

Curve Fitting and MO Calculation Demo with XLMATH v3.0
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*This worksheet demonstrates the custom functions in XLMATH.XLL.
 All function calls are hi-lighted in magenta color.*

Polynomial Curve Fitting (view Polyde.xlc)

Change the order below and watch the chart

Double click for Notes:

2 Order <= 18

For row ver

Index	IndVar	DepVar	Yest	Resid		For Order 2
0	2	619.7151	Err:511	Err:511	Err:511	polynomial coefficients
1	2.1	254.9522	Err:511	Err:511	Err:511	
2	2.2	504.8611	Err:511	Err:511	Err:511	standard errors of coefficients
3	2.3	690.3672	Err:511	Err:511	Err:511	
4	2.4	638.3767	Err:511	Err:511	Err:511	see
5	2.5	805.3697	Err:511	Err:511	Err:511	
6	2.6	471.9897	Err:511	Err:511	Err:511	rsqrval
7	2.7	566.8193	Err:511	Err:511	Err:511	
8	2.8	383.0008	Err:511	Err:511	Err:511	rval
9	2.9	398.7258	Err:511	Err:511	Err:511	
10	3	759.1758	Err:511	Err:511	Err:511	cferror
11	3.1	1132.11	Err:511	Err:511	Err:511	
12	3.2	743.4951	Err:511	Err:511	Err:511	empty
13	3.3	821.8927	Err:511	Err:511	Err:511	
14	3.4	1352.934	Err:511	Err:511	Err:511	
15	3.5	889.918	Err:511	Err:511	Err:511	
16	3.6	921.1335	Err:511	Err:511	Err:511	
17	3.7	1808.001	Err:511	Err:511	Err:511	
18	3.8	1047.614	Err:511	Err:511	Err:511	
19	3.9	1245.865	Err:511	Err:511	Err:511	

Cubic Splines (view Splinede.xlc)

*Demo function is 3*cos(x) where x is from 0 to 2*pi
 X-values of 2.3 and 4.4 are altered*

*SplineX contains 100 x-values
 SplineY contains interpolated Y values f*

For row ver

Index	IndVarS	DepVarS	CoefS				SplineX	SplineY	OriginalY
0	0	3	Err:508	Err:508	Err:508	Err:508	0	Err:508	3
1	0.628319	2.427051	Err:508	Err:508	Err:508	Err:508	0.062832	Err:508	
2	1.256637	0.927051	Err:508	Err:508	Err:508	Err:508	0.125664	Err:508	
3	1.884956	-0.927051	Err:508	Err:508	Err:508	Err:508	0.188496	Err:508	
4	2.3	1.5	Err:508	Err:508	Err:508	Err:508	0.251327	Err:508	

5	3.141593	-3	Err:508	Err:508	Err:508	Err:508	0.314159	Err:508	
6	3.769911	-2.427051	Err:508	Err:508	Err:508	Err:508	0.376991	Err:508	
7	4.4	2	Err:508	Err:508	Err:508	Err:508	0.439823	Err:508	
8	5.026548	0.927051	Err:508	Err:508	Err:508	Err:508	0.502655	Err:508	
9	5.654867	2.427051	Err:508	Err:508	Err:508	Err:508	0.565487	Err:508	
10	6.283185	3					0.628319	Err:508	2.427051
11							0.69115	Err:508	
12							0.753982	Err:508	
13							0.816814	Err:508	
14							0.879646	Err:508	
15							0.942478	Err:508	
16							1.00531	Err:508	
17							1.068142	Err:508	
18							1.130973	Err:508	
19							1.193805	Err:508	
20							1.256637	Err:508	0.927051
21							1.319469	Err:508	
22							1.382301	Err:508	
23							1.445133	Err:508	
24							1.507964	Err:508	
25							1.570796	Err:508	
26							1.633628	Err:508	
27							1.69646	Err:508	
28							1.759292	Err:508	
29							1.822124	Err:508	
30							1.884956	Err:508	-0.927051
31							1.947787	Err:508	
32							2.010619	Err:508	
33							2.073451	Err:508	
34							2.136283	Err:508	
35							2.199115	Err:508	
36							2.261947	Err:508	
37							2.3	Err:508	1.5
38							2.38761	Err:508	
39							2.450442	Err:508	
40							2.513274	Err:508	
41							2.576106	Err:508	
42							2.638938	Err:508	
43							2.70177	Err:508	
44							2.764602	Err:508	
45							2.827433	Err:508	
46							2.890265	Err:508	
47							2.953097	Err:508	
48							3.015929	Err:508	

49		3.078761	Err:508	
50		3.141593	Err:508	-3
51		3.204425	Err:508	
52		3.267256	Err:508	
53		3.330088	Err:508	
54		3.39292	Err:508	
55		3.455752	Err:508	
56		3.518584	Err:508	
57		3.581416	Err:508	
58		3.644247	Err:508	
59		3.707079	Err:508	
60		3.769911	Err:508	-2.427051
61		3.832743	Err:508	
62		3.895575	Err:508	
63		3.958407	Err:508	
64		4.021239	Err:508	
65		4.08407	Err:508	
66		4.146902	Err:508	
67		4.209734	Err:508	
68		4.272566	Err:508	
69		4.335398	Err:508	
70	4.4	4.4	Err:508	2
71		4.461062	Err:508	
72		4.523893	Err:508	
73		4.586725	Err:508	
74		4.649557	Err:508	
75		4.712389	Err:508	
76		4.775221	Err:508	
77		4.838053	Err:508	
78		4.900885	Err:508	
79		4.963716	Err:508	
80		5.026548	Err:508	0.927051
81		5.08938	Err:508	
82		5.152212	Err:508	
83		5.215044	Err:508	
84		5.277876	Err:508	
85		5.340708	Err:508	
86		5.403539	Err:508	
87		5.466371	Err:508	
88		5.529203	Err:508	
89		5.592035	Err:508	
90		5.654867	Err:508	2.427051
91		5.717699	Err:508	
92		5.78053	Err:508	

93
94
95
96
97
98
99

5.843362 Err:508
5.906194 Err:508
5.969026 Err:508
6.031858 Err:508
6.09469 Err:508
6.157522 Err:508
6.220353 Err:508

Index	Data	Smooth Smooth	
		SG	Wts
0	0.424047	Err:508	Err:508
1	0.426167	Err:508	Err:508
2	0.588218	Err:508	Err:508
3	0.298215	Err:508	Err:508
4	0.655027	Err:508	Err:508
5	0.311573	Err:508	Err:508
6	0.672289	Err:508	Err:508
7	0.560037	Err:508	Err:508
8	0.026531	Err:508	Err:508
9	0.213634	Err:508	Err:508
10	0.899942	Err:508	Err:508
11	0.367753	Err:508	Err:508
12	0.468984	Err:508	Err:508
13	0.627856	Err:508	Err:508
14	0.079983	Err:508	Err:508
15	0.290841	Err:508	Err:508
16	0.409883	Err:508	Err:508
17	0.457373	Err:508	Err:508
18	0.598791	Err:508	Err:508
19	0.52675	Err:508	Err:508
20	0.3876	Err:508	Err:508
21	0.455432	Err:508	Err:508
22	0.778475	Err:508	Err:508
23	0.796244	Err:508	Err:508
24	0.08509	Err:508	Err:508
25	0.994466	Err:508	Err:508
26	0.324838	Err:508	Err:508
27	-0.007341	Err:508	Err:508
28	0.667727	Err:508	Err:508
29	0.341793	Err:508	Err:508
30	0.339821	Err:508	Err:508
31	0.975367	Err:508	Err:508
32	0.106476	Err:508	Err:508
33	0.270673	Err:508	Err:508
34	0.877473	Err:508	Err:508
35	0.730755	Err:508	Err:508
36	0.248515	Err:508	Err:508

Weights	
1	
2	
3	
2	
1	
9 Divisor	

2 SmoothNum
0 DerivNum

For row ver

37	0.90489	Err:508	Err:508
38	0.54678	Err:508	Err:508
39	1.016805	Err:508	Err:508
40	0.578917	Err:508	Err:508
41	0.295606	Err:508	Err:508
42	0.240673	Err:508	Err:508
43	1.017725	Err:508	Err:508
44	0.989523	Err:508	Err:508
45	0.197795	Err:508	Err:508
46	0.308024	Err:508	Err:508
47	0.243192	Err:508	Err:508
48	0.029114	Err:508	Err:508
49	0.633745	Err:508	Err:508
50	0.747063	Err:508	Err:508
51	0.500093	Err:508	Err:508
52	0.077143	Err:508	Err:508
53	0.624355	Err:508	Err:508
54	0.43396	Err:508	Err:508
55	0.088871	Err:508	Err:508
56	0.559792	Err:508	Err:508
57	0.513646	Err:508	Err:508
58	0.918661	Err:508	Err:508
59	0.551599	Err:508	Err:508
60	0.016619	Err:508	Err:508
61	0.961202	Err:508	Err:508
62	0.942313	Err:508	Err:508
63	0.331129	Err:508	Err:508
64	0.683808	Err:508	Err:508
65	0.786607	Err:508	Err:508
66	0.808009	Err:508	Err:508
67	0.850055	Err:508	Err:508
68	0.75776	Err:508	Err:508
69	0.379798	Err:508	Err:508
70	0.958668	Err:508	Err:508
71	0.393922	Err:508	Err:508
72	0.856866	Err:508	Err:508
73	0.015407	Err:508	Err:508
74	0.381266	Err:508	Err:508
75	0.663137	Err:508	Err:508
76	0.762058	Err:508	Err:508
77	0.474249	Err:508	Err:508
78	0.153008	Err:508	Err:508
79	0.253495	Err:508	Err:508
80	0.166244	Err:508	Err:508

81	0.135595	Err:508	Err:508
82	0.987579	Err:508	Err:508
83	0.996722	Err:508	Err:508
84	-0.016731	Err:508	Err:508
85	0.453525	Err:508	Err:508
86	0.744685	Err:508	Err:508
87	0.441727	Err:508	Err:508
88	0.980077	Err:508	Err:508
89	0.695799	Err:508	Err:508
90	0.650383	Err:508	Err:508
91	-0.043253	Err:508	Err:508
92	-0.002745	Err:508	Err:508
93	0.625888	Err:508	Err:508
94	0.96763	Err:508	Err:508
95	1.045383	Err:508	Err:508
96	0.083841	Err:508	Err:508
97	0.619348	Err:508	Err:508
98	0.76099	Err:508	Err:508
99	0.62342	Err:508	Err:508

Huckel MO Calculations with Diagonalize & MODensity

Benzene

0	1	0	0	0	1
1	0	1	0	0	0
0	1	0	1	0	0
0	0	1	0	1	0
0	0	0	1	0	1
1	0	0	0	1	0

Coefficients

Charges & Bond Orders

###	###	###	###	###	###	###	###	###	###
###	###	###	###	###	###	###	###	###	###
###	###	###	###	###	###	###	###	###	###
###	###	###	###	###	###	###	###	###	###
###	###	###	###	###	###	###	###	###	###
###	###	###	###	###	###	###	###	###	###
###	###	###	###	###	###	2	2	2	0

Orbital Energies

Occupancies

allyl

CycloPropene

0	1	1	0	1	1
1	0	1	1	0	1
0	1	0	1	1	0

Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	###	###	###
Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	###	###	###
Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	###	###	###
Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	2	0.5	0.5

Butene

0	1	0	0
1	0	1	0
0	1	0	1
0	0	1	1

Err:508	Err:508	Err:508	Err:508	###	###	###	###
Err:508	Err:508	Err:508	Err:508	###	###	###	###
Err:508	Err:508	Err:508	Err:508	###	###	###	###
Err:508	Err:508	Err:508	Err:508	###	###	###	###
Err:508	Err:508	Err:508	Err:508	2	2	0	0

Napthalene

0	1	0	0	0	0	0	0	0	0	1
1	0	1	0	0	0	1	0	0	0	0
0	1	0	1	0	0	0	0	0	0	0
0	0	1	0	1	0	0	0	0	0	0
0	0	0	1	0	1	0	0	0	0	0
0	0	0	0	1	0	1	0	0	0	0
0	1	0	0	0	1	0	1	0	0	0
0	0	0	0	0	0	1	0	1	0	0
0	0	0	0	0	0	0	1	0	1	0
1	0	0	0	0	0	0	0	1	0	0

Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508
Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508
Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508
Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508
Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508
Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508
Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508
Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508
Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508
Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508

2	2	2	2	2	0	0	0	0	0
###	###	###	###	###	###	###	###	###	###
###	###	###	###	###	###	###	###	###	###

###	###	###	###	###	###	###	###	###	###
###	###	###	###	###	###	###	###	###	###
###	###	###	###	###	###	###	###	###	###
###	###	###	###	###	###	###	###	###	###
###	###	###	###	###	###	###	###	###	###
###	###	###	###	###	###	###	###	###	###
###	###	###	###	###	###	###	###	###	###
###	###	###	###	###	###	###	###	###	###
###	###	###	###	###	###	###	###	###	###
###	###	###	###	###	###	###	###	###	###

Note:

ctors see =>

Index	0	1	2	3	4	5	6
IndVarH	2	2.1	2.2	2.3	2.4	2.5	2.6
DepVarH	619.7151	254.9522	504.8611	690.3672	638.3767	805.3697	471.9897
Yest	Err:511	Err:511	Err:511	Err:511	Err:511	Err:511	Err:511
Resid	Err:511	Err:511	Err:511	Err:511	Err:511	Err:511	Err:511
	Err:511	Err:511	Err:511	Err:511	Err:511	Err:511	Err:511

for the 100 x-values

ctors see =>

Note:

Diff
Err:508
Err:508
Err:508
Err:508
Err:508

Index	0	1	2	3	4	5
IndVarSH	0	0.628319	1.256637	1.884956	2.3	3.141593
DepVarSH	3	2.427051	0.927051	-0.927051	1.5	-3
	0	Err:508	Err:508	Err:508	Err:508	
	1	Err:508	Err:508	Err:508	Err:508	
	2	Err:508	Err:508	Err:508	Err:508	

Err:508
Err:508
Err:508
Err:508
Err:508
Err:508
Err:508

Note:

Index	0	1	2	3	4	5	6
DataH	0.776904	0.203105	0.709906	0.151812	0.421547	0.030714	0.24274
SmoothSG	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508
SmoothWT	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508

ctors see =>

###	###
###	###
###	###
###	###
###	###
###	###
###	###
0	0

7	8	9	10	11	12	13	14	15	16
2.7	2.8	2.9	3	3.1	3.2	3.3	3.4	3.5	3.6
566.8193	383.0008	398.7258	759.1758	1132.11	743.4951	821.8927	1352.934	889.918	921.1335
Err:511	Err:511	Err:511	Err:511	Err:511	Err:511	Err:511	Err:511	Err:511	Err:511
Err:511	Err:511	Err:511	Err:511	Err:511	Err:511	Err:511	Err:511	Err:511	Err:511
Err:511	Err:511	Err:511	Err:511	Err:511	Err:511	Err:511	Err:511	Err:511	Err:511

6	7	8	9	10
3.769911	4.4	5.026548	5.654867	6.283185
-2.427051	2	0.927051	2.427051	3

array is always
ray regardless of the input

7	8	9	10	11	12	13	14	15	16
0.320401	0.794019	0.639079	0.607136	0.070191	0.573441	0.860871	0.319506	0.506149	0.161321
Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508
Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508

17	18	19
3.7	3.8	3.9
1808.001	1047.614	1245.865
Err:511	Err:511	Err:511
Err:511	Err:511	Err:511
Err:511	Err:511	Err:511

17	18	19	20	21	22	23	24	25	26
0.359509	0.164336	0.588703	0.56226	0.823118	0.142391	-0.021943	0.941548	0.342674	0.886321
Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508
Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508

27	28	29	30	31	32	33	34	35	36
0.012024	0.205209	0.180247	0.602979	1.004531	0.155333	0.083096	0.35354	0.426795	0.726994
Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508
Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508

37	38	39	40	41	42	43	44	45	46
0.909162	0.191538	0.578417	-0.058198	0.00415	0.255656	0.643731	0.403512	0.69889	0.360633
Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508
Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508

47	48	49	50	51	52	53	54	55	56
0.170547	0.649684	1.028354	0.125304	0.818227	0.576102	0.196654	0.647845	0.247754	0.965824
Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508
Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508

57	58	59	60	61	62	63	64	65	66
0.917358	0.821328	0.657967	0.479046	0.326288	0.096917	0.723525	0.064801	0.884314	0.826019
Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508
Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508

67	68	69	70	71	72	73	74	75	76
0.563658	0.832665	0.174537	0.467583	0.02896	0.677702	0.009262	0.044813	0.506984	0.520551
Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508
Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508

77	78	79	80	81	82	83	84	85	86
0.569844	0.011874	0.077337	0.957093	0.923507	0.16537	0.788495	0.547063	0.646579	0.042451
Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508
Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508

87	88	89	90	91	92	93	94	95	96
0.696442	0.141966	1.029331	0.270877	0.884844	0.431714	0.704621	0.832303	0.361255	0.395356
Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508
Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508	Err:508

97	98	99
0.454599	0.534566	0.95616
Err:508	Err:508	Err:508
Err:508	Err:508	Err:508

Xlmath v3.0 Custom Fitting Examples

The Xlmath CustomFit tool has been significantly revised. To use the revised tool, you must define a column of calculated Y values adjacent to and to the right of the column which contains the measured Y values. In example 1 below, the measured values are in column E the calculated in column C. When defining the calculated values, refer to the parameters n you will input into CustomFit. DO NOT refer to the output parameters in columns D to F. CustomFit works by changing the parameters on the sheet, waiting for Excel to recalculate Y values, and then reading the newly evaluated Y values. You will not see this on the screen since the screen echo is turned off. When the calculation is complete, you will be prompted before overwriting the parameters.

Example 1 -- $Y = p_0 + p_1 \cdot \text{EXP}(p_2 \cdot x)$

IndVar	Measured Y	Calculated Y	
-5	127	#NAME?	523.305536 -156.94784 -0.1996646 Final parameter
-3	151	#NAME?	100.066637 111.315698 0.10692545 Std. deviations
-1	379	#NAME?	2.43047611 0.56344331 0.00608058 Eigenvalues
1	421	#NAME?	2.44948974 3.64375345 2339.5307 Scale vectors
3	460	#NAME?	
5	426	#NAME?	

_p01	_p11	_p21	
523.305536	-156.94784	-0.1996646	Initial values
10000	10000	10000	Upper bounds
-1000	-1000	-1000	Lower bounds
400	-140	-0.13	start parameters

Example 2 -- $Y = p_0 \cdot x / (p_1 + x)$

IndVar	Measured Y	Calculated Y		Deviations
1.68	0.172	0.29577465	0.42380958 2.45193659 Final parameter	0.01532016346
3.33	0.25	0.45429741	0.00829087 0.16742349 Std. deviations	0.04173743088
5	0.286	0.55555556	1.88955331 0.11044669 Eigenvalues	0.07266019753
6.67	0.303	0.62511715	1.7088967 0.08462518 Scale vectors	0.1037594589
10	0.334	0.71428571		0.14461722449

20	0.384	0.83333333	
_p02	_p12		
1	4	Initial parameters	
10000	10000	Upper bounds	
0.000001	0.000001	Lower bounds	
1	4	start parameters	

0.20190044444
0.5799949197
0.17982144213

Example 3 -- $Y = p_0 + (p_1 - p_0) * \exp(-p_2 * x)$

This example can be found in "C curve fitting" by Jens-Georg Reich, ISBN 0-07-051761-4

IndVar	Measured Y	Calculated Y				
0.0707	0.9411	0.98263376	0.39996858	1.00001637	1.99984956	Final parameter
0.1	0.9011	0.97561471	0.0069376	0.00972573	0.06905219	Std. deviations
0.1414	0.8266	0.96587069	2.29314005	0.58822552	0.11863442	Eigenvalues
0.166	0.829	0.96017557	2.66798472	1.91540946	0.28415285	Scale vectors
0.2	0.7774	0.95241871				
0.31	0.7311	0.92820759				
0.4	0.68	0.90936538				
0.5657	0.5697	0.87681641				
0.69	0.5868	0.85411018				
0.8	0.5455	0.83516002				
1.1314	0.4356	0.78398122				
1.6	0.3912	0.72466448				
1.96	0.4021	0.68765555				
2.2627	0.4304	0.66129873				
2.42	0.4174	0.64909864				

_p03	_p13	_p23
0.5	1	0.5
10000	10000	10000
0.000001	0.000001	0.000001
0.5	1	0.5 start



Example 4 -- $Y = (x1*p3)/(p4*(p1*(p0/x1+1)+x1)/x2+x1+p2)$

This is an example of a two variable problem contributed by "julehto@polaris.cc.utu.fi"

X1	X2	Measured Y	Calculated Y	Dev	Dev^2
80	300	3.38595991	#VALUE!	#VALUE!	#VALUE!
80	150	3.5768975	#VALUE!	#VALUE!	#VALUE!
80	50	3.61508502	#VALUE!	#VALUE!	#VALUE!
80	10	2.80041797	#VALUE!	#VALUE!	#VALUE!
80	5	2.29125107	#VALUE!	#VALUE!	#VALUE!
80	3	1.98575093	#VALUE!	#VALUE!	#VALUE!
80	1	1.04379215	#VALUE!	#VALUE!	#VALUE!
80	0.5	0.53462525	#VALUE!	#VALUE!	#VALUE!
60	300	3.2968557	#VALUE!	#VALUE!	#VALUE!
60	150	3.2968557	#VALUE!	#VALUE!	#VALUE!
60	50	3.0677306	#VALUE!	#VALUE!	#VALUE!
60	10	2.74950128	#VALUE!	#VALUE!	#VALUE!
60	5	2.35489693	#VALUE!	#VALUE!	#VALUE!
60	3	2.10031348	#VALUE!	#VALUE!	#VALUE!
60	1	1.22200057	#VALUE!	#VALUE!	#VALUE!
60	0.5	0.61100028	#VALUE!	#VALUE!	#VALUE!
40	300	2.42393321	#VALUE!	#VALUE!	#VALUE!
40	150	3.6478	#VALUE!	#VALUE!	#VALUE!
40	50	3.4983	#VALUE!	#VALUE!	#VALUE!
40	10	3.1694	#VALUE!	#VALUE!	#VALUE!
40	5	2.76575	#VALUE!	#VALUE!	#VALUE!
40	3	2.3023	#VALUE!	#VALUE!	#VALUE!
40	1	1.382875	#VALUE!	#VALUE!	#VALUE!
40	0.5	0.725075	#VALUE!	#VALUE!	#VALUE!
30	300	2.47572665	#VALUE!	#VALUE!	#VALUE!
30	150	2.5275201	#VALUE!	#VALUE!	#VALUE!

6.3046832971006

8.2617871705051

3.4685115170004

0.0795004704043

30	50	2.49644403	#VALUE!	#VALUE!	#VALUE!
30	20	2.26855288	#VALUE!	#VALUE!	#VALUE!
30	10	2.14424861	#VALUE!	#VALUE!	#VALUE!
30	5	1.89564007	#VALUE!	#VALUE!	#VALUE!
30	2	1.50200989	#VALUE!	#VALUE!	#VALUE!
30	0.5	0.60080396	#VALUE!	#VALUE!	#VALUE!
20	300	1.91020574	#VALUE!	#VALUE!	#VALUE!
20	150	2.37519003	#VALUE!	#VALUE!	#VALUE!
20	50	2.14898145	#VALUE!	#VALUE!	#VALUE!
20	20	1.96047431	#VALUE!	#VALUE!	#VALUE!
20	10	1.80966859	#VALUE!	#VALUE!	#VALUE!
20	5	1.59602716	#VALUE!	#VALUE!	#VALUE!
20	2	1.10590858	#VALUE!	#VALUE!	#VALUE!
20	0.5	0.41471572	#VALUE!	#VALUE!	#VALUE!
15	300	1.93707483	#VALUE!	#VALUE!	#VALUE!
15	150	1.82312925	#VALUE!	#VALUE!	#VALUE!
15	50	1.76097712	#VALUE!	#VALUE!	#VALUE!
15	20	1.5952381	#VALUE!	#VALUE!	#VALUE!
15	10	1.39842301	#VALUE!	#VALUE!	#VALUE!
15	5	1.19124923	#VALUE!	#VALUE!	#VALUE!
15	3	0.87012987	#VALUE!	#VALUE!	#VALUE!
15	1	0.40398887	#VALUE!	#VALUE!	#VALUE!
10	300	1.55832573	#VALUE!	#VALUE!	#VALUE!
10	150	1.63372859	#VALUE!	#VALUE!	#VALUE!
10	50	1.54575859	#VALUE!	#VALUE!	#VALUE!
10	20	1.26928144	#VALUE!	#VALUE!	#VALUE!
10	10	1.05564001	#VALUE!	#VALUE!	#VALUE!
10	5	0.82943144	#VALUE!	#VALUE!	#VALUE!
10	3	0.57808858	#VALUE!	#VALUE!	#VALUE!
10	1	0.34559643	#VALUE!	#VALUE!	#VALUE!
5	300	1.11847573	#VALUE!	#VALUE!	#VALUE!
5	150	1.10590858	#VALUE!	#VALUE!	#VALUE!
5	50	0.9928043	#VALUE!	#VALUE!	#VALUE!
5	20	0.86713287	#VALUE!	#VALUE!	#VALUE!
5	10	0.71632715	#VALUE!	#VALUE!	#VALUE!
5	5	0.42728286	#VALUE!	#VALUE!	#VALUE!
5	3	0.36444715	#VALUE!	#VALUE!	#VALUE!
5	1	0.20107429	#VALUE!	#VALUE!	#VALUE!
3	300	0.82869511	#VALUE!	#VALUE!	#VALUE!
3	150	0.77690167	#VALUE!	#VALUE!	#VALUE!
3	50	0.69403216	#VALUE!	#VALUE!	#VALUE!
3	20	0.58008658	#VALUE!	#VALUE!	#VALUE!
3	10	0.40398887	#VALUE!	#VALUE!	#VALUE!
3	5	0.2796846	#VALUE!	#VALUE!	#VALUE!

3	3	0.21753247	#VALUE!	#VALUE!	#VALUE!
3	1	0.09115646	#VALUE!	#VALUE!	#VALUE!
2	300	0.73829201	#VALUE!	#VALUE!	#VALUE!
2	300	0.62809917	#VALUE!	#VALUE!	#VALUE!
2	150	0.57300275	#VALUE!	#VALUE!	#VALUE!
2	100	0.66115702	#VALUE!	#VALUE!	#VALUE!
2	50	0.45179063	#VALUE!	#VALUE!	#VALUE!
2	20	0.41873278	#VALUE!	#VALUE!	#VALUE!
2	10	0.34710744	#VALUE!	#VALUE!	#VALUE!
2	5	0.21157025	#VALUE!	#VALUE!	#VALUE!
2	3	0.13553719	#VALUE!	#VALUE!	#VALUE!
2	1	0.05399449	#VALUE!	#VALUE!	#VALUE!
1	300	0.41763085	#VALUE!	#VALUE!	#VALUE!
1	150	0.44628099	#VALUE!	#VALUE!	#VALUE!
1	50	0.36253444	#VALUE!	#VALUE!	#VALUE!
1	20	0.32286501	#VALUE!	#VALUE!	#VALUE!
1	10	0.22369146	#VALUE!	#VALUE!	#VALUE!
1	5	0.14876033	#VALUE!	#VALUE!	#VALUE!
1	4	0.12451791	#VALUE!	#VALUE!	#VALUE!
1	3	0.09917355	#VALUE!	#VALUE!	#VALUE!

#VALUE! SSQ

#VALUE! SSQ as % of mean Y value

_p04	_p14	_p24	_p34	_p44
0.3	111.2509	9.739352	3.538908	0.7553023
1000000	1000000	1000000	1000000	1000000
-1000000	-1000000	-1000000	-1000000	-1000000

0.3 111.2509 9.739352 3.538908 0.7553023 start
 6.3046833 24.472388 16.412666 4.2223401 1.6000616 CustomFit
 6.3048492 24.472065 16.412665 4.2223405 1.6000673 Solver: auto scale, quadratic,central,Newton

Example 5 -- $Y = (x1*p3)/(p4*(p1*(p0/x1+1)+x1)/x2+x1+p2)$

This is an exact fit contributed by Oliver - "cf15@ictibm2.chemie.uni-karlsruhe.de"

IndVar	Measured Y	Calculated Y	Output values				
298	37.4686297	#NAME?	42.364066	0.0121423	-736912	-2.42846E-06	Final parameters
300	37.6002835	#NAME?	1.1905E-18	9.6795E-22	2.8799E-13	6.103823E-25	Std. deviations
400	42.2267324	#NAME?	2.92361945	0.98847764	0.0867833	0.0011196127	Eigenvalues
500	44.880453	#NAME?	4.35889894	5360.85851	1.8018E-05	8501340.2561	Scale vectors
600	46.7282226	#NAME?					
700	48.1698286	#NAME?					
800	49.3722666	#NAME?					
900	50.4153155	#NAME?					
1000	51.340994	#NAME?					

1100	52.1731412	#NAME?
1200	52.9260992	#NAME?
1300	53.608916	#NAME?
1400	54.2275289	#NAME?
1500	54.7859646	#NAME?
1600	55.2870322	#NAME?
1700	55.7327397	#NAME?
1800	56.1245536	#NAME?
1900	56.4635647	#NAME?
2000	56.750598	#NAME?

_p05	_p15	_p25	_p35	
39	0.01023	0	0	Initial values
1000000	1000000	1000000	1000000	Upper bounds
-1000000	-1000000	-1000000	-1000000	Lower bounds
39.024	0.01023	0	0	initial values

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Deviations

#NAME?
#NAME?
#NAME?
#NAME?
#NAME?
#NAME?


#NAME? SSQ

#NAME? SSQ as % of mean Y value



SSQ

SSQ as % of mean Y value



Dev^2
0.00172505
0.00555244
0.01939632
0.01720703
0.03063155
0.0388514
0.05260848
0.09432049
0.07145473
0.08390293
0.12136947
0.11119856
0.08154197
0.05331422
0.05368426

0.83675891 SSQ

0.02495364 SSQ as % of mean Y value



24.47238767	16.4126655	4.2223401019798	1.600061606	Final parameters
21.37547631	1.85528087	0.16850570000147	0.482980839	Std. deviations
1.033761356	0.416992515	0.0645399593173925	0.016194653	Eigenvalues
0.062083024	0.312342152	3.8011438146552	1.970171433	Scale vectors



Deviations

- #NAME?
- #NAME?
- #NAME?
- #NAME?
- #NAME?
- #NAME?
- #NAME?
- #NAME?
- #NAME?

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#NAME?
#NAME?
#NAME?

#NAME? SSQ

#NAME? SSQ as % of mean Y value

Dialog Box Curve Fitting and MO Calculation Demo with XLMATH v3.0

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This worksheet demonstrates the dialog box commands in XLMATH.XLL.
 Input values are hi-lited in green & output in magenta

Polynomial Curve Fitting

Double click for Notes:

Index	IndVar	DepVar	Yest	Resid		For Order 2
0	2	414.841497	518.524792	103.683295	1385.47624	polynomial
1	2.1	573.596586	519.384578	-54.212009	-854.49819	coefficients
2	2.2	432.31411	524.454589	92.1404784	210.511233	
3	2.3	384.331612	533.734824	149.403212	1845.75154	standard
4	2.4	889.992239	547.225284	-342.76695	1284.31115	errors of
5	2.5	884.364063	564.925969	-319.43809	216.859077	coefficients
6	2.6	365.843123	586.836879	220.993756	287.336231	see
7	2.7	412.530905	612.958013	200.427108	0.4340472	rsqrval
8	2.8	743.2976	643.289371	-100.00823	0.65882259	rval
9	2.9	812.530967	677.830955	-134.70001	0	cferror
10	3	397.261869	716.582763	319.320894	0	empty
11	3.1	784.136899	759.544796	-24.592103	0	
12	3.2	699.318422	806.717053	107.398631	0	
13	3.3	1189.58915	858.099535	-331.48962	0	
14	3.4	1142.22196	913.692242	-228.52972	0	
15	3.5	1155.84058	973.495173	-182.3454	0	
16	3.6	674.155962	1037.50833	363.352367	0	
17	3.7	645.668253	1105.73171	460.063457	0	
18	3.8	924.644885	1178.16532	253.52043	0	
19	3.9	1807.03063	1254.80914	-552.22149	0	

Cubic Splines

Demo function is $3 \cdot \cos(x)$ where x is from 0 to $2 \cdot \pi$
 X-values of 2.3 and 4.4 are altered

SplineX contains 100 x-values
 SplineY contains interpolated values

Index	IndVarS	DepVarS	CoefS				SplineX
0	0	3	3	-0.8089001	0	-0.2608426	0
1	0.62831853	2.42705098	2.42705098	-1.1178298	-0.4916768	-2.4331389	0.06283185
2	1.25663706	0.92705098	0.92705098	-4.6173833	-5.0780356	12.3032089	0.12566371
3	1.88495559	-0.927051	-0.927051	3.57270557	18.1129668	-30.434487	0.18849556

4	2.3	1.5	1.5	2.87997291	-19.782024	11.8900002	0.25132741
5	3.14159265	-3	-3	-5.1525547	10.237587	-0.9322416	0.31415927
6	3.76991118	-2.427051	-2.427051	6.60827383	8.48035294	-12.406617	0.37699112
7	4.4	2	2	2.51830041	-14.971459	13.1178146	0.43982297
8	5.02654825	0.92705098	0.92705098	-0.7936882	9.68537199	-7.3571498	0.50265482
9	5.65486678	2.42705098	2.42705098	2.6638502	-4.1825287	2.21890038	0.56548668
10	6.28318531	3					0.62831853
11							0.69115038
12							0.75398224
13							0.81681409
14							0.87964594
15							0.9424778
16							1.00530965
17							1.0681415
18							1.13097336
19							1.19380521
20							1.25663706
21							1.31946891
22							1.38230077
23							1.44513262
24							1.50796447
25							1.57079633
26							1.63362818
27							1.69646003
28							1.75929189
29							1.82212374
30							1.88495559
31							1.94778745
32							2.0106193
33							2.07345115
34							2.136283
35							2.19911486
36							2.26194671
37							2.3
38							2.38761042
39							2.45044227
40							2.51327412
41							2.57610598
42							2.63893783
43							2.70176968
44							2.76460154
45							2.82743339
46							2.89026524
47							2.95309709

48	3.01592895
49	3.0787608
50	3.14159265
51	3.20442451
52	3.26725636
53	3.33008821
54	3.39292007
55	3.45575192
56	3.51858377
57	3.58141563
58	3.64424748
59	3.70707933
60	3.76991118
61	3.83274304
62	3.89557489
63	3.95840674
64	4.0212386
65	4.08407045
66	4.1469023
67	4.20973416
68	4.27256601
69	4.33539786
70	4.4
71	4.46106157
72	4.52389342
73	4.58672527
74	4.64955713
75	4.71238898
76	4.77522083
77	4.83805269
78	4.90088454
79	4.96371639
80	5.02654825
81	5.0893801
82	5.15221195
83	5.2150438
84	5.27787566
85	5.34070751
86	5.40353936
87	5.46637122
88	5.52920307
89	5.59203492
90	5.65486678
91	5.71769863

92
93
94
95
96
97
98
99

5.78053048
5.84336234
5.90619419
5.96902604
6.03185789
6.09468975
6.1575216
6.22035345

Data Smoothing

Index	Data	Smooth SG	Smooth Wts	Weights
0	0.84067272	0.66374887	0.78234375	1
1	0.98038652	0.66374887	0.78234375	2
2	0.91486494	0.66374887	0.78234375	3
3	0.69867428	0.66374887	0.64902688	2
4	0.09770457	0.46779949	0.48198523	1
5	0.73969356	0.39252303	0.45958717	
6	0.25315277	0.44239762	0.4220618	
7	0.51681489	0.45664181	0.41711432	
8	0.42837644	0.27731051	0.33281791	
9	0.10083223	0.31873628	0.28142729	
10	0.22178488	0.2052047	0.24670788	
11	0.41321142	0.18765161	0.2687165	
12	0.09855251	0.3899329	0.33713585	
13	0.43730722	0.42237752	0.42348643	
14	0.81574299	0.50656802	0.50652381	
15	0.2576538	0.58134268	0.48643656	
16	0.62301079	0.39480537	0.43188642	
17	0.29015287	0.32034728	0.35688939	
18	0.1065891	0.34945589	0.34677031	
19	0.62469231	0.34029306	0.41357847	
20	0.34846438	0.57450761	0.495515	
21	0.64786949	0.58749957	0.53431036	
22	0.76252917	0.41207775	0.47319859	
23	0.01850534	0.40779482	0.38695093	
24	0.28998573	0.41095797	0.39920061	
25	0.67414309	0.36696611	0.43413832	
26	0.57502226	0.46793345	0.46744204	
27	0.13629431	0.51545795	0.46431236	
28	0.571051	0.51990444	0.51085218	

29	0.80363869	0.48513845	0.52676475
30	0.42962833	0.52244086	0.49895001
31	0.19231366	0.48791366	0.46683652
32	0.6387094	0.46796648	0.50164064
33	0.68427352	0.50413465	0.5300417
34	0.41583488	0.58546848	0.53725704
35	0.41615249	0.52379819	0.52869974
36	0.74824727	0.49334138	0.56337668
37	0.4974024	0.67629324	0.61813795
38	0.58270368	0.69601944	0.64529655
39	0.99297993	0.56628535	0.63414274
40	0.33054597	0.60006833	0.58254349
41	0.40444318	0.65489232	0.59449777
42	0.87370362	0.56227186	0.59934328
43	0.73567128	0.53481398	0.55598532
44	0.16220373	0.51900963	0.47743194
45	0.32059614	0.40083405	0.45544732
46	0.82403778	0.51977308	0.54212857
47	0.42908314	0.64224382	0.56092151
48	0.74548155	0.48336973	0.52878454
49	0.3014094	0.49192858	0.47739919
50	0.23759339	0.48922747	0.46772616
51	0.99713153	0.49567718	0.50967918
52	0.15419183	0.47348742	0.40548375
53	0.51073817	0.29300505	0.30571469
54	-0.0665545	0.02300735	0.15243238
55	0.04681156	0.19575205	0.22314157
56	0.3022637	0.33381775	0.38458187
57	0.88568292	0.67268018	0.63268635
58	0.75601124	0.83570091	0.74979917
59	0.87376693	0.83862223	0.76462262
60	0.65899545	0.67241141	0.65673175
61	0.54460651	0.54696212	0.52979338
62	0.34084129	0.29416219	0.3778871
63	0.26088046	0.318504	0.33600847
64	0.10849059	0.30779654	0.33959441
65	0.79816461	0.46307163	0.45731246
66	0.27194647	0.45976435	0.4546941
67	0.69956373	0.51991896	0.50707633
68	0.17246022	0.43494185	0.48031301
69	0.77801775	0.65858426	0.6091003
70	0.57832696	0.6339764	0.62385048
71	0.94671133	0.68105126	0.64196161
72	0.2577551	0.51820457	0.51288491

73	0.48733865	0.46678185	0.46264521
74	0.39627198	0.37851713	0.39934828
75	0.44702546	0.37612892	0.3613798
76	0.27883529	0.25382862	0.27765546
77	0.07378865	0.22669168	0.22133583
78	0.22449311	0.1886848	0.2079501
79	0.31697428	0.11801307	0.21152622
80	0.13771045	0.31035336	0.28905167
81	0.15461742	0.40857474	0.39217221
82	1.02065718	0.50544926	0.5553414
83	0.43198811	0.74714643	0.62161283
84	0.62517954	0.64793661	0.60463662
85	0.85226024	0.44009414	0.53029611
86	-0.0229629	0.48348716	0.45386984
87	0.57946295	0.50188916	0.50183431
88	0.66509151	0.50440647	0.52385856
89	0.64160255	0.59645186	0.52149926
90	0.30028444	0.36289075	0.39166082
91	0.25847082	0.25005276	0.32584627
92	0.15885584	0.38674887	0.37091596
93	0.59732087	0.47957614	0.46820064
94	0.84980834	0.50281192	0.50917382
95	0.14604396	0.52869258	0.44402438
96	0.38755386	0.3291642	0.37942219
97	0.48604229	0.3291642	0.37074377
98	0.1381573	0.3291642	0.37074377
99	0.68110082	0.3291642	0.37074377

Huckel MO Calculations with Diagonalize & MODensity

Benzene

0	1	0	0	0	1
1	0	1	0	0	0
0	1	0	1	0	0
0	0	1	0	1	0
0	0	0	1	0	1
1	0	0	0	1	0

Coefficients

Charges & Bond Orders

0.40824828	0.2036262	-0.5402497	-0.5716132	0.08118999	0.4082481	1	0.66666668
0.40824828	-0.3660568	-0.4464703	0.35611951	0.45443655	-0.4082479	0.66666668	1
0.40824829	-0.5696831	0.09377935	0.21549355	-0.5356268	0.40824805	8.4106E-09	0.66666666
0.4082483	-0.2036262	0.54024966	-0.5716129	0.08119047	-0.4082485	-0.33333333	-1.309E-08
0.4082483	0.36605682	0.4464703	0.35611915	0.45443607	0.40824872	-1.31E-08	-0.33333333

0.40824829	0.56968305	-0.0937794	0.2154939	-0.5356263	-0.4082485	0.66666666	4.6796E-09
2	1	1	-1	-1	-2	2	2
Orbital Energies						Occupancies	

allyl

0	1	0
1	0	1
0	1	0

0.50000001	-0.7071068	0.5	1	0.70710679	-1.051E-13
0.70710678	8.7025E-09	-0.7071068	0.70710679	1	0.70710677
0.49999999	0.70710679	0.5	-1.051E-13	0.70710677	1
1.41421356	2.3112E-16	-1.4142136	2	1	0
Orbital energies			Occupancies		

CycloPropene

0	1	1
1	0	1
1	1	0

Charges & Bond Orders

0.57735027	0.70710678	-0.4082483	1	0.5	0.5
0.57735027	-0.7071068	-0.4082483	0.5	1	0.5
0.57735027	0	0.81649658	0.5	0.5	1
2	-1	-1	2	0.5	0.5
Orbital energies			Occupancies		

For horizontal see =>

Sample Calc'n
518.524792

IndVarH	2	2.1
DepVarH	414.841497	573.596586
	518.524792	519.384578
	103.683295	-54.212009
	1385.47624	-854.49819

alues
ated Y values for the 100 x-values

Horizontal
below

Spline-Y	Original-Y	Diff						
3	3	0	IndVarSH	0	0.62831853	1.25663706	1.88495559	
2.9491106		0.04496958	DepVarSH	3	2.42705098	0.92705098	-0.927051	
2.89783299		0.07851111						
2.84577896		0.10108279						

2.79256029		0.11318919	0.92705098	-4.6173833	-5.0780356	12.3032089
2.73778877		0.11538078		-0.927051	3.57270557	18.1129668 -30.434487
2.68107619		0.10825327		1.5	2.87997291	-19.782024 11.8900002
2.62203433		0.09244683		-3	-5.1525547	10.237587 -0.9322416
2.56027498		0.06864506		-2.427051	6.60827383	8.48035294 -12.406617
2.49540994		0.03757384		2	2.51830041	-14.971459 13.1178146
2.42705098	2.42705098	0		0.92705098	-0.7936882	9.68537199 -7.3571498
2.35427106		-0.0427313		2.42705098	2.6638502	-4.1825287 2.21890038
2.27398778		-0.0870819				
2.18257988		-0.1289386				
2.07642612		-0.1641542				
1.95190527		-0.1885495				
1.80539607		-0.1979157				
1.63327729		-0.1880163				
1.43192768		-0.1545898				
1.19772599		-0.0933523				
0.92705098	0.92705098	0				
0.61993677		0.12613289				
0.29103888		0.27110507				
-0.0413318		0.41733152				
-0.3588644		0.54723599				
-0.6432481		0.64324807				
-0.8761719		0.68780031				
-1.0393249		0.66332524				
-1.1143964		0.55225246				
-1.0830754		0.33700572				
-0.927051	-0.927051	0				
-0.6386134		-0.4657602				
-0.2524573		-1.0248806				
0.18612171		-1.6313827				
0.63182791		-2.2393083				
1.03936563		-2.8027214				
1.36343918		-3.2757111				
1.5	1.5	-3.4988281				
1.60847259		-3.7953785				
1.52603032		-3.83757				
1.32976587		-3.7568169				
1.03737515		-3.5703589				
0.66655404		-3.2954741				
0.23499847		-2.9494796				
-0.2395957		-2.5497338				
-0.7395325		-2.1136371				
-1.2471161		-1.6586334				
-1.7446505		-1.2022112				

-2.2144399		-0.7619042
-2.6387884		-0.3552918
-3	-3	0
-3.2835594		0.28947924
-3.4876736		0.51132946
-3.6137299		0.66686812
-3.6631158		0.75736632
-3.6372188		0.78404926
-3.5374263		0.74809689
-3.3651259		0.65064472
-3.1217049		0.49278482
-2.8085507		0.27556696
-2.427051	-2.427051	0
-1.9814393		-0.3301005
-1.4873341		-0.6995717
-0.9632004		-1.0904409
-0.4275029		-1.4847691
0.10129375		-1.8646495
0.60472462		-2.212205
1.06432497		-2.509586
1.46163001		-2.7389679
1.77817496		-2.8825486
2	2	-2.9219986
2.10093658		-2.8470062
2.10714155		-2.6692855
2.03363307		-2.4096328
1.8999344		-2.088306
1.72556881		-1.7255688
1.53005954		-1.341688
1.33292986		-0.9569302
1.15370304		-0.5915591
1.01190232		-0.2658327
0.92705098	0.92705098	0
0.91359345		0.1907802
0.9656589		0.31167897
1.07229767		0.37296335
1.22256011		0.38492028
1.40549655		0.35785921
1.61015735		0.30211462
1.82559285		0.22804847
2.04085339		0.14605249
2.24498932		0.06655041
2.42705098	2.42705098	0
2.57846406		-0.0454803

2.70015562	-0.0712356
2.79542803	-0.0809469
2.8675837	-0.0782542
2.91992501	-0.0667555
2.95575436	-0.0500049
2.97837414	-0.0315124
2.99108675	-0.0147426
2.99719457	-0.0031144

For row vectors see =>

DataH	0.84067272	0.98038652	0.91486494	0.69867428
SmoothSG	0.66374887	0.66374887	0.66374887	0.66374887
SmoothWt	0.78234375	0.78234375	0.78234375	0.64902688

8.4106E-09	-0.3333333	-1.31E-08	0.66666666
0.66666666	-1.309E-08	-0.3333333	4.6796E-09
	1 0.66666666	4.679E-09	-0.3333334
0.66666666		1 0.66666668	8.4117E-09
4.679E-09	0.66666668		1 0.66666666

-0.3333334	8.4117E-09	0.66666666	1
2	0	0	0

2.2	2.3	2.4	2.5	2.6	2.7	2.8	2.9
432.31411	384.331612	889.992239	884.364063	365.843123	412.530905	743.2976	812.530967
524.454589	533.734824	547.225284	564.925969	586.836879	612.958013	643.289371	677.830955
92.1404784	149.403212	-342.76695	-319.43809	220.993756	200.427108	-100.00823	-134.70001
210.511233	1845.75154	1284.31115	216.859077	287.336231	0.4340472	0.65882259	0

2.3	3.14159265	3.76991118	4.4	5.02654825	5.65486678	6.28318531
1.5	-3	-2.427051	2	0.92705098	2.42705098	3

0.09770457 0.73969356 0.25315277 0.51681489 0.42837644 0.10083223 0.22178488 0.41321142
0.46779949 0.39252303 0.44239762 0.45664181 0.27731051 0.31873628 0.2052047 0.18765161
0.48198523 0.45958717 0.4220618 0.41711432 0.33281791 0.28142729 0.24670788 0.2687165

3	3.1	3.2	3.3	3.4	3.5	3.6	3.7
397.261869	784.136899	699.318422	1189.58915	1142.22196	1155.84058	674.155962	645.668253
716.582763	759.544796	806.717053	858.099535	913.692242	973.495173	1037.50833	1105.73171
319.320894	-24.592103	107.398631	-331.48962	-228.52972	-182.3454	363.352367	460.063457
0	0	0	0	0	0	0	0

0.09855251 0.43730722 0.81574299 0.2576538 0.62301079 0.29015287 0.1065891 0.62469231
0.3899329 0.42237752 0.50656802 0.58134268 0.39480537 0.32034728 0.34945589 0.34029306
0.33713585 0.42348643 0.50652381 0.48643656 0.43188642 0.35688939 0.34677031 0.41357847

3.8	3.9
924.644885	1807.03063
1178.16532	1254.80914
253.52043	-552.22149
0	0

0.34846438 0.64786949 0.76252917 0.01850534 0.28998573 0.67414309 0.57502226 0.13629431
0.57450761 0.58749957 0.41207775 0.40779482 0.41095797 0.36696611 0.46793345 0.51545795
0.495515 0.53431036 0.47319859 0.38695093 0.39920061 0.43413832 0.46744204 0.46431236

0.571051 0.80363869 0.42962833 0.19231366 0.6387094 0.68427352 0.41583488 0.41615249
0.51990444 0.48513845 0.52244086 0.48791366 0.46796648 0.50413465 0.58546848 0.52379819
0.51085218 0.52676475 0.49895001 0.46683652 0.50164064 0.5300417 0.53725704 0.52869974

0.74824727 0.4974024 0.58270368 0.99297993 0.33054597 0.40444318 0.87370362 0.73567128
0.49334138 0.67629324 0.69601944 0.56628535 0.60006833 0.65489232 0.56227186 0.53481398
0.56337668 0.61813795 0.64529655 0.63414274 0.58254349 0.59449777 0.59934328 0.55598532

0.16220373 0.32059614 0.82403778 0.42908314 0.74548155 0.3014094 0.23759339 0.99713153
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0.15419183 0.51073817 -0.0665545 0.04681156 0.3022637 0.88568292 0.75601124 0.87376693
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0.65899545 0.54460651 0.34084129 0.26088046 0.10849059 0.79816461 0.27194647 0.69956373
0.67241141 0.54696212 0.29416219 0.318504 0.30779654 0.46307163 0.45976435 0.51991896
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0.27883529 0.07378865 0.22449311 0.31697428 0.13771045 0.15461742 1.02065718 0.43198811
0.25382862 0.22669168 0.1886848 0.11801307 0.31035336 0.40857474 0.50544926 0.74714643
0.27765546 0.22133583 0.2079501 0.21152622 0.28905167 0.39217221 0.5553414 0.62161283

0.62517954 0.85226024 -0.0229629 0.57946295 0.66509151 0.64160255 0.30028444 0.25847082
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0.15885584 0.59732087 0.84980834 0.14604396 0.38755386 0.48604229 0.1381573 0.68110082
0.38674887 0.47957614 0.50281192 0.52869258 0.3291642 0.3291642 0.3291642 0.3291642
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