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Supplement of

Best performances of visible–near-infrared models in soils with little carbonate – a field study in Switzerland

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Supplementary material

Table S1: Data distribution statistics for each of the six fields (A-F) and the combined data set (All). Concentrations in soil organic C (SOC), total N, total C and inorganic C are indicated in g kg^{-1}, permanganate oxidizable C (POXC) in mg kg^{-1} and soil texture in %.

Field	Property	n	Mean	SD	CV [%]	Min	1 Quant.	Median	3 Quant.	Max	Skew	Kurtosis
A	SOC	70	22.4	3.7	16.5	15.0	19.7	22.0	24.9	32.1	0.28	-0.32
	POXC		789	108	13.7	524	731	782	863	1047	-0.24	0.01
	Total N		2.25	0.29	13.1	1.66	2.06	2.24	2.42	2.97	0.36	-0.27
	Total C		29.5	9.0	30.6	16.4	21.8	27.3	34.9	50.0	0.67	-0.78
	pH		7.21	0.13	1.8	6.91	7.13	7.22	7.29	7.50	-0.04	-0.34
	Inorganic C		7.1	6.7	94.6	1.1	1.8	4.1	9.3	25.3	1.14	3.03
	Sand		50.0	5.4	10.8	40.3	46.6	50.5	52.3	60.5	0.18	2.69
	Silt		29.5	2.6	8.9	24.6	28.2	29.5	30.9	34.0	-0.11	2.49
	Clay		20.5	2.1	10.5	16.2	19.4	20.6	21.6	24.6	-0.05	2.78
B	SOC	70	18.7	4.3	22.7	11.7	15.6	18.4	21.1	30.6	0.65	-0.07
	POXC		720	115	15.9	441	634	728	794	1059	0.10	-0.03
	Total N		2.03	0.37	18.2	1.46	1.80	1.96	2.20	3.05	0.84	0.23
	Total C		20.1	4.9	24.3	12.5	16.5	19.4	22.8	33.7	0.68	-0.13
	pH		6.63	0.47	7.1	5.72	6.15	6.84	7.01	7.28	-0.41	-1.32
	Inorganic C		1.3	1.0	73.5	0.0	0.6	0.9	1.5	4.3	1.27	3.56
	Sand		44.5	3.5	7.8	39.8	41.7	43.8	46.1	51.8	76.8	2.66
	Silt		35.2	1.98	5.6	30.9	34.3	35.5	36.8	38.1	-0.75	2.82
	Clay		20.3	1.6	7.8	16.9	19.5	20.6	21.5	22.9	-0.50	2.51
C	SOC	70	28.8	3.2	11.1	23.2	26.0	28.5	31.5	28.5	0.19	-1.10
	POXC		890	101	11.3	644	830	899	967	1076	-0.35	-0.54
	Total N		2.84	0.27	9.7	2.23	2.66	2.86	3.03	3.42	-0.16	-0.42
	Total C		32.6	5.2	16.1	24.7	28.6	32.6	35.9	46.5	0.75	-0.08
	pH		7.19	0.16	2.2	6.64	7.14	7.24	7.29	7.4	-1.74	3.40
	Inorganic C		3.9	4.0	96.6	0.6	1.2	2.3	3.8	14.8	1.46	3.65
	Sand		26.8	3.8	14.2	20.6	24.4	25.7	27.8	35.7	0.94	3.26
	Silt		35.2	1.89	5.4	30.6	34.9	35.8	36.4	37.6	-1.26	3.68
	Clay		38.0	3.5	9.3	31.7	35.5	38.4	39.8	46.0	0.15	2.96
D	SOC	70	20.7	4.9	23.6	12.0	17.9	20.2	24.5	30.7	0.15	-0.84
	POXC		799	154	19.2	424	709	772	953	1034	-0.20	-0.90
	Total N		2.38	0.47	19.6	1.40	2.16	2.35	2.73	3.36	0.02	-0.65
	Total C		24.2	6.2	25.8	13.0	19.9	24.4	29.2	38.2	0.01	-0.89
	pH		6.80	0.59	8.7	5.52	6.26	7.11	7.30	7.49	-0.58	-1.14
	Inorganic C		3.5	3.8	107.8	0.5	0.7	1.7	5.9	18.2	1.43	4.77
	Sand		28.3	2.2	7.6	24.9	27.0	28.2	29.3	33.7	0.62	3.21
	Silt		43.6	2.1	4.8	38.8	42.3	43.7	45.4	46.4	-0.45	2.55
	Clay		28.3	2.2	7.6	24.9	27.0	28.2	29.3	33.7	0.62	3.21
E	SOC	53	15.2	2.9	15.1	9.8	12.4	15.1	17.5	21.3	0.04	-1.08
	POXC		635	118	18.5	396	552	655	719	911	-0.29	-0.68
	Total N		1.77	0.31	17.3	1.16	1.47	1.79	2.03	2.30	-0.22	-1.21
	Total C		21.3	9.4	44.0	10.2	12.7	18.4	29.1	39.7	0.55	-1.20
	pH		6.77	0.68	10.1	5.48	6.15	6.99	7.37	7.47	-0.55	-1.29
	Inorganic C		6.11	7.9	129.4	0.0	0.4	0.9	12.4	21.9	0.95	2.24
	Sand		29.7	4.6	15.5	15.8	27.7	30.0	32.5	35.6	-1.37	5.16
	Silt		47.7	2.3	4.7	44.9	46.1	47.4	48.6	54.5	1.40	5.07

		n										
	Clay		22.6	1.8	7.9	20.3	21.1	22.8	23.4	27.4	0.84	3.67
F	SOC	53	28.6	2.7	9.6	22.4	26.8	29.1	30.7	33.3	-0.51	-0.63
	POXC		661	72	11.0	479	615	664	707	790	-0.18	-0.61
	Total N		1.92	0.22	11.5	1.44	1.73	1.97	2.09	2.30	-0.29	-1.05
	Total C		50.3	2.4	4.8	45.0	48.3	50.5	52.3	54.0	-0.47	-0.85
	pH		7.49	0.04	0.5	7.38	7.47	7.50	7.53	7.56	-0.68	0.15
	Inorganic C		21.7	1.9	8.9	18.5	20.5	21.5	23.2	26.4	0.56	2.64
	Sand		38.8	9.2	23.6	26.5	31.5	35.3	46.4	53.6	0.19	1.47
	Silt		42.8	5.7	13.3	33.6	38.0	44.9	47.3	50.3	-0.20	1.48
	Clay		18.4	3.4	18.3	13.1	15.4	19.8	21.3	23.1	-0.15	1.43
All	SOC	386	22.4	6.1	27.1	9.8	17.7	22.4	27.3	35.2	0.00	-1.02
	POXC		758	142	18.8	396	661	752	861	1076	0.01	-0.50
	Total N		2.23	0.48	21.6	1.16	1.88	2.17	2.60	3.42	0.32	-0.62
	Total C		29.1	11.6	39.9	10.2	20.0	27.5	35.5	54.0	0.57	-0.64
	pH		7.00	0.51	7.3	5.48	6.88	7.20	7.35	7.56	-1.30	0.60
	Inorganic C		6.7	7.9	117.8	0.0	0.9	2.6	10.4	26.4	1.12	2.69
	Sand		36.3	10.3	28.4	15.8	27.7	32.7	45.1	60.5	0.37	1.99
	Silt		39.0	17.7	24.6	24.6	34.4	37.1	45.8	54.5	0.04	1.97
	Clay		24.7	7.2	29.1	13.1	20.3	22.1	28.2	46.0	1.00	3.26

Table S2: Example of model performance with different pre-processing options for total C on field C. Model metrics of Cross-validation are indicated as mean with the standard deviation across the repeats in brackets.

Range of wavelengths / interval [nm]	Pre-processing	Latent variables	n	Calibration				Cross-validation			
				R^2_{cal}	bias	$RMSE_{cal}$	RPD_{cal}	R^2	bias	RMSE	RPD
350-2500 / 1	None	9	70	0.84	0.00	2.10	2.50	0.66 (0.16)	0.04 (1.11)	3.18 (0.74)	1.71 (0.44)
350-2500 / 1	Refl., SG (m = 1, w=5)	6	70	0.99	0.00	0.62	8.48	0.91	0.00 (0.55)	1.61 (0.30)	3.31 (0.62)
350-2500 / 3	Refl., SG (m = 1, w=5)	6	70	0.97	0.00	0.83	6.31	0.91 (0.06	0.02 (0.55)	1.56 (0.27)	3.39 (0.64)
350-2500 / 1	Refl., SG (m = 1, w=35)	6	70	0.96	0.00	1.06	4.94	0.92 (0.06)	-0.04 (0.48)	1.52 (0.32)	3.55 (0.84)
350-2500 / 1	Abs., SG (m = 1, w=35)	5	70	0.93	0.00	1.37	3.84	0.89 (0.04)	0.04 (0.47)	1.82 (0.31)	2.91 (0.56)
350-2500 / 3	Refl., SG (m = 1, w=35)	6	70	0.94	0.00	1.23	4.28	0.92 (0.05)	-0.04 (0.46)	1.50 (0.30)	3.57 (0.81)
350-2500 / 3	Refl., SG (m = 2, w=5)	3	70	095	0.00	1.12	4.70	0.74 (0.15)	-0.01 (0.81)	2.89 (0.69)	1.87 (0.41)
350-2500 / 3	Abs., SG (m=2, w=21)	4	70	0.93	0.00	1.38	3.79	0.88 (0.06)	-0.04 (0.53)	1.91 (0.38)	2.83 (0.72)
350-2500 / 3	Abs. SNV, GSD (m=2, w=21, s=1)	10	70	0.97	0.00	0.95	5.53	0.92 (0.04)	0.04 (0.40)	1.53 (0.28)	3.51 (0.83)
350-2500 / 1	Refl., SNV, GSD (m=2, w=21, s=1)	4	70	0.94	0.00	1.22	4.29	0.90 (0.05)	-0.03 (0.51)	1.83 (0.32)	2.91 (0.636)
350-2500 / 3	Refl., SNV, GSD (m=2, w=21, s=1)	6	70	0.94	0.00	1.24	4.24	0.91 (0.04)	0.00 (0.45)	1.70 (0.30)	3.17 (0.83)
390-2500 / 3	Refl., SNV, GSD (m=2, w=21, s=1)	7	70	0.95	0.00	1.18	4.46	0.91 (0.03)	0.02 (0.40)	1.62 (0.21)	3.26 (0.68)
350-2500 / 6	Refl., SNV, GSD (m=2, w=21, s=1)	5	70	0.92	0.00	1.47	3.58	0.89 (0.04)	-0.01 (0.49)	1.80 (0.30)	2.94 (0.48)
350-2500 / 1	Refl., Abs., GSD (m=2, w=21, s=1)	5	70	0.94	0.00	1.33	3.96	0.90 (0.04)	-0.04 (0.49)	1.74 (0.31)	3.10 (0.80)
350-2500 / 3	Refl., Abs., GSD (m=2, w=21, s=1)	6	70	0.92	0.00	1.46	3.59	0.90 (0.04)	0.05 (0.46)	1.78 (0.32)	2.99 (0.57)
350-2500 / 6	Refl., Abs., GSD (m=2, w=21, s=1)	11	70	0.89	0.00	1.75	3.00	0.80 (0.11)	0.10 (0.64)	2.33 (0.49)	2.35 (0.75)
350-2500 / 3	Refl., SG (m=1, w=21), MSC	10	70	0.97	0.00	0.83	6.31	0.93 (0.03)	-0.07 (0.33)	1.45 (0.24)	3.69 (0.85)
350-2500 / 5	**Refl., SG (m=1, w=21), MSC**	**10**	**70**	**0.97**	**0.00**	**0.92**	**5.69**	**0.93 (0.03)**	**-0.07 (0.33)**	**1.44 (0.29)**	**3.74 (0.98)**
350-2500 / 5	Abs., SG (m=1, w=21), MSC	5	70	0.93	0.00	1.40	3.74	0.91 (0.04)	0.01 (0.47)	1.71 (0.32)	3.11 (0.62)
350-2500 / 3	Refl., SG (m=2, w=21), MSC	3	70	0.97	0.00	0.87	6.06	0.74 (0.14)	0.03 (0.88)	2.92 (0.75)	1.87 (0.43)
350-2500 / 5	Refl., SG (m=2, w=21), MSC	6	70	0.96	0.00	0.98	5.33	0.93 (0.03)	1.48 (0.23)	2.01 (0.44)	3.55 (0.59)

Table S3: Mean, standard deviation and coefficient of variation (CV) of soil texture measured on 20 samples per field with Laser-diffraction analysis (LDA) and the measurement of the improved integral suspension pressure (IPS+) method (one composite sample) with the CV of the LDA-measurement and adjusted standard deviation (SDnew)

| Field	Texture class (%)	LDA			IPS+		
		mean	SD	CV (%)	Mean	SDnew	CV (%)
A	Sand	43.7	4.7	10.8	50.0	5.4	10.8
	Silt	47.0	4.2	8.9	29.5	2.6	8.9
	Clay	9.4	1.0	10.5	20.5	2.1	10.5
B	Sand	42.9	3.3	7.8	44.5	3.5	7.8
	Silt	47.6	2.7	5.6	35.2	2.0	5.6
	Clay	9.4	0.7	7.8	20.3	1.6	7.8
C	Sand	29.5	4.2	14.3	26.8	3.8	14.3
	Silt	56.6	3.0	5.4	35.2	1.9	5.4
	Clay	13.9	1.3	9.3	38.0	3.5	9.3
D	Sand	26.0	3.7	14.3	28.1	4.0	14.3
	Silt	62.1	3.0	4.8	43.6	2.1	4.8
	Clay	11.9	0.9	7.6	28.3	2.2	7.6
E	Sand	24.5	3.8	15.5	29.7	4.6	15.5
	Silt	64.6	3.1	4.7	47.7	2.3	4.7
	Clay	10.8	0.9	7.9	22.6	1.8	7.9
F	Sand	37.3	8.8	23.6	38.8	9.2	23.6
	Silt	53.6	7.2	13.3	42.8	5.7	13.3
	Clay	9.2	1.7	18.3	18.4	3.4	18.3

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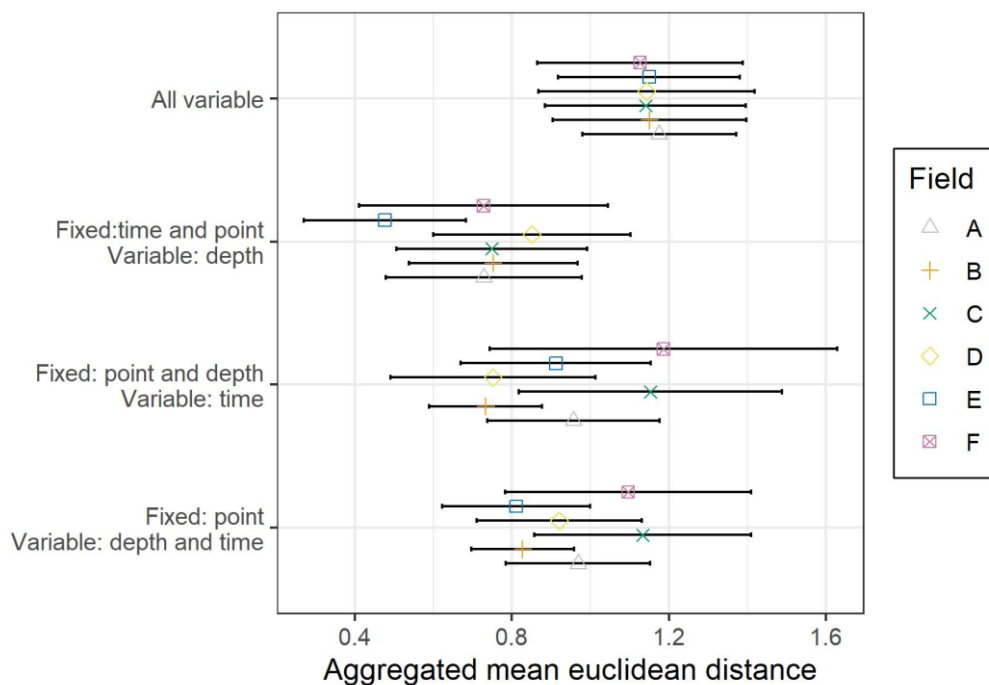
Figure S1: Aggregated mean Euclidean distance of pre-processed reflectance spectra per field between all samples (all variable),
between samples at same time and point but different depths (fixed: time and point, variable: depth), between samples at same point
and depth but different sampling times (fixed: point and depth, variable. Time) and between samples at the same point but different
depth and sampling times (fixed: point, variable: depth and time). All spectra were pre-processed using a Savitzky-Golay filter on
first order derivative with window width 21 and multiplicative scatter correction (Refl., sg (m = 1, w = 21), MSC)

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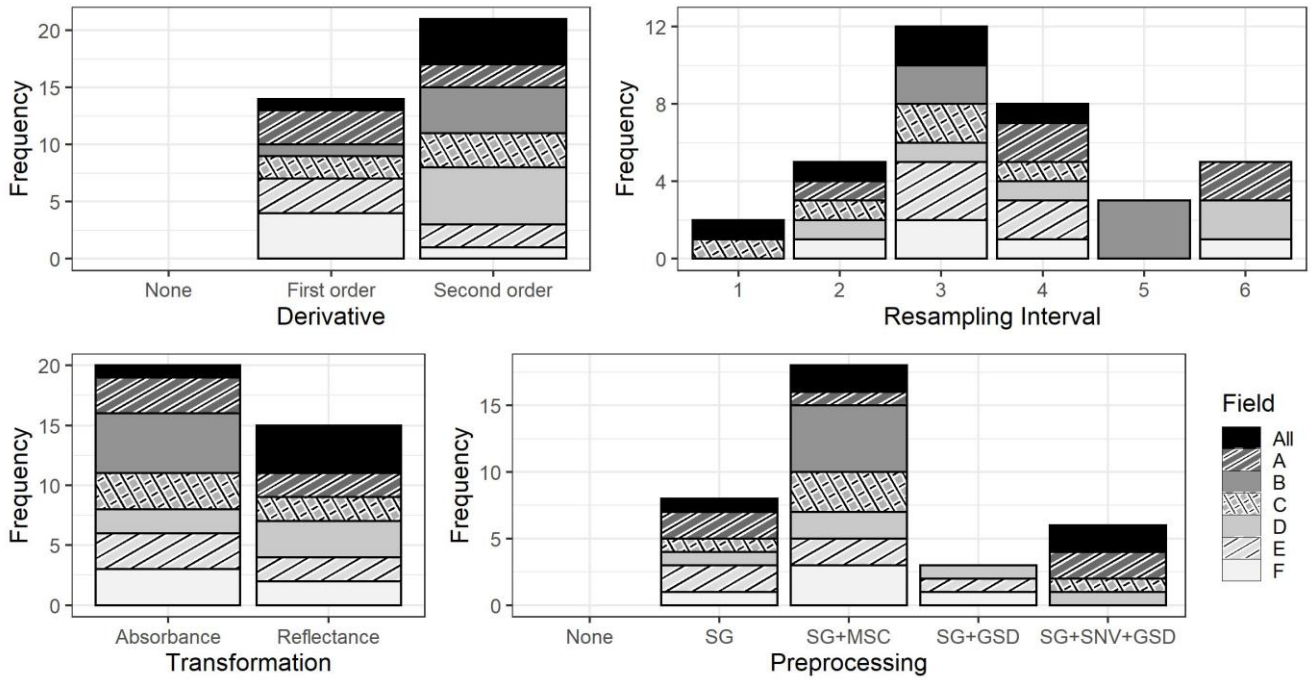
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Figure S2: Frequency of applied pre-processing steps to obtain the best model for SOC, total C, total N, POXC and pH for datasets of the six fields and a combined general (All) dataset. Window widths from 5 to 51 were tested. SG = Savitzky-Golay filter (m = order of derivative, w = window width), SNV = standard normal variate, GSD = gap segment derivative (m = derivative, w = window width, s = segment size), MSC = multiplicative scatter correction

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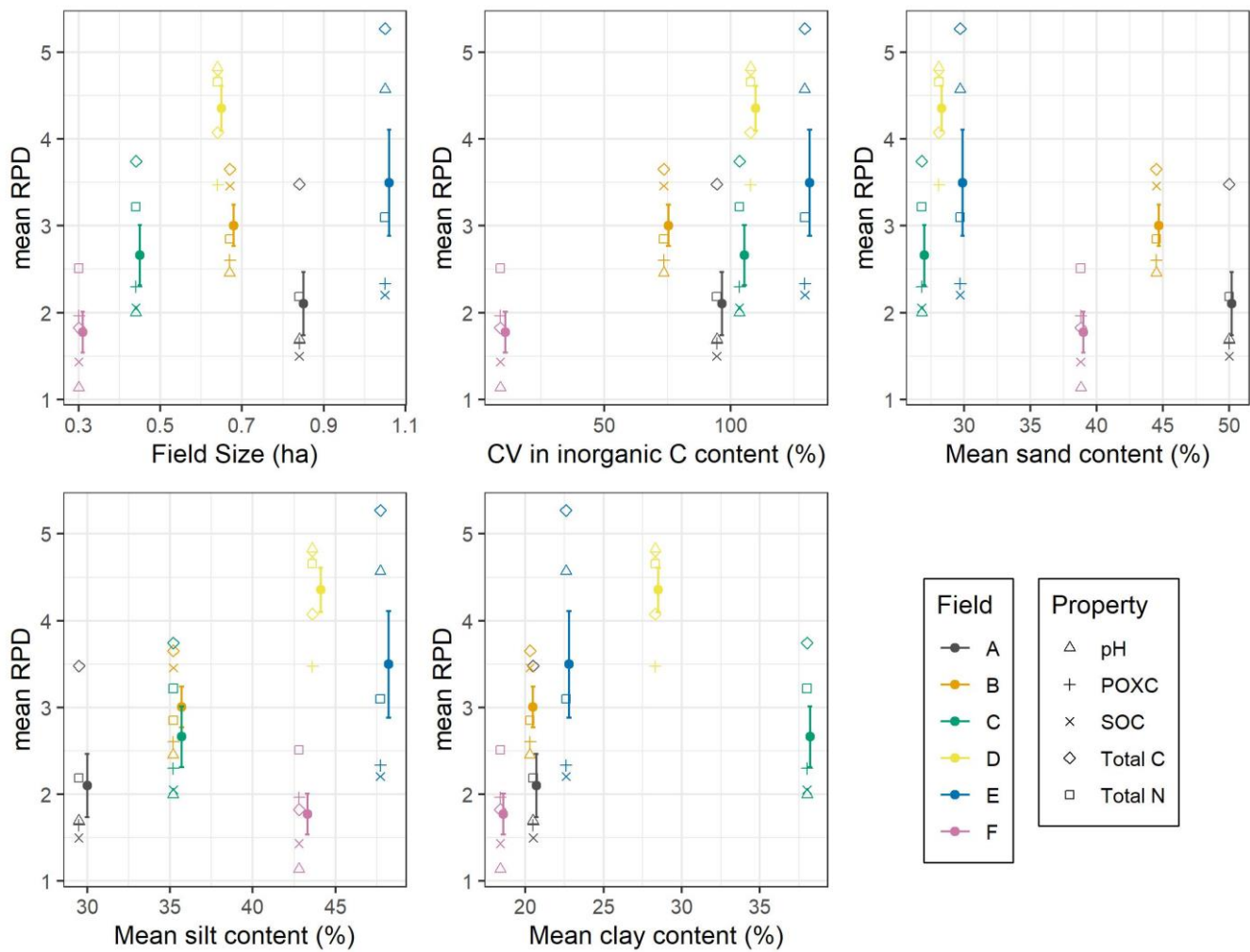
Figure S3: Ratio of performance to deviation (RPD) from the local models for SOC, total C, total N, POXC, and pH aggregated (mean and standard error) per field (A-F) in dependence of field size, coefficient of variation (CV) in inorganic C content, mean sand content, mean silt content and mean clay content. The error bars represent standard deviations across the repeats in the cross-validation
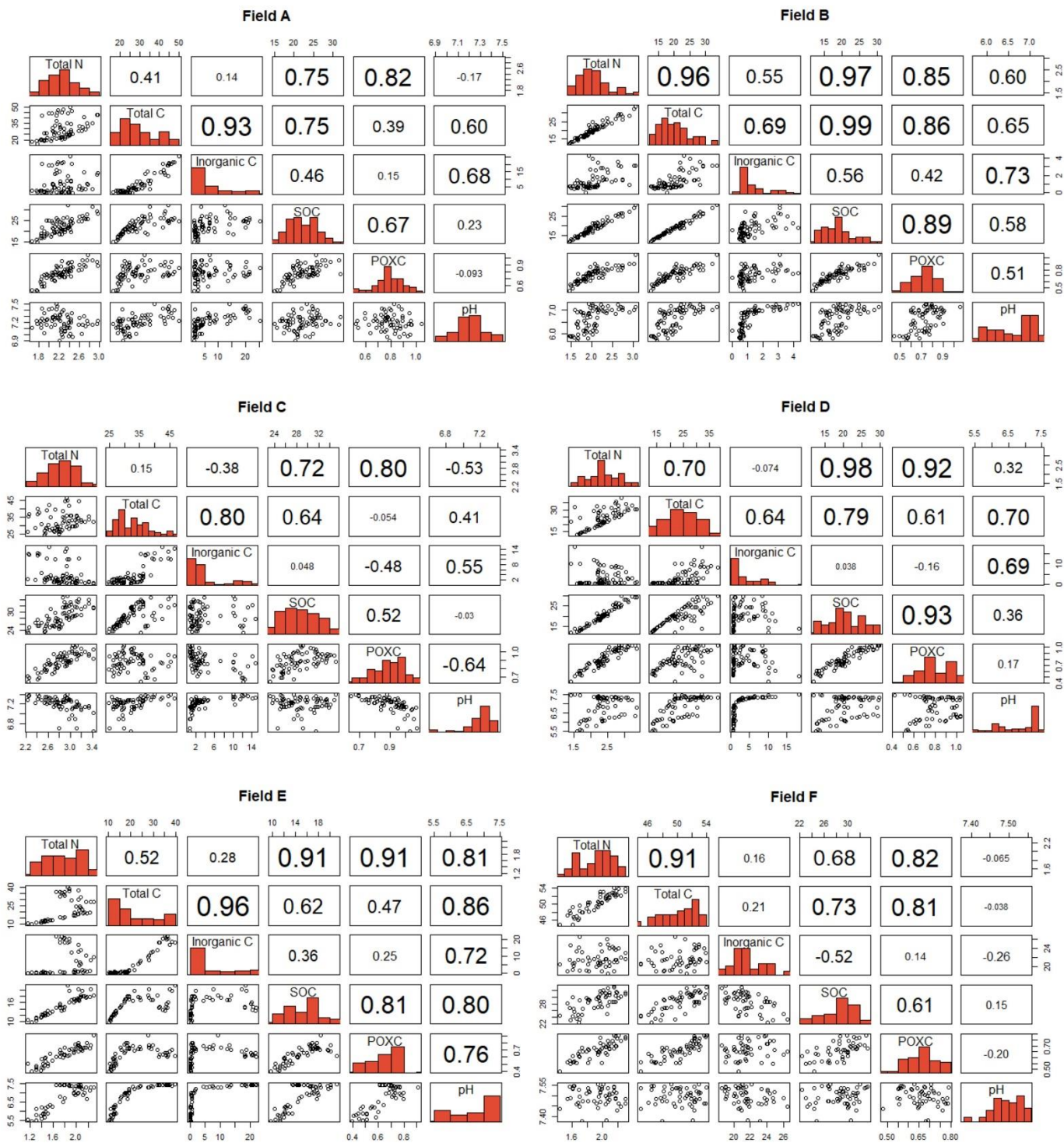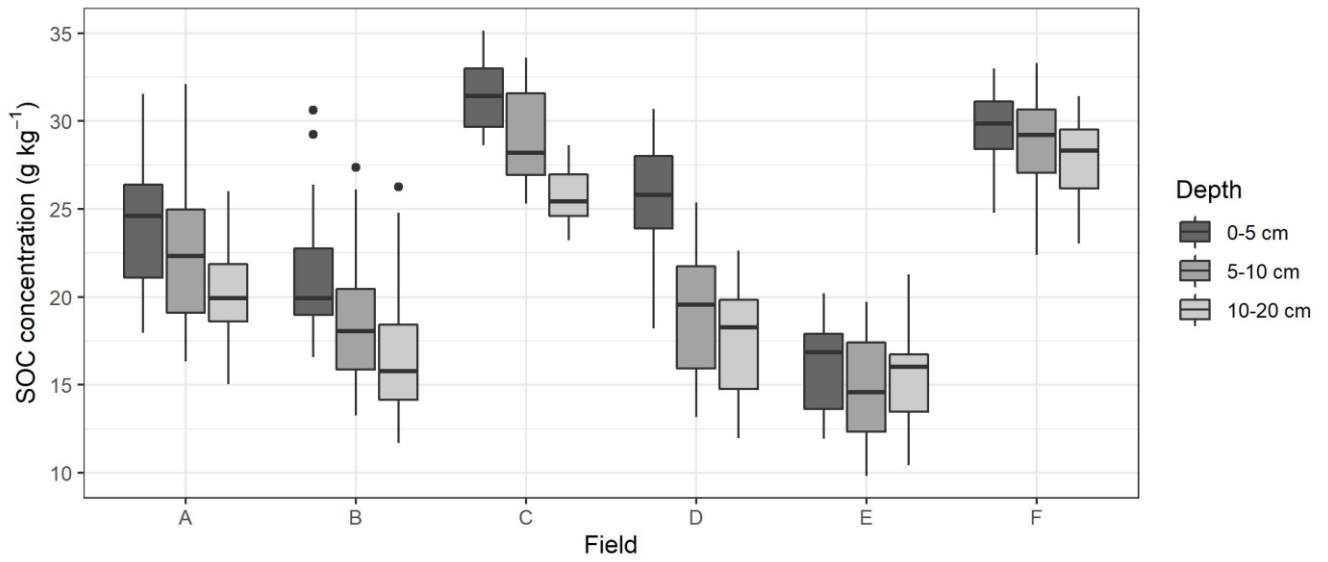
Figure S4: Pairwise correlation matrices between target soil properties and inorganic C for all Fields (A-F)

Figure S5: SOC concentration per soil depth in the reference dataset for fields A-F. Fields A, B, C and D have 70 samples and fields E and F 53 samples

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