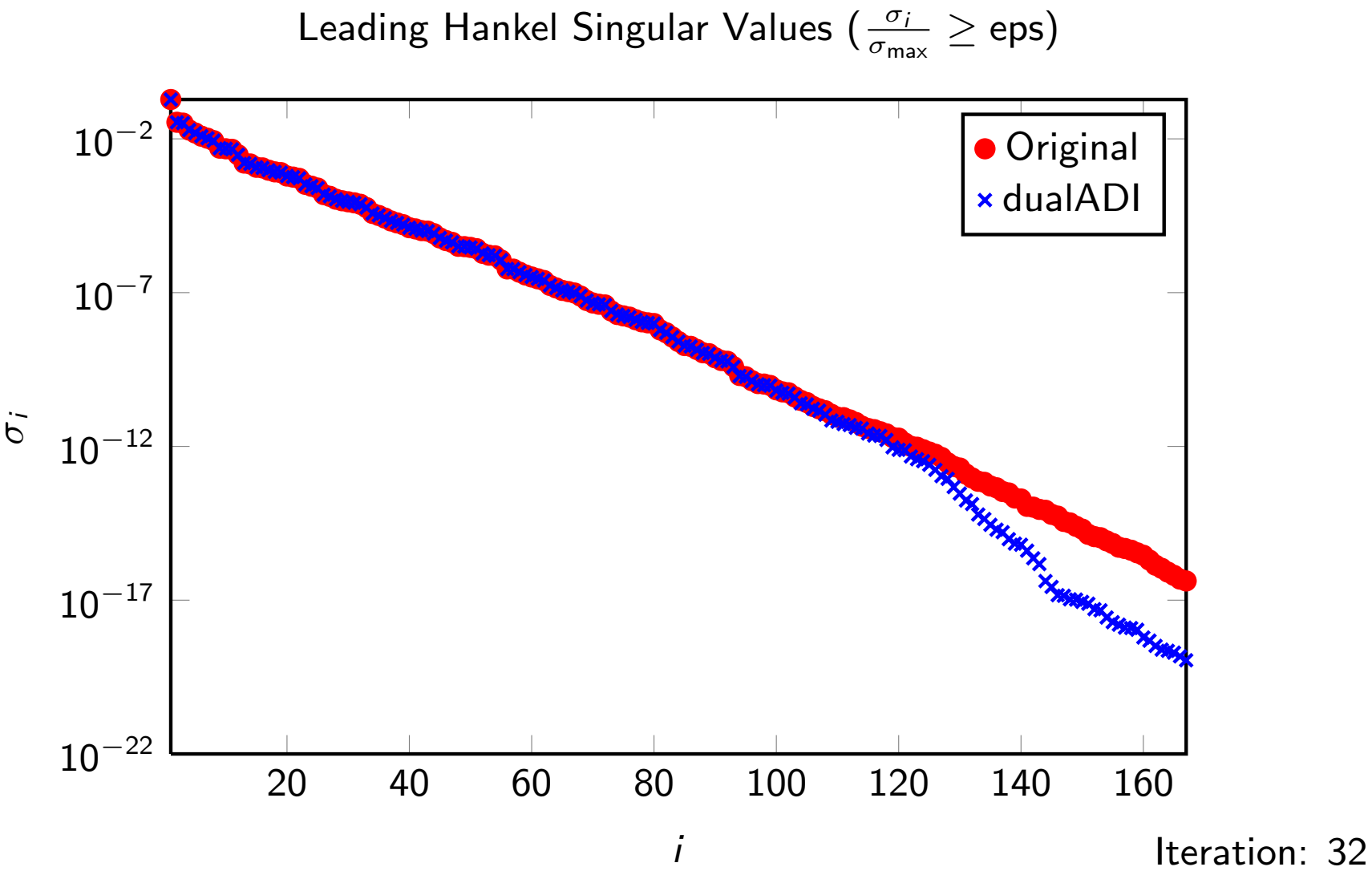

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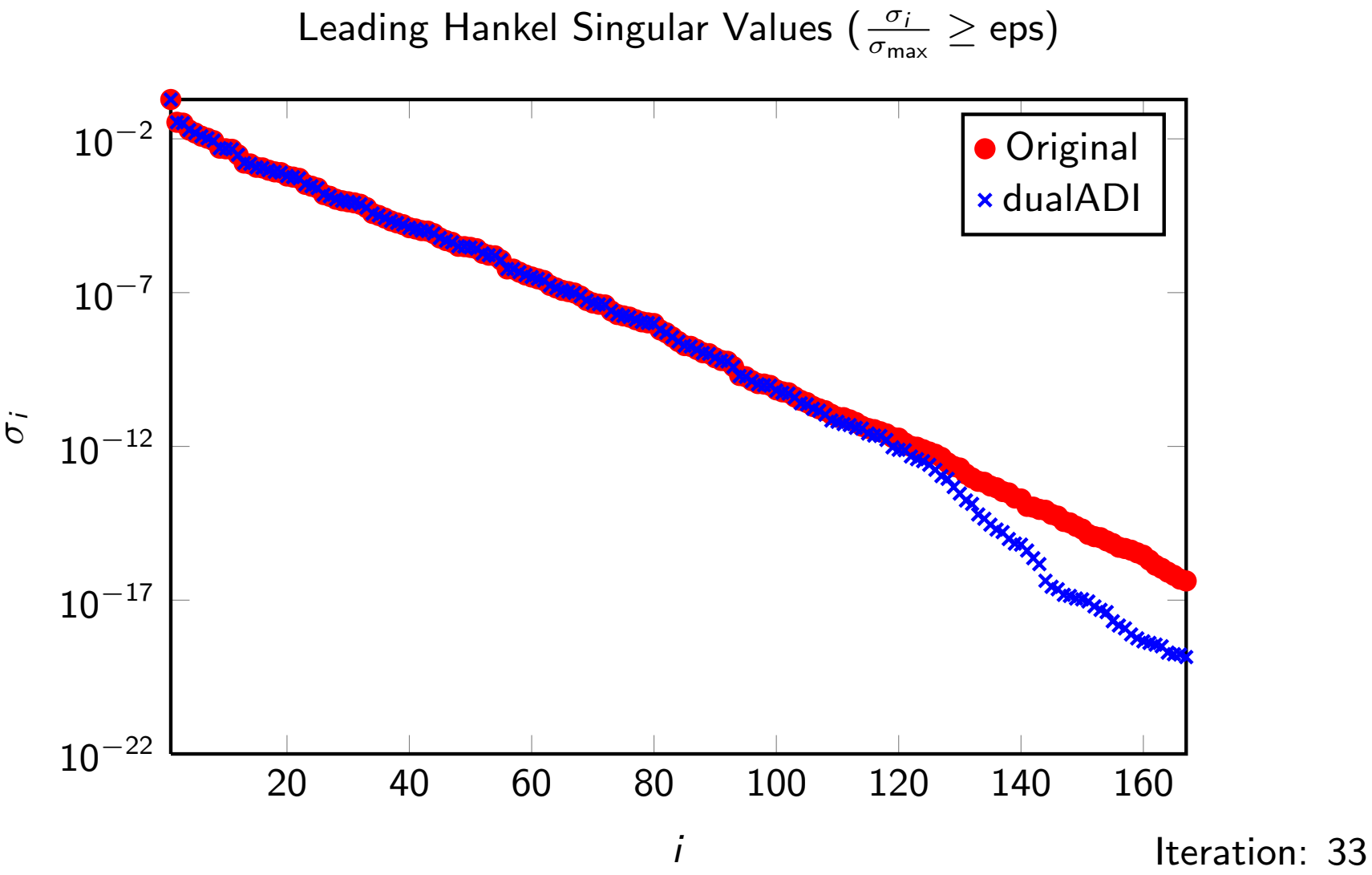

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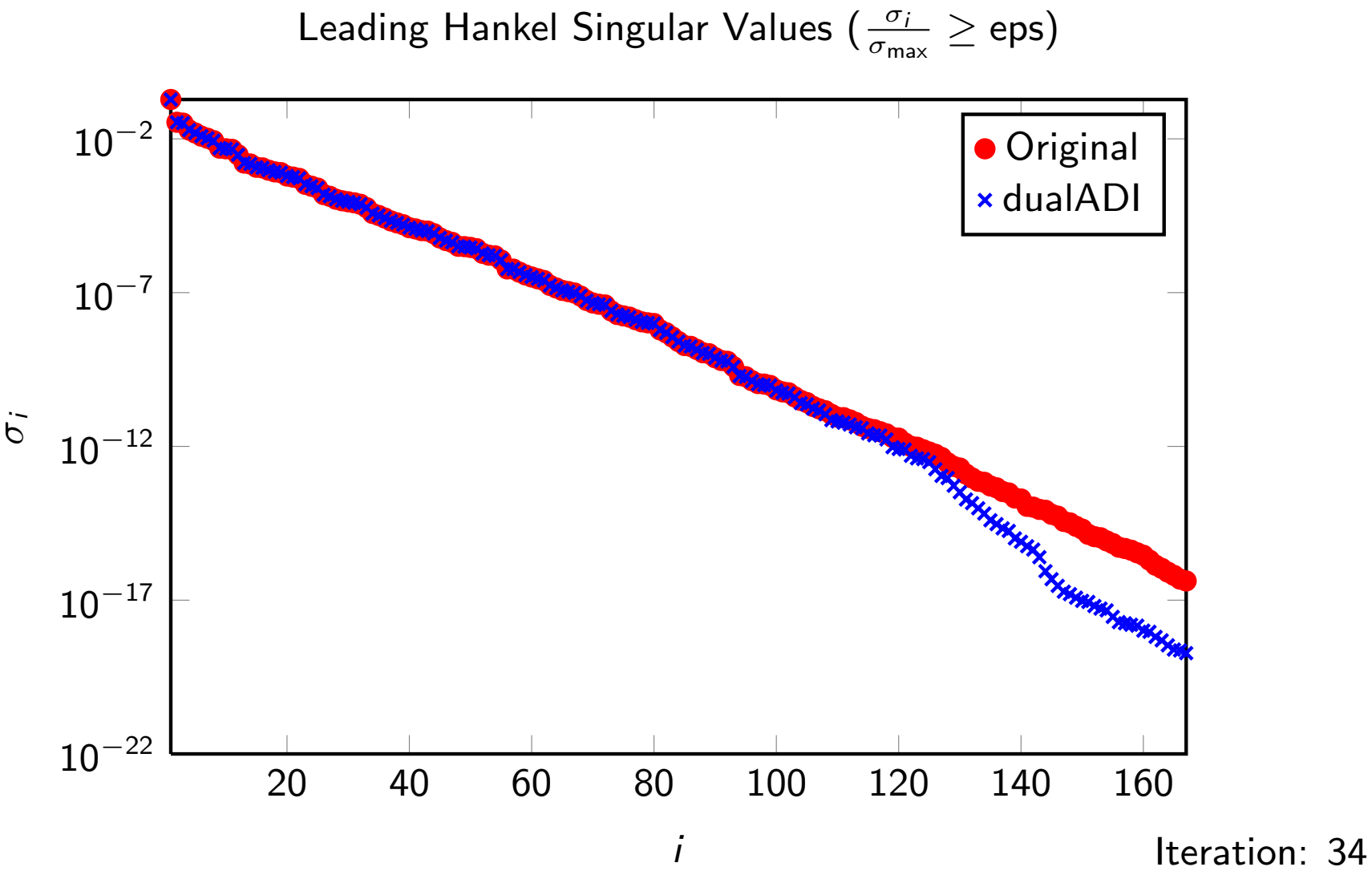

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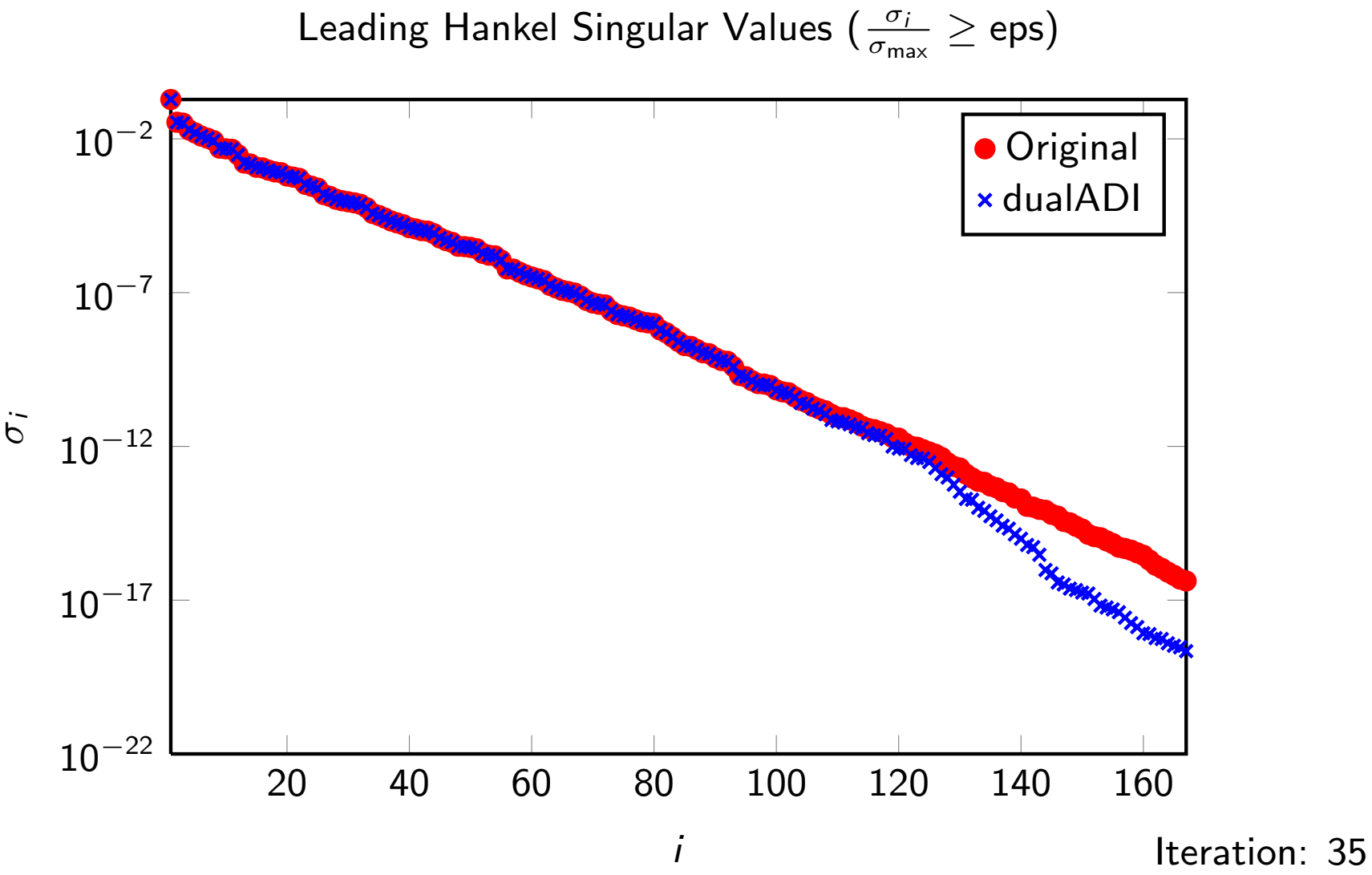

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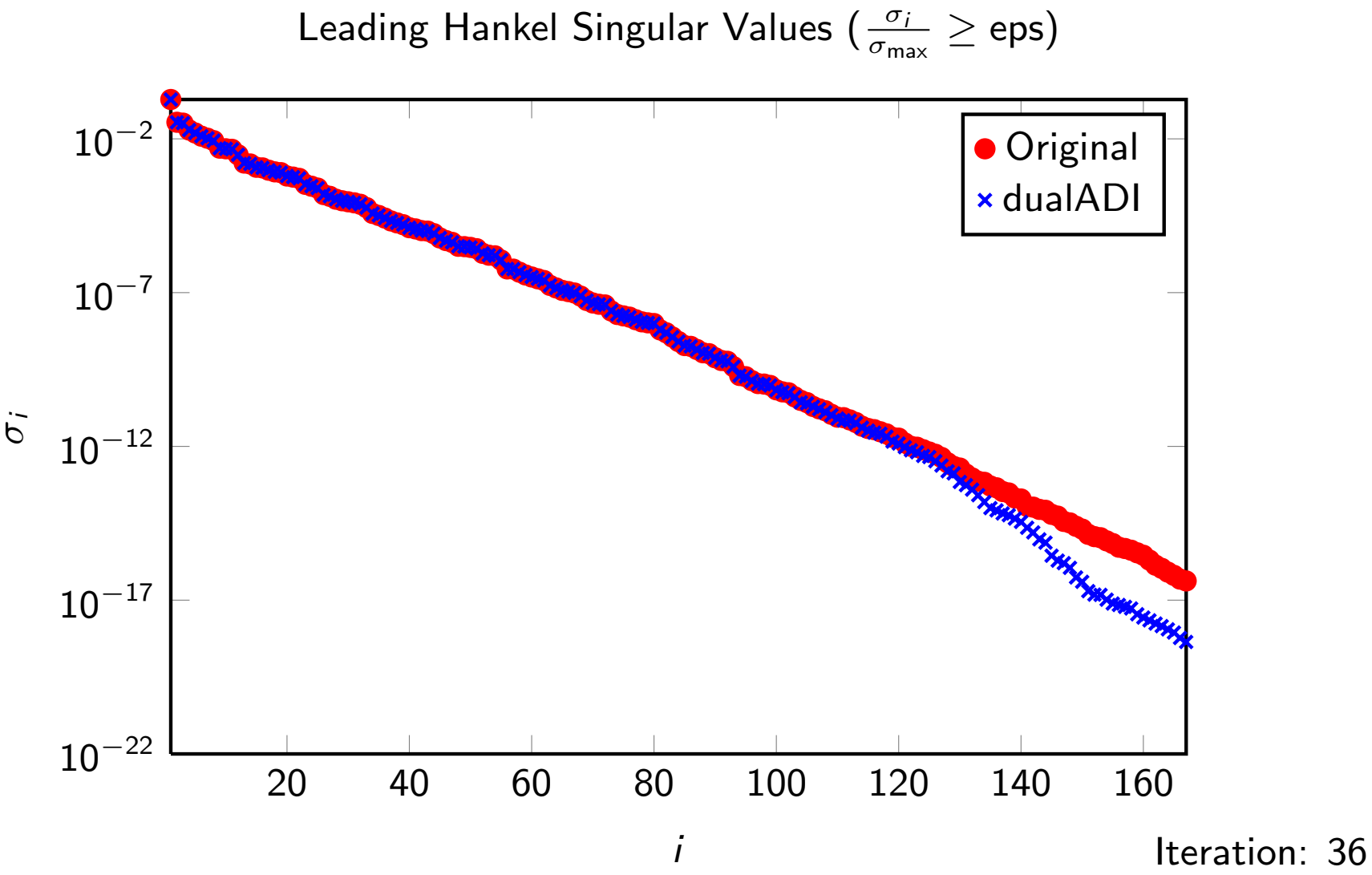

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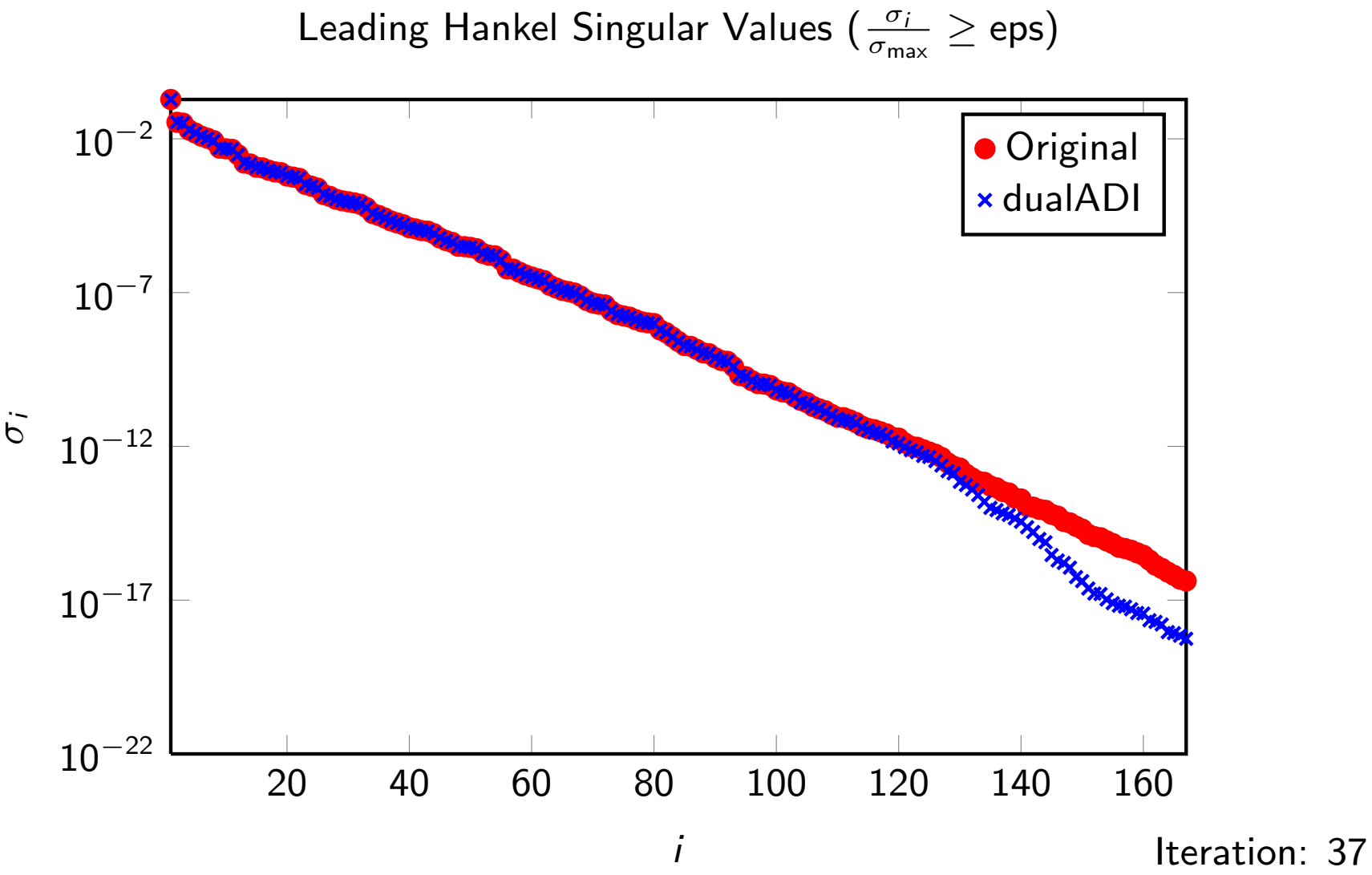

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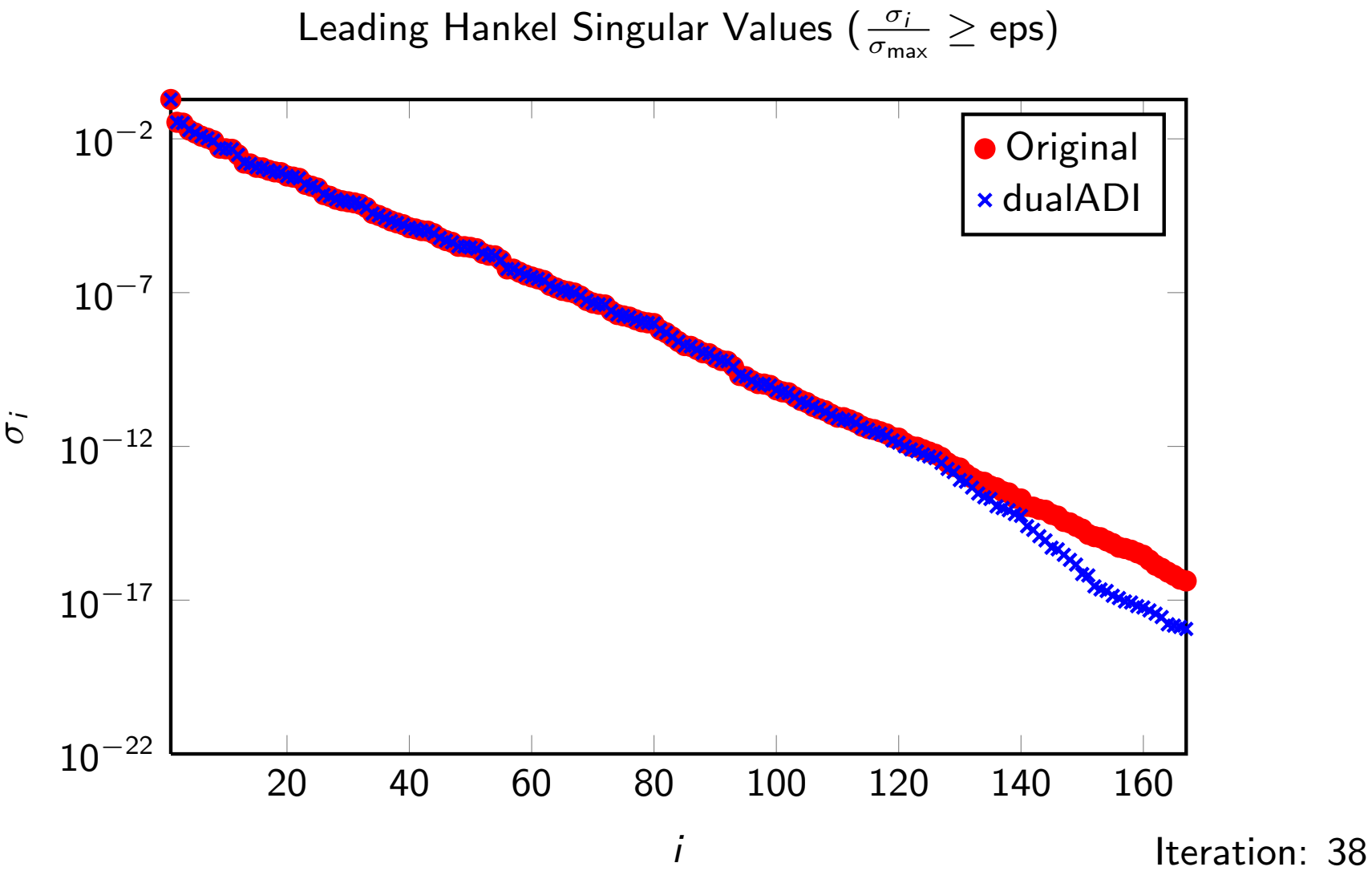

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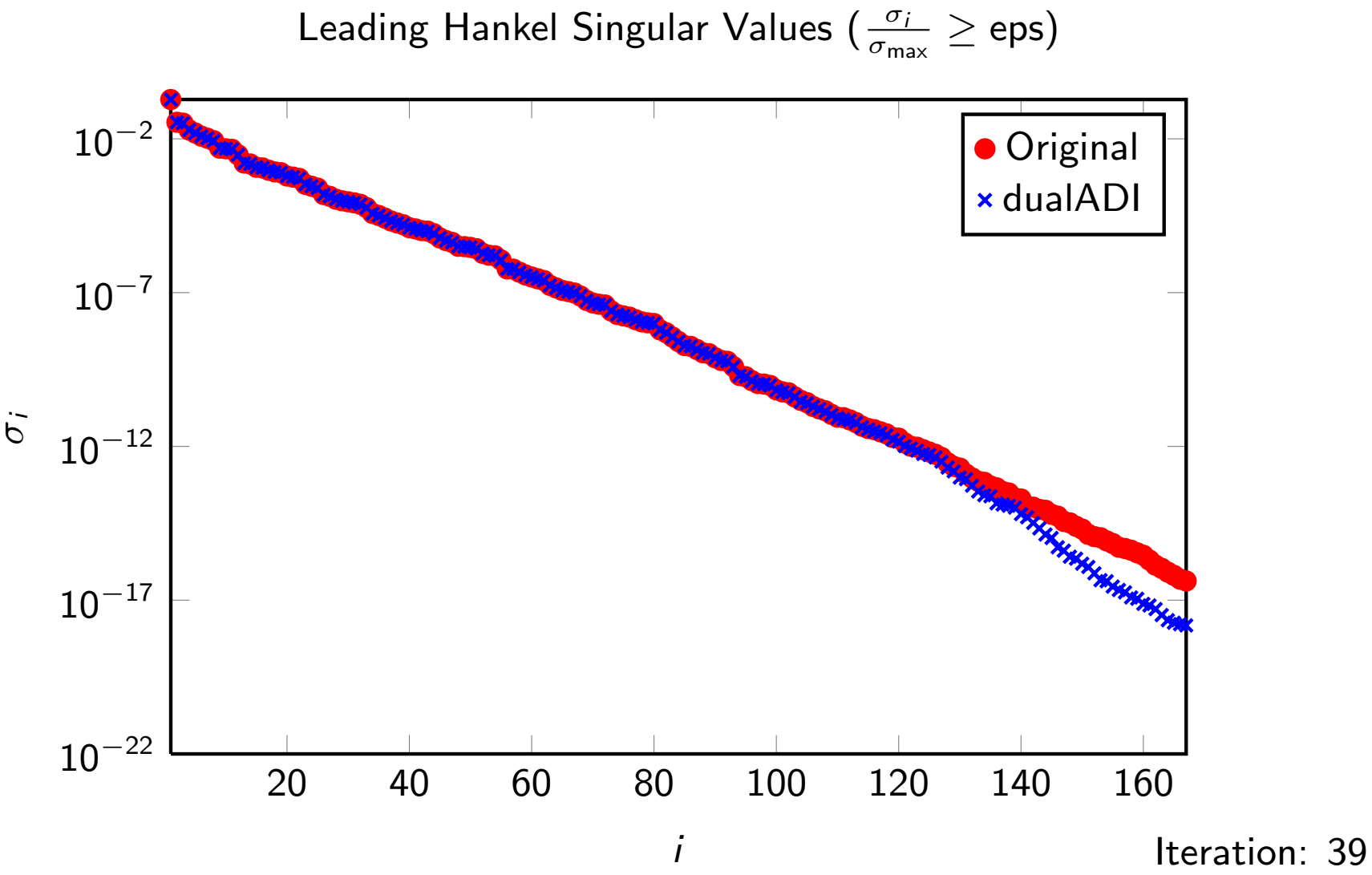
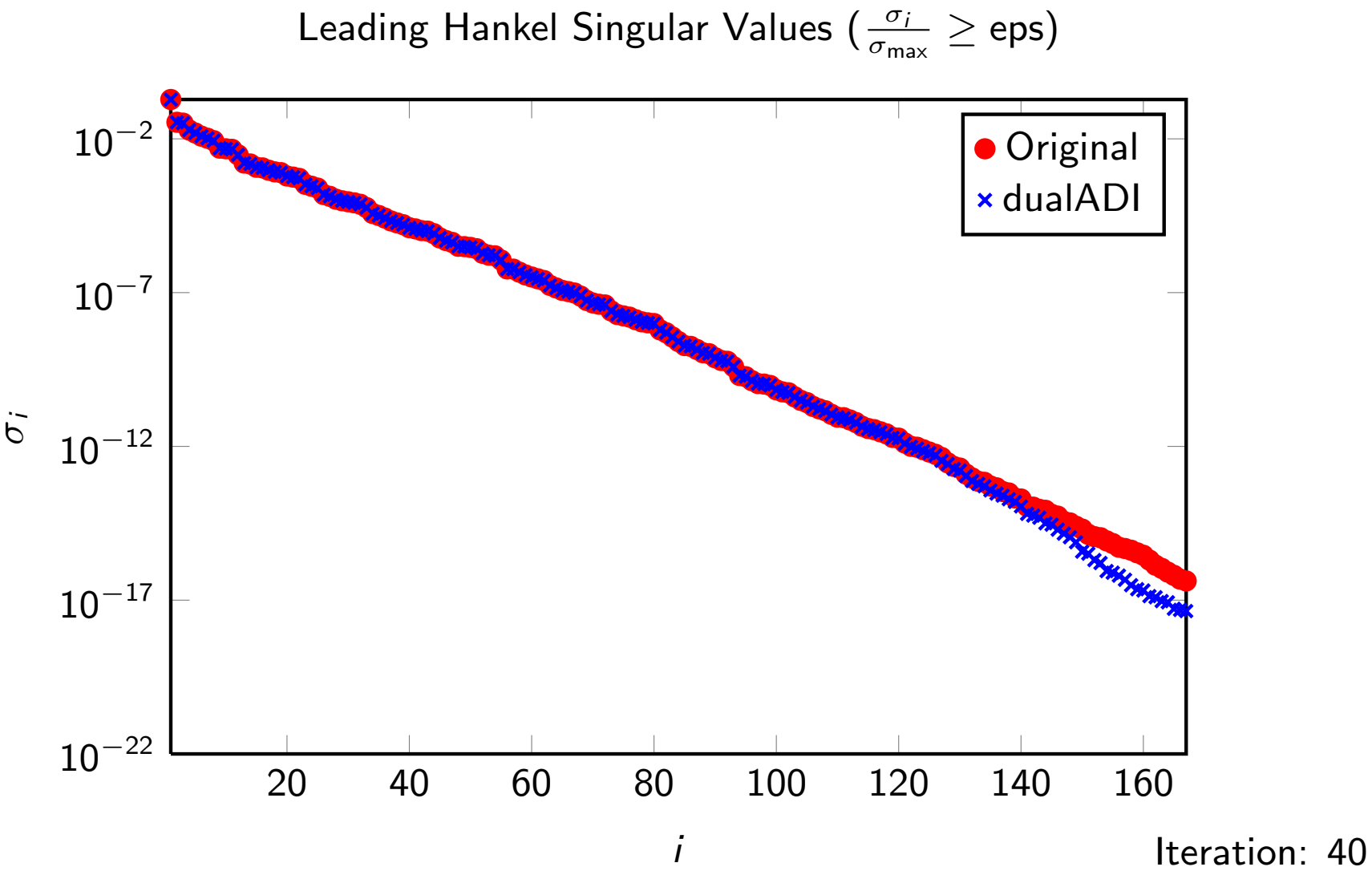


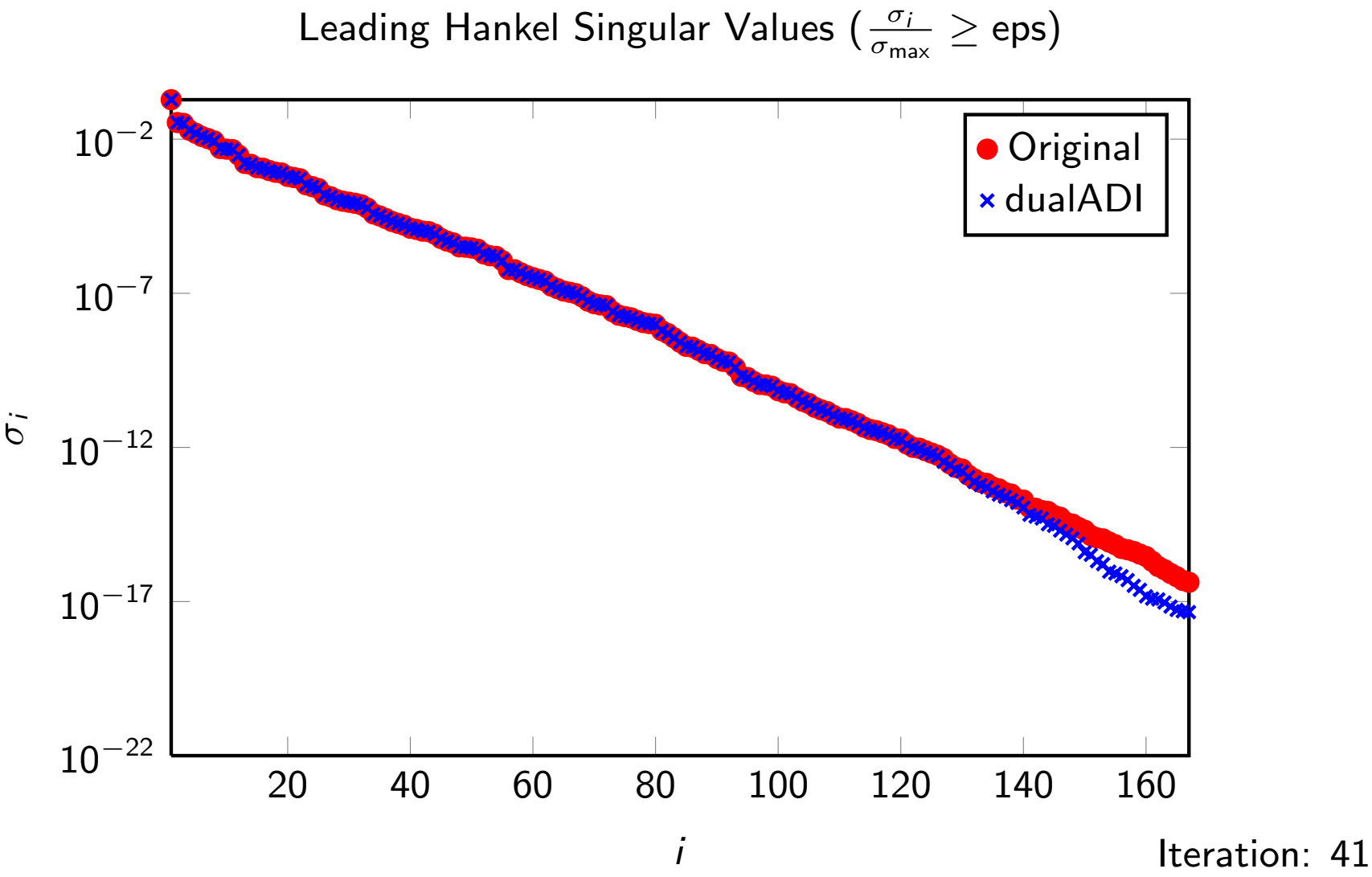
Numerical Results

Rail Model



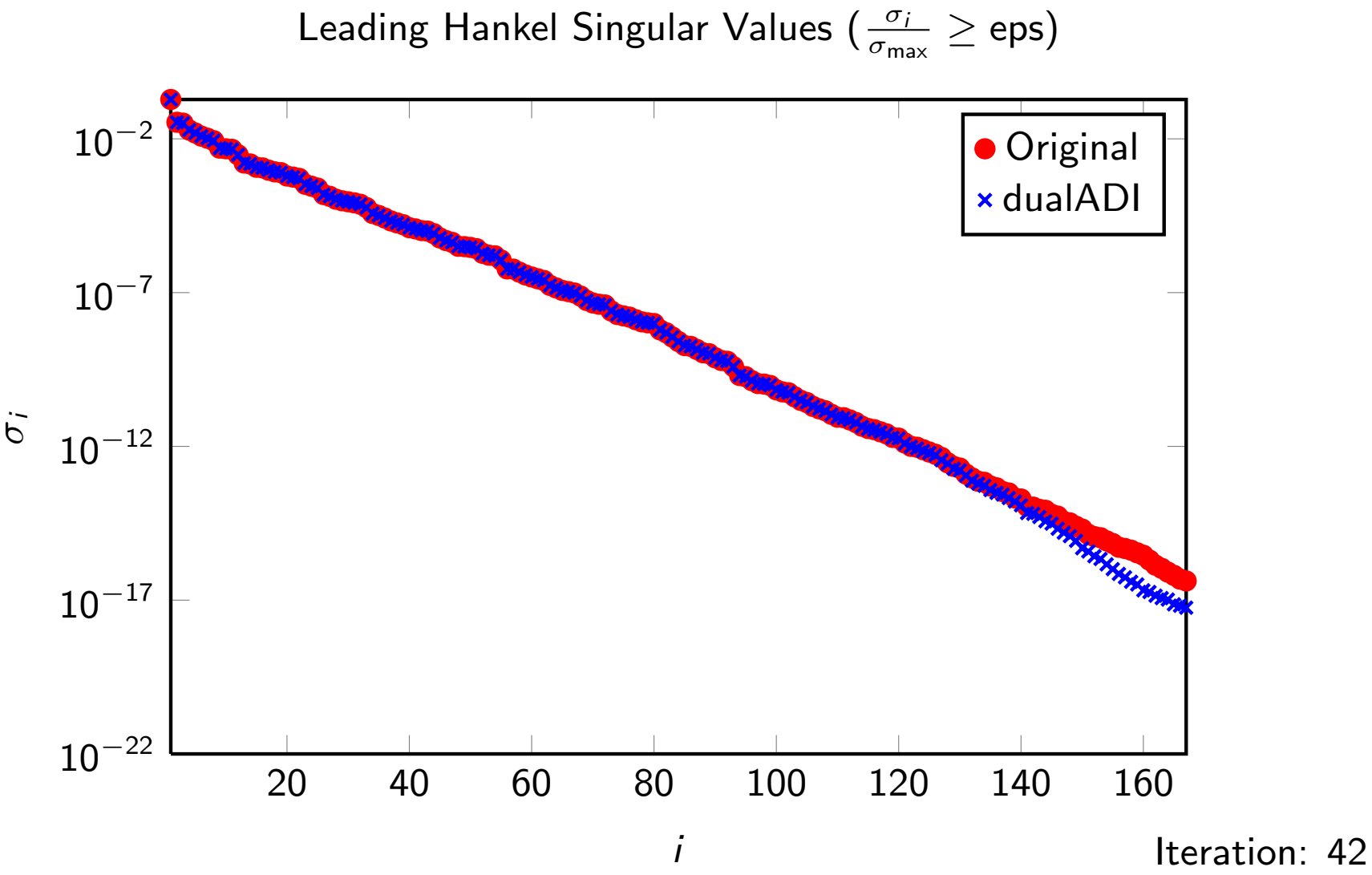
Numerical Results

Rail Model



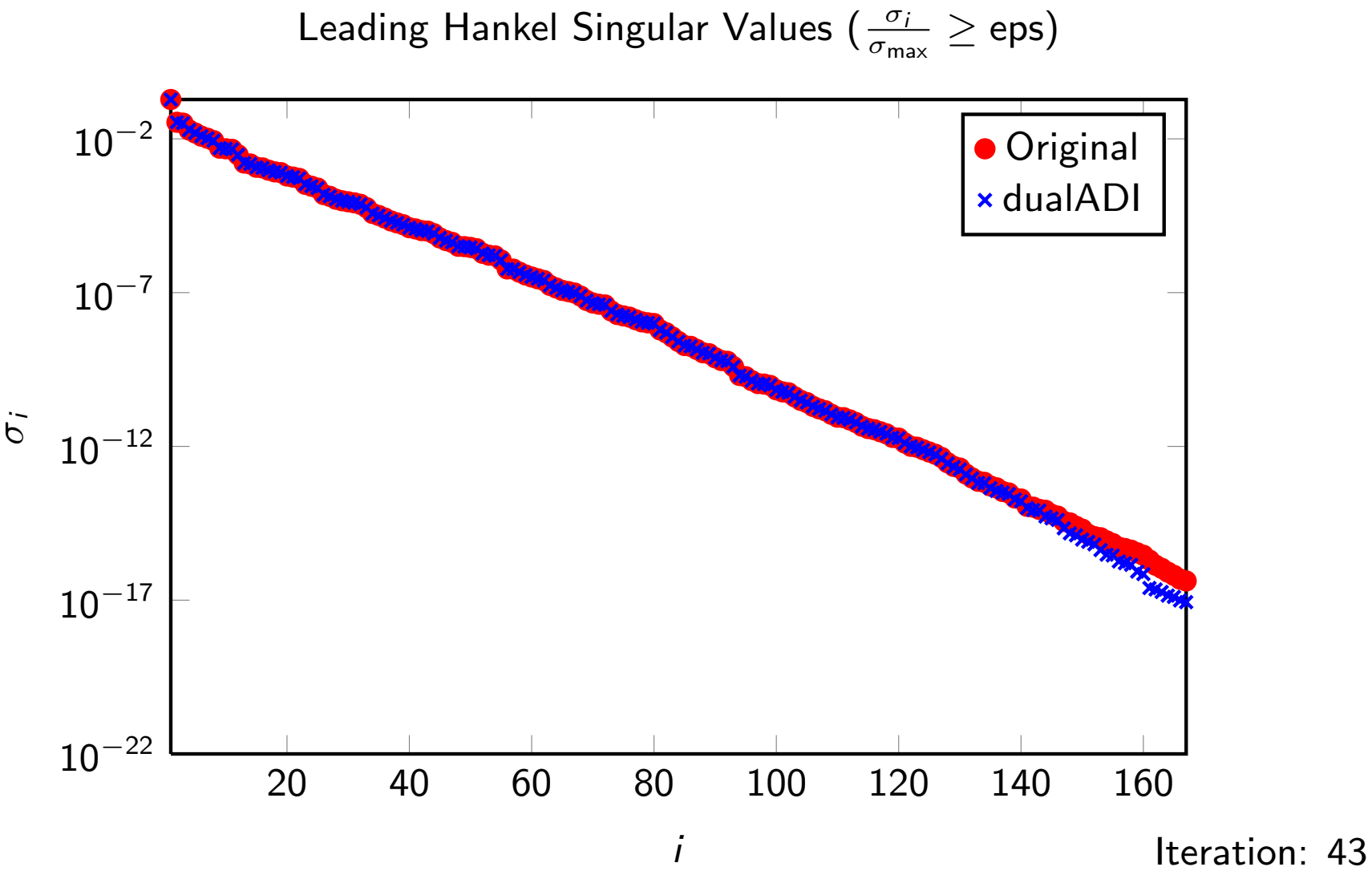
Numerical Results

Rail Model



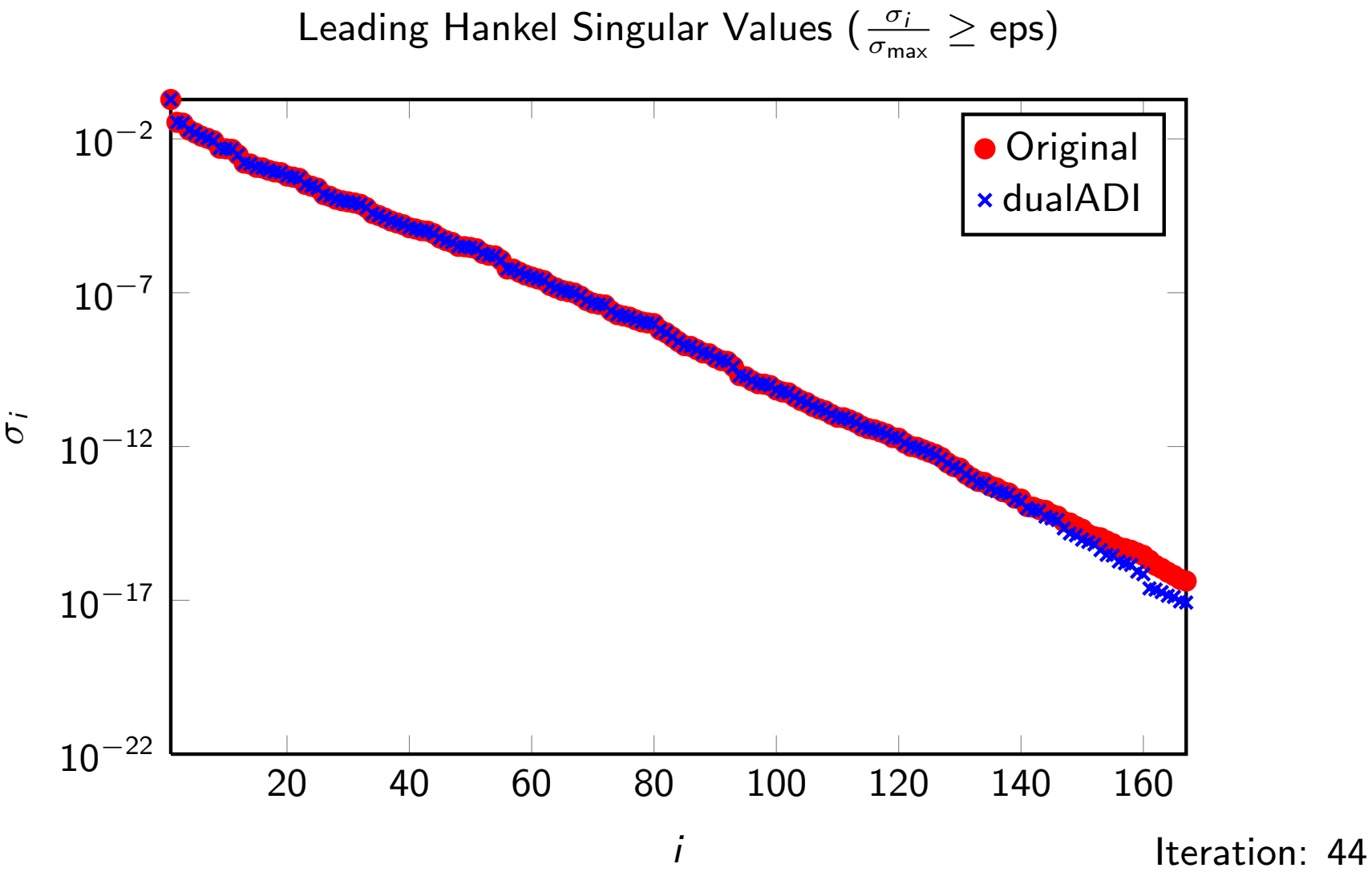
Numerical Results

Rail Model



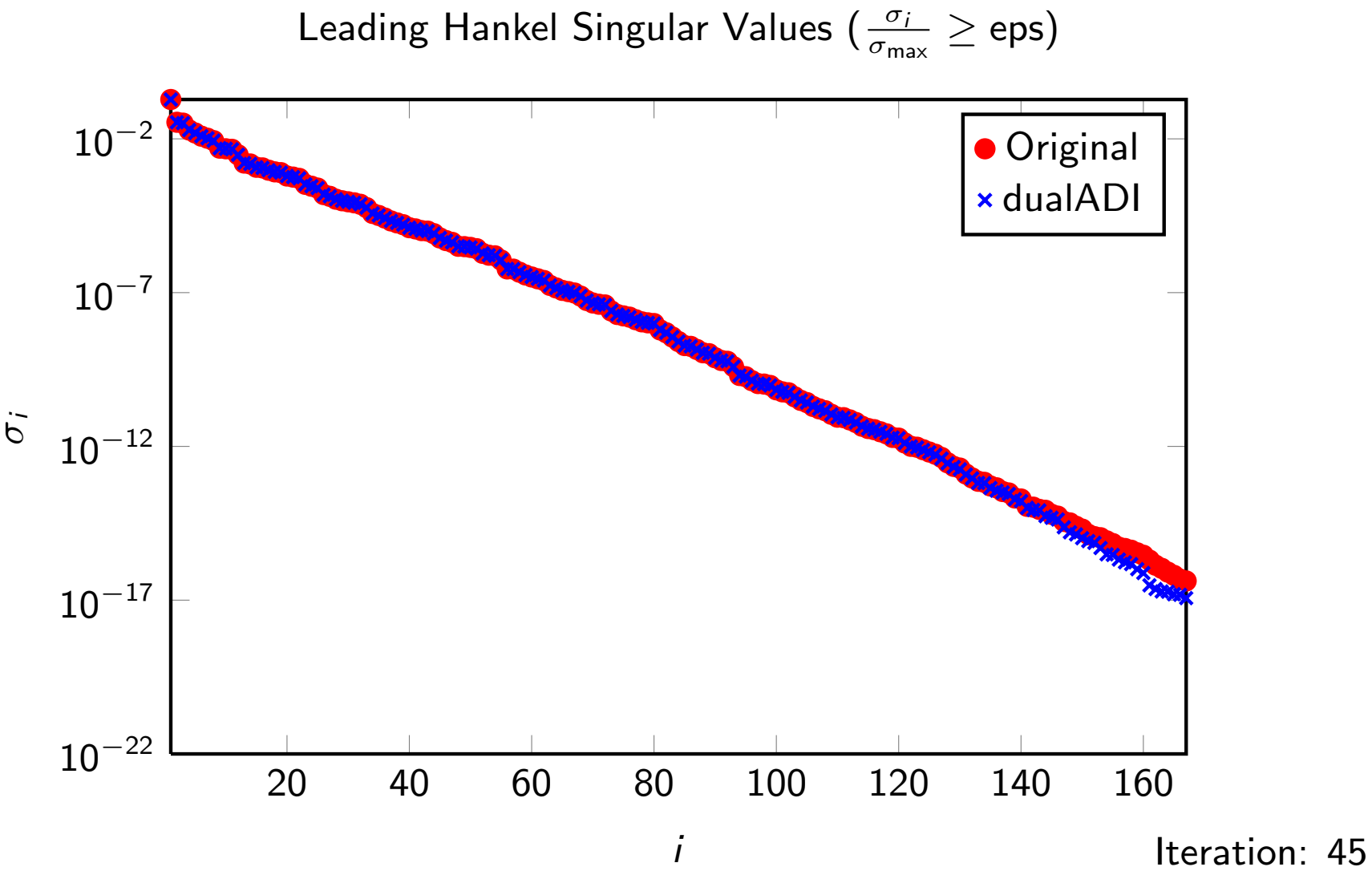
Numerical Results

Rail Model



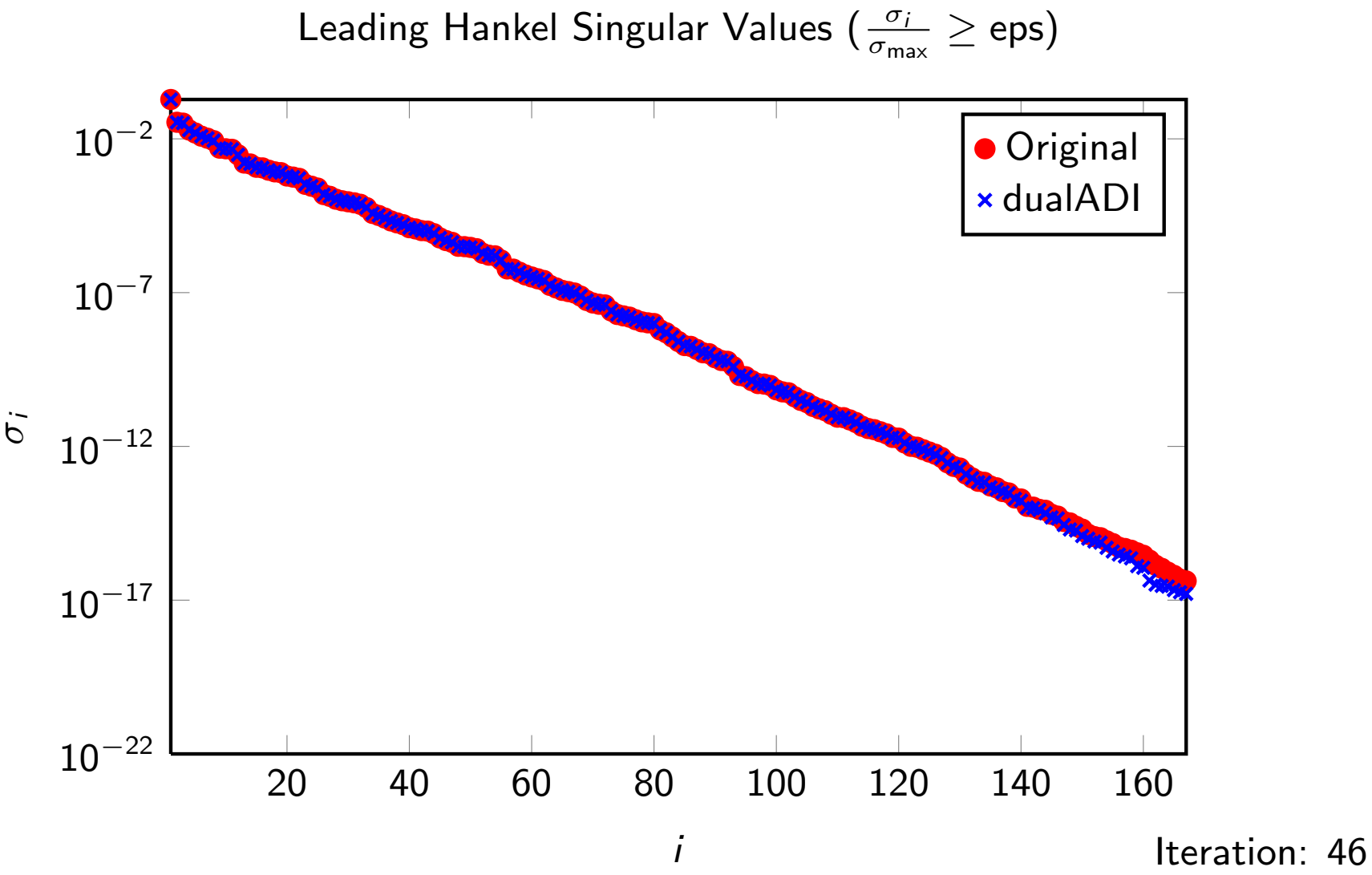
Numerical Results

Rail Model



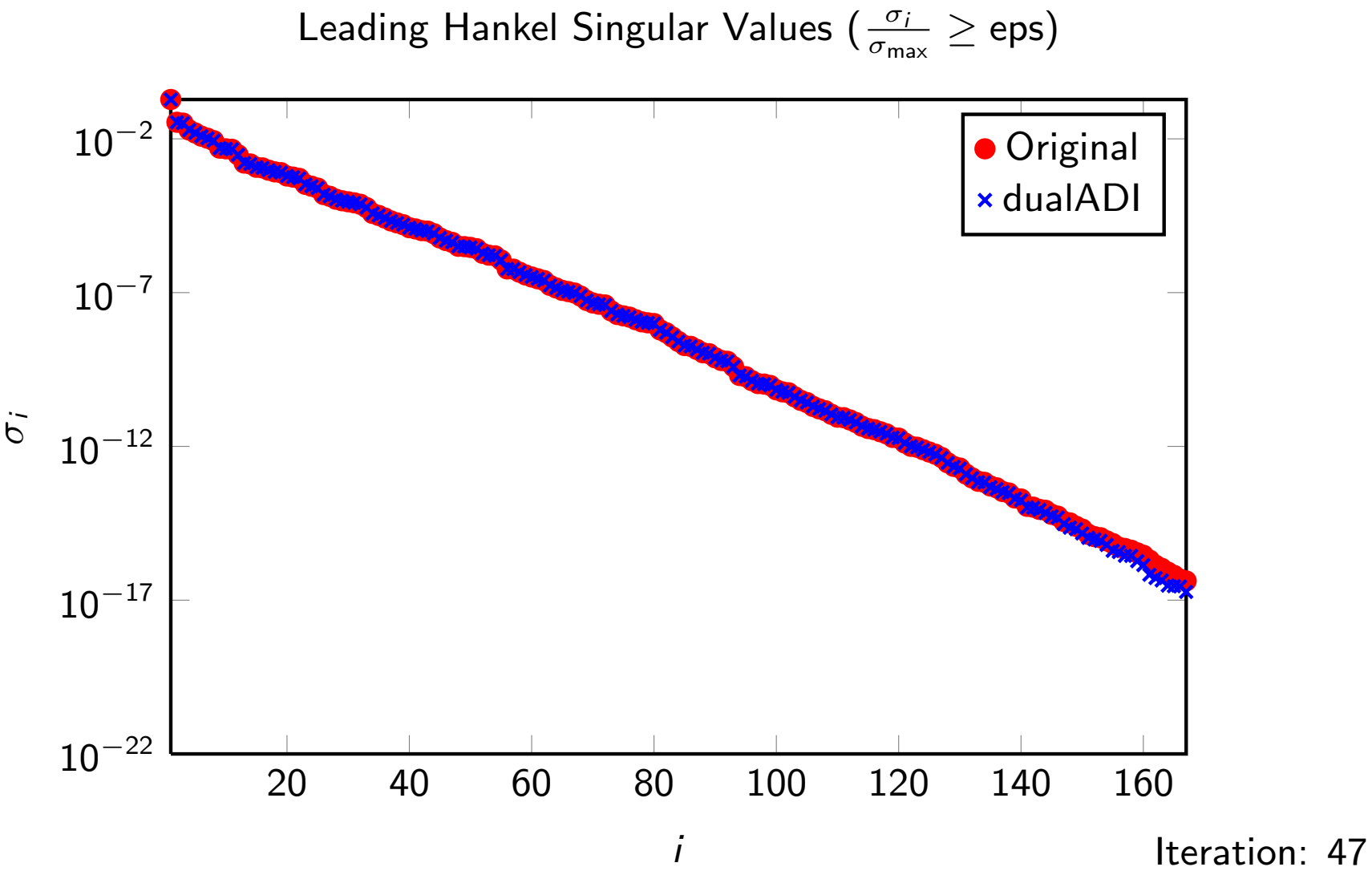
Numerical Results

Rail Model



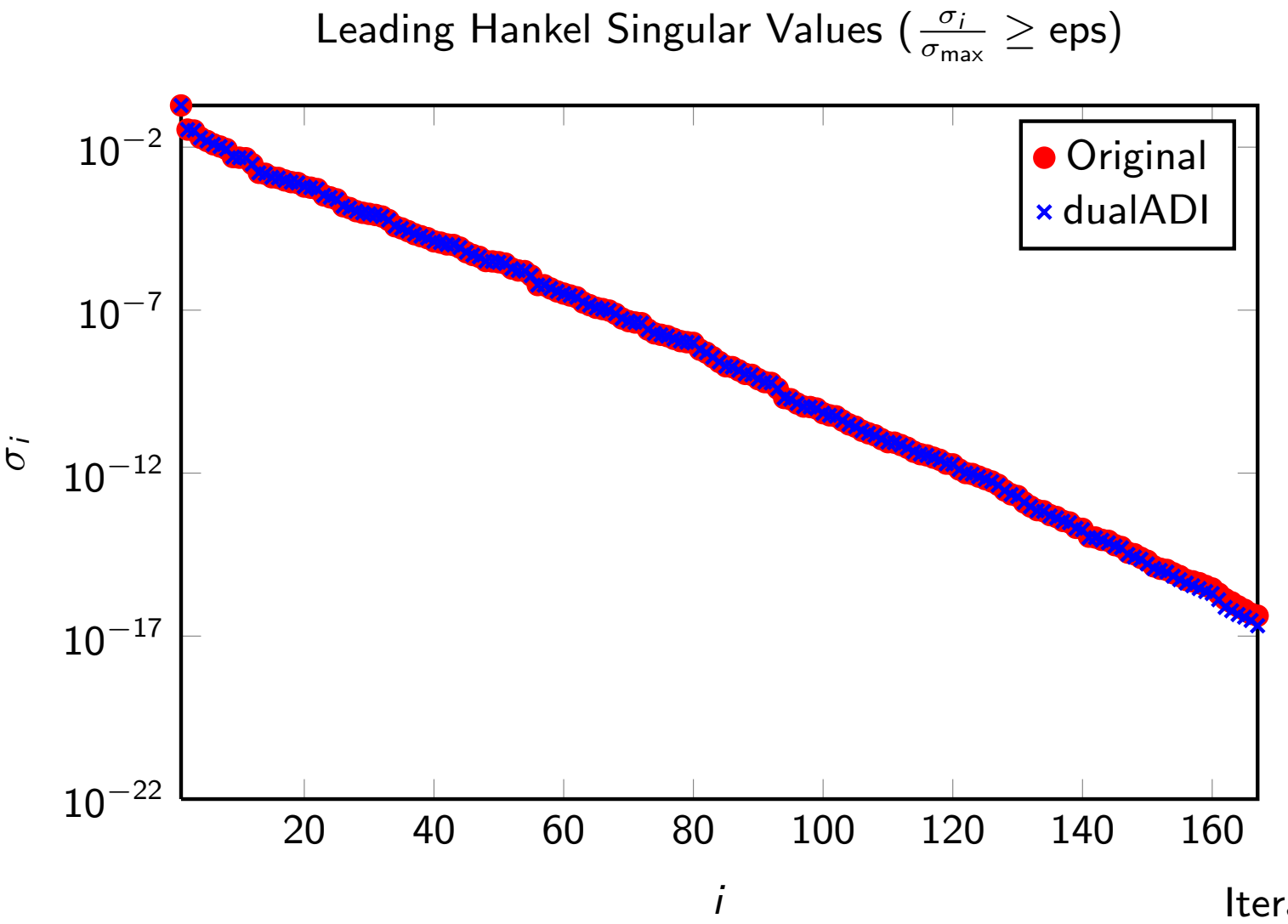
Numerical Results

Rail Model



Numerical Results

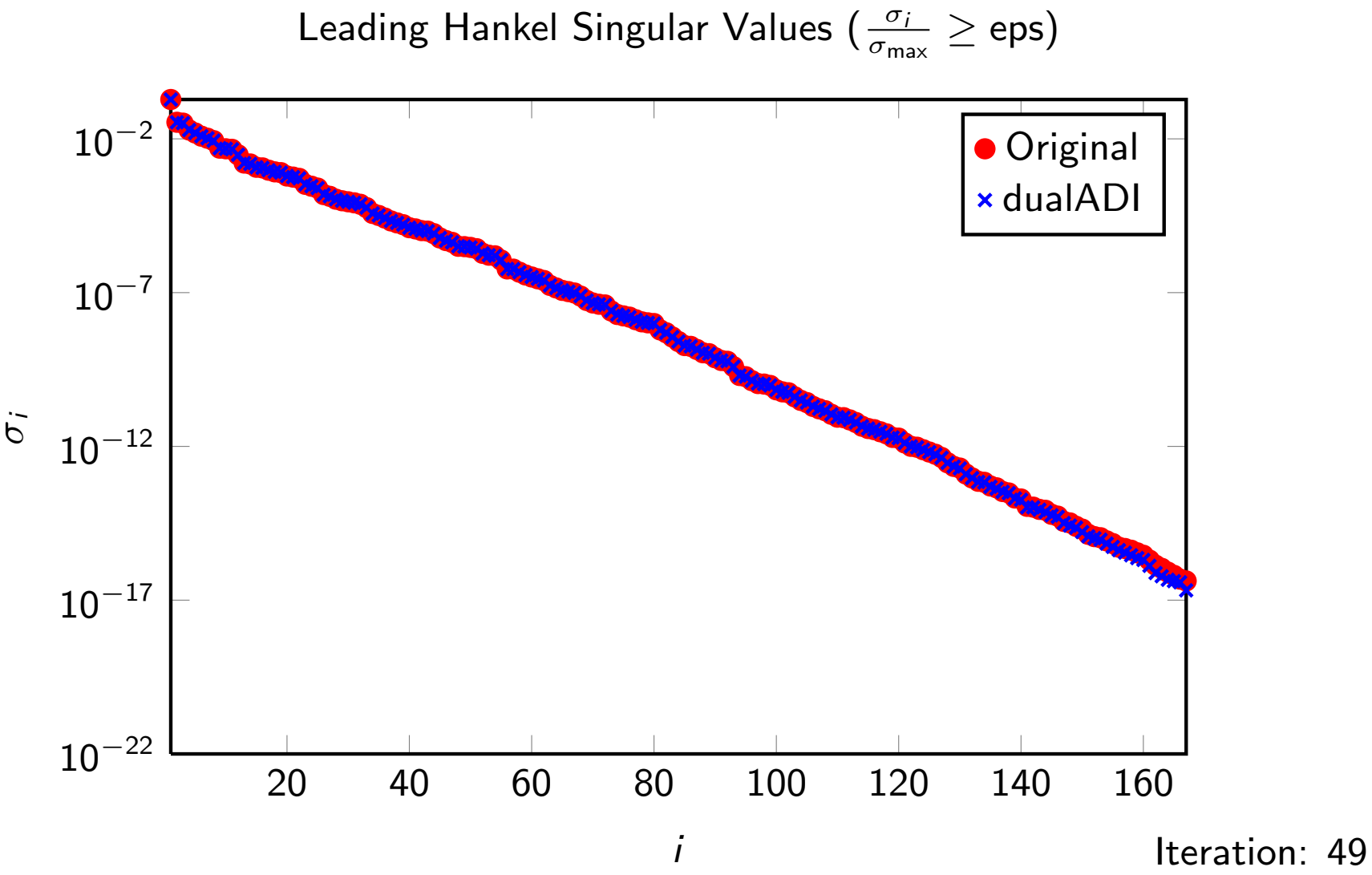
Rail Model



Iteration: 48

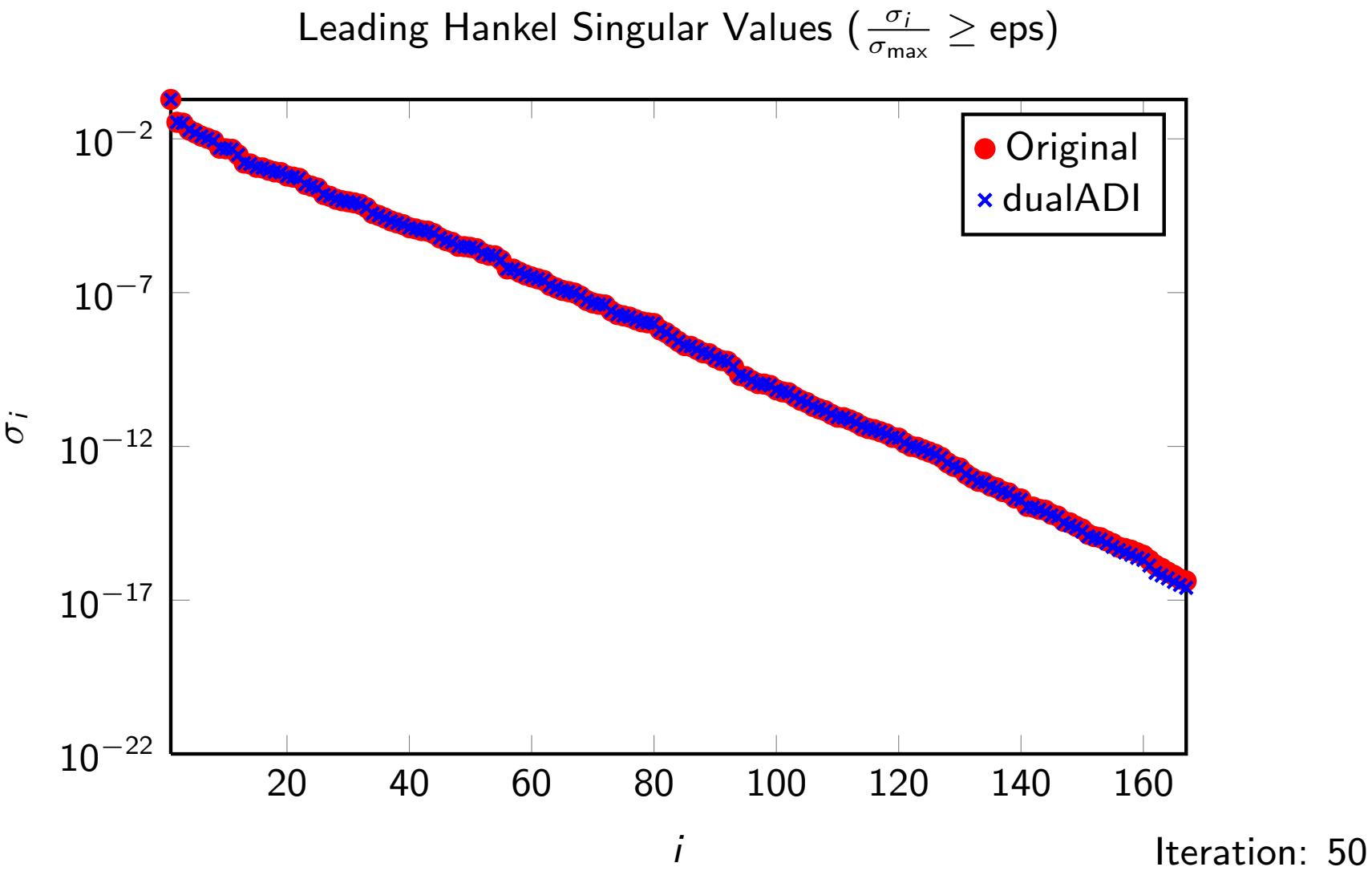
Numerical Results

Rail Model



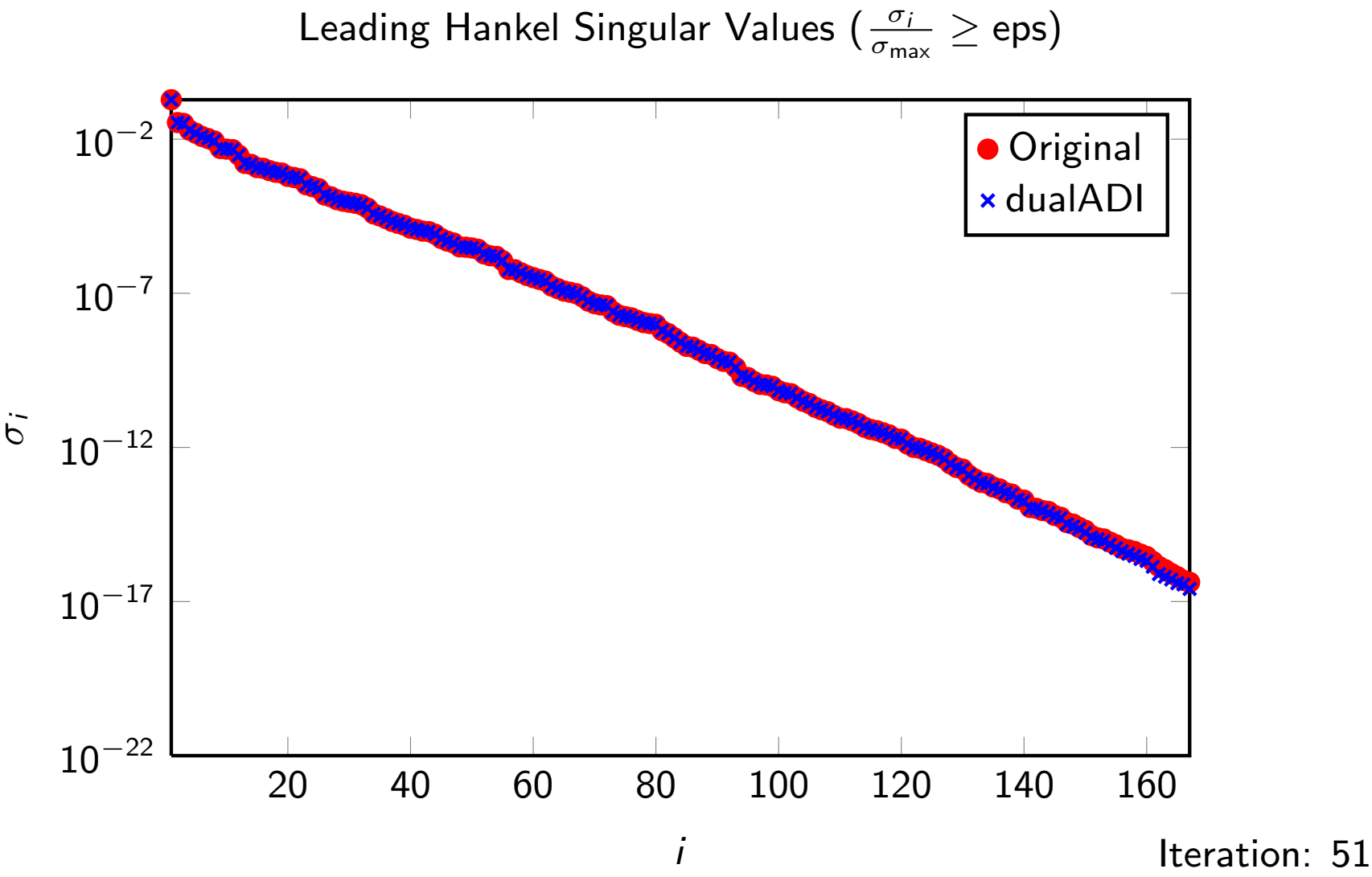
Numerical Results

Rail Model



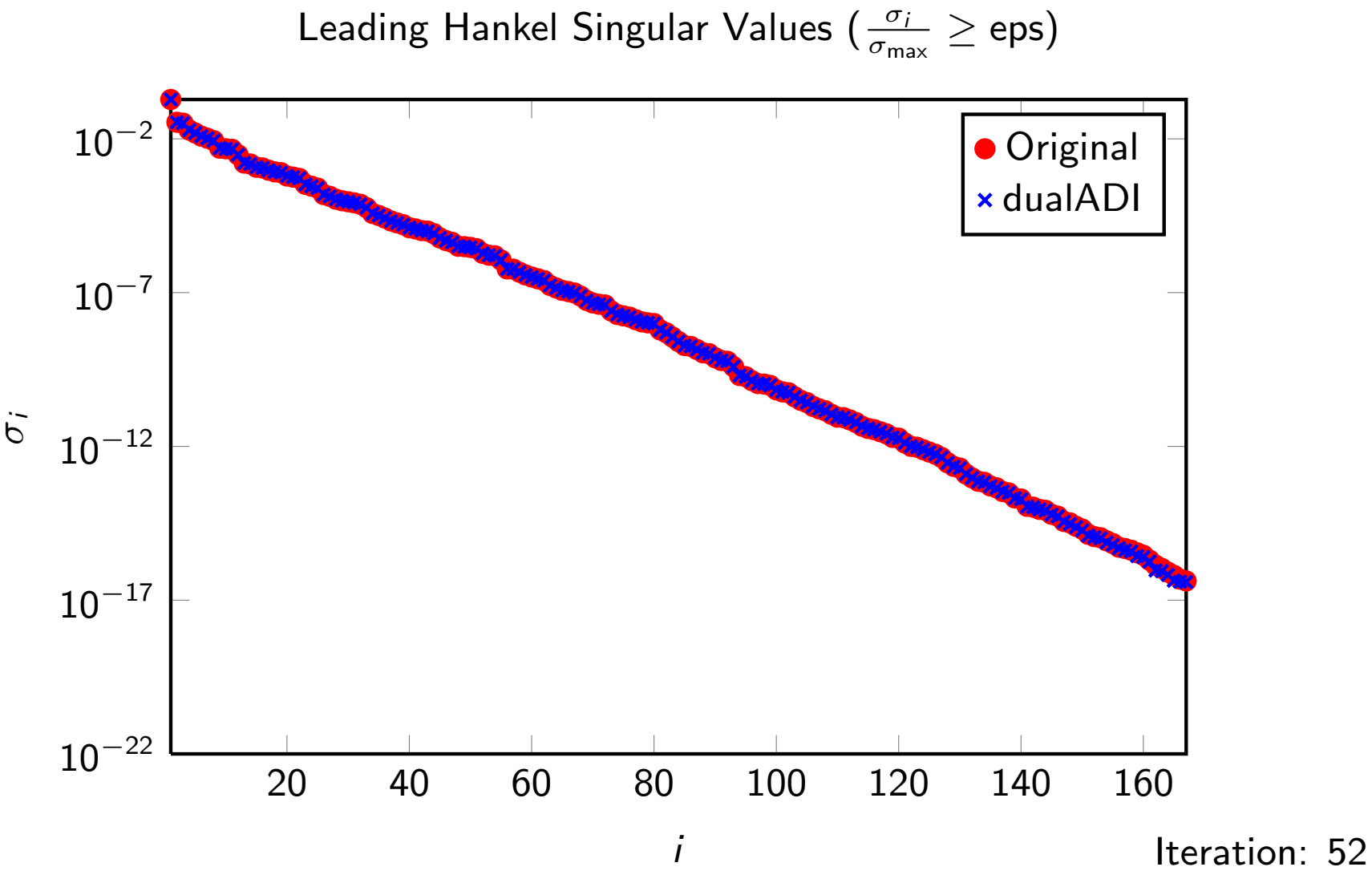
Numerical Results

Rail Model



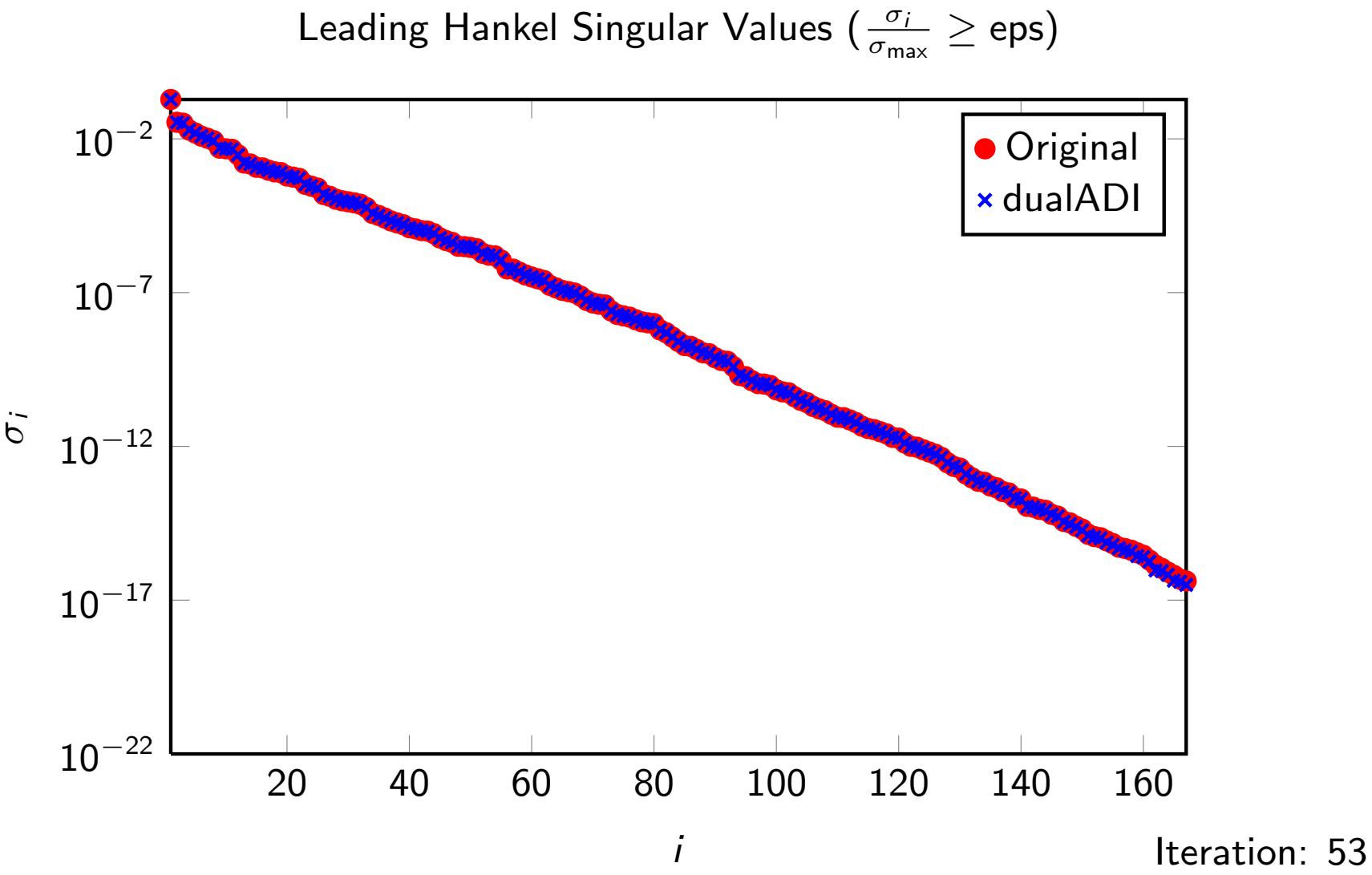
Numerical Results

Rail Model



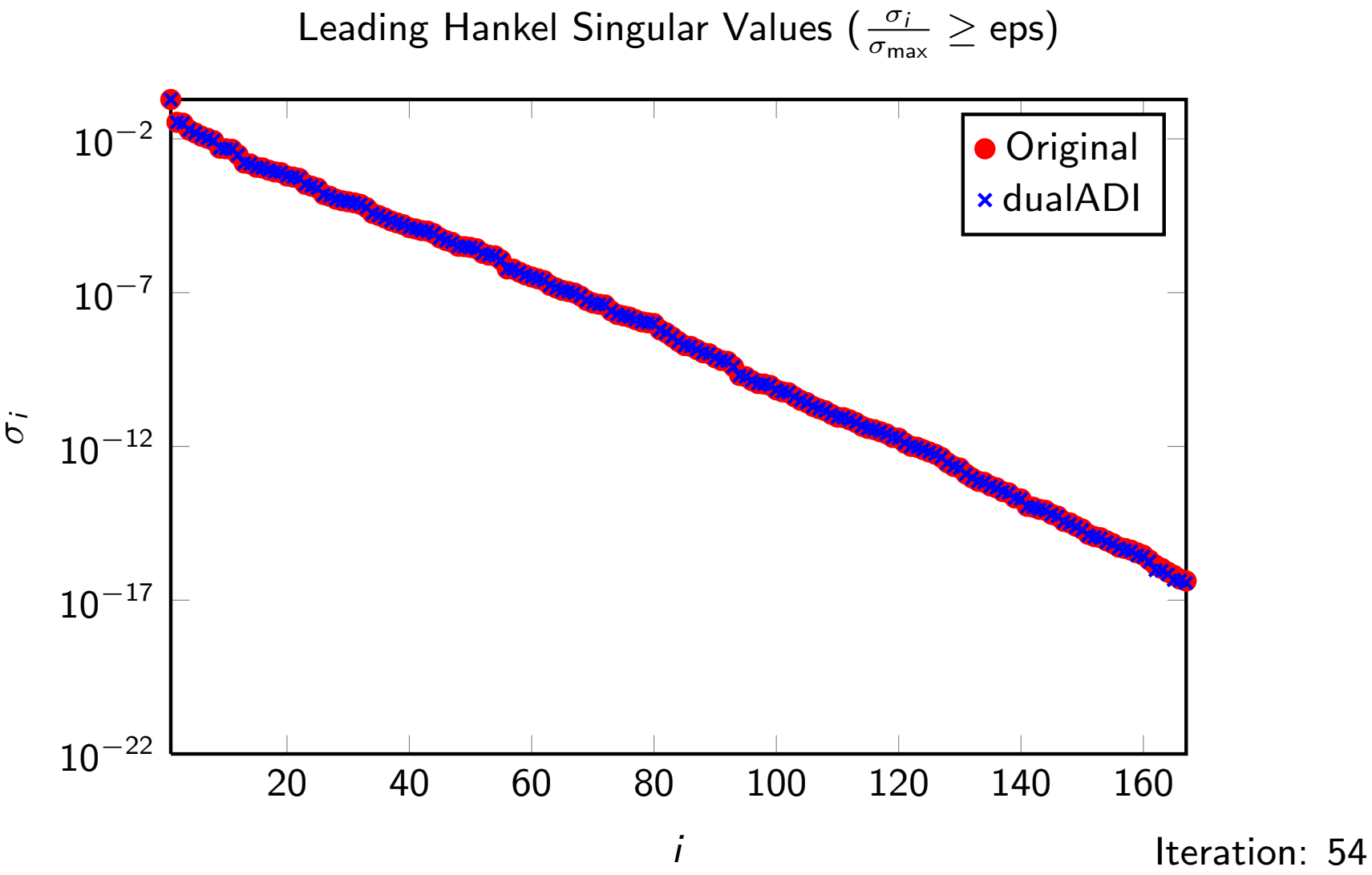
Numerical Results

Rail Model



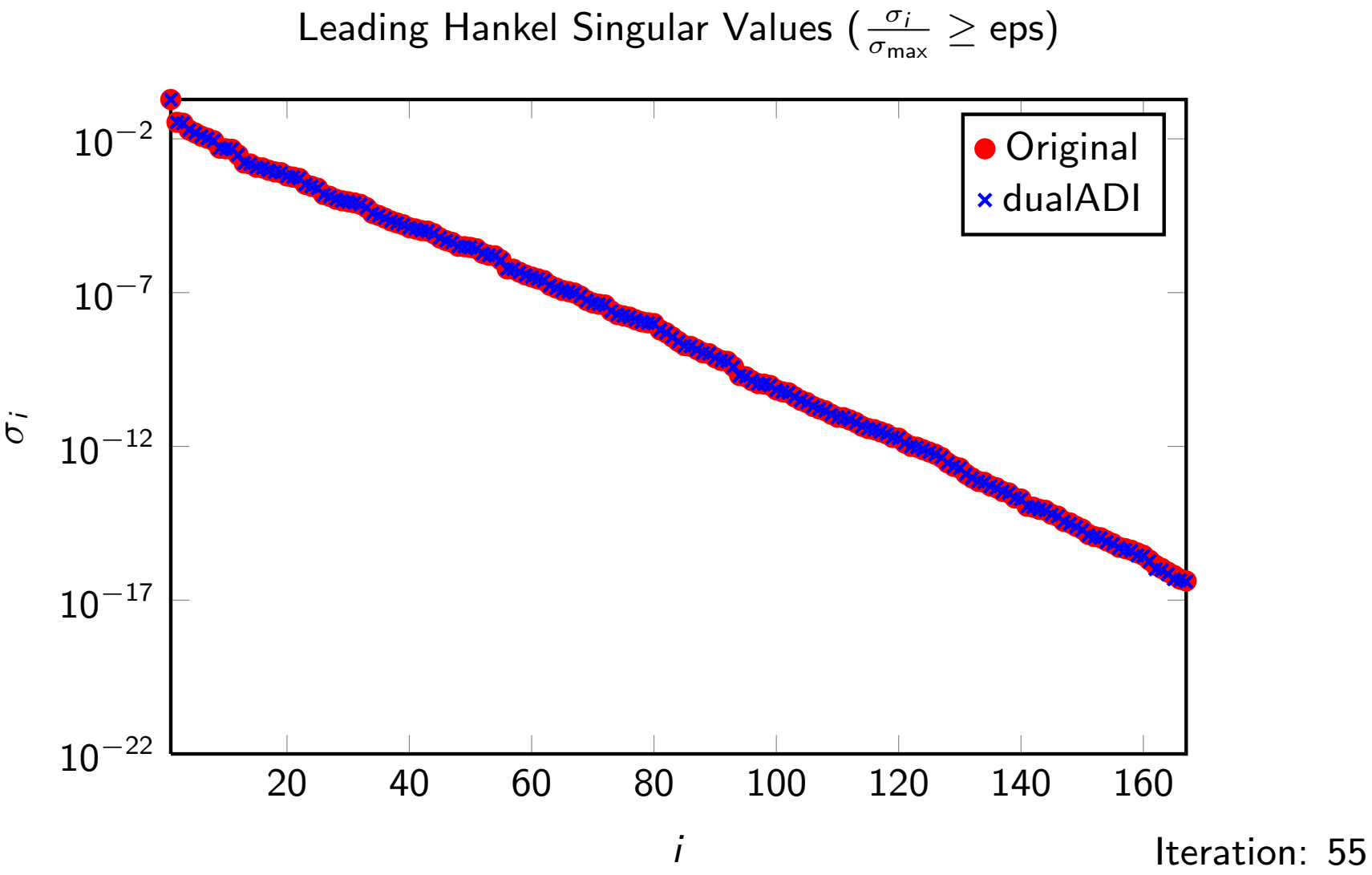
Numerical Results

Rail Model



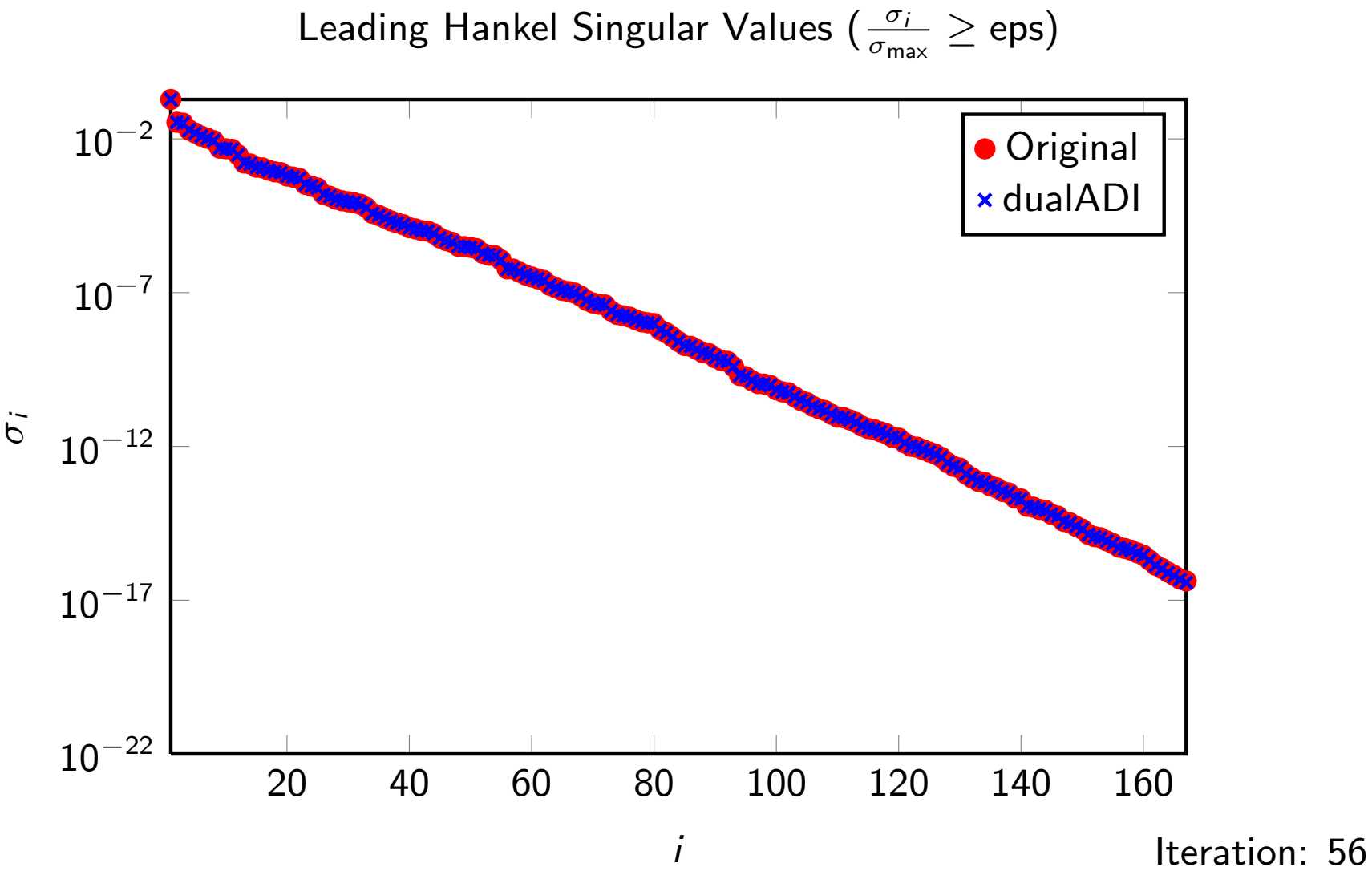
Numerical Results

Rail Model



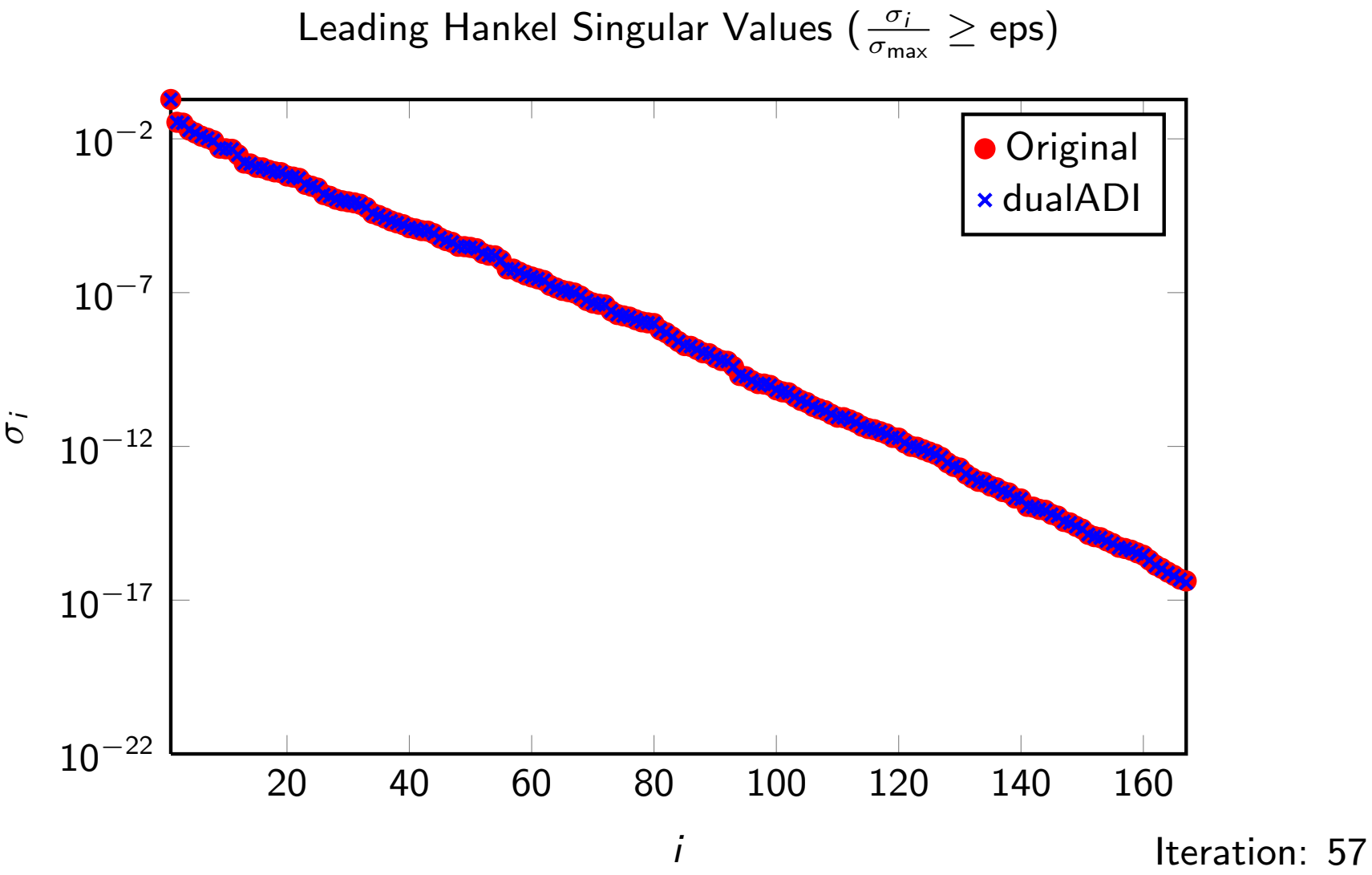
Numerical Results

Rail Model



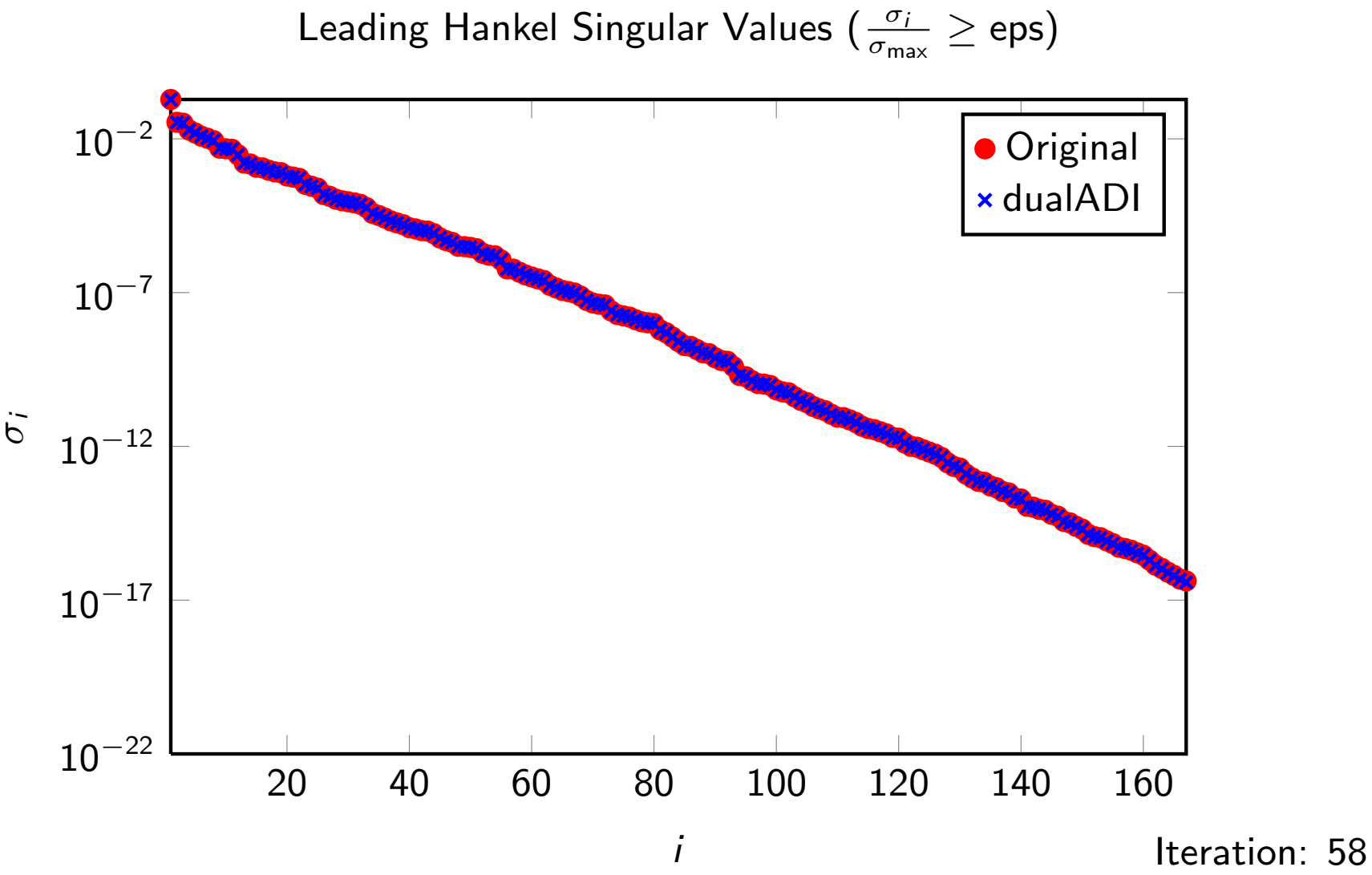
Numerical Results

Rail Model



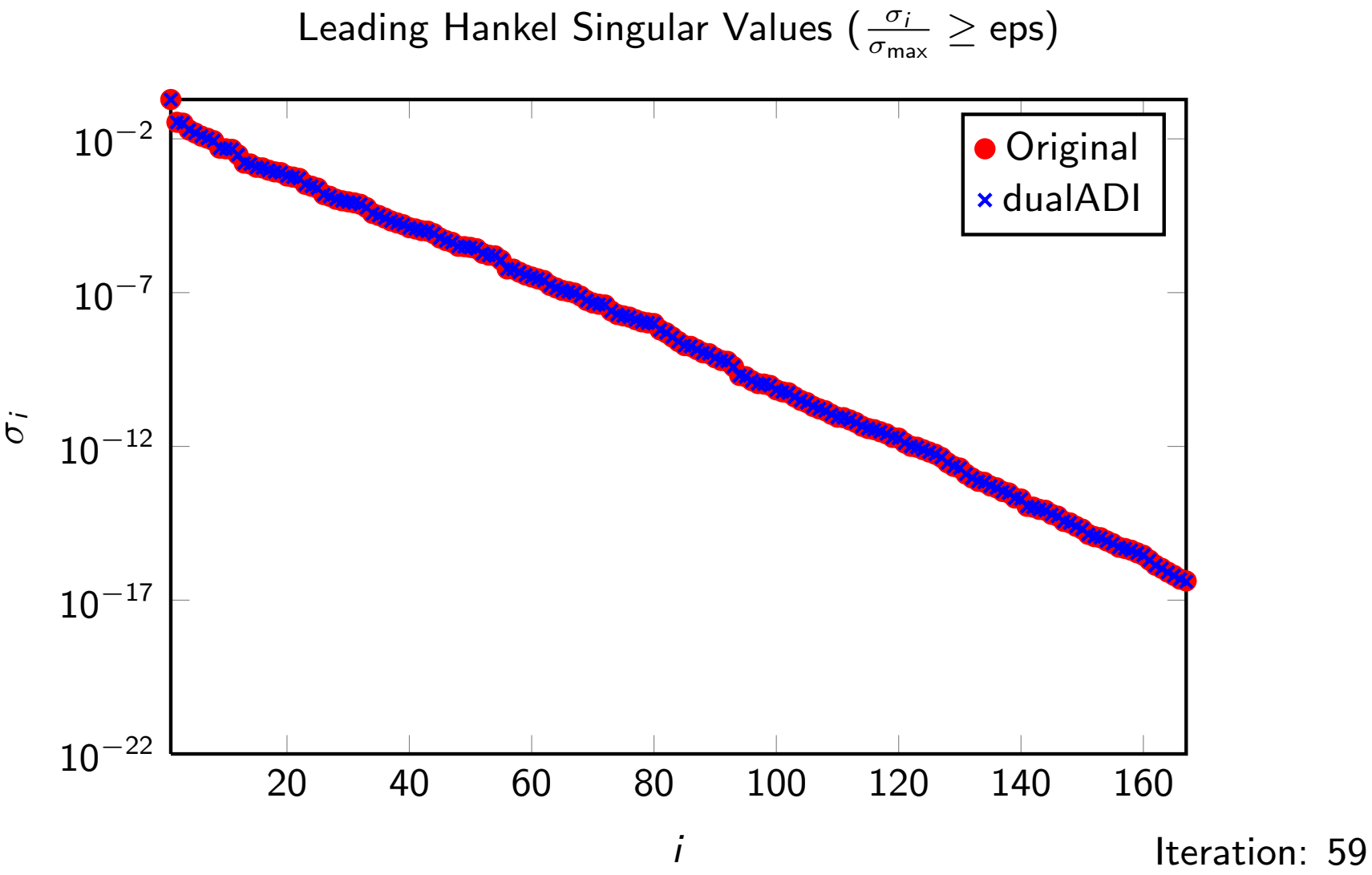
Numerical Results

Rail Model



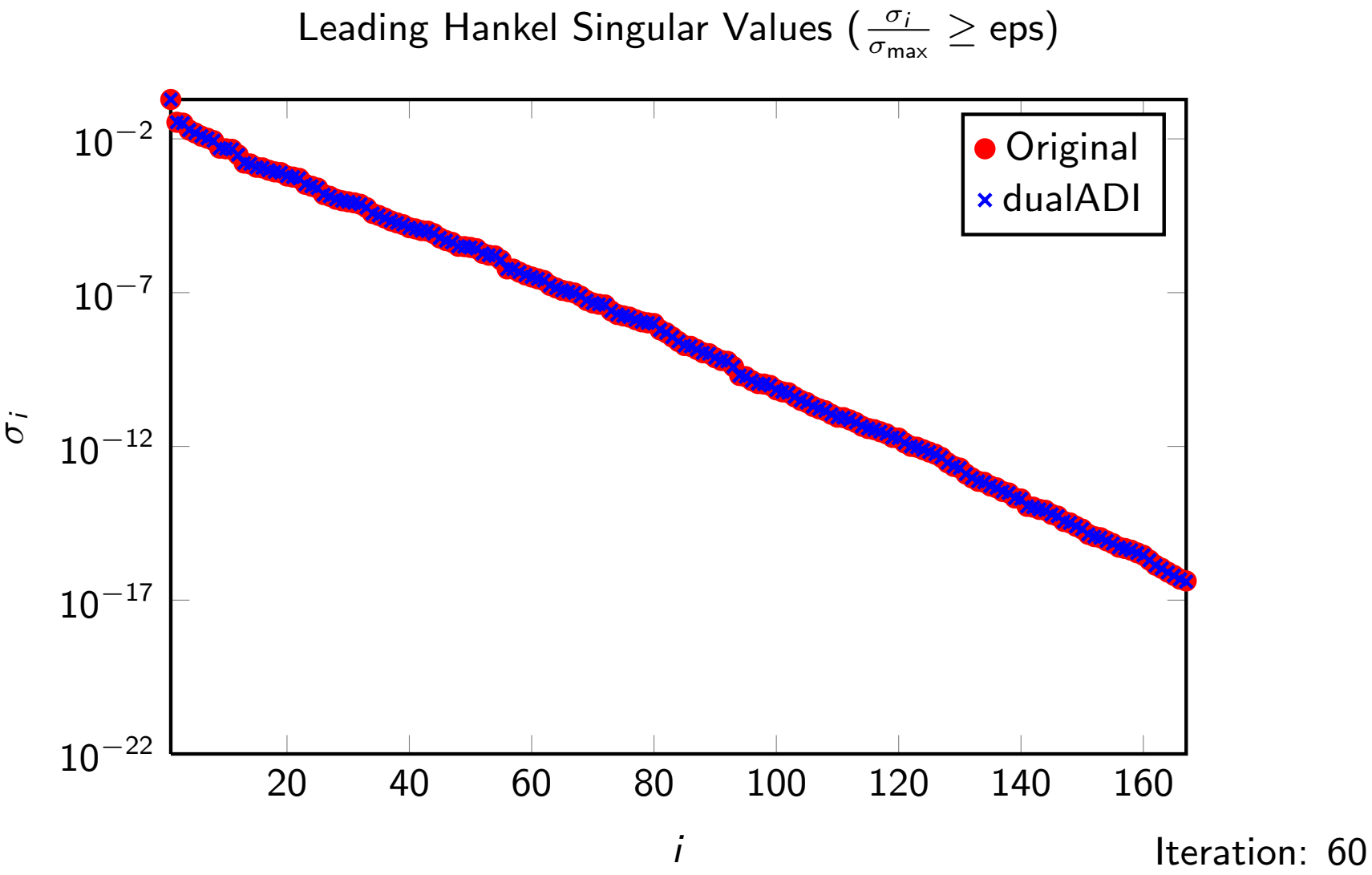
Numerical Results

Rail Model



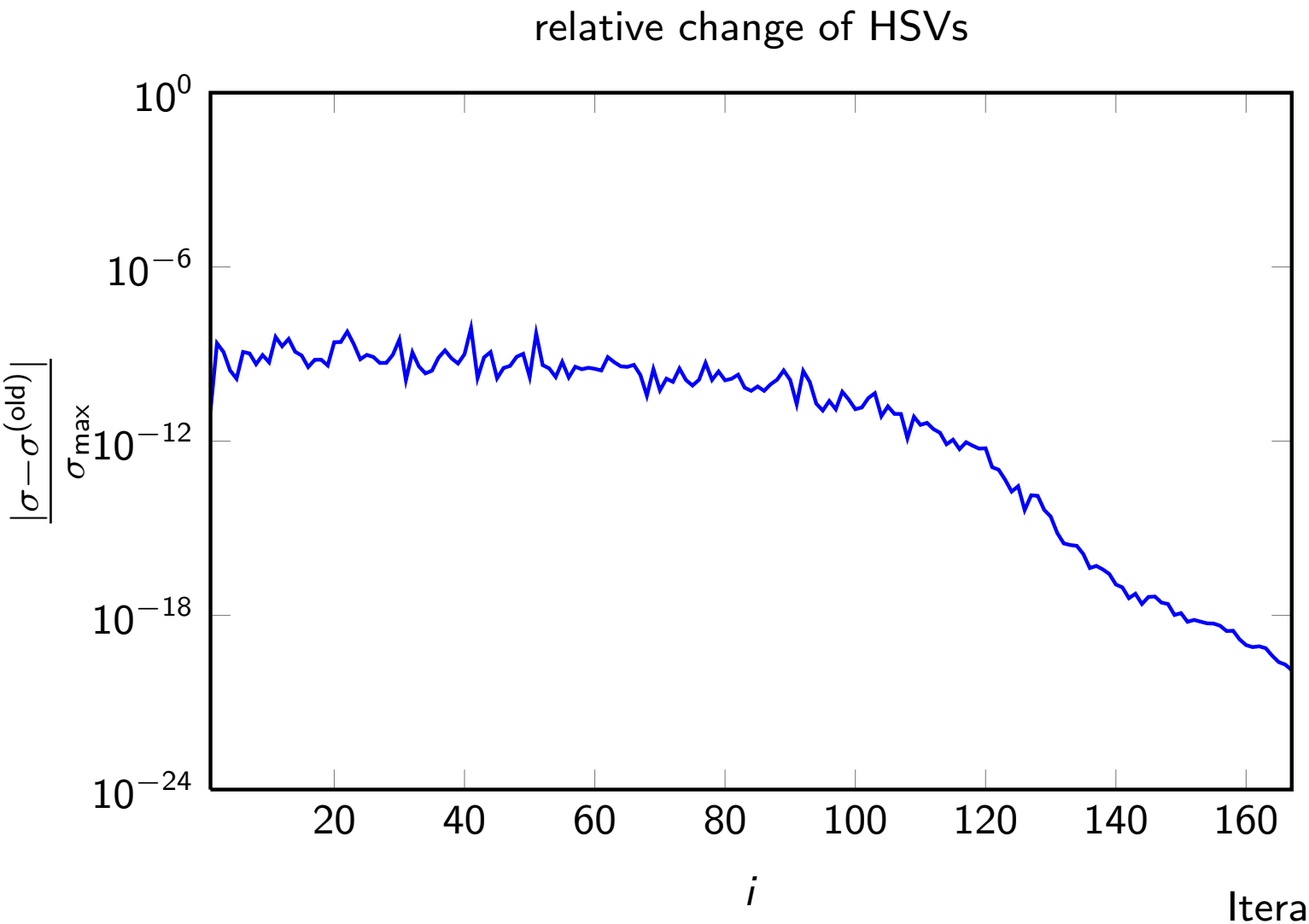
Numerical Results

Rail Model



Numerical Results

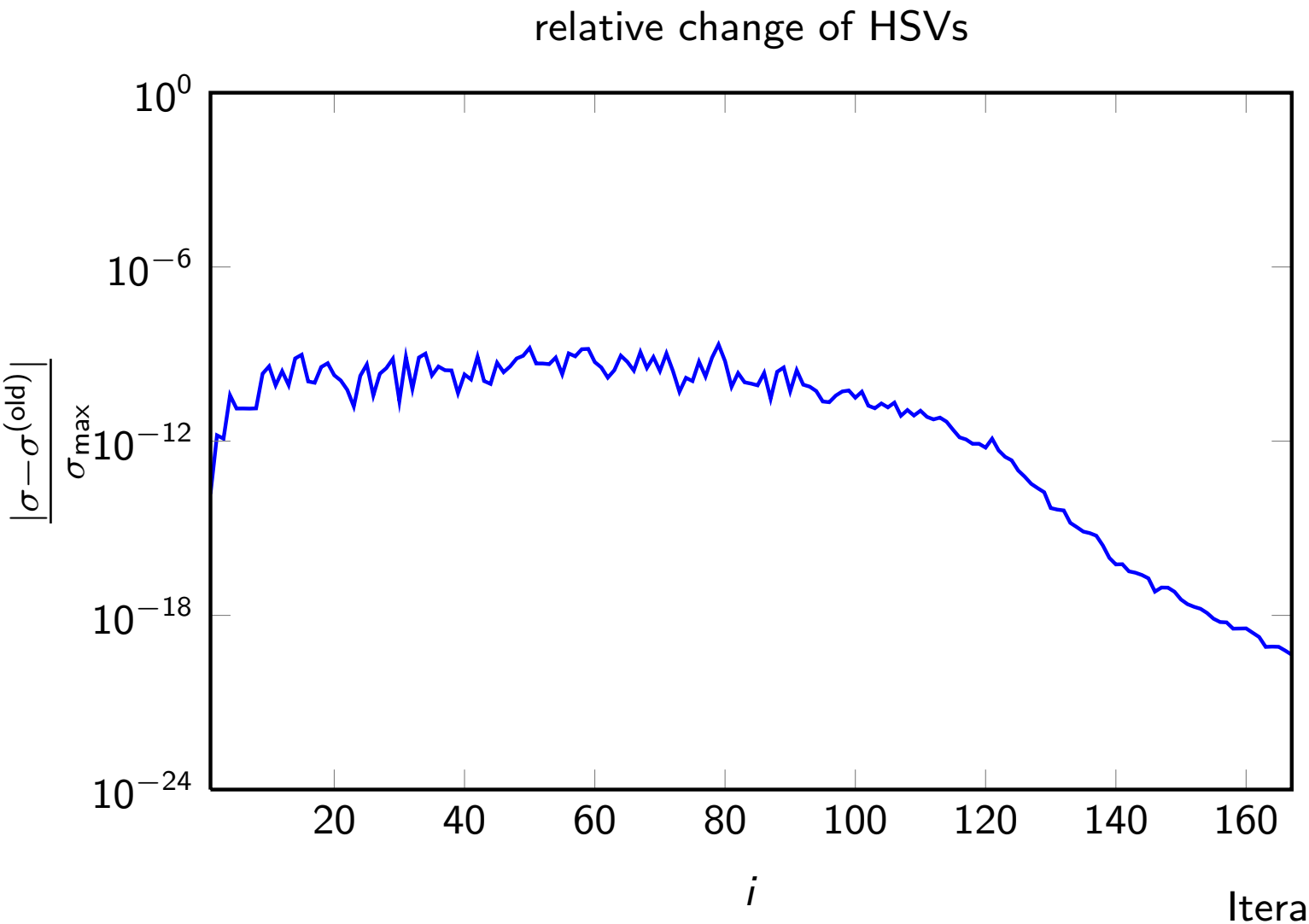
Rail Model



Iteration: 29

Numerical Results

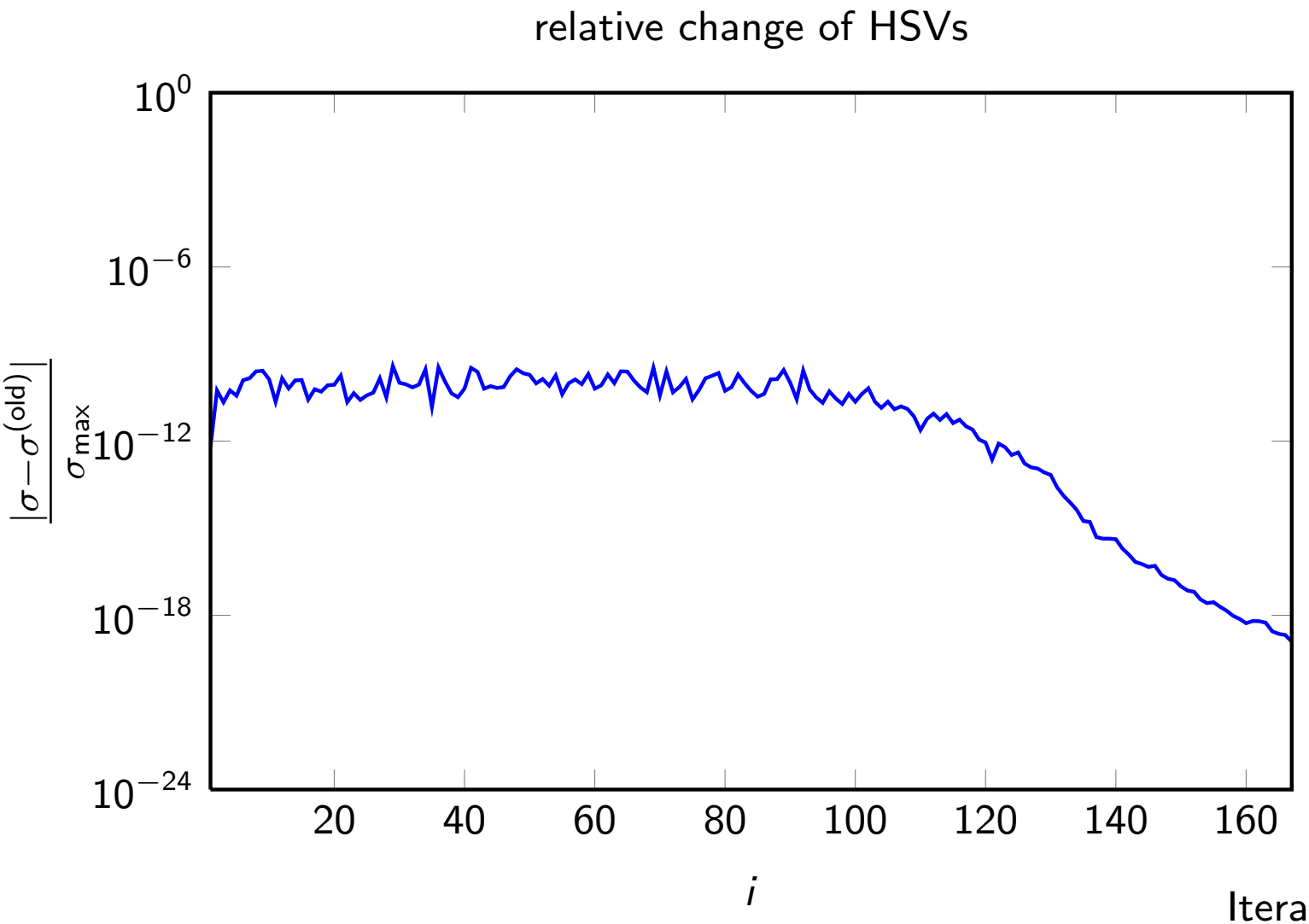
Rail Model



Iteration: 30

Numerical Results

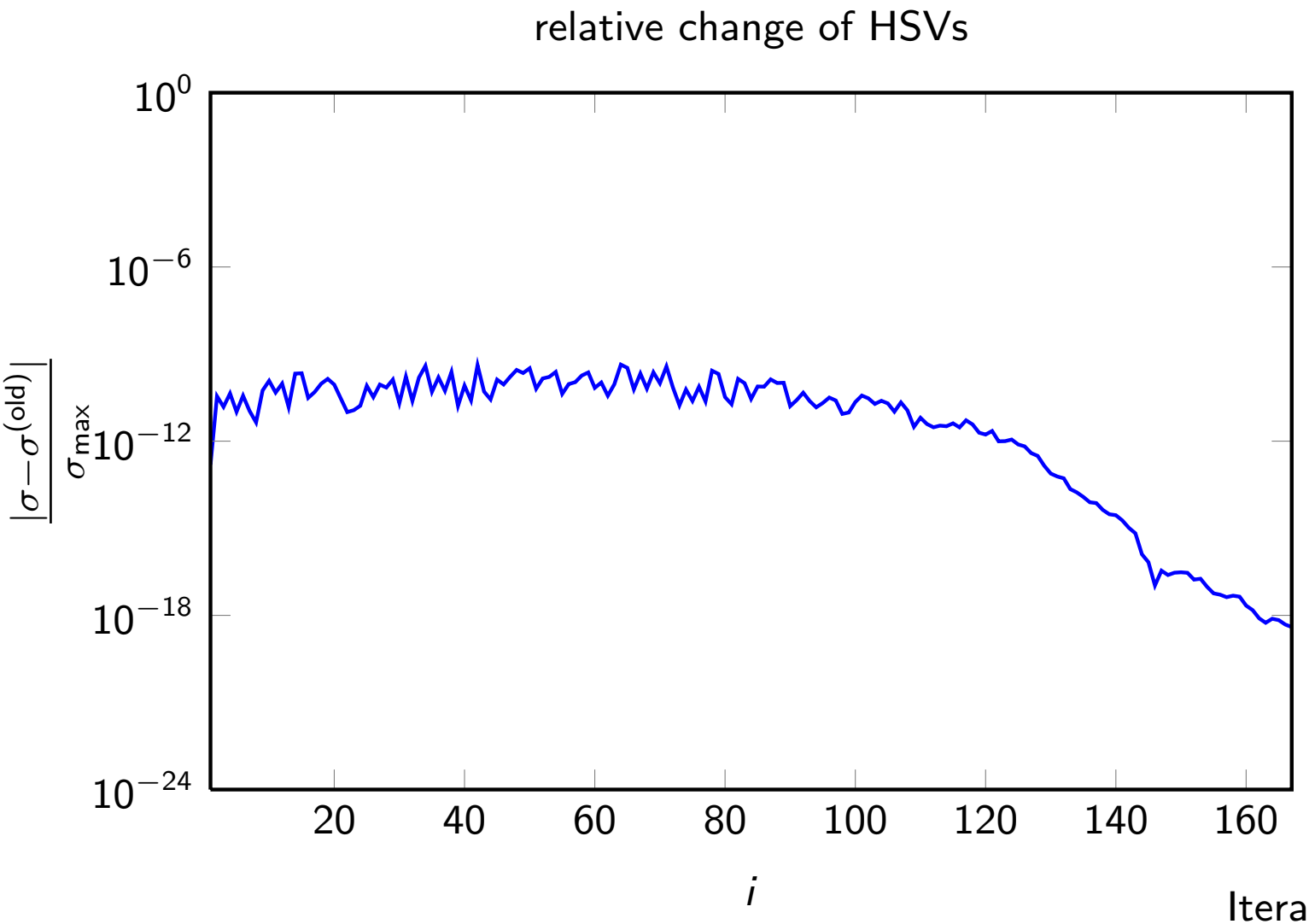
Rail Model



Iteration: 31

Numerical Results

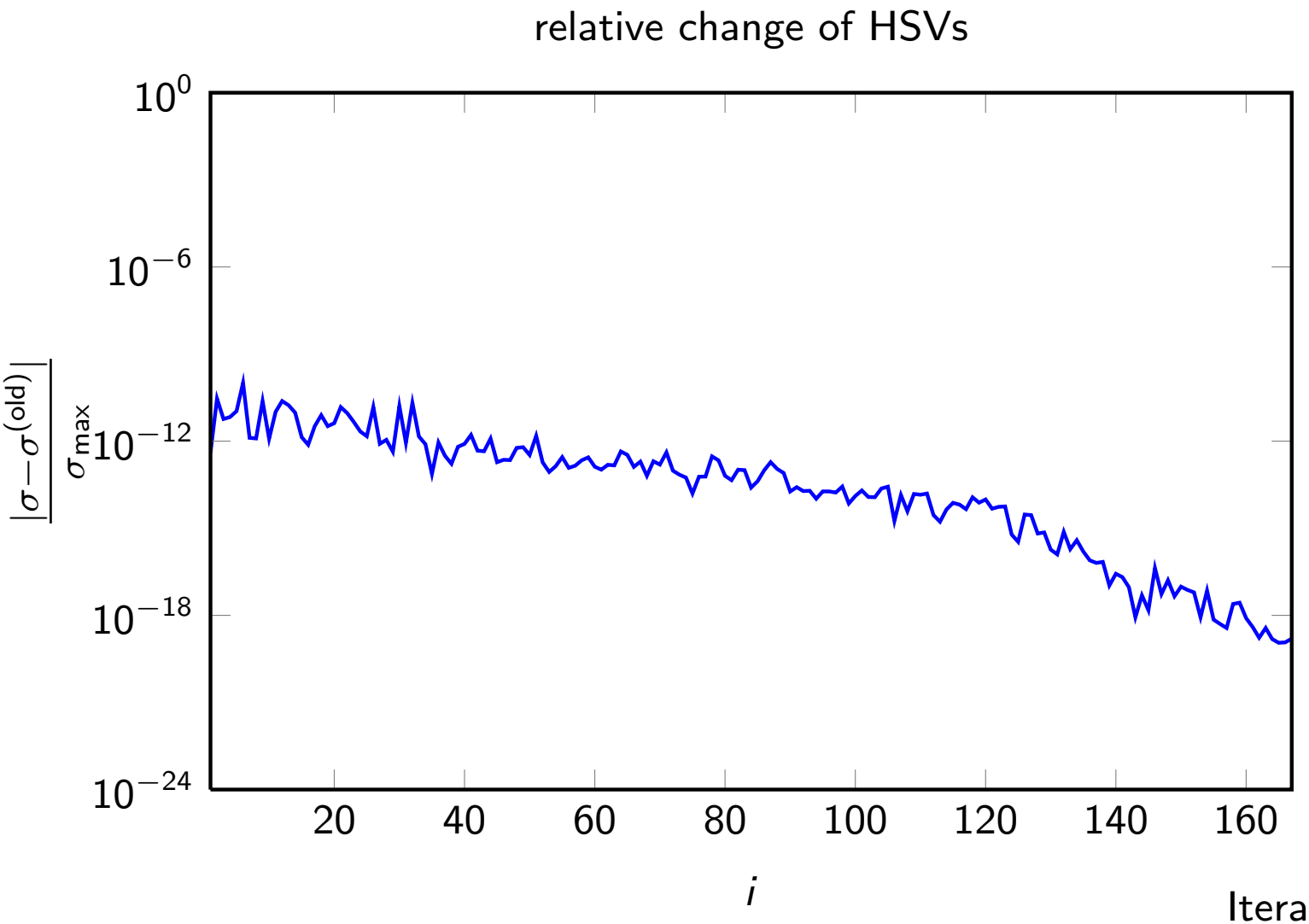
Rail Model



Iteration: 32

Numerical Results

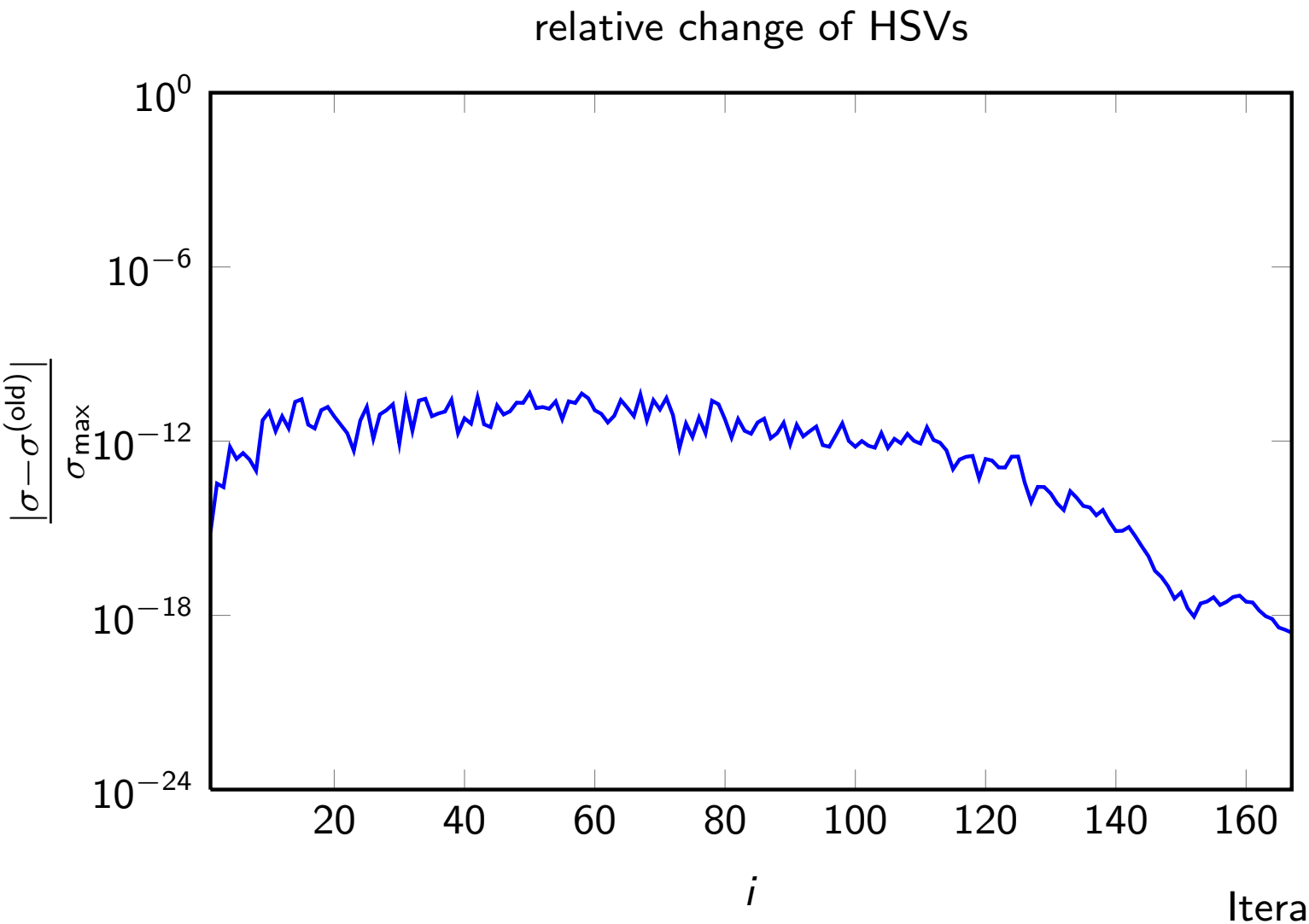
Rail Model



Iteration: 33

Numerical Results

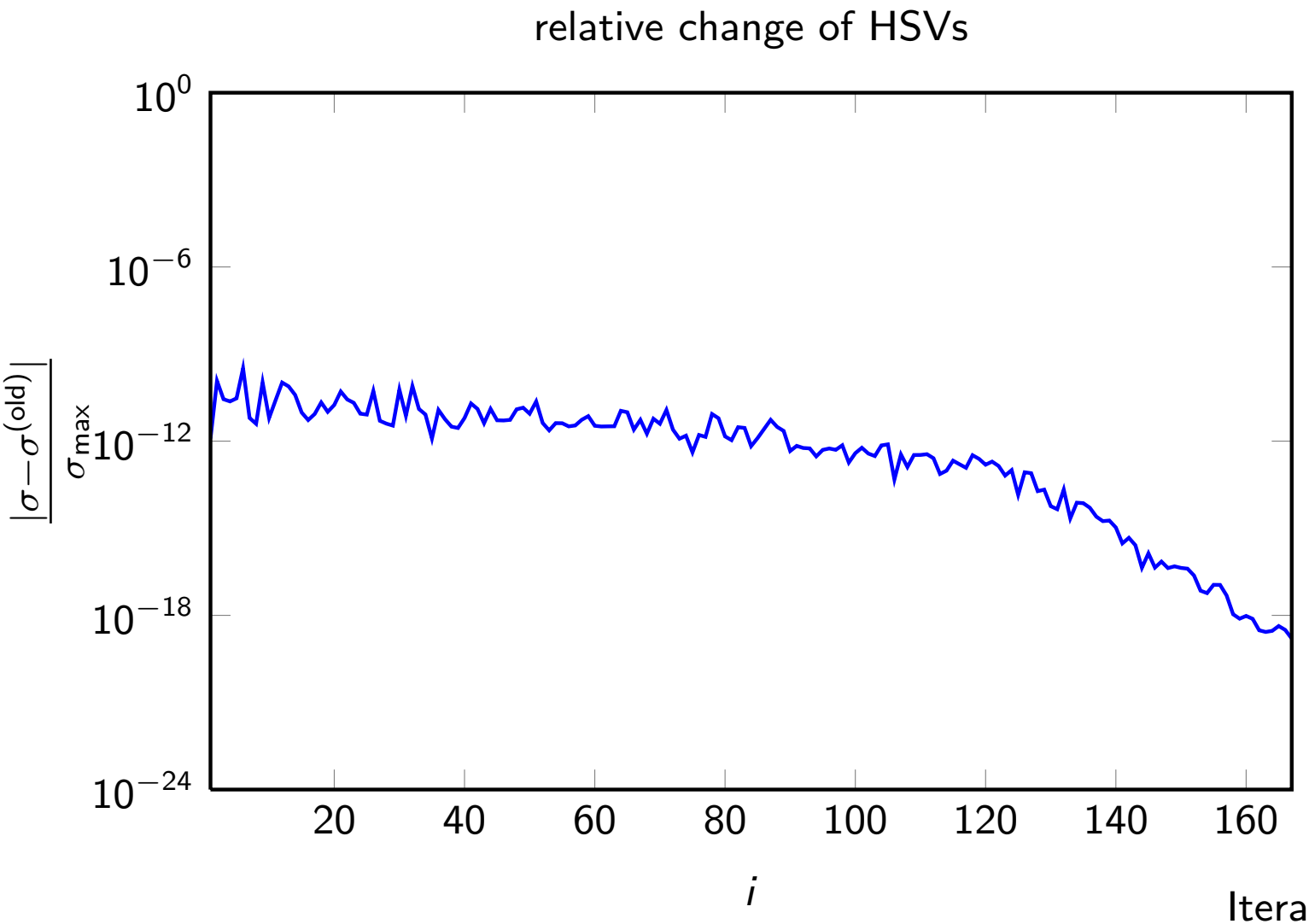
Rail Model



Iteration: 34

Numerical Results

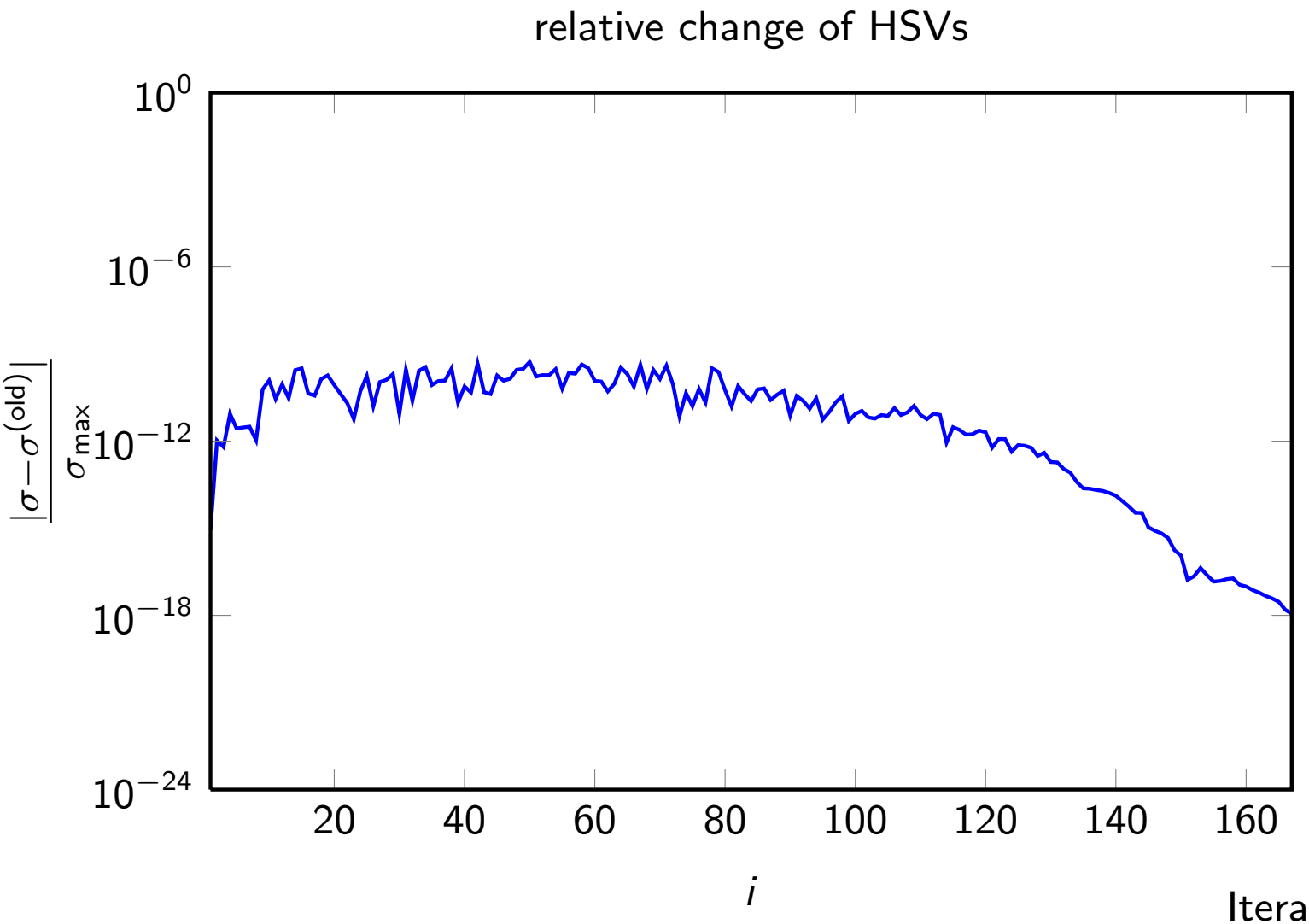
Rail Model



Iteration: 35

Numerical Results

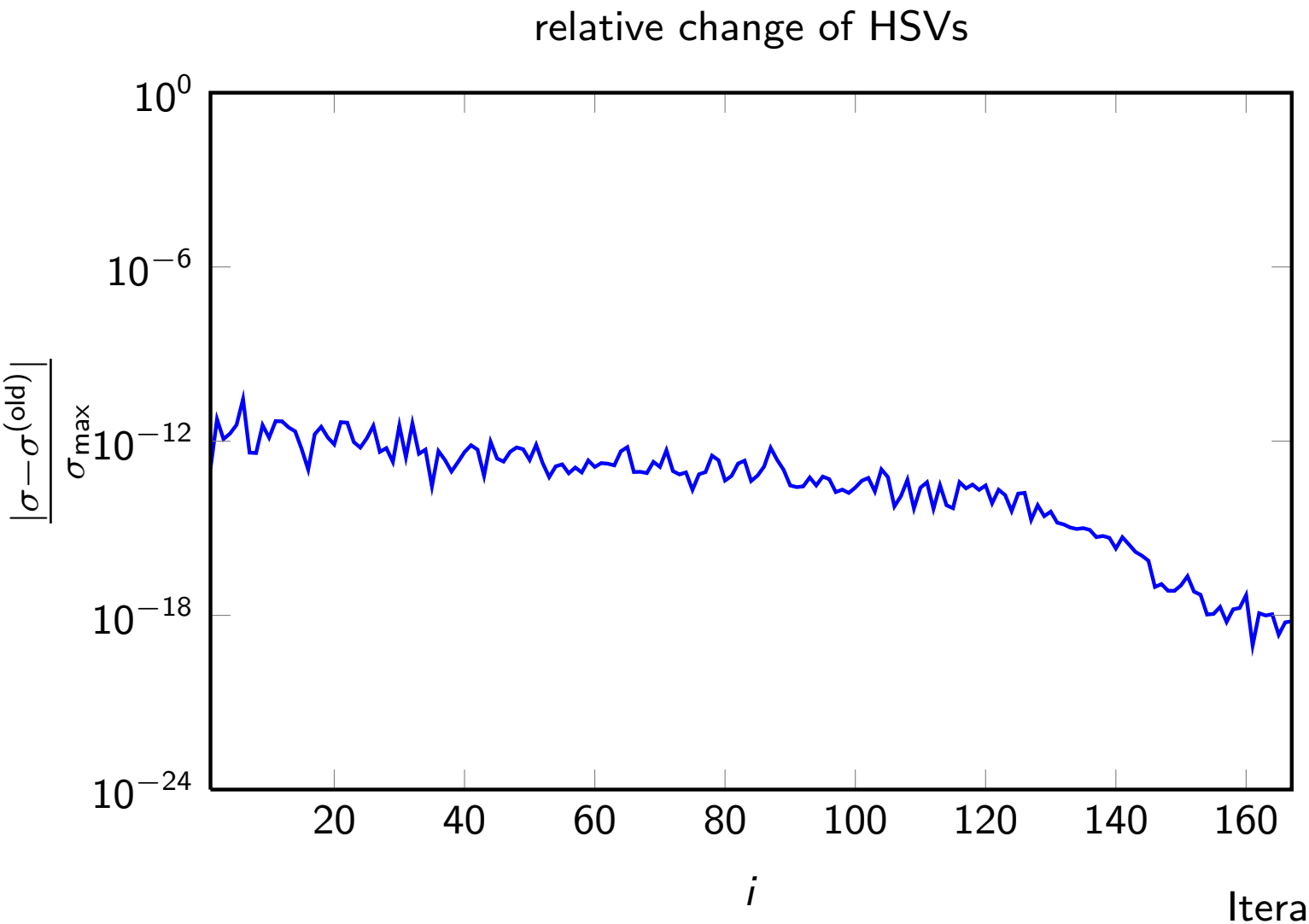
Rail Model



Iteration: 36

Numerical Results

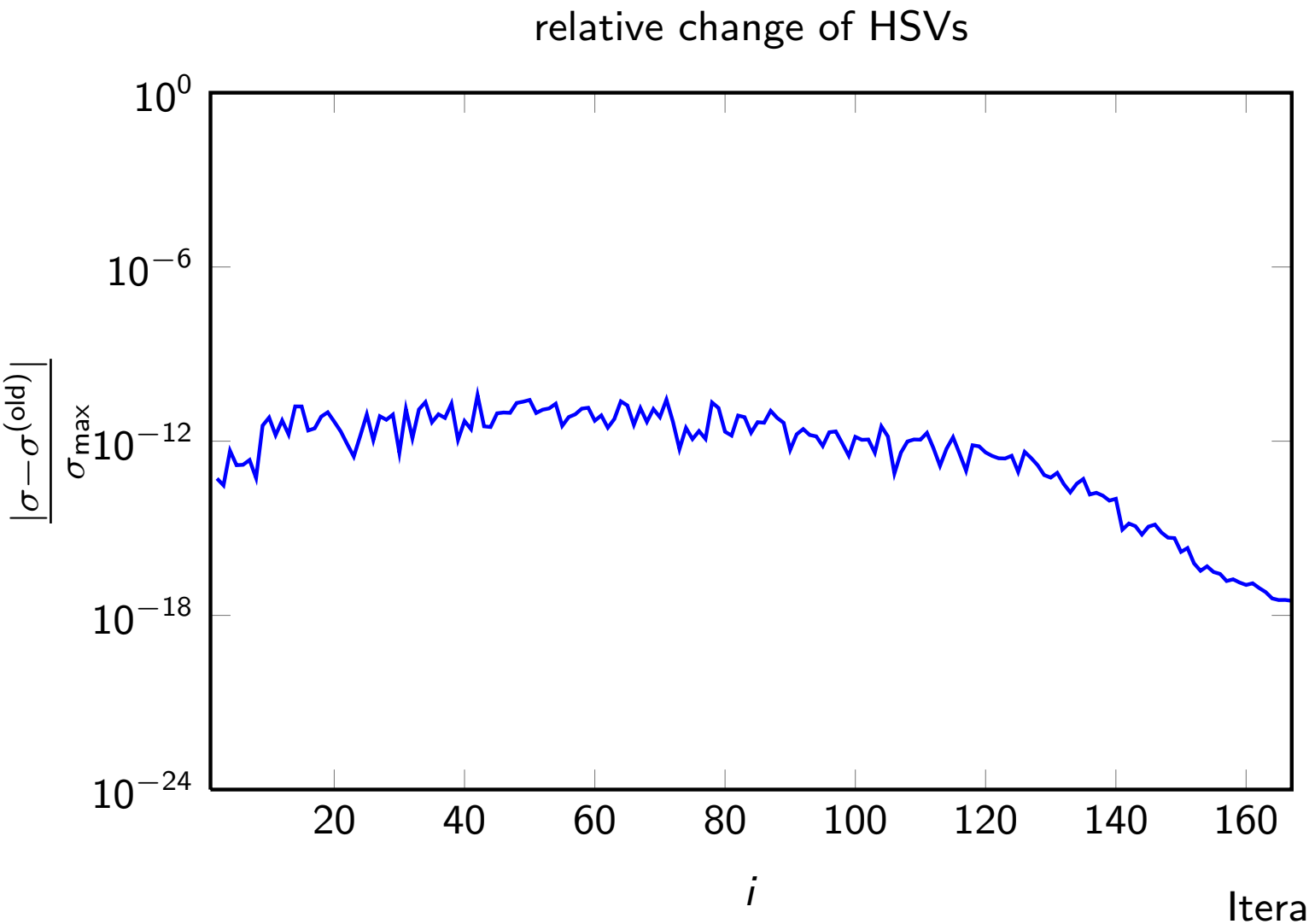
Rail Model



Iteration: 37

Numerical Results

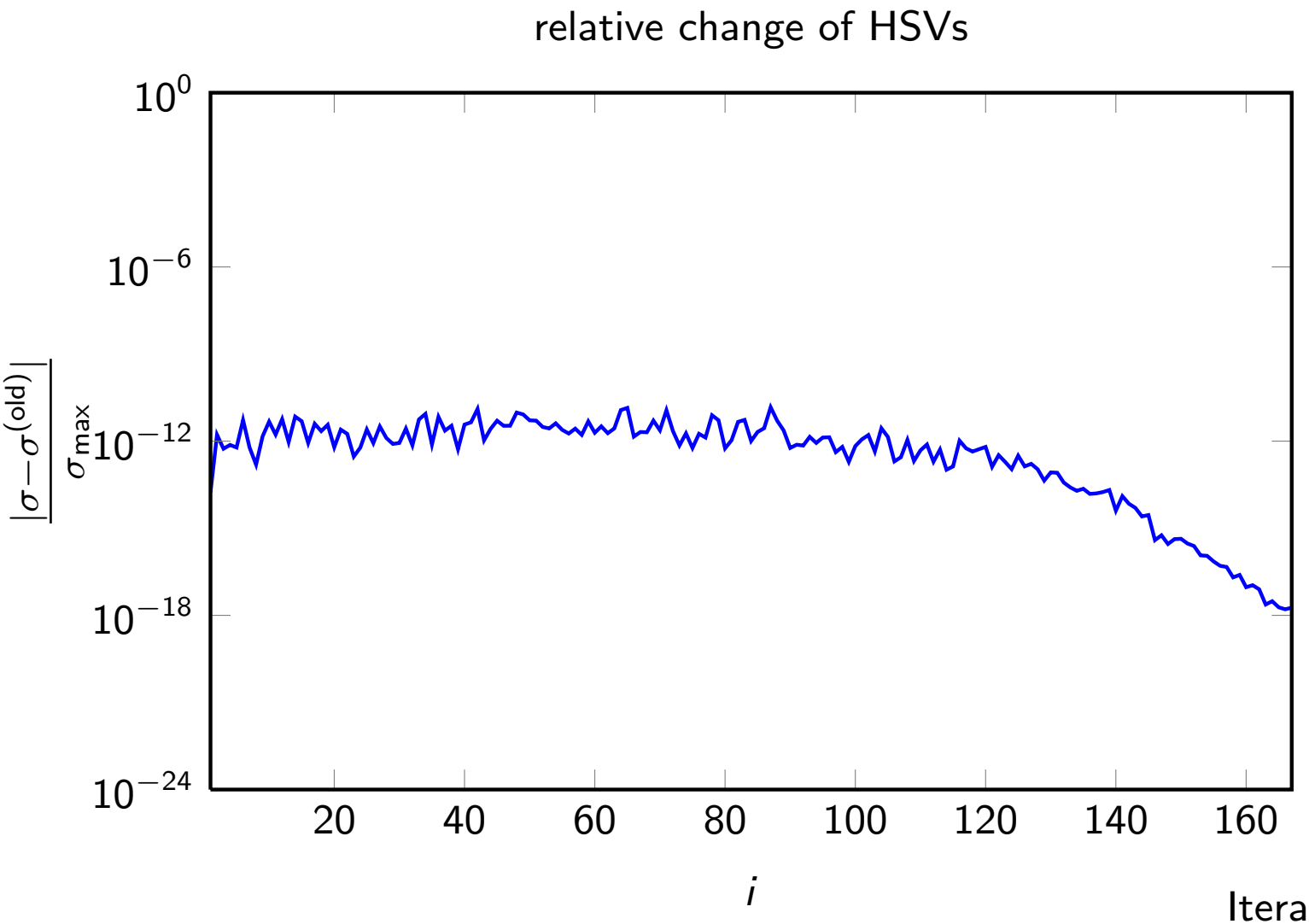
Rail Model



Iteration: 38

Numerical Results

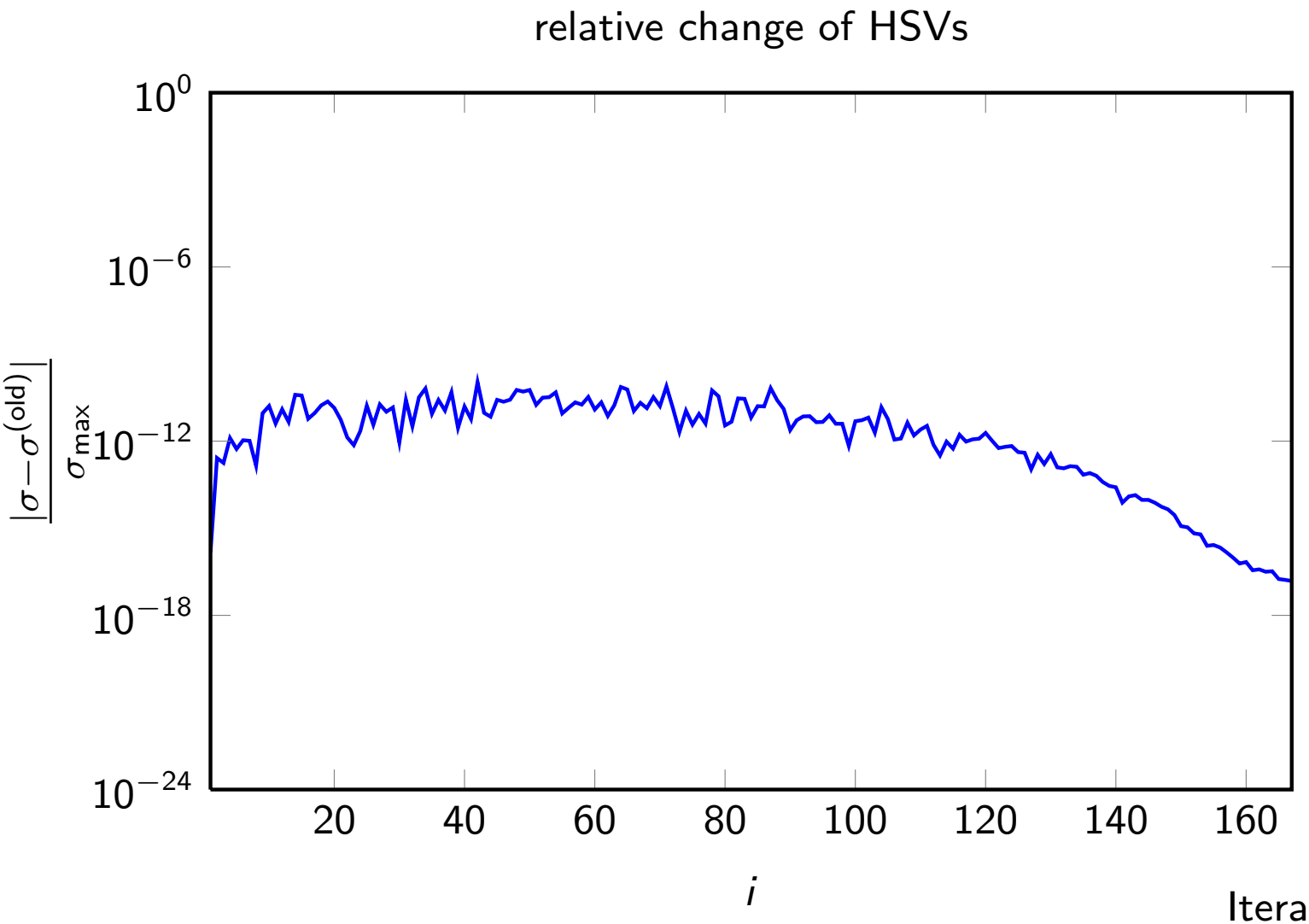
Rail Model



Iteration: 39

Numerical Results

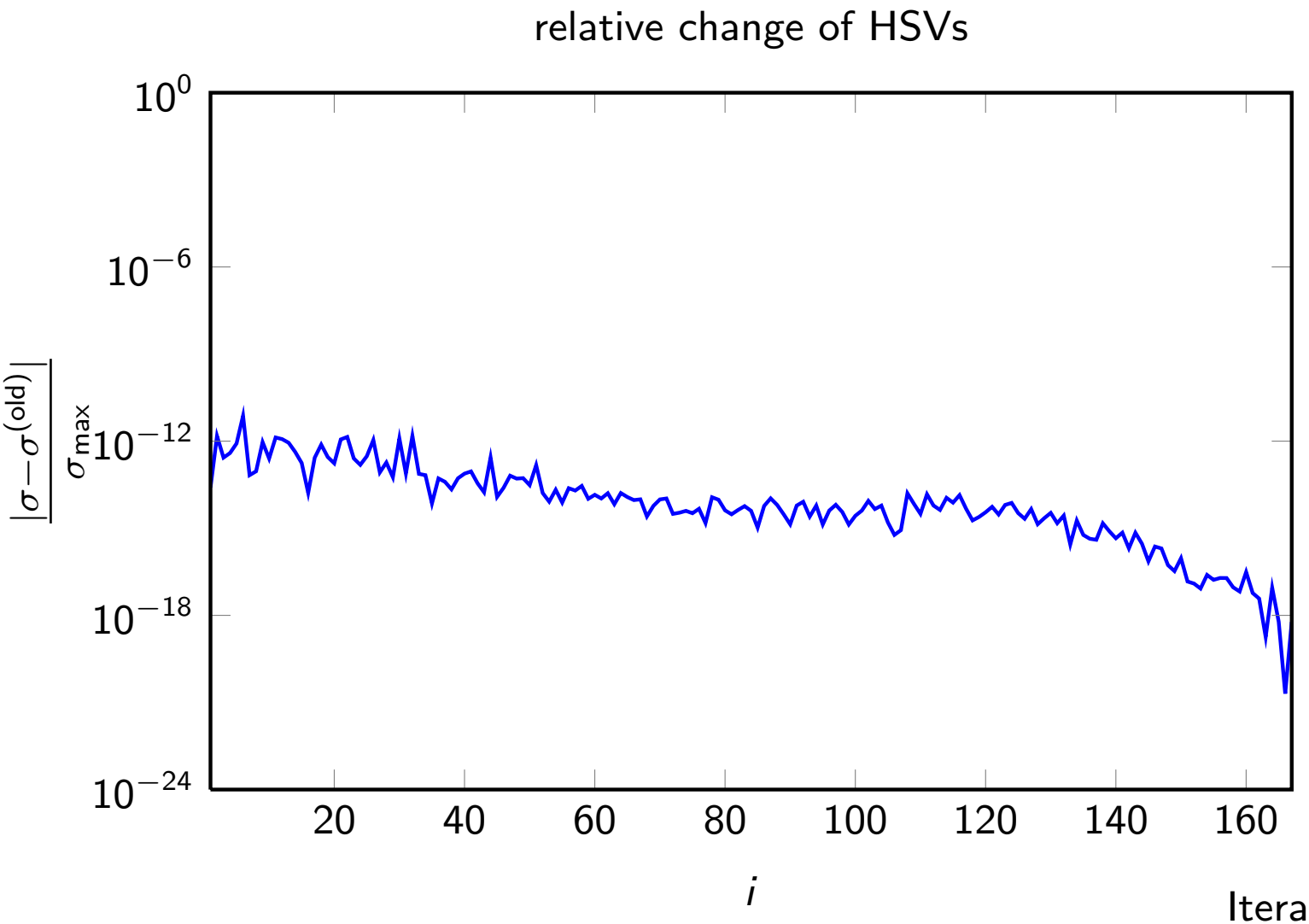
Rail Model



Iteration: 40

Numerical Results

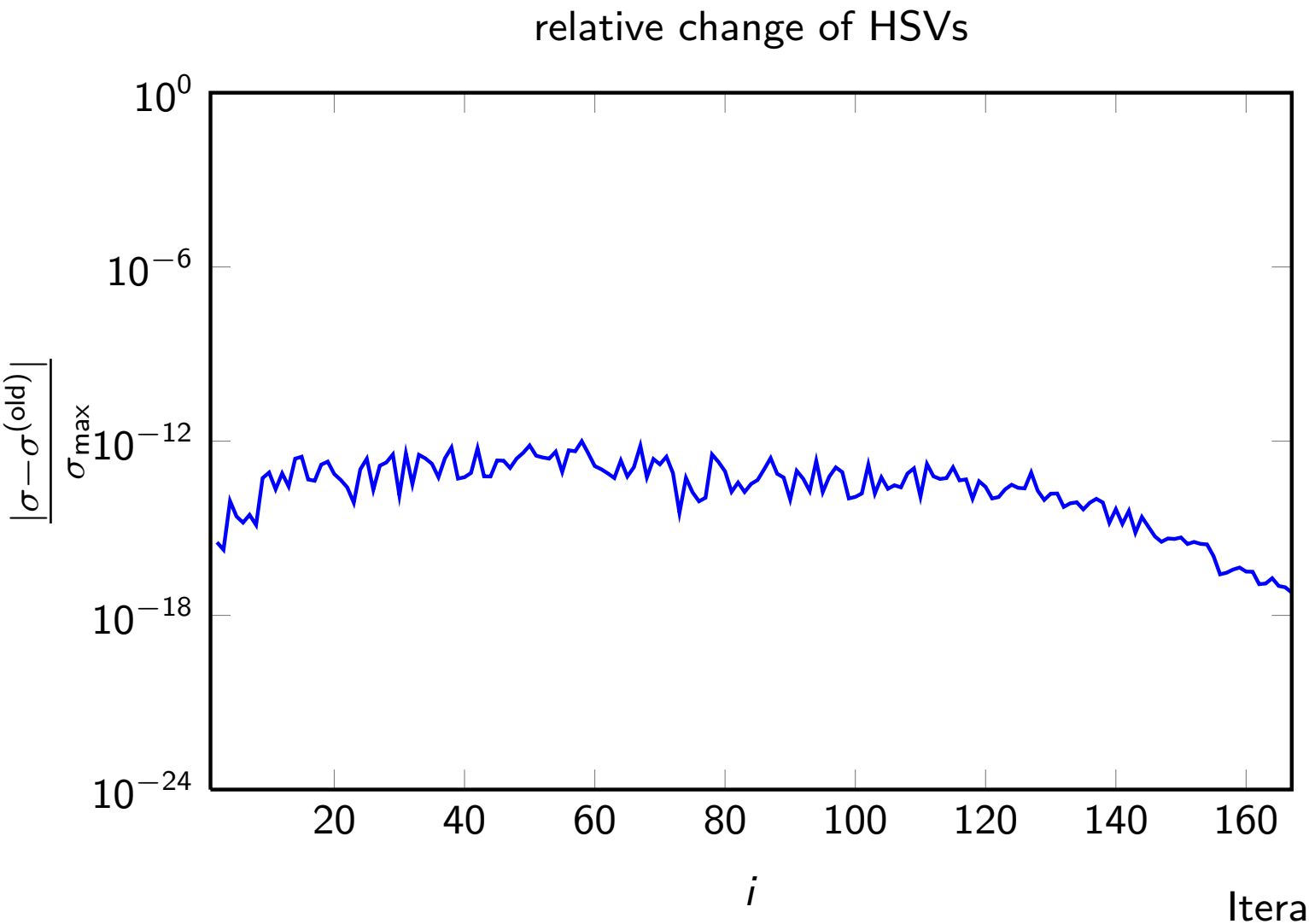
Rail Model



Iteration: 41

Numerical Results

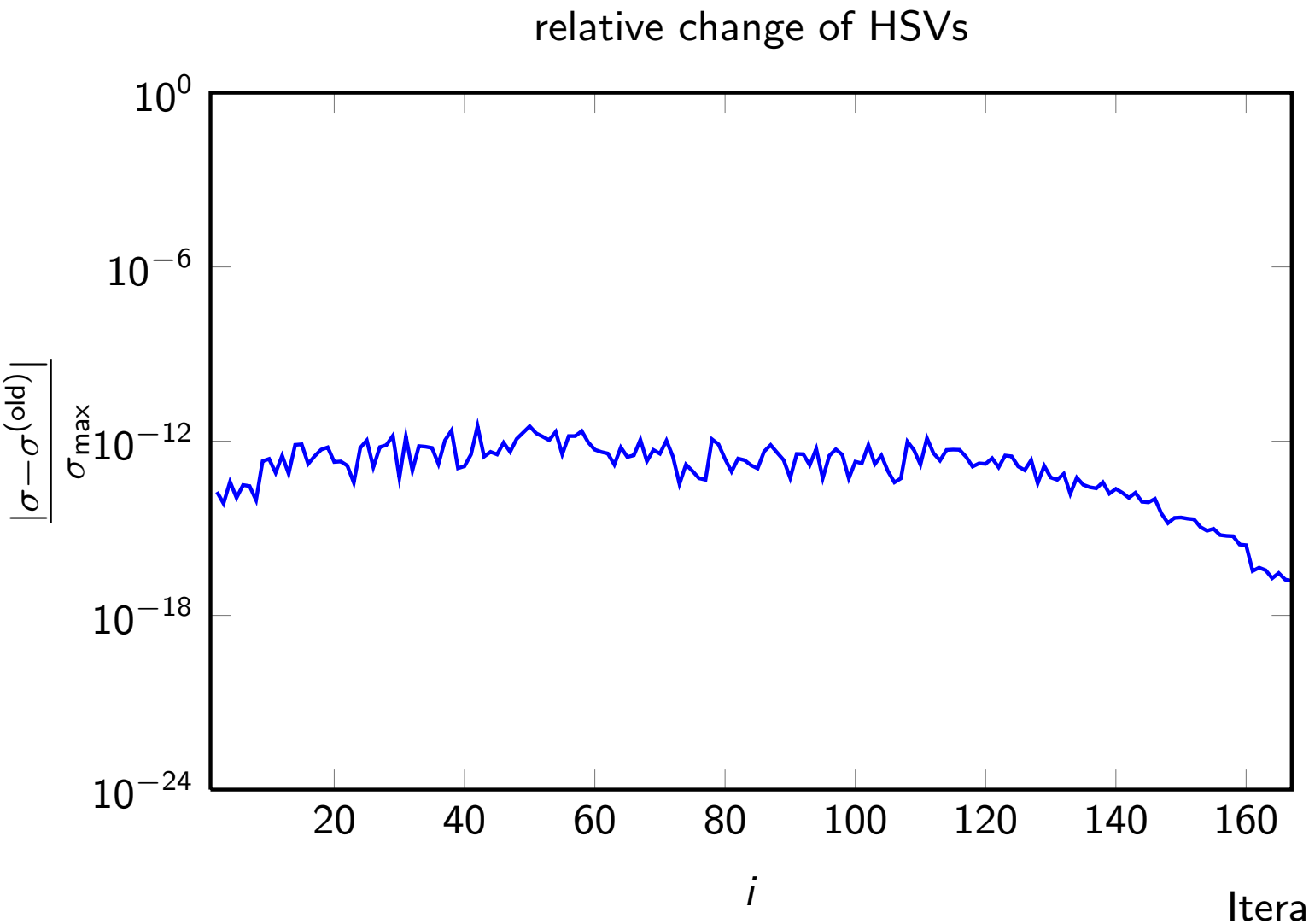
Rail Model



Iteration: 42

Numerical Results

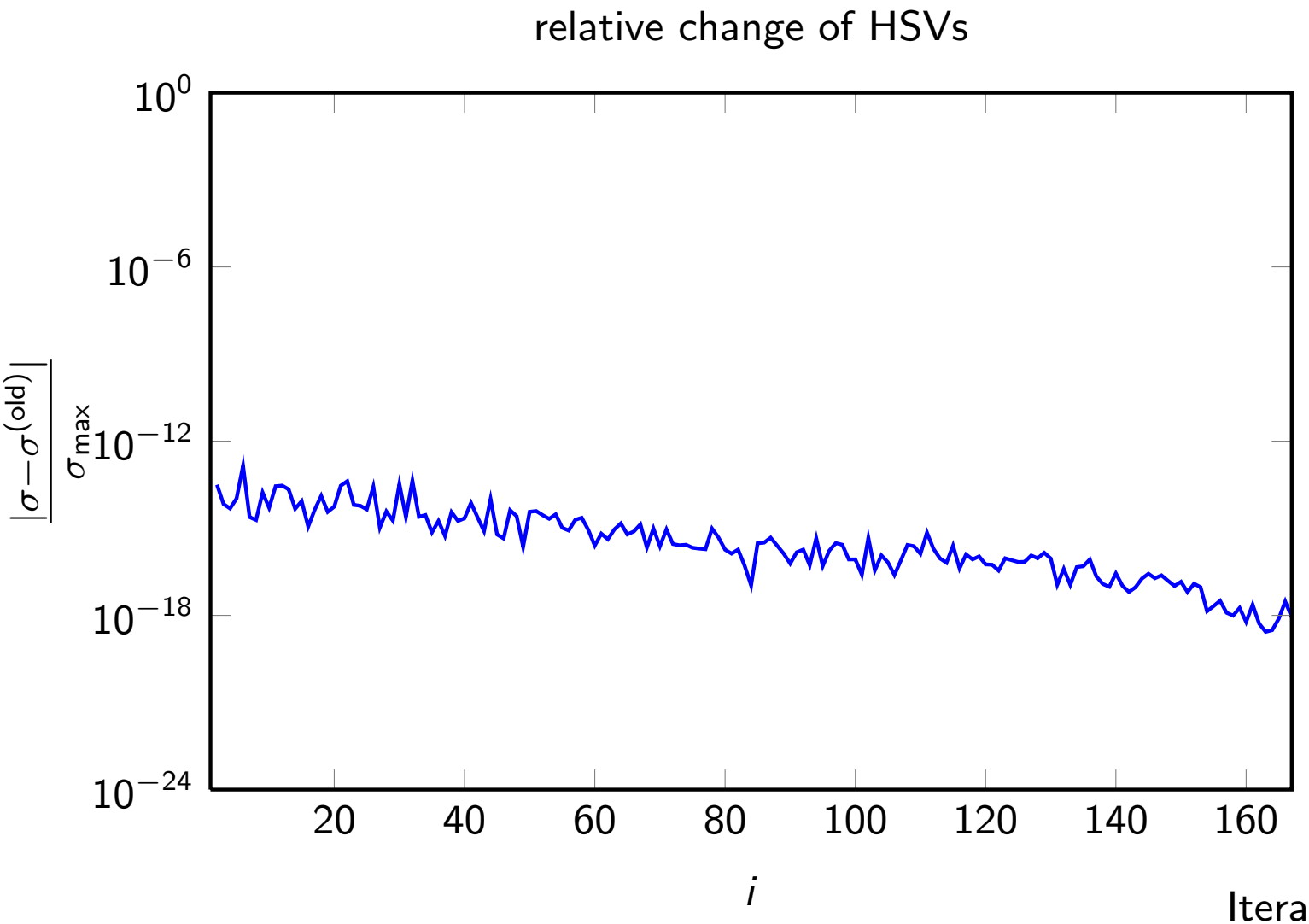
Rail Model



Iteration: 43

Numerical Results

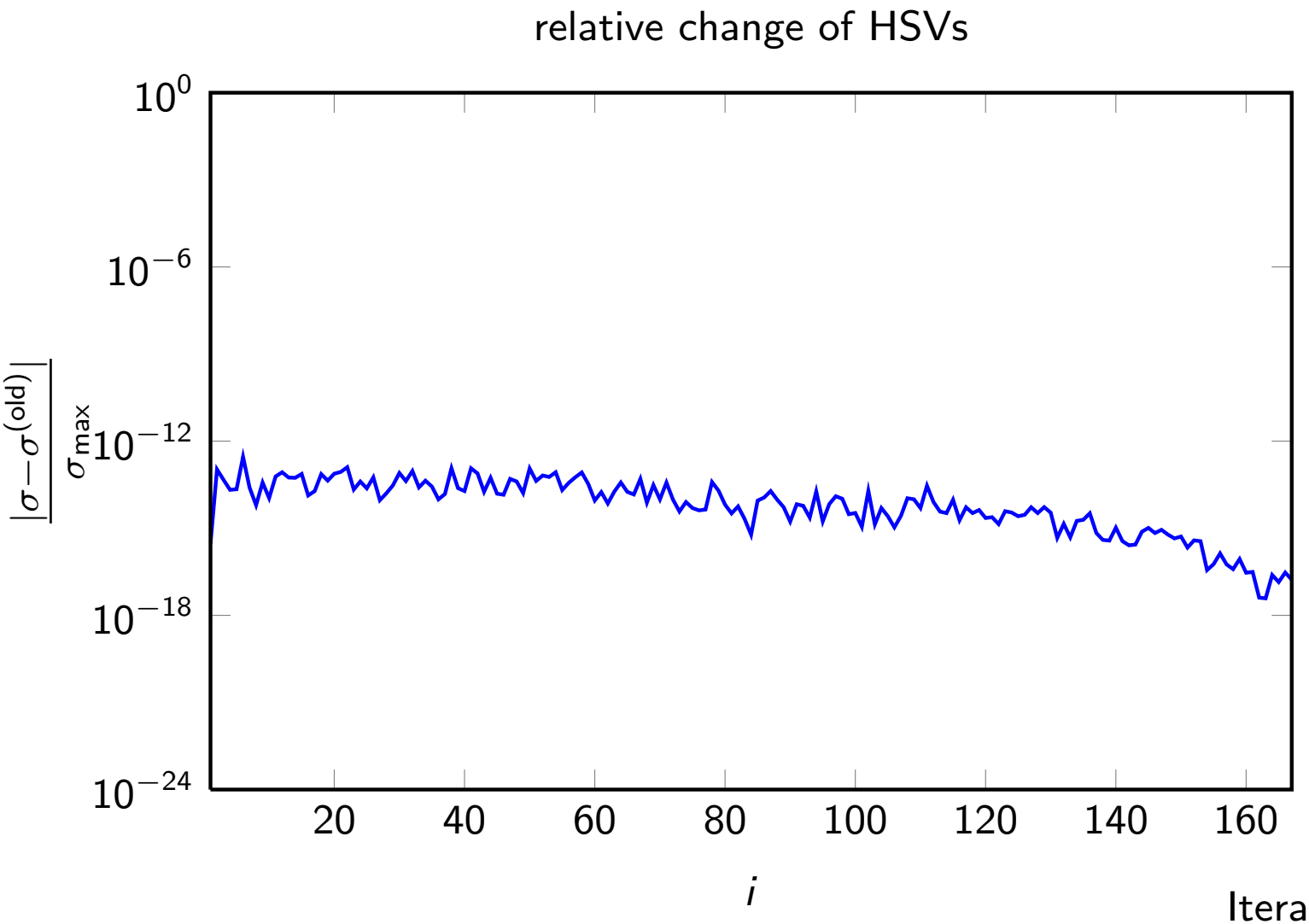
Rail Model



Iteration: 44

Numerical Results

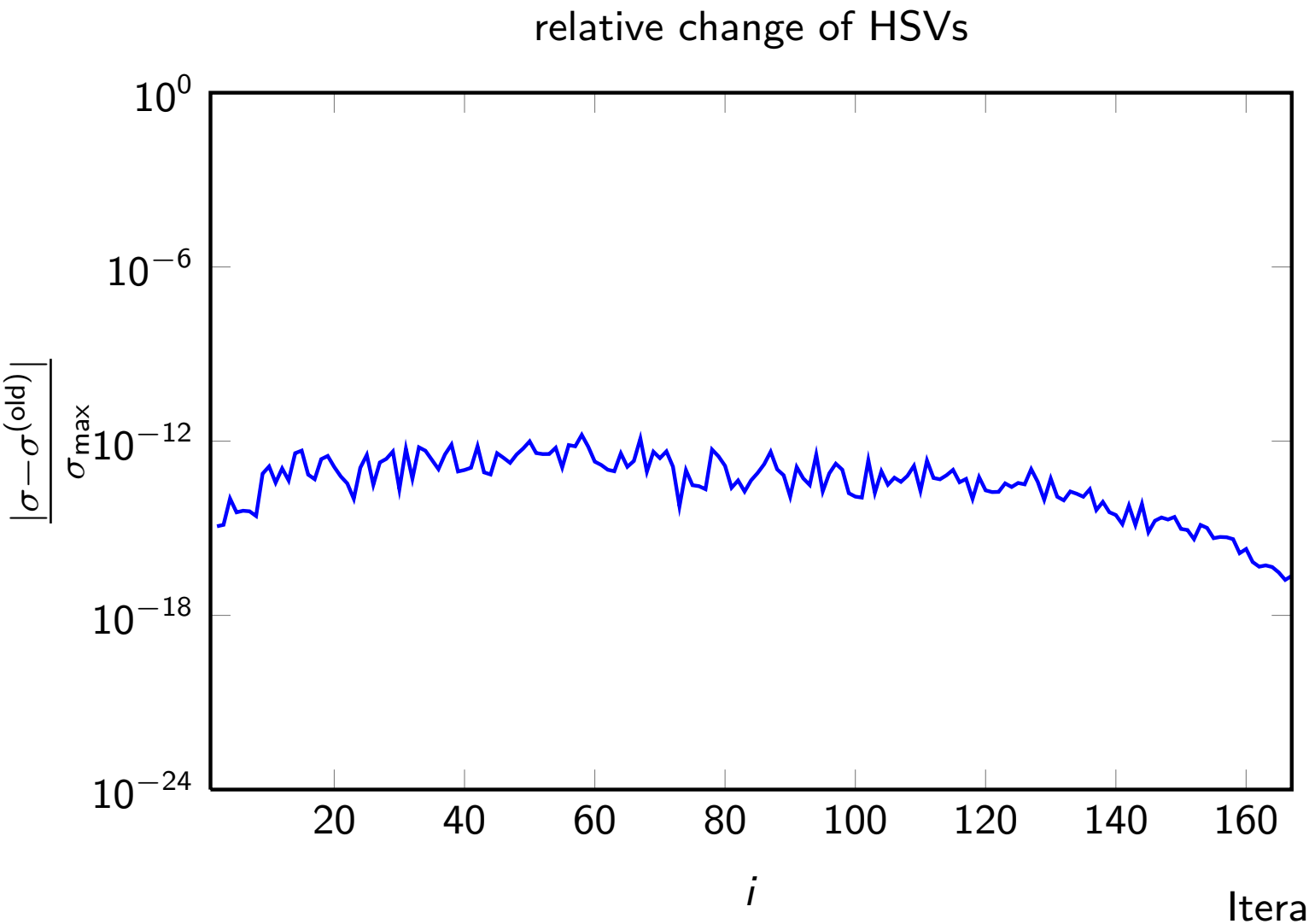
Rail Model



Iteration: 45

Numerical Results

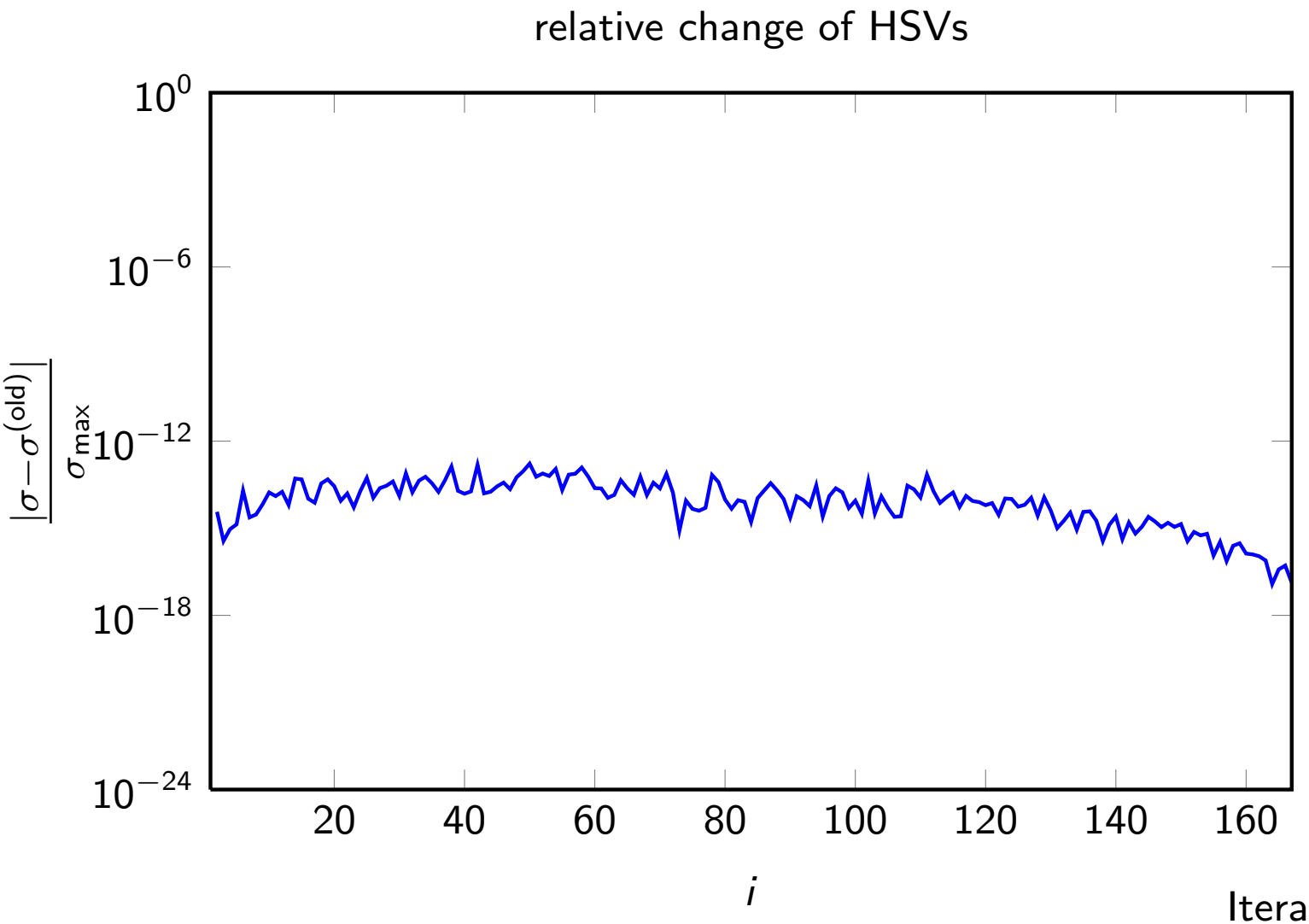
Rail Model



Iteration: 46

Numerical Results

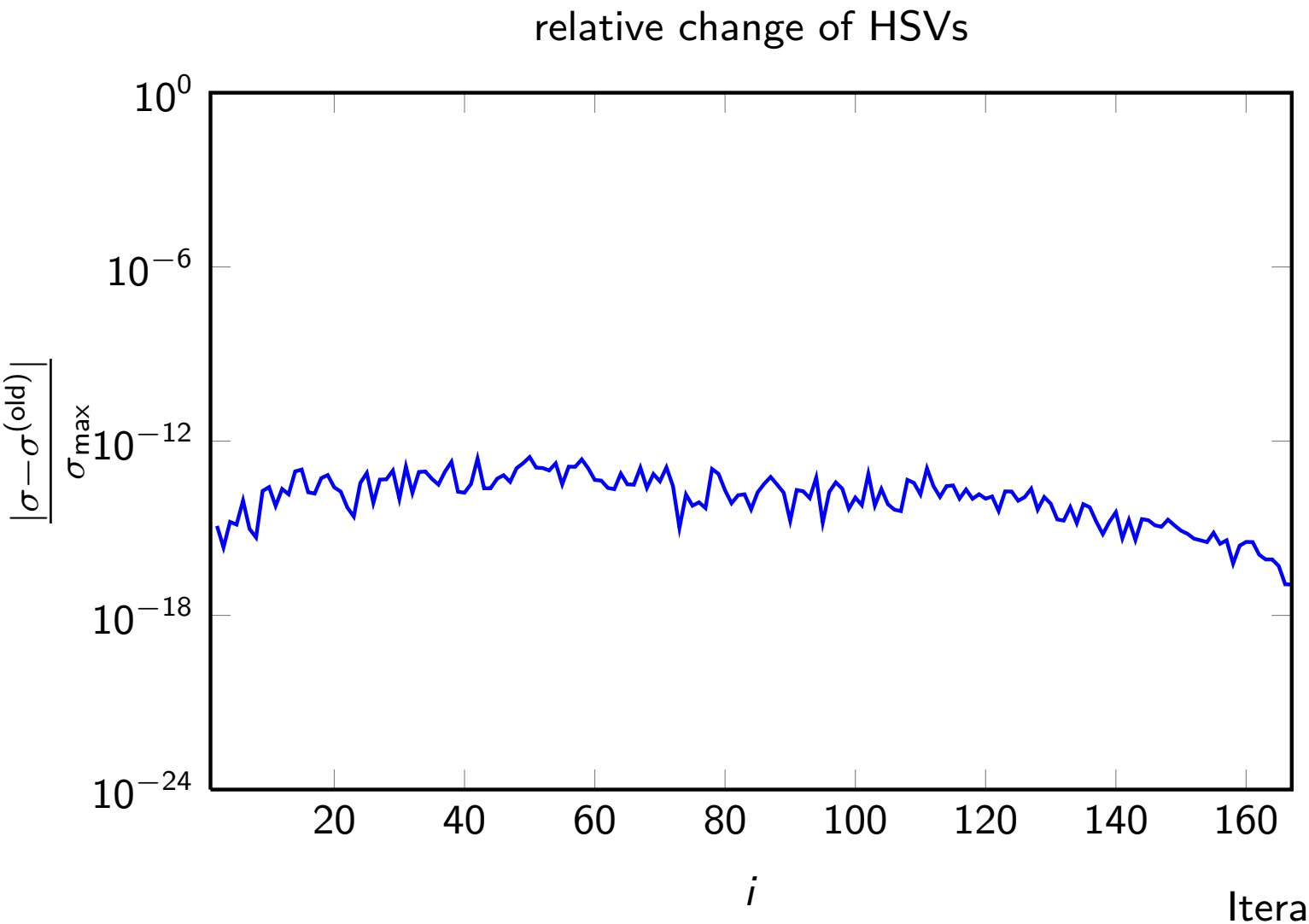
Rail Model



Iteration: 47

Numerical Results

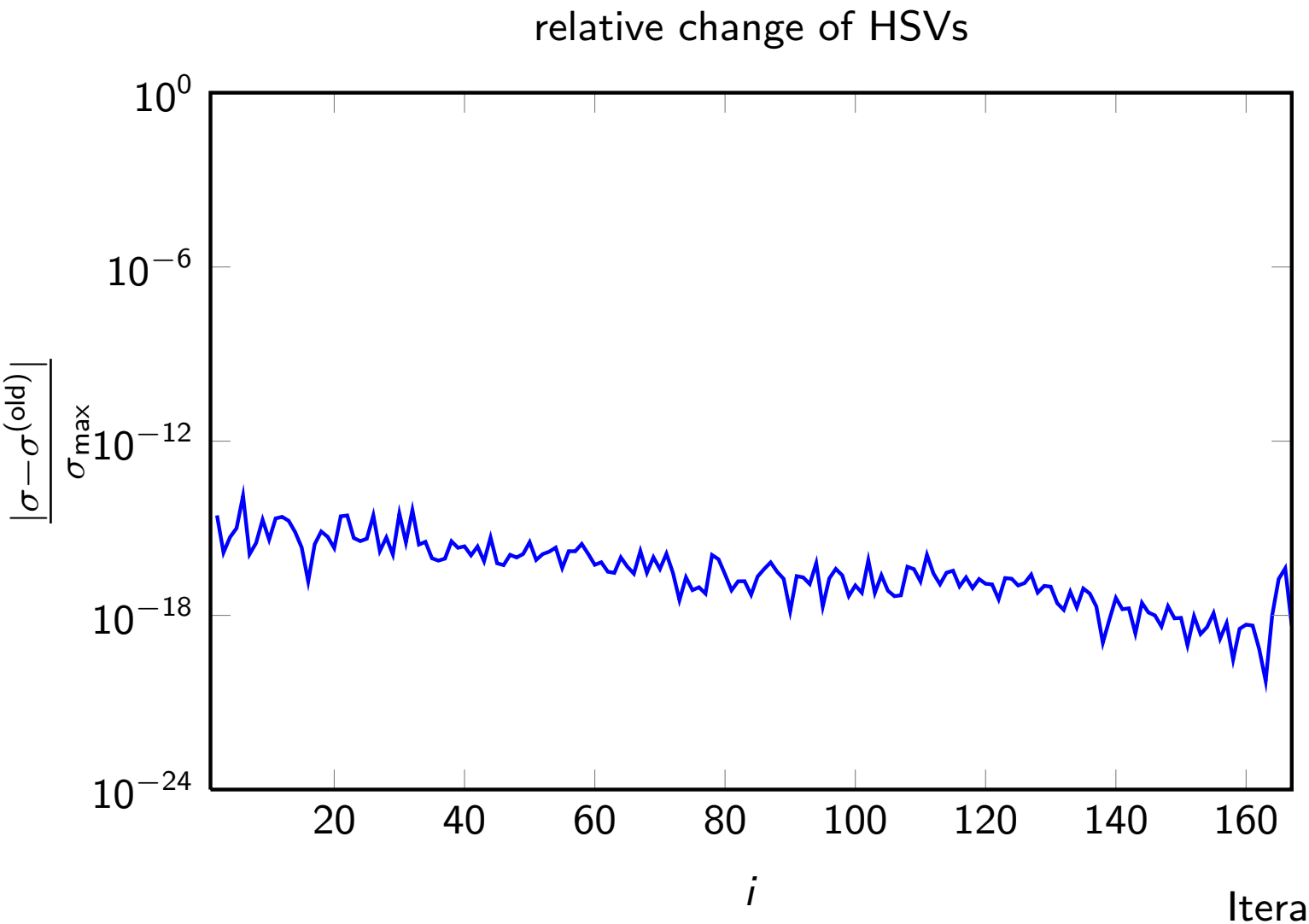
Rail Model



Iteration: 48

Numerical Results

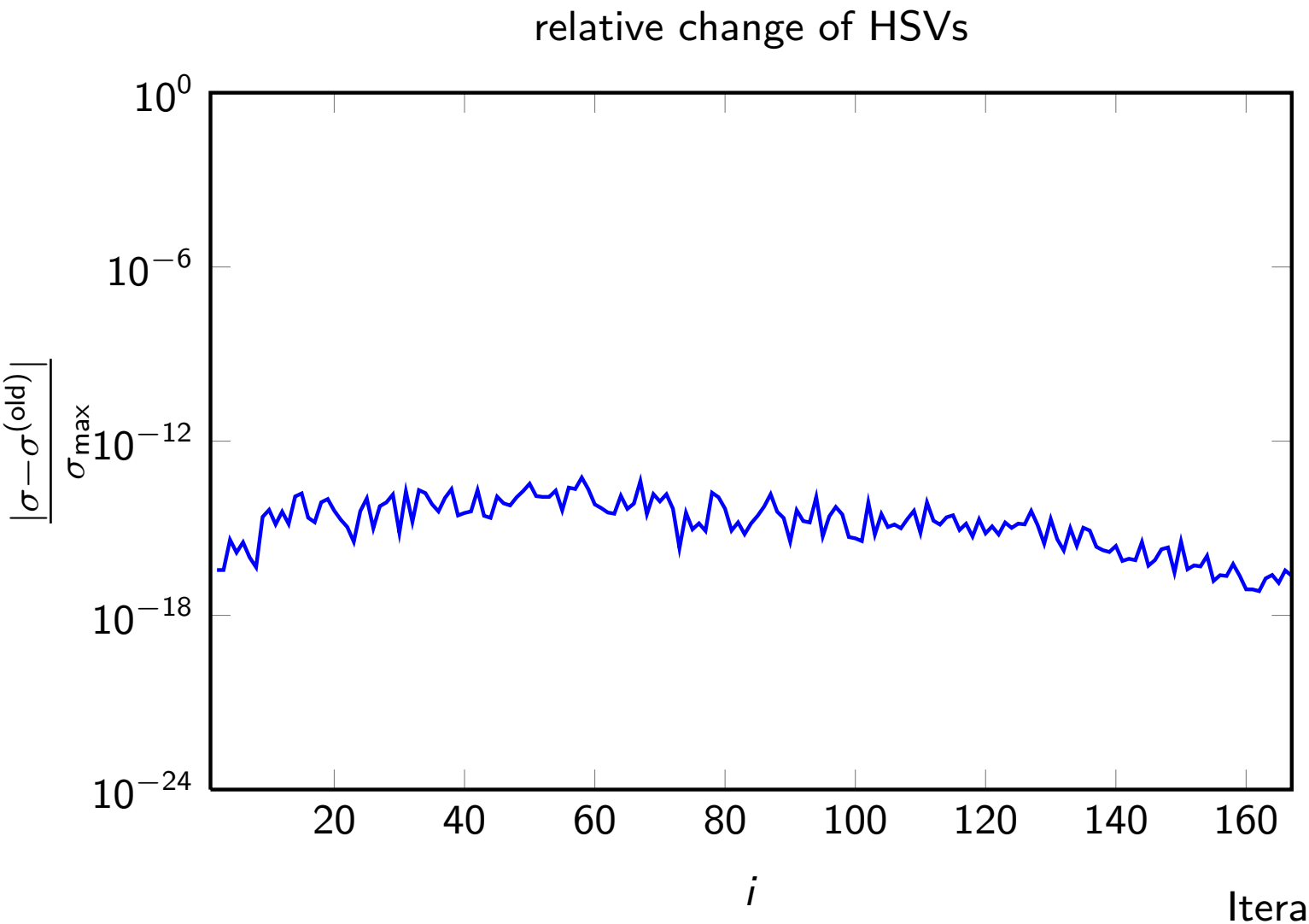
Rail Model



Iteration: 49

Numerical Results

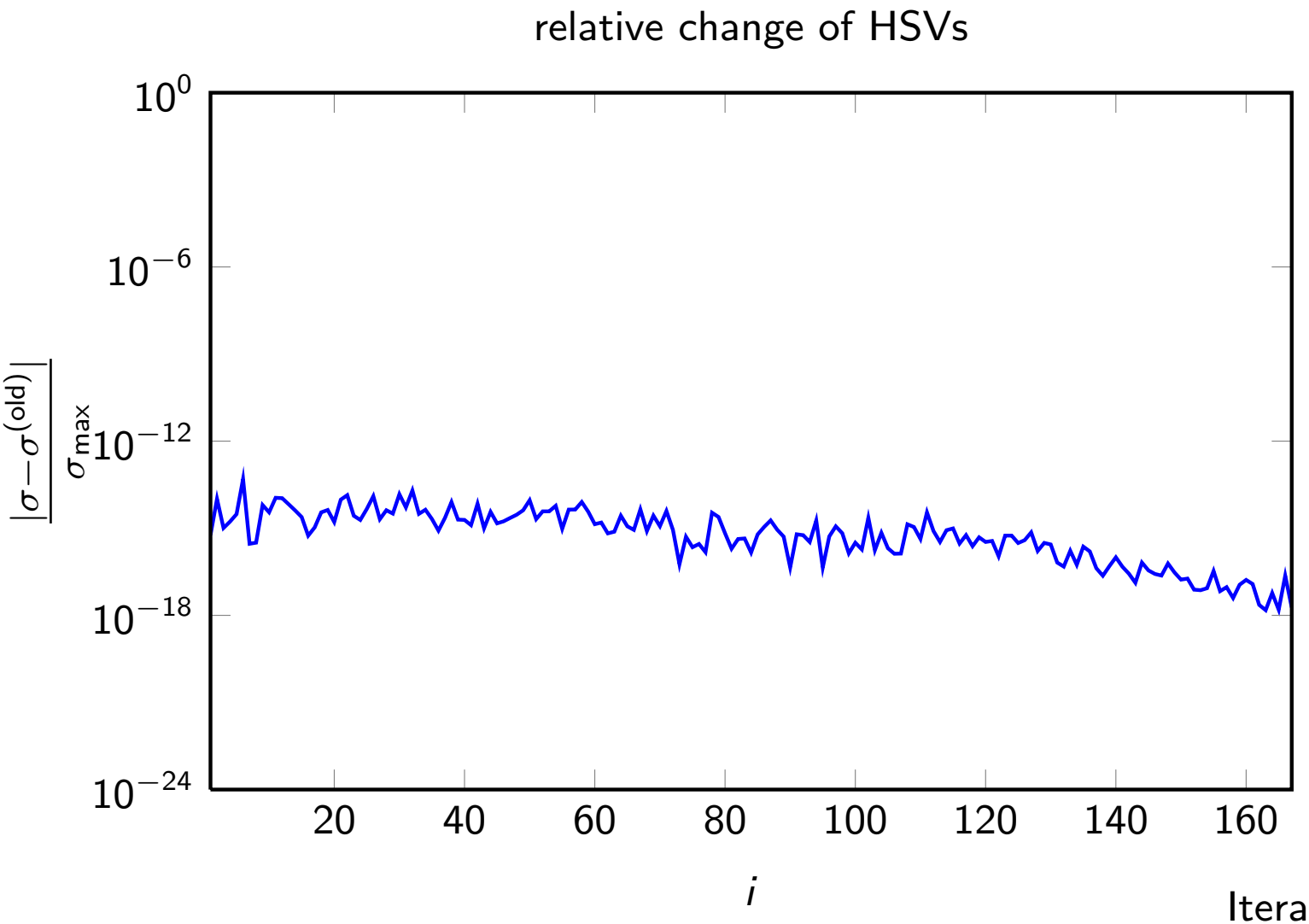
Rail Model



Iteration: 50

Numerical Results

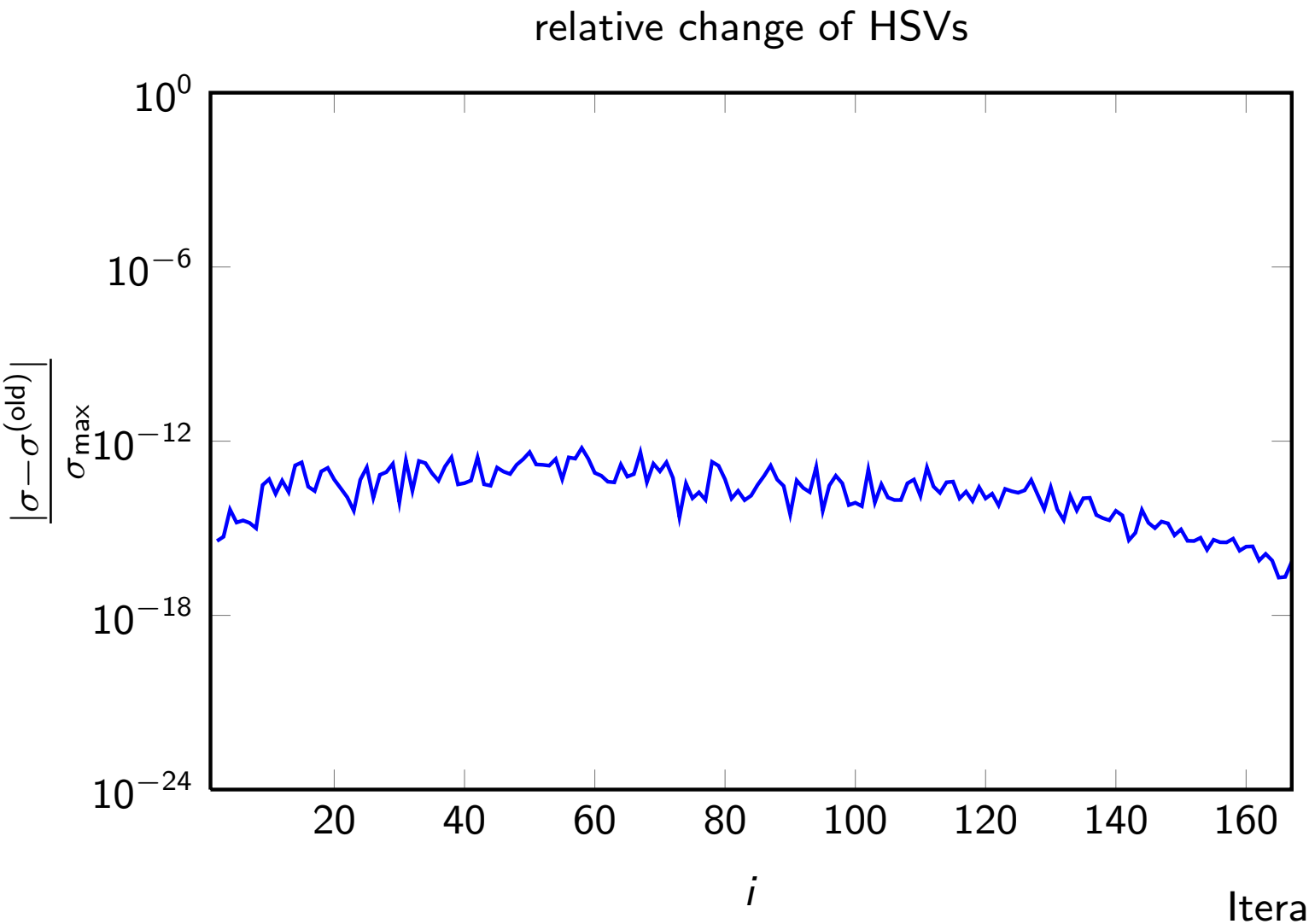
Rail Model



Iteration: 51

Numerical Results

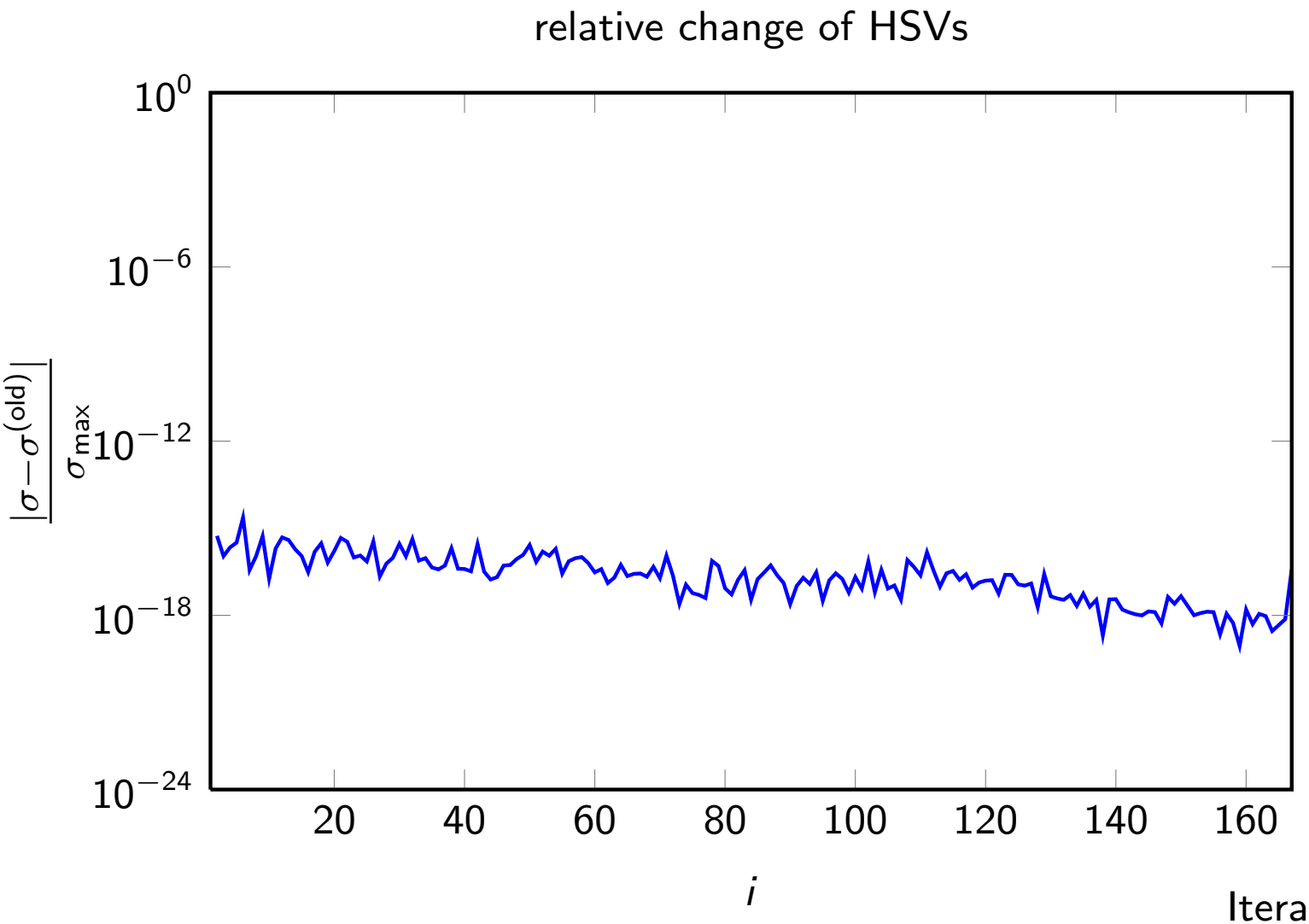
Rail Model



Iteration: 52

Numerical Results

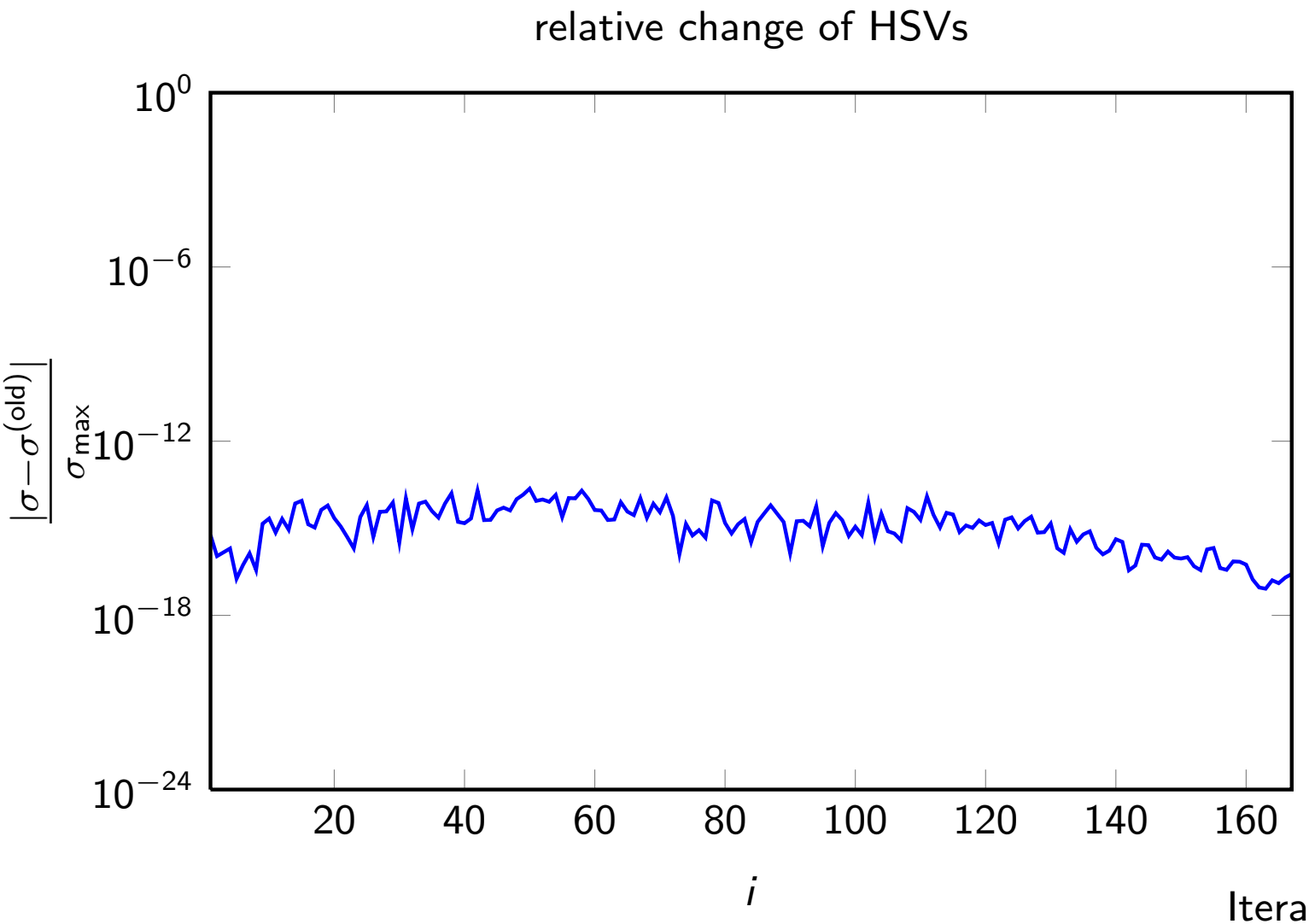
Rail Model



Iteration: 53

Numerical Results

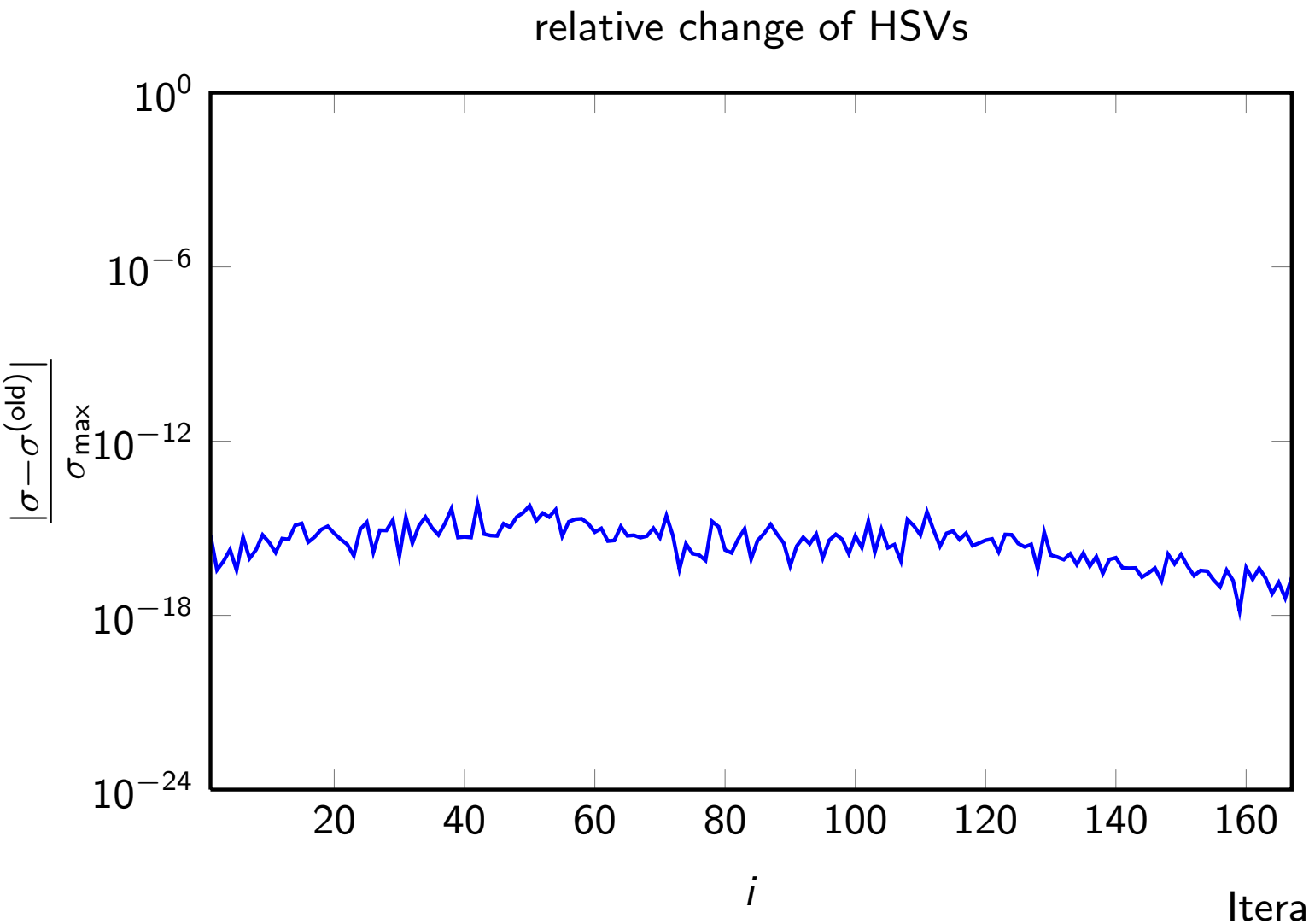
Rail Model



Iteration: 54

Numerical Results

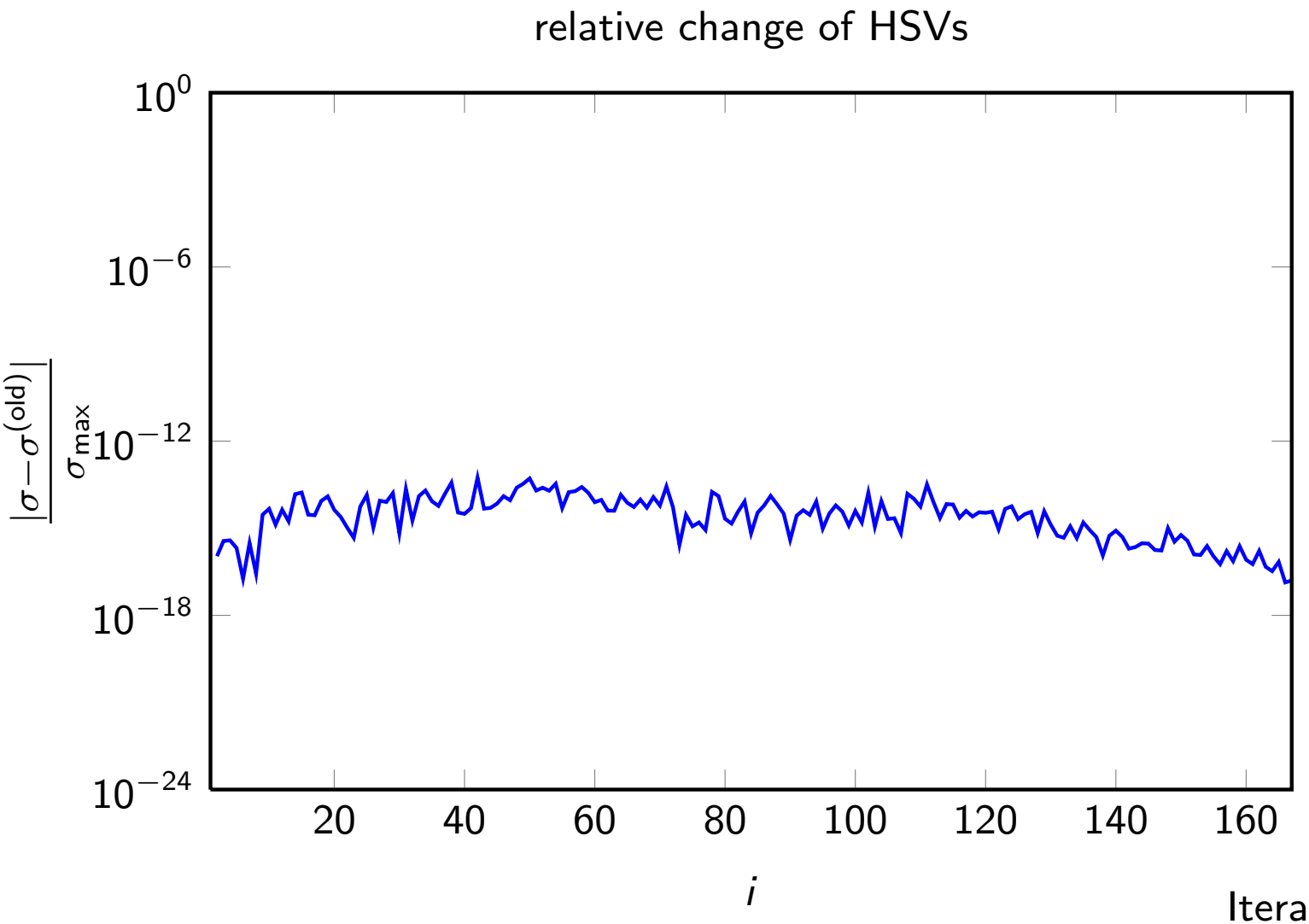
Rail Model



Iteration: 55

Numerical Results

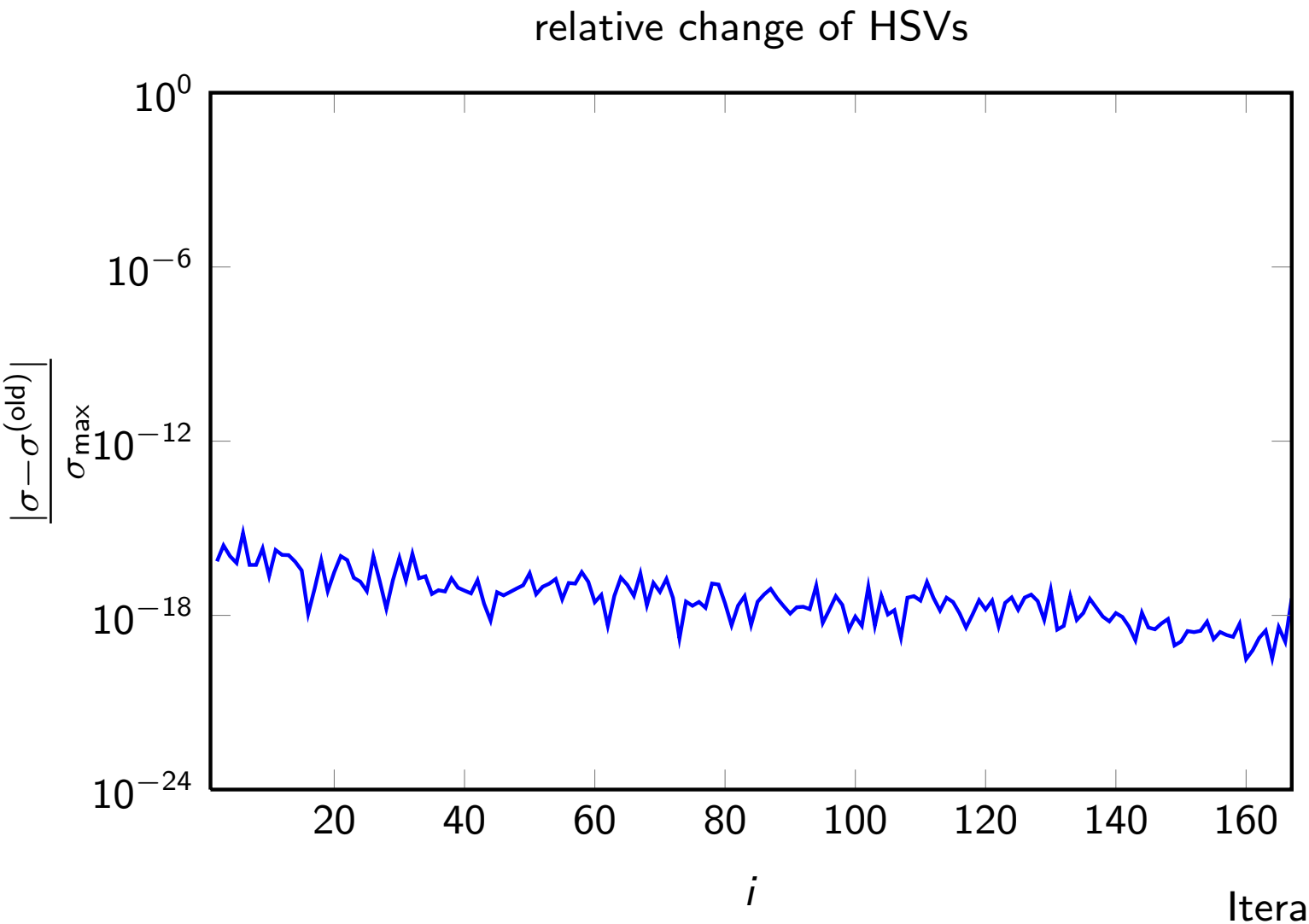
Rail Model



Iteration: 56

Numerical Results

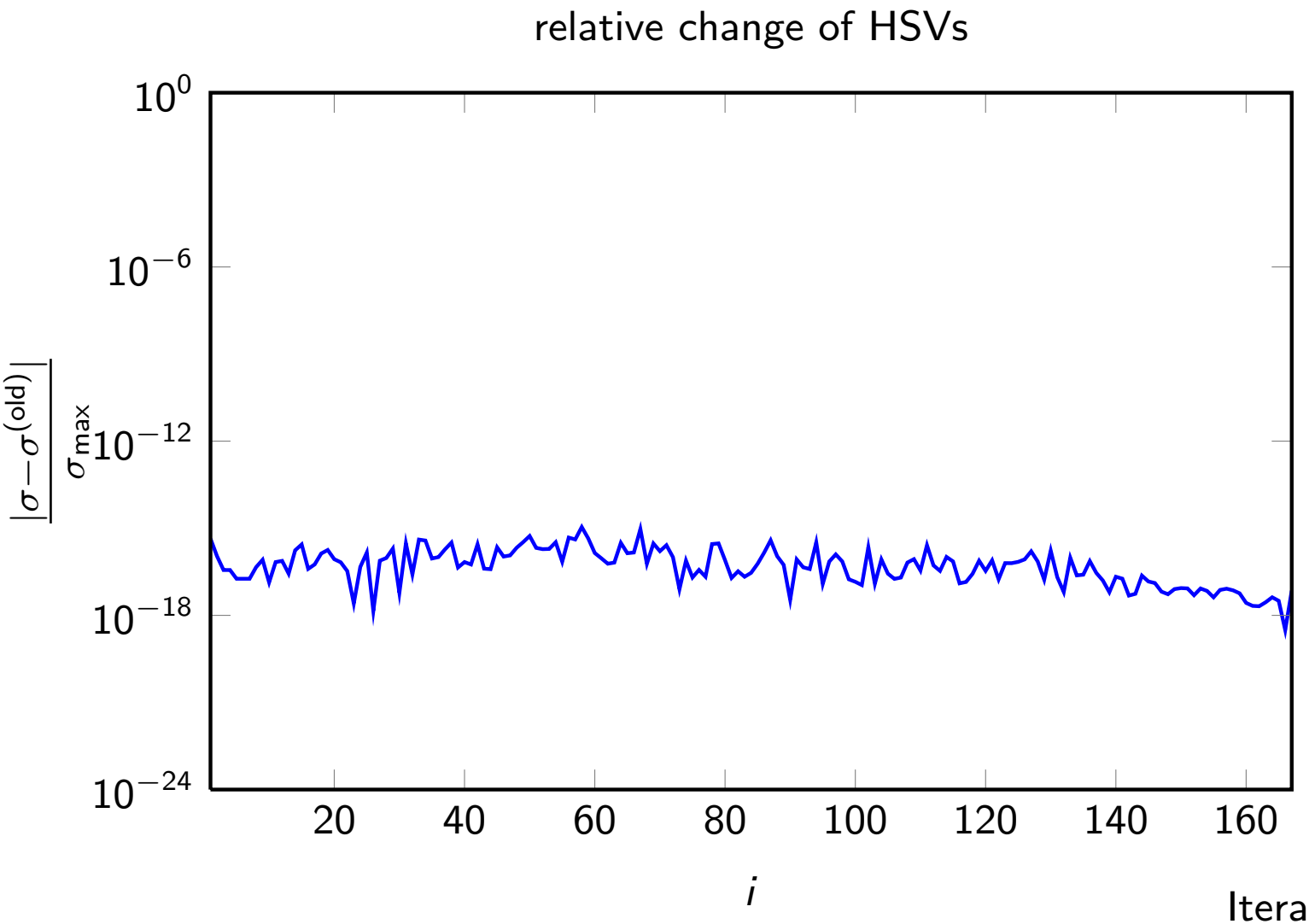
Rail Model



Iteration: 57

Numerical Results

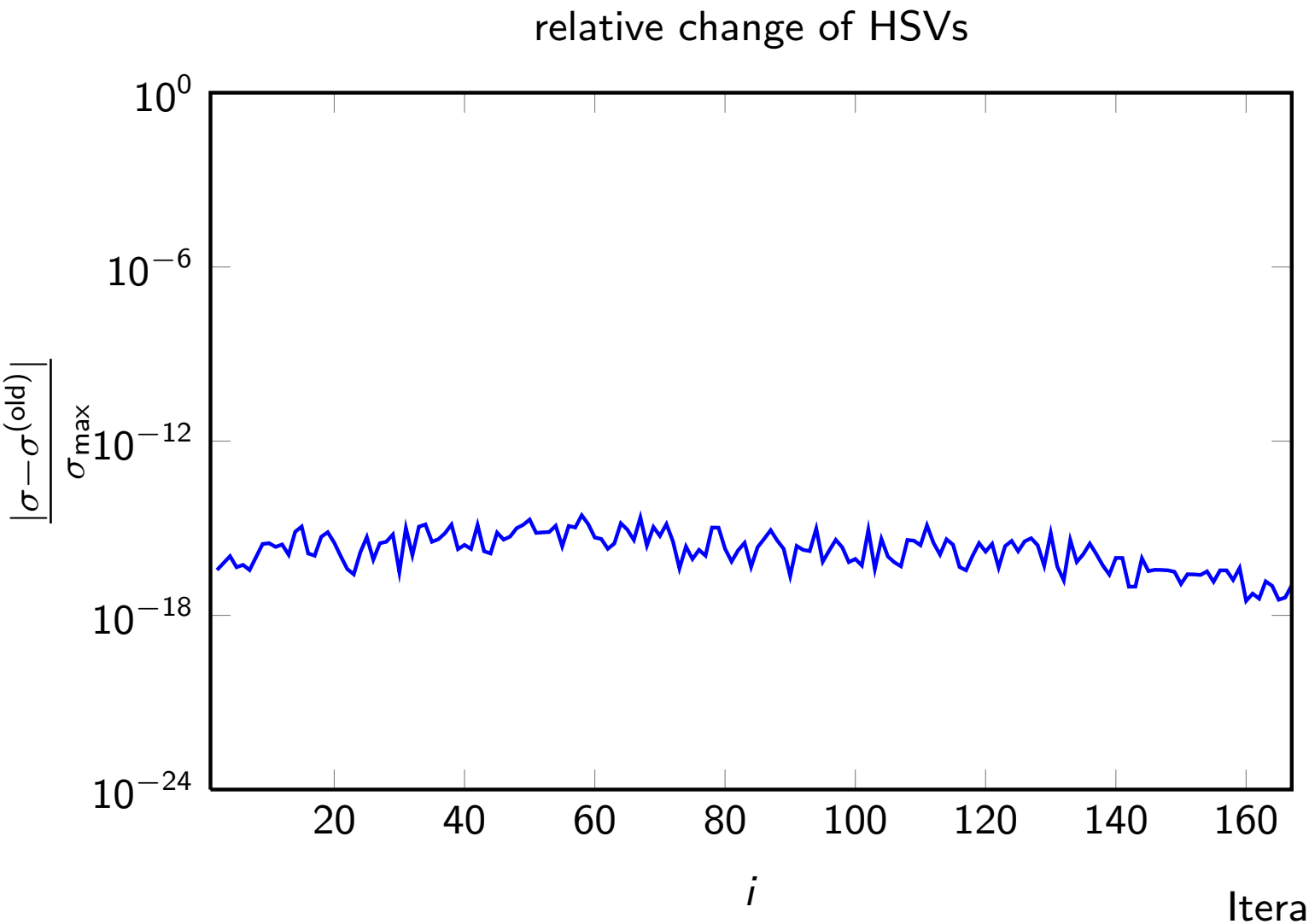
Rail Model



Iteration: 58

Numerical Results

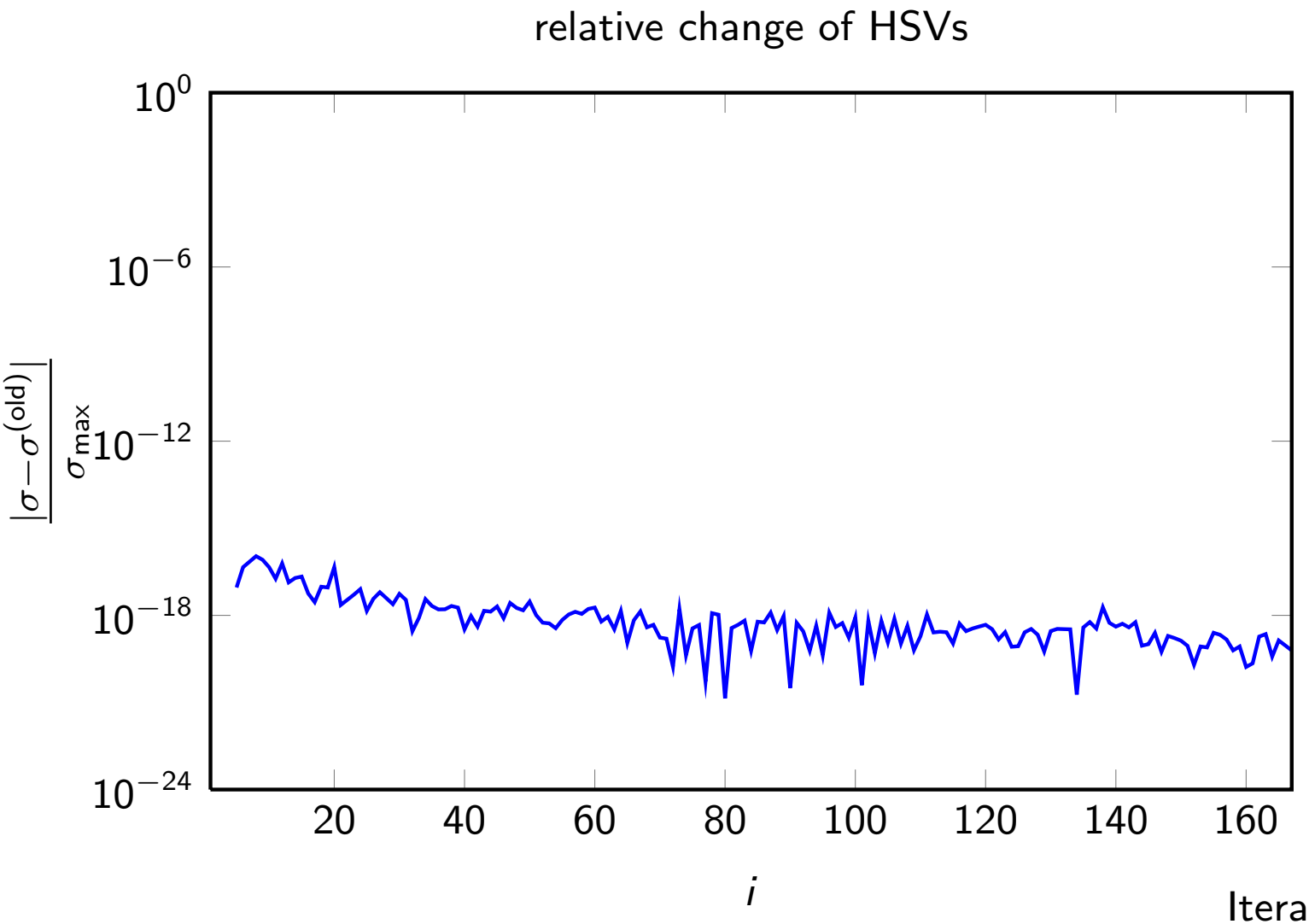
Rail Model



Iteration: 59

Numerical Results

Rail Model



Iteration: 60

Numerical Results

Rail Model

Observation

Leading HSVs converge from below.

Qualitative explanation:

- LRCF-ADI is a shifted rational Arnoldi process.
- HSVs are thus approximated via Ritz values.
- Ritz values converge to the eigenvalues from the inside of the spectrum.

Quantitative analysis: work in progress.

Numerical Results

BIPS07

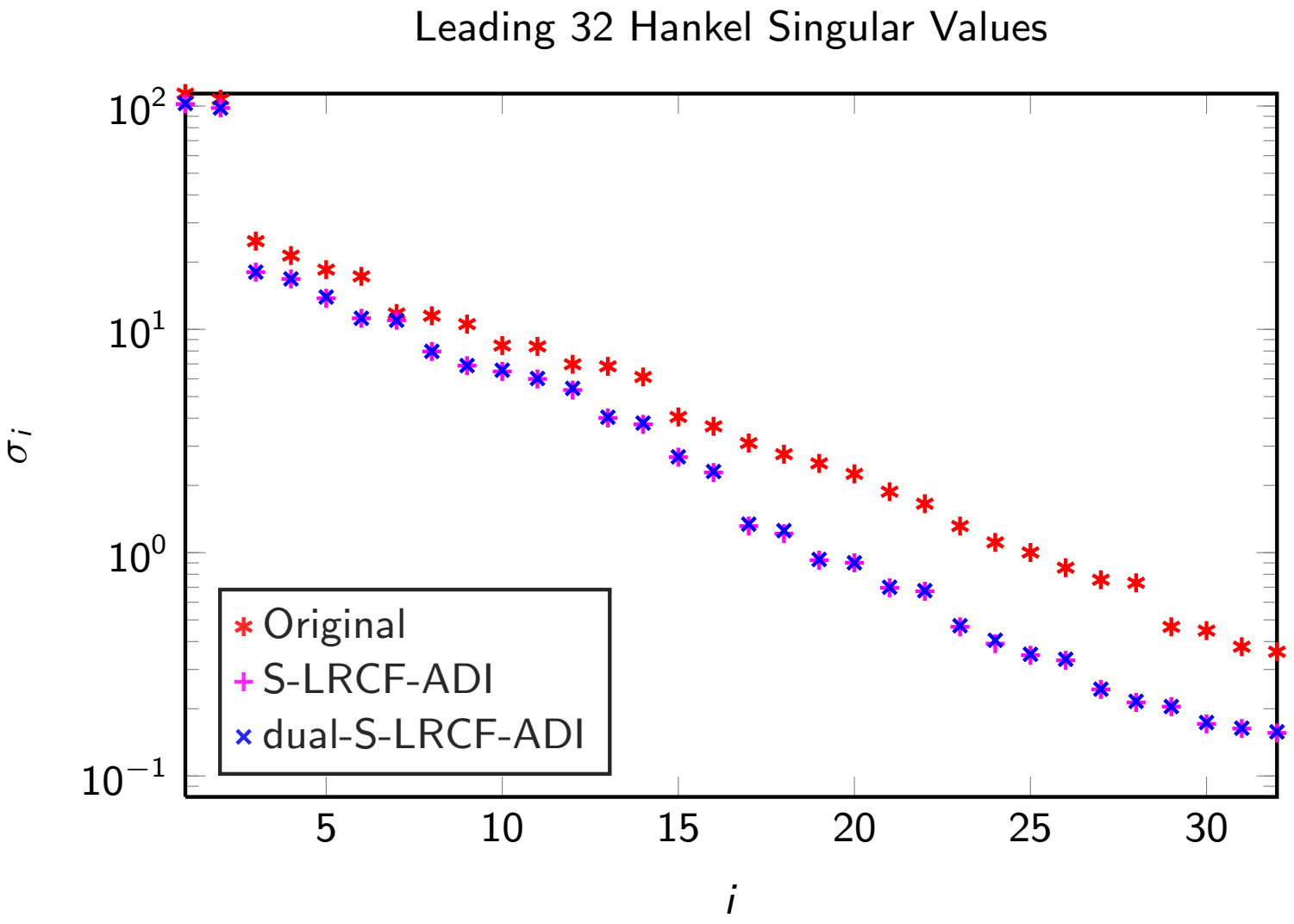
Test Setup

We take the same settings as in [Freitas/Rommes/Martins '08], i.e.:

- shift parameters
  - 50 Penzl shifts
  - from 80 Ritz values and 80 harmonic Ritz values
- reduced order model dimension 32
- maximum iteration number 80
- α-shifted S-LRCF-ADI with $\alpha = 0.05$

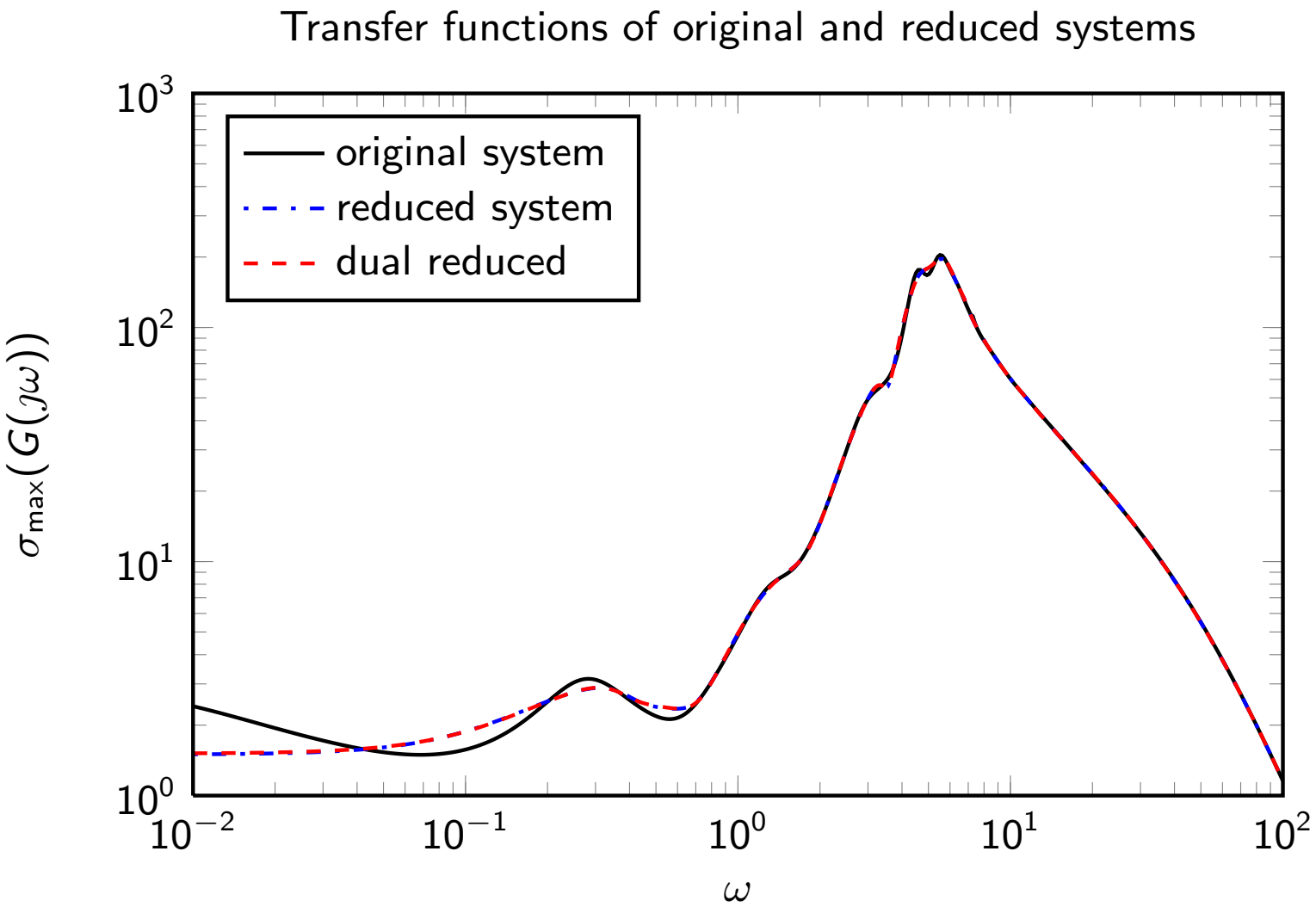
Numerical Results

BIPS07



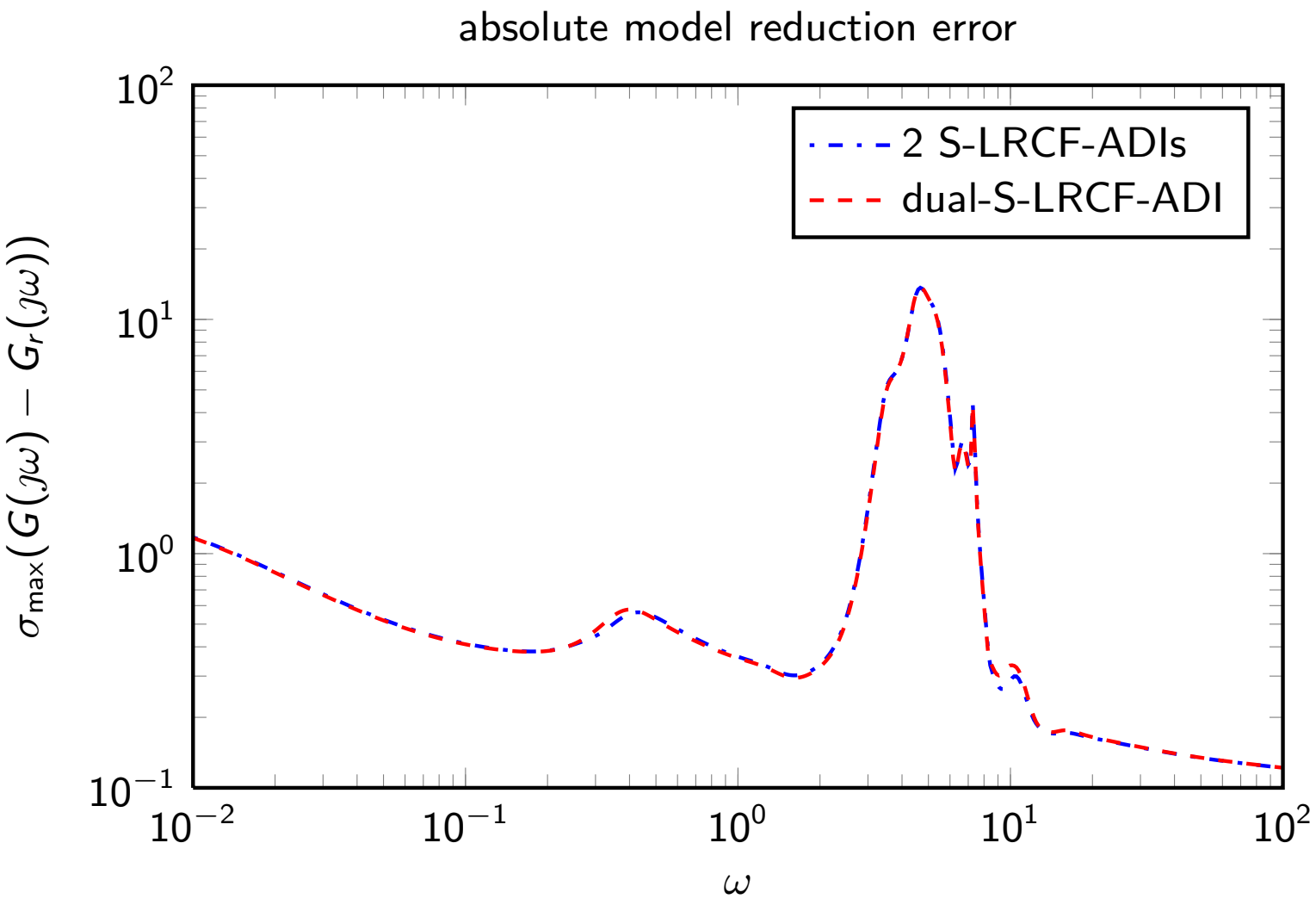
Numerical Results

BIPS07



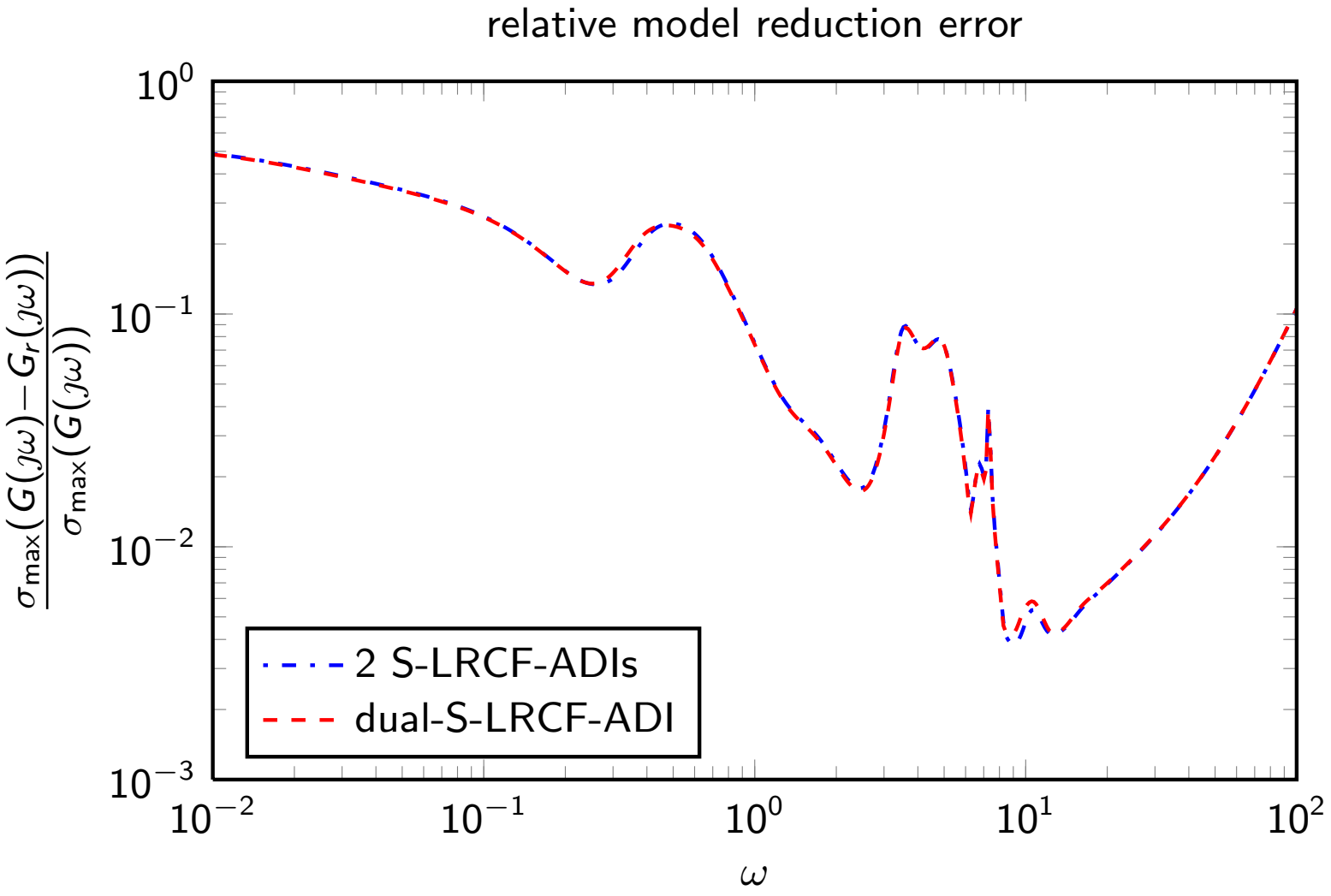
Numerical Results

BIPS07



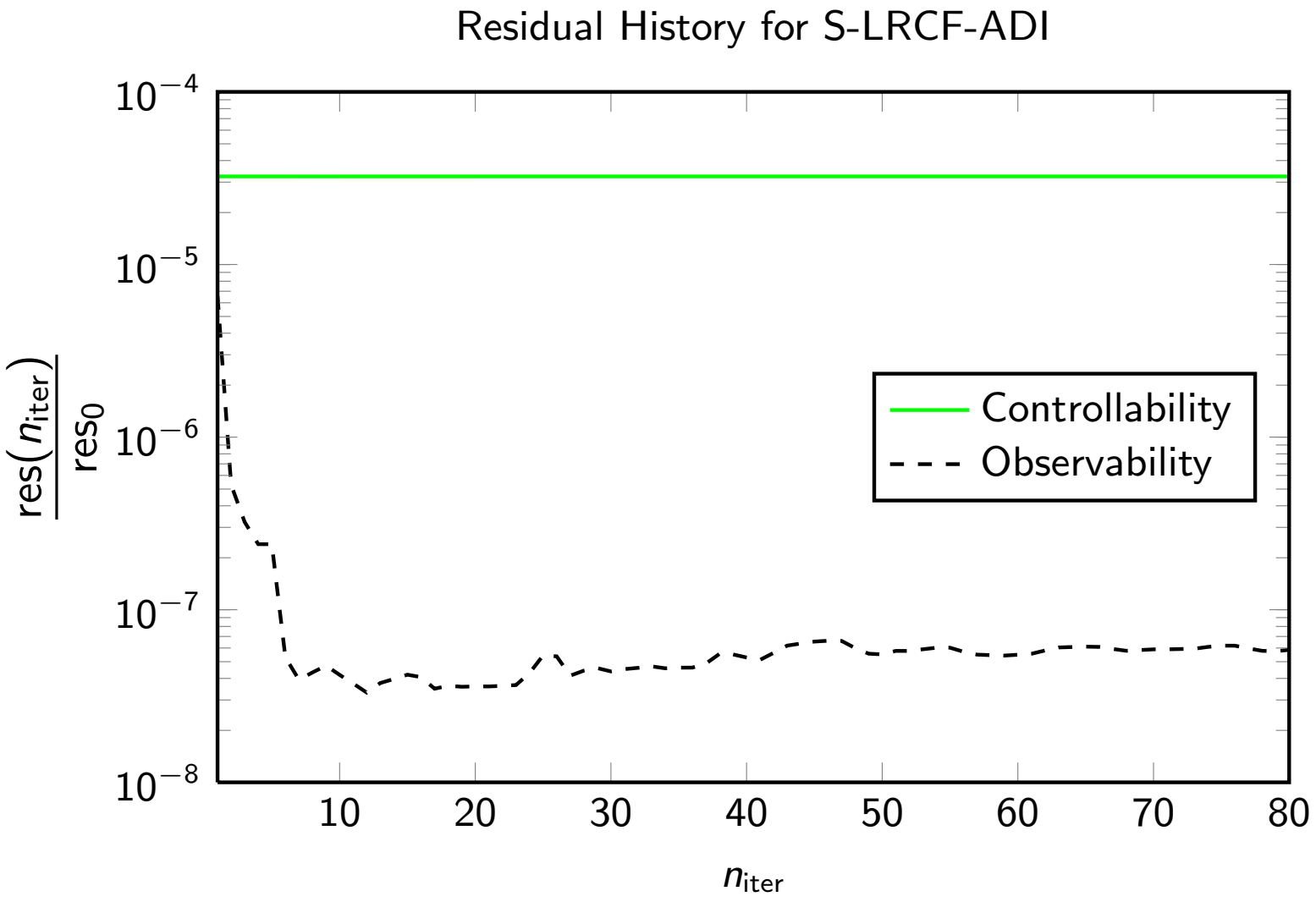
Numerical Results

BIPS07



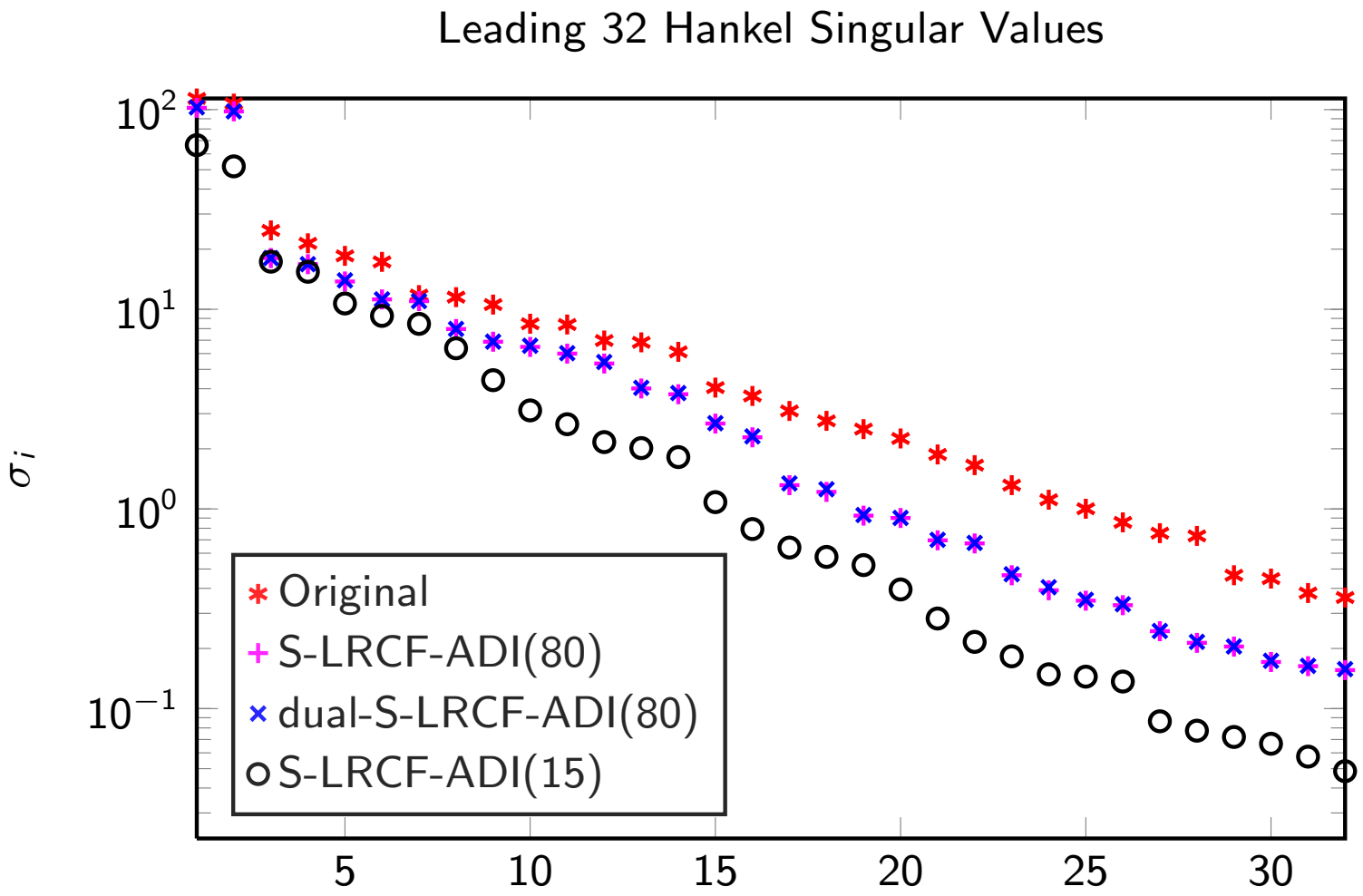
Numerical Results

BIPS07



Numerical Results

BIPS07



Do not trust residuals!

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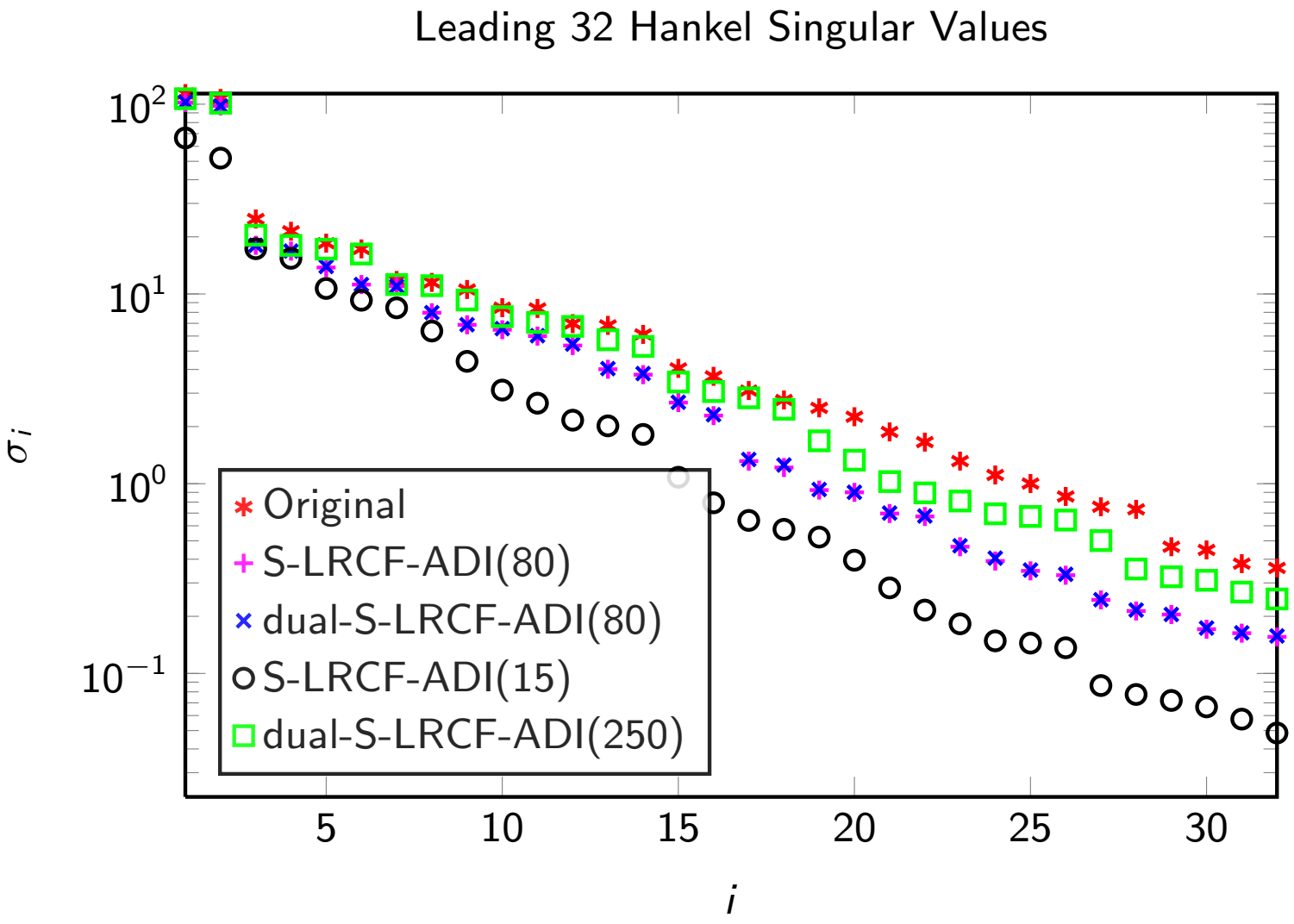
BIPS07



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BIPS07

maxiter	50	75	100	125	150
t_{dual} in s	2.97	5.22	7.31	10.33	14.72
$t_{\text{S-LRCF-ADI}}$ in s	19.87	27.82	37.03	47.65	58.97
speedup	6.68	5.33	5.06	4.61	4.01
change HSV	2.151e-1	1.123e-1	7.440e-2	6.579e-2	6.438e-2
final res. B	3.237e-5	3.237e-5	3.237e-5	3.237e-5	3.237e-5
final res. C	5.513e-8	6.194e-8	5.900e-8	5.778e-8	5.710e-8

	175	200	225	250
	20.20	29.99	39.34	52.51
	72.16	86.32	98.50	111.7
	3.57	2.88	2.50	2.13
	6.389e-2	6.282e-2	6.189e-2	6.058e-2
	3.237e-5	3.237e-5	3.237e-5	3.237e-5
	5.703e-8	5.706e-8	5.707e-8	5.710e-8

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Column compression via RRQR can reduce the SVD cost in the dual method:

$$\text{maxiter} = 250,\ \text{CC-frequency}{=}20,\ \text{RRQR-tolerance}{=}\text{eps} \rightsquigarrow t_{dual} \approx 37\text{s}$$

Conclusions and Future Perspectives

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- Simultaneous handling of the dual Lyapunov equations can drastically improve the performance.
- Goal oriented stopping criteria enhance the reliability of the results.

Future Work

- Quantify convergence results.
- Investigate reliable adaptive ROM dimension control.
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Thank you very much for listening.