

Electronic Supplementary Information (ESI)

A sparse modeling for small data: Case studies in controlled syntheses of 2D materials

Yuri Haraguchi,¹ Yasuhiko Igarashi^{2,3}, Hiroaki Imai,¹ Yuya Oaki*^{1,3},

¹ Department of Applied Chemistry, Faculty of Science and Technology, Keio University, 3-14-1 Hiyoshi, Kohoku-ku, Yokohama 223-8522, Japan

² Faculty of Engineering, Information and Systems, University of Tsukuba, 1-1-1 Tennodai, Tsukuba 305-8573, Japan

³ JST, PRESTO, 4-1-8 Honcho, Kawaguchi, Saitama 332-0012, Japan

E-mail: oakiyuya@aplc.keio.ac.jp

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†**Note:** All the training and test datasets in Tables S3–S7 are available as csv file.

Characteristics of objective variables in the datasets

Table S1. Characteristics of objective variables in the datasets.

Datasets		$y_1, y_1'' / \%$	$y_2, y_2'' / -$	$y_3, y_3'' / -$
Training	Mean	34.1	0.267	0.266
	SD	21.3	0.115	0.162
	n	30	48	54
Test	Mean	17.4	0.298	0.210
	SD	20.7	0.256	0.167
	n	79	64	43
Merged ^a (Training + Test)	Mean	22.0	0.285	0.241
	SD	22.1	0.208	0.166
	n	109	112	97

^a The merged dataset was used for the 10-segmentalized validation in Fig. 5.

Table S2. Training dataset for y1 (yield).²⁵

No.	x1	x2	x3	x4	x5	x6	x7	x8	x9	x10	x11	x12	x13	x14	x15	x16	x17	x18	x19	x20	x21	x22	x23	x24	x25	x26	x28	x29	x30	x31	x32	x34	x36	x39	x40	y1
y1_train_1	99.1	0.531	-24.4	202	1.03	32.2	0.3	1.67	1.47	40.8	24.7	81.4	91.7	4.30	1.02E-39	18	12.3	7.2	213.4	2.80E-39	1.24	72.2	157.4	286.0	1.95	2.90	0.585	0.93	16.1	2.3	4.1	1.78E-39	3.06	47.5	11.1	13.6
y1_train_2	73.1	0.429	-60.4	153	0.94	36.7	3.7	0.80	1.43	37.1	19.9	75.8	68.1	4.37	7.23E-40	17.4	13.7	11.3	213.4	2.80E-39	1.24	72.2	157.4	286.0	1.95	2.90	0.585	0.93	16.1	2.3	4.1	2.07E-39	3.14	52.3	13.7	22.5
y1_train_3	18.0	0.149	0.0	100	1.00	78.5	23.8	0.89	1.33	72.6	6.0	46.5	14.7	2.43	8.64E-41	15.5	16	42.3	122.2	1.46E-39	1.26	33.9	90.7	107.6	0.78	1.64	0.582	1.27	19.9	7	12.2	1.38E-39	1.17	27.9	32.6	62.1
y1_train_4	41.1	0.319	-43.8	82	0.78	35.9	88.8	0.34	1.34	31.8	10.3	60.2	30.8	3.93	3.89E-40	15.3	18	6.1	122.2	1.46E-39	1.26	33.9	90.7	107.6	0.78	1.64	0.582	1.27	19.9	7	12.2	1.07E-39	2.67	23.7	15.6	10.8
y1_train_5	99.1	0.531	-24.4	202	1.03	32.2	0.3	1.67	1.47	40.8	24.7	81.4	91.7	4.30	1.02E-39	18	12.3	7.2	122.2	1.46E-39	1.26	33.9	90.7	107.6	0.78	1.64	0.582	1.27	19.9	7	12.2	4.43E-40	3.04	9.2	8.2	12.0
y1_train_6	73.1	0.429	-60.4	153	0.94	36.7	3.7	0.80	1.43	37.1	19.9	75.8	68.1	4.37	7.23E-40	17.4	13.7	11.3	122.2	1.46E-39	1.26	33.9	90.7	107.6	0.78	1.64	0.582	1.27	19.9	7	12.2	7.40E-40	3.12	14.0	8.4	52.7
y1_train_7	78.1	0.471	18.5	189	1.10	46.5	0.6	1.99	1.48	45.7	20.1	76.5	53.0	5.16	7.93E-40	18.4	16.4	10.2	122.2	1.46E-39	1.26	33.9	90.7	107.6	0.78	1.64	0.582	1.27	19.9	7	12.2	6.69E-40	3.90	13.8	10.1	36.6
y1_train_8	18.0	0.149	0.0	100	1.00	78.5	23.8	0.89	1.33	72.6	6.0	46.5	14.7	2.43	8.64E-41	15.5	16	42.3	121.2	1.50E-39	1.17	33.4	95.2	114.7	0.80	1.70	0.451	0.92	18.8	4.8	6.6	1.41E-39	1.26	27.4	38.0	10.0
y1_train_9	32.0	0.287	-97.7	65	0.79	32.7	127.0	0.55	1.33	24.0	8.8	56.8	34.0	2.11	2.65E-40	15.1	12.3	22.3	121.2	1.50E-39	1.17	33.4	95.2	114.7	0.80	1.70	0.451	0.92	18.8	4.8	6.6	1.23E-39	0.94	24.6	18.9	14.1
y1_train_10	32.0	0.287	-97.7	65	0.79	32.7	127.0	0.55	1.33	24.0	8.8	56.8	34.0	2.11	2.65E-40	15.1	12.3	22.3	107.2	1.28E-39	1.49	27.4	83.5	96.3	0.70	1.34	0.483	1.41	18.8	4.6	7.1	1.01E-39	0.62	18.6	18.6	21.5
y1_train_11	58.1	0.436	-94.7	58	0.78	20.6	231.1	0.30	1.36	26.2	16.6	73.8	56.0	3.23	5.90E-40	15.5	10.4	7	107.2	1.28E-39	1.49	27.4	83.5	96.3	0.70	1.34	0.483	1.41	18.8	4.6	7.1	6.89E-40	1.74	10.8	8.8	12.2
y1_train_12	99.1	0.531	-24.4	202	1.03	32.2	0.3	1.67	1.47	40.8	24.7	81.4	91.7	4.30	1.02E-39	18	12.3	7.2	125.2	1.28E-39	3.61	30.6	88.1	91.5	0.72	1.58	0.481	1.15	18.7	6.2	7.3	2.60E-40	0.69	5.9	6.3	25.3
y1_train_13	73.1	0.429	-60.4	153	0.94	36.7	3.7	0.80	1.43	37.1	19.9	75.8	68.1	4.37	7.23E-40	17.4	13.7	11.3	125.2	1.28E-39	3.61	30.6	88.1	91.5	0.72	1.58	0.481	1.15	18.7	6.2	7.3	5.56E-40	0.77	10.7	8.9	21.8
y1_train_14	18.0	0.149	0.0	100	1.00	78.5	23.8	0.89	1.33	72.6	6.0	46.5	14.7	2.43	8.64E-41	15.5	16	42.3	123.2	1.36E-39	1.83	32.2	89.1	99.3	0.77	1.32	0.451	1.56	19.6	7.2	13.4	1.28E-39	0.60	26.2	31.3	65.8
y1_train_15	32.0	0.287	-97.7	65	0.79	32.7	127.0	0.55	1.33	24.0	8.8	56.8	34.0	2.11	2.65E-40	15.1	12.3	22.3	123.2	1.36E-39	1.83	32.2	89.1	99.3	0.77	1.32	0.451	1.56	19.6	7.2	13.4	1.10E-39	0.27	23.4	13.6	48.8
y1_train_16	46.1	0.411	-114.5	78	0.78	24.6	59.0	1.08	1.36	24.0	13.4	64.4	52.8	1.94	4.56E-40	15.8	8.8	19.4	123.2	1.36E-39	1.83	32.2	89.1	99.3	0.77	1.32	0.451	1.56	19.6	7.2	13.4	9.08E-40	0.11	18.8	9.8	45.4
y1_train_17	99.1	0.531	-24.4	202	1.03	32.2	0.3	1.67	1.47	40.8	24.7	81.4	91.7	4.30	1.02E-39	18	12.3	7.2	123.2	1.36E-39	1.83	32.2	89.1	99.3	0.77	1.32	0.451	1.56	19.6	7.2	13.4	3.45E-40	2.47	7.5	8.6	57.1
y1_train_18	73.1	0.429	-60.4	153	0.94	36.7	3.7	0.80	1.43	37.1	19.9	75.8	68.1	4.37	7.23E-40	17.4	13.7	11.3	123.2	1.36E-39	1.83	32.2	89.1	99.3	0.77	1.32	0.451	1.56	19.6	7.2	13.4	6.42E-40	2.54	12.3	8.1	67.1
y1_train_19	78.1	0.471	18.5	189	1.10	46.5	0.6	1.99	1.48	45.7	20.1	76.5	53.0	5.16	7.93E-40	18.4	16.4	10.2	123.2	1.36E-39	1.83	32.2	89.1	99.3	0.77	1.32	0.451	1.56	19.6	7.2	13.4	5.71E-40	3.32	12.0	10.0	73.0
y1_train_20	18.0	0.149	0.0	100	1.00	78.5	23.8	0.89	1.33	72.6	6.0	46.5	14.7	2.43	8.64E-41	15.5	16	42.3	113.2	1.19E-39	2.09	25.9	83.0	74.7	0.60	1.39	0.437	1.23	19.3	5.6	10.1	1.11E-39	0.34	19.9	34.7	59.7
y1_train_21	32.0	0.287	-97.7	65	0.79	32.7	127.0	0.55	1.33	24.0	8.8	56.8	34.0	2.11	2.65E-40	15.1	12.3	22.3	113.2	1.19E-39	2.09	25.9	83.0	74.7	0.60	1.39	0.437	1.23	19.3	5.6	10.1	9.29E-40	0.01	17.2	16.3	21.1
y1_train_22	99.1	0.531	-24.4	202	1.03	32.2	0.3	1.67	1.47	40.8	24.7	81.4	91.7	4.30	1.02E-39	18	12.3	7.2	113.2	1.19E-39	2.09	25.9	83.0	74.7	0.60	1.39	0.437	1.23	19.3	5.6	10.1	1.74E-40	2.21	1.2	7.7	14.3
y1_train_23	73.1	0.429	-60.4	153	0.94	36.7	3.7	0.80	1.43	37.1	19.9	75.8	68.1	4.37	7.23E-40	17.4	13.7	11.3	113.2	1.19E-39	2.09	25.9	83.0	74.7	0.60	1.39	0.437	1.23	19.3	5.6	10.1	4.71E-40	2.28	6.1	9.0	22.1
y1_train_24	78.1	0.471	18.5	189	1.10	46.5	0.6	1.99	1.48	45.7	20.1	76.5	53.0	5.16	7.93E-40	18.4	16.4	10.2	113.2	1.19E-39	2.09	25.9	83.0	74.7	0.60	1.39	0.437	1.23	19.3	5.6	10.1	4.00E-40	3.07	5.8	10.9	15.4
y1_train_25	18.0	0.149	0.0	100	1.00	78.5	23.8	0.89	1.33	72.6	6.0	46.5	14.7	2.43	8.64E-41	15.5	16	42.3	171.2	2.23E-39	1.45	44.4	100.9	146.0	0.83	1.84	0.502	1.26	19.5	4	5.9	2.15E-39	0.98	38.3	39.2	10.4
y1_train_26	32.0	0.287	-97.7	65	0.79	32.7	127.0	0.55	1.33	24.0	8.8	56.8	34.0	2.11	2.65E-40	15.1	12.3	22.3	171.2	2.23E-39	1.45	44.4	100.9	146.0	0.83	1.84	0.502	1.26	19.5	4	5.9	1.97E-39	0.66	35.6	20.4	62.1
y1_train_27	46.1	0.411	-114.5	78	0.78	24.6	59.0	1.08	1.36	24.0	13.4	64.4	52.8	1.94	4.56E-40	15.8	8.8	19.4	171.2	2.23E-39	1.45	44.4	100.9	146.0	0.83	1.84	0.502	1.26	19.5	4	5.9	1.78E-39	0.49	30.9	16.1	32.0
y1_train_28	58.1	0.436	-94.7	58	0.78	20.6	231.1	0.30	1.36	26.2	16.6	73.8	56.0	3.23	5.90E-40	15.5	10.4	7	171.2	2.23E-39	1.45	44.4	100.9	146.0	0.83	1.84	0.502	1.26	19.5	4	5.9	1.64E-39	1.78	27.8	10.3	13.0
y1_train_29	119.4	0.287	-63.5	61	1.48	4.8	194.8	0.54	1.44	29.9	14.3	73.6	15.0	1.53	6.53E-40	17.8	3.1	5.7	171.2	2.23E-39	1.45	44.4	100.9	146.0	0.83	1.84	0.502	1.26	19.5	4	5.9	1.58E-39	0.08	30.1	3.5	55.3
y1_train_30	73.1	0.429	-60.4	153	0.94	36.7	3.7	0.80	1.43	37.1	19.9	75.8	68.1	4.37	7.23E-40	17.4	13.7	11.3	171.2	2.23E-39	1.45	44.4	100.9	146.0	0.83	1.84	0.502	1.26	19.5	4	5.9	1.51E-39	2.93	24.5	11.9	44.1

