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Supplementary Material

Supplementary Material for "NestedAE: Interpretable Nested Autoencoders for Multi-Scale Materials Characterization"

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In this supplementary material, we provide the functions and associated parameters of the synthetic dataset reported in the main article, a comparison of the latent structures between the NestedAE and single AE results, and a latent split analysis for the NestedAE architecture.

S1 ANALYTICAL FUNCTIONS COMPRISING THE SYNTHETIC DATASET

The 13 analytical functions that comprise the synthetic dataset are:

$$
\begin{aligned}
f_1(z_1, z_2; \epsilon_1) &= z_1^2 + z_2^2 - 2\, z_1 z_2 + \epsilon_1, \\
f_2(z_1, z_2; \epsilon_2) &= \sin z_1 + \cos z_1 + \sin 2z_1 + \cos 2z_1 + \sin z_2 + \cos z_2 + \sin 2z_2 + \cos 2z_2 + \epsilon_2, \\
f_3(z_1, z_2; \epsilon_3) &= \exp -z_1 + \exp -z_2 + \epsilon_3, \\
f_4(z_1, z_2; \epsilon_4) &= \tanh z_1 + \tanh z_2 + \epsilon_4, \\
f_5(\vec{z}; \epsilon_5) &= z_1 z_2 - z_3 - z_4 + \epsilon_5, \\
f_6(z_1, z_2, z_5; \epsilon_6) &= \sin z_1 z_2 + \sin 2z_5 + \epsilon_6, \\
f_7(z_3, z_4, z_5; \epsilon_7) &= \exp -\frac{(z_3^2 + z_4^2 + z_5^2)}{z_3 + z_4 + z_5} + \epsilon_7, \\
f_8(z_1, z_2, z_3; \epsilon_8) &= \tanh z_1 + \tanh z_2 + \tanh z_3 + \tanh z_4 + \tanh z_5 + \epsilon_8, \\
f_9(\vec{z}; \epsilon_9) &= \log z_1 + \log |z_2| + \log z_3 + \log z_4 + \log z_5 + \epsilon_9, \\
f_{10}(\vec{z}; \epsilon_{10}) &= z_1^2 + z_2^2 - 2\, z_1 z_2 + z_3^2 + z_4^2 + z_5^2 - z_3 z_4 z_5 + \epsilon_{10}, \\
f_{11}(z_1, z_5; \epsilon_{11}) &= \sin z_1 + \sin z_5 + \epsilon_{11}, \\
f_{12}(\vec{z}; \epsilon_{12}) &= \frac{1}{24}\left(z_1^4 - 16\, z_1^3 + 72\, z_1^2 - 96\, z_1 + 24\right) + \\
&\quad \frac{1}{24}\left(z_2^4 - 16\, z_2^3 + 72\, z_2^2 - 96\, z_2 + 24\right) + \\
&\quad \frac{1}{24}\left(z_3^4 - 16\, z_3^3 + 72\, z_3^2 - 96\, z_3 + 24\right) + \\
&\quad \frac{1}{24}\left(z_4^4 - 16\, z_4^3 + 72\, z_4^2 - 96\, z_4 + 24\right) + \\
&\quad \frac{1}{24}\left(z_5^4 - 16\, z_5^3 + 72\, z_5^2 - 96\, z_5 + 24\right) + \epsilon_{12}, \\
f_{13}(\vec{z}; \epsilon_{13}) &= z_1^2 + z_2^2 + z_3^2 + z_4^2 + z_5^2 + \epsilon_{13}.
\end{aligned}
$$

where the ϵ_i represent noise. In the noiseless limit, $\epsilon_i = 0$ for all i. We also considered a Gaussian noise case in which $\epsilon_i \in \mathcal{N}(0, \sigma_i)$ where $\mathcal{N}$ represents a Gaussian distribution with width σ_i. In this work, we set $\sigma_i = 0.5$ for $i \in (1, \ldots, 4)$ and $\sigma_i = 1.0$ for $i \in (5, \ldots, 13)$.

The range for z_1 through z_5 is set to:

$$
\begin{aligned}
z1 &= [0.01, 5.0], \\
z2 &= [2.0, 5.0], \\
z3 &= [0.5, 10], \\
z4 &= [0.5, 10], \\
z5 &= 10 * \mathrm{U}(0, 1),
\end{aligned}
$$

where $\mathrm{U}(0, 1)$ represents a uniform distribution between (0,1).

S2 LATENT SPACE ANALYSIS FOR SYNTHETIC DATASET

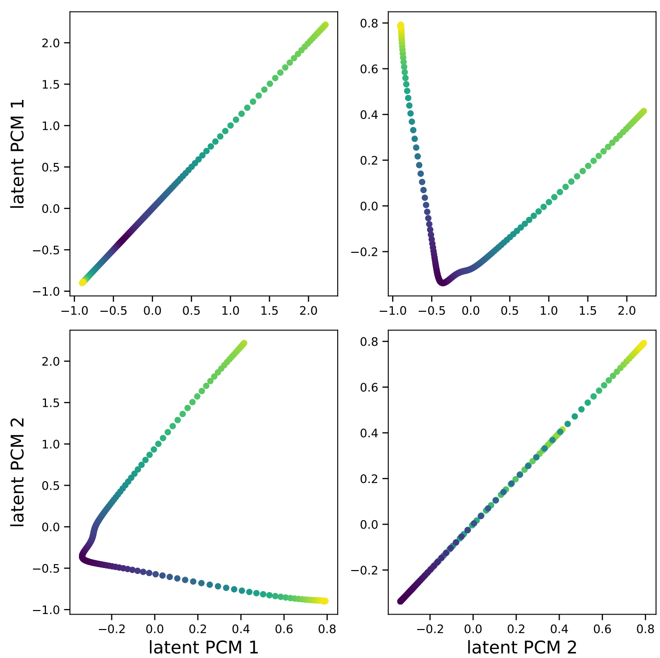

Figure S1: Latent space structures obtained from training the first autoencoder in the NestedAE architecture. The latent space is colored based on the L_2 norm of the 13 analytical functions described in Sec. S1. The x- and y-axes denote the Principal Component Modes (PCMs) of the latent space.

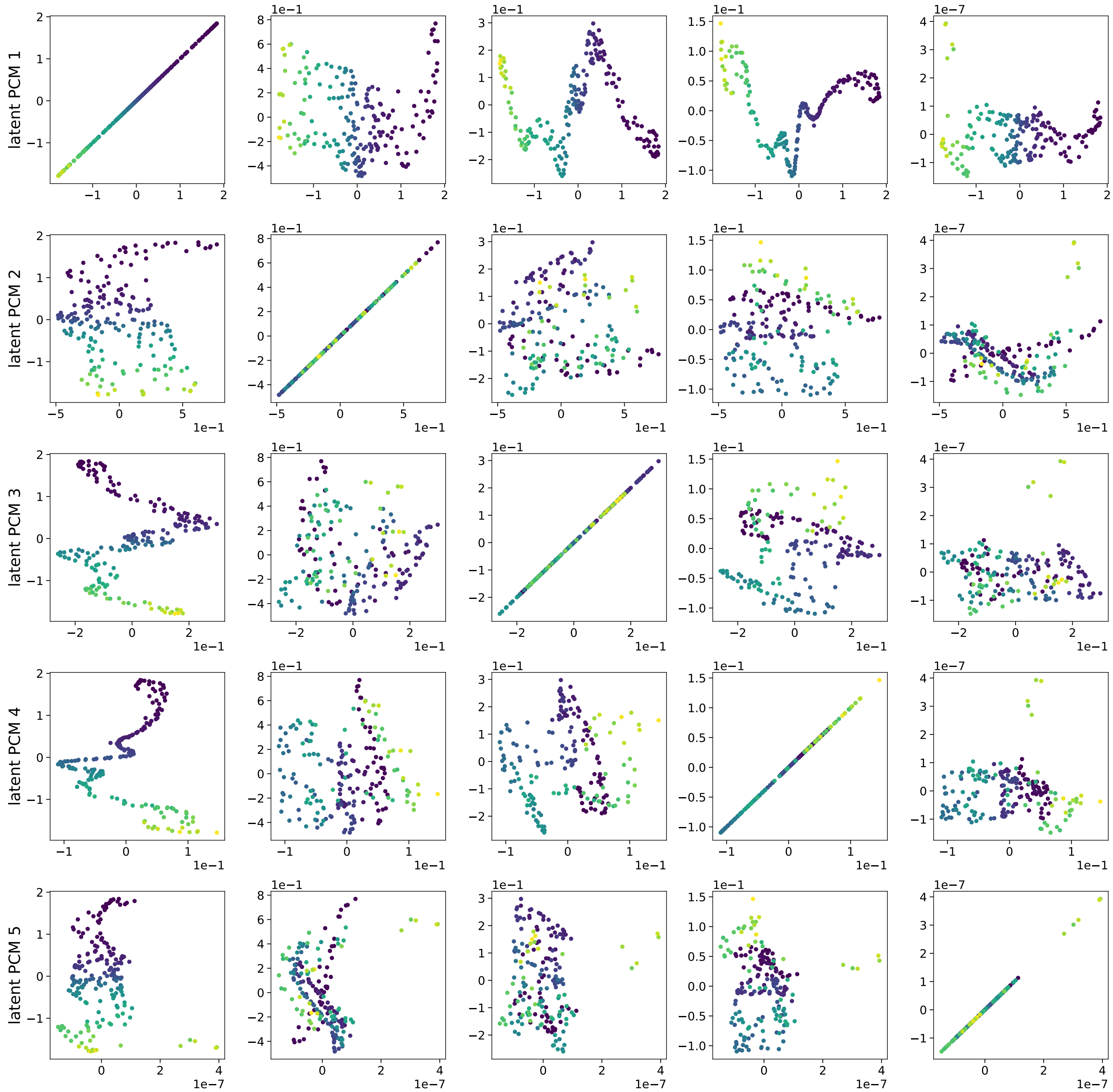

Figure S2: Latent space structures obtained from training the second autoencoder in the NestedAE architecture. The latent space is colored based on the L_2 Norm of the 13 analytical functions described in Sec. S1. The x- and y-axes denote the PCMs of the latent space.

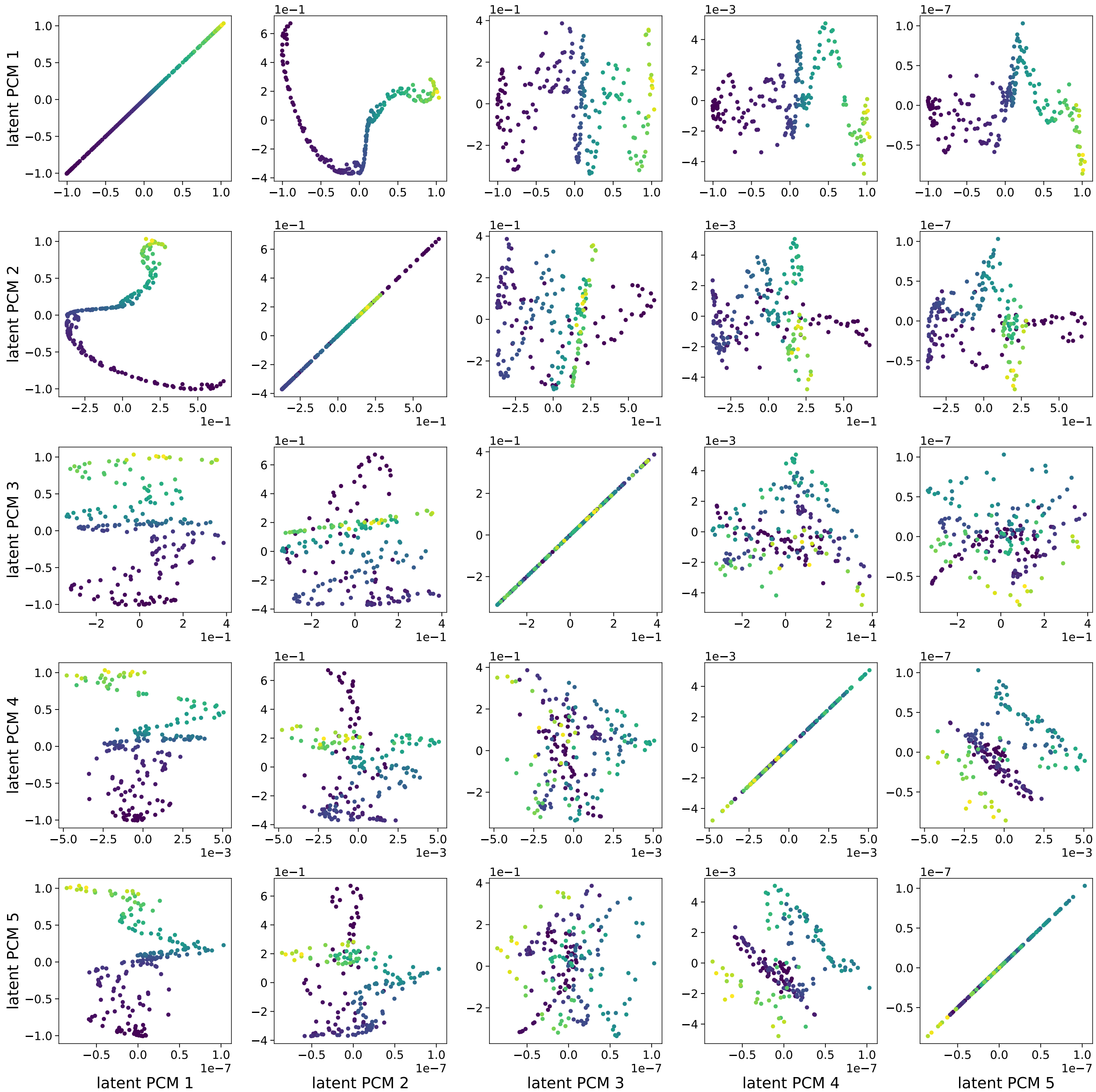

Figure S3: Latent space structures obtained from training a single autoencoder on the constructed synthetic dataset. The latent space is colored based on the L_2 Norm of the 13 analytical functions described in Sec. S1. The x- and y-axes denote the PCMs of the latent space.