Estimation of groundwater age distributions from hydrochemistry: Comparison of two metamodelling algorithms in the Heretaunga Plains aquifer system, New Zealand

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Spreadsheets (Table S2 and Table S3, attached): Input data and model results (Table S2); and time series data used for predictions, and predicted results, (Table S3)
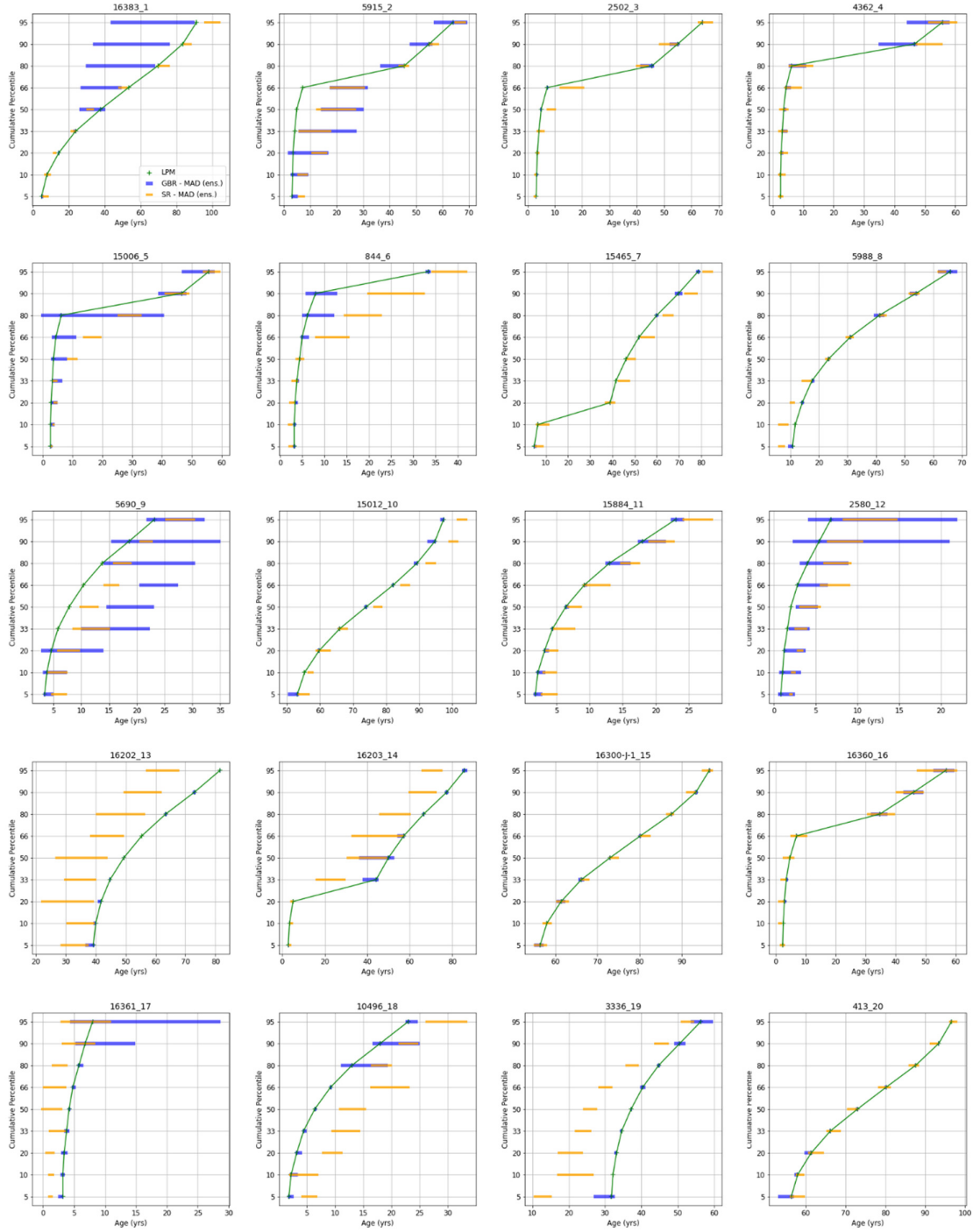
Figure S1: Age distributions for samples 1-20 based on LPMs (green) (Morgenstern et al. 2018) compared to the chained SR (orange) and GBR (blue) models developed in this study (bars represent ensemble MAD). The map ID following the underscore links with the location of the site on Fig. 3.

Figure S2: Age distributions for samples 21-40 based on LPMs (green) (Morgenstern et al. 2018) compared to the chained SR (orange) and GBR (blue) models developed in this study (bars represent ensemble MAD). The map ID following the underscore links with the location of the site on Fig. 3.

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Figure S3: Age distributions for samples 41-60 based on LPMs (green) (Morgenstern et al. 2018) compared to the chained SR (orange) and GBR (blue) models developed in this study (bars represent ensemble MAD). The map ID following the underscore links with the location of the site on Fig. 3.
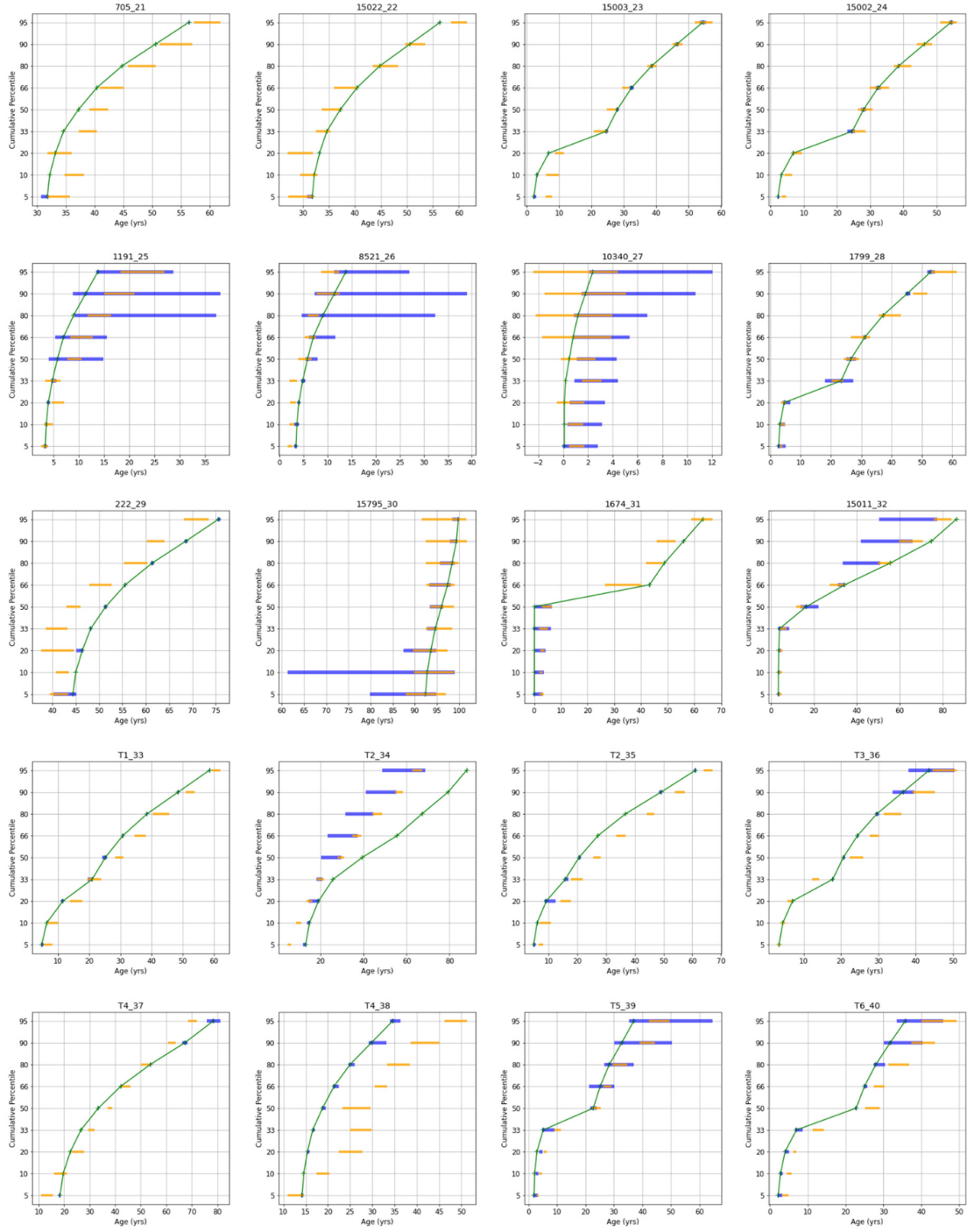
Figure S4: Age distributions for samples 61-76 based on LPMs (green) (Morgenstern et al. 2018) compared to the chained SR (orange) and GBR (blue) models developed in this study (bars represent ensemble MAD). The map ID following the underscore links with the location of the site on Fig. 3.
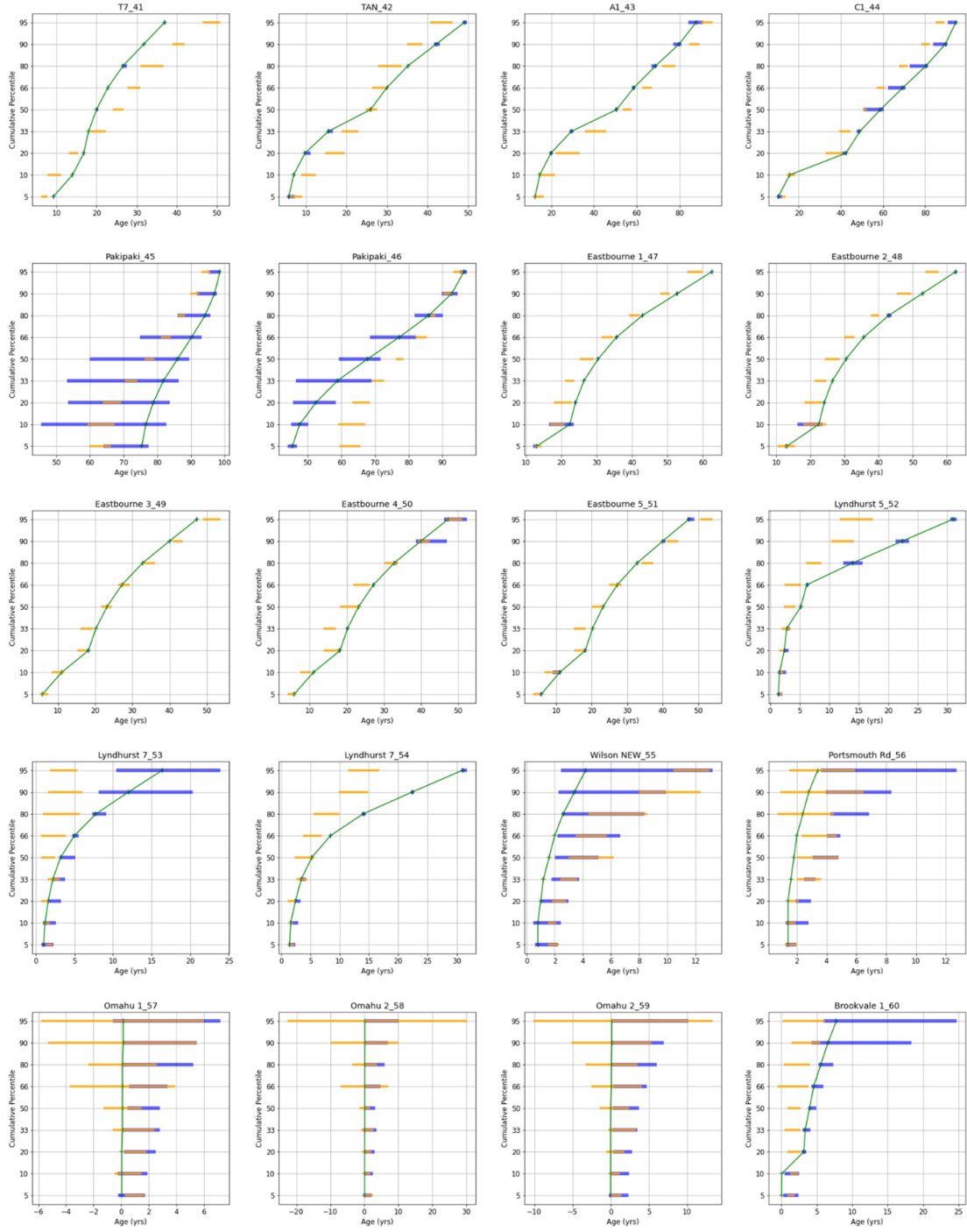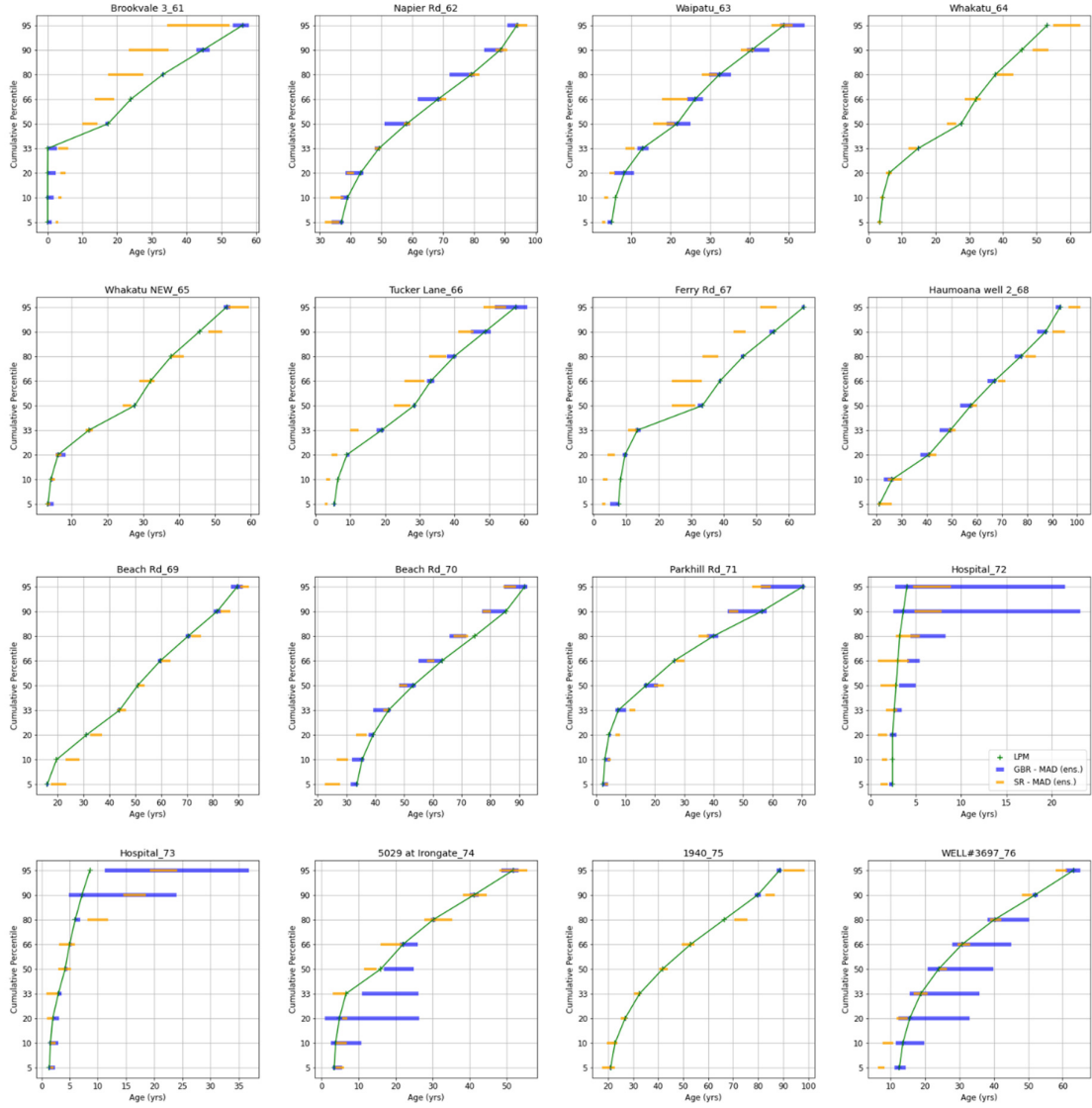
Table S1. Goodness of fit metrics for the 40-member ensembles of SR and GBR models at each of nine percentiles.

	Percentile	Unchained models										Chained models									
		R²		Absolute Error (Years)						Relative Error (%)		R²		Absolute Error (Years)						Relative Error (%)	
		Ensemble Mean		Ensemble Mean		Ensemble Min		Ensemble Max		Ensemble Mean		Ensemble Mean		Ensemble Mean		Ensemble Min		Ensemble Max		Ensemble Mean	
		Train	Test	Train	Test	Train	Test	Train	Test	Train	Test	Train	Test	Train	Test	Train	Test	Train	Test	Train	Test
Symbolic Regression	5	0.88	0.77	6.2	9.0	3.3	3.4	8.7	14.5	26.5	22.5	0.97	0.88	2.4	4.8	1.3	2.9	5.7	8.1	5.8	6.3
	10	0.90	0.73	4.9	7.8	2.2	3.7	9.3	16.0	16.8	13.9	0.97	0.91	2.2	4.6	1.6	2.5	2.6	7.2	3.7	4.7
	20	0.91	0.75	4.3	6.9	2.9	3.6	6.9	11.7	6.4	8.6	0.97	0.91	2.4	4.6	1.3	2.6	4.3	6.9	3.5	5.5
	33	0.91	0.76	4.7	8.0	3.3	4.3	6.2	12.0	3.2	4.1	0.96	0.91	2.9	4.7	2.0	2.0	4.5	6.1	1.1	2.0
	50	0.92	0.77	5.2	8.7	3.7	5.5	7.6	12.5	3.4	5.4	0.96	0.92	3.2	5.1	2.2	3.7	4.9	6.6	1.5	2.6
	66	0.89	0.73	6.4	10.0	4.8	6.6	9.5	13.7	1.8	3.4	0.95	0.89	3.9	6.5	2.5	4.7	5.2	8.9	1.0	2.2
	80	0.87	0.72	7.3	11.6	5.7	6.9	10.7	16.3	2.2	2.4	0.95	0.88	4.2	7.3	2.8	4.6	5.2	10.2	0.9	3.0
	90	0.85	0.65	8.1	13.7	6.0	11.6	11.5	16.4	1.7	3.6	0.94	0.88	4.9	7.9	3.5	5.8	7.0	10.3	0.6	2.2
	95	0.84	0.62	8.6	15.4	6.4	10.8	11.6	19.9	1.8	4.5	0.93	0.87	5.4	8.9	3.9	6.4	7.3	11.9	0.6	3.1
	All	0.83		7.5						7.3		0.94		4.4						2.6	
Gradient Boosted Regression	5	0.99	0.76	1.04	5.32	0.00	0.05	4.75	31.8	4.17	7.02	1	0.51	0.44	7.69	0.01	0.05	2.69	43.8	2.42	6.48
	10	1	0.76	0.48	5.28	0.00	0.04	2.04	31.0	2.52	7.35	1	0.53	0.43	8.24	0.00	0.02	2.80	41.6	2.82	6.90
	20	1	0.82	0.47	5.48	0.00	0.09	2.05	34.2	2.82	7.42	0.99	0.70	0.71	7.34	0.00	0.03	8.29	34.5	3.60	7.54
	33	1	0.81	0.37	6.43	0.00	0.05	1.64	27.5	0.47	3.51	0.98	0.78	1.13	7.03	0.00	0.04	11.92	28.8	1.21	4.72
	50	1	0.80	0.20	7.37	0.00	0.19	0.59	26.3	0.19	4.81	0.98	0.79	1.41	7.65	0.00	0.19	16.88	28.1	1.87	6.23
	66	1	0.81	0.18	8.43	0.00	0.01	0.51	24.9	0.06	2.04	0.97	0.80	1.61	8.41	0.00	0.17	25.40	28.0	0.62	1.80
	80	1	0.82	0.34	8.86	0.00	0.07	0.85	24.6	0.15	2.15	0.96	0.80	2.11	9.42	0.00	0.09	29.12	31.7	0.78	2.26
	90	1	0.73	0.30	11.09	0.00	0.43	1.05	39.8	0.14	1.72	0.95	0.78	2.67	10.20	0.00	0.14	31.25	39.7	0.57	1.93
	95	1	0.74	0.41	12.18	0.02	0.36	1.02	29.78	0.13	1.90	0.96	0.77	2.66	10.19	0.00	0.58	29.22	49.2	0.65	2.12
	All	0.98		1.16						1.47		0.95		2.16						1.90	