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Online Supplement for ”shape invariant mixture model for clustering non-linear longitudinal growth trajectories”

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Table E1. Comparison of candidates SITAR mixture models for pregnant women dataset

	Constrained variance			Unconstrained variance		
Number of clusters	$\bar{D}$	p_D	DIC	$\bar{D}$	p_D	DIC
1	1225.13	12.632	1237.76	-	-	-
2	1230.39	90.1415	1320.53	**1087.9**	**51.2841**	**1139.19**
3	1244.98	36.7511	1281.73	1194.27	44.6451	1238.91

Table E2. Clustering performance of Mixture SITAR using different number of knots and knots locations

	Equally spaced of the sample quantiles		Equally time spaced	
Number of Knots	cRate	aRand	cRate	aRand
2	0.83	0.32	0.83	0.32
3	0.86	0.45	0.88	0.49
4	0.88	0.50	0.88	0.50
5	0.88	0.50	0.86	0.46
6	0.88	0.52	0.88	0.52
7	0.88	0.52	0.88	0.52
8	0.88	0.52	0.88	0.52

cRate: correct classification rate
aRand: adjusted rand index

Table E3. Parameter settings in Simulation I

	Scenario 1		Scenario 2		Scenario 3	
	$k=1$	$k=2$	$k=1$	$k=2$	$k=1$	$k=2$
μ_{k1}	-1	3	0	4	1	2
μ_{k2}	-1	-3	0	-5	0	-5
μ_{k3}	-0.05	-0.5	-0.05	-0.2	0	-0.2
$\Sigma_{k_{11}}$	0.0114	0.06	0.0114	0.06	0.0114	0.06
$\Sigma_{k_{12}}$	0.0119	-0.081	0.0119	-0.081	0.0119	-0.081
$\Sigma_{k_{13}}$	0.0054	-0.027	0.0054	-0.027	0.0054	-0.027
$\Sigma_{k_{22}}$	0.0137	0.1301	0.0137	0.1301	0.0137	0.1301
$\Sigma_{k_{23}}$	0.0067	0.0245	0.0067	0.0245	0.0067	0.0245
$\Sigma_{k_{33}}$	0.0035	0.0326	0.0035	0.0326	0.0035	0.0326
γ_{k1}	9.8	4.2	9.8	7	9.8	7
γ_{k2}	10.5	5.6	10.5	7	10.5	7
γ_{k3}	7.7	7	7.7	5.6	7.7	5.6
γ_{k4}	17.5	5.6	17.5	2.1	17.5	2.1
γ_{k5}	6.3	4.2	6.3	1.4	6.3	1.4
σ_k^2	1.5	1.5	1.5	1.5	1.5	1.5

$\Sigma_{k_{ij}}$ indicates the i^{th} row and j^{th} column of Σ_k

Table E4. Percentage of correctly selecting the number of clusters using DIC in different scenarios of Simulation I

Sample size	max.obs	Proportion	Scenario 1 (Low separation)	Scenario 2 (Median separation)	Scenario 3 (High separation)
100	4	(0.5, 0.5)	0	0	93.3
		(0.7, 0.3)	0	0	93.3
	8	(0.5, 0.5)	0	16.7	100
		(0.7, 0.3)	3.3	13.3	100
	12	(0.5, 0.5)	46.7	60	100
		(0.7, 0.3)	16.7	53.3	100
200	4	(0.5, 0.5)	0	0	100
		(0.7, 0.3)	0	0	100
	8	(0.5, 0.5)	0	3.3	100
		(0.7, 0.3)	0	10	96.7
	12	(0.5, 0.5)	20	76.7	100
		(0.7, 0.3)	0	86.7	96.7

Table E5. Percentage of correctly selecting the number of clusters using R & M criteria in different scenarios of Simulation I

			Scenario 1 (Low separation)					
			$\delta = 1$		$\delta = 2$		$\delta = 4$	
Sample size	max.obs	Proportion	$\varphi = 0.05$	$\varphi = 0.1$	$\varphi = 0.05$	$\varphi = 0.1$	$\varphi = 0.05$	$\varphi = 0.1$
100	4	(0.5, 0.5)	86.7	96.7	16.7	20.0	6.7	10.0
		(0.7, 0.3)	0.0	0.0	16.7	10.0	20.0	26.7
	8	(0.5, 0.5)	100.0	100.0	56.7	70.0	60.0	63.3
		(0.7, 0.3)	70.0	70.0	60.0	70.0	66.7	86.7
	12	(0.5, 0.5)	96.7	100.0	93.3	100.0	46.7	66.7
		(0.7, 0.3)	100.0	86.7	96.7	83.3	43.3	66.7
200	4	(0.5, 0.5)	100	100	100	100	100	60
		(0.7, 0.3)	30.0	0.0	40.0	0.0	46.7	63.3
	8	(0.5, 0.5)	73.3	80.0	46.7	63.3	40.0	56.7
		(0.7, 0.3)	60.0	80.0	80.0	90.0	56.7	76.7
	12	(0.5, 0.5)	100.0	100.0	90.0	100.0	90.0	93.3
		(0.7, 0.3)	100.0	100.0	100.0	96.7	93.3	100.0
			Scenario 2 (Median separation)					
			$\delta = 1$		$\delta = 2$		$\delta = 4$	
Sample size	max.obs	Proportion	$\varphi = 0.05$	$\varphi = 0.1$	$\varphi = 0.05$	$\varphi = 0.1$	$\varphi = 0.05$	$\varphi = 0.1$
100	4	(0.5, 0.5)	33.3	23.3	30.0	20.0	33.3	20.0
		(0.7, 0.3)	30.0	23.3	16.7	10.0	30.0	23.3
	8	(0.5, 0.5)	66.7	60.0	43.3	56.7	43.3	73.3
		(0.7, 0.3)	90.0	63.3	56.7	70.0	33.3	63.3
	12	(0.5, 0.5)	20.0	56.7	3.3	43.3	16.7	46.7
		(0.7, 0.3)	40.0	86.7	36.7	50.0	23.3	46.7
200	4	(0.5, 0.5)	100.00	96.67	100.00	100.00	83.33	90.00
		(0.7, 0.3)	86.67	0.00	93.33	3.33	96.67	13.33
	8	(0.5, 0.5)	26.67	73.33	26.67	60.00	10.00	33.33
		(0.7, 0.3)	76.67	83.33	63.33	80.00	60.00	80.00
	12	(0.5, 0.5)	0.00	36.67	0.00	26.67	0.00	30.00
		(0.7, 0.3)	26.67	83.33	30.00	80.00	26.67	80.00
			Scenario 3 (High separation)					
			$\delta = 1$		$\delta = 2$		$\delta = 4$	
Sample size	max.obs	Proportion	$\varphi = 0.05$	$\varphi = 0.1$	$\varphi = 0.05$	$\varphi = 0.1$	$\varphi = 0.05$	$\varphi = 0.1$
100	4	(0.5, 0.5)	96.7	100.0	100.0	20.0	23.3	30.0
		(0.7, 0.3)	100.0	100.0	46.7	46.7	23.3	23.3
	8	(0.5, 0.5)	63.3	80.0	36.7	16.7	6.7	6.7
		(0.7, 0.3)	76.7	93.3	13.3	33.3	3.3	10.0
	12	(0.5, 0.5)	23.3	3.3	0.0	0.0	0.0	0.0
		(0.7, 0.3)	0.0	16.7	6.7	16.7	6.7	23.3
200	4	(0.5, 0.5)	96.7	100.0	93.3	100.0	6.7	10.0
		(0.7, 0.3)	100.0	100.0	96.7	63.3	30.0	43.3
	8	(0.5, 0.5)	33.3	80.0	26.7	60.0	13.3	43.3
		(0.7, 0.3)	56.7	90.0	40.0	80.0	36.7	83.3
	12	(0.5, 0.5)	0.0	23.3	3.3	20.0	0.0	23.3
		(0.7, 0.3)	10.0	50.0	20.0	56.7	10.0	56.7

Table E6. Parameter setting in Simulation II

	Scenario 1 (Two clusters)		Scenario 2 (Three clusters)			Scenario 3 (Four clusters)			
	$k=1$	$k=2$	$k=1$	$k=2$	$k=3$	$k=1$	$k=2$	$k=3$	$k=4$
μ_{k1}	-2	3	-2	3	1	-2	3	1	6
μ_{k2}	-1	0	-1	0	0.8	-1	0	0.8	0.2
μ_{k3}	-0.2	0.5	-0.2	0.5	-0.5	-0.2	0.5	-0.5	-0.1
$\Sigma_{k_{11}}$	0.0525	0.81	0.0525	0.81	0.65	0.0525	0.81	0.65	0.17
$\Sigma_{k_{12}}$	0.0425	-0.521	0.0425	-0.521	-0.001	0.0425	-0.521	-0.001	0.05
$\Sigma_{k_{13}}$	0.016	-0.099	0.016	-0.099	-0.085	0.016	-0.099	-0.085	-0.005
$\Sigma_{k_{22}}$	0.0525	0.4101	0.0525	0.4101	0.0901	0.0525	0.4101	0.0901	0.0225
$\Sigma_{k_{23}}$	0.016	0.0465	0.016	0.0465	0.0035	0.016	0.0465	0.0035	-0.006
$\Sigma_{k_{33}}$	0.0054	0.0326	0.0054	0.0326	0.0126	0.0054	0.0326	0.0126	0.0029
γ_{k1}	9	18	9	18	6	9	18	6	10
γ_{k2}	8	8	8	8	8	8	8	8	4
γ_{k3}	-2	-5	-2	-5	-2	-2	-5	-2	4
γ_{k4}	12	8	12	8	8	12	8	8	10
γ_{k5}	8	10	8	10	-8	8	10	-8	-1
γ_{k6}	15	8	15	8	0	15	8	0	2
γ_{k7}	-8	10	-8	10	8	-8	10	8	2
σ_k^2	1.5	1.5	1.5	1.5	1.5	1.5	1.5	1.5	1.5

$\Sigma_{k_{ij}}$ indicates the i^{th} row and j^{th} column of Σ_k

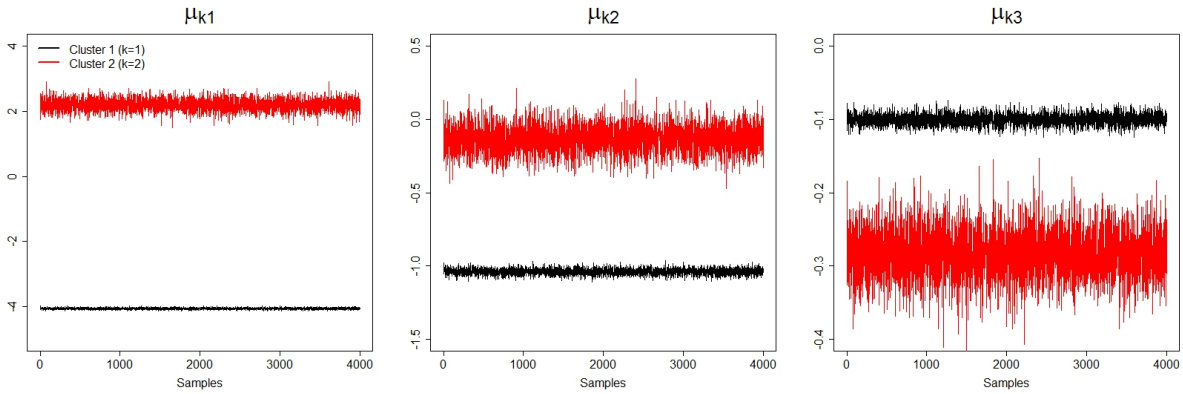

Figure E1. Trace plots of μ_k for Hormone profile dataset

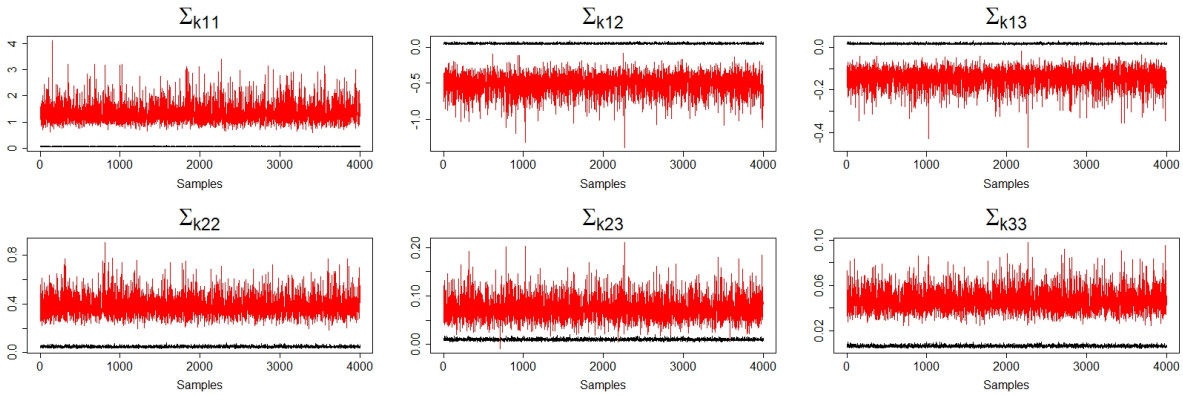

Figure E2. Trace plots of elements of Σ_k for Hormone profile dataset

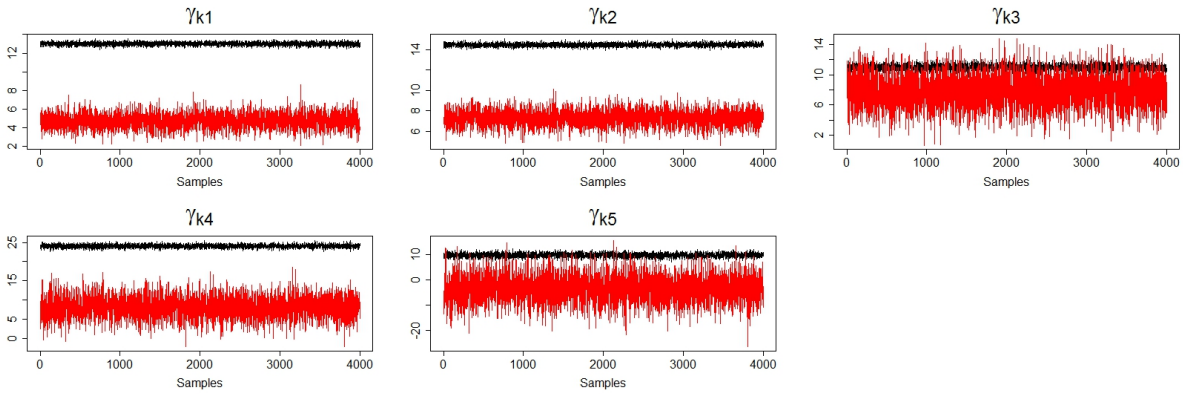

Figure E3. Trace plots of γ_k for Hormone profile dataset