行政院國家科學委員會專題研究計畫　成果報告

具偵測界限及遺漏值之環境資料的貝氏與非貝氏估計

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計畫主持人：鄭宗記

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In this project, I conduct a simulation study to compare some methods for the problem of detection limit. Shumway, Azari and Johnson (1989) propose a method based on the maximum likelihood (ML) for estimating the mean using small samples of nonnormal environmental data that are subject to censoring because of lower detection limits. Recently, Korn and Tyler (2001) propose a family of M-estimators for censored data, which include the maximum likelihood estimates of location and scale for censored t-distribution. Shumway, Azari and Kayhanian (2002) compare the ML estimation and regression on order statistics (ROS) for data with nondects. Hsieh and Cheng (2003) propose a robust moment estimator for environmental data with one-sided detection limit, in which the concept of the extreme value theory is employed.

1 Simulation study

Four distributions are generated: (a) double exponential distribution, (b) standard normal distribution, t distributions (c) with 1 degree of freedom, and (d) with 5 degrees of freedom, and a mixture normal distribution $0.8 * N(0,1) + 0.2 * N(5,1)$. Tables 1 and 2 show the simulation results of sample sizes 50 and 100, respectively. The values in these tables are the mean of the estimates form 1000 simulated data set, and those values at the second line for each cell are the sample standard deviations of the estimates. Note that the first 6 columns use the approaches proposed by Hsieh and Cheng (2003) under different settings, "DL/2" denotes the observations with detection limits replaced by half of the reported values, "ROS" denotes ROS approach, "EM" denotes the method proposed by Shumway *et al.* (1989), and "M" denotes the M estimate using t distribution with df=3 (Korn and Tyler, 2001).

Table 1 $n = 50$

(a) Double exponential distribution

censoring (%)		Fill-in power	Fill-in exp	Fill-in weibull	power	exp	weibull	DL/2	ROS	EM	M
10	μ	0.002	0.011	0.010	0.021	0.015	0.015	0.087	0.023	-0.050	-0.007
		0.191	0.135	0.134	0.135	0.135	0.134	0.131	0.127	0.140	0.112
	σ	0.969	0.947	0.947	0.943	0.952	0.951	0.836	0.929	1.081	0.820
		0.439	0.173	0.172	0.174	0.177	0.175	0.138	0.162	0.171	0.125
20	μ	-0.141	0.009	0.010	0.014	0.013	0.017	0.131	0.010	-0.131	-0.009
		0.738	0.126	0.126	0.128	0.126	0.124	0.124	0.117	0.141	0.112
	σ	1.205	0.928	0.926	1.109	0.957	0.958	0.791	0.943	1.188	0.796
		1.432	0.179	0.179	0.233	0.191	0.194	0.137	0.183	0.187	0.128
30	μ	-2.155	0.008	0.010	0.017	0.013	0.02	0.158	-0.027	-0.249	-0.007
		36.958	0.118	0.125	0.111	0.118	0.118	0.117	0.113	0.144	0.111
	σ	0.986	0.906	0.905	0.986	0.962	0.980	0.773	0.981	1.312	0.788
		57.016	0.182	0.185	0.302	0.199	0.218	0.137	0.211	0.205	0.134
40	μ	-1.072	0.025	0.016	0.052	0.030	0.036	0.186	-0.072	-0.404	0.003
		18.418	0.096	0.132	0.090	0.096	0.107	0.106	0.119	0.146	0.097
	σ	2.298	0.884	0.894	1.350	0.967	1.050	0.771	1.042	1.467	0.811
		22.772	0.184	0.201	0.371	0.203	0.296	0.136	0.248	0.222	0.150

(b) Normal distribution

censoring (%)		Fill-in power	Fill-in exp	Fill-in weibull	power	exp	weibull	DL/2	ROS	EM	M
10	μ	0.012	0.012	0.011	0.018	0.015	0.014	0.087	0.003	-0.045	0.003
		0.147	0.146	0.146	0.146	0.146	0.145	0.137	0.146	0.144	0.153
	σ	0.966	0.965	0.966	0.962	0.966	0.967	0.860	0.984	1.076	0.977
		0.112	0.109	0.108	0.110	0.109	0.109	0.091	0.111	0.108	0.114
20	μ	-0.007	0.015	0.017	0.019	0.019	0.020	0.138	0.003	-0.123	0.003
		0.177	0.148	0.147	0.148	0.148	0.147	0.130	0.150	0.145	0.153
	σ	0.986	0.949	0.947	0.965	0.965	0.963	0.803	0.983	1.187	0.978
		0.198	0.117	0.115	0.141	0.121	0.120	0.087	0.124	0.119	0.125
30	μ	-0.245	0.016	0.021	0.014	0.020	0.027	0.173	0.003	-0.237	0.004
		1.226	0.155	0.154	0.153	0.154	0.152	0.123	0.156	0.145	0.154
	σ	1.331	0.934	0.927	1.118	0.975	0.971	0.774	0.984	1.320	0.980
		1.835	0.128	0.126	0.239	0.138	0.141	0.085	0.138	0.132	0.139
40	μ	-1.072	0.039	0.044	0.052	0.043	0.056	0.207	0.026	-0.390	0.025
		4.247	0.141	0.166	0.132	0.141	0.146	0.104	0.147	0.137	0.142
	σ	2.298	0.908	0.903	1.350	0.984	1.014	0.764	0.978	1.485	0.982
		5.235	0.132	0.154	0.328	0.147	0.242	0.083	0.153	0.149	0.151

(c) t distribution with 1 degree of freedom

censoring (%)					Fill-in						
		power	exp	weibull	power	exp	weibull	DL/2	ROS	EM	M
10	μ	-0.995	0.067	-1.444	0.319	0.239	1.528	1.213	1.302	-2.999	-0.063
		6.037	0.500	22.271	0.770	1.022	10.805	15.164	6.160	25.163	0.241
	σ	8.228	19.587	22.812	5.146	20.358	18.835	25.134	18.066	36.355	2.054
		19.207	99.536	138.804	4.397	103.435	91.221	104.789	93.121	149.125	0.501
20	μ	-4.189	0.030	0.961	0.303	0.127	1.558	1.322	-0.366	-6.545	-0.078
		37.860	0.320	8.718	0.765	0.560	11.254	15.163	2.814	36.743	0.245
	σ	12.925	18.670	18.172	4.955	19.418	18.615	25.089	19.121	38.689	1.894
		76.773	95.249	90.882	5.190	98.228	90.508	104.796	97.868	158.001	0.442
30	μ	-6.603	0.020	1.228	0.267	0.089	1.593	1.381	-2.837	-10.986	-0.083
		30.417	0.253	10.287	0.611	0.400	11.421	15.160	15.519	53.353	0.232
	σ	13.835	18.277	17.819	4.588	18.943	18.481	25.057	20.748	41.431	1.909
		46.966	93.777	90.285	4.014	96.049	90.288	104.799	105.136	168.711	0.495
40	μ	-4.518	0.056	1.855	0.534	0.121	2.247	2.091	-8.176	-18.237	-0.111
		12.993	0.198	23.351	1.621	0.507	24.370	27.206	69.580	92.198	0.202
	σ	10.497	22.753	22.266	5.869	23.461	23.140	29.600	29.087	50.979	2.112
		19.392	189.506	183.464	11.513	193.179	183.406	190.676	236.876	278.006	0.645

(d) t distribution with 5 degrees of freedom

censoring (%)					Fill-in						
		power	exp	weibull	power	exp	weibull	DL/2	ROS	EM	M
10	μ	0.017	0.020	0.019	0.032	0.024	0.024	0.117	0.023	-0.056	-0.002
		0.185	0.180	0.179	0.181	0.18	0.179	0.175	0.177	0.188	0.175
	σ	1.225	1.219	1.221	1.212	1.224	1.225	1.085	1.217	1.386	1.120
		0.240	0.224	0.222	0.219	0.23	0.227	0.182	0.206	0.241	0.143
20	μ	-0.052	0.020	0.020	0.027	0.025	0.026	0.175	0.007	-0.159	-0.003
		0.412	0.177	0.176	0.181	0.177	0.175	0.166	0.174	0.192	0.175
	σ	1.320	1.197	1.197	0.020	1.226	1.228	1.025	1.236	1.523	1.112
		0.725	0.231	0.231	0.279	0.245	0.248	0.183	0.237	0.260	0.152
30	μ	-0.552	0.018	0.021	0.020	0.023	0.031	0.213	-0.022	-0.308	-0.002
		5.912	0.175	0.177	0.167	0.174	0.172	0.157	0.178	0.199	0.174
	σ	2.038	1.176	1.172	1.442	1.236	1.244	0.996	1.266	1.687	1.117
		9.114	0.231	0.233	0.375	0.249	0.264	0.184	0.271	0.284	0.167
40	μ	-3.215	0.406	0.426	0.047	0.424	0.467	1.150	0.400	0.428	0.355
		114.566	0.170	0.192	0.200	0.169	0.178	0.125	0.168	0.147	0.171
	σ	4.873	2.868	2.844	1.352	3.144	3.216	2.107	2.978	2.945	2.290
		176.756	0.202	0.221	0.746	0.233	0.317	0.124	0.203	0.171	0.181

(e) Mixture distribution $0.8 * N(0,1) + 0.2 * N(5,1)$

censoring (%)		Fill-in									
		power	exp	weibull	power	exp	weibull	DL/2	ROS	EM	M
10	μ	0.992	0.991	0.988	0.998	0.996	0.990	1.081	0.826	0.875	0.383
		0.148	0.148	0.147	0.147	0.147	0.147	0.137	0.146	0.144	0.167
	σ	2.257	2.257	2.262	2.256	2.258	2.264	2.162	2.512	2.422	1.879
		0.138	0.138	0.138	0.138	0.138	0.138	0.129	0.155	0.141	0.156
20	μ	0.103	0.814	0.803	0.871	0.825	0.812	1.125	0.630	0.690	0.390
		0.389	0.177	0.158	0.200	0.175	0.156	0.131	0.154	0.145	0.168
	σ	2.493	2.454	2.465	2.505	2.519	2.525	2.125	2.742	2.655	2.053
		0.619	0.182	0.165	0.345	0.207	0.181	0.126	0.177	0.155	0.167
30	μ	-21.934	0.406	0.426	0.193	0.424	0.467	1.150	0.400	0.428	0.355
		114.566	0.170	0.192	0.200	0.169	0.178	0.125	0.168	0.147	0.171
	σ	37.016	2.868	2.844	4.816	3.144	3.216	2.107	2.978	2.945	2.290
		176.756	0.202	0.221	0.746	0.233	0.317	0.124	0.203	0.171	0.181
40	μ	-3.215	0.025	0.016	0.047	0.030	0.036	0.186	-0.072	-0.404	0.003
		18.418	0.096	0.132	0.090	0.096	0.107	0.106	0.119	0.146	0.097
	σ	4.813	0.884	0.894	1.352	0.967	1.050	0.771	1.042	1.467	0.811
		22.772	0.184	0.201	0.371	0.203	0.296	0.136	0.248	0.222	0.150

Table 2 $n = 100$

(a) Double exponential distribution

censoring (%)		Fill-in power	Fill-in exp	Fill-in weibull	power	exp	weibull	DL/2	ROS	EM	M
10	μ	0.000	0.009	0.009	0.012	0.011	0.012	0.093	0.027	-0.045	-0.003
		0.103	0.099	0.098	0.099	0.099	0.098	0.095	0.094	0.103	0.084
	σ	0.977	0.959	0.958	0.983	0.972	0.9715	0.835	0.931	1.087	0.821
		0.144	0.126	0.125	0.144	0.132	0.132	0.099	0.116	0.124	0.090
20	μ	-0.087	0.008	0.010	-0.012	0.010	0.013	0.136	0.012	-0.127	-0.005
		0.242	0.093	0.093	0.102	0.093	0.093	0.090	0.087	0.104	0.084
	σ	1.090	0.937	0.934	1.123	0.975	0.978	0.792	0.948	1.194	0.797
		0.428	0.130	0.130	0.236	0.141	0.145	0.098	0.133	0.135	0.094
30	μ	-3.605	0.006	0.009	-0.051	0.009	0.015	0.161	-0.027	-0.247	-0.004
		59.502	0.089	0.090	0.098	0.089	0.089	0.086	0.085	0.107	0.083
	σ	6.403	0.913	0.910	1.506	0.979	1.002	0.774	0.989	1.319	0.788
		91.334	0.131	0.132	0.381	0.144	0.160	0.098	0.152	0.148	0.097
40	μ	-3.173	0.011	0.001	-0.044	0.014	0.013	0.178	-0.088	-0.415	-0.006
		10.696	0.076	0.108	0.073	0.076	0.094	0.079	0.091	0.112	0.077
	σ	4.773	0.887	0.897	1.916	0.980	1.106	0.769	1.050	1.472	0.803
		13.150	0.130	0.145	0.446	0.145	0.285	0.097	0.176	0.162	0.107

(b) Normal distribution

censoring (%)		Fill-in power	Fill-in exp	Fill-in weibull	power	exp	weibull	DL/2	ROS	EM	M
10	μ	0.002	0.004	0.004	0.006	0.005	0.005	0.086	-0.001	-0.049	-0.001
		0.102	0.102	0.102	0.102	0.102	0.101	0.095	0.102	0.100	0.107
	σ	0.986	0.981	0.981	0.989	0.986	0.986	0.865	0.995	1.089	0.991
		0.078	0.076	0.076	0.079	0.078	0.077	0.064	0.079	0.078	0.081
20	μ	-0.025	0.005	0.008	-0.006	0.007	0.010	0.138	-0.001	-0.127	-0.001
		0.123	0.105	0.104	0.110	0.105	0.104	0.091	0.105	0.100	0.107
	σ	1.012	0.967	0.963	1.052	0.990	0.985	0.808	0.994	1.201	0.991
		0.117	0.084	0.083	0.127	0.089	0.088	0.062	0.088	0.086	0.091
30	μ	-0.525	0.004	0.012	-0.052	0.006	0.015	0.171	-0.001	-0.244	-0.001
		5.738	0.108	0.107	0.128	0.108	0.107	0.086	0.109	0.101	0.108
	σ	1.729	0.951	0.941	1.352	1.001	0.996	0.779	0.995	1.336	0.992
		8.784	0.091	0.089	0.318	0.099	0.101	0.061	0.098	0.095	0.099
40	μ	-3.089	0.011	0.013	-0.070	0.013	0.022	0.194	0.003	-0.412	0.004
		9.970	0.108	0.148	0.120	0.108	0.125	0.078	0.113	0.100	0.108
	σ	4.747	0.925	0.923	1.993	1.014	1.078	0.767	0.994	1.502	0.990
		12.236	0.095	0.132	0.487	0.108	0.306	0.061	0.109	0.108	0.110

(c) t distribution with 1 degree of freedom

censoring (%)					Fill-in						
		power	exp	weibull	power	exp	weibull	DL/2	ROS	EM	M
10	μ	-2.871	0.035	1.020	0.306	0.137	1.758	1.724	1.314	-3.317	-0.061
		16.144	0.312	10.948	0.821	0.606	13.578	15.659	6.001	18.104	0.161
	σ	15.278	27.788	27.132	7.571	28.871	27.584	34.333	26.467	47.561	2.035
		50.344	154.661	147.920	7.989	159.489	147.205	153.333	150.009	183.177	0.340
20	μ	-6.140	0.019	1.567	1.320	0.074	1.842	1.829	-0.855	-7.971	-0.075
		66.105	0.211	13.16	18.076	0.341	13.826	15.658	5.777	30.735	0.162
	σ	30.537	26.905	26.295	18.032	27.732	27.123	34.303	27.638	50.610	1.868
		221.525	151.061	146.82	180.924	154.018	146.843	153.338	154.945	194.713	0.308
30	μ	-17.419	0.014	1.717	2.673	0.053	1.893	1.880	-4.046	-13.818	-0.082
		134.503	0.169	13.627	29.051	0.250	13.929	15.657	22.611	51.205	0.157
	σ	60.105	26.540	26.054	31.931	27.225	26.907	34.293	29.441	54.265	1.878
		351.164	149.844	146.736	290.442	151.954	146.737	153.339	162.746	208.734	0.336
40	μ	-3.031	0.014	1.690	0.377	0.045	1.890	1.929	-8.795	-21.373	-0.139
		2.008	0.147	13.755	0.816	0.203	13.975	15.657	47.553	79.128	0.150
	σ	9.094	26.430	26.088	7.632	27.037	27.268	34.382	32.333	58.926	2.048
		8.530	149.216	146.699	8.087	150.852	146.655	153.319	175.338	226.262	0.431

(d) t distribution with 5 degrees of freedom

censoring (%)					Fill-in						
		power	exp	weibull	power	exp	weibull	DL/2	ROS	EM	M
10	μ	0.005	0.011	0.011	0.017	0.014	0.014	0.118	0.022	-0.056	-0.003
		0.129	0.126	0.125	0.127	0.126	0.125	0.124	0.124	0.131	0.122
	σ	1.256	1.243	1.243	1.263	1.257	1.258	1.091	1.230	1.402	1.128
		0.183	0.172	0.171	0.185	0.180	0.181	0.139	0.158	0.178	0.106
20	μ	-0.048	0.01	0.011	-0.004	0.013	0.015	0.177	0.004	-0.160	-0.004
		0.178	0.122	0.122	0.130	0.122	0.121	0.118	0.122	0.133	0.122
	σ	1.309	1.22	1.218	1.373	1.260	1.262	1.032	1.252	1.541	1.120
		0.285	0.175	0.176	0.258	0.188	0.193	0.140	0.181	0.193	0.112
30	μ	-0.552	0.008	0.013	-0.002	0.011	0.018	0.214	-0.029	-0.313	-0.005
		1.937	0.124	0.123	0.144	0.124	0.122	0.113	0.128	0.137	0.123
	σ	1.996	1.196	1.189	1.773	1.267	1.277	1.004	1.286	1.707	1.124
		2.928	0.173	0.174	0.438	0.188	0.201	0.141	0.208	0.211	0.122
40	μ	-7.418	0.019	0.019	-0.061	0.022	0.030	0.240	-0.07	-0.529	0.001
		75.020	0.118	0.146	0.127	0.118	0.133	0.101	0.137	0.143	0.118
	σ	10.301	1.162	1.162	2.433	1.274	1.367	0.994	1.330	1.913	1.130
		92.313	0.173	0.188	0.580	0.190	0.336	0.140	0.242	0.231	0.134

(e) Mixture distribution $0.8 * N(0,1) + 0.2 * N(5,1)$

censoring (%)		Fill-in power	Fill-in exp	Fill-in weibull	power	exp	weibull	DL/2	ROS	EM	M
10	μ	0.978	0.979	0.979	0.982	0.981	0.980	1.080	0.822	0.872	0.386
		0.104	0.104	0.104	0.104	0.104	0.103	0.096	0.104	0.100	0.121
	σ	2.266	2.264	2.265	2.271	2.270	2.270	2.156	2.512	2.430	1.897
		0.100	0.099	0.098	0.101	0.100	0.099	0.091	0.110	0.100	0.108
20	μ	0.651	0.754	0.779	0.741	0.761	0.785	1.125	0.630	0.687	0.393
		0.405	0.137	0.123	0.203	0.136	0.122	0.091	0.109	0.101	0.121
	σ	2.689	2.521	2.488	2.860	2.627	2.576	2.118	2.738	2.664	2.070
		0.659	0.146	0.128	0.582	0.180	0.155	0.089	0.125	0.110	0.117
30	μ	-96.556	0.398	0.417	-0.118	0.407	0.439	1.150	0.406	0.424	0.358
		1378.201	0.124	0.140	0.189	0.123	0.134	0.086	0.120	0.103	0.123
	σ	151.317	2.868	2.845	6.888	3.183	3.306	2.10	2.967	2.955	2.301
		2115.842	0.145	0.159	0.975	0.172	0.258	0.087	0.143	0.121	0.127
40	μ	-18.546	0.342	0.335	-0.123	0.350	0.360	1.157	0.153	0.045	0.256
		25.326	0.127	0.152	0.165	0.127	0.143	0.082	0.139	0.108	0.130
	σ	25.738	2.814	2.821	7.301	3.174	3.458	2.095	3.199	3.329	2.609
		31.143	0.142	0.160	0.937	0.166	0.312	0.086	0.165	0.136	0.144

2 Conclusion

From the simulation studies, we can the proposed method work well. However, there are several related issues required to be examined further. Also, the real data analysis has not been explored yet. The completed results on related work will be done in the future.

3 References

Hseih, P. H. and Cheng, T.-C. (2003) "Robust Estimation of Moments of Environmental Data With One-Sided Detection Limit," 2003 ASA meeting, San Francisco.

Korn, L. R. and Tyler, D. E. (2001) "Robust Estimation for Chemical Concentration Data Subject to Detection Limits," *Statistics in Genetics and in the Environmental Sciences*, ed. by L. Fernholz, S. Morgenthaler and W. Stahel, Basel: Birkhauser-Verlag, pp. 41-63.

Shummay, R. H., Azari, A. S. and Johnson, P. (1989) "Estimating Mean Concentrations Under Transformation for Environmental Data With Detection Limits", *Technometrics*, **31**, 347-356.

Shummay, R. H., Azari, A. S. and Kayhanian, M. (2002) "Statistical Approaches to Estimating Mean Water Quality Concentrations with Detection Limits", *Environmental Science & Technology*, **36**, 3345-3353.