Supporting Information for "Quantifying complex microstructures of earth materials: Reconstructing higher-order spatial correlations using deep generative adversarial networks"

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Introduction

This supporting information provides three tables and one text about the their contents. Tables are referenced in the main text. The introduction gives a brief overview of the supporting information. You should include information

Text S1. Model's architecture and hyperparameters

Table S1 presents the architectures used for the generator and the discriminator. Note that no batch normalisation should be applied in the discriminator's layers, otherwise WGAN-GP does not improve the stability as reported by Guan (2018). This is critical in

WGAN-GP as the norm of the discriminator's gradient is penalized according to each image instead of the entire batch (Gulrajani et al., 2017). A convolution layer is also added before the last layer in the generator to avoid checkerboard pattern artefacts created by the uneven overlap in the transpose convolution layers (Odena et al., 2016). In generator, However, batch normalisation is followed at each layer by applying a rectified linear unit (ReLU) or leaky ReLU as activation functions. Please read Shang, Sohn, Almeida, and Lee (2016) and Maas, Hannun, Ng, et al. (2013) for more information. Our investigation indicates better results are obtained when no activation function is applied in the discriminator's last layer.

Table S2 provides the parameters for training the WGAN-GP in both case studies. Network weights were first randomly initialised and then were updated at each iteration by the Adam optimiser (Kingma & Ba, 2014) using the reported learning rate and momentums. Discriminator repeats are the number of times the discriminator's weights were updated for each generator update.

Table S3 reports the mean square errors (MSEs) between scaled spatial-correlation functions derived from original and reconstructed microstructures using SA and WGAN-GP methods. It can be seen that the MSE associated with WGAN-GP is two to three orders of magnitude less than SA, except for the two-point correlation function.

References

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Table S1. Generator and discriminator architecture in this study.[a]

Layer	Type	Filters	Kernel	Stride	Padding	Batch	Activation
Generator							
1	ConvTrans2D	1024	4×4	1	0	Yes	ReLU
2	ConvTrans2D	512	4×4	2	1	Yes	ReLU
3	ConvTrans2D	256	4×4	2	1	Yes	ReLU
4	ConvTrans2D	128	4×4	2	1	Yes	ReLU
5	ConvTrans2D	64	4×4	2	1	Yes	ReLU
6	Conv2D	64	1×1	1	0	Yes	ReLU
7	ConvTrans2D	1	4×4	2	1	No	Tanh
Discriminator							
1	Conv2D	64	4×4	2	1	No	LeakyReLU
2	Conv2D	128	4×4	2	1	No	LeakyReLU
3	Conv2D	256	4×4	2	1	No	LeakyReLU
4	Conv2D	512	4×4	2	1	No	LeakyReLU
5	Conv2D	1024	4×4	2	1	No	LeakyReLU
6	Conv2D	1	4×4	1	0	No	None

[a] Conv2D = convolutional; ConvTrans2D. = transpose convolutional

; ReLU = Rectified Linear Unit.

Table S2. Training parameters used in this study.

Image size	128^2
Batch size	128
Noise vector (z) dimension	512
Generator filters	64
Discriminator filters	64
Learning rate (α)	0.0001
Momenta(β_1, β_2)	(0.5, 0.999)
Discriminator repeats	5
Coefficient(λ)	10

Table S3. The assessment of image reconstruction quality using SA and our WGAN-GP. The values are mean square errors (MSEs) calculated between correlation functions of original and reconstructed images as shown in Figs. 4-5.

Correlation function	Meta-igneous		Serpentinite	
	SA	WGAN-GP	SA	WGAN-GP
S_2	8.26×10^{-6}	2.16×10^{-5}	5.94×10^{-5}	4.42×10^{-5}
P_{3H}	5.23×10^{-5}	2.96×10^{-7}	1×10^{-3}	2.13×10^{-6}
P_{3V}	7.69×10^{-5}	4.72×10^{-7}	1.27×10^{-3}	3.78×10^{-6}
P_4	6×10^{-5}	1.61×10^{-6}	1.33×10^{-3}	5.74×10^{-6}
P_6	2.98×10^{-5}	2.56×10^{-7}	1.19×10^{-3}	1.44×10^{-6}