TABLE 1

Summary of Tajima's D coalescent simulations with various demographic parameters

Equilibrium (n=10)

theta	alpha	strength	time since	E(D)	V(D)	Pr(D>TajUp)	Pr(D<TajLo)	% Reject	Upper 2.5%	Lower 2.5%
1				-0.0297	0.863	0.0101	0.00998	2.0%	1.83	-1.56
10				-0.0778	0.802	0.00742	0.0256	3.3%	1.66	-1.74
50				-0.0831	0.758	0.00527	0.0217	2.7%	1.60	-1.71

Population Growth (n=10)

theta	alpha	strength	time since	E(D)	V(D)	Pr(D>TajUp)	Pr(D<TajLo)	% Reject	Upper 2.5%	Lower 2.5%
1	0.1			-0.130	0.758	0.00345	0.00403	0.7%	1.64	-1.56
1	0.5			-0.142	0.733	0.00252	0.00287	0.5%	1.59	-1.56
1	1.0			-0.153	0.715	0.00177	0.00230	0.4%	1.46	-1.56
1	2.0			-0.176	0.688	0.00096	0.00170	0.3%	1.46	-1.56
1	5.0			-0.199	0.638	0.00064	0.00087	0.2%	1.46	-1.40
10	0.1			-0.239	0.643	0.00284	0.0207	2.4%	1.38	-1.70
10	0.5			-0.260	0.598	0.00145	0.0182	2.0%	1.30	-1.67
10	1.0			-0.289	0.566	0.00106	0.0166	1.8%	1.23	-1.66
10	2.0			-0.327	0.526	0.00085	0.0158	1.7%	1.13	-1.65
10	5.0			-0.399	0.473	0.00055	0.0153	1.6%	1.01	-1.65
50	0.1			-0.253	0.575	0.00145	0.0156	1.7%	1.23	-1.65
50	0.5			-0.282	0.525	0.00053	0.0119	1.3%	1.17	-1.62
50	1.0			-0.309	0.481	0.00015	0.00959	1.0%	1.06	-1.59
50	2.0			-0.352	0.429	0.00004	0.00828	0.8%	0.923	-1.58
50	5.0			-0.433	0.348	0.00000	0.00565	0.6%	0.723	-1.54

TABLE 1 (continued)

Weak Bottleneck (n=10)

theta	alpha	strength	time since	E(D)	V(D)	Pr(D>TajUp)	Pr(D<TajLo)	% Reject	Upper 2.5%	Lower 2.5%
1		0.5	0.00	0.284	0.786	0.0207	0.00661	2.7%	1.95	-1.56
1		0.5	0.01	0.249	0.805	0.0206	0.00682	2.7%	1.95	-1.56
1		0.5	0.05	0.118	0.853	0.0164	0.00813	2.5%	1.84	-1.56
1		0.5	0.10	0.0174	0.856	0.0137	0.00853	2.2%	1.84	-1.56
1		0.5	0.25	-0.105	0.833	0.00967	0.00881	1.8%	1.77	-1.56
1		0.5	0.50	-0.134	0.805	0.00694	0.00808	1.5%	1.64	-1.56
10		0.5	0.00	0.578	1.61	0.147	0.0693	21.6%	2.47	-1.98
10		0.5	0.01	0.446	1.60	0.120	0.0732	19.3%	2.43	-1.98
10		0.5	0.05	0.0917	1.63	0.00603	0.127	13.3%	2.21	-2.10
10		0.5	0.10	-0.00845	1.33	0.00327	0.0941	9.7%	2.06	-1.99
10		0.5	0.25	-0.281	1.02	0.0110	0.0669	7.8%	1.75	-1.91
10		0.5	0.50	-0.269	0.787	0.00636	0.0315	3.8%	1.59	-1.78
50		0.5	0.00	0.652	1.90	0.186	0.0903	27.6%	2.67	-2.11
50		0.5	0.01	0.466	1.87	0.144	0.0999	24.4%	2.50	-2.12
50		0.5	0.05	0.0917	1.63	0.0603	0.127	18.7%	2.21	-2.10
50		0.5	0.10	-0.121	1.41	0.0280	0.124	15.2%	2.00	-2.07
50		0.5	0.25	-0.318	1.00	0.00821	0.0707	7.9%	1.70	-1.91
50		0.5	0.50	-0.292	0.731	0.00468	0.0255	3.0%	1.55	-1.74

TABLE 1 (continued)

Strong Bottleneck (n=10)

theta	alpha	strength	time since	E(D)	V(D)	Pr(D>TajUp)	Pr(D<TajLo)	% Reject	Upper 2.5%	Lower 2.5%
1		1.0	0.00	0.200	0.581	0.0160	0.00524	2.1%	1.84	-1.40
1		1.0	0.01	0.155	0.611	0.0152	0.00584	2.1%	1.84	-1.40
1		1.0	0.05	0.0138	0.681	0.0126	0.00599	1.9%	1.84	-1.56
1		1.0	0.10	-0.0938	0.711	0.0104	0.00624	1.7%	1.83	-1.56
1		1.0	0.25	-0.217	0.722	0.00640	0.00700	1.3%	1.64	-1.56
1		1.0	0.50	-0.211	0.739	0.00533	0.00555	1.1%	1.60	-1.56
10		1.0	0.00	0.458	1.61	0.157	0.0885	24.6%	2.53	-2.02
10		1.0	0.01	0.224	1.71	0.124	0.0912	21.5%	2.46	-2.02
10		1.0	0.05	-0.246	1.63	0.0587	0.113	17.2%	2.25	-2.03
10		1.0	0.10	-0.468	1.38	0.0287	0.141	17.0%	2.02	-2.01
10		1.0	0.25	-0.557	0.944	0.00909	0.0874	9.6%	1.65	-1.93
10		1.0	0.50	-0.423	0.665	0.00349	0.0727	7.6%	1.43	-1.75
50		1.0	0.00	0.544	2.09	0.209	0.127	33.6%	2.78	-2.14
50		1.0	0.01	0.0507	2.44	0.158	0.154	31.2%	2.60	-2.14
50		1.0	0.05	-0.421	2.02	0.0616	0.280	34.2%	2.25	-2.13
50		1.0	0.10	-0.590	1.56	0.0254	0.234	25.9%	1.98	-2.10
50		1.0	0.25	-0.620	0.925	0.00677	0.0839	9.1%	1.61	-1.93
50		1.0	0.50	-0.458	0.595	0.00277	0.0193	2.0%	1.37	-1.69

TABLE 1 (continued)

n=50 (selected cases)

theta	alpha	strength	time since	E(D)	V(D)	Pr(D>TajUp)	Pr(D<TajLo)	% Reject	Upper 2.5%	Lower 2.5%
10				-0.0995	0.801	0.0143	0.0137	2.8%	1.81	-1.65
10	1			-0.542	0.435	0.00024	0.0160	1.6%	0.842	-1.71
10		0.5	0.01	0.962	2.08	0.255	0.0301	28.5%	3.48	-1.87
10		0.5	0.25	-0.466	1.10	0.169	0.0734	24.2%	1.87	-2.04
10		1.0	0.01	0.383	2.88	0.208	0.0729	28.1%	3.56	-2.10
10		1.0	0.25	-0.864	1.05	0.0123	0.151	16.3%	1.69	-2.14

Explanation of column headings

Parameters:

theta	The population mutation rate.
alpha	The initial effective population size multiplied by the population growth rate.
strength	The strength of the bottleneck, modeled as time without mutation, in units of 2N generations.
time since	The time since occurrence of the bottleneck, scaled in units of 2N generations.

Results:

E(D)	Mean value of Tajima's D
V(D)	Variance of Tajima's D
Pr(D>TajUp)	Proportion of D values above published upper 2.5% critical values. For n=10, 1.975. For n=50, 2.044.
Pr(D<TajLo)	Proportion of D values below published lower 2.5% critical values. For n=10, -1.733. For n=50, -1.800.
% Reject	The total percentage of D values that fall outside published upper and lower 2.5% critical values.
Upper 2.5%	The corrected upper 2.5% critical value, based on these simulations.
Lower 2.5%	The corrected lower 2.5% critical value, based on these simulations.

Note: each run included 100,000 cycles

Figure 2: The 5 period moving average is a sliding window of histogram values. It serves to smooth out the chaotic nature of the theta = 1 graph.

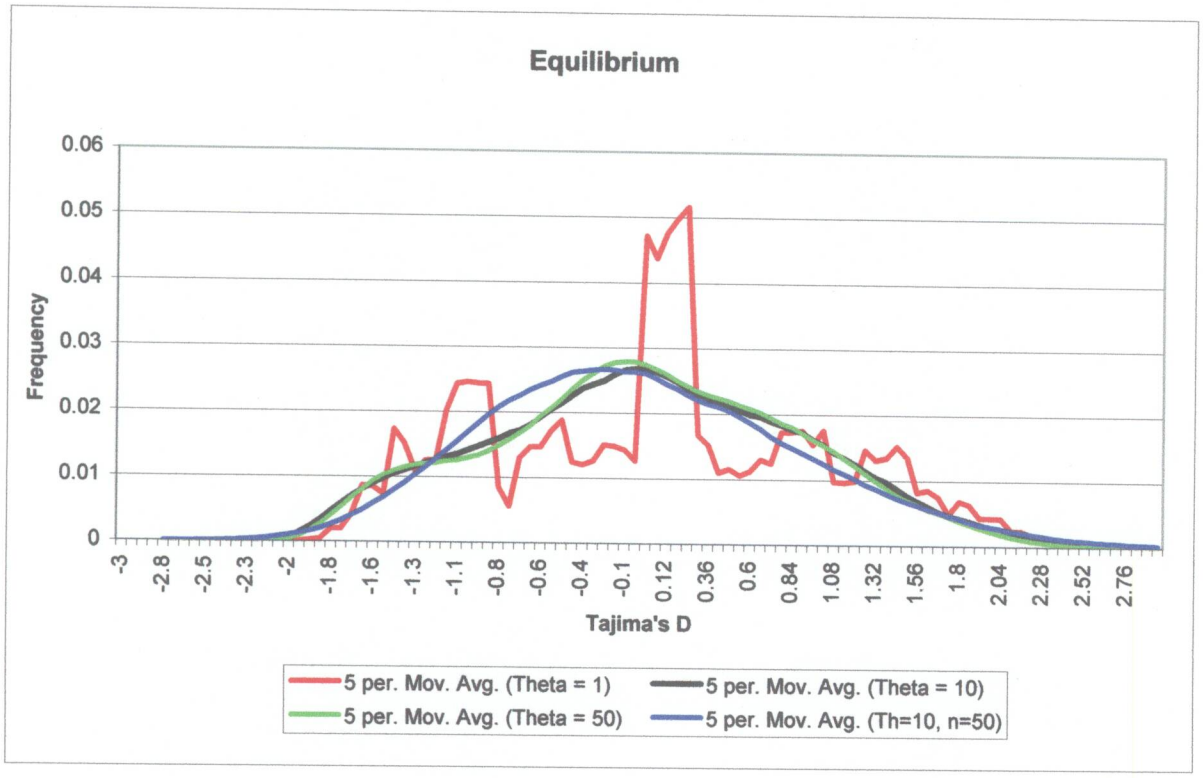

Figure 3:

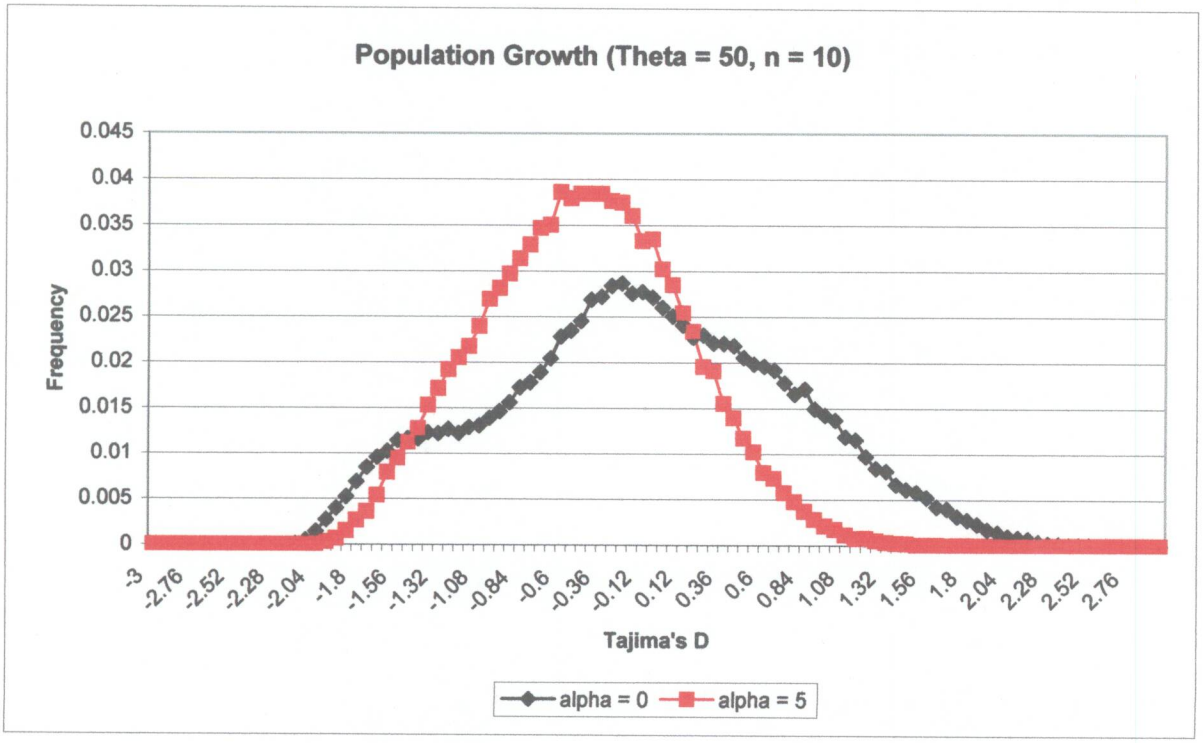

Figure 4: Change in mean value of Tajima's D through time after weak and strong bottlenecks (Theta = 50)

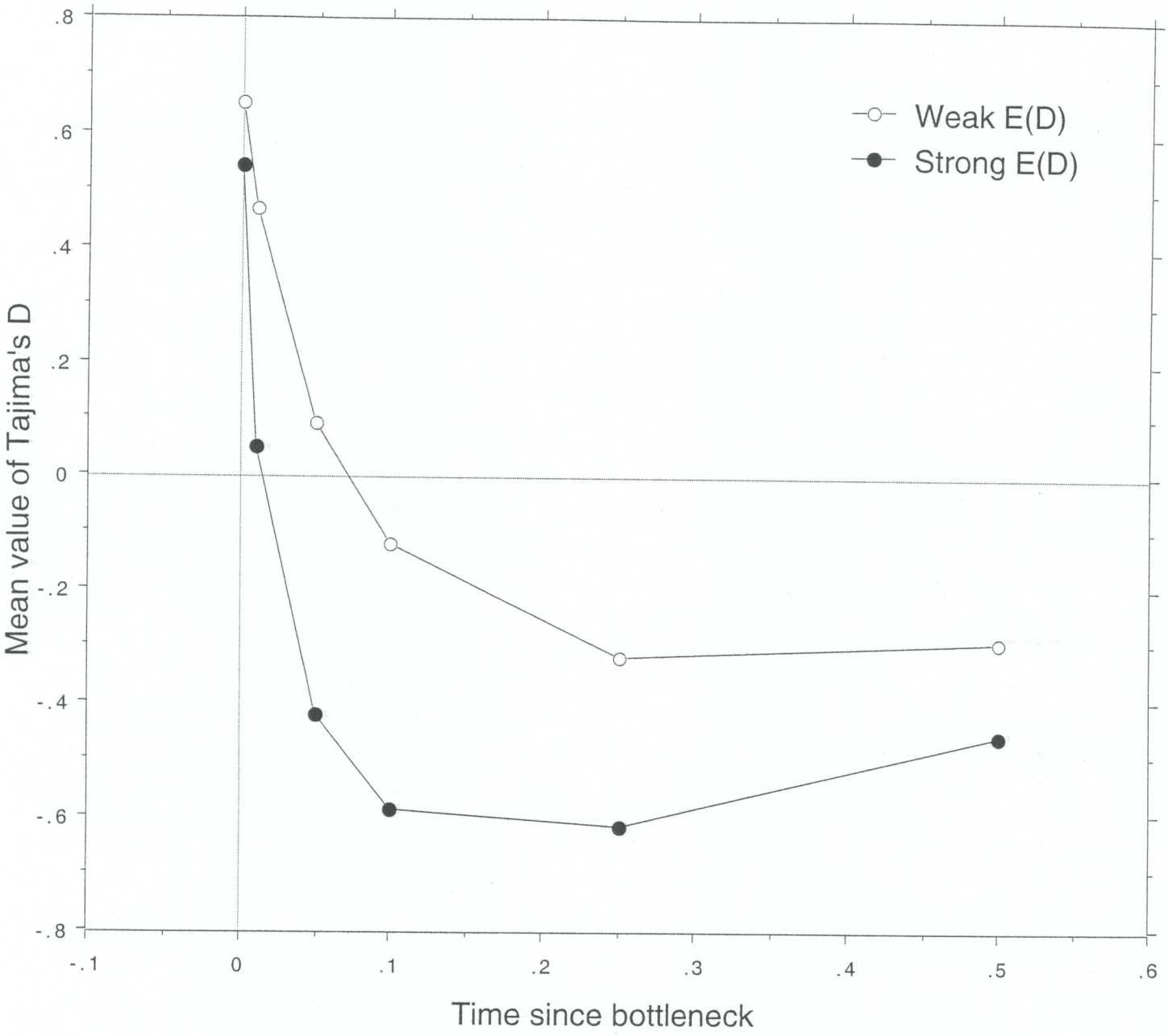

Figure 5:

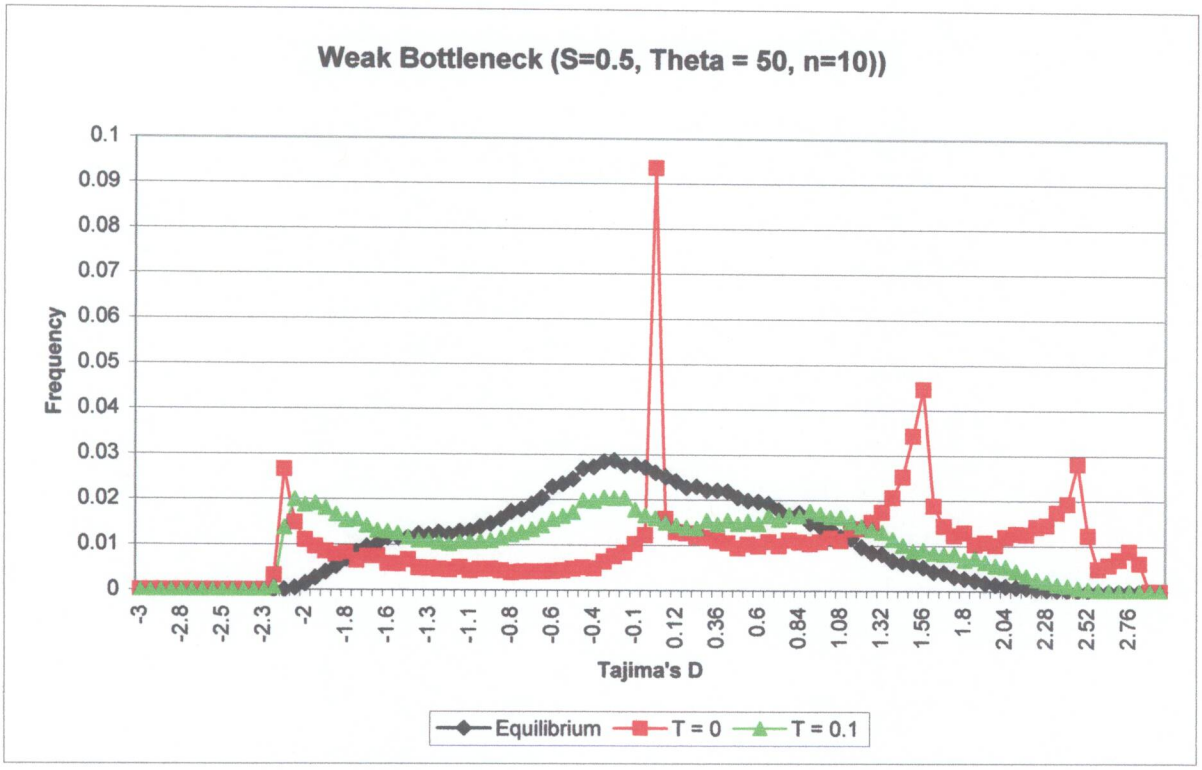

Figure 6:

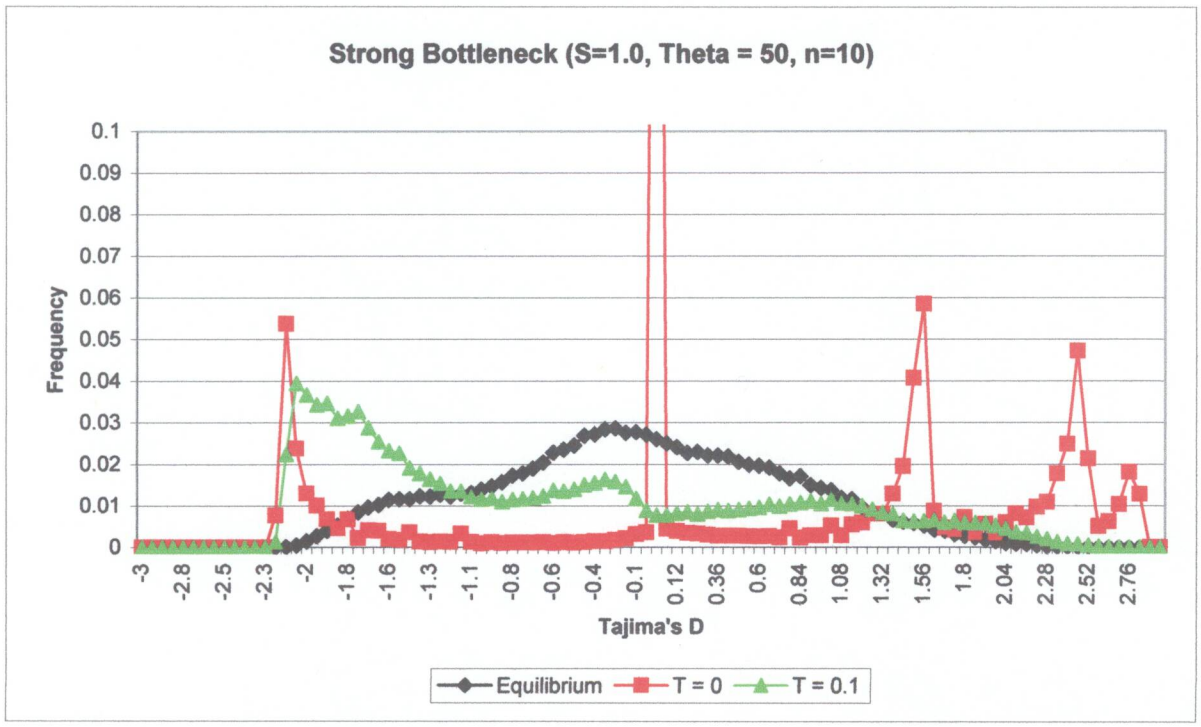

Figure 7: Distribution of Tajima's D at a sequence of times after a weak bottleneck (histograms) vs. equilibrium (line)

Parameters: S = 0.5, Theta = 50, n = 10

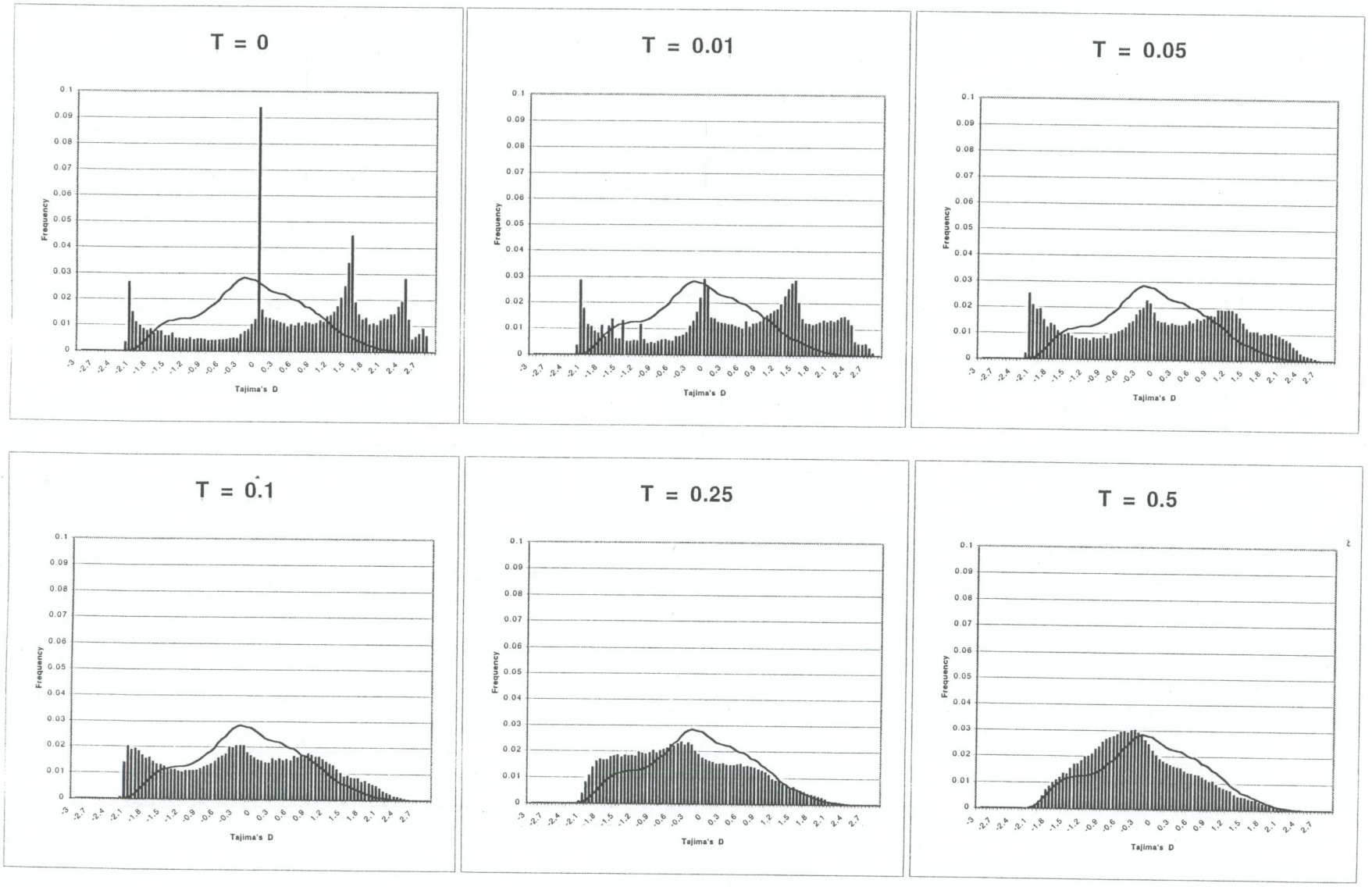

Figure 8: Distribution of Tajima's D at a sequence of times after a strong bottleneck (histograms) vs. equilibrium (line)

Parameters: S = 1, Theta = 50, n = 10