AI-Based Digital Rocks Augmentation and Assessment Metrics

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Abstract

Reliable uncertainty model calculation in subsurface engineering from pore- and grain-scale to field-scale relies on sufficient data, but subsurface dataset acquisition remains a challenge, particularly in domains where data collection is expensive or time-consuming, such as Computed Topography (CT) imaging for digital rock images. While AI-based data augmentation may assist the model training, it still requires many training images as well as the quality assessment of generated data. Yet, most data quantitative metrics flatten spatial data into vectors; therefore, removing the essential spatial relationships within the data. We evaluate topology-based metrics for quality assessment of AI-based image augmentation, coupled with digital rocks augmentation practice using the Single image Generative Adversarial Network (SinGAN) for binarized (segmented) images. Compared to most traditional dimensionality reduction methods that process images into a flattened vector, we propose topological image analysis for dimensionality reduction while preserving the essential geometric and topological features of the high-dimensional data. To demonstrate our proposed approach, we evaluate the generated images starting from four distinct digital rock samples, sorted sandstone, synthetic sphere pack, limestone, and poorly sorted sandstone, using Minkowski functionals, image graph network-based measures, graph Laplacian-based measures, local trend maps, and a homogeneity-heterogeneity classifier. Our workflow suggests that AI-based digital rock augmentation, combined with topological dimensionality reduction offers a powerful tool for enhanced quality assessment and diagnostic of digital rock augmentation and improved interpretation to support decision-making.
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Key Points:
- The single-image GAN shows good performance for digital rock augmentation.
- We recommend Minkowski functionals, pore-throat graph network measures, and Laplacian graph measures for the assessment of AI-based digital rocks image augmentation.
- Topological and graph connectivity measures are important for assessing imaged spatial datasets.

Abstract
Reliable uncertainty model calculation in subsurface engineering from pore- and grain-scale to field-scale relies on sufficient data, but subsurface dataset acquisition remains a challenge, particularly in domains where data collection is expensive or time-consuming, such as Computed Topography (CT) imaging for digital rock images. While AI-based data augmentation may assist the model training, it still requires many training images as well as the quality assessment of generated data. Yet, most data quantitative metrics flatten spatial data into vectors; therefore, removing the essential spatial relationships within the data. We evaluate topology-based metrics for quality assessment of AI-based image augmentation, coupled with digital rocks augmentation practice using the Single image Generative Adversarial Network (SinGAN) for binarized (segmented) images. Compared to most traditional dimensionality reduction methods that process images into a flattened vector, we propose topological image analysis for dimensionality reduction while preserving the essential geometric and topological features of the high-dimensional data. To demonstrate our proposed approach, we evaluate the generated images starting from four distinct digital rock samples, sorted sandstone, synthetic sphere pack, limestone, and poorly sorted sandstone, using Minkowski functionals, image graph network-based measures, graph Laplacian-based measures, local trend maps, and a homogeneity-heterogeneity classifier. Our workflow suggests that AI-based digital rock augmentation, combined with topological dimensionality reduction offers a powerful tool for enhanced quality assessment and diagnostic of digital rock augmentation and improved interpretation to support decision-making.

1 Introduction

Training data acquisition has been a challenge for AI model training, because of the general lack of training data, the increasing demand for training data with the wider application of AI, and the high cost to acquire data (Li et al., 2021; Roh et al., 2021). While this is the case for many
types of AI modeling, one important example relevant to digital rock physics is high-resolution imaging of porous media, such as X-ray Micro-computed tomography (Micro-CT, see review in Wildenschild & Sheppard, 2013), which is time-consuming especially for high-resolution scans and results in limited data acquisition with scanning one sample at a time.

The development of generative AI has made it possible to generate similar-looking data due to its ability to learn complex image patterns, motivating the application of AI for image augmentation. AI-generated data mimics real-world data but is not sampled from natural observations. A common architecture for image generation is the Generative Adversarial Network (GAN), composed of a generator and a discriminator, both are made up of neural networks (Goodfellow et al., 2014). The GAN-related developments have been applied for image augmentation in various fields, such as in the medical imaging domain to improve disease diagnosis (Frid-Adar et al., 2018), in agriculture to increase production efficiency (Bird et al., 2022), and in petroleum engineering to interpret the petrophysical properties (Mosser et al., 2017).

A common pitfall of these practices is that these GAN-related developments require many training images for training the architecture. The emergence of Single-image GAN (SinGAN) brought the idea of training with a single image to generate multiple images statistically similar to the original one (Shaham et al., 2019).

While GANs have been widely applied for digital porous data augmentation, one of the unsolved problems is assessing how similar the generated images are to the real images, and it appears that the definitions or metrics of “similar” are somewhat different for different researchers. The current practices apply various dimensionality reduction methods to visualize the similarity between generated images and real images (Feng et al., 2019; Fokina et al., 2020; L. Mosser et al., 2018; Phan et al., 2024; Sahimi & Tahmasebi, 2021). A common image processing method is to flatten the high-dimensional image to a one-dimensional vector and then lower the dimensionality, which removes the geometric and topological information associated with the images. Porous materials, whether in subsurface or material sciences (e.g., batteries) are special because they are bi-continuous in 3D, that is, both solid and pore spaces span across the sample. They further interact through a complex interface of a large specific area. Those two factors profoundly affect all types of transport through fluid and solid phases in porous materials and are important to reproduce in data augmentation and account for in imaged data metrics.

Table 1. Summary of previous work: goals, methods, and metrics.

<table>
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<tr>
<th>Methods and dimensionality</th>
<th>Data metrics for assessing similarity</th>
<th>Citation</th>
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<tr>
<td>CDBN, reconstruct 2D pore samples using 2D pore structure images</td>
<td>Visual interpretation</td>
<td>Cang et al. (2017)</td>
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<tr>
<td>DCGAN, generate 3D realistic porous media representations similar to the 3D training dataset</td>
<td>Two-point probability function; grain and pore chord length; Minkowski functionals, flow simulation (permeability and velocity distributions)</td>
<td>Mosser et al. (2017)</td>
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GAN, case study on 3D porous media samples generation using 3D images

<table>
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<th>Method</th>
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<td>GAN</td>
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<td>Liu et al. (2019)</td>
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<td>CGAN, generate 2D images using 2D training data</td>
<td>Visual interpretation, porosity, two-point correlation function, linear path function, chord-length distribution function, two-point cluster function</td>
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<tr>
<td>StyleGAN, generate more realistic-looking 2D porous media images using 2D training data</td>
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<td>Fokina et al. (2020)</td>
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<tr>
<td>GAN Auto-Encoder (GAN-AE), reconstruct 3D multi-scale porous media images based on 3D training data</td>
<td>Porosity, two-point correlation function, flow simulation (permeability)</td>
<td>Shams et al. (2020)</td>
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Table 1 shows a concise summary of metrics previously applied to check AI-based generated data. Cang et al. (2017) propose a Convolutional Deep Belief Network (CDBN) for microstructure reconstruction. They reconstruct porous samples by training four different microstructure samples (Ti-6Al-4V alloy, Pb-Sn alloy, sandstone, and spherical colloids) and check the results with visual inspection. Mosser et al. (2017) demonstrate the use of GAN for 3D porous media image reconstruction. They extract overlapped subsets from the original volumetric data as training images and generate random samples through Deep Convolutional GAN (DCGAN). Their evaluation criteria include metrics based on two-point statistics and Minkowski functionals. A similar 3D porous media image reconstruction is conducted by Liu et al. (2019) where they conduct a visual inspection of the generated data. Fokina et al. (2020) generate Alporas aluminum foam images using Style-based GAN (StyleGAN) which incorporates the style transfer method in the GAN architecture (Karras et al., 2019) and compare the Minkowski functionals between generated images and original images. Shams et al. (2020) use porosity, auto-correlation function, and permeability to evaluate the quality of reconstructed sandstone through GAN.

Feng et al. (2019) provide a comprehensive assessment of image reconstruction and experiment with AI generation of 2D images of a silica sample, battery material, sandstone sample, and an artificial anisotropic porous material sample through conditional GAN (CGAN) and check the performance using porosity and morphological functions, including two-point correlation function, lineal path function, chord-length distribution function, and two-point cluster function, which mainly focus on two-point statistical relationships. This previous work demonstrates dimensionality reduction metrics do not generally account for the topology (including connectivity of the phases) of the image and more accurate topological metrics are needed for the quality assessment of AI-based generated images of porous materials.

We propose the adoption of SinGAN for digital rock data augmentation and the use of topological dimensionality reduction metrics for AI-based digital rock augmentation that preserve essential spatial structural information. We demonstrate our proposed workflow through data
augmentation for four typical digital rock samples using SinGAN. The four samples are sorted sandstone, silica sphere packing, limestone, and fluvial graded sandstone, all open data available on the Digital Rocks Portal (Sheppard & Schroeder-Turk, 2015). We evaluate the quality of generated images using topological and geometric metrics: Minkowski functionals, graph network-based measures, Laplacian graph-based measures, local trend measures, homogeneity-heterogeneity classifier, and principal component analysis (PCA), all contributing to dimensionality reduction, quality and similarity analysis of AI-based data augmentation.

The materials and methods section introduces details of the assessment metrics, followed by the data sources. The results and discussion section presents the assessment results of four training image cases and related analysis. Finally, the conclusions section summarizes the main contributions of this work and gives recommendations for future work.

2 Materials and Methods

Beginning from binarized (segmented) images, i.e. those where image pixels have been classified into two different phases (referred to as 0 or 1, foreground or background, pore and solid, etc. in literature), one has a choice of working with either phase when calculating different measures described below. The topological quality assessment metrics start with the Minkowski functionals of a selected phase, and extend to graph network-based measures, graph Laplacian-based measures, local trend map, homogeneity-heterogeneity classifier, and eventually assisted with dimensionality reduction analysis using principal component analysis (PCA). We work with the solid phase except for porosity. Below are details about the calculation of some of the imaged data assessment metrics.

Minkowski functionals

Minkowski functionals is a family of morphological measures to describe geometry and topology. In d-dimensional space, there exists a basis set of d + 1 intrinsic values that quantify geometry (Hadjwiger, 2013; Mecke & Stoyan, 2000), and more recent reviews for their use as descriptors of porous materials are available (Armstrong et al., 2018; Arns et al., 2010). For 2D images, the three measures \( M_i \) are the area (A in Equation 1) which implies porosity, contour length of the boundaries between pores and solids (L in Equation 2), and Euler characteristic (Equation 3), an indicator of connectedness (topology) of a system. We use QuantImPy, an opensource Python package to perform Minkowski functionals calculation (Boelens & Tchelepi, 2021).

\[
\begin{align*}
M_0 &= \int_{\Omega} dA' = A \\
M_1 &= \int_{\delta X} dL' = L \\
M_2 &= \int_{\delta X} \frac{1}{r} dL' = 2\pi \chi
\end{align*}
\]

where \( \Omega \) is the total image area, \( \delta X \) represents the boundary of the foreground pixels, \( r \) is the local connected pixel radius, and \( \chi \) is the Euler number.
Graph network-based measures

The graph network-based measures are topological calculations based on the pore-throat (or solids and grains) network of the image (the left of Figure 1 is a grain network example). The geometry of the pore space can often be simplified as pores (larger openings) that are connected by throats (tight spots). The history of pore network analysis in porous media dates back to the bundle of tubes models in the 1920s for flow (Blunt, 2017), and a historical review of the approaches that reduce imaged pore space to a pore-throat network can be found in Mehmani et al (2019). Once we have a network, we have a graph of grain centers (nodes) connected by links, and the graph can be quantified using different graph theory measures. The offdiagonal complexity (OdC) is used to measure the network complexity (Claussen, 2007; Mehmani & Prodanović, 2014). In other words, the OdC of a pore network model is indicative of pore connectivity and the complexity of those connections. High OdC suggests there may be many pathways between pores; OdC was successfully used to characterize the connectivity of different types of complex porous media with microporosity arising from partial dissolution of grains vs. microporosity within original pores (Mehmani & Prodanović, 2014). To accomplish the calculation of OdC, the pore throat network is first extracted using the Python implementation of the SNOW algorithm from Porespy (Gostick et al., 2019) based on the watershed segmentation (Gostick, 2017). Then the adjacency matrix (Figure 1, right) is calculated based on the pore throat network, where the main diagonal elements represent self-connections and the off-diagonal elements represent the connections between different nodes. Then the complexity can be proxied by the entropy of the off-diagonal elements.

Another classical, graph network-related measure is the cost of the minimum spanning tree. The minimum spanning tree (MST) is a subset of the graph that connects all vertices together with the minimum possible total edge weights, and the cost is the sum of the weights of all the edges of a MST (Kruskal, 1956). The cost of MST can be indicative of the similarities in network design (Tewarie et al., 2015). In our application, we assign all edges the weight of one.

The third measure is the average degree of the graph, which reflects the ratio of the total number of edges and the total number of nodes in the graph (Equation 4).

![Figure 1](image_url)

**Figure 1.** The graph network of the grain (white) phase in an image and its associated adjacency matrix (left and right, respectively).

\[
\text{average degree} = \frac{2E}{N} \tag{4}
\]

where E refers to the total number of edges and N refers to the total number of nodes in a graph.
The Laplacian graph-based measures are from the eigenvectors of the graph Laplacian matrix \( L \), a subtraction of the adjacency matrix \( A \) from the degree matrix \( D \) of the graph (Equation 5).

\[
L = D - A
\]  

where \( D \) is a diagonal matrix where each element \( D_{ii} \) on the diagonal equals the degree of vertex \( i \), which is the number of edges connected to \( i \). The graph Laplacian summarizes the network and the associated eigenvalues provide useful information summarization, including the number of clusters to separate the graph based on its connections (Merris, 1998). Figure 2 shows a Laplacian matrix example given the pore throat network in Figure 1, and curve ACB in the right figure shows the ordered eigenvectors. We calculate the Lorenz coefficient of the eigenvalues curve, the ratio of area ABCA and area ACBDA, as an indicator of the connectedness of the graph.

Figure 2. For the grain network in Figure 1, the graph Laplacian matrix of the pore throat network (left) and its associated eigenvalues (right).

e-type measures

The local trend measures are described by the local mean map and the local proportion map defined at every pixel. The mean map is the average value at the same pixel location over all generated images. The proportional map is calculated following Figure 3. The phase proportion distribution within a window is obtained along all generated sand-pack images. The phase proportion of the training image at the same window size and location is calculated and its percentile in the phase proportion distribution of generated images is decided to be the value in the proportional map. For example, the first pixel (up left corner) in the sand-pack proportional map is calculated as 75.
Figure 3. The schematic illustration for calculating the local trend map.

**Homogeneity-heterogeneity classifier**

The homogeneity-heterogeneity classifier is a scale-independent classifier for binarized CT rock images (Mohamed & Prodanović, 2023). Figure 4 presents a schematic plot for calculating this classifier. Given a sandpack 2D image as an example, a moving window with radius $r$ is placed in $n$ random locations within the image and the variance in window porosity is computed. This process is repeated with different radii ranging from $r_{\text{min}}$ to $r_{\text{max}}$. The minimum radius is decided based on the maximum of the Euclidean distance transform of the image, the maximum radius can be as large as the image because the resulting porosity variance tends to 0. Then we plot the porosity variance with respect to the relative radius (number of radius increases). The relative radius concept is introduced to compare different images together that may have different resolution. We first find the radius corresponding to the maximal disk that can be inscribed into the pore space: this is equivalent to the maximum Euclidian distance transform for the pore space. Then this defines the starting $r_{\text{min}}$ and this value is different for different images. Relative radius is reported as the difference of actual radius of the window and $r_{\text{min}}$. This algorithm is tested on different types of homogeneous and heterogeneous benchmarking data and shows a robust classification performance. We use 30 radii and place the window 500 times per radius.

![Schematic illustration for homogeneity-heterogeneity classifier](image)

Figure 4. The schematic illustration for homogeneity-heterogeneity classifier.

3 Training Data

We train SinGAN model on four segmented rock images from Digital Rocks Portal (Sheppard & Schroeder-Turk, 2015) shown in Figure 5: a random slice of Castlegate outcrop fine sandstone (Ss), a slice of packing of silica spheres (Sp), a fossiliferous outcrop carbonate Mt Gambier limestone (Ls), a poorly sorted unconsolidated fluvial sandstone (S). The original Castlegate sandstone has dimensions of $512 \times 512 \times 512$ voxels with a voxel size of 5.6 micrometers. The silica sphere packing has dimensions of $512 \times 512 \times 512$ voxels with a voxel size of 17.4 micrometers. The original Gambier limestone sample has the dimensions of $512 \times 512 \times 512$ voxels with a voxel size of 3.024 micrometers. The fluvial sandpack has dimensions of $512 \times 512 \times 512$ voxels with a voxel size of 9.184 micrometers. Figure 5 shows the downscaled slice examples from the same original volumetric dataset labeled as real and generated image examples labeled as fake with dimensions of $128 \times 128$ voxels. We generate 100 fake images per training image. The detailed introduction to SinGAN architecture is available in Liu et al (2024; 2024).
Figure 5. The original volumetric dataset, four slices of training images from the volumetric dataset, the real slices from the same volumetric dataset, and the generated image examples labeled as fake (from left to right). The training images are sandstone (Ss), sandpack (Sp), limestone (Ls), and poorly sorted sandstone (S) from above to below. Pore space is shown in black and solid space in white.

4 Results and Discussion

We have a choice of working with solid or pore space in the image. The Minkowski functionals results are calculated for the solid phase (except porosity) as shown in Figure 6. The porosity distributions show that generated images tend to have smaller porosity distributions than the original dataset, and the porosity of the training image is closer to the distribution of real slices than the generated images. As for the contour length, Sp has better reproduction than other training image cases. Ss and Ls have worse reproduction: Ss is a more consolidated sandstone slice, leaving limited information of pores (black pixels) for the SinGAN model to learn representations. Ls is a slice of limestone, having more variability to be learned compared to the Sp and Ss. The Euler characteristic reflects the connectedness of the grains. The generated images overall show similar
connectedness to the training images (TIs) except that S-generated images show more complex connected structure.

Figure 7 shows the graph network-based measures: complexity, average degree, and cost of MST. Here we grab the grain throat network for analysis. The graph networks of generated images tend to be slightly more complex than the real slices, however, the complexity of generated images aligns well with the complexity of the TIs. The average degree of the Sp and the Ls cases show better reproduction than Ss and S cases, similarly in the MST reproduction. We are working with images downscaled from the originals, and while we do not mix different resolutions of the same image, we briefly evaluate the sensitivity of the measures to scaling in Appendix A.

Figure 6. Minkowski functionals results of the generated images, real images, and training images.

Figure 7. Graph network-based measures.
There are some common patterns of reproduction observed in the four training image cases. As shown in the mean map of Figure 8, the features at the corners are highly reproduced, similar to the subsurface geological modeling with SinGAN (Liu et al., 2024). Another observation is that the highly-reproduced features show a square shape, which may result from the SinGAN pyramid architecture and accumulated edge learning at each scale. The proportional map indicates an idea about the percentile of TI phase proportion in the phase proportions distribution of the generated images. For example, the yellow region implies that TI facies proportion is mainly at the tails of the distribution of the generated images. Note that the phases proportion in pore scale digital images are equivalent to the concept of facies proportion on reservoir scale, commonly used in geostatistics (Ma & Zhang, 2019).

The Lorenz coefficient-like calculation for the ordered eigenvector of graph Laplacian (Figure 9) demonstrates that the graph structure of the Ss, Sp, and Ls-generated images have
inherent clusters similar to that of their training image and real images from the same volumetric data. We observe a slight difference for the S case.

Figure 9. The Lorenz coefficient-like calculation of the ordered eigenvector of graph Laplacian.

Lastly, we use some of the demonstrated metric results for dimensionality reduction and visualization of all images in a 2-dimensional space. We first visualize all images using average degree and offdiagonal complexity as classifiers (Figure 10). The Ss, Sp, and Ls cases show a good mixing between generated and real images. The S case shows a little separation between generated and real images. We then apply the PCA to project porosity, contour length, Euler characteristic, offdiagonal complexity, average degree, and cost of MST to two principal components, and the PCA loading result is shown in Figure 11. The explained variance of PC1 and PC2 are 3.51 and 1.99, respectively. This implies that the cost of MST, average degree, Euler characteristic, and porosity have more influence on PC1, from the perspective of PC1. The PCs can provide reference on contributable features when analyzing digital rock-augmented images.

Figure 10. The scatter plot between offdiagonal complexity and average degree of all images’ graph network.
We further apply the homogeneity-heterogeneity classifier algorithm to our generated images. We first calculate the porosity variance of each generated image and compare it with the training image and real slices. For better visualization, we plot the confidence interval (P25-P75) of the relationships rather than the individual curves (Figure 12). The 2D curves show similar variance changes with slight differences over very small window sizes, which assures that the fake images are similar to the real ones though they are not duplicates as the SinGAN model introduces fine details to the generated images.

Figure 11. The PCA loading plot.

Figure 12. The scale-independent variance of generated images and real slices compared with the training image.
5 Conclusions

The current AI-based images mainly use visual inspection to check the quality of generated images or some dimensionality reduction methods that may destroy the image topology and spatial structure. We propose topological dimensionality reduction using Minkowski functionals, pore network-based measures, Laplacian graph-related measures, and other measures including the homogeneity-heterogeneity classifier and local trend maps. We demonstrate this workflow based on SinGAN-generated images on four porous media training samples. Our results demonstrate detailed comparisons and diagnostics of generated images and real images. The demonstrated metrics eventually help the dimensionality reduction and analysis of the AI-generated images, which may guide future porous media research such as the incorporation of proposed metrics during model training to improve the quality of data augmentation. Lastly, this study was conducted on 2D image slices as presently would be difficult to evaluate all the measures as extensively in 3D as it was done here. The concepts do extend directly to 3D and this will be part of our future work.

Appendix A: data resolution sensitivity test on topological and geometric metrics

We conduct a geometrical and topological metric sensitivity test on the effect of image resolution, using Minkowski functionals as an example. We compare the Minkowski functionals at three different data resolutions in the process of downsampling the images with bilinear interpolation: 512x512, 256x256, and 128x128. We start with the original 3D data (512x512x512) and downscale each slice using the nearest-neighbor downscaling method to obtain 512 slices of 2D images of size 256x256 and 128x128, respectively.

Figure A1 shows slice examples of the original dataset with a resolution of 512, and differences between these slices and their downscaled slices with resolutions of 256 and 128 (second and third rows, respectively). The differences are obtained by upscaling the downscaled images to the original resolution. This process can not fully recover the original details lost during downsampling. As a result, we observe that downscaled images lose part of the information specifically at the contours of grains in the original high-resolution images (black refers to no differences and white shows differences).

Figure A2 shows Minkowski functional results of original slices with the resolution of 512, and downscaled resolutions of 256 and 128. Overall, the porosity distribution is not affected by the resolution. As for the contour length, we use a scaled metric (contour length divided by the image resolution) for comparisons due to different resolutions. The scaled contour length decreases for both downscaled images and sphere packing (Sp) shows the smallest decrease (reflected by the smaller gaps between green-colored distributions). Euler characteristic distributions change differently for each image type and are most affected as they are also affected by the number of disconnected components in the images.
Figure A1. Original dataset slice examples (first row) and downscaled slice differences (shown in white color in the second and third rows). The difference between the original 512 and downscaled 256 resolution is denoted as 256_diff, the difference for resolution 128 is denoted as 128_diff. The squared labels of red, green, blue, and orange colors respond to sandstone (Ss), sand pack (Sp), limestone (Ls), and poorly sorted sandstone (S).
**Figure A2.** Minkowski functionals results of the original datasets (resolution of 512 in solid line) and downscaled images (resolutions of 256 in dash-dotted line and 128 in dash line). The colors respond to different samples in Figure A1.

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**Open Research**

The digital rock data used for image augmentation are available at Digital Rocks Portal through Sheppard and Schroeder-Turk (2015).
References


