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Techniques of Water-Resources Investigations
of the United States Geological Survey

Chapter B4

REGRESSION MODELING OF GROUND-WATER FLOW

By Richard L. Cooley and Richard L. Naff

Book 3
APPLICATIONS OF HYDRAULICS

2.10 Tables of Probability Distributions

[All tables modified from Walpole and Myers (1972), with permission from the publisher]

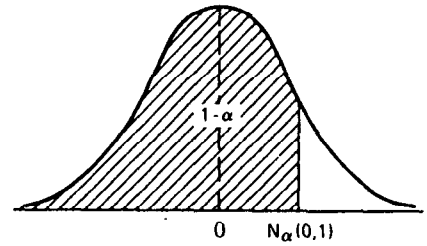

Table 2.10-1

Areas, $1-\alpha$, Under the Normal Curve

$N_\alpha(0,1)$	0.00	0.01	0.02	0.03	0.04	0.05	0.06	0.07	0.08	0.09
−3.4	0.0003	0.0003	0.0003	0.0003	0.0003	0.0003	0.0003	0.0003	0.0003	0.0002
−3.3	0.0005	0.0005	0.0005	0.0004	0.0004	0.0004	0.0004	0.0004	0.0004	0.0003
−3.2	0.0007	0.0007	0.0006	0.0006	0.0006	0.0006	0.0006	0.0005	0.0005	0.0005
−3.1	0.0010	0.0009	0.0009	0.0009	0.0008	0.0008	0.0008	0.0008	0.0007	0.0007
−3.0	0.0013	0.0013	0.0013	0.0012	0.0012	0.0011	0.0011	0.0011	0.0010	0.0010
−2.9	0.0019	0.0018	0.0017	0.0017	0.0016	0.0016	0.0015	0.0015	0.0014	0.0014
−2.8	0.0026	0.0025	0.0024	0.0023	0.0023	0.0022	0.0021	0.0021	0.0020	0.0019
−2.7	0.0035	0.0034	0.0033	0.0032	0.0031	0.0030	0.0029	0.0028	0.0027	0.0026
−2.6	0.0047	0.0045	0.0044	0.0043	0.0041	0.0040	0.0039	0.0038	0.0037	0.0036
−2.5	0.0062	0.0060	0.0059	0.0057	0.0055	0.0054	0.0052	0.0051	0.0049	0.0048
−2.4	0.0082	0.0080	0.0078	0.0075	0.0073	0.0071	0.0069	0.0068	0.0066	0.0064
−2.3	0.0107	0.0104	0.0102	0.0099	0.0096	0.0094	0.0091	0.0089	0.0087	0.0084
−2.2	0.0139	0.0136	0.0132	0.0129	0.0125	0.0122	0.0119	0.0116	0.0113	0.0110
−2.1	0.0179	0.0174	0.0170	0.0166	0.0162	0.0158	0.0154	0.0150	0.0146	0.0143
−2.0	0.0228	0.0222	0.0217	0.0212	0.0207	0.0202	0.0197	0.0192	0.0188	0.0183
−1.9	0.0287	0.0281	0.0274	0.0268	0.0262	0.0256	0.0250	0.0244	0.0239	0.0233
−1.8	0.0359	0.0352	0.0344	0.0336	0.0329	0.0322	0.0314	0.0307	0.0301	0.0294
−1.7	0.0446	0.0436	0.0427	0.0418	0.0409	0.0401	0.0392	0.0384	0.0375	0.0367
−1.6	0.0548	0.0537	0.0526	0.0516	0.0505	0.0495	0.0485	0.0475	0.0465	0.0455
−1.5	0.0668	0.0655	0.0643	0.0630	0.0618	0.0606	0.0594	0.0582	0.0571	0.0559
−1.4	0.0808	0.0793	0.0778	0.0764	0.0749	0.0735	0.0722	0.0708	0.0694	0.0681
−1.3	0.0968	0.0951	0.0934	0.0918	0.0901	0.0885	0.0869	0.0853	0.0838	0.0823
−1.2	0.1151	0.1131	0.1112	0.1093	0.1075	0.1056	0.1038	0.1020	0.1003	0.0985
−1.1	0.1357	0.1335	0.1314	0.1292	0.1271	0.1251	0.1230	0.1210	0.1190	0.1170
−1.0	0.1587	0.1562	0.1539	0.1515	0.1492	0.1469	0.1446	0.1423	0.1401	0.1379
−0.9	0.1841	0.1814	0.1788	0.1762	0.1736	0.1711	0.1685	0.1660	0.1635	0.1611
−0.8	0.2119	0.2090	0.2061	0.2033	0.2005	0.1977	0.1949	0.1922	0.1894	0.1867
−0.7	0.2420	0.2389	0.2358	0.2327	0.2296	0.2266	0.2236	0.2206	0.2177	0.2148
−0.6	0.2743	0.2709	0.2676	0.2643	0.2611	0.2578	0.2546	0.2514	0.2483	0.2451
−0.5	0.3085	0.3050	0.3015	0.2981	0.2946	0.2912	0.2877	0.2843	0.2810	0.2776
−0.4	0.3446	0.3409	0.3372	0.3336	0.3300	0.3264	0.3228	0.3192	0.3156	0.3121
−0.3	0.3821	0.3783	0.3745	0.3707	0.3669	0.3632	0.3594	0.3557	0.3520	0.3483
−0.2	0.4207	0.4168	0.4129	0.4090	0.4052	0.4013	0.3974	0.3936	0.3897	0.3859
−0.1	0.4602	0.4562	0.4522	0.4483	0.4443	0.4404	0.4364	0.4325	0.4286	0.4247
−0.0	0.5000	0.4960	0.4920	0.4880	0.4840	0.4801	0.4761	0.4721	0.4681	0.4641
0.0	0.5000	0.5040	0.5080	0.5120	0.5160	0.5199	0.5239	0.5279	0.5319	0.5359
0.1	0.5398	0.5438	0.5478	0.5517	0.5557	0.5596	0.5636	0.5675	0.5714	0.5753
0.2	0.5793	0.5832	0.5871	0.5910	0.5948	0.5987	0.6026	0.6064	0.6103	0.6141
0.3	0.6179	0.6217	0.6255	0.6293	0.6331	0.6368	0.6406	0.6443	0.6480	0.6517
0.4	0.6554	0.6591	0.6628	0.6664	0.6700	0.6736	0.6772	0.6808	0.6844	0.6879
0.5	0.6915	0.6950	0.6985	0.7019	0.7054	0.7088	0.7123	0.7157	0.7190	0.7224
0.6	0.7257	0.7291	0.7324	0.7357	0.7389	0.7422	0.7454	0.7486	0.7517	0.7549
0.7	0.7580	0.7611	0.7642	0.7673	0.7704	0.7734	0.7764	0.7794	0.7823	0.7852
0.8	0.7881	0.7910	0.7939	0.7967	0.7995	0.8023	0.8051	0.8078	0.8106	0.8133
0.9	0.8159	0.8186	0.8212	0.8238	0.8264	0.8289	0.8315	0.8340	0.8365	0.8389
1.0	0.8413	0.8438	0.8461	0.8485	0.8508	0.8531	0.8554	0.8577	0.8599	0.8621
1.1	0.8643	0.8665	0.8686	0.8708	0.8729	0.8749	0.8770	0.8790	0.8810	0.8830
1.2	0.8849	0.8869	0.8888	0.8907	0.8925	0.8944	0.8962	0.8980	0.8997	0.9015
1.3	0.9032	0.9049	0.9066	0.9082	0.9099	0.9115	0.9131	0.9147	0.9162	0.9177
1.4	0.9192	0.9207	0.9222	0.9236	0.9251	0.9265	0.9278	0.9292	0.9306	0.9319
1.5	0.9332	0.9345	0.9357	0.9370	0.9382	0.9394	0.9406	0.9418	0.9429	0.9441
1.6	0.9452	0.9463	0.9474	0.9484	0.9495	0.9505	0.9515	0.9525	0.9535	0.9545
1.7	0.9554	0.9564	0.9573	0.9582	0.9591	0.9599	0.9608	0.9616	0.9625	0.9633
1.8	0.9641	0.9649	0.9656	0.9664	0.9671	0.9678	0.9686	0.9693	0.9699	0.9706
1.9	0.9713	0.9719	0.9726	0.9732	0.9738	0.9744	0.9750	0.9756	0.9761	0.9767
2.0	0.9772	0.9778	0.9783	0.9788	0.9793	0.9798	0.9803	0.9808	0.9812	0.9817
2.1	0.9821	0.9826	0.9830	0.9834	0.9838	0.9842	0.9846	0.9850	0.9854	0.9857
2.2	0.9861	0.9864	0.9868	0.9871	0.9875	0.9878	0.9881	0.9884	0.9887	0.9890
2.3	0.9893	0.9896	0.9898	0.9901	0.9904	0.9906	0.9909	0.9911	0.9913	0.9916
2.4	0.9918	0.9920	0.9922	0.9925	0.9927	0.9929	0.9931	0.9932	0.9934	0.9936
2.5	0.9938	0.9940	0.9941	0.9943	0.9945	0.9946	0.9948	0.9949	0.9951	0.9952
2.6	0.9953	0.9955	0.9956	0.9957	0.9959	0.9960	0.9961	0.9962	0.9963	0.9964
2.7	0.9965	0.9966	0.9967	0.9968	0.9969	0.9970	0.9971	0.9972	0.9973	0.9974
2.8	0.9974	0.9975	0.9976	0.9977	0.9977	0.9978	0.9979	0.9979	0.9980	0.9981
2.9	0.9981	0.9982	0.9982	0.9983	0.9984	0.9984	0.9985	0.9985	0.9986	0.9986
3.0	0.9987	0.9987	0.9987	0.9988	0.9988	0.9989	0.9989	0.9989	0.9990	0.9990
3.1	0.9990	0.9991	0.9991	0.9991	0.9992	0.9992	0.9992	0.9992	0.9993	0.9993
3.2	0.9993	0.9993	0.9994	0.9994	0.9994	0.9994	0.9994	0.9995	0.9995	0.9995
3.3	0.9995	0.9995	0.9995	0.9996	0.9996	0.9996	0.9996	0.9996	0.9996	0.9997
3.4	0.9997	0.9997	0.9997	0.9997	0.9997	0.9997	0.9997	0.9997	0.9997	0.9998

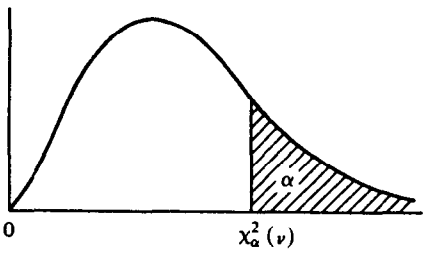

Table 2.10-2

Critical Values of the Chi-Square Distribution

	α							
ν	0.995	0.99	0.975	0.95	0.05	0.025	0.01	0.005
1	0.0^4393	0.0^3157	0.0^3982	0.0^2393	3.841	5.024	6.635	7.879
2	0.0100	0.0201	0.0506	0.103	5.991	7.378	9.210	10.597
3	0.0717	0.115	0.216	0.352	7.815	9.348	11.345	12.838
4	0.207	0.297	0.484	0.711	9.488	11.143	13.277	14.860
5	0.412	0.554	0.831	1.145	11.070	12.832	15.086	16.750
6	0.676	0.872	1.237	1.635	12.592	14.449	16.812	18.548
7	0.989	1.239	1.690	2.167	14.067	16.013	18.475	20.278
8	1.344	1.646	2.180	2.733	15.507	17.535	20.090	21.955
9	1.735	2.088	2.700	3.325	16.919	19.023	21.666	23.589
10	2.156	2.558	3.247	3.940	18.307	20.483	23.209	25.188
11	2.603	3.053	3.816	4.575	19.675	21.920	24.725	26.757
12	3.074	3.571	4.404	5.226	21.026	23.337	26.217	28.300
13	3.565	4.107	5.009	5.892	22.362	24.736	27.688	29.819
14	4.075	4.660	5.629	6.571	23.685	26.119	29.141	31.319
15	4.601	5.229	6.262	7.261	24.996	27.488	30.578	32.801
16	5.142	5.812	6.908	7.962	26.296	28.845	32.000	34.267
17	5.697	6.408	7.564	8.672	27.587	30.191	33.409	35.718
18	6.265	7.015	8.231	9.390	28.869	31.526	34.805	37.156
19	6.844	7.633	8.907	10.117	30.144	32.852	36.191	38.582
20	7.434	8.260	9.591	10.851	31.410	34.170	37.566	39.997
21	8.034	8.897	10.283	11.591	32.671	35.479	38.932	41.401
22	8.643	9.542	10.982	12.338	33.924	36.781	40.289	42.796
23	9.260	10.196	11.689	13.091	35.172	38.076	41.638	44.181
24	9.886	10.856	12.401	13.848	36.415	39.364	42.980	45.558
25	10.520	11.524	13.120	14.611	37.652	40.646	44.314	46.928
26	11.160	12.198	13.844	15.379	38.885	41.923	45.642	48.290
27	11.808	12.879	14.573	16.151	40.113	43.194	46.963	49.645
28	12.461	13.565	15.308	16.928	41.337	44.461	48.278	50.993
29	13.121	14.256	16.047	17.708	42.557	45.722	49.588	52.336
30	13.787	14.953	16.791	18.493	43.773	46.979	50.892	53.672

Abridged from Table 8 of *Biometrika Tables for Statisticians*, Vol. I, by permission of E. S. Pearson and the Biometrika Trustees.

2.10 Tables of Probability Distributions—Continued

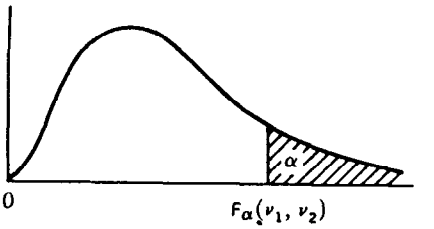

Table 2.10-3

Critical Values of the F Distribution

$F_{0.05}(\nu_1, \nu_2)$

	ν_1								
ν_2	1	2	3	4	5	6	7	8	9
1	161.4	199.5	215.7	224.6	230.2	234.0	236.8	238.9	240.5
2	18.51	19.00	19.16	19.25	19.30	19.33	19.35	19.37	19.38
3	10.13	9.55	9.28	9.12	9.01	8.94	8.89	8.85	8.81
4	7.71	6.94	6.59	6.39	6.26	6.16	6.09	6.04	6.00
5	6.61	5.79	5.41	5.19	5.05	4.95	4.88	4.82	4.77
6	5.99	5.14	4.76	4.53	4.39	4.28	4.21	4.15	4.10
7	5.59	4.74	4.35	4.12	3.97	3.87	3.79	3.73	3.68
8	5.32	4.46	4.07	3.84	3.69	3.58	3.50	3.44	3.39
9	5.12	4.26	3.86	3.63	3.48	3.37	3.29	3.23	3.18
10	4.96	4.10	3.71	3.48	3.33	3.22	3.14	3.07	3.02
11	4.84	3.98	3.59	3.36	3.20	3.09	3.01	2.95	2.90
12	4.75	3.89	3.49	3.26	3.11	3.00	2.91	2.85	2.80
13	4.67	3.81	3.41	3.18	3.03	2.92	2.83	2.77	2.71
14	4.60	3.74	3.34	3.11	2.96	2.85	2.76	2.70	2.65
15	4.54	3.68	3.29	3.06	2.90	2.79	2.71	2.64	2.59
16	4.49	3.63	3.24	3.01	2.85	2.74	2.66	2.59	2.54
17	4.45	3.59	3.20	2.96	2.81	2.70	2.61	2.55	2.49
18	4.41	3.55	3.16	2.93	2.77	2.66	2.58	2.51	2.46
19	4.38	3.52	3.13	2.90	2.74	2.63	2.54	2.48	2.42
20	4.35	3.49	3.10	2.87	2.71	2.60	2.51	2.45	2.39
21	4.32	3.47	3.07	2.84	2.68	2.57	2.49	2.42	2.37
22	4.30	3.44	3.05	2.82	2.66	2.55	2.46	2.40	2.34
23	4.28	3.42	3.03	2.80	2.64	2.53	2.44	2.37	2.32
24	4.26	3.40	3.01	2.78	2.62	2.51	2.42	2.36	2.30
25	4.24	3.39	2.99	2.76	2.60	2.49	2.40	2.34	2.28
26	4.23	3.37	2.98	2.74	2.59	2.47	2.39	2.32	2.27
27	4.21	3.35	2.96	2.73	2.57	2.46	2.37	2.31	2.25
28	4.20	3.34	2.95	2.71	2.56	2.45	2.36	2.29	2.24
29	4.18	3.33	2.93	2.70	2.55	2.43	2.35	2.28	2.22
30	4.17	3.32	2.92	2.69	2.53	2.42	2.33	2.27	2.21
40	4.08	3.23	2.84	2.61	2.45	2.34	2.25	2.18	2.12
60	4.00	3.15	2.76	2.53	2.37	2.25	2.17	2.10	2.04
120	3.92	3.07	2.68	2.45	2.29	2.17	2.09	2.02	1.96
∞	3.84	3.00	2.60	2.37	2.21	2.10	2.01	1.94	1.88

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Table 2.10-3 continued

$F_{0.05}(\nu_1, \nu_2)$

ν_2	ν_1									
	10	12	15	20	24	30	40	60	120	∞
1	241.9	243.9	245.9	248.0	249.1	250.1	251.1	252.2	253.3	254.3
2	19.40	19.41	19.43	19.45	19.45	19.46	19.47	19.48	19.49	19.50
3	8.79	8.74	8.70	8.66	8.64	8.62	8.59	8.57	8.55	8.53
4	5.96	5.91	5.86	5.80	5.77	5.75	5.72	5.69	5.66	5.63
5	4.74	4.68	4.62	4.56	4.53	4.50	4.46	4.43	4.40	4.36
6	4.06	4.00	3.94	3.87	3.84	3.81	3.77	3.74	3.70	3.67
7	3.64	3.57	3.51	3.44	3.41	3.38	3.34	3.30	3.27	3.23
8	3.35	3.28	3.22	3.15	3.12	3.08	3.04	3.01	2.97	2.93
9	3.14	3.07	3.01	2.94	2.90	2.86	2.83	2.79	2.75	2.71
10	2.98	2.91	2.85	2.77	2.74	2.70	2.66	2.62	2.58	2.54
11	2.85	2.79	2.72	2.65	2.61	2.57	2.53	2.49	2.45	2.40
12	2.75	2.69	2.62	2.54	2.51	2.47	2.43	2.38	2.34	2.30
13	2.67	2.60	2.53	2.46	2.42	2.38	2.34	2.30	2.25	2.21
14	2.60	2.53	2.46	2.39	2.35	2.31	2.27	2.22	2.18	2.13
15	2.54	2.48	2.40	2.33	2.29	2.25	2.20	2.16	2.11	2.07
16	2.49	2.42	2.35	2.28	2.24	2.19	2.15	2.11	2.06	2.01
17	2.45	2.38	2.31	2.23	2.19	2.15	2.10	2.06	2.01	1.96
18	2.41	2.34	2.27	2.19	2.15	2.11	2.06	2.02	1.97	1.92
19	2.38	2.31	2.23	2.16	2.11	2.07	2.03	1.98	1.93	1.88
20	2.35	2.28	2.20	2.12	2.08	2.04	1.99	1.95	1.90	1.84
21	2.32	2.25	2.18	2.10	2.05	2.01	1.96	1.92	1.87	1.81
22	2.30	2.23	2.15	2.07	2.03	1.98	1.94	1.89	1.84	1.78
23	2.27	2.20	2.13	2.05	2.01	1.96	1.91	1.86	1.81	1.76
24	2.25	2.18	2.11	2.03	1.98	1.94	1.89	1.84	1.79	1.73
25	2.24	2.16	2.09	2.01	1.96	1.92	1.87	1.82	1.77	1.71
26	2.22	2.15	2.07	1.99	1.95	1.90	1.85	1.80	1.75	1.69
27	2.20	2.13	2.06	1.97	1.93	1.88	1.84	1.79	1.73	1.67
28	2.19	2.12	2.04	1.96	1.91	1.87	1.82	1.77	1.71	1.65
29	2.18	2.10	2.03	1.94	1.90	1.85	1.81	1.75	1.70	1.64
30	2.16	2.09	2.01	1.93	1.89	1.84	1.79	1.74	1.68	1.62
40	2.08	2.00	1.92	1.84	1.79	1.74	1.69	1.64	1.58	1.51
60	1.99	1.92	1.84	1.75	1.70	1.65	1.59	1.53	1.47	1.39
120	1.91	1.83	1.75	1.66	1.61	1.55	1.50	1.43	1.35	1.25
∞	1.83	1.75	1.67	1.57	1.52	1.46	1.39	1.32	1.22	1.00

2.11 Appendices

2.11.1 Correlation of Two Linearly Related Random Variables

Consider a linear relationship between two random variables X and Y such that

$$Y=a+bX+\varepsilon \qquad (2.11\text{-}1)$$

where ε represents a zero-mean random error (independent of X). Then

$$\sigma_Y^2=b^2\sigma_X^2+\sigma_\varepsilon^2 \qquad (2.11\text{-}2)$$

because $\sigma_{X\varepsilon}=E[(X-\mu_X)\varepsilon]=0$. By direct calculation of σ_{XY} from equation 2.11-1, one obtains

$$\begin{aligned}\sigma_{XY}&=E[(X-\mu_X)(Y-\mu_Y)]\\&=E[(X-\mu_X)(b(X-\mu_X)+\varepsilon)]\\&=b\sigma_X^2 \ .\end{aligned} \qquad (2.11\text{-}3)$$

Upon squaring both sides of equation 2.11-3 and dividing by $\sigma_X^2\sigma_Y^2$, one obtains

$$\rho_{XY}^2=b^2\frac{\sigma_X^2}{\sigma_Y^2} \qquad (2.11\text{-}4)$$

which, from equation 2.11-2, can be put in the form

$$\rho_{XY}^2=1-\frac{\sigma_\varepsilon^2}{\sigma_Y^2} \ . \qquad (2.11\text{-}5)$$

Again from equation 2.11-2, it is seen that

$$b^2\sigma_X^2=\sigma_Y^2-\sigma_\varepsilon^2 \qquad (2.11\text{-}6)$$

and as $b^2\sigma_X^2$ is a nonnegative quantity, σ_Y^2 must be greater than or equal to σ_ε^2. This shows that, for a linear relationship, ρ_{XY}^2 is either less than unity or equal to one if σ_ε^2 is equal to zero.

2.11.2 Expected Value of Variance Estimator

The sample statistic S_X^{*2} is defined as

$$S_X^{*2}=\frac{1}{n}\sum_{i=1}^{n}(X_i-\bar{X})^2 \ . \qquad (2.11\text{-}7)$$

By taking expected values of both sides, one sees that

$$\begin{aligned}E\left[S_X^{*2}\right]&=\frac{1}{n}E\left[\sum_{i=1}^{n}(X_i-\bar{X})^2\right]\\&=\frac{1}{n}E\left[\sum_{i=1}^{n}(X_i-\mu_X-(\bar{X}-\mu_X))^2\right]\\&=\frac{1}{n}\left[\sum_{i=1}^{n}E[(X_i-\mu_X)^2]-E[n(\bar{X}-\mu_X)^2]\right]\end{aligned} \qquad (2.11\text{-}8)$$

where use is made of the fact that $\sum_{i=1}^{n}(X_i-\mu_X)=n(\bar{X}-\mu_X)$. Now the second expected value in equation 2.11-8 becomes

$$\begin{aligned}E[n(\bar{X}-\mu_X)^2]&=\frac{1}{n}E\left[\sum_{i=1}^{n}(X_i-\mu_X)\sum_{j=1}^{n}(X_j-\mu_X)\right]\\&=\frac{1}{n}E\left[\sum_{i=1}^{n}\sum_{j=1}^{n}(X_i-\mu_X)(X_j-\mu_X)\right]\\&=\frac{1}{n}\sum_{i=1}^{n}\sum_{j=1}^{n}\mathrm{Cov}[X_i,X_j] \ .\end{aligned} \qquad (2.11\text{-}9)$$

As X_i and X_j are randomly selected and therefore independent,

$$\mathrm{Cov}[X_i,X_j]=\begin{cases}\sigma_X^2 & i=j\\ 0 & i\neq j\end{cases} \ . \qquad (2.11\text{-}10)$$

Thus, equation 2.11-9 becomes

$$E[n(\bar{X}-\mu_X)^2]=\sigma_X^2 \qquad (2.11\text{-}11)$$

which allows us to write equation 2.11-8 as

$$\begin{aligned}E\left[S_X^{*2}\right]&=\frac{1}{n}\left[\left(\sum_{i=1}^{n}\sigma_X^2\right)-\sigma_X^2\right]\\&=\frac{n-1}{n}\sigma_X^2\end{aligned} \qquad (2.11\text{-}12)$$

and demonstrates the desired result. Note that equation 2.11-11 also demonstrates that

$$\sigma_{\bar{X}}^2=\sigma_X^2/n \qquad (2.11\text{-}13)$$

as $\sigma_{\bar{X}}^2=E[(\bar{X}-\mu_X)^2]$.

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Additional Reading

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3 Regression Solution of Modeling Problems

3.1 Introduction and Background

Ground-water flow models are members of a class of models known as mathematical models, in which the physical model of the flow system is replaced by mathematical expressions containing mathematical variables, parameters, and constants (Krumbein and Graybill, 1965, p. 15). Mathematical models always involve simplification of the actual (true) physical system. Krumbein and Graybill (1965, p. 15) argued that mathematical models can be classified into several types, including deterministic models, statistical models, and stochastic-process models.

A deterministic model is one in which the dependent variable(s) can be exactly computed from an expression involving independent variables, parameters, and constants. Note that deterministic models do not have to be physically based but may instead be completely empirical. The classical and inverse flow models discussed in section 1 are of the physically based deterministic type. In contrast, a statistical model is a deterministic model that has one or more random components added. These random components frequently involve measurement or other errors, but may involve separate sources of random variability as well. Incorporation of the errors in both observed heads and estimated parameters discussed in section 1 converts the deterministic flow model into a statistical model.

The term "stochastic model" can be considered to be synonymous with the term "statistical model" (Krumbein and Graybill, 1965, p. 19). A stochastic-process model may consider random effects such as those contained in the statistical model but in addition has a stochastic process built into it. Generation of a spatially varying permeability field in an aquifer has been considered to be a stochastic process by Bakr and others (1978), Gutjahr and others (1978), and Smith and Freeze (1979a, 1979b). Recently, this type of process has been incorporated into a parameter estimation scheme for a steady-state ground-water flow model (Kitanidis and Vomvoris, 1983). Stochastic-process models are not considered further here.

3.1.1 Assumed Model Structure

Consider an experiment where two variables, ξ and Y, are measured repeatedly. The independent variable, ξ, is considered to be a precisely defined quantity, whereas the dependent variable, Y, whose values depend upon values of the independent variable, contains some error resulting from the experimental process. A scatter diagram of the data might appear as in figure 3.1-1.

From the scatter diagram or from physical considerations, the experimentalist may decide that an appropriate model equation for the data is

$$Y_i=\beta_1+\beta_2\xi_i+\epsilon_i \qquad (3.1\text{-}1)$$

where β_1 and β_2 are the intercept and slope of the equation for a straight line, subscript i represents the ith observation of (ξ,Y), and ϵ_i is the true error in Y for observation i. The quantity $\beta_1+\beta_2\xi$ is the deterministic part of the equation (the computed value of the dependent variable), and, because ϵ_i is the true error, parameters β_1 and β_2 are the true parameters representing the deterministic part of the model response. True error ϵ_i, often called a disturbance, is a random variable and, thus, represents the stochastic part of the model response. Note that if the model is correct and no other source of bias in ϵ_i exists, $E(\epsilon_i)=0$.

Equation 3.1-1 is linear in parameters β_1 and β_2. Another example of a model equation that is linear in the parameters is

$$Y_i=\beta_1+\beta_2\xi_i+\beta_3\xi_i^2+\epsilon_i \qquad (3.1\text{-}2)$$

which is the equation for a second degree polynomial. In equation 3.1-2 there is still only one independent variable, ξ, although the equation has two terms containing ξ. An alternate form for equation 3.1-2 is

$$Y_i=X_{i1}\beta_1+X_{i2}\beta_2+X_{i3}\beta_3+\epsilon_i \quad , \qquad (3.1\text{-}3)$$

where

$$\left.\begin{aligned} X_1&=1\\ X_2&=\xi\\ X_3&=\xi^2 \end{aligned}\right\} \quad . \qquad (3.1\text{-}4)$$

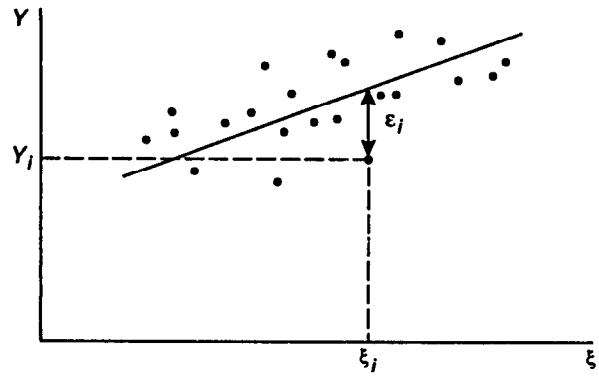

Figure 3.3-1

In general, any equation that is linear in parameters $\beta_1, \beta_2, \ldots, \beta_p$, where there are p parameters for the system, can be written in the form

$$Y_i = X_{i1}\beta_1 + X_{i2}\beta_2 + \ldots + X_{ip}\beta_p + \epsilon_i \quad (3.1\text{-}5)$$

where

$$X_{ij} = X_{ij}(\xi_{i1}, \xi_{i2}, \ldots, \xi_{ik}) \quad (3.1\text{-}6)$$

is a function of k independent variables that multiplies the jth parameter and does not contain the parameters. Because

$$\frac{\partial}{\partial \beta_j}\left(X_{i1}\beta_1 + X_{i2}\beta_2 + \ldots + X_{ip}\beta_p\right) = X_{ij}, \quad (3.1\text{-}7)$$

the X terms are often called sensitivity coefficients or, simply, sensitivities. They indicate the change in the model response (the computed value of the dependent variable) at observation point i for a unit change in parameter β_j. Equation 3.1-5 can be written compactly in matrix form as

$$\underline{Y} = \underline{X}\underline{\beta} + \underline{\epsilon} \quad (3.1\text{-}8)$$

where

$$\underline{Y} = \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{bmatrix} \quad (3.1\text{-}9)$$

$$\underline{X} = \begin{bmatrix} X_{11} & X_{12} & \cdots & X_{1p} \\ X_{21} & X_{22} & \cdots & X_{2p} \\ \vdots & & & \vdots \\ X_{n1} & \cdots & & X_{np} \end{bmatrix} \quad (3.1\text{-}10)$$

$$\underline{\beta} = \begin{bmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_p \end{bmatrix} \quad (3.1\text{-}11)$$

$$\underline{\epsilon} = \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{bmatrix} \quad (3.1\text{-}12)$$

and n observations are assumed.

Often we are faced with models where the equation is no longer linear in the parameters, $\underline{\beta}$. For example, suppose that the model equation is

$$Y_i = \sqrt{\beta_1 + \beta_2}\, \tan\left(\frac{\sqrt{\beta_1 + \beta_2}}{\beta_1}\, \xi_i\right) + \epsilon_i \; . \quad (3.1\text{-}13)$$

Equation 3.1-13 cannot be reduced to the form of equation 3.1-5, and, thus, is not linear in the parameters. Equations of this type are written in the general vector form

$$\underline{Y} = \underline{f}(\underline{\xi}_1, \underline{\xi}_2, \ldots, \underline{\xi}_k; \beta_1, \beta_2, \ldots, \beta_p) + \underline{\epsilon} \quad (3.1\text{-}14)$$

or, in more compact form,

$$\underline{Y} = \underline{f}(\underline{\xi}, \underline{\beta}) + \underline{\epsilon} \quad (3.1\text{-}15)$$

where $\underline{f}$ is an n-vector, each element f_i of which is a general function of the k independent variables, $\xi_{i\ell}$ ($\ell = 1,2,\ldots,k$), and p parameters, β_j ($j = 1,2,\ldots,p$). Equation 3.1-15 incorporates equation 3.1-8 because 3.1-8 is simply the special case where $\underline{f}(\underline{\xi}, \underline{\beta}) = \underline{\underline{X}}(\underline{\xi})\underline{\beta}$.

Some equations may be nonlinear in $\underline{\beta}$ but linear in some transformation of $\underline{\beta}$. For example, the model

$$Y_i = \beta_1 (\beta_2)^{X_i} \epsilon_i \quad (3.1\text{-}16)$$

in which the error ϵ_i is multiplicative, is nonlinear in β_1 and β_2. However, equation 3.1-16 may be written as

$$\log Y_i = \log \beta_1 + X_i \log \beta_2 + \log \epsilon_i \quad (3.1\text{-}17)$$

which is linear in $\log \beta_1$ and $\log \beta_2$ and has an additive error term. Thus, it is of the standard linear form. Equations such as 3.1-16 are frequently best utilized in their transformed, thus linearized, form. However, all model analyses (to be discussed further on) would probably be made in terms of the transformed variables, and this would have to be remembered when results were interpreted.

Types of models other than the linear and nonlinear ones discussed above also exist. Some types involve a complex model equation that cannot be solved explicitly for the dependent variable. In other cases the function $f(\underline{\xi},\underline{\beta})$, which is assumed to be a known function of $\underline{\xi}$ and $\underline{\beta}$, cannot be obtained and, therefore, must be replaced by a numerical formulation. However, the basic model structure of equation 3.1-15, where the error $\underline{\epsilon}$ in $\underline{Y}$ is assumed to be additive to a deterministic dependent variable vector, is always assumed. Additional complexities of the other types of models are handled by auxiliary equations appended to equation 3.1-15. The other models are introduced at appropriate places further on.

3.1.2 Least-Squares Estimation

Because the true parameter set $\underline{\beta}$ and true error set $\underline{\epsilon}$ are generally unknown, the true model equation 3.1-15 must be regarded as unknown, even though the form of the model is known (or, at least assumed). We do, however, have measurements to make up the independent variable set $\underline{\xi}$ and observation set $\underline{Y}$. We would like to use these measurements and the form of the model to obtain estimates of $\underline{\beta}$ and $\underline{\epsilon}$. The method explained in the following paragraphs is based on the idea that, if estimates of $\underline{\beta}$ and $\underline{\epsilon}$ can be found such that the error structure of the true model is duplicated as closely as possible, then the resulting model should, in some sense, be the best possible approximation of the true model.

Assume that all ϵ_i $(i=1,2,\ldots,n)$ as random variables have finite common variance σ^2 and that ϵ_i and ϵ_j, $i \neq j$, are uncorrelated. Then

$$\mathrm{Var}(\underline{\epsilon}) = \underline{I}\sigma^2 \quad . \quad (3.1\text{-}18)$$

The scalar variance σ^2 can be solved for by taking the trace of both sides of equation 3.1-18:

$$\mathrm{tr}[\mathrm{Var}(\underline{\epsilon})] = \mathrm{tr}(\underline{I})\sigma^2$$

or

$$\mathrm{tr}[E((\underline{\epsilon}-E(\underline{\epsilon}))(\underline{\epsilon}-E(\underline{\epsilon}))^T)] = n\sigma^2$$

or

$$E[(\underline{\epsilon}-E(\underline{\epsilon}))^T(\underline{\epsilon}-E(\underline{\epsilon}))] = n\sigma^2$$

from which

$$\sigma^2 = \frac{E[(\underline{\epsilon}-E(\underline{\epsilon}))^T(\underline{\epsilon}-E(\underline{\epsilon}))]}{n} \quad . \quad (3.1\text{-}19)$$

Ordinarily the assumptions would be made that the model being used is the correct one and that no other source of bias in $\underline{\epsilon}$ exists, so that $E(\underline{\epsilon}) = \underline{0}$ and

$$\sigma^2 = \frac{E(\underline{\epsilon}^T\underline{\epsilon})}{n} \quad . \quad (3.1\text{-}20)$$

Equation 3.1-20 indicates that the sum of squared disturbances over all observations, averaged over many sets of observations, divided by n yields σ^2.

As indicated previously, the investigator only has available the data and the form of the model, so that $\underline{\epsilon}$, σ^2, and $\underline{\beta}$ must all be considered as unknowns. However, a good approximation of the true model would produce estimates of $\underline{\epsilon}$ that, for many observations, would yield a variance approaching σ^2. Let $\underline{b}$ be an estimator of $\underline{\beta}$. Then a linear model incorporating $\underline{b}$ is

$$\underline{Y} = \underline{X}\underline{b} + \underline{e} \quad (3.1\text{-}21)$$

where the vector $\underline{e}$ is an estimate of $\underline{\epsilon}$ called the residual vector. From equations 3.1-20 and 3.1-21, an estimate of σ^2 is

$$\tilde{\sigma}^2 = \frac{\underline{e}^T\underline{e}}{n} \quad (3.1\text{-}22)$$

Most arbitrary parameter sets are expected to yield values of $\tilde{s}^2$ that are larger than σ^2 because they would yield models that do not fit the data well. Of all possible parameter sets $\underline{b}$, the one that fits the data the best and at the same time minimizes $\tilde{s}^2$ is the set that minimizes the sum of squares function $S(\underline{b})$,

$$S(\underline{b})=\underline{e}^T\underline{e} \qquad (3.1\text{-}23)$$

with respect to $\underline{b}$. The process of finding estimates of σ^2 and $\underline{\beta}$ by minimizing $S(\underline{b})$ is termed least squares estimation. It is developed fully in sections 3.2 and 3.3.

Recall that equation 3.1-18 and, hence, equations 3.1-22 and 3.1-23 assume that the ϵ_i all come from the same distribution having variance σ^2 and that ϵ_i and ϵ_j, $i\neq j$, are uncorrelated. In some instances ϵ_i and ϵ_j have different variances, say σ_i^2 and σ_j^2, and they may even be correlated so that they have nonzero covariance σ_{ij}. In this case, equation 3.1-18 must be written in the more general form

$$\text{Var}(\underline{\epsilon})=\underline{\underline{V}}\sigma^2 \qquad (3.1\text{-}24)$$

where $\underline{\underline{V}}\sigma^2$ is a symmetric, positive definite variance-covariance matrix defined as

$$\underline{\underline{V}}\sigma^2=\begin{bmatrix}\sigma_1^2 & \sigma_{12} & \sigma_{13} & \cdots & \sigma_{1n}\\ \sigma_{21} & \sigma_2^2 & \sigma_{23} & \cdots & \sigma_{2n}\\ & & \cdots & & \\ \sigma_{n1} & \sigma_{n2} & \sigma_{n3} & \cdots & \sigma_n^2\end{bmatrix}. \qquad (3.1\text{-}25)$$

In equation 3.1-24, σ^2 is no longer the common variance of all ϵ_i but is instead another type of common variance. Its exact meaning can be discerned as follows. Define $\underline{\underline{V}}^{1/2}$ as the nonsingular symmetric matrix such that $\underline{\underline{V}}^{1/2}\underline{\underline{V}}^{1/2}=\underline{\underline{V}}$. Then, from equation 3.1-24,

$$\underline{\underline{V}}^{-1/2}\,\text{Var}(\underline{\epsilon})\underline{\underline{V}}^{-1/2}=\underline{\underline{V}}^{-1/2}\underline{\underline{V}}\underline{\underline{V}}^{-1/2}\sigma^2$$

or

$$\text{Var}(\underline{\underline{V}}^{-1/2}\underline{\epsilon})=\underline{\underline{I}}\sigma^2 \qquad (3.1\text{-}26)$$

from which σ^2 is seen to be the constant or common variance of the transformed disturbances $\underline{\underline{V}}^{-1/2}\underline{\epsilon}$. Equation 3.1-26 shows that these disturbances are uncorrelated.

The more general conditions represented by equation 3.1-24 may easily be incorporated into the least squares procedure. All developments through equation 3.1-20 are repeated using $\underline{\underline{V}}^{-1/2}\underline{\epsilon}$ instead of $\underline{\epsilon}$. The result is

$$\sigma^2=\frac{E[(\underline{\underline{V}}^{-1/2}\underline{\epsilon})^T(\underline{\underline{V}}^{-1/2}\underline{\epsilon})]}{n}$$

$$=\frac{E(\underline{\epsilon}^T\underline{\underline{V}}^{-1}\underline{\epsilon})}{n} \qquad (3.1\text{-}27)$$

which suggests that

$$S(\underline{b})=\underline{e}^T\underline{\underline{V}}^{-1}\underline{e} \qquad (3.1\text{-}28)$$

be minimized instead of equation 3.1-23.

If equation 3.1-23 is minimized to find the parameter estimates when the more general error structure given by equation 3.1-24 is correct, then the incorrect error structure will be reflected in parameter estimates that are less precise than if equation 3.1-28 were used. The proper sum of squares function to minimize when equation 3.1-24 represents the correct error structure is equation 3.1-28.

Even more general cases can be postulated to yield $S(\underline{b})$ in the form

$$S(\underline{b})=\underline{e}^T\underline{\underline{\omega}}\underline{e} \qquad (3.1\text{-}29)$$

where $\underline{\underline{\omega}}$ is a general symmetric positive definite weight matrix that subsumes $\underline{\underline{V}}^{-1}$. To apply equation 3.1-29, $\underline{\underline{\omega}}$ does not necessarily reflect the error structure of $\underline{\epsilon}$. Instead it may reflect the investigator's desire to emphasize (or deemphasize) certain components of $S(\underline{b})$. Equation 3.1-29 is used in all developments to follow in which the general form is applicable.

As a final note, least-squares estimation should be viewed as more than simply a parameter estimation procedure. The development given in this section is intended to show that the procedure is an attempt to reproduce the true model structure: the variance, σ^2, the distribution of $\underline{\epsilon}$, and $\underline{\beta}$. Although it is possible to use least-squares estimation as just an algebraic process, making no assumptions

about structure, considerably more information can be gained by taking the more general approach to make model analysis, including analysis of assumptions initially made concerning model structure, an integral part of the regression process.

3.1.3 Inclusion of Prior Information

The model structure given by equation 3.1-15 is general. Nothing is implied about the nature of $\underline{Y}$ except that it is a dependent variable vector, in error by the amount $\underline{\epsilon}$. A very general interpretation of equation 3.1-15 is to assume that $\underline{Y}$, $\underline{f}$, and $\underline{\epsilon}$ are each composed of two partitions, one giving sample information and one giving prior information on parameters. This viewpoint amounts to an expansion of the original formulation given in the previous section where only sample information was considered (Theil, 1963).

For example, suppose that an investigator collects data (ξ, Y) on a process for which the model equation is given by equation 3.1-2. However, suppose that he or she also has developed methods to collect some data directly on parameters β_1 and β_3 and suppose that these data can be represented by the equations

$$\left.\begin{aligned} P_1 &= a_{11}\beta_1 + u_1 \\ P_2 &= a_{21}\beta_1 + a_{23}\beta_3 + u_2 \end{aligned}\right\} \qquad (3.1\text{-}30)$$

where a_{ij} is a constant and u_i is a random error. If $a_{11}=1$, then P_1 is a direct observation, subject to error u_1, of β_1. The entire set of equations representing the system, then, can be written

$$\left.\begin{aligned} Y_1 &= \beta_1 + \xi_1\beta_2 + \xi_1^2\beta_3 + \epsilon_1 \\ Y_2 &= \beta_1 + \xi_2\beta_2 + \xi_2^2\beta_3 + \epsilon_2 \\ &\cdots \\ Y_n &= \beta_1 + \xi_n\beta_2 + \xi_n^2\beta_3 + \epsilon_n \\ P_1 &= a_{11}\beta_1 + u_1 \\ P_2 &= a_{21}\beta_1 + a_{23}\beta_3 + u_2 \end{aligned}\right\} . \qquad (3.1\text{-}31)$$

If $\underline{Y}$, $\underline{X}$, and $\underline{\epsilon}$ are augmented to include the prior information, then equation 3.1-31 is of the form 3.1-8 where

$$\underline{Y} = \begin{bmatrix} Y_1 \\ Y_2 \\ \cdots \\ Y_n \\ P_1 \\ P_2 \end{bmatrix} \qquad \underline{\epsilon} = \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \cdots \\ \epsilon_n \\ u_1 \\ u_2 \end{bmatrix}$$

$$\underline{X} = \begin{bmatrix} 1 & \xi_1 & \xi_1^2 \\ 1 & \xi_2 & \xi_2^2 \\ & \cdots & \\ 1 & \xi_n & \xi_n^2 \\ a_{11} & 0 & 0 \\ a_{21} & 0 & a_{23} \end{bmatrix} .$$

Note that the number of observations is now the number of equations giving sample information (n) plus the number of equations giving prior information (2).

Although the equations giving prior information are often linear, they do not need to be. Hence, a general form of equation 3.1-15 to include the prior information may be assumed:

$$\underline{Y} = \underline{f}(\underline{\xi}, \underline{\beta}) + \underline{\epsilon} \qquad (3.1\text{-}32)$$

where

$$\underline{Y} = \begin{bmatrix} \underline{Y}_s \\ \underline{Y}_p \end{bmatrix} \qquad \underline{f} = \begin{bmatrix} \underline{f}_s \\ \underline{f}_p \end{bmatrix} \qquad \underline{\epsilon} = \begin{bmatrix} \underline{\epsilon}_s \\ \underline{\epsilon}_p \end{bmatrix} \qquad (3.1\text{-}33)$$

and subscripts s and p indicate partitions of the respective vectors pertaining to sample and prior information, respectively. Corresponding to these partitions, it is convenient to redefine n as the total number of observations, $n=n_s+n_p$, where n_s is the number of items (or equations) of sample information and n_p is the number of items (or equations) of prior information.

To apply the least squares procedure to equation 3.1-15 as augmented by the prior information, it is assumed for now that

$$\mathrm{Var}(\underline{\epsilon}_s) = \underline{V}_s\sigma^2 \qquad (3.1\text{-}34)$$

$$\mathrm{Var}(\underline{\epsilon}_p) = \underline{V}_p\sigma^2 \qquad (3.1\text{-}35)$$

$$\text{Cov}(\underline{\epsilon}_s, \underline{\epsilon}_p)=\underline{0} \qquad (3.1\text{-}36)$$

where $\underline{\underline{V}}_s$ is symmetric, positive definite and of order n_s, and $\underline{\underline{V}}_p$ is symmetric, positive definite and of order n_p. Equation 3.1-36 indicates that sample disturbances $\underline{\epsilon}_s$ and prior information disturbances $\underline{\epsilon}_p$ are not correlated with each other. With use of equations 3.1-34 through 3.1-36, equation 3.1-24 becomes

$$\text{Var}\begin{bmatrix}\underline{\epsilon}_s\\ \underline{\epsilon}_p\end{bmatrix}=\begin{bmatrix}\text{Var}(\underline{\epsilon}_s) & \underline{0}\\ \underline{0} & \text{Var}(\underline{\epsilon}_p)\end{bmatrix}$$

$$=\sigma^2\begin{bmatrix}\underline{\underline{V}}_s & \underline{0}\\ \underline{0} & \underline{\underline{V}}_p\end{bmatrix}$$

$$=\underline{\underline{V}}\sigma^2 \qquad . \qquad (3.1\text{-}37)$$

With use of equation 3.1-37, 3.1-28 becomes

$$S(\underline{b})=\underline{e}^T\underline{\underline{V}}^{-1}\underline{e}$$

$$=\begin{bmatrix}\underline{e}_s^T, & \underline{e}_p^T\end{bmatrix}\begin{bmatrix}\underline{\underline{V}}_s^{-1} & \underline{0}\\ \underline{0} & \underline{\underline{V}}_p^{-1}\end{bmatrix}\begin{bmatrix}\underline{e}_s\\ \underline{e}_p\end{bmatrix}$$

$$=\underline{e}_s^T\underline{\underline{V}}_s^{-1}\underline{e}_s+\underline{e}_p^T\underline{\underline{V}}_p^{-1}\underline{e}_p \qquad (3.1\text{-}38)$$

where the residual vector is defined as

$$\underline{e}=\begin{bmatrix}\underline{e}_s\\ \underline{e}_p\end{bmatrix} \qquad (3.1\text{-}39)$$

and

$$\underline{\underline{V}}^{-1}=\begin{bmatrix}\underline{\underline{V}}_s^{-1} & \underline{0}\\ \underline{0} & \underline{\underline{V}}_p^{-1}\end{bmatrix}. \qquad (3.1\text{-}40)$$

The least-squares procedure may be generalized even further by using equation 3.1-29 instead of equation 3.1-28 to define $S(\underline{b})$. In this case the weight matrix $\underline{\underline{\omega}}$ is defined by

$$\underline{\underline{\omega}}=\begin{bmatrix}\underline{\underline{\omega}}_s & \underline{0}\\ \underline{0} & \underline{\underline{\omega}}_p\end{bmatrix} \qquad (3.1\text{-}41)$$

where $\underline{\underline{\omega}}_s$ is a symmetric positive definite submatrix of order n_s that pertains to the sample information and $\underline{\underline{\omega}}_p$ is a symmetric positive definite submatrix of order n_p that pertains to the prior information. Because equation 3.1-41 is of block diagonal form like equation 3.1-37, zero correlation of sample and prior information is again assumed. Thus, $S(\underline{b})$ may be written in the same form as equation 3.1-38, or as

$$S(\underline{b})=\underline{e}_s^T\underline{\underline{\omega}}_s\underline{e}_s+\underline{e}_p^T\underline{\underline{\omega}}_p\underline{e}_p \qquad . \qquad (3.1\text{-}42)$$

Problem 3.1-1

You are charged with a ground-water study in the vicinity of Lake Ohpupu (figure 1). Estimates of transmissivity and recharge for the confined aquifer surrounding the lake are necessary for the completion of your report. Taking advantage of the unusually colinear equipotential contours on the west side of the lake (constructed from an unbiased source, of course), you decide that estimates based on a uniform stream tube will suffice. Recharge to the aquifer is largely from precipitation and is uniform over the region. Assume that the boundary heads at the range front and the lake are imprecisely known; estimates of these parameters will also be necessary. Your project has limited funds to bore n_s holes along the stream tube and obtain measurements of head at n_s locations of distance, s, from the range front.

The steady-state flow equation for a stream tube is

$$\frac{d}{ds}\left(TD\frac{dh}{ds}\right)+WD=0 \qquad (1)$$

where

T=transmissivity (ft^2/d);
W=recharge (ft/d);
D=width of stream tube (ft);
h=hydraulic head (ft); and
s=distance along tube from the range front (ft).

The boundary conditions are taken to be

$$\left.\begin{aligned}h&=h_0 \text{ at } s=0\\ h&=h_b \text{ at } s=s_b\end{aligned}\right\} \qquad . \qquad (2)$$

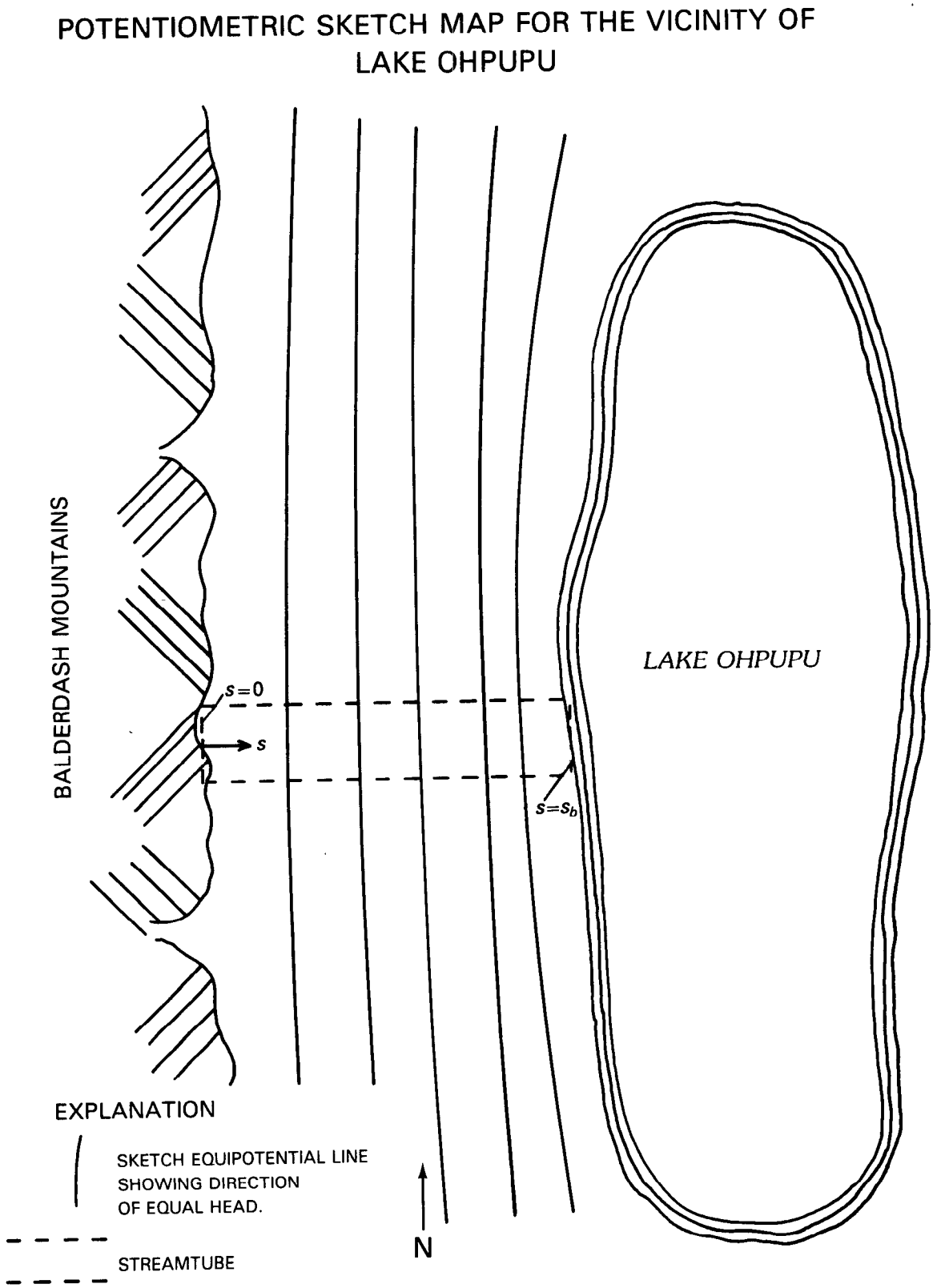
POTENTIOMETRIC SKETCH MAP FOR THE VICINITY OF LAKE OHPUPU
BALDERDASH MOUNTAINS
LAKE OHPUPU
s=0
s
s=s_b
EXPLANATION
SKETCH EQUIPOTENTIAL LINE SHOWING DIRECTION OF EQUAL HEAD.
STREAMTUBE
N

Figure 1

By integrating the flow equation twice with respect to s (assuming T, D, and W to be constant) and using the above boundary conditions, the solution for hydraulic head h along the stream tube is found to be:

$$h=\frac{W}{2T}(s_b-s)s+h_b\frac{s}{s_b}+h_o\left(\frac{s_b-s}{s_b}\right). \qquad (3)$$

Let

$$\left.\begin{array}{lll}\beta_1=h_o & \beta_3=W/T & X_2=\dfrac{s}{s_b}\\ \beta_2=h_b & X_1=\dfrac{s_b-s}{s_b} & X_3=\dfrac{(s_b-s)s}{2}\end{array}\right\} \qquad (4)$$

and write the above solution (equation 3) to the flow equation using the definitions of β_i and X_i (i=1,2,3). Then write the system of n_s linear regression equations in the three unknown parameters using matrix notation and indicate the contents of each matrix. Identify dependent variable(s), independent variable(s), sensitivities, and parameters.

Let b_i be an estimate of β_i, and:

a. Assume that $\mathrm{Var}(\underline{\epsilon})=\underline{I}\sigma^2$. Write $S(\underline{b})$ using the matrix form of the model equation 3.1-21 with the estimated parameters b_i. Write a few terms of $S(\underline{b})$ using algebraic notation.

b. Assume that a unique estimate of the variance of the error associated with every head observation is available and that these errors are uncorrelated. Indicate the contents of the resulting weight matrix $\underline{\omega}=\underline{V}^{-1}$. Write $S(\underline{b})$ using the matrix form of the model equation with parameters b_i. Write a few terms of $S(\underline{b})$ using weights ω_{jj} and algebraic notation.

c. Assume case a above, except that there is a prior estimate of h_b having a standard deviation of σ_{h_b}. Indicate the contents of the resulting weight matrix $\underline{\omega}=\underline{V}^{-1}$. Write $S(\underline{b})$ using the matrix form of the model equation with parameters b_i. Write a few terms of $S(\underline{b})$ using algebraic notation. Include the term involving the prior information.

3.2 Regression When the Model is Linear

3.2.1 Derivation of Solution

The linear model assumed is

$$Y=X_1\beta_1+X_2\beta_2+\ldots+X_p\beta_p+\epsilon \qquad (3.2\text{-}1)$$

where the X_i are not functions of the parameters. If n observations are used, then an equation of the form of equation 3.2-1 is written for each observation, so that the system can be written in matrix form as

$$\underline{Y}=\underline{X}\underline{\beta}+\underline{\epsilon}\ . \qquad (3.2\text{-}2)$$

To find estimates of $\underline{\beta}$ and $\underline{\epsilon}$, the weighted error sum of squares $S(\underline{b})$,

$$\begin{aligned}S(\underline{b})&=\underline{e}^T\underline{\omega}\underline{e}\\&=(\underline{Y}-\underline{X}\underline{b})^T\underline{\omega}(\underline{Y}-\underline{X}\underline{b})\end{aligned} \qquad (3.2\text{-}3)$$

is minimized with respect to $\underline{b}$.

To minimize $S(\underline{b})$ with respect to $\underline{b}$ means to take the derivative of $S(\underline{b})$ with respect to each element of $\underline{b}$, b_j (j=1,2,...,p), and set the results to zero, or

$$\begin{aligned}\frac{\partial}{\partial b_j}S(\underline{b})\Big|_{\underline{b}=\hat{\underline{b}}}&=\frac{\partial}{\partial b_j}[(\underline{Y}-\underline{X}\underline{b})^T\underline{\omega}(\underline{Y}-\underline{X}\underline{b})]\Big|_{\underline{b}=\hat{\underline{b}}}\\&=0,\ j=1,2,\ldots,p,\end{aligned} \qquad (3.2\text{-}4)$$

where $|_{\underline{b}=\hat{\underline{b}}}$ signifies that $\hat{\underline{b}}$ is the set of parameters that causes the derivatives of $S(\underline{b})$ to be zero. By employing the rule of differentiating a product and noting that $\underline{\omega}$ is independent of $\underline{b}$, it can be seen that

$$\begin{aligned}\frac{\partial}{\partial b_j}[(\underline{Y}-\underline{X}\underline{b})^T\underline{\omega}(\underline{Y}-\underline{X}\underline{b})]&=[\frac{\partial}{\partial b_j}(\underline{Y}-\underline{X}\underline{b})^T]\underline{\omega}(\underline{Y}-\underline{X}\underline{b})\\&+(\underline{Y}-\underline{X}\underline{b})^T\underline{\omega}\frac{\partial}{\partial b_j}(\underline{Y}-\underline{X}\underline{b}).\end{aligned} \qquad (3.2\text{-}5)$$

To evaluate $\frac{\partial}{\partial b_j}(\underline{Y}-\underline{X}\underline{b})^T$, note that taking the derivative of a vector, $\underline{Y}-\underline{X}\underline{b}$, with respect to a scalar, b_j, means taking the derivative of each

entry of the vector and, thus, yields a new vector. Therefore, because observations $\underline{Y}$ are independent of $\underline{b}$,

$$\frac{\partial}{\partial b_j}(\underline{Y}-\underline{X}\underline{b})^T=\frac{\partial}{\partial b_j}\left\{\begin{bmatrix}Y_1\\Y_2\\\vdots\\Y_n\end{bmatrix}-[\underline{X}_1,\underline{X}_2,\ldots,\underline{X}_p]\begin{bmatrix}b_1\\b_2\\\vdots\\b_p\end{bmatrix}\right\}^T$$

$$=-\underline{X}_j^T, \qquad (3.2\text{-}6)$$

where $\underline{X}_j$ is the jth column vector of matrix $\underline{X}$. Also, the first and second terms on the right side of equation 3.2-5 are equal because the transpose of a scalar is the scalar, and $\underline{\omega}$ is symmetric so that $\underline{\omega}=\underline{\omega}^T$. Hence, transposing the second term on the right side of equation 3.2-5 gives

$$(\underline{Y}-\underline{X}\underline{b})^T\underline{\omega}\frac{\partial}{\partial b_j}(\underline{Y}-\underline{X}\underline{b})=[(\underline{Y}-\underline{X}\underline{b})^T\underline{\omega}\frac{\partial}{\partial b_j}(\underline{Y}-\underline{X}\underline{b})]^T$$

$$=[\frac{\partial}{\partial b_j}(\underline{Y}-\underline{X}\underline{b})^T]\underline{\omega}(\underline{Y}-\underline{X}\underline{b}). \qquad (3.2\text{-}7)$$

The combination of equstions 3.2-4 through 3.2-7 yields

$$-2\underline{X}_j^T\underline{\omega}(\underline{Y}-\underline{X}\hat{\underline{b}})=0 \qquad (3.2\text{-}8)$$

or

$$\underline{X}_j^T\underline{\omega}\underline{X}\hat{\underline{b}}=\underline{X}_j^T\underline{\omega}\underline{Y},\ j=1,2,\ldots,p. \qquad (3.2\text{-}9)$$

The system of equations implied by equation 3.2-9 can be written as

$$\begin{bmatrix}\underline{X}_1^T\\\underline{X}_2^T\\\vdots\\\underline{X}_p^T\end{bmatrix}\underline{\omega}\underline{X}\hat{\underline{b}}=\begin{bmatrix}\underline{X}_1^T\\\underline{X}_2^T\\\vdots\\\underline{X}_p^T\end{bmatrix}\underline{\omega}\underline{Y}. \qquad (3.2\text{-}10)$$

Each vector $\underline{X}_j^T$ in equation 3.2-10 is a row vector, so that, by definition,

$$\begin{bmatrix}\underline{X}_1^T\\\underline{X}_2^T\\\vdots\\\underline{X}_p^T\end{bmatrix}=\underline{X}^T \qquad (3.2\text{-}11)$$

and equation 3.2-10 becomes

$$\underline{X}^T\underline{\omega}\underline{X}\hat{\underline{b}}=\underline{X}^T\underline{\omega}\underline{Y}. \qquad (3.2\text{-}12)$$

The set of equations symbolized in matrix form by equation 3.2-12 are called the normal equations, and parameters $\hat{\underline{b}}$ are called the estimates of β. The estimates are found from

$$\hat{\underline{b}}=(\underline{X}^T\underline{\omega}\underline{X})^{-1}\underline{X}^T\underline{\omega}\underline{Y}. \qquad (3.2\text{-}13)$$

Students not comfortable with the preceding development should read Draper and Smith (1981, p. 5-17, 70-80, 85-87). This material covers fitting a straight line without and with matrix nomenclature, and then extends the results to the general linear situation. Weighted least squares (where $\underline{\omega}\neq\underline{I}$) is covered in Draper and Smith (1981, p. 108-116).

Elements of $\underline{X}$ are often of vastly differing magnitudes. Thus, when working with a calculator or computer, round-off error can cause serious errors to develop when solving equation 3.2-13. It is often useful to scale equation 3.2-12 with respect to a matrix $\underline{C}$, which is a diagonal matrix defined as follows: Let $\underline{X}^T\underline{\omega}\underline{X}=\underline{A}$. Then $\underline{C}=\text{diag}\{1/A_{11}^{1/2},1/A_{22}^{1/2},\ldots,1/A_{pp}^{1/2}\}$, where A_{ii} is a diagonal entry of $\underline{A}$. Thus, equation 3.2-12 can be transformed to become

$$\underline{C}^T\underline{X}^T\underline{\omega}\underline{X}\underline{C}\underline{C}^{-1}\hat{\underline{b}}=\underline{C}^T\underline{X}^T\underline{\omega}\underline{Y} \qquad (3.2\text{-}14)$$

or

$$\underline{S}^T\underline{\omega}\underline{S}\hat{\underline{a}}=\underline{S}^T\underline{\omega}\underline{Y} \qquad (3.2\text{-}15)$$

where

$$\underline{S}=\underline{X}\underline{C} \qquad (3.2\text{-}16)$$

$$\hat{\underline{a}}=\underline{C}^{-1}\hat{\underline{b}}. \qquad (3.2\text{-}17)$$

The effect of the scaling is to preserve the symmetry of $\underline{X}^T\underline{\omega}\underline{X}$ while at the same time to produce a matrix having all diagonal entries equal to unity. Thus, variability from entry to entry of the $\underline{S}^T\underline{\omega}\underline{S}$ matrix is usually reduced considerably over that of $\underline{X}^T\underline{\omega}\underline{X}$.

It is also sometimes useful to transform equation 3.2-2 and equation 3.2-12 to incremental form. By definition

$$\underline{f}(\underline{\xi},\underline{b})=\underline{X}\underline{b} \quad . \tag{3.2-18}$$

Then, subtracting equation 3.2-18 from equation 3.2-2 results in

$$\underline{Y}-\underline{f}(\underline{\xi},\underline{b})=\underline{X}(\underline{\beta}-\underline{b})+\underline{\epsilon} \tag{3.2-19}$$

which is an incremental linear model. To obtain the analog to equation 3.2-12, premultiply equation 3.2-18 by $\underline{X}^T\underline{\omega}$ and subtract the result from equation 3.2-12 to obtain

$$\underline{X}^T\underline{\omega}\underline{X}(\hat{\underline{b}}-\underline{b})=\underline{X}^T\underline{\omega}(\underline{Y}-\underline{f}(\underline{\xi},\underline{b})) \quad . \tag{3.2-20}$$

Equation 3.2-20 can be transformed to obtain a result analogous to equation 3.2-15:

$$\underline{S}^T\underline{\omega}\underline{S}\hat{\underline{\delta}}=\underline{S}^T\underline{\omega}(\underline{Y}-\underline{f}(\underline{\xi},\underline{b})) \tag{3.2-21}$$

where

$$\hat{\underline{\delta}}=\underline{C}^{-1}(\hat{\underline{b}}-\underline{b}) \quad . \tag{3.2-22}$$

If $\hat{\underline{b}}$ as calculated initially using equations 3.2-15 and 3.2-17 is in error because of round-off, then $\hat{\underline{b}}$ can be used to calculate $\underline{f}(\underline{\xi},\hat{\underline{b}})$ which then can be substituted into equation 3.2-21 to calculate $\hat{\underline{\delta}}$. By using equation 3.2-22, a new improved estimate of $\hat{\underline{b}}$ can be obtained. Writing equation 3.2-2 in incremental form also provides a basis for procedures, involving statistical analysis of the model, that apply for both linear and (with restrictions) nonlinear models. These are discussed later on.

3.2.2 Solution Algorithm

Sequential steps to follow are:

1. Form $\underline{X}^T\underline{\omega}\underline{X}$ and $\underline{X}^T\underline{\omega}\underline{Y}$.
2. Transform equation 3.2-12 to 3.2-15.
3. Solve equation 3.2-15 (or 3.2-21) for $\hat{\underline{a}}$.
4. Solve equation 3.2-17 for $\hat{\underline{b}}$.

Problem 3.2-1

a. By using $\underline{\omega}$ from case c, problem 3.1-1, write out the normal equations used to estimate parameters $\underline{\beta}$ explicitly in sum-of-product (algebraic) form. (Use equation 3.2-12.)

b. By using either data set 1 (table 1) or 2 (table 2), generate the least squares coefficient matrix ($\underline{X}^T\underline{\omega}\underline{X}$) and then compute its inverse. Do not round off any intermediate calculations or the final inverse. To aid in the calculations, table 3 gives the sums of products for the sample information from the two data sets. You must add the prior information to complete the sums of products.

c. Find the vector $\hat{\underline{b}}$. Do not round off the results.

Table 1.—Data set 1

s_j (ft)	X_{j1}	X_{j2}	X_{j3}	Observed head, Y_j (ft)
50	0.95	0.05	23,750	48.33
150	.85	.15	63,750	45.76
250	.75	.25	93,750	42.08
350	.65	.35	113,750	38.34
450	.55	.45	123,750	35.30
550	.45	.55	123,750	31.00
650	.35	.65	113,750	25.85
750	.25	.75	93,750	21.76
850	.15	.85	63,750	16.11
950	.05	.95	23,750	12.48

Assume $\sigma^2=0.25$ ft^2, $s_b=1{,}000$ ft, and prior information as follows: $h_b=11$ ft and $\sigma_{h_b}=1.1$ ft.

Table 2.—Data set 2

s_j (ft)	X_{j1}	X_{j2}	X_{j3}	Observed head, Y_j (ft)
100	0.9	0.1	45,000	47.13
200	.8	.2	80,000	44.14
300	.7	.3	105,000	39.89
400	.6	.4	120,000	36.36
500	.5	.5	125,000	32.48
600	.4	.6	120,000	29.70
700	.3	.7	105,000	24.33
800	.2	.8	80,000	19.10
900	.1	.9	45,000	14.96

Assume $\sigma^2=0.25$ ft^2, $s_b=1{,}000$ ft, and prior information as follows: $h_b=9.5$ ft and $\sigma_{h_b}=0.95$ ft.

Table 3.—Sums of products of sample information

	Data Set 1	Data Set 2
$\sum_j X_{j1}X_{j1}$	3.3250	2.8500
$\sum_j X_{j1}X_{j2}$	1.6750	1.6500
$\sum_j X_{j1}X_{j3}$	418,750	412,500
$\sum_j X_{j2}X_{j2}$	3.3250	2.8500
$\sum_j X_{j2}X_{j3}$	418,750	412,500
$\sum_j X_{j3}X_{j3}$	83,340,625,000	83,325,000,000
$\sum_j X_{j1}Y_j$	192.18350	168.2030
$\sum_j X_{j2}Y_j$	124.82650	119.8870
$\sum_j X_{j3}Y_j$	26,879,687.5	26,583,550

3.2.3 Singularity and Conditioning

Singularity of the least-squares coefficient matrix occurs whenever columns of the sensitivity matrix, $\underline{X}$, are linearly dependent because this causes rows (or columns) of the coefficient matrix $\underline{X}^T\underline{\omega}\underline{X}$ to be linearly dependent. Linear dependence in $\underline{X}$ may be stated as

$$\underline{X}\underline{c}=\underline{0} \qquad (3.2\text{-}23)$$

where not all components of the vector $\underline{c}$ of order p are zero. By premultiplying equation 3.2-23 by $\underline{X}^T\underline{\omega}$,

$$\underline{X}^T\underline{\omega}\underline{X}\underline{c}=\underline{0} \qquad (3.2\text{-}24)$$

which shows that columns of $\underline{X}^T\underline{\omega}\underline{X}$ (or rows since $\underline{X}^T\underline{\omega}\underline{X}$ is symmetric) are linearly dependent. Note that transformation of $\underline{X}^T\underline{\omega}\underline{X}$ to $\underline{S}^T\underline{\omega}\underline{S}$ alters only the form of $\underline{c}$.

Near-singularity, also referred to as ill-conditioning, occurs whenever the columns of $\underline{X}$ (or $\underline{S}$) are almost linearly dependent. Often, this condition is indicated by a high degree of correlation among two or more parameter estimates. This correlation reflects the redundancy in the problem. As a result of ill-conditioning, computed parameters can be affected greatly by accumulation of round-off error generated by solving the normal equations. Also, computed variances of the parameters, which are proportional to the diagonal elements of $(\underline{X}^T\underline{\omega}\underline{X})^{-1}$, will be large.

A common form of ill-conditioning results if a column of $\underline{X}$ approaches zero so that $\underline{c}=[0,0,\ldots,1,0,\ldots,0]^T$, where the one appears in the row corresponding to the zero column in $\underline{X}$. This condition indicates that the model is insensitive to the parameter corresponding to the zero column in $\underline{X}$ and that the parameter should be eliminated from the model. The problem is readily detected by examining the $\underline{X}$ matrix. Another readily detected form of ill-conditioning results if two columns of $\underline{X}$ are nearly proportional, or

$$\alpha\underline{X}_i \cong \underline{X}_j \qquad (3.2\text{-}25)$$

so that $\underline{c}=[0,0,\ldots,\alpha,0,\ldots,-1,0,\ldots,0]^T$, where α appears in row i and -1 appears in row j of $\underline{c}$. In this case

$$\underline{X}_j^T\underline{\omega}\underline{X}_j \cong \alpha\underline{X}_i^T\underline{\omega}\underline{X}_j$$

$$\cong \frac{1}{\alpha}\underline{X}_j^T\underline{\omega}\underline{X}_j$$

so that

$$\underline{S}_i^T\underline{\omega}\underline{S}_j = \frac{\underline{X}_i^T\underline{\omega}\underline{X}_j}{\sqrt{(\underline{X}_i^T\underline{\omega}\underline{X}_i)(\underline{X}_j^T\underline{\omega}\underline{X}_j)}}$$

$$\cong \pm 1 \qquad . \qquad (3.2\text{-}26)$$

Thus, to detect this problem, one need only examine the $\underline{S}^T\underline{\omega}\underline{S}$ matrix for an off-diagonal entry nearly equal to ± 1. This type of linear dependence indicates that parameters b_i, and b_j should be combined because the model can be written as

$$Y=X_1b_1+\ldots+X_ib_i+\ldots+X_jb_j+\ldots+X_pb_p$$

$$\cong X_1b_1+\ldots+X_i(b_i+\alpha b_j)+\ldots+X_pb_p$$

$$=X_1b_1+\ldots+X_ib_i^*+\ldots+X_{p-1}b_{p-1} \qquad (3.2\text{-}27)$$

where b_i^* replaces $b_i+\alpha b_j$, and all subsequent variables are shifted by one so that the last variable number is $p-1$.

An excellent way to detect general ill-conditioned (or completely linearly dependent) problems is to orthogonalize the columns of the scaled sensitivity matrix, $\underline{S}$ (Draper and Smith, 1981, p. 275-278). If the columns are all linearly independent, then they can all be transformed

so as to be orthogonal to one another; that is, such that

$$\underline{\underline{Q}}^T\underline{\underline{Q}}=\underline{\underline{D}} \tag{3.2-28}$$

where $\underline{\underline{Q}}$ is the nonzero transformation of $\underline{\underline{S}}$, and $\underline{\underline{D}}$ is a full-rank diagonal matrix. If linear dependence exists in $\underline{\underline{S}}$, then equation 3.2-28 is replaced by a similar diagonal form except that one or more diagonal entries will be zero. The technique is to successively transform columns such that each new column is orthogonal to all of the previously transformed columns. If column dependence exists, then eventually a column will be calculated that exists entirely of very small numbers (theoretically all zeros for a linearly dependent problem). This column, then, is almost (or completely) linearly dependent on one or more of the previous columns.

The transformation procedure is called Gram-Schmidt orthogonalization and takes the following form:

$$\left.\begin{aligned}\underline{Q}_1&=\underline{S}_1\\ \underline{Q}_j&=\underline{S}_j-\sum_{i=1}^{j-1}c_{ij}\underline{Q}_i,\ j=2,3,\ldots,p\end{aligned}\right\} \tag{3.2-29}$$

where

$$c_{ij}=\frac{\underline{Q}_i^T\underline{S}_j}{\underline{Q}_i^T\underline{Q}_i},$$

$\underline{Q}_i$=the transformed vector orthogonal to vectors already in $\underline{\underline{Q}}$,

$\underline{S}_j$=the next column vector of $\underline{\underline{S}}$ to be transformed.

3.3 Regression When the Model is Nonlinear

3.3.1 Modified Gauss-Newton Method

If the model is nonlinear in the parameters but is linear in the dependent variable, then the model may be written in the standard form for nonlinear regression:

$$Y=f(\xi_1,\xi_2,\ldots,\xi_k;\beta_1,\beta_2,\ldots\beta_p)+\epsilon\ . \tag{3.3-1}$$

Because of the nonlinearity, f cannot be written in the form $f=X_1\beta_1+X_2\beta_2+\ldots+X_p\beta_p$. The case more complicated than equation 3.3-1, where the model is nonlinear in both the parameters and the dependent variable, is treated in section 6.1. When there are n observations, equation 3.3-1 may be written in matrix form as

$$\underline{Y}=\underline{f}(\underline{\xi},\underline{\beta})+\underline{\epsilon} \tag{3.3-2}$$

or, in terms of general estimate $\underline{b}$ of $\underline{\beta}$ and estimate $\underline{e}$ of $\underline{\epsilon}$,

$$\underline{Y}=\underline{f}(\underline{\xi},\underline{b})+\underline{e}\ . \tag{3.3-3}$$

As for the linear case, the regression solution of equation 3.3-3 is obtained by minimizing the weighted error sum of squares:

$$\begin{aligned}S(\underline{b})&=\underline{e}^T\underline{\underline{\omega}}\underline{e}\\ &=(\underline{Y}-\underline{f}(\underline{\xi},\underline{b}))^T\underline{\underline{\omega}}(\underline{Y}-\underline{f}(\underline{\xi},\underline{b}))\ .\end{aligned} \tag{3.3-4}$$

However, because equation 3.3-3 is nonlinear, solution of the problem is not as direct as it was for the linear case.

A convenient and robust solution method is obtained by linearizing equation 3.3-3 around an initial estimate of parameters, then proceeding as if the problem were linear. This yields a new set of parameters that minimizes equation 3.3-4 where $\underline{f}$ is replaced by the linear approximation. The new parameters are then substituted for the initial set, and the process is repeated to yield a better set of parameters. The iterative process stops whenever the change in calculated parameters from one iteration to the next is small. At that point the minimum of equation 3.3-4 has been found.

To derive the method, first $\underline{f}(\underline{\xi},\underline{b})$ is expanded about the initial set of parameters $\underline{b}_0$ by using a truncated Taylor series to obtain a linear approximation for $\underline{f}(\underline{\xi},\underline{b})$:

$$\underline{f}(\underline{\xi},\underline{b})\cong\underline{f}(\underline{\xi},\underline{b}_0)+\underline{\underline{X}}_0(\underline{b}-\underline{b}_0) \tag{3.3-5}$$

where

$$\underline{\underline{X}}_0=\{X_{ij}^0\}=\left\{\left.\frac{\partial f_i}{\partial b_j}\right|_{\underline{b}=\underline{b}_0}\right\}(n\times p) \tag{3.3-6}$$

and f_i *is* f calculated at the ith observation point. The components of $\underline{X}_0$ are recognized as sensitivity coefficients, or simply sensitivities.

By using equation 3.3-5, equation 3.3-3 may be written as

$$\underline{Y}-\underline{f}(\underline{\xi},\underline{b}_0) \cong \underline{X}_0(\underline{b}-\underline{b}_0)+\underline{e} \qquad (3.3\text{-}7)$$

which is of the form of the incremental linear model of section 3.2. Note that if the model is linear so that $\underline{f}(\underline{\xi},\underline{b})=\underline{X}(\underline{\xi})\underline{b}$, then the truncated Taylor series and hence equation 3.3-7 are exact. In this case expansion in a Taylor series is another way of deriving the incremental linear model. If the model is nonlinear, equation 3.3-7 is the approximate (linearized) model for parameters in the vicinity of $\underline{b}_0$, as illustrated by a simple one-parameter example in figure 3.3-1.

An approximate best estimate of $\underline{\beta}$ (which is exact for a linear model) can be obtained by minimizing $S(\underline{b})=\underline{e}^T\underline{\omega}\underline{e}\cong(\underline{Y}-\underline{f}(\underline{\xi},\underline{b}_0)-\underline{X}_0(\underline{b}-\underline{b}_0))^T \cdot\underline{\omega}(\underline{Y}-\underline{f}(\underline{\xi},\underline{b}_0)-\underline{X}_0(\underline{b}-\underline{b}_0))$ with respect to $\underline{b}$. This process is carried out exactly like it was for the linear model and yields the set of normal equations

$$\underline{X}_0^T\underline{\omega}\underline{X}_0\underline{d}_1=\underline{X}_0^T\underline{\omega}(\underline{Y}-\underline{f}(\underline{\xi},\underline{b}_0)) \qquad (3.3\text{-}8)$$

where subscript 1 indicates the first approximate solution and

$$\underline{d}_1=\underline{b}_1-\underline{b}_0\,. \qquad (3.3\text{-}9)$$

To reduce round-off error in nonlinear regression, it is generally useful to scale equation

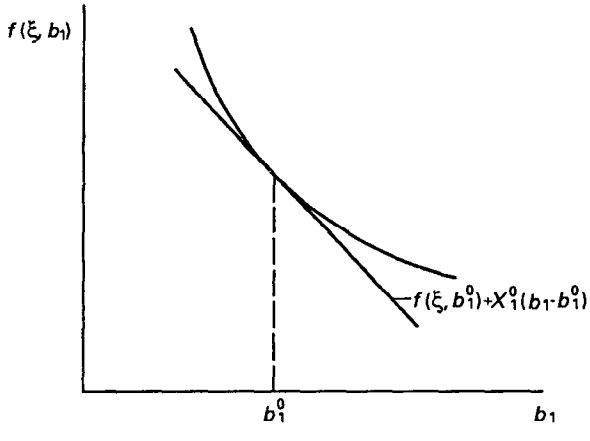

Figure 3.3-1

3.3-8 in the same manner as for linear regression (equations 3.2-14 through 3.2-17), although another type of scaling that is useful for some types of problems is introduced in problem 3.3-1. Scaling equation 3.3-8 produces

$$\underline{S}_0^T\underline{\omega}\underline{S}_0\underline{\delta}_1=\underline{S}_0^T\underline{\omega}(\underline{Y}-\underline{f}(\underline{\xi},\underline{b}_0)) \qquad (3.3\text{-}10)$$

where

$$\underline{S}_0=\underline{X}_0\underline{C}_0 \qquad (3.3\text{-}11)$$

$$\underline{\delta}=\underline{C}_0^{-1}\underline{d}_1 \qquad (3.3\text{-}12)$$

$$\underline{C}_0=\text{diag}\{(A_{11}^0)^{-1/2},(A_{22}^0)^{-1/2},\ldots,(A_{pp}^0)^{-1/2}\} \qquad (3.3\text{-}13)$$

$$\underline{A}_0=\underline{X}_0^T\underline{\omega}\underline{X}_0 \qquad (3.3\text{-}14)$$

and A_{ii}^0 is a diagonal component of $\underline{A}_0$.

Because equation 3.3-8 is not exact, equation 3.3-4 is not truly minimized, and $\underline{b}_1$ is not actually the optimal set. Hence, $\underline{b}_1$ is substituted for $\underline{b}_0$, and the entire process is repeated to yield another, hopefully improved, estimate. As a general iteration equation, 3.3-10 may be written in the form

$$\underline{S}_r^T\underline{\omega}\underline{S}_r\underline{\delta}_{r+1}=\underline{S}_r^T\underline{\omega}(\underline{Y}-\underline{f}(\underline{\xi},\underline{b}_r)) \qquad (3.3\text{-}15)$$

where

$$\underline{S}_r=\underline{X}_r\underline{C}_r \qquad (3.3\text{-}16)$$

$$\underline{\delta}_{r+1}=\underline{C}_r^{-1}(\underline{b}_{r+1}-\underline{b}_r)=\underline{C}_r^{-1}\underline{d}_{r+1} \qquad (3.3\text{-}17)$$

$$\underline{C}_r=\text{diag}\{(A_{11}^r)^{-1/2},(A_{22}^r)^{-1/2},\ldots,(A_{pp}^r)^{-1/2}\} \qquad (3.3\text{-}18)$$

and A_{ii}^r is defined analogously to A_{ii}^0. As the process converges, $\underline{\delta}_{r+1}\rightarrow\underline{0}$ and equation 3.3-7 becomes $\underline{Y}-\underline{f}(\underline{\xi},\hat{\underline{b}})=\hat{\underline{e}}$. At the same point, $\hat{\underline{b}}$ minimizes $S(\underline{b})$ in equation 3.3-4, or $S(\hat{\underline{b}})=(\underline{Y}-\underline{f}(\underline{\xi},\hat{\underline{b}}))^T\underline{\omega}(\underline{Y}-\underline{f}(\underline{\xi},\hat{\underline{b}}))$, which is a minimum for the nonlinear equation. This process for finding the minimum of $S(\underline{b})$ is known as the Gauss-Newton method.

A sketch of progression of the iterations to the minimum for a hypothetical two-parameter problem is given in figure 3.3-2. As diagrammed

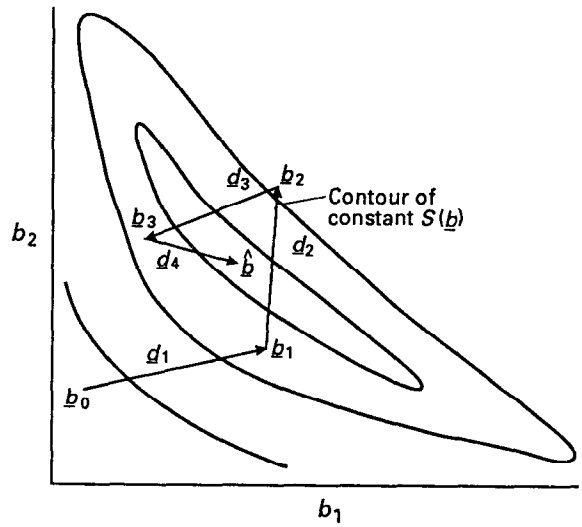

Figure 3.3-2

in figure 3.3-2, the solution often does not progress directly toward the minimum.

Modifications to the Basic Procedure. It is well known that the Gauss-Newton method as defined by equation 3.3-15, does not always converge. To help induce convergence, a damping parameter, ρ, is introduced by modifying equation 3.3-17 to give

$$\underline{b}_{r+1}=\rho\underline{d}_{r+1}+\underline{b}_r \ . \qquad (3.3\text{-}19)$$

where $\underline{d}_{r+1}=\underline{C}_r\underline{\delta}_{r+1}$. If $0<\rho<1$, the changes in computed parameters are less than would result for $\rho=1$; thus the method is an interpolation method. Similarly, if $\rho>1$, the method is an extrapolation method.

Inspection of equation 3.3-19 reveals that ρ changes the magnitude of the displacement from $\underline{b}_r$ to $\underline{b}_{r+1}$. However, because all components of the displacement vector $\underline{d}_{r+1}$ are scaled by the same multiplier ρ, the direction of the displacement vector is not altered. If the displacement vector $\underline{d}_{r+1}$ is oriented in a direction nearly parallel to a contour in the sum of squares surface ($S(\underline{b})$), then little, if any, improvement (in terms of reducing $S(\underline{b})$) can result from solution of equation 3.3-15. In this case it would be desirable to alter the direction of $\underline{d}_{r+1}$ to point closer to a down-gradient direction. For example, in figure 3.3-3 vector $\underline{d}_{r+1}$ yields no improvement in estimates $\underline{b}_r$, but vector $\underline{d}'_{r+1}$ yields a significant improvement in the estimates.

A modification that accomplishes the desired alteration of direction of $\underline{d}_{r+1}$, and reduces its magnitude as well, consists of adding a positive parameter μ, known as the Marquardt parameter (Marquardt, 1963), to the main diagonal of the coefficient matrix $\underline{S}_r^T\underline{\omega}\underline{S}_r$ of equation 3.3-15. Scaling is needed so that μ can have the same effect on each entry of the main diagonal of the coefficient matrix. The scaling accomplishes this effect because each entry of the main diagonal of the scaled matrix $\underline{S}_r^T\underline{\omega}\underline{S}_r$ is unity. Mathematically, the Marquardt modification can be stated as follows.

$$(\underline{S}_r^T\underline{\omega}\underline{S}_r+\mu\underline{I})\underline{\delta}_{r+1}=\underline{S}_r^T\underline{\omega}(\underline{Y}-\underline{f}(\underline{\xi},\underline{b}_r)) \ . \qquad (3.3\text{-}20)$$

Solution Algorithm. The sequential steps implementing the modified Gauss-Newton procedure are:

1. Calculate $\underline{f}(\underline{\xi},\underline{b}_r)$ and $\underline{S}_r$ using initial parameters $\underline{b}_r$ and the combination of equation 3.3-6 (with index r replacing 0) and equation 3.3-16.
2. Solve equation 3.3-20 for $\underline{\delta}_{r+1}$.
3. Solve equation 3.3-17 for $\underline{d}_{r+1}$.
4. Solve equation 3.3-19 for $\underline{b}_{r+1}$.
5. Test to determine if $|d_i^{r+1}/c|>\epsilon$, where ϵ is

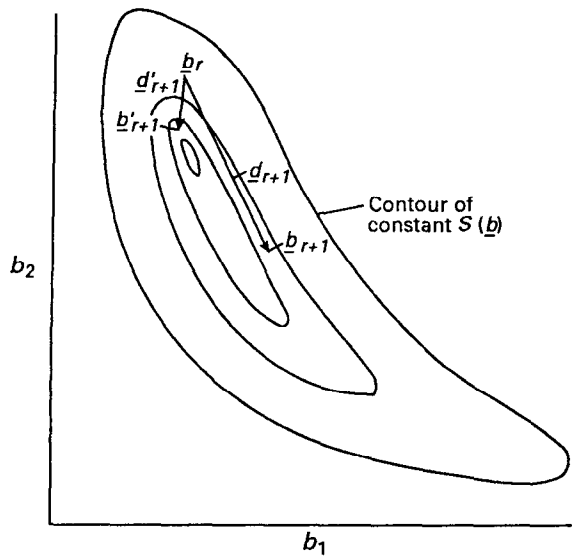

Figure 3.3-3

a small number such as 0.01, $c=b_i^r$ for $b_i^r \neq 0$, and $c=1$ for $b_i^r=0$.

6. If $|d_i^{r+1}/c|>\epsilon$, increment r by one and return to 1. If not, then the process has converged.

Problem 3.3-1

The Theis equation for flow to a well in a confined, nonleaky aquifer is

$$s=\frac{Q}{4\pi T}\int_{r_o^2S/4Tt}^{\infty}\frac{e^{-z}}{z}\,dz \qquad (1)$$

where t=time (d);
s=drawdown (ft);
r_o=radial distance to observation well (ft);
Q=discharge (ft^3/s);
T=transmissivity (ft^2/s); and
S=storage coefficient.

The integral can be evaluated by summing the infinite series

$$\int_u^{\infty}\frac{e^{-z}}{z}\,dz=-0.577216-\ln u+u-\frac{u^2}{2\cdot 2!}+\frac{u^3}{3\cdot 3!}-\frac{u^4}{4\cdot 4!}+\ldots \qquad (2)$$

where $n!=n\cdot(n-1)\cdot(n-2)\ldots 3\cdot 2\cdot 1$.

The Theis equation is nonlinear in the parameters T and S. Using the information in section 3.3.1, develop an algorithm for solving this equation for T and S, given time and drawdown data.

a. Let

$$f(t, r_o; T, S)=\frac{Q}{4\pi T}W(u) \qquad (3)$$

where $u=r_o^2S/4Tt$ and W(u) is the integral in equation 2. Find the sensitivities for T and S. (See equation 3.3-6. Hint:

$$\frac{d}{d\alpha}\int_{u(\alpha)}^{\infty}f(x)dx=-f(u(\alpha))\,\frac{du(\alpha)}{d\alpha}.)$$

b. Assume that initial estimates of transmissivity and storage coefficient, T_0 and S_0, exist. In equation 3.3-6 let $j=T$ indicate the sensitivity for T, and $j=S$ indicate the sensitivity for S. Then note that X_{iT}^0 can be scaled to become $Z_{iT}^0=X_{iT}^0T_0$, and X_{iS}^0 can be scaled to become $Z_{iS}^0=X_{iS}^0S_0$. Modify the functions for X_{iT}^0 and X_{iS}^0 computed in step a to become the scaled functions Z_{iT}^0 and Z_{iS}^0. Do you see any resulting simplifications in arithmetic? Do you think that the scaled sensitivities Z_{iT}^0 and Z_{iS}^0 might be more nearly uniform in value for any fixed i than X_{iT}^0 and X_{iS}^0? What do you think this uniformity in value accomplishes?

c. Construct, for n time observations at a single spatial location, the incremental linear model (equation 3.3-7). Then transform this model so that scaled sensitivities Z_{iT} and Z_{iS} are used instead of X_{iT} and X_{iS}. How does the parameter displacement vector $\underline{d}$ transform? How can you recover $\underline{d}$ from the transformed displacement vector? (Hint: equations 3.3-10 through 3.3-14 are analogous to the present scaling problem.)

Figure 1 is a flow diagram for programming the steps indicated in section 3.3.1. Obtain a coding sheet and proceed to write code according to this flow diagram. Helpful hints, numbered on the flow diagram, follow:

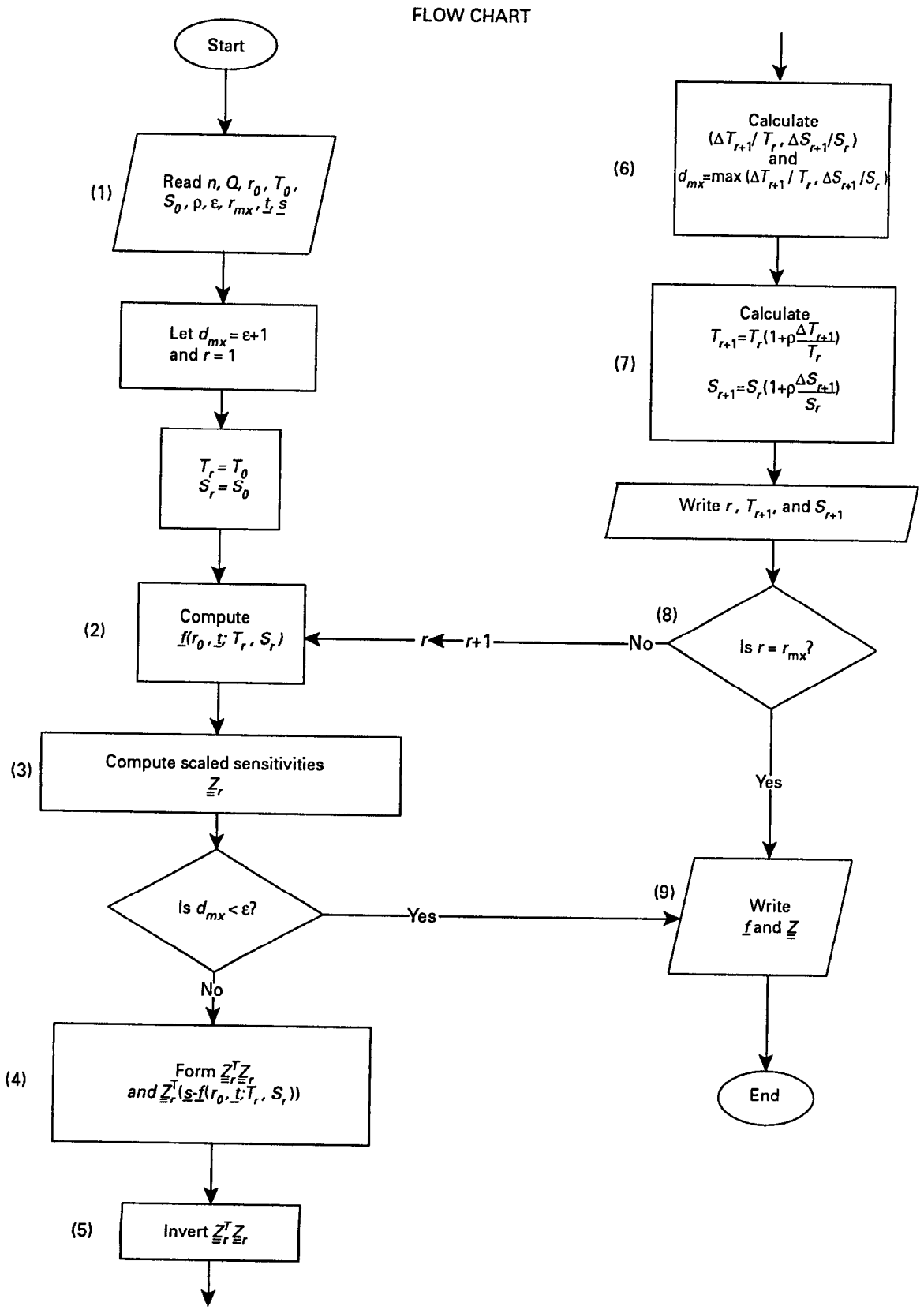
FLOW CHART
Start
(1)
Read n, Q, r_0, T_0, S_0, ρ, ε, r_{mx}, $\underline{t}$, $\underline{s}$
Let d_{mx} = ε+1 and r = 1
$T_r = T_0$
$S_r = S_0$
(2)
Compute $\underline{f}(r_0, \underline{t}; T_r, S_r)$
(3)
Compute scaled sensitivities $\underline{\underline{Z}}_r$
Is $d_{mx} < \varepsilon$?
Yes
No
(4)
Form $\underline{\underline{Z}}_r^T \underline{\underline{Z}}_r$ and $\underline{Z}_r^T(\underline{s}-\underline{f}(r_0, \underline{t}; T_r, S_r))$
(5)
Invert $\underline{\underline{Z}}_r^T \underline{\underline{Z}}_r$
$r \leftarrow r+1$
No
(8)
Is $r = r_{mx}$?
Yes
(9)
Write $\underline{f}$ and $\underline{\underline{Z}}$
End
(6)
Calculate $(\Delta T_{r+1}/T_r, \Delta S_{r+1}/S_r)$ and d_{mx}=max $(\Delta T_{r+1}/T_r, \Delta S_{r+1}/S_r)$
(7)
Calculate $T_{r+1} = T_r(1+\rho\frac{\Delta T_{r+1}}{T_r})$
$S_{r+1} = S_r(1+\rho\frac{\Delta S_{r+1}}{S_r})$
Write r, T_{r+1}, and S_{r+1}

Figure 1

1. n=number of observations;
   r_0=radial distance to observation well;
   t_i=time of each observation;
   s_i=observed drawdown for each time t_i;
   T_0=initial guess, transmissivity;
   S_0=initial guess, storage coefficient;
   Q=discharge;
   ρ=damping parameter;
   ϵ=convergence criterion;
   r_{mx}=maximum number of iterations.

2. $f_i(r_0,t_i;T_r,S_r)=\frac{Q}{4\pi T_r}W(r_0,t_i;T_r,S_r)$.

   You will have to program a finite number of terms of the infinite series to evaluate $W(r_0,t_i;T_r,S_r)$. Note that one computation of f_i will occur for every time observation t_i. These computations form the column vector $\underline{f}$.
3. The sensitivities will form an $n\times 2$ array (one sensitivity for each parameter T and S; sensitivities are evaluated for each observation). Use the information in parts a and b above.
4. Matrix multiplication is done with the basic algorithm

$$c_{ij}=\sum_{k=1}^{n} a_{ik}b_{kj}$$

   where a_{ik}, b_{kj}, and c_{ij} are elements of matrices $\underline{A}$, $\underline{B}$, and $\underline{C}$, respectively, and $\underline{C}=\underline{AB}$. If $\underline{A}=\underline{B}^T$, then

$$c_{ij}=\sum_{k=1}^{n} b_{ki}b_{kj}$$

   because $b_{ik}^T=b_{ki}$. Similarly, if $\underline{A}=\underline{D}^T$, then $\underline{C}=\underline{AB}$ becomes

$$c_{ij}=\sum_{k=1}^{n} d_{ki}b_{kj}\ .$$

   Note that the model error variance Var($\underline{\epsilon}$) is assumed to be $\underline{I}\sigma^2$.
5. Use the definition of the inverse to construct the inverse.
6. See part c above. Also, note that $\underline{d}_{r+1}=[\Delta T_{r+1},\Delta S_{r+1}]$.
7. Include the damping parameter ρ in your calculation of the new regression parameters. If convergence does not occur, then you may be best advised to set ρ to a value less than one.
8. This is the end of the iteration loop.
9. You may wish to compute the final estimate of residuals $\underline{e}=\underline{f}-\underline{s}$, then print them also.

Because convergence problems may arise, limit the number of passes that can be made through the algorithm. Test your code using the following data.

36-Hour Pumping Test

Test starts: 12 February 1976, 0805 h.
Test ends: 13 February 1976, 2005 h.
Production well was pumped varying between 517 gal/min and 530 gal/min. Time and drawdown data at observation well 175 ft from production well appear in table 1.

Table 1

[Data from S.P. Larson, presently of S.S. Papadopulos and Associates (formerly U.S. Geological Survey), 1978]

Time (s)	Drawdown (ft)
480	1.71
1,020	2.23
1,500	2.54
2,040	2.77
2,700	3.04
3,720	3.25
4,920	3.56

To aid in debugging your computer program, some example calculations follow. Assume that T_0=0.1 ft^2/s, S_0=0.0005, Q=1.16 ft^3/s, and r_o=175 ft. Then

$$u_i^0=\frac{r_o^2S_0}{4T_0t_i}=\frac{(175)^2(0.0005)}{4(0.1)t_i}=38.28125/t_i$$

$$f_i^0=\frac{Q}{4\pi T_0}W(u_i^0)=\frac{1.16}{4\pi(0.1)}W(u_i^0)=0.923099W(u_i^0)$$

Use of these values for u_i^0 and f_i^0 allows for calculation of the following data.

t_i	u_i^0	$W(u_i^0)$	f_i^0
480	0.0797526	2.02980	1.87371
1,020	.0375306	2.74256	2.53165
1,500	.0255208	3.11640	2.87675
2,040	.0187653	3.41721	3.15442
2,700	.0141782	3.69296	3.40897
3,720	.0102907	4.00957	3.70123
4,920	.00778074	4.28665	3.95700

Data for u_i^0 and f_i^0 are used to compute Z_{iT}^0 and Z_{iS}^0.

$$Z_{iT}^0 = -f_i^0 + \frac{Q}{4\pi T_0} e^{-u_i^0} = -f_i^0 + 0.923099\ e^{-u_i^0}$$

$$Z_{iS}^0 = -\frac{Q}{4\pi T_0} e^{-u_i^0} = -0.923099 e^{-u_i^0}$$

Note that $Z_{iT}^0 = X_{iT}^0 T_0$ and $Z_{iS}^0 = X_{iS}^0 S_0$ are calculated directly, without first calculating sensitivities X_{iT}^0 and X_{iS}^0, then formally making the multiplication. These scaled sensitivities result from the following scaled linearized model.

$$f_i^1 = f_i^0 + X_{iT}^0 \Delta T_1 + X_{iS}^0 \Delta S_1$$

$$= f_i^0 + X_{iT}^0 T_0 \left|\frac{\Delta T_1}{T_0}\right| + X_{iS}^0 S_0 \left|\frac{\Delta S_1}{S_0}\right|$$

$$= f_i^0 + Z_{iT}^0 \frac{\Delta T_1}{T_0} + Z_{iS}^0 \frac{\Delta S_1}{S_0}$$

The computed values for Z_{iT}^0 and Z_{iS}^0 are:

Z_{iT}^0	Z_{iS}^0
-1.02137	-0.852339
-1.64255	-.889097
-1.97691	-.899839
-2.24848	-.905938
-2.49887	-.910103
-2.78758	-.913648
-3.04106	-.915944

Use of the computed values for Z_{iT}^0 and Z_{iS}^0 yields the entries in the $\underline{Z}^T\underline{Z}$ matrix:

$$\sum_i \left(Z_{iT}^0\right)^2 = 35.96800209 \quad \sum_i \left(Z_{iS}^0\right)^2 = 5.649402682$$

$$\sum_i Z_{iT}^0 Z_{iS}^0 = 13.75336059$$

Elements of the $\underline{Z}^T(\underline{s}-\underline{f}_0)$ vector are computed in the following manner.

Z_{iT}^0	s_i	f_i^0	$Z_{iT}^0(s_i - f_i^0)$
-1.02137	1.71	1.87371	0.1672084827
-1.64255	2.23	2.53165	.4954752075
-1.97691	2.54	2.87675	.6657244425
-2.24848	2.77	3.15442	.8643606816
-2.49887	3.04	3.40897	.9220080639
-2.78758	3.25	3.70123	1.257839723
-3.04106	3.56	3.95700	1.20730082

$$\sum_i Z_{iT}^0 \left(s_i - f_i^0\right) = 5.579917421$$

Z_{iS}^0	s_i	f_i^0	$Z_{iS}^0(s_i - f_i^0)$
-0.852339	1.71	1.87371	0.1395364177
-.889097	2.23	2.53165	.2681961101
-.899839	2.54	2.87675	.3030207833
-.905938	2.77	3.15442	.3482606860
-.910103	3.04	3.40897	.3358007039
-.913648	3.25	3.70123	.4122653870
-.915944	3.56	3.95700	.3636297680

$$\sum_i Z_{iS}^0 \left(s_i - f_i^0\right) = 2.170709856$$

Finally, the two elements of the scaled displacement vector $(\Delta T_1/T_0, \Delta S_1/S_0)$ are computed and used to compute T_1 and S_1, the new estimates for T and S.

$$\frac{\Delta S_1}{S_0} = (2.170709856 - (13.75336059) \cdot (5.579917421)/35.96800209) / (5.649402682 - (13.75336059)^2 / 35.96800209)$$

$$= \frac{0.03707407158}{0.3904247981} = 0.09495829097$$

$$\frac{\Delta T_1}{T_0} = (5.579917421 - (0.09495829097)(13.75336059)) / 35.96800209$$

$$= 0.1188256660$$

$$S_1 = (1 + 0.0949583)(0.0005) = 0.000547479$$

$$T_1 = (1 + 0.118826)(0.1) = 0.111883$$

Some similar calculations for the second iteration are:

$$u_i^1 = \frac{(175)^2(0.000547479)}{4(0.111883)t_i} = 37.4645/t_i$$

$$f_i^1 = \frac{1.16}{4\pi(0.111883)} W(u_i^1) = 0.825057 W(u_i^1)$$

t_i	u_i^1	$W(u_i^1)$	f_i^1
480	0.0780510	2.04973	1.69114
1020	.0367299	2.76334	2.27991
1500	.0249763	3.13743	2.58856
2040	.0183650	3.43838	2.83686
2700	.0138757	3.71423	3.06445
3720	.0100711	4.03091	3.32573
4920	.00761474	4.30805	3.55439

$$Z_{iT}^1 = -f_i^1 + 0.825057e^{-u^1{}_i}$$

$$Z_{iS}^1 = -0.825057e^{-u^1{}_i}$$

Z_{iT}^1	Z_{iS}^1
-0.928031	-0.763109
-1.48461	-.795303
-1.78385	-.804705
-2.02682	-.810043
-2.25076	-.813688
-2.50894	-.816789
-2.73559	-.818798

3.3.2 Nonlinear Regression When the Model Is Numerical

The basic model equations assumed in all previous developments have been of the closed form or analytical type where the dependent variable f is a known function of $\underline{\xi}$ and $\underline{\beta}$. In many cases such models may either not exist or be too complicated for practical use. In these cases the basic equation relating the dependent variable to the independent variables and parameters may be a numerical solution that can be stated in the general form

$$\underline{\underline{D}}(\underline{h},\underline{\xi},\underline{\beta})\underline{h} = \underline{q}(\underline{h},\underline{\xi},\underline{\beta}) \quad . \qquad (3.3\text{-}21)$$

Equation 3.3-21 is a nonlinear matrix equation in which $\underline{h}$ is the solution (dependent variable) vector of order m; $\underline{\underline{D}}$ is a nonsingular coefficient matrix of order m that is a function of $\underline{h}$, $\underline{\xi}$, and $\underline{\beta}$; and $\underline{q}$ is a vector of order m that is a function of $\underline{h}$, $\underline{\xi}$, and $\underline{\beta}$. Order m is not related to the number of observations n, but instead is simply the order required to give a good numerical approximation to the solution of the problem.

If equation 3.3-21 is linear in $\underline{h}$ so that $\underline{\underline{D}}$ and $\underline{q}$ are not functions of $\underline{h}$, then equation 3.3-21 may be solved directly for $\underline{h}$. In this case the Gauss-Newton method may be used to obtain the regression solution. (The nonlinear case is considered in section 6.1.2.) The procedure is as follows. First write equation 3.3-21 in the form

$$\underline{h} = \underline{\underline{D}}^{-1}\underline{q} \qquad (3.3\text{-}22)$$

which is explicit in the dependent variable $\underline{h}$. Next, note that $\underline{h}$ in equation 3.3-22 and $\underline{f}$ in equation 3.3-2 (or, as an estimate, equation 3.3-3) are expressions of the same quantity, the only difference between them being that elements of $\underline{h}$ are values of the dependent variable computed at points defined by the numerical solution, and elements of $\underline{f}$ are values of the dependent variable computed at observation points. If all n_s observation points are contained in the set of points required for the numerical solution, which implies that $m \geq n_s$, then $\underline{f}$ is obtained from $\underline{h}$ simply by eliminating those entries in $\underline{h}$ not corresponding to observation points. In other instances the points in m may not correspond to those in n_s. For these instances an interpolation scheme would be used to obtain $\underline{f}$ from $\underline{h}$. In either case, the vector $\underline{f}(\underline{\xi}, \underline{b}_r)$ is obtained by using $\underline{h}$ computed from equation 3.3-22 in which $\underline{b}_r$ was used to evaluate $\underline{\underline{D}}$ and $\underline{q}$.

The final step in forming the Gauss-Newton solution is to derive the sensitivity matrix $\underline{\underline{X}}$. To accomplish this step, write equation 3.3-21 in terms of a general parameter set $\underline{b}$, then differentiate it with respect to $\underline{b}$ to yield

$$\underline{\underline{D}}\frac{\partial \underline{h}}{\partial b_j} + \frac{\partial \underline{\underline{D}}}{\partial b_j}\underline{h} = \frac{\partial \underline{q}}{\partial b_j}, j = 1,2,\ldots,p \qquad (3.3\text{-}23)$$

or

$$\frac{\partial \underline{h}}{\partial b_j} = \underline{\underline{D}}^{-1}\left(\frac{\partial \underline{q}}{\partial b_j} - \frac{\partial \underline{\underline{D}}}{\partial b_j}\underline{h}\right), j = 1,2,\ldots,p. \qquad (3.3\text{-}24)$$

The quantity $\partial \underline{h}/\partial b_j$ forms a column of the sensitivity matrix for points in m. Sensitivity

matrix $\underline{X}_r$ would be found by first computing $\partial \underline{h}/\partial b_j$ using equation 3.3-24 written in terms of $\underline{h}_r$ and $\underline{b}_r$, then following one of the two procedures described above for obtaining $\underline{f}$ from $\underline{h}$. By incorporating the procedures to compute numerical estimates of $\underline{f}(\underline{\xi},\underline{b}_r)$ and $\underline{X}_r$, the algorithm given for the Gauss-Newton method may be followed exactly to find the regression solution of equation 3.3-22.

By studying the sequence of calculations in the solution algorithm carefully, it will be noted that to calculate $\underline{h}_r$ and $\underline{X}_r$, $\underline{D}_r$ ($\underline{D}$ computed using $\underline{b}_r$) must already have been computed. This requires one of two possible calculation schemes. Either $\underline{D}_r$ and p matrices of the form $(\partial \underline{D}/\partial b_j)_r$ must be formed at the same time and stored before $\underline{h}_r$ and $\underline{X}_r$ are calculated, or $\underline{D}_r$ must be formed before $\underline{h}_r$ is calculated and then each matrix $(\partial \underline{D}/\partial b_j)_r$ formed as needed to calculate each column (that is, $\underline{X}_j^r$) of $\underline{X}_r$. The first alternative could require a considerable amount of computer memory or the use of scratch files, whereas the second alternative could require repetitive calculation because many arithmetic operations could be the same for forming both $\underline{D}_r$ and $(\partial \underline{D}/\partial b_j)_r$. Often, however, matrices $(\partial \underline{D}/\partial b_j)_r$ can be written in a condensed or decomposed form to conserve computer memory. In this way $\underline{D}_r$ and the decomposed form of $(\partial \underline{D}/\partial b_j)_r$ can be computed together without using a significant amount of extra memory. Then each matrix $(\partial \underline{D}/\partial b_j)_r$ may be assembled as needed without performing numerous repetitive calculations.

A significant amount of computer memory can also be wasted unless care is taken when forming $\underline{X}_r$. The general procedure is to form the column vector $(\partial \underline{q}/\partial b_j)_r - (\partial \underline{D}/\partial b_j)_r \underline{h}_r$, then use equation 3.3-24 to form the vector $(\partial \underline{h}/\partial b_j)_r$, which replaces the first vector in central computer memory. From this, vector $\underline{X}_j^r$ is immediately formed and stored. The matrix composed of vectors $(\partial \underline{h}/\partial b_j)_r$ should not be stored in central computer memory because it is often large. If desired, it may be stored column by column on a scratch file for later retrieval and printing.

Problem 3.3-2

Assume the finite difference representation of a flow problem shown in figure 1.

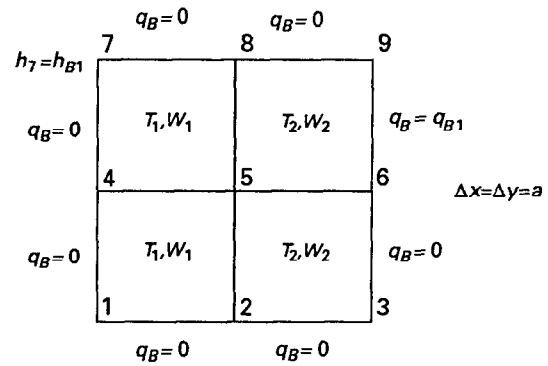

Figure 1

Finite difference equations for this problem can be written as follows.

1. $\frac{1}{2}\Delta y T_1(h_2-h_1)/\Delta x+\frac{1}{2}\Delta x T_1(h_4-h_1)/\Delta y = -\frac{1}{2}\Delta x \frac{1}{2}\Delta y W_1.$
2. $\frac{1}{2}\Delta y T_2(h_3-h_2)/\Delta x-\frac{1}{2}\Delta y T_1(h_2-h_1)/\Delta x +\frac{1}{2}\Delta x T_1(h_5-h_2)/\Delta y+\frac{1}{2}\Delta x T_2(h_5-h_2)/\Delta y = -\frac{1}{2}\Delta x \frac{1}{2}\Delta y W_1-\frac{1}{2}\Delta x \frac{1}{2}\Delta y W_2.$
3. $-\frac{1}{2}\Delta y T_2(h_3-h_2)/\Delta x+\frac{1}{2}\Delta x T_2(h_6-h_3)/\Delta y = -\frac{1}{2}\Delta x \frac{1}{2}\Delta y W_2.$
4. $\Delta y T_1(h_5-h_4)/\Delta x+\frac{1}{2}\Delta x T_1(h_{B1}-h_4)/\Delta y -\frac{1}{2}\Delta x T_1(h_4-h_1)/\Delta y = -\frac{1}{2}\Delta x \Delta y W_1.$
5. $\Delta y T_2(h_6-h_5)/\Delta x-\Delta y T_1(h_5-h_4)/\Delta x +\frac{1}{2}\Delta x T_1(h_8-h_5)/\Delta y+\frac{1}{2}\Delta x T_2(h_8-h_5)/\Delta y -\frac{1}{2}\Delta x T_1(h_5-h_2)/\Delta y-\frac{1}{2}\Delta x T_2(h_5-h_2)/\Delta y = -\frac{1}{2}\Delta x \Delta y W_1-\frac{1}{2}\Delta x \Delta y W_2.$
6. $-\Delta y T_2(h_6-h_5)/\Delta x+\frac{1}{2}\Delta x T_2(h_9-h_6)/\Delta y -\frac{1}{2}\Delta x T_2(h_6-h_3)/\Delta y = -\frac{1}{2}\Delta x \Delta y W_2-\frac{1}{2}\Delta y q_{B1}.$
7. $h_7=h_{B1}.$
8. $\frac{1}{2}\Delta y T_2(h_9-h_8)/\Delta x-\frac{1}{2}\Delta y T_1(h_8-h_{B1})/\Delta x -\frac{1}{2}\Delta x T_1(h_8-h_5)/\Delta y-\frac{1}{2}\Delta x T_2(h_8-h_5)/\Delta y = -\frac{1}{2}\Delta x \frac{1}{2}\Delta y W_1-\frac{1}{2}\Delta x \frac{1}{2}\Delta y W_2.$
9. $-\frac{1}{2}\Delta y T_2(h_9-h_8)/\Delta x-\frac{1}{2}\Delta x T_2(h_9-h_6)/\Delta y = -\frac{1}{2}\Delta x \frac{1}{2}\Delta y W_2-\frac{1}{2}\Delta y q_{B1}.$

Or, by assuming that $\Delta x=\Delta y=a$,

1. $T_1(h_2-h_1)+T_1(h_4-h_1)=-\frac{1}{2}a^2 W_1.$
2. $T_2(h_3-h_2)-T_1(h_2-h_1)+(T_1+T_2)(h_5-h_2) = -\frac{1}{2}a^2(W_1+W_2).$
3. $-T_2(h_3-h_2)+T_2(h_6-h_3)=-\frac{1}{2}a^2 W_2.$
4. $2T_1(h_5-h_4)+T_1(h_{B1}-h_4)-T_1(h_4-h_1) = -a^2 W_1.$
5. $2T_2(h_6-h_5)-2T_1(h_5-h_4)+(T_1+T_2)(h_8-h_5) -(T_1+T_2)(h_5-h_2)=-a^2(W_1+W_2).$
6. $-2T_2(h_6-h_5)+T_2(h_9-h_6)-T_2(h_6-h_3) = -a^2 W_2-a q_{B1}.$
7. $h_7=h_{B1}.$
8. $T_2(h_9-h_8)-T_1(h_8-h_{B1})-(T_1+T_2)(h_8-h_5) = -\frac{1}{2}a^2(W_1+W_2).$
9. $-T_2(h_9-h_8)-T_2(h_9-h_6)=-\frac{1}{2}a^2 W_2-a q_{B1}.$

a. Verify the finite difference equations so that you understand their physical basis. (Hint: read appendix, section 4.3.1.)
b. Write the equations in matrix form:

$$\underline{\underline{D}}\,\underline{h}=\underline{q}$$

by explicitly writing out $\underline{\underline{D}}$, $\underline{h}$, and $\underline{q}$.
c. Let vectors $(\partial \underline{q}/\partial b_j)_r-(\partial \underline{\underline{D}}/\partial b_j)_r\underline{h}_r=\underline{J}_j^r$, and develop $\underline{J}_j^r$ $(j=1,2,3,4)$ for the parameters $\beta_1=T_1$, $\beta_2=T_2$, $\beta_3=W_1$, and $\beta_4=q_{B1}$.
d. Using the modified Gauss-Newton method, develop the algorithm (not computer program) to solve for the parameters. Assume that all nodes except number 7 are observation points.

3.3.3 Convergence and Conditioning

A value of ρ, $0<\rho\leq 1$, can be shown to exist for which the Gauss-Newton procedure, as modified using equation 3.3-19, will converge to the global minimum value of $S(\underline{b})$ provided that:

1. An initial estimate of the parameters can be found such that they lie within a parameter region R bounded by sets of parameters $\underline{b}^*$ defined by

$$S(\underline{b}_0)\leq \min_{\underline{b}^*} S(\underline{b}^*) \qquad (3.3\text{-}25)$$

and the global minimum point lies within this region.
2. For all $\underline{b}$ belonging to R, $\underline{\underline{X}}$ is a continuous and unique matrix function.
3. The matrix $\underline{\underline{S}}^T\underline{\underline{\omega}}\,\underline{\underline{S}}$ is nonsingular and is a continuous function of $\underline{b}$.

Condition 2 is almost always met. Condition 1 requires that the system be well enough understood that intelligent initial estimates of parameters can be made. Difficulties frequently arise in connection with condition 3. Unless the problem is correctly specified, the least squares coefficient matrix (for example, $\underline{\underline{S}}^T\underline{\underline{\omega}}\,\underline{\underline{S}}$) can be singular. Moreover, problems often arise because of ill-conditioning (that is, near-singularity) of the matrix. Although the addition of the Marquardt parameter, μ, is intended to help these cases, convergence can be difficult to obtain. In the following paragraphs, the general question of convergence is considered first. This is followed by discussions of singularity and ill-conditioning.

In general, the rate of convergence has been found to be related to the number of parameters being estimated, as predicted by theory. That is, the greater the number of parameters, the slower the rate, all other things being equal. It is also related to the conditioning of the problem and to the nearness of the initial set of parameters to the optimum set, in that the rate of convergence is usually much faster near a minimum of $S(\underline{b})$. As a rule of thumb, one may often expect convergence within a number of iterations equal to either 5 or twice the number of parameters, whichever is greater. Fewer iterations are required for well-conditioned problems.

A problem that frequently retards the convergence rate, or even causes divergence, is overshoot. This happens when the parameter correction vector $\rho\underline{\delta}_{r+1}$ has a favorable orientation but is much longer than an ideal value. The result is that the new set of parameters $\underline{b}_{r+1}$ is almost as far as (or even further than) the old set $\underline{b}_r$ from the optimum value. A two-parameter example is illustrated in figure 3.3-4.

Overshoot is detected as large oscillations with accompanying changes in sign of components of $\rho\underline{\delta}_{r+1}$ from one iteration to the next. The remedy is to decrease the value of ρ such that $0<\rho<1$. In figure 3.3-4, a good value would be $\rho=0.5$, which would give $\underline{b}_{r+1}$ at point 1.

Care must be taken not to make ρ too small so that undershoot becomes a problem. Undershoot occurs when $\rho\underline{\delta}_{r+1}$ is too small, and it manifests itself as small steps $\rho\underline{\delta}_{r+1}$, the components of which usually do not change sign. The remedy is to increase the value of ρ, in rare occasions such that $\rho>1$. As a practical guide, the best value of ρ is one that causes some

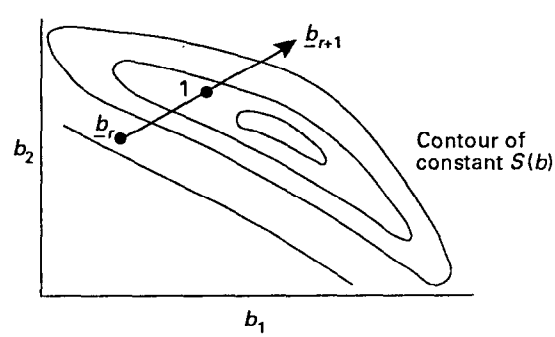

Figure 3.3-4

oscillations in sign of a few components of $\rho\underline{\delta}_{r+1}$ from one iteration to the next.

Sometimes the solution may converge to a local minimum instead of the global minimum. Most commonly this can occur (1) if ρ is too large and the overshoot causes the search vector $\rho\underline{\delta}_{r+1}$ to escape from the region defined by equation 3.3-25, or (2) if the initial estimate $\underline{b}_0$ is not in the region defined by equation 3.3-25. Detection of this problem is accomplished through adequate knowledge of the system so that the wrong solution can be recognized. If the computed parameter vector $\hat{\underline{b}}$ is physically illogical or the model analysis discussed in section 5 suggests that the model is not correct, then one might suspect that a local minimum has been reached. The remedy to the problem is to decrease ρ and (or) choose another initial estimate $\underline{b}_0$. If $\underline{b}_0$ is changed, usually the distance between $\underline{b}_0$ and the vector $\hat{\underline{b}}$ computed for the local minimum should be increased. Thus, if some components of $\hat{\underline{b}}$ are far too large to be realistic, then the same components of $\underline{b}_0$ should be reduced in value. If several attempts at changing ρ and (or) $\underline{b}_0$ do not produce a change in $\hat{\underline{b}}$, then the cause of the poor results is probably not a local minimum.

As for the linear case, singularity of the least-squares coefficient matrix occurs whenever columns of the sensitivity matrix are linearly dependent. Near-singularity, caused by near-linear dependence, is a more frequent occurrence. As a result of ill-conditioning, step sizes $\underline{\delta}_{r+1}$ can be highly erratic, appearing to head toward no well-defined point and can be dominated by overshoot. In addition, some problems may start fairly well conditioned for the initial parameters but may become progressively more poorly conditioned during the iterative solution process.

The same techniques for analysis of poorly conditioned problems as are used for linear problems may be used for nonlinear problems as well. Whenever a problem is poorly conditioned, the sensitivity matrix $\underline{\underline{X}}$ may be examined for a near-zero column, and $\underline{\underline{S}}^T\underline{\underline{\omega}}\underline{\underline{S}}$ may be examined for off-diagonal components near unity. Also, the orthogonal transformation may be used to indicate that ill-conditioning exists and to point out possible columns where linear dependency occurs.

Use of the Marquardt parameter, μ, is intended to improve conditioning by adding a small quantity to the main diagonal of the least-squares coefficient matrix. Although conditioning is always artificially improved by employing μ, the parameters resulting from applying the least squares process to a very poorly conditioned problem may be considerably in error unless the actual causes of the poor conditioning are discovered and the conditioning improved without using μ.

3.3.4 Computation of μ and ρ

For best efficiency, both μ and ρ should be recomputed at each iteration, r. A number of schemes exist in the literature for making these computations, but virtually all schemes involve assuming several trial values of μ and ρ, then performing all of the calculations for iteration r for each of the trial values. The best values to use are then computed so as to minimize or substantially decrease $S(\underline{b})$. The problem with these schemes is that they require so much time that one is often much better off settling for approximate values of μ and ρ computed by using a much simpler scheme.

The scheme adopted here is derived from the considerations discussed in section 3.3.3. Parameter μ is used only when the problem is so poorly conditioned that the search direction $\underline{\delta}$ must be altered. Overshoot and undershoot are controlled primarily through use of ρ.

Because the Marquardt parameter is used with a scaled problem formulation, computations must be made using scaled quantities (see equation 3.3-16). By direct computation, it can be verified that the scaled gradient $(\partial S(\underline{b})/\partial b_j) \cdot C_{jj}$ $(j=1,2,...,p)$ of the sum of squares $S(\underline{b})$ is given by

$$\underline{\underline{C}}^T \frac{\partial S(\underline{b})}{\partial \underline{b}} = -\underline{g} = -\underline{\underline{S}}^T \underline{\underline{\omega}} (\underline{Y} - \underline{f}(\underline{\xi}, \underline{b})) . \qquad (3.3\text{-}26)$$

Thus, by definition (Spiegel, 1959, p. 16), the angle between g, which points directly down the sum of squares surface, and displacement vector $\underline{\delta}$ is given for the rth iteration by

$$\cos\Theta = \frac{\underline{\delta}_{r+1}^T \underline{g}_r}{\sqrt{(\underline{\delta}_{r+1}^T \underline{\delta}_{r+1})(\underline{g}_r^T \underline{g}_r)}} . \qquad (3.3\text{-}27)$$

For two parameters, b_1 and b_2, the relationships given by equation 3.3-27 are illustrated in figure 3.3-5. (Note the use of scaled parameters; see equation 3.3-17.)

If $\Theta=90°$, then, as discussed in section 3.3.1, no improvement in parameters is likely to result from application of the Gauss-Newton procedure. However, application of the Marquardt parameter, $\mu>0$, will result in $\Theta<90°$ (Marquardt, 1963) because vector $\underline{\delta}$ is shifted progressively toward $\underline{g}$ as μ increases. Thus, a viable scheme for choosing μ is to define a maximum value of Θ, $\Theta_{mx}<90°$, and compute μ so that Θ never exceeds Θ_{mx}. This can be accomplished rather simply. At the beginning of the regression set $\mu_0=0$. Then at each iteration r, check and recompute μ as necessary:

$$\left.\begin{aligned}&\mu_r=\mu_\ell\\&\text{if } \underline{\delta}_{r+1}^T\underline{g}_r\geq\cos\Theta_{mx}\sqrt{(\underline{\delta}_{r+1}^T\underline{\delta}_{r+1})(\underline{g}_r^T\underline{g}_r)} \text{ or}\\&\mu_{\ell+1}=\frac{3}{2}\mu_\ell+0.001\\&\text{if } \underline{\delta}_{r+1}^T\underline{g}_r<\cos\Theta_{mx}\sqrt{(\underline{\delta}_{r+1}^T\underline{\delta}_{r+1})(\underline{g}_r^T\underline{g}_r)}\end{aligned}\right\} \quad (3.3\text{-}28)$$

At the beginning of iteration r, $\ell=1$ and $\mu_\ell=\mu_{r-1}$. Then equation 3.3-20 is solved and equation 3.3-28 is applied. If the second part of equation 3.3-28 is employed, equation 3.3-20 is resolved using $\mu_{\ell+1}$, ℓ is incremented by one, and equation 3.3-28 is used again. This process is continued until the first part of equation 3.3-28 is used, at which point the appropriate value of μ for iteration r has been found. The formula for computing $\mu_{\ell+1}$ from μ_ℓ is empirical but gives what experience has shown to be a good range in values of μ. For each resolution of equation 3.3-20, $\underline{S}_r^T\underline{\omega}\,\underline{S}_r$ and $\underline{g}_r$ are not recomputed. Thus, the calculations are not extensive.

Computation of ρ is designed to prevent disastrous overshoot and to keep $\rho\underline{\delta}$ within the region R defined by equation 3.3-25. A simple but usually effective scheme is to estimate the maximum fraction that any of the parameters could change and still remain within R and then to prevent any parameter from changing any more than this amount over any iteration. Let t_{mx} be this maximum fractional change. Then at iteration r, ρ is calculated as follows:

$$t=\max_i|d_i^{r+1}/c| \quad (3.3\text{-}29)$$

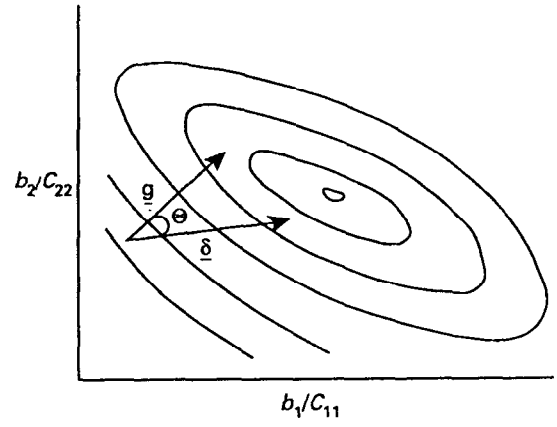

Figure 3.3-5

$$\left.\begin{aligned}&\rho=1 \text{ if } t\leq t_{mx} \text{ or}\\&\rho=t_{mx}/t \text{ if } t>t_{mx}\end{aligned}\right\} \quad (3.3\text{-}30)$$

where $c=b_i^r$ if $b_i^r\neq 0$ and $c=1$ if $b_i^r=0$.

3.4 Regression Including Prior Information

3.4.1 Model Structure

Recall that the standard nonlinear regression model including prior information on the parameters may be written in the form (equation 3.1-32)

$$\underline{Y}=\underline{f}(\underline{\xi},\underline{\beta})+\underline{\epsilon} \quad (3.4\text{-}1)$$

where

$$\underline{Y}=\begin{bmatrix}\underline{Y}_s\\ \underline{Y}_p\end{bmatrix} \quad (3.4\text{-}2)$$

$$\underline{f}(\underline{\xi},\underline{\beta})=\begin{bmatrix}\underline{f}_s(\underline{\xi},\underline{\beta})\\ \underline{f}_p(\underline{\xi},\underline{\beta})\end{bmatrix} \quad (3.4\text{-}3)$$

$$\underline{\epsilon}=\begin{bmatrix}\underline{\epsilon}_s\\ \underline{\epsilon}_p\end{bmatrix} \quad (3.4\text{-}4)$$