

Supplementary materials

Here, we provide supplementary information to the article: “Interpreting neural networks trained to predict plasma temperature from optical emission spectra”.

Synthetic spectra

The chemical composition of the ChemCam sample used for generating the synthetic spectra.

Table S1: The 29 considered target compositions.

Sample number	Sample Composition (wt. %)										
	Si	Ti	Al	Fe	Mn	Mg	Ca	Na	K	P	O
1	22.38	0.42	10.55	12.20	0.00	5.80	9.12	0.64	0.05	0.00	41.74
2	45.81	1.06	0.06	0.71	0.00	0.01	0.03	0.00	0.00	0.26	53.48
3	20.37	0.26	8.92	15.92	0.00	6.74	6.40	1.28	0.08	0.00	40.22
4	23.68	1.68	9.73	8.95	0.13	4.12	8.27	0.95	0.43	0.12	42.07
5	33.13	0.15	12.26	0.96	0.02	0.28	2.14	2.47	1.03	0.02	47.61
6	39.69	0.02	8.35	0.84	0.12	1.27	0.01	0.06	0.02	0.00	49.68
7	34.41	0.20	9.85	1.41	0.03	0.22	0.81	1.42	4.65	0.03	47.02
8	35.12	0.04	9.62	0.77	0.02	0.02	0.07	2.17	4.10	0.00	47.92
9	34.60	0.87	4.89	4.69	0.07	2.04	4.23	0.46	0.22	0.33	47.42
10	23.63	1.30	20.25	7.80	0.07	1.92	1.44	0.92	1.15	0.00	41.28
11	23.52	1.69	9.36	12.62	0.21	1.79	4.82	1.40	1.75	0.82	41.73
12	29.07	0.55	12.79	2.84	0.06	0.58	1.34	2.30	5.32	0.11	44.66
13	32.30	0.25	11.30	3.22	0.07	1.73	1.21	1.17	2.30	0.00	46.03
14	29.45	0.43	12.24	5.11	0.14	3.26	1.36	0.48	3.03	0.00	44.08
15	29.89	0.35	12.57	3.29	0.06	1.19	3.59	2.00	1.10	0.06	45.44
16	22.54	0.02	23.02	0.78	0.01	0.14	10.96	1.11	0.03	0.01	40.91
17	37.82	0.08	9.07	3.74	0.14	0.35	0.07	0.04	0.10	0.00	48.12
18	22.63	0.25	7.80	13.57	0.00	3.85	10.21	0.66	0.09	0.00	40.43
19	34.47	0.02	11.77	0.40	0.05	0.01	0.17	1.70	3.31	0.20	47.38
20	37.95	0.19	6.61	2.38	0.02	0.74	0.89	0.87	0.93	0.00	48.87
21	22.60	0.70	12.49	7.23	0.13	5.10	8.70	0.90	0.16	0.06	41.38
22	22.30	0.58	11.08	7.92	0.14	5.85	9.58	0.76	0.02	0.01	41.16
23	23.31	0.96	12.05	7.37	0.11	4.45	6.24	1.61	0.93	0.20	42.14
24	35.30	0.11	9.55	0.65	0.02	0.10	0.56	1.50	4.03	0.04	47.45
25	36.37	0.14	7.41	2.52	0.06	1.98	0.01	0.06	3.45	0.02	47.28
26	38.90	0.08	6.54	0.86	0.01	0.45	0.91	0.79	1.49	0.00	49.24
27	34.77	0.02	10.21	1.22	0.02	0.04	0.31	1.88	3.37	0.00	47.42
28	24.96	0.15	20.39	0.78	0.01	0.11	7.64	2.17	0.13	0.02	42.90
29	24.87	0.71	10.54	10.03	0.15	2.81	7.07	0.85	0.35	0.04	41.81

Artificial neural network

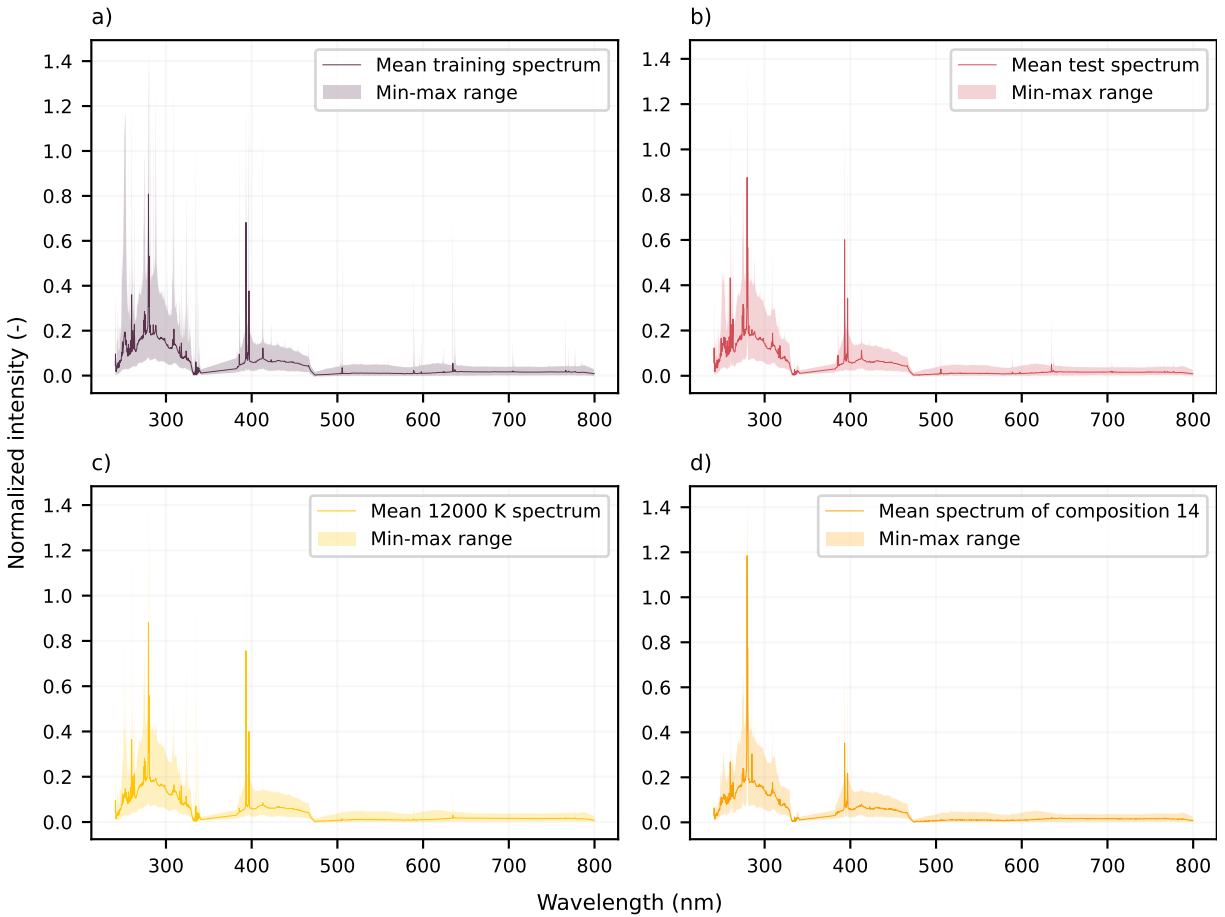


Figure S1: Summary representation of the dataset: a) mean of the training dataset; b) mean of the testing dataset; c) mean of all spectra generated at 12000 K, *i.e.*, averaged over all compositions; d) mean of all spectra of the target composition 14, *i.e.*, the average over, all temperature values. The shaded areas represent the corresponding standard deviation.

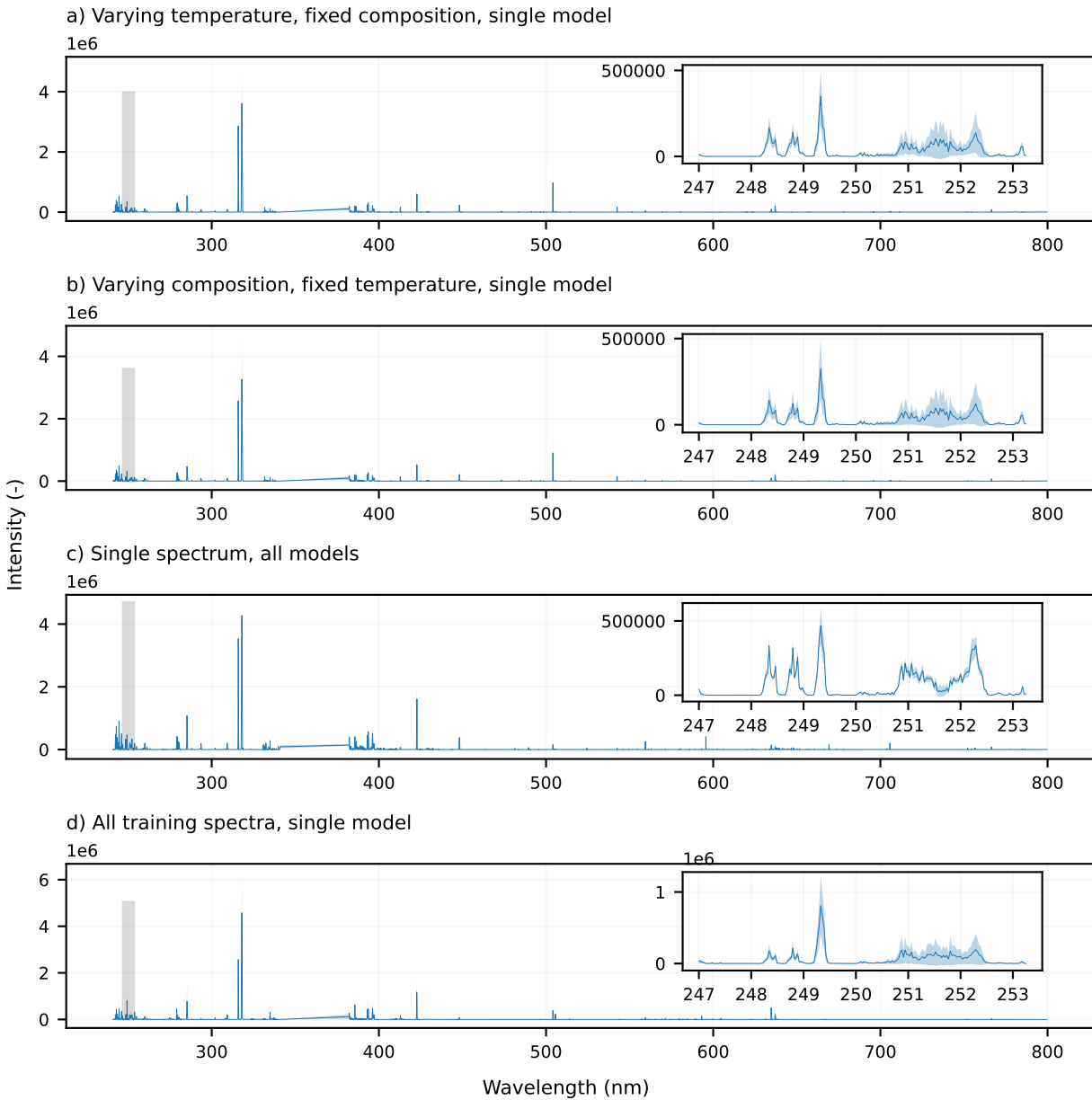


Figure S2: Summary of the relevance scores analysis: a) mean relevance scores across all temperatures with fixed composition; b) mean relevance scores overall compositions at a fixed temperature; c) mean relevance score of a single spectrum over all models (which were identical in architecture and training but differed in initialization); and d) mean relevance scores over the whole training dataset. The shaded areas represent the standard deviation. The transparent rectangle corresponds to the inset's position.

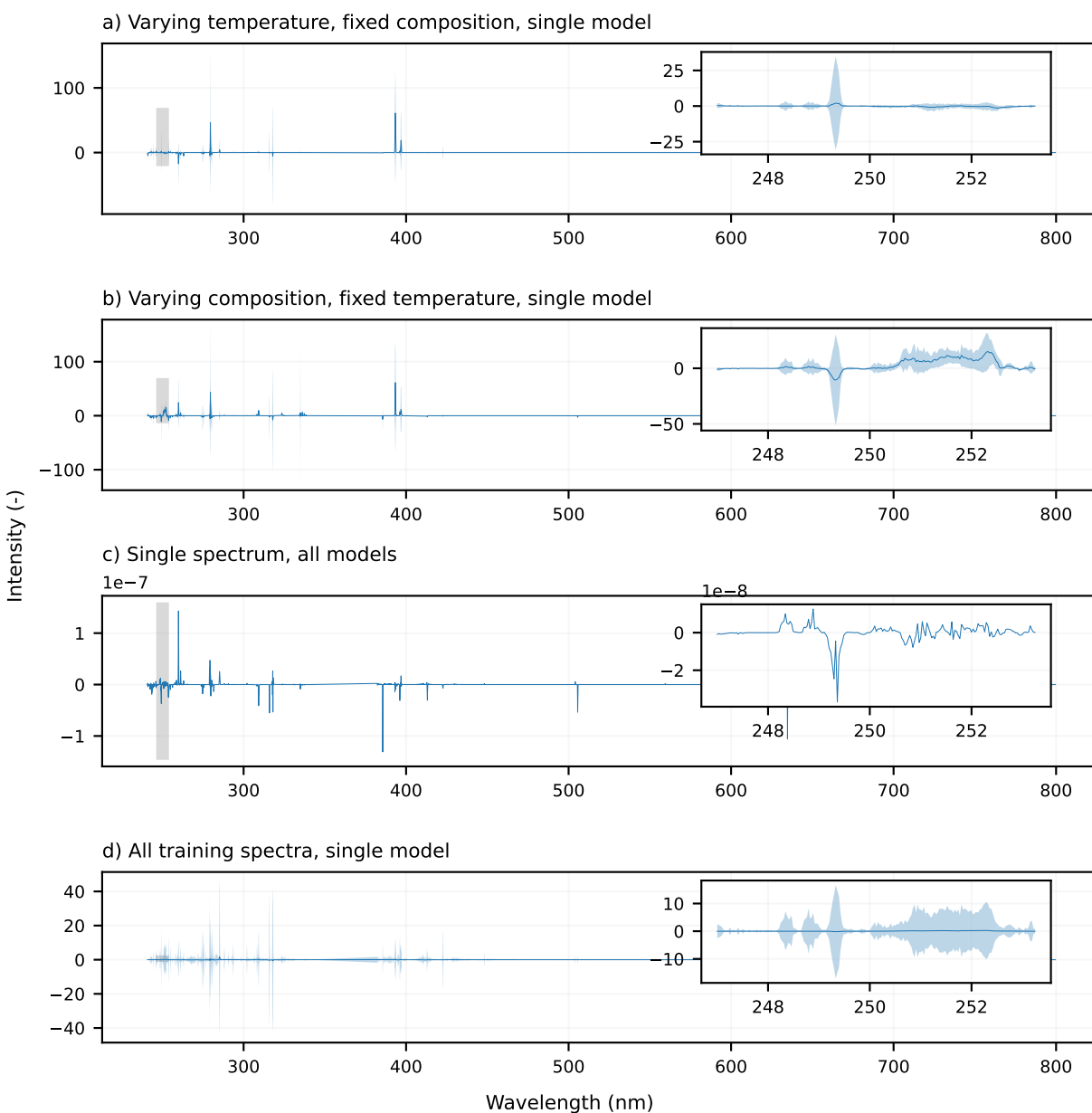


Figure S3: Summary of the first order Taylor approximation analysis: a) mean Taylor spectrum (second term on the right-hand side of Eq. 16 in the main text) across all temperatures with a fixed composition; b) Taylor spectrum averaged over all compositions at a fixed temperature; c) mean Taylor spectrum of a single spectrum over all models (which were identical in architecture and training but differed in initialization); and d) mean relevance scores over the whole training dataset. The shaded areas represent the standard deviation. The transparent rectangle corresponds to the inset's position.