

# Supplement To “Bayesian Nonparametric Monotone Regression”

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## 1 Additional Simulation Results

### 1.1 More detailed tables

Tables 1 and 2 show additional simulation results for estimation of  $f$ . The table includes BNMR and BISOREG with additional choices for order of the basis expansion and additional metrics to summarize the results.

Tables 3 and 4 show additional simulation results for estimation of the derivative  $f'$ . The table includes BNMR and BISOREG with additional choices for order of the basis expansion and additional metrics to summarize the results.

### 1.2 Sensitivity to choice of $\mu$ and $\phi$

Additional simulation results to assess the sensitivity to the choice of  $\mu$  and  $\phi$ , the prior mean and standard deviation of the base measure on the Dirichlet process. All results are for sample size  $n = 100$  and based on 100 simulated datasets for each scenario and each combination of parameter levels. All other details are the same as described in the main simulation study presented in the main text.

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Figures 1 and 2 show that the root mean square error (RMSE) on the estimated regression function and its derivative are fairly robust to the choice of priors. Figure 3 shows that in the flat scenario the posterior probability of a flat response (no association) is sensitive to this choice. Specifically, the posterior probability of a flat response decreases as the prior variance increases. Hence, the regression function does not change a lot but the inference on no association is sensitive. Figure 4 shows that the number of unique non-zero regression parameters (the number of clusters) increases as  $\phi$  increases.

## 2 Additional Data Analysis Results

Figures 5-10 show the estimated pressure differential with each of the six methods. Figures 11-16 show the time-resolved  $\text{PM}_{2.5}$  concentration estimated with each of the six methods. Figures 17 and 18 shows the posterior mode basis with BNMR and BISOREG for each sample.

## 3 Additional Details of Computation

Table 5 shows the results for the MCMC efficiency for both BNMR and BISOREG from the data analysis. The two methods use the same Bernstein polynomial basis. The effective sample size and autocorrelation function were calculated for the estimation of  $f(x)$  for each observation in the data. We then calculated the mean across all observations as a summary measure for each of the 12 samples. The table presents means, medians, and standard errors for the means across all 12 samples. Note that the posterior was thinned so that every 10<sup>th</sup> iteration was retained and the autocorrelation and effective sample size was computed after thinning. Hence, the lag 1 autocorrelation in the table is really the lag 10 from the unthinned posterior sample and the lag 10 autocorrelation in the table is really the lag 100 from the unthinned posterior sample.

Figure 19 shows the computation time for the simulation study as a function of sample size

and order of the Bernstein polynomial used. All computing was done on Intel Xeon E5-2680 v3 @2.50GHz (2 CPUs/node, 24 cores/node) processor using a single node. Specifically, the figure shows median computation time and the 25<sup>th</sup> to 75<sup>th</sup> percentiles. All MCMC chains in the simulated data sets were run for 150,000 iterations.

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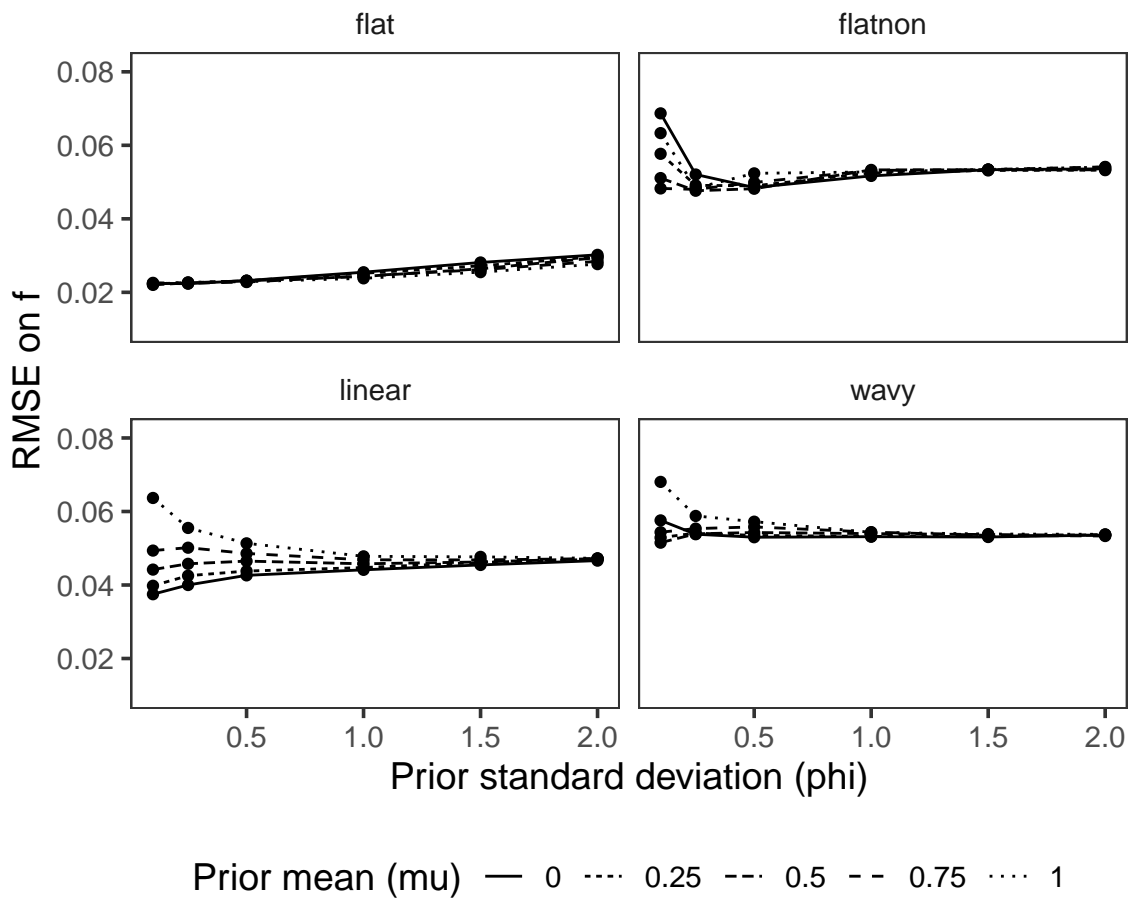


Figure 1: RMSE on the estimated function  $f$  as a function of  $\mu$  and  $\phi$ .

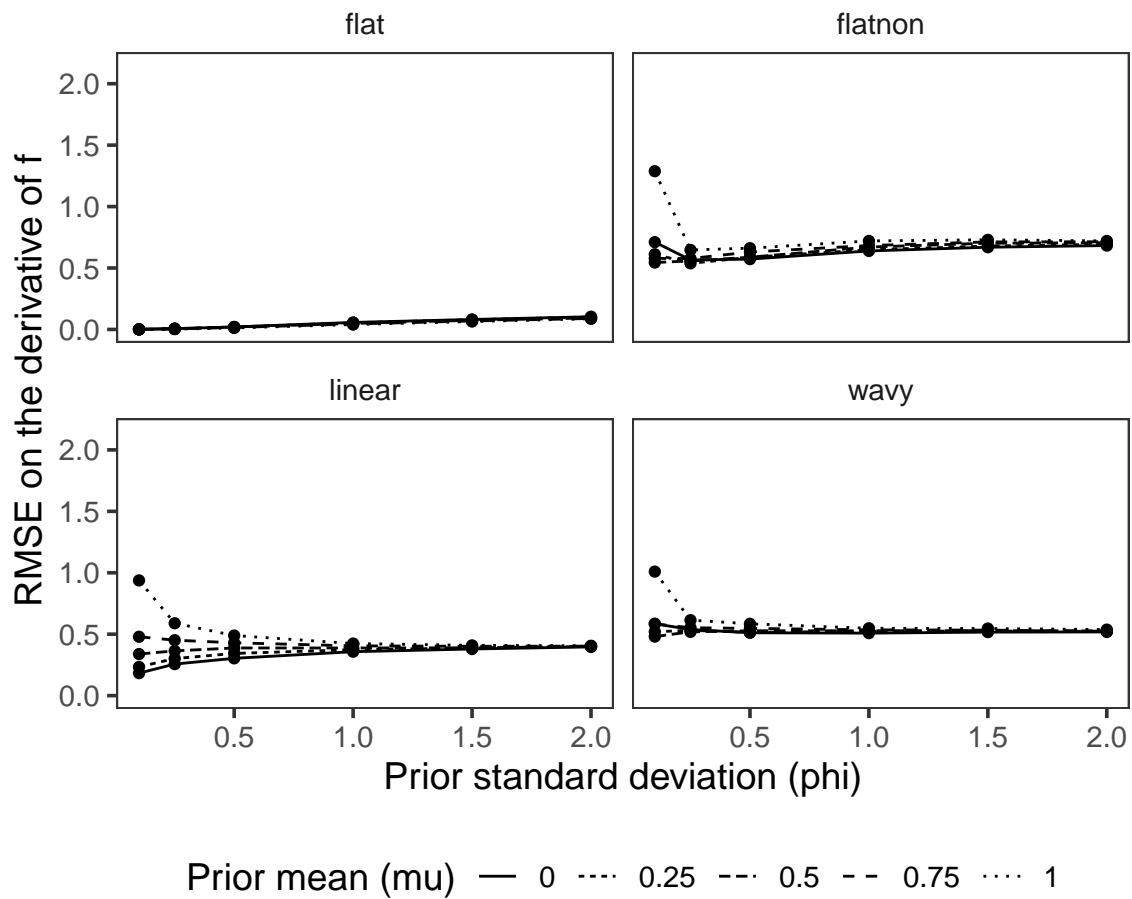


Figure 2: RMSE on the estimated derivative of the function  $f$  as a function of  $\mu$  and  $\phi$ .

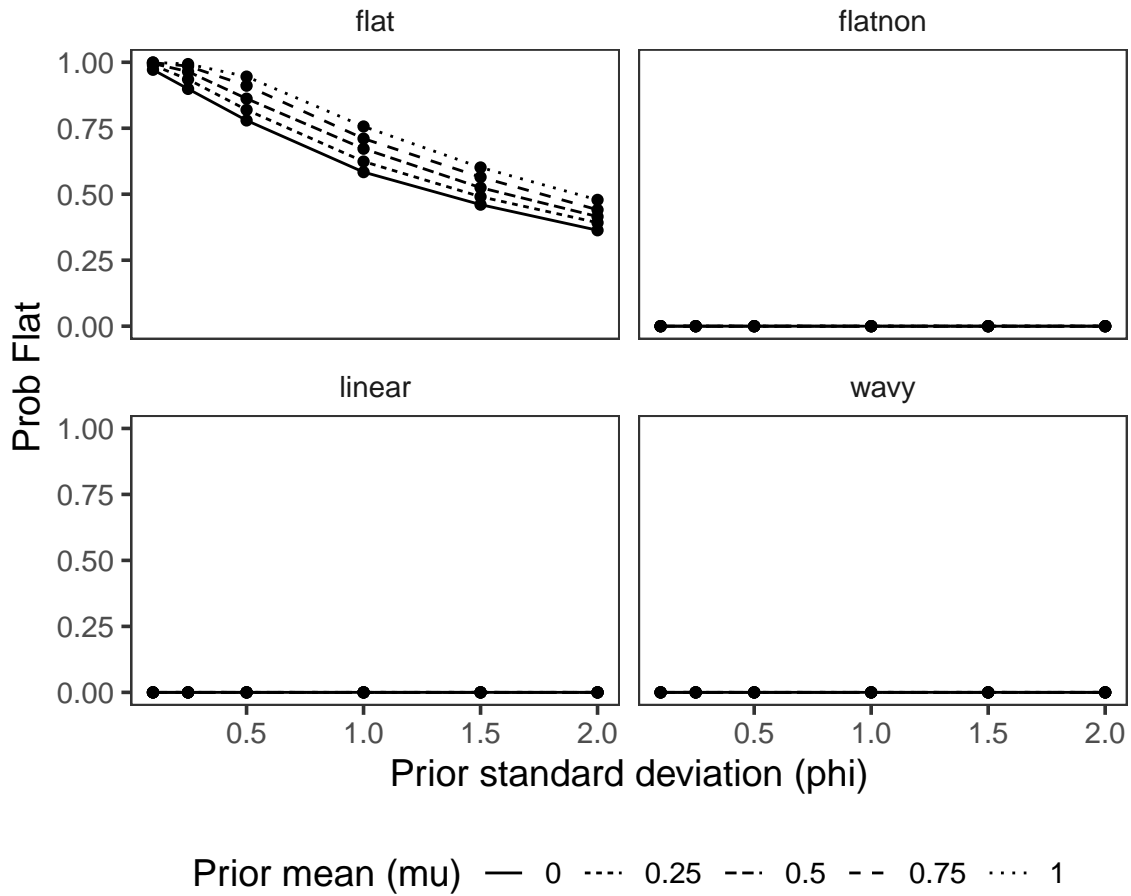


Figure 3: Mean posterior probability of a flat response (no association) as a function of  $\mu$  and  $\phi$ .

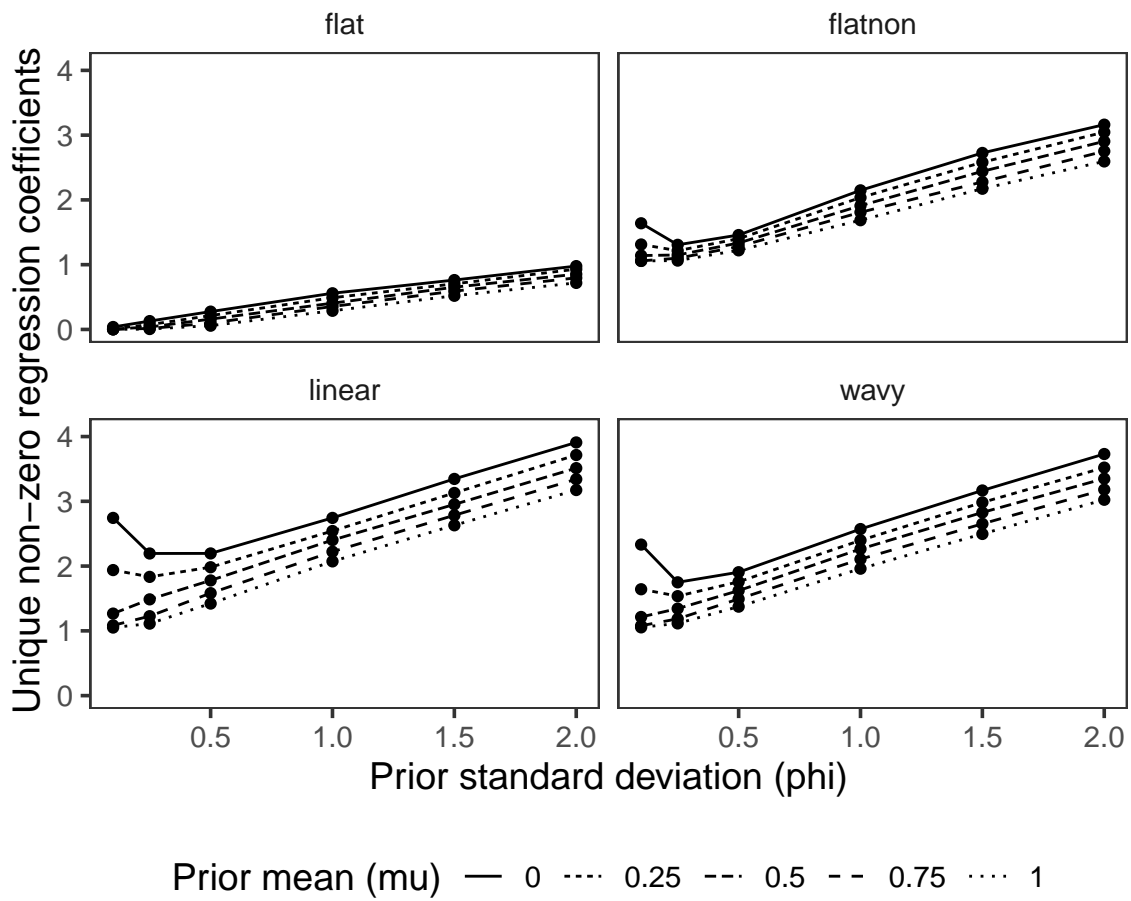


Figure 4: Mean number of unique non-zero regression parameters as a function of  $\mu$  and  $\phi$ .



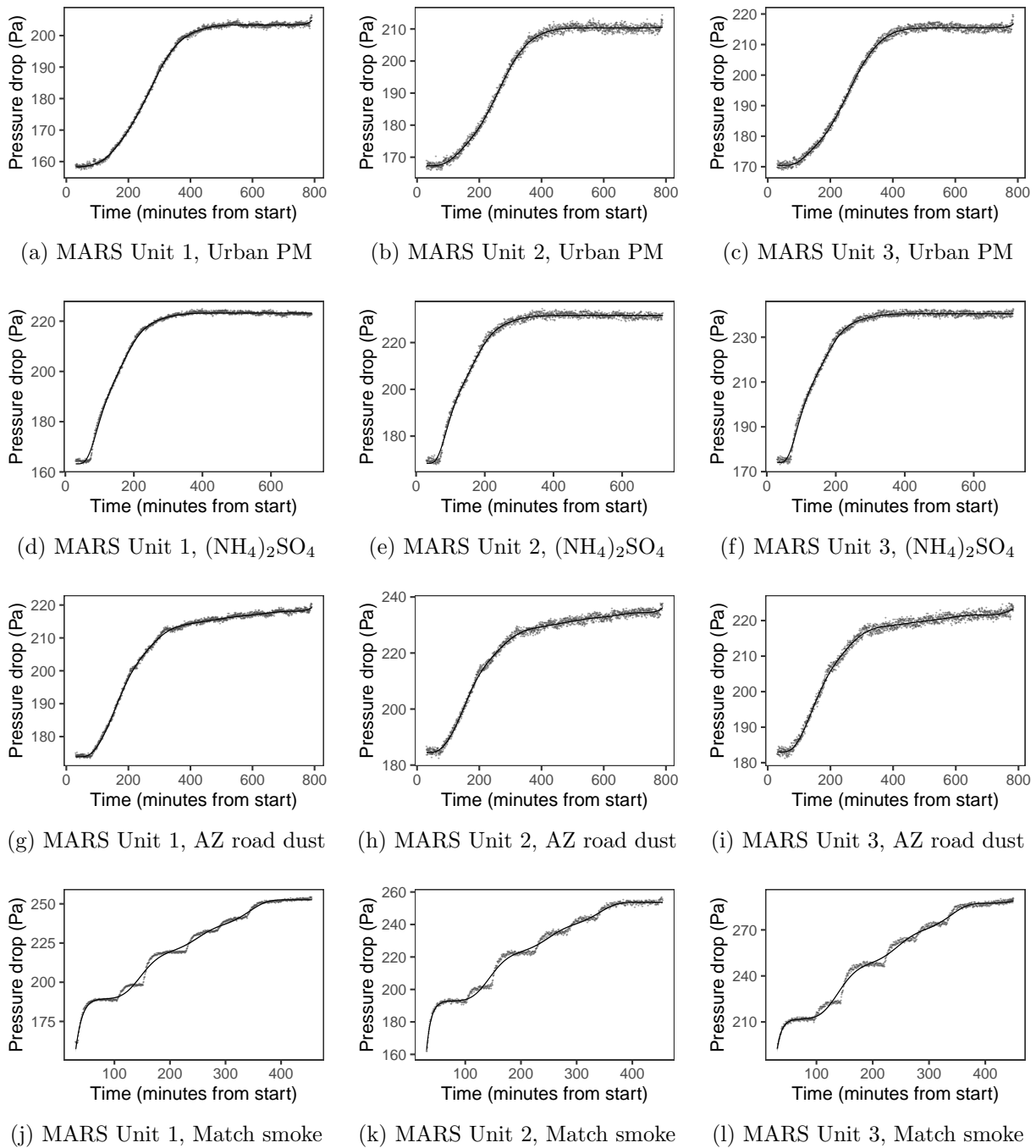


Figure 5: Estimated pressure differential with BNMR for each of the 12 samples.

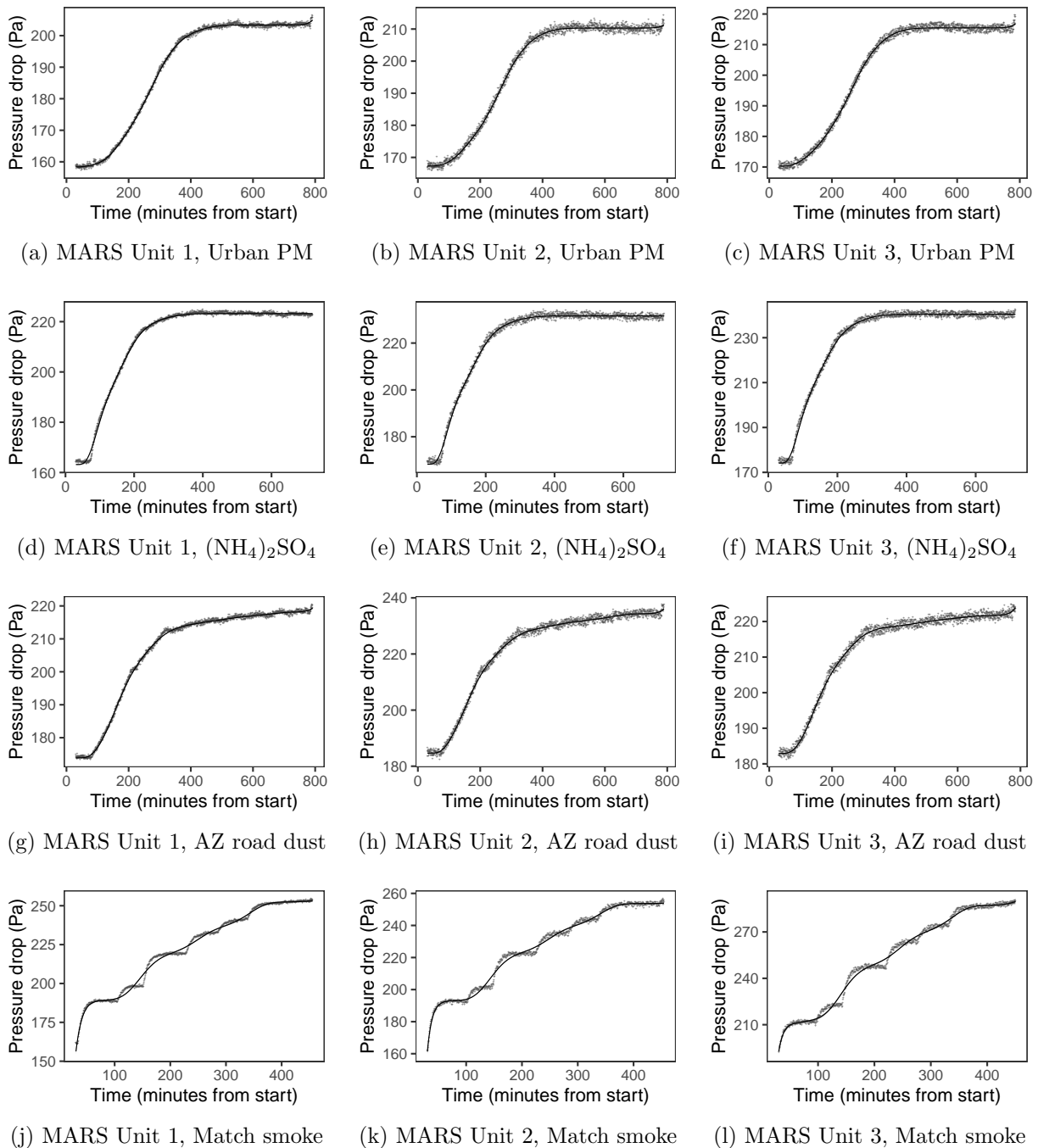


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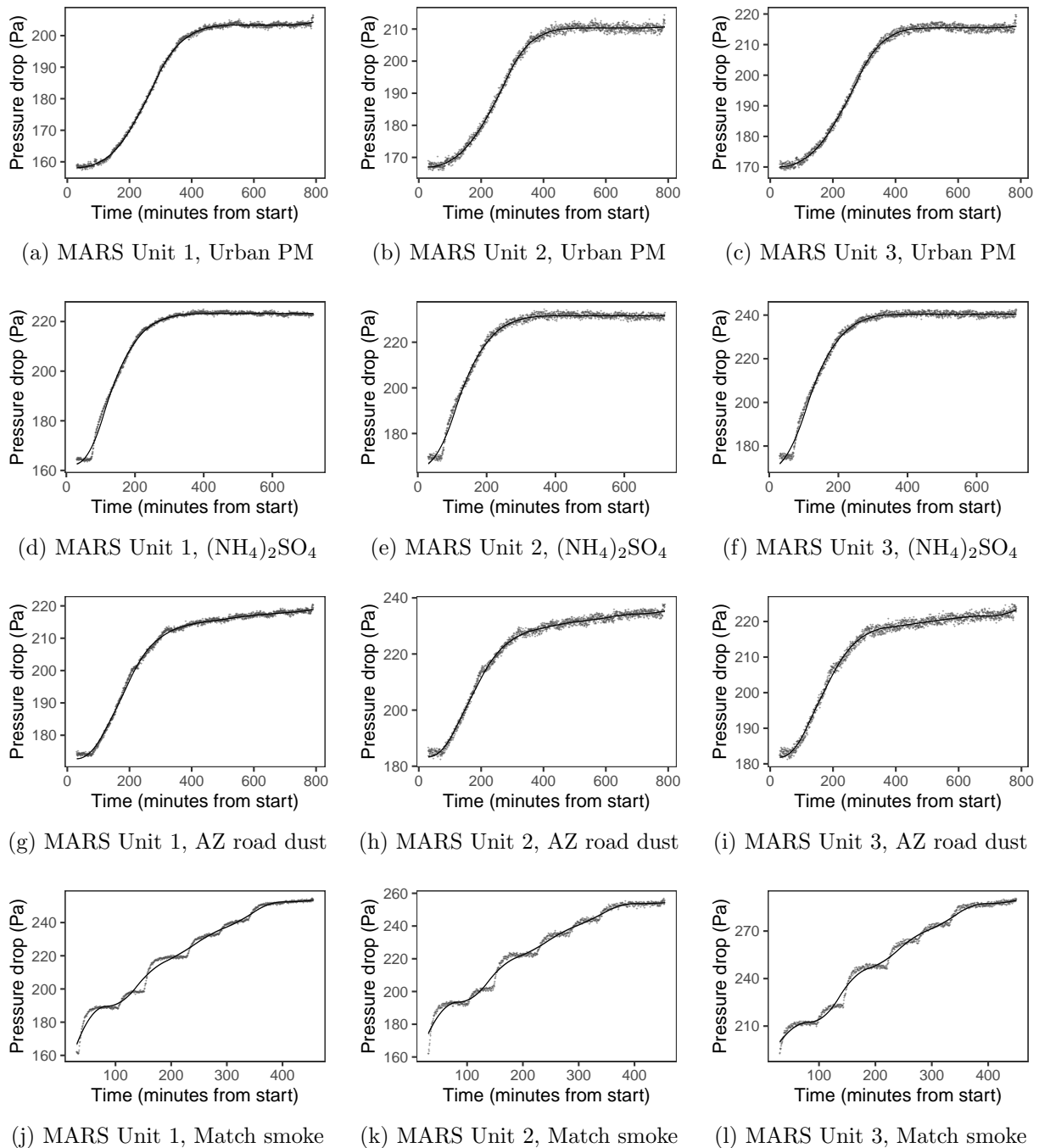


Figure 7: Estimated pressure differential with CGAM for each of the 12 samples.

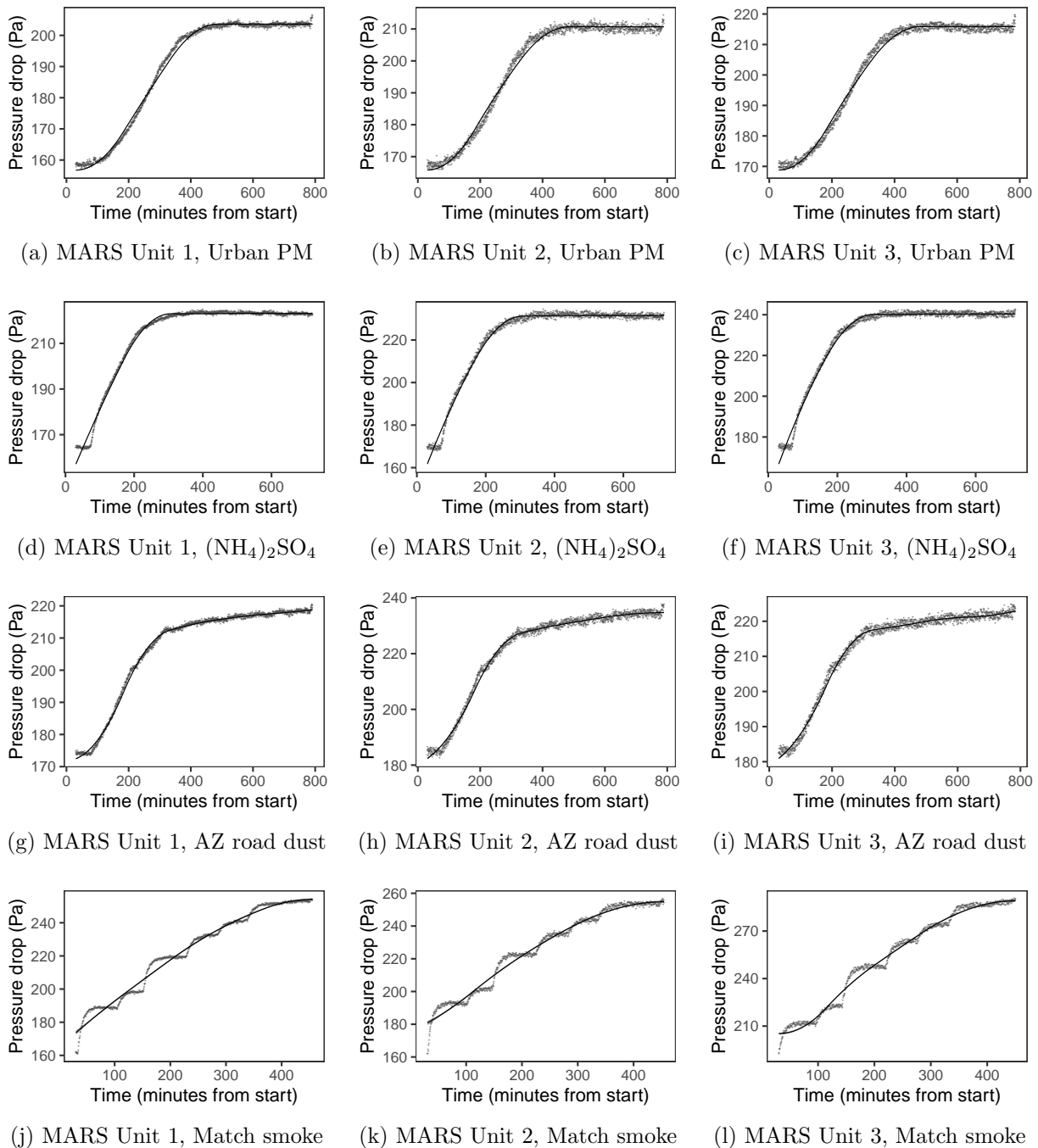


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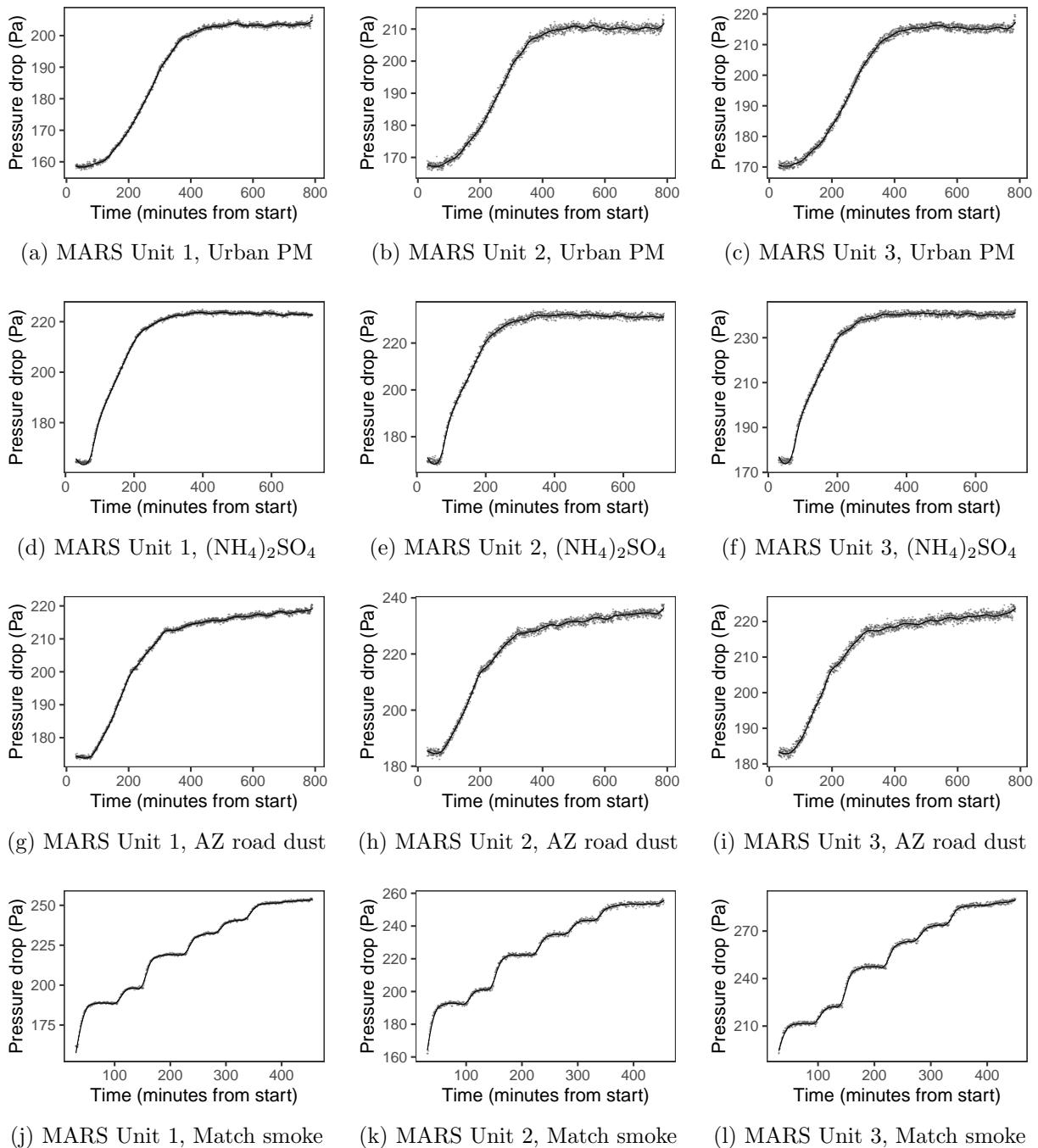


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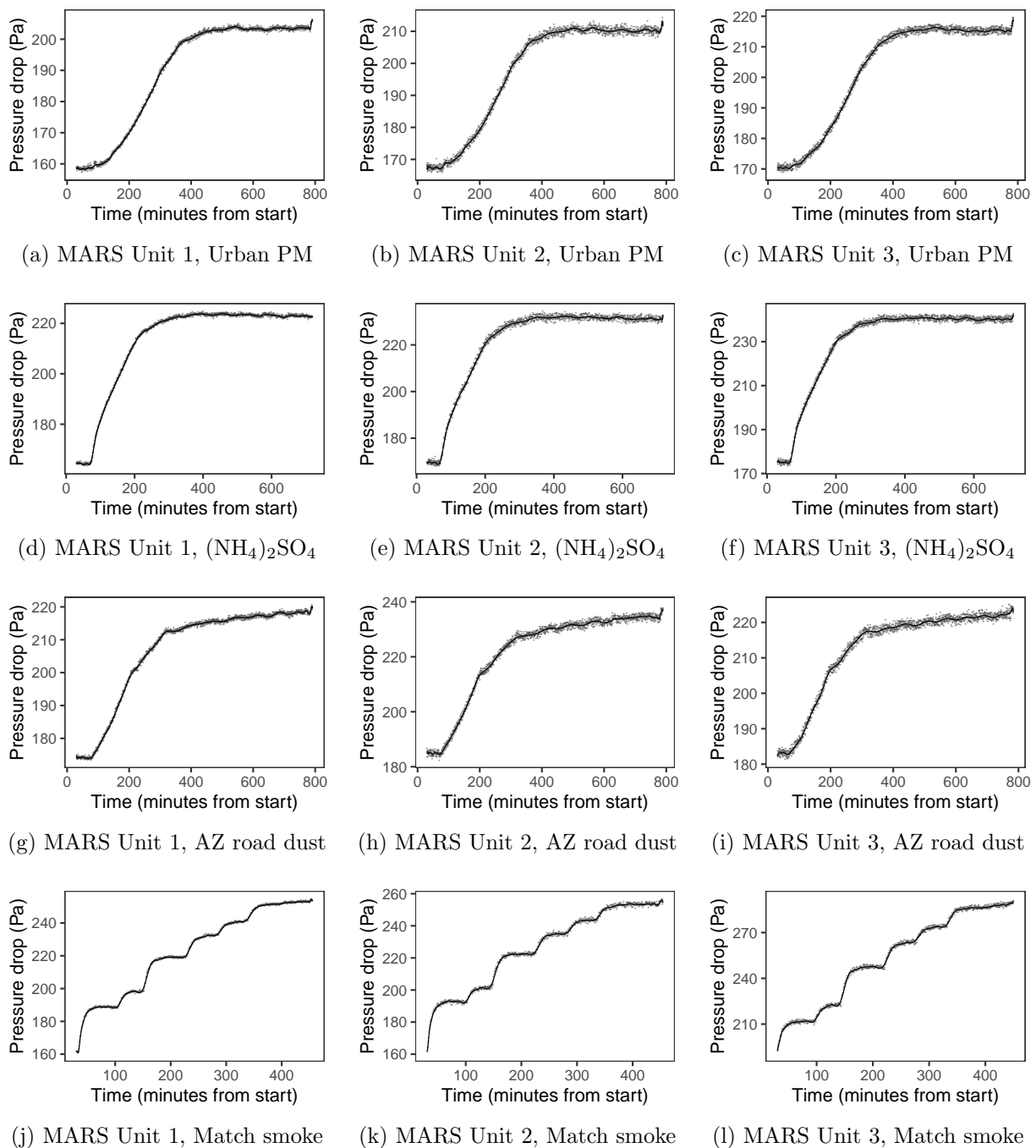


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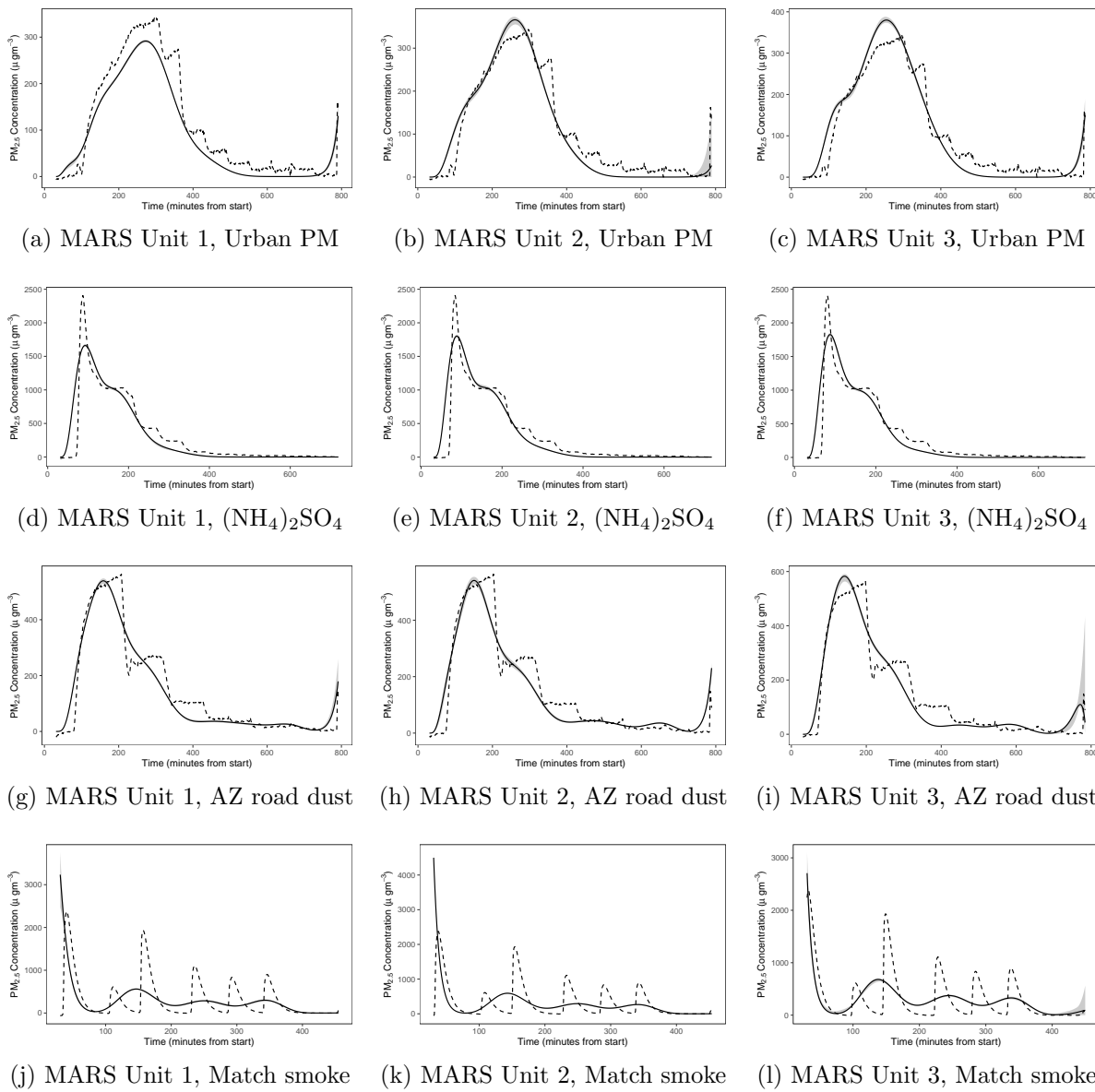


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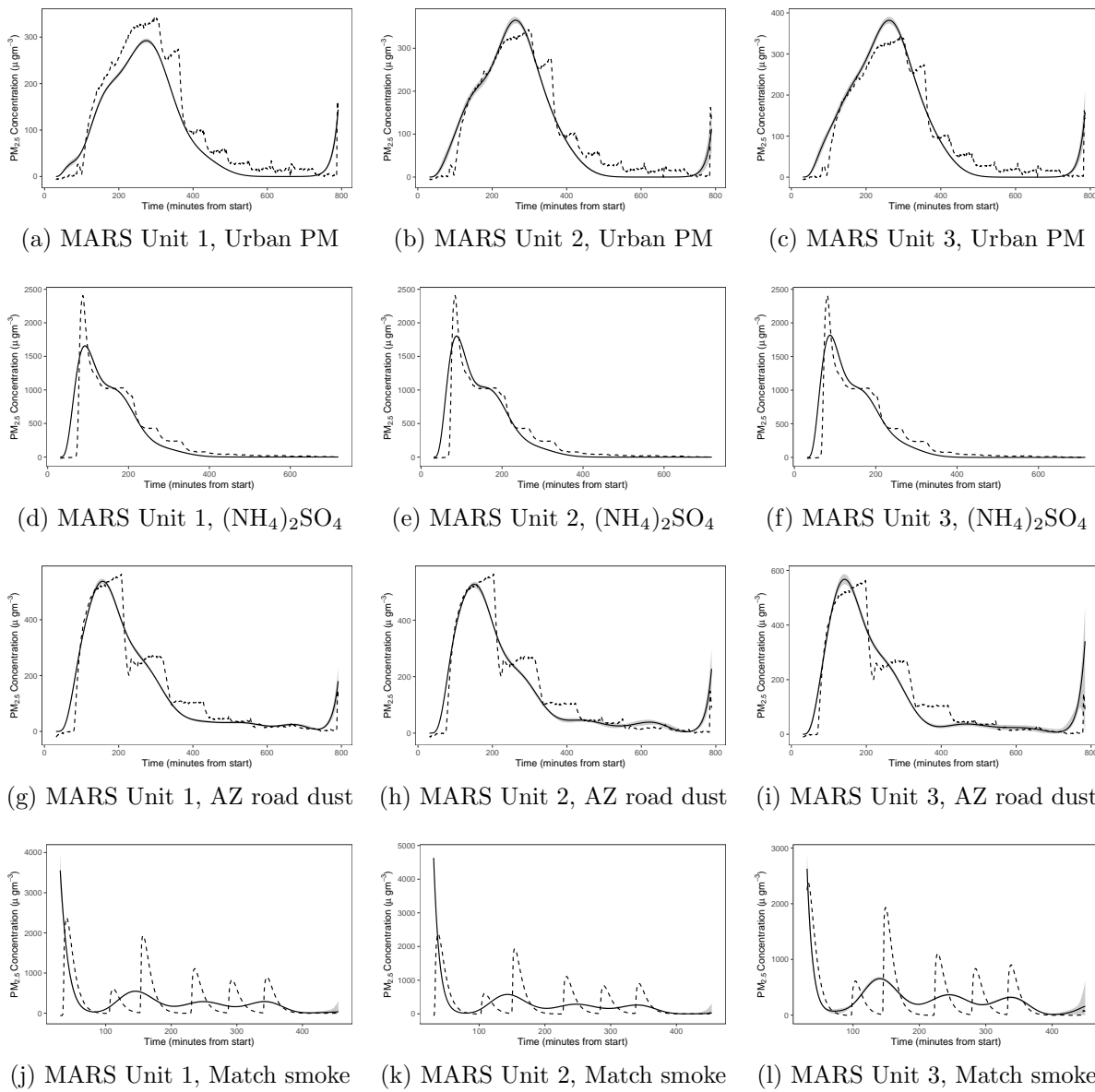


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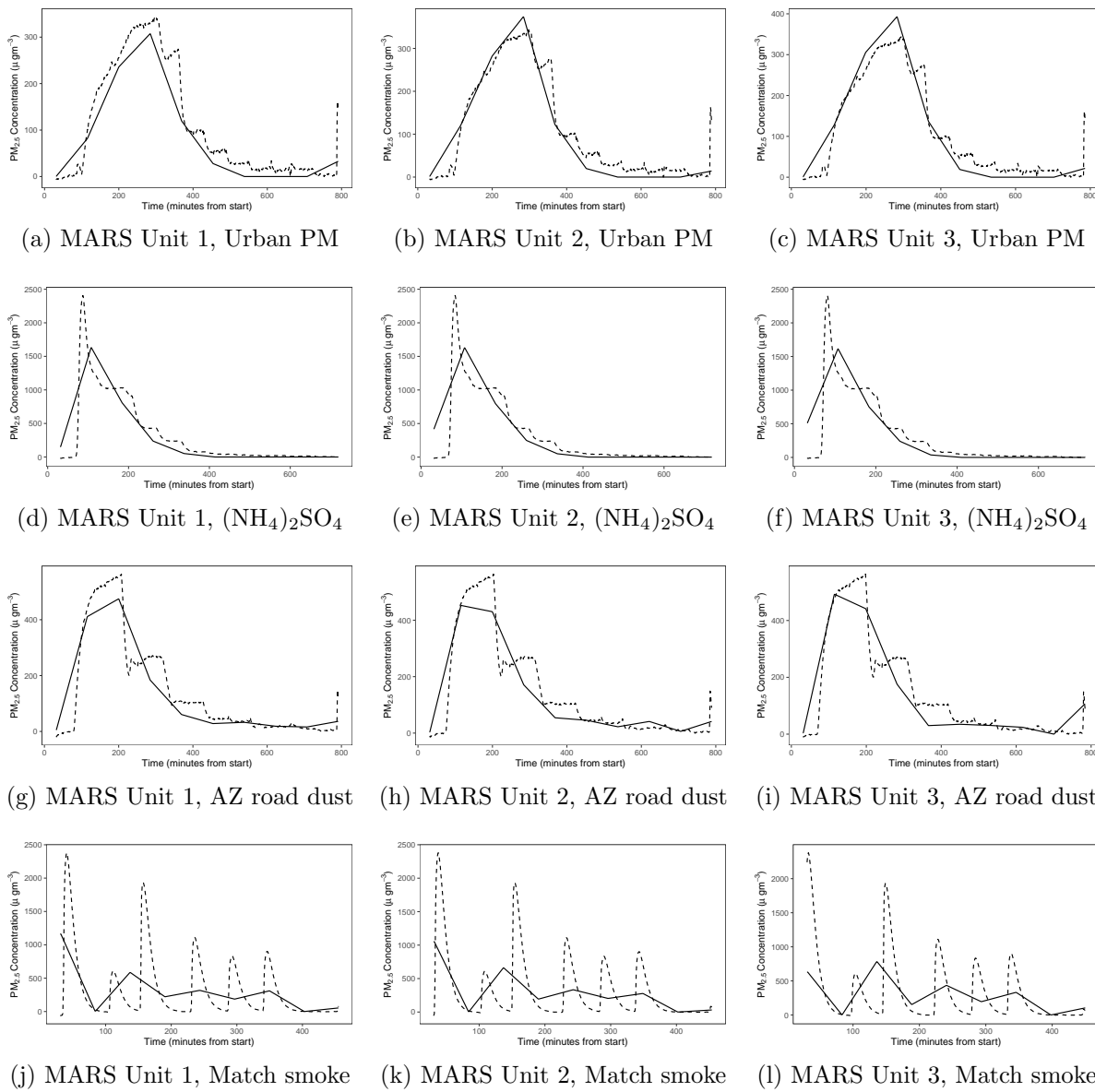


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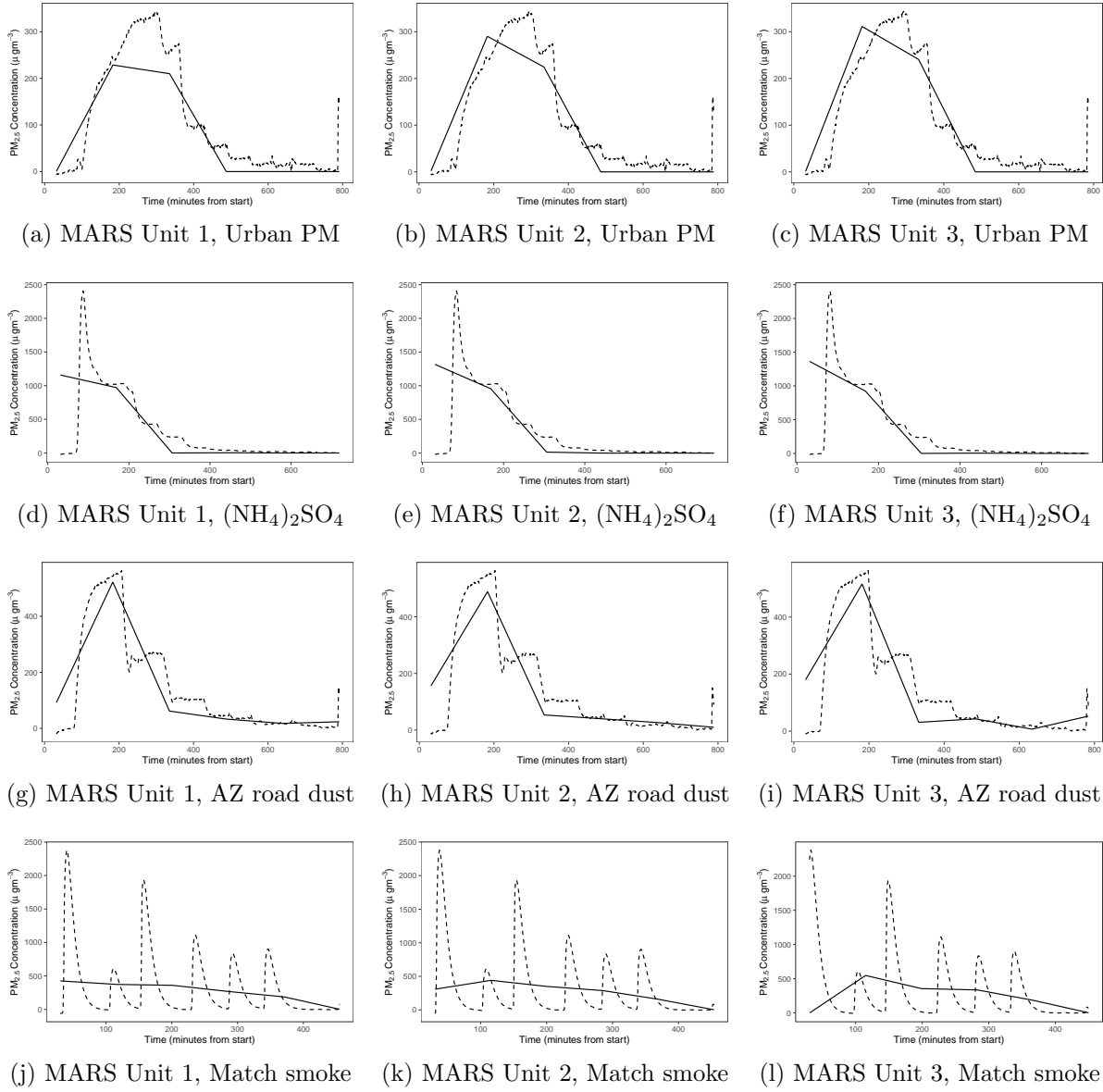


Figure 14: Estimated PM<sub>2.5</sub> with with BCGAM for each of the 12 samples.

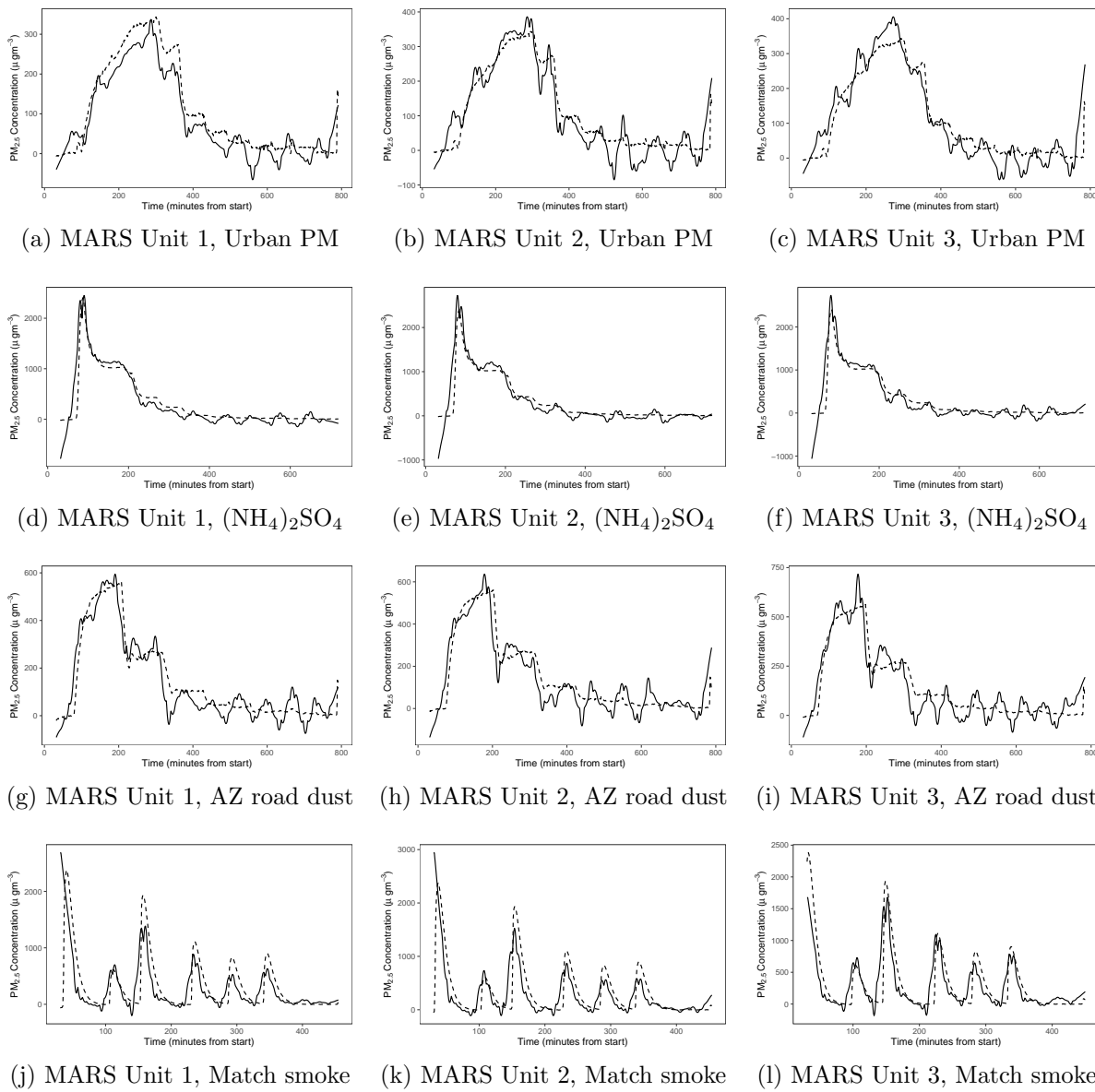


Figure 15: Estimated  $\text{PM}_{2.5}$  with with LOESS for each of the 12 samples.

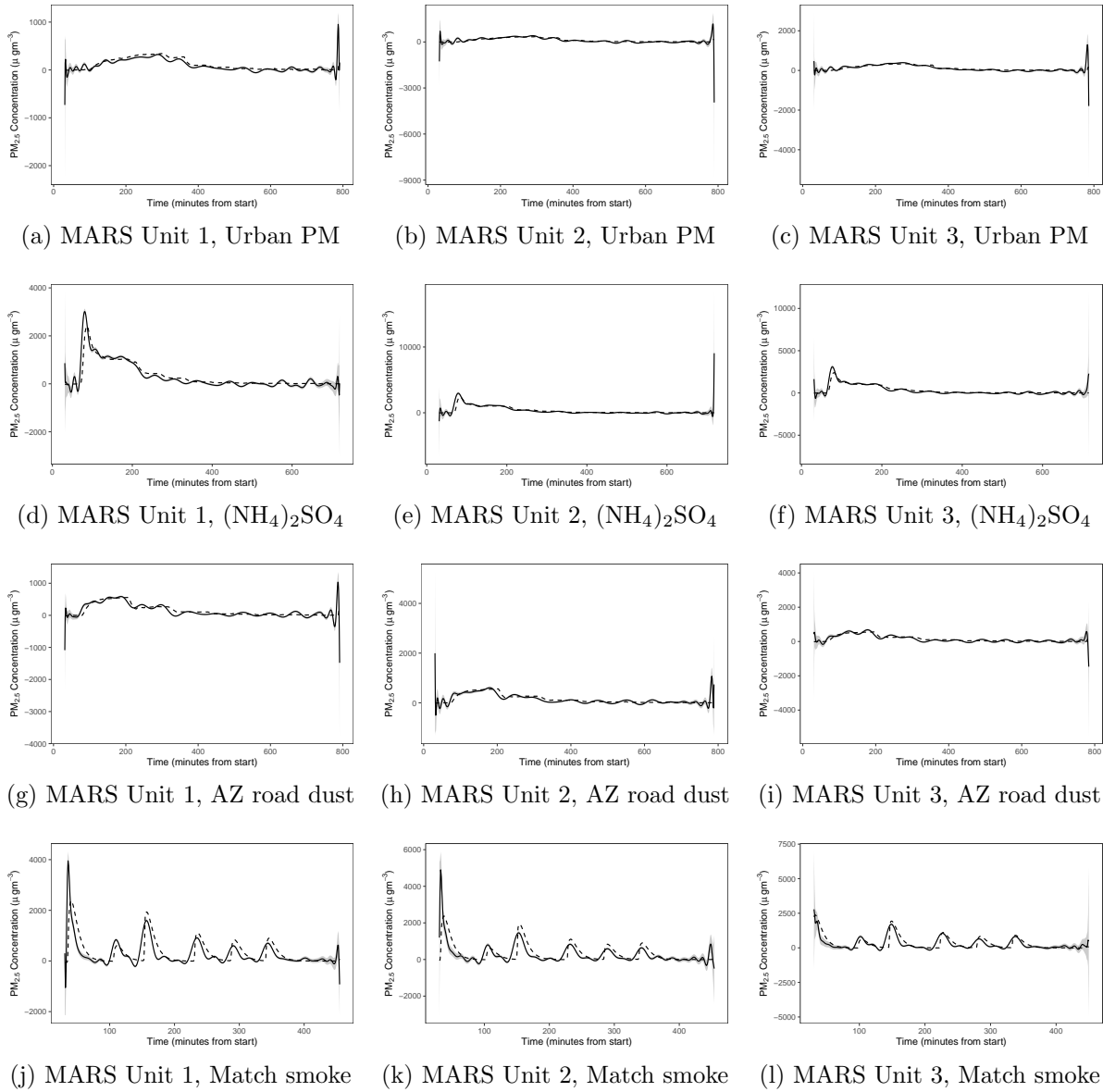


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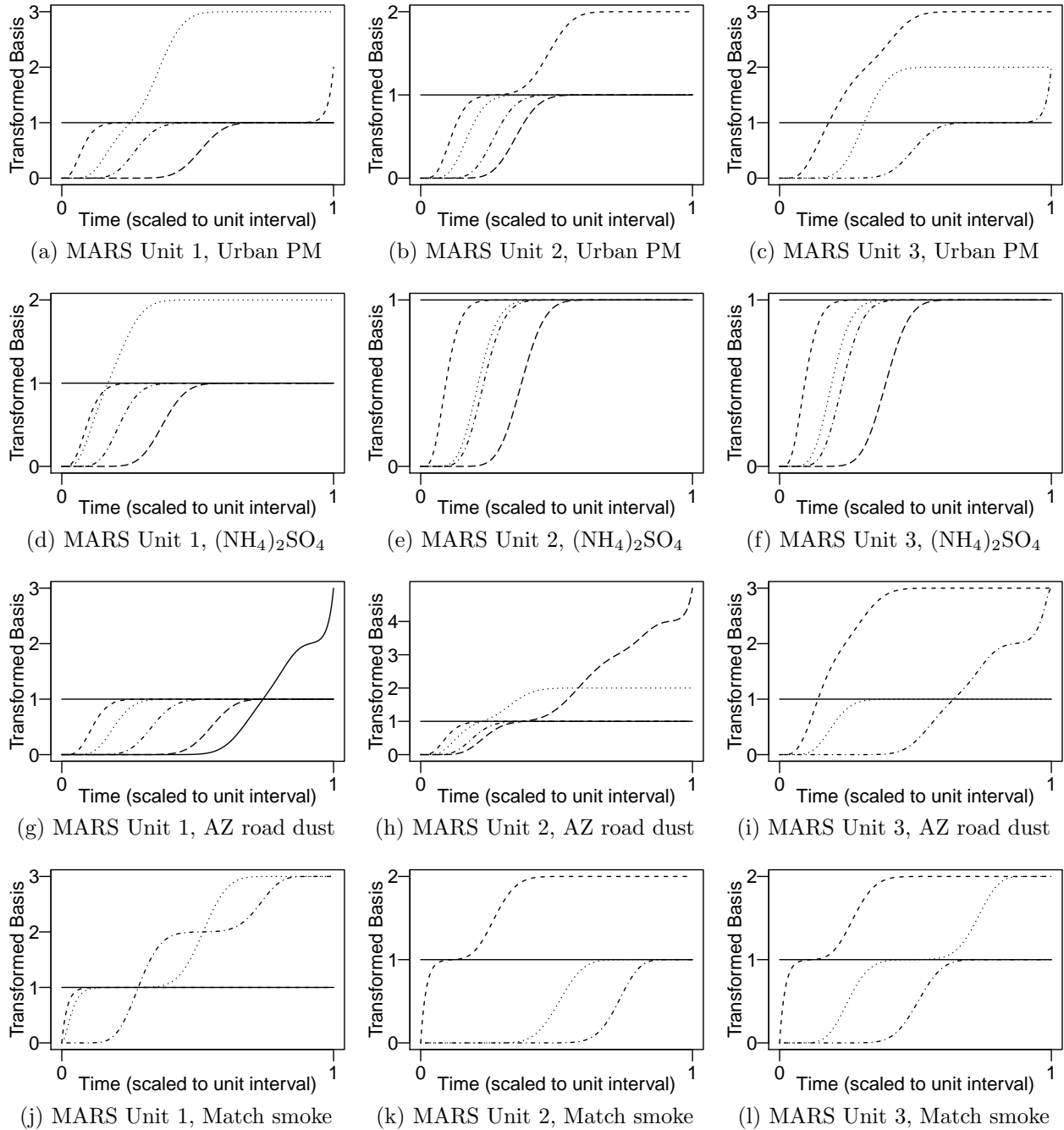


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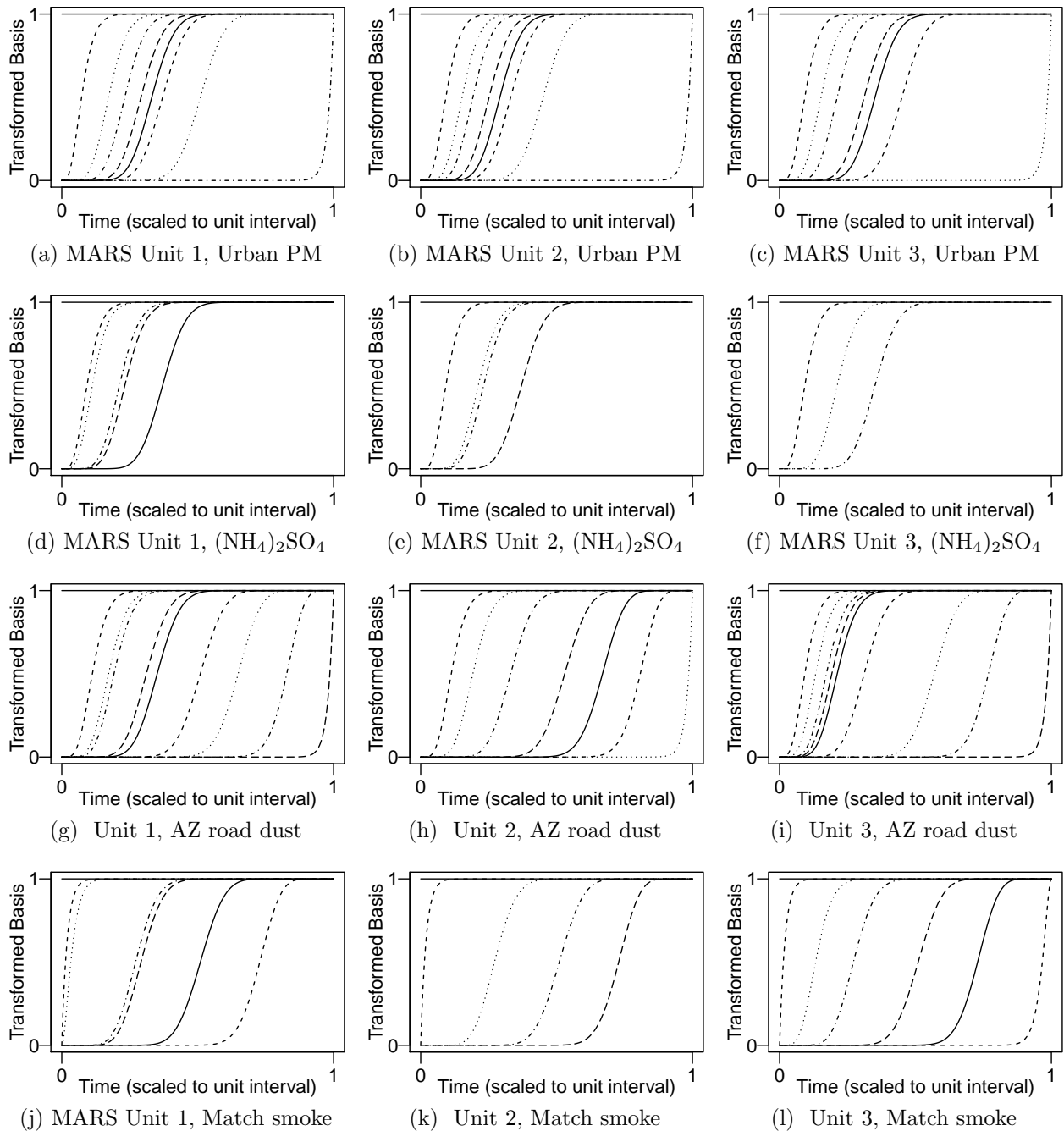


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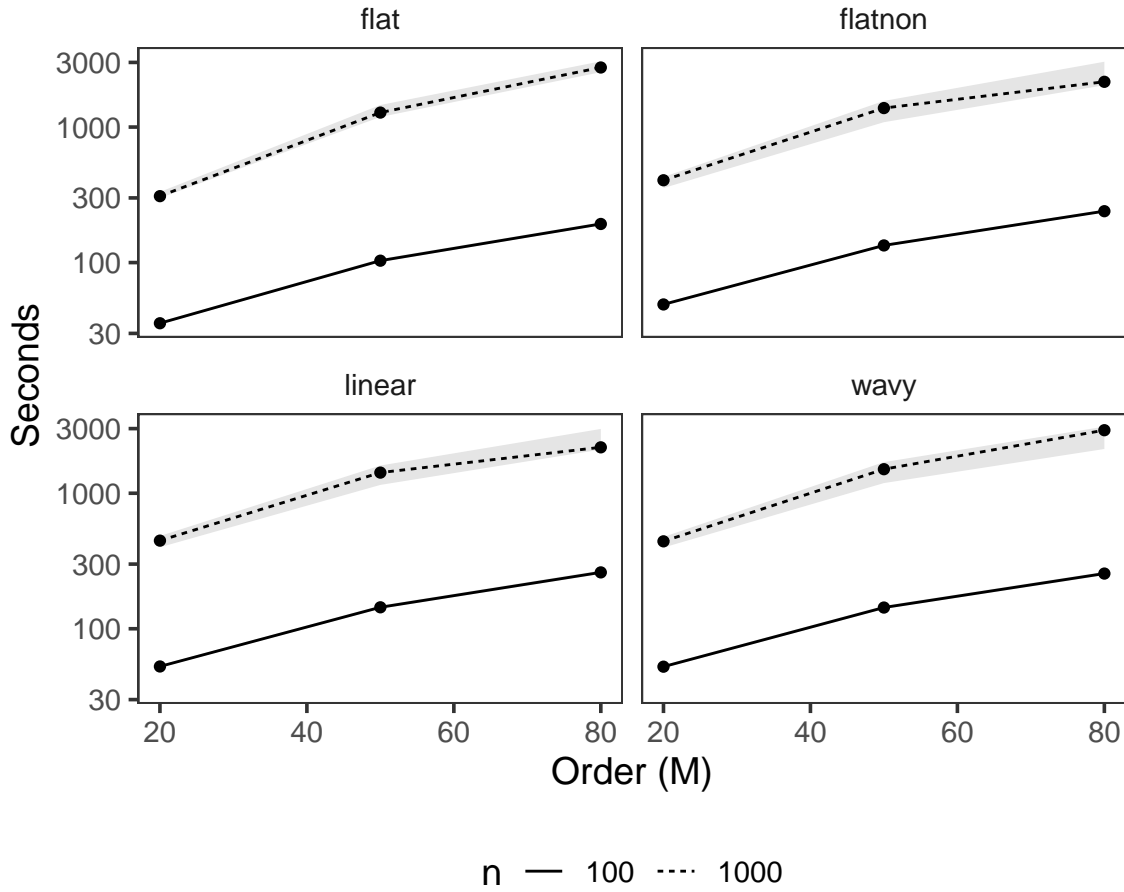


Figure 19: Computation time in seconds for the simulation by sample size ( $n$ ) and the order of the Bernstein polynomial ( $M$ ). The line is the median computation time and the ribbon spans the 25<sup>th</sup> to 75<sup>th</sup> percentiles of computation time. The ribbon for time at the smaller sample size is not visible due to a very small range. Each simulated dataset was run for 150,000 iterations.

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Table 1: Additional simulation results for function  $f$  with  $n = 100$ . The table shows RMSE, the standard error of RMSE, 95% interval coverage, and 95% interval width evaluated pointwise on a grid of 100 evenly spaced points. The column labeled  $\text{Pr}(\text{ linear })$  is the posterior probability that the estimated function is linear. The column labeled  $\text{Pr}(\text{ flat })$  is the posterior probability of a flat response or, for OLS and CGAM, the mean  $p$ -value for rejecting the null of association. RMSE and its standard error are multiplied by 100 to ease interpretability.

	RMSE	SE RMSE	Coverage	CI Width	$\text{Pr}(\text{ linear })$	$\text{Pr}(\text{ flat })$
<i>Scenario 1: Flat</i>						
BCGAM	2.22	0.07	0.95	0.11	0.00	0.00
BISOREG, M=20	2.19	0.07	0.96	0.11	0.87	0.87
BISOREG, M=50	2.19	0.07	0.97	0.11	0.86	0.86
BISOREG, M=80	2.19	0.07	0.96	0.11	0.86	0.86
BNMR, M=20	2.09	0.07	0.96	0.11	0.94	0.94
BNMR, M=50	2.08	0.07	0.96	0.11	0.94	0.94
BNMR, M=80	2.09	0.07	0.96	0.11	0.94	0.94
CGAM	3.57	0.09	0.98	0.17	0.00	0.49
LOESS	5.15	0.11	0.93	0.20	NA	NA
OLS	3.11	0.07	0.95	0.14	1.00	0.50
UBP	5.23	0.10	0.93	0.20	0.00	0.00
<i>Scenario 2: Linear</i>						
BCGAM	6.42	0.08	0.84	0.20	0.00	0.00
BISOREG, M=20	5.43	0.07	0.96	0.23	0.00	0.00
BISOREG, M=50	5.99	0.07	0.96	0.25	0.00	0.00
BISOREG, M=80	6.26	0.07	0.96	0.26	0.00	0.00
BNMR, M=20	4.51	0.07	0.97	0.21	0.00	0.00
BNMR, M=50	4.72	0.07	0.98	0.22	0.00	0.00
BNMR, M=80	4.78	0.07	0.98	0.23	0.00	0.00
CGAM	5.79	0.07	0.96	0.24	0.00	0.00
LOESS	5.15	0.11	0.93	0.20	NA	NA
OLS	3.11	0.07	0.95	0.14	1.00	0.00
UBP	5.28	0.10	0.93	0.20	0.00	0.00
<i>Scenario 3: Wavy</i>						
BCGAM	6.57	0.08	0.84	0.19	0.00	0.00
BISOREG, M=20	5.52	0.08	0.95	0.22	0.00	0.00
BISOREG, M=50	5.98	0.08	0.95	0.24	0.00	0.00
BISOREG, M=80	6.23	0.08	0.95	0.25	0.00	0.00
BNMR, M=20	5.46	0.07	0.94	0.21	0.00	0.00
BNMR, M=50	5.30	0.07	0.96	0.22	0.00	0.00
BNMR, M=80	5.34	0.07	0.97	0.23	0.00	0.00
CGAM	5.67	0.07	0.96	0.23	0.00	0.00
LOESS	6.44	0.09	0.89	0.22	NA	NA
OLS	8.02	0.03	0.56	0.14	1.00	0.00
UBP	6.38	0.09	0.90	0.22	0.00	0.00
<i>Scenario 4: Flat-nonlinear</i>						
BCGAM	5.33	0.09	0.90	0.17	0.00	0.00
BISOREG, M=20	4.93	0.07	0.96	0.19	0.00	0.00
BISOREG, M=50	5.60	0.07	0.95	0.21	0.00	0.00
BISOREG, M=80	5.87	0.08	0.95	0.22	0.00	0.00
BNMR, M=20	4.65	0.08	0.95	0.18	0.00	0.00
BNMR, M=50	4.95	0.08	0.96	0.20	0.00	0.00
BNMR, M=80	5.12	0.08	0.96	0.20	0.00	0.00
CGAM	5.29	0.07	0.96	0.21	0.00	0.00
LOESS	5.70	0.10	0.91	0.20	NA	NA
OLS	16.11	0.04	0.32	0.16	1.00	0.00
UBP	5.42	0.10	0.93	0.20	0.00	0.00

Table 2: Additional simulation results for function  $f$  with  $n = 1000$ . The table shows RMSE, the standard error of RMSE, 95% interval coverage, and 95% interval width evaluated pointwise on a grid of 100 evenly spaced points. The column labeled  $\text{Pr}(\text{ linear })$  is the posterior probability that the estimated function is linear. The column labeled  $\text{Pr}(\text{ flat })$  is the posterior probability of a flat response or, for OLS and CGAM, the mean  $p$ -value for rejecting the null of association. RMSE and its standard error are multiplied by 100 to ease interpretability.

	RMSE	SE RMSE	Coverage	CI Width	$\text{Pr}(\text{ linear })$	$\text{Pr}(\text{ flat })$
<i>Scenario 1: Flat</i>						
BCGAM	0.65	0.02	0.96	0.03	0.00	0.00
BISOREG, M=20	0.61	0.02	0.97	0.03	0.96	0.96
BISOREG, M=50	0.61	0.02	0.97	0.03	0.95	0.95
BISOREG, M=80	0.61	0.02	0.97	0.03	0.95	0.95
BNMR, M=20	0.60	0.02	0.96	0.03	0.99	0.99
BNMR, M=50	0.60	0.02	0.96	0.03	0.99	0.99
BNMR, M=80	0.60	0.02	0.96	0.03	0.99	0.99
CGAM	1.17	0.03	0.99	0.06	0.00	0.50
LOESS	1.61	0.04	0.95	0.06	NA	NA
OLS	0.93	0.02	0.96	0.04	1.00	0.53
UBP	1.60	0.03	0.95	0.06	0.00	0.00
<i>Scenario 2: Linear</i>						
BCGAM	2.58	0.03	0.84	0.08	0.00	0.00
BISOREG, M=20	2.08	0.02	0.96	0.08	0.00	0.00
BISOREG, M=50	2.42	0.02	0.95	0.10	0.00	0.00
BISOREG, M=80	2.59	0.02	0.95	0.10	0.00	0.00
BNMR, M=20	1.85	0.02	0.97	0.08	0.00	0.00
BNMR, M=50	2.14	0.02	0.96	0.09	0.00	0.00
BNMR, M=80	2.29	0.02	0.96	0.09	0.00	0.00
CGAM	2.30	0.02	0.95	0.09	0.00	0.00
LOESS	1.61	0.04	0.95	0.06	NA	NA
OLS	0.93	0.02	0.96	0.04	1.00	0.00
UBP	1.60	0.03	0.95	0.06	0.00	0.00
<i>Scenario 3: Wavy</i>						
BCGAM	2.17	0.02	0.88	0.07	0.00	0.00
BISOREG, M=20	1.94	0.02	0.94	0.07	0.00	0.00
BISOREG, M=50	2.25	0.02	0.95	0.09	0.00	0.00
BISOREG, M=80	2.45	0.02	0.95	0.09	0.00	0.00
BNMR, M=20	1.86	0.02	0.95	0.07	0.00	0.00
BNMR, M=50	2.25	0.02	0.94	0.08	0.00	0.00
BNMR, M=80	2.42	0.02	0.93	0.09	0.00	0.00
CGAM	2.15	0.02	0.96	0.09	0.00	0.00
LOESS	2.14	0.03	0.93	0.08	NA	NA
OLS	7.22	0.00	0.19	0.04	1.00	0.00
UBP	2.30	0.02	0.90	0.07	0.00	0.00
<i>Scenario 4: Flat-nonlinear</i>						
BCGAM	1.93	0.03	0.89	0.06	0.00	0.00
BISOREG, M=20	1.75	0.02	0.95	0.06	0.00	0.00
BISOREG, M=50	2.12	0.02	0.96	0.07	0.00	0.00
BISOREG, M=80	2.26	0.03	0.96	0.08	0.00	0.00
BNMR, M=20	1.55	0.02	0.96	0.06	0.00	0.00
BNMR, M=50	1.82	0.02	0.96	0.07	0.00	0.00
BNMR, M=80	1.98	0.02	0.95	0.07	0.00	0.00
CGAM	1.91	0.02	0.97	0.08	0.00	0.00
LOESS	1.88	0.03	0.93	0.07	NA	NA
OLS	16.24	0.00	0.09	0.05	1.00	0.00
UBP	1.91	0.02	0.91	0.06	0.00	0.00

Table 3: Additional simulation results for the derivative  $f'$  with  $n = 100$ . The table shows RMSE, the standard error of RMSE, 95% interval coverage, and 95% interval width evaluated pointwise on a grid of 100 evenly spaced points. Intervals for the derivative with BCGAM, CGAM and LOESS are not available. RMSE and its standard error are multiplied by 100 to ease interpretability.

	RMSE	SE RMSE	Coverage	CI Width
<i>Scenario 1: Flat</i>				
BCGAM	3.24	0.37	NA	NA
BISOREG, M=20	3.18	0.31	0.00	0.16
BISOREG, M=50	4.90	0.77	0.00	0.18
BISOREG, M=80	5.56	0.84	0.00	0.18
BNMR, M=20	1.04	0.12	1.00	0.06
BNMR, M=50	1.12	0.13	1.00	0.06
BNMR, M=80	1.15	0.13	1.00	0.06
CGAM	22.80	0.97	NA	NA
LOESS	53.81	3.38	NA	NA
UBP	55.26	2.99	0.92	1.55
<i>Scenario 2: Linear</i>				
BCGAM	61.68	0.78	NA	NA
BISOREG, M=20	49.45	0.89	0.97	2.13
BISOREG, M=50	65.54	1.47	0.96	2.85
BISOREG, M=80	74.41	1.72	0.95	3.24
BNMR, M=20	32.66	0.47	0.99	1.75
BNMR, M=50	39.57	0.61	1.00	2.41
BNMR, M=80	42.39	0.69	1.00	2.76
CGAM	68.85	1.07	NA	NA
LOESS	53.81	3.38	NA	NA
UBP	56.90	3.02	0.91	1.57
<i>Scenario 3: Wavy</i>				
BCGAM	64.03	0.90	NA	NA
BISOREG, M=20	55.72	0.92	0.91	1.93
BISOREG, M=50	70.78	1.48	0.95	2.65
BISOREG, M=80	80.32	1.70	0.95	3.06
BNMR, M=20	53.97	0.68	0.88	1.72
BNMR, M=50	55.00	0.68	0.97	2.38
BNMR, M=80	57.81	0.70	0.98	2.76
CGAM	69.21	1.09	NA	NA
LOESS	87.54	3.44	NA	NA
UBP	97.38	3.13	0.78	2.07
<i>Scenario 4: Flat-nonlinear</i>				
BCGAM	62.08	1.42	NA	NA
BISOREG, M=20	71.05	1.12	0.46	1.63
BISOREG, M=50	92.18	1.73	0.46	2.33
BISOREG, M=80	103.23	1.85	0.46	2.69
BNMR, M=20	48.84	0.89	0.53	1.31
BNMR, M=50	61.45	0.91	0.68	1.98
BNMR, M=80	67.80	0.92	0.77	2.35
CGAM	66.95	1.31	NA	NA
LOESS	65.11	3.38	NA	NA
UBP	62.59	3.14	0.88	1.60

Table 4: Additional simulation results for the derivative  $f'$  with  $n = 1000$ . The table shows RMSE, the standard error of RMSE, 95% interval coverage, and 95% interval width evaluated pointwise on a grid of 100 evenly spaced points. Intervals for the derivative with BCGAM, CGAM and LOESS are not available. RMSE and its standard error are multiplied by 100 to ease interpretability.

	RMSE	SE RMSE	Coverage	CI Width
<i>Scenario 1: Flat</i>				
BCGAM	0.85	0.10	NA	NA
BISOREG, M=20	0.35	0.04	0.00	0.02
BISOREG, M=50	0.61	0.07	0.00	0.02
BISOREG, M=80	0.77	0.08	0.00	0.02
BNMR, M=20	0.14	0.01	1.00	0.01
BNMR, M=50	0.19	0.02	1.00	0.00
BNMR, M=80	0.21	0.02	1.00	0.00
CGAM	9.92	0.41	NA	NA
LOESS	18.49	1.58	NA	NA
BP	16.61	0.87	0.93	0.47
<i>Scenario 2: Linear</i>				
BCGAM	39.98	0.55	NA	NA
BISOREG, M=20	31.97	0.46	0.95	1.13
BISOREG, M=50	44.91	0.67	0.94	1.65
BISOREG, M=80	53.90	1.00	0.94	1.98
BNMR, M=20	27.31	0.37	0.98	1.06
BNMR, M=50	38.21	0.48	0.95	1.50
BNMR, M=80	44.72	0.54	0.94	1.74
CGAM	40.79	0.54	NA	NA
LOESS	18.49	1.58	NA	NA
BP	16.60	0.89	0.93	0.47
<i>Scenario 3: Wavy</i>				
BCGAM	32.05	0.48	NA	NA
BISOREG, M=20	33.35	0.56	0.82	0.85
BISOREG, M=50	46.53	0.60	0.91	1.36
BISOREG, M=80	56.83	0.94	0.91	1.67
BNMR, M=20	30.57	0.38	0.82	0.80
BNMR, M=50	45.13	0.50	0.85	1.21
BNMR, M=80	51.83	0.60	0.83	1.47
CGAM	37.04	0.60	NA	NA
LOESS	35.18	1.59	NA	NA
BP	52.52	1.12	0.68	0.88
<i>Scenario 4: Flat-nonlinear</i>				
BCGAM	28.82	0.63	NA	NA
BISOREG, M=20	44.81	0.83	0.45	0.79
BISOREG, M=50	65.44	1.15	0.45	1.21
BISOREG, M=80	74.40	1.48	0.46	1.49
BNMR, M=20	29.44	0.64	0.48	0.63
BNMR, M=50	46.91	0.74	0.61	1.01
BNMR, M=80	55.22	0.70	0.66	1.22
CGAM	34.57	0.67	NA	NA
LOESS	28.99	1.57	NA	NA
BP	28.39	0.78	0.66	0.52

Table 5: Comparison of computational efficiency of the MCMC algorithm for the data analysis. The results show the summaries of the effective sample size (ESS) and the autocorrelation (AC) at lag 1 for BNMR and BISOREG. The mean, SE for the mean, and median shown below are taken across the 12 samples.

	ESS			AC lag 1		
	Mean	SE	Median	Mean	SE	Median
BNMR	1164	400	757	0.273	0.041	0.278
BISOREG	1066	228	814	0.375	0.026	0.375