Supplementary material for

HER: an information theoretic alternative for geostatistics

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Supplement S1: Summary statistics of the resampled datasets

Table S1.1 and Table S1.2 summarize the statistics of the learning, validation, test and full datasets.

Table S1.1: Summary statistics of the resampled datasets – Short-range dataset (SR0 and SR1).

Sample size	200	400	600	800	1000	1500	2000	2000 (val. set)	2000 (test set)	10000 (full set)
					SR0					
mean	-0.57	-0.59	-0.58	-0.59	-0.59	-0.58	-0.57	-0.53	-0.56	-0.55
sd.	1.05	1.06	1.02	1.01	0.99	0.99	0.99	0.99	1.00	0.99
H	4.27	4.38	4.34	4.33	4.31	4.32	4.32	4.31	4.34	4.34
max.	1.76	1.92	1.92	1.92	1.92	1.92	2.05	2.08	2.02	2.08
median	-0.42	-0.50	-0.51	-0.56	-0.54	-0.52	-0.52	-0.46	-0.50	-0.49
min.	-3.68	-3.68	-3.68	-3.68	-3.68	-3.68	-3.68	-3.67	-3.71	-3.71
kur.	3.21	3.04	3.12	3.15	3.17	3.14	3.12	3.18	3.07	3.09
sk.	-0.62	-0.43	-0.41	-0.35	-0.35	-0.32	-0.30	-0.36	-0.33	-0.34
					SR1					
mean	-0.52	-0.54	-0.55	-0.57	-0.57	-0.57	-0.56	-0.54	-0.54	-0.55
sd.	1.17	1.17	1.14	1.12	1.11	1.10	1.10	1.11	1.12	1.11
H	4.46	4.54	4.51	4.50	4.49	4.49	4.49	4.49	4.52	4.50
max.	2.50	2.70	2.70	2.70	2.70	2.70	2.99	2.96	2.86	2.99
median	-0.36	-0.51	-0.51	-0.55	-0.56	-0.54	-0.53	-0.51	-0.48	-0.51
min.	-3.66	-3.66	-3.66	-3.84	-3.84	-4.01	-4.01	-4.63	-4.25	-4.63
kur.	2.82	2.83	2.93	2.94	2.99	3.03	3.04	3.24	3.09	3.11
sk.	-0.40	-0.15	-0.19	-0.19	-0.18	-0.20	-0.20	-0.28	-0.26	-0.25

sd. = standard deviation; *H* = entropy; max. = maximum; min. = minimum; kur. = kurtosis; sk. = skewness.

Table S1.2: Summary statistics of the resampled datasets – Long-range dataset (LR0 and LR1).

Sample size	200	400	600	800	1000	1500	2000	2000 (val. set)	2000 (test set)	10000 (full set)
					LR0					
mean	-0.98	-0.96	-1.03	-1.01	-1.01	-1.01	-1.02	-1.00	-1.02	-1.01
sd.	0.90	0.88	0.89	0.89	0.90	0.91	0.91	0.90	0.91	0.90
H	3.99	4.02	4.07	4.09	4.09	4.11	4.11	4.11	4.12	4.12
max.	1.04	1.15	1.23	1.23	1.23	1.23	1.23	1.28	1.27	1.28
median	-0.77	-0.81	-0.92	-0.92	-0.91	-0.91	-0.92	-0.88	-0.89	-0.89
min.	-2.78	-2.78	-3.07	-3.07	-3.07	-3.08	-3.08	-3.00	-3.07	-3.08
kur.	2.11	2.18	2.26	2.24	2.21	2.16	2.20	2.22	2.16	2.20
sk.	-0.09	-0.07	0.02	0.02	0.03	0.03	0.03	-0.03	0.00	-0.01
					LR1					
mean	-0.92	-0.91	-0.99	-1.00	-1.00	-1.01	-1.01	-1.01	-1.00	-1.00
sd.	0.98	1.00	1.01	1.02	1.03	1.04	1.03	1.05	1.03	1.03
H	4.21	4.31	4.34	4.37	4.38	4.40	4.39	4.41	4.39	4.40
max.	1.40	1.87	1.87	1.87	1.96	1.96	2.00	2.29	2.14	2.29
median	-0.88	-0.91	-0.97	-0.98	-0.99	-0.99	-0.98	-0.98	-0.96	-0.96
min.	-3.19	-3.65	-3.65	-3.74	-3.74	-3.74	-3.95	-4.02	-3.75	-4.02
kur.	2.51	2.67	2.56	2.56	2.59	2.50	2.53	2.59	2.44	2.53
sk.	-0.09	0.02	0.06	0.04	0.06	0.05	0.04	-0.02	0.02	0.00

sd. = standard deviation; H = entropy; max. = maximum; min. = minimum; kur. = kurtosis; sk. = skewness.

Supplement S2: Parameter tuning

This supplement consolidates the final parameters used in the models presented in Sec. 4.2. Particularly for HER, Figure S2.1 presents the final weights optimized for Eqs. (4) and (5). It was limited to 18 grid units (nine distance classes), due to the small contribution of the faraway classes. Similarly, Figure S2.2 shows α and β weights of Eq. (7). Finally, Table S2.1 and Table S2.2 summarize the calibrated parameters obtained for each model (varying method, sample size and dataset type).

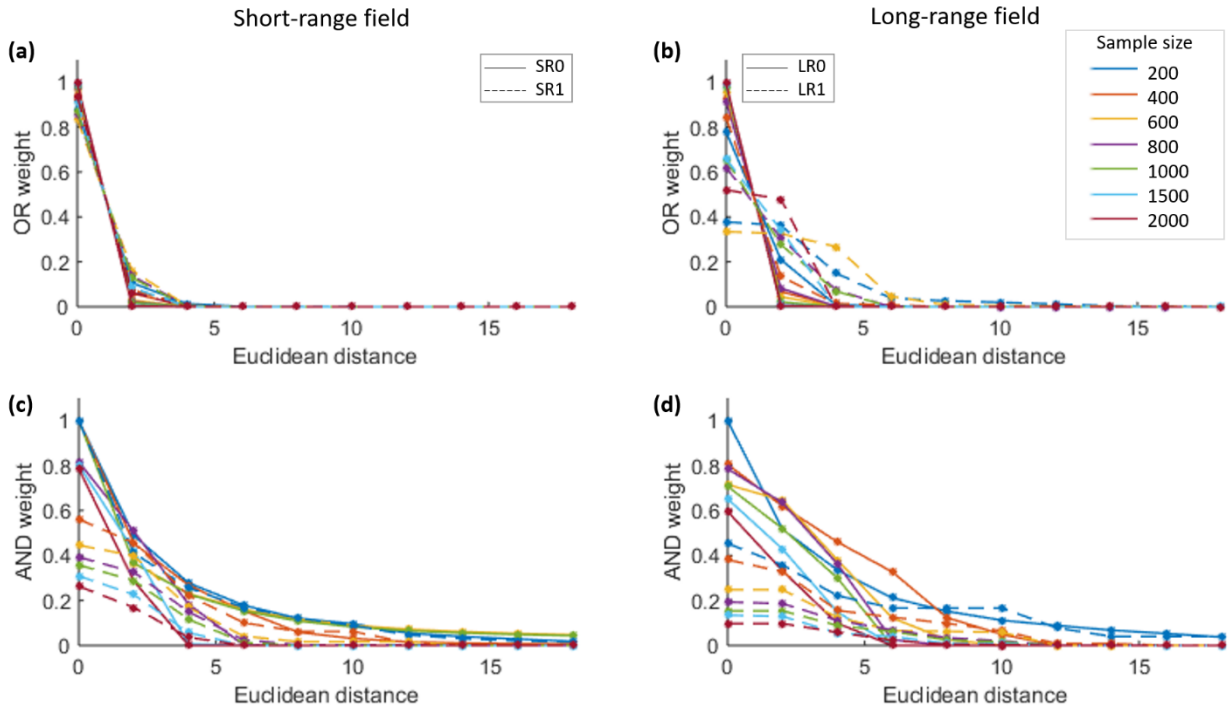

Figure S2.1: HER optimized weights by distance class: a,b) w_{OR}, Eq. (4), and c,d) w_{AND} Eq. (5). SR datasets on the left panel and LR datasets on the right panel. Continuous line refers to datasets without noise and dashed lines to datasets with noise.

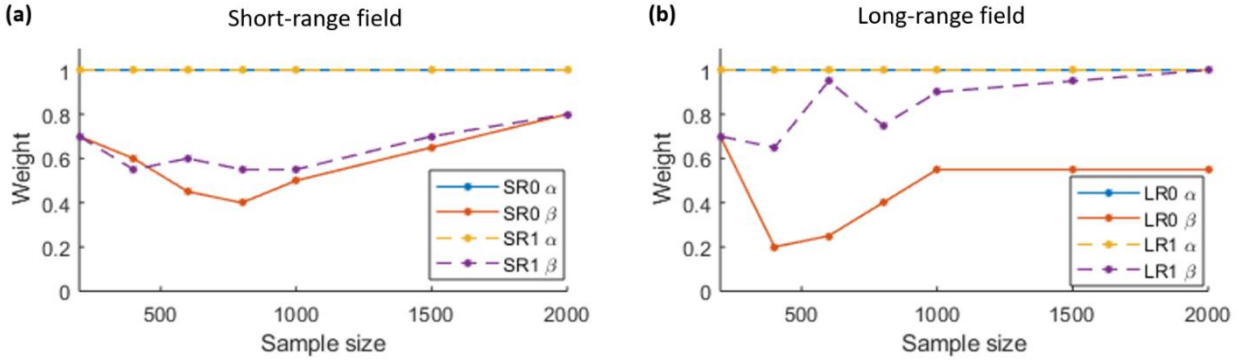

Figure S2.2. HER α and β weights by sample size, Eq. (7): a) SR datasets on the left panel, and b) LR datasets on the right panel. Continuous line refers to datasets without noise and dashed lines to datasets with noise.

Table S2.1: Method calibration by sample size – Parameters of the models for the short-range dataset (SR0 and SR1).

Model sample size		200	400	600	800	1000	1500	2000
Method	**Parameter**[1]				**SR0**			
NN	n.n.	1	1	1	1	1	1	1
IDS	exp.	2	2	2	2	2	2	2
OK	n.n.	12	12	12	12	12	12	12
	lag width	2	2	2	2	2	2	2
	variogram	Spherical	Spherical	Spherical	Spherical	Spherical	Spherical	Spherical
	eff. range	35.99	35.43	33.63	33.50	33.13	33.21	33.65
	nugget	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	sill	1.24	1.28	1.16	1.13	1.11	1.09	1.08
	max. lag	60	60	60	60	60	60	60
	n.n. [min.,max.]	[3,20]	[3,20]	[3,20]	[3,20]	[3,20]	[3,20]	[3,20]
HER	n.n.	12	12	12	12	12	12	12
	class width	2	2	2	2	2	2	2
	bin widths (z, Δz)	0.2	0.2	0.2	0.2	0.2	0.2	0.2
	model range	36.00	24.00	26.00	26.00	26.00	26.00	26.00
	α	1.00	1.00	1.00	1.00	1.00	1.00	1.00
	β	0.70	0.60	0.45	0.40	0.50	0.65	0.80
Method	**Parameter**[1]				**SR1**			
NN	n.n.	1	1	1	1	1	1	1
IDS	exp.	2	2	2	2	2	2	2
OK	n.n.	12	12	12	12	12	12	12
	lag width	2	2	2	2	2	2	2
	variogram	Spherical	Spherical	Spherical	Spherical	Spherical	Spherical	Spherical
	eff. range	43.53	35.81	35.43	34.69	32.70	32.18	33.30
	nugget	0.28	0.15	0.18	0.18	0.17	0.17	0.20
	sill	1.29	1.39	1.25	1.22	1.19	1.16	1.12
	max. lag	60	60	60	60	60	60	60
	n.n. [min.,max.]	[3,20]	[3,20]	[3,20]	[3,20]	[3,20]	[3,20]	[3,20]
HER	n.n.	12	12	12	12	12	12	12
	class width	2	2	2	2	2	2	2
	bin widths (z, Δz)	0.2	0.2	0.2	0.2	0.2	0.2	0.2
	model range	38.00	26.00	26.00	26.00	26.00	26.00	26.00
	α	1.00	1.00	1.00	1.00	1.00	1.00	1.00
	β	0.70	0.55	0.60	0.55	0.55	0.70	0.80

[1]n.n. = number of neighbors; exp. = exponent of the weighting function; eff. range = effective range; max. = maximum; min. = minimum

Table S2.2: Method calibration by sample size – Parameters of the models for the long-range dataset (LR0 and LR1).

Model sample size		200	400	600	800	1000	1500	2000
Method	**Parameter**[1]				**LR0**			
NN	n.n.	1	1	1	1	1	1	1
IDS	exp.	2	2	2	2	2	2	2
OK	n.n.	12	12	12	12	12	12	12
	lag width	2	2	2	2	2	2	2
	variogram	Gaussian	Gaussian	Gaussian	Gaussian	Gaussian	Gaussian	Gaussian
	eff. range	67.47	66.93	69.10	68.23	69.12	71.82	73.01
	nugget	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	sill	1.06	0.99	1.03	1.03	1.05	1.10	1.10
	max. lag	100	100	100	100	100	100	100
	n.n. [min.,max.]	[3,20]	[3,20]	[3,20]	[3,20]	[3,20]	[3,20]	[3,20]
HER[2]	n.n.	12	12	12	12	12	12	12
	class width	2	2	2	2	2	2	2
	bin widths (z, Δz)	0.2	0.2	0.2	0.2	0.2	0.2	0.2
	model range	46.00	48.00	48.00	46.00	46.00	48.00	48.00
	α	1.00	1.00	1.00	1.00	1.00	1.00	1.00
	β	0.70	0.20	0.25	0.40	0.55	0.55	0.55
Method	**Parameter**[1]				**LR1**			
NN	n.n.	1	1	1	1	1	1	1
IDS	exp.	2	2	2	2	2	2	2
OK	n.n.	12	12	12	12	12	12	12
	lag width	2	2	2	2	2	2	2
	variogram	Gaussian	Gaussian	Gaussian	Gaussian	Gaussian	Gaussian	Gaussian
	eff. range	81.79	76.14	71.43	69.02	74.43	78.75	78.05
	nugget	0.29	0.31	0.29	0.28	0.30	0.29	0.29
	sill	0.99	0.95	0.98	1.00	1.03	1.10	1.08
	max. lag	100	100	100	100	100	100	100
	n.n. [min.,max.]	[3,20]	[3,20]	[3,20]	[3,20]	[3,20]	[3,20]	[3,20]
HER	n.n.	12	12	12	12	12	12	12
	class width	2	2	2	2	2	2	2
	bin widths (z, Δz)	0.2	0.2	0.2	0.2	0.2	0.2	0.2
	model range	48.00	46.00	44.00	44.00	44.00	46.00	46.00
	α	1.00	1.00	1.00	1.00	1.00	1.00	1.00
	β	0.70	0.65	0.95	0.75	0.90	0.95	1.00

[1]n.n. = number of neighbors; exp. = exponent of the weighting function; eff. range = effective range; max. = maximum; min. = minimum

Supplement S3: Summary statistics of the model predictions

This supplement summarizes the statistics of the deterministic predictions (mean of z) for the test set by method and learning sets (from 200 to 2000 observations). HER outcomes refer to the AND/OR aggregation. The four random fields types are presented from Table S3.1 to Table S3.4. Finally, Figure S3.1 illustrates their residue correlation.

Table S3.1: Summary statistics of the prediction on test set by model – Short-range dataset without noise (SR0).

Method	Statistics[1]	200	400	600	800	1000	1500	2000
				SR0				
NN	mean	-0.54	-0.55	-0.56	-0.56	-0.56	-0.56	-0.56
	sd.	1.01	1.03	1.01	1.00	1.00	1.01	1.00
	H	4.17	4.33	4.31	4.31	4.31	4.34	4.33
	max.	1.76	1.92	1.92	1.91	1.91	1.91	1.91
	median	-0.44	-0.47	-0.57	-0.57	-0.53	-0.53	-0.52
	min.	-3.68	-3.68	-3.68	-3.68	-3.68	-3.68	-3.68
	kur.	3.37	3.13	3.06	3.04	3.07	3.08	3.08
	sk.	-0.56	-0.43	-0.36	-0.30	-0.32	-0.30	-0.32
IDS	mean	-0.54	-0.57	-0.58	-0.59	-0.57	-0.57	-0.57
	sd.	0.79	0.88	0.89	0.90	0.91	0.93	0.94
	H	3.96	4.13	4.16	4.19	4.21	4.24	4.26
	max.	1.58	1.80	1.79	1.80	1.80	1.79	1.80
	median	-0.55	-0.53	-0.53	-0.56	-0.53	-0.54	-0.53
	min.	-3.49	-3.49	-3.51	-3.53	-3.54	-3.56	-3.58
	kur.	3.56	3.28	3.27	3.17	3.15	3.13	3.10
	sk.	-0.44	-0.37	-0.37	-0.32	-0.32	-0.30	-0.30
OK	mean	-0.53	-0.56	-0.56	-0.57	-0.56	-0.56	-0.56
	sd.	0.86	0.92	0.93	0.94	0.95	0.97	0.97
	H	4.11	4.21	4.24	4.26	4.27	4.30	4.30
	max.	1.63	1.86	1.90	1.90	1.90	1.90	1.90
	median	-0.47	-0.49	-0.49	-0.52	-0.51	-0.51	-0.51
	min.	-3.60	-3.56	-3.57	-3.63	-3.66	-3.67	-3.67
	kur.	3.46	3.18	3.13	3.09	3.08	3.08	3.08
	sk.	-0.46	-0.41	-0.39	-0.34	-0.35	-0.32	-0.33
HER	mean	-0.54	-0.56	-0.58	-0.57	-0.57	-0.57	-0.57
	sd.	0.87	0.95	0.92	0.96	0.94	0.98	0.98
	H	4.08	4.23	4.21	4.26	4.24	4.31	4.31
	max.	1.70	1.82	1.81	1.83	1.82	1.83	1.86
	median	-0.50	-0.51	-0.54	-0.57	-0.54	-0.53	-0.53
	min.	-3.55	-3.55	-3.57	-3.61	-3.58	-3.59	-3.61
	kur.	3.54	3.18	3.22	3.10	3.13	3.10	3.07
	sk.	-0.54	-0.43	-0.37	-0.31	-0.32	-0.30	-0.31

[1]sd. = standard deviation; *H* = entropy; max. = maximum; min. = minimum; kur. = kurtosis; sk. = skewness.

Table S3.2: Summary statistics of the prediction on test set by model – Short-range dataset with noise (SR1).

Method	Statistics[1]	200	400	600	800	1000	1500	2000
				SR1				
NN	mean	-0.50	-0.52	-0.55	-0.55	-0.56	-0.55	-0.56
	sd.	1.15	1.16	1.14	1.14	1.13	1.11	1.11
	H	4.45	4.51	4.49	4.50	4.50	4.48	4.49
	max.	2.50	2.70	2.70	2.70	2.70	2.70	2.99
	median	-0.43	-0.51	-0.53	-0.54	-0.54	-0.53	-0.54
	min.	-3.66	-3.66	-3.66	-3.84	-3.84	-3.84	-4.00
	kur.	2.86	2.79	2.92	2.91	2.90	2.97	2.97
	sk.	-0.27	-0.05	-0.05	-0.09	-0.14	-0.13	-0.18
IDS	mean	-0.49	-0.53	-0.55	-0.58	-0.56	-0.56	-0.56
	sd.	0.85	0.92	0.92	0.95	0.95	0.96	0.96
	H	4.09	4.22	4.24	4.28	4.27	4.29	4.30
	max.	2.19	2.37	2.34	2.28	2.27	2.19	2.07
	median	-0.47	-0.47	-0.50	-0.53	-0.51	-0.53	-0.52
	min.	-3.42	-3.30	-3.29	-3.50	-3.52	-3.59	-3.55
	kur.	3.17	2.84	2.97	2.86	2.91	2.98	2.92
	sk.	-0.23	-0.13	-0.19	-0.21	-0.21	-0.22	-0.23
OK	mean	-0.49	-0.52	-0.54	-0.57	-0.55	-0.56	-0.56
	sd.	0.79	0.90	0.91	0.93	0.93	0.94	0.94
	H	3.99	4.20	4.21	4.24	4.25	4.25	4.25
	max.	1.58	2.30	2.22	2.20	2.21	2.17	1.90
	median	-0.48	-0.46	-0.48	-0.51	-0.49	-0.49	-0.49
	min.	-3.17	-3.16	-3.19	-3.31	-3.44	-3.51	-3.45
	kur.	3.22	2.82	2.84	2.76	2.85	2.94	2.89
	sk.	-0.22	-0.19	-0.24	-0.25	-0.26	-0.27	-0.26
HER	mean	-0.50	-0.53	-0.54	-0.57	-0.55	-0.56	-0.56
	sd.	0.90	0.96	0.98	0.98	0.97	0.97	0.97
	H	4.16	4.28	4.31	4.33	4.31	4.31	4.30
	max.	2.24	2.31	2.35	2.28	2.28	2.26	2.00
	median	-0.47	-0.48	-0.50	-0.54	-0.51	-0.53	-0.52
	min.	-3.32	-3.32	-3.38	-3.46	-3.45	-3.55	-3.54
	kur.	3.11	2.70	2.89	2.82	2.85	2.98	2.89
	sk.	-0.27	-0.13	-0.14	-0.16	-0.20	-0.19	-0.24

[1]sd. = standard deviation; *H* = entropy; max. = maximum; min. = minimum; kur. = kurtosis; sk. = skewness.

Table S3.3: Summary statistics of the prediction on test set by model – Long-range dataset without noise (LR0).

Method	Statistics[1]	200	400	600	800	1000	1500	2000
				LR0				
NN	mean	-1.03	-1.02	-1.01	-1.02	-1.02	-1.01	-1.02
	sd.	0.91	0.91	0.91	0.91	0.91	0.91	0.91
	H	3.98	4.06	4.10	4.11	4.11	4.12	4.11
	max.	1.04	1.15	1.15	1.23	1.23	1.23	1.23
	median	-0.92	-0.91	-0.90	-0.90	-0.90	-0.90	-0.90
	min.	-2.78	-2.78	-3.07	-3.07	-3.07	-3.08	-3.08
	kur.	2.10	2.13	2.20	2.18	2.20	2.15	2.16
	sk.	0.00	0.02	0.03	0.02	0.03	0.01	0.00
IDS	mean	-1.04	-1.02	-1.02	-1.02	-1.02	-1.02	-1.02
	sd.	0.85	0.87	0.88	0.89	0.89	0.90	0.90
	H	3.91	3.98	4.05	4.07	4.07	4.08	4.09
	max.	0.99	1.08	1.14	1.15	1.16	1.14	1.14
	median	-0.86	-0.88	-0.89	-0.88	-0.88	-0.88	-0.89
	min.	-2.72	-2.71	-3.01	-3.01	-3.01	-3.02	-3.02
	kur.	1.95	2.01	2.11	2.12	2.12	2.11	2.13
	sk.	-0.12	-0.03	-0.03	-0.01	-0.01	-0.02	-0.01
OK	mean	-1.04	-1.02	-1.02	-1.02	-1.02	-1.02	-1.02
	sd.	0.91	0.91	0.91	0.91	0.91	0.91	0.91
	H	4.11	4.11	4.12	4.12	4.12	4.12	4.12
	max.	1.34	1.28	1.24	1.28	1.27	1.27	1.27
	median	-0.93	-0.88	-0.89	-0.89	-0.89	-0.89	-0.89
	min.	-2.89	-2.97	-3.08	-3.08	-3.07	-3.07	-3.07
	kur.	2.12	2.15	2.17	2.17	2.16	2.16	2.16
	sk.	0.01	0.01	0.01	0.01	0.01	0.00	0.00
HER	mean	-1.04	-1.02	-1.02	-1.02	-1.02	-1.02	-1.02
	sd.	0.88	0.88	0.89	0.90	0.90	0.90	0.91
	H	3.98	4.03	4.07	4.09	4.09	4.09	4.09
	max.	1.02	1.13	1.14	1.22	1.20	1.15	1.15
	median	-0.89	-0.90	-0.90	-0.90	-0.90	-0.90	-0.90
	min.	-2.77	-2.78	-3.06	-3.07	-3.07	-3.08	-3.07
	kur.	2.02	2.09	2.17	2.16	2.16	2.13	2.14
	sk.	-0.05	0.00	0.00	0.00	0.01	-0.01	-0.01

[1]sd. = standard deviation; *H* = entropy; max. = maximum; min. = minimum; kur. = kurtosis; sk. = skewness.

Table S3.4: Summary statistics of the prediction on test set by model – Long-range dataset with noise (LR1).

Method	Statistics[1]	200	400	600	800	1000	1500	2000
				LR1				
NN	mean	-1.00	-0.99	-1.00	-1.01	-1.01	-1.00	-1.01
	sd.	1.00	1.02	1.03	1.03	1.04	1.05	1.05
	H	4.23	4.33	4.36	4.35	4.39	4.40	4.40
	max.	1.40	1.87	1.87	1.87	1.87	1.87	1.87
	median	-0.90	-0.94	-0.97	-0.99	-0.99	-0.99	-0.98
	min.	-3.19	-3.65	-3.65	-3.65	-3.65	-3.65	-3.87
	kur.	2.50	2.66	2.56	2.57	2.57	2.51	2.49
	sk.	-0.11	0.03	0.02	0.10	0.08	0.06	0.03
IDS	mean	-0.99	-0.98	-0.99	-1.01	-1.00	-1.01	-1.01
	sd.	0.86	0.90	0.91	0.92	0.92	0.93	0.93
	H	4.04	4.14	4.14	4.16	4.18	4.17	4.16
	max.	1.21	1.76	1.48	1.45	1.61	1.54	1.43
	median	-0.79	-0.85	-0.85	-0.88	-0.90	-0.88	-0.90
	min.	-3.04	-3.12	-3.12	-3.12	-3.05	-3.15	-3.25
	kur.	2.21	2.39	2.28	2.31	2.32	2.26	2.26
	sk.	-0.26	0.01	0.04	0.06	0.05	0.05	0.03
OK	mean	-0.98	-0.96	-0.98	-1.00	-1.00	-1.01	-1.01
	sd.	0.79	0.83	0.85	0.86	0.87	0.88	0.89
	H	3.89	4.01	4.00	4.02	4.02	4.04	4.05
	max.	0.81	1.29	1.25	1.32	1.30	1.14	1.19
	median	-0.78	-0.81	-0.81	-0.84	-0.84	-0.86	-0.88
	min.	-2.85	-2.82	-2.74	-2.76	-2.69	-2.84	-2.92
	kur.	2.28	2.38	2.17	2.18	2.18	2.13	2.13
	sk.	-0.40	-0.10	-0.04	-0.01	-0.01	-0.01	-0.01
HER	mean	-0.99	-0.97	-0.98	-1.01	-1.00	-1.01	-1.01
	sd.	0.85	0.89	0.89	0.90	0.90	0.92	0.91
	H	4.01	4.11	4.07	4.11	4.11	4.12	4.11
	max.	1.20	1.64	1.32	1.33	1.36	1.30	1.30
	median	-0.80	-0.83	-0.83	-0.86	-0.89	-0.89	-0.89
	min.	-3.00	-2.98	-2.82	-2.90	-2.83	-2.98	-3.13
	kur.	2.21	2.46	2.23	2.28	2.27	2.23	2.23
	sk.	-0.28	0.03	0.02	0.05	0.04	0.05	0.02

[1]sd. = standard deviation; *H* = entropy; max. = maximum; min. = minimum; kur. = kurtosis; sk. = skewness.

Figure S3.1 illustrates for the residue correlation of the models calculated using the test set. The more negative the residue correlation, the greater the tendency of true z values being overestimated in low-valued regions of the field and underestimated in high-valued regions.

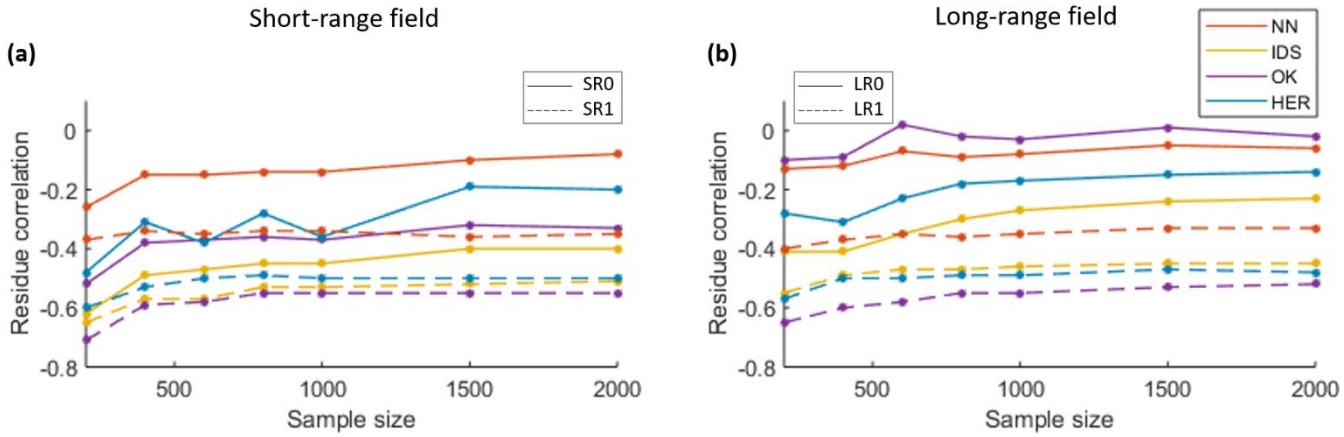

Figure S3.1: Performance comparison of NN, IDS, OK and HER: a) residual correlation for SR datasets, and b) residual correlation for LR datasets. Continuous line refers to datasets without noise and dashed lines to datasets with noise.

45