Curve Fitting and MO Calculation Demo with XLMATH v3.0

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 ve

Index	IndVar	DepVar	Yest	Resid		For Order 2
0	2	551.5619	Err:511	Err:511	Err:511	**polynomial**
1	2.1	129.1071	Err:511	Err:511	Err:511	**coefficients**
2	2.2	555.4033	Err:511	Err:511	Err:511	
3	2.3	444.4936	Err:511	Err:511	Err:511	**standard**
4	2.4	449.3654	Err:511	Err:511	Err:511	**errors of**
5	2.5	906.933	Err:511	Err:511	Err:511	**coefficients**
6	2.6	508.4154	Err:511	Err:511	Err:511	**see**
7	2.7	636.6257	Err:511	Err:511	Err:511	**rsqrval**
8	2.8	527.4107	Err:511	Err:511	Err:511	**rval**
9	2.9	615.9052	Err:511	Err:511	Err:511	**cferror**
10	3	1375.393	Err:511	Err:511	Err:511	**empty**
11	3.1	1011.526	Err:511	Err:511	Err:511	
12	3.2	1219.58	Err:511	Err:511	Err:511	
13	3.3	836.7245	Err:511	Err:511	Err:511	
14	3.4	567.9705	Err:511	Err:511	Err:511	
15	3.5	1150.735	Err:511	Err:511	Err:511	
16	3.6	1568.287	Err:511	Err:511	Err:511	
17	3.7	1144.808	Err:511	Err:511	Err:511	
18	3.8	1790.906	Err:511	Err:511	Err:511	
19	3.9	1153.442	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 ve

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	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	5.843362	Err:508
94	5.906194	Err:508
95	5.969026	Err:508
96	6.031858	Err:508
97	6.09469	Err:508
98	6.157522	Err:508
99	6.220353	Err:508

Data Smoothing (view Smoothde.xlc)

Index	Data	Smooth SG	Smooth Wts
0	0.348113	Err:508	Err:508
1	0.843827	Err:508	Err:508
2	0.931143	Err:508	Err:508
3	0.243752	Err:508	Err:508
4	0.650825	Err:508	Err:508
5	0.658509	Err:508	Err:508
6	0.881206	Err:508	Err:508
7	1.042289	Err:508	Err:508
8	0.244818	Err:508	Err:508
9	0.115211	Err:508	Err:508
10	0.179857	Err:508	Err:508
11	0.668893	Err:508	Err:508
12	0.132307	Err:508	Err:508
13	0.473247	Err:508	Err:508
14	0.529464	Err:508	Err:508
15	0.636849	Err:508	Err:508
16	0.517833	Err:508	Err:508
17	0.294681	Err:508	Err:508
18	0.999608	Err:508	Err:508
19	0.635492	Err:508	Err:508
20	0.926744	Err:508	Err:508
21	-0.006448	Err:508	Err:508
22	0.214272	Err:508	Err:508
23	0.571256	Err:508	Err:508
24	0.348888	Err:508	Err:508
25	0.365365	Err:508	Err:508
26	0.257492	Err:508	Err:508
27	0.224511	Err:508	Err:508
28	0.430575	Err:508	Err:508
29	-0.000872	Err:508	Err:508
30	0.413887	Err:508	Err:508
31	0.758211	Err:508	Err:508
32	0.303606	Err:508	Err:508
33	0.992028	Err:508	Err:508
34	0.739105	Err:508	Err:508
35	0.119292	Err:508	Err:508
36	0.627548	Err:508	Err:508

Weights	
1	
2	
3	
2	
1	
9	**Divisor**

2	**SmoothNum**
0	**DerivNum**

For row ve

37	0.448252	Err:508	Err:508
38	0.421743	Err:508	Err:508
39	0.547954	Err:508	Err:508
40	0.866306	Err:508	Err:508
41	0.630292	Err:508	Err:508
42	0.090851	Err:508	Err:508
43	0.64689	Err:508	Err:508
44	0.835912	Err:508	Err:508
45	0.145741	Err:508	Err:508
46	0.293715	Err:508	Err:508
47	0.176848	Err:508	Err:508
48	0.561907	Err:508	Err:508
49	0.135043	Err:508	Err:508
50	0.92767	Err:508	Err:508
51	0.522215	Err:508	Err:508
52	0.90148	Err:508	Err:508
53	0.899504	Err:508	Err:508
54	0.116659	Err:508	Err:508
55	0.273061	Err:508	Err:508
56	0.648853	Err:508	Err:508
57	1.076578	Err:508	Err:508
58	0.471867	Err:508	Err:508
59	0.554389	Err:508	Err:508
60	0.697223	Err:508	Err:508
61	0.582502	Err:508	Err:508
62	0.127623	Err:508	Err:508
63	0.145518	Err:508	Err:508
64	0.521535	Err:508	Err:508
65	0.084733	Err:508	Err:508
66	0.793326	Err:508	Err:508
67	0.619911	Err:508	Err:508
68	0.673846	Err:508	Err:508
69	0.771519	Err:508	Err:508
70	0.209717	Err:508	Err:508
71	0.234276	Err:508	Err:508
72	0.660965	Err:508	Err:508
73	0.777663	Err:508	Err:508
74	0.369176	Err:508	Err:508
75	0.341882	Err:508	Err:508
76	0.439528	Err:508	Err:508
77	0.785114	Err:508	Err:508
78	0.891676	Err:508	Err:508
79	0.369776	Err:508	Err:508
80	0.444786	Err:508	Err:508

81	0.210055	Err:508	Err:508
82	0.763656	Err:508	Err:508
83	0.320389	Err:508	Err:508
84	0.28817	Err:508	Err:508
85	-0.035966	Err:508	Err:508
86	0.167545	Err:508	Err:508
87	0.912208	Err:508	Err:508
88	0.381193	Err:508	Err:508
89	0.110337	Err:508	Err:508
90	-0.040849	Err:508	Err:508
91	0.373662	Err:508	Err:508
92	0.031034	Err:508	Err:508
93	0.270504	Err:508	Err:508
94	0.358416	Err:508	Err:508
95	0.230094	Err:508	Err:508
96	0.217914	Err:508	Err:508
97	-0.039631	Err:508	Err:508
98	0.094376	Err:508	Err:508
99	0.988511	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

0	1	1
1	0	1
0	1	0

CycloPropene

0	1	1
1	0	1
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	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	1
1	0	1	0	0	0	1	0	0	0
0	1	0	1	0	0	0	0	0	0
0	0	1	0	1	0	0	0	0	0
0	0	0	1	0	1	0	0	0	0
0	0	0	0	1	0	1	0	0	0
0	1	0	0	0	1	0	1	0	0
0	0	0	0	0	0	1	0	1	0
0	0	0	0	0	0	0	1	0	1
1	0	0	0	0	0	0	0	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	Err:508	Err:508
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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
###	###	###	###	###	###	###	###	###	###
###	###	###	###	###	###	###	###	###	###

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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	551.5619	129.1071	555.4033	444.4936	449.3654	906.933	508.4154
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

or the 100 x-values

Note:

ctors see =>

Diff
Err:508
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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	3	Err:508	Err:508	Err:508	Err:508	
Err:508	4	Err:508	Err:508	Err:508	Err:508	NOTE:
Err:508	5	Err:508	Err:508	Err:508	Err:508	Returned a
Err:508	6	Err:508	Err:508	Err:508	Err:508	an N x 4 ar
Err:508	7	Err:508	Err:508	Err:508	Err:508	
Err:508	8	Err:508	Err:508	Err:508	Err:508	
Err:508	9	Err:508	Err:508	Err:508	Err:508	
Err:508	10					
Err:508						
Err:508						
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Note:

Index	0	1	2	3	4	5	6
DataH	0.14244	0.650586	0.190905	0.052192	-0.02933	0.814142	0.644965
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
636.6257	527.4107	615.9052	1375.393	1011.526	1219.58	836.7245	567.9705	1150.735	1568.287
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

rray is always
ray regardless of the input

7	8	9	10	11	12	13	14	15	16
0.156071	0.835976	0.832931	0.685248	0.559938	0.253136	0.768463	0.672517	0.095485	0.549048
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
1144.808	1790.906	1153.442
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
0.387095	0.395232	0.856101	0.388312	0.161841	0.08847	0.199952	0.567666	0.443302	0.35645
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
0.867032	0.247757	0.162659	0.715552	0.175791	0.649746	0.587777	0.298379	0.51543	0.422555
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
0.123907	1.053925	0.965801	0.407348	0.22059	0.62246	0.87978	0.41424	0.125638	0.865452
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
0.551402	0.023844	0.924998	0.533609	0.625331	0.524295	0.412671	0.748065	0.950059	0.491901
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
0.960849	0.865561	0.822847	0.608886	0.362208	0.990218	0.267656	0.950054	0.207734	0.316877
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
0.579721	0.522302	0.867158	0.536117	0.190422	0.054883	-0.033708	0.589021	0.325855	0.240016
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
0.418279	0.492058	-0.063856	0.140257	1.04192	0.866459	0.761712	0.28498	0.13783	0.785707
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
0.455995	0.564765	0.952351	0.88681	0.779576	0.544146	0.901075	0.638736	0.468194	0.655127
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
0.800479	-0.064734	0.328755
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 mus
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 w
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 scree
since the screen echo is turned off. When the calculation is complete, you will be prompted
before overwritting the parameters.

Example 1 -- Y = p0 + p1*EXP(p2*x)

IndVar	Measured Y	Calculated Y
-5	127	#NAME?
-3	151	#NAME?
-1	379	#NAME?
1	421	#NAME?
3	460	#NAME?
5	426	#NAME?

523.305536	-156.94784	-0.1996646	Final parameter
100.066637	111.315698	0.10692545	Std. deviations
2.43047611	0.56344331	0.00608058	Eigenvalues
2.44948974	3.64375345	2339.5307	Scale vectors

_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 = p0*x/(p1 + x)

IndVar	Measured Y	Calculated Y
1.68	0.172	0.29577465
3.33	0.25	0.45429741
5	0.286	0.55555556
6.67	0.303	0.62511715
10	0.334	0.71428571

0.42380958	2.45193659	Final parame
0.00829087	0.16742349	Std. deviations
1.88955331	0.11044669	Eigenvalues
1.7088967	0.08462518	Scale vectors

Deviations
0.01532016346
0.04173743088
0.07266019753
0.1037594589
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 = p0 + (p1 - p0) * exp(-p2 * 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
0.1	0.9011	0.97561471
0.1414	0.8266	0.96587069
0.166	0.829	0.96017557
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

0.39996858	1.00001637	1.99984956	Final parameter
0.0069376	0.00972573	0.06905219	Std. deviations
2.29314005	0.58822552	0.11863442	Eigenvalues
2.66798472	1.91540946	0.28415285	Scale vectors

_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 paramete
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?

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

#NAME?	SSQ
#NAME?	SSQ as % of mean Y value

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

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*cos(x) where x is from 0 to 2*pi

X-values of 2.3 and 4.4 are altered

SplineX contains 100 x-va

SplineY contains interpola

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	5.78053048
93	5.84336234
94	5.90619419
95	5.96902604
96	6.03185789
97	6.09468975
98	6.1575216
99	6.22035345

Data Smoothing

		Smooth	Smooth		
Index	Data	SG	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	-0.3333333	-1.309E-08
0.4082483	0.36605682	0.4464703	0.35611915	0.45443607	0.40824872	-1.31E-08	-0.3333333

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
2.9491106		0.04496958
2.89783299		0.07851111
2.84577896		0.10108279

IndVarSH	0	0.62831853	1.25663706	1.88495559
DepVarSH	3	2.42705098	0.92705098	-0.927051
	3	-0.8089001	0	-0.2608426
	2.42705098	-1.1178298	-0.4916768	-2.4331389

2.79256029		0.11318919
2.73778877		0.11538078
2.68107619		0.10825327
2.62203433		0.09244683
2.56027498		0.06864506
2.49540994		0.03757384
2.42705098	2.42705098	0
2.35427106		-0.0427313
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

0.92705098	-4.6173833	-5.0780356	12.3032089
-0.927051	3.57270557	18.1129668	-30.434487
1.5	2.87997291	-19.782024	11.8900002
-3	-5.1525547	10.237587	-0.9322416
-2.427051	6.60827383	8.48035294	-12.406617
2	2.51830041	-14.971459	13.1178146
0.92705098	-0.7936882	9.68537199	-7.3571498
2.42705098	2.6638502	-4.1825287	2.21890038

-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
0.47348742 0.29300505 0.02300735 0.19575205 0.33381775 0.67268018 0.83570091 0.83862223
0.40548375 0.30571469 0.15243238 0.22314157 0.38458187 0.63268635 0.74979917 0.76462262

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
0.65673175	0.52979338	0.3778871	0.33600847	0.33959441	0.45731246	0.4546941	0.50707633

0.17246022 0.77801775 0.57832696 0.94671133 0.2577551 0.48733865 0.39627198 0.44702546
0.43494185 0.65858426 0.6339764 0.68105126 0.51820457 0.46678185 0.37851713 0.37612892
0.48031301 0.6091003 0.62385048 0.64196161 0.51288491 0.46264521 0.39934828 0.3613798

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
0.64793661 0.44009414 0.48348716 0.50188916 0.50440647 0.59645186 0.36289075 0.25005276
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0.38674887 0.47957614 0.50281192 0.52869258 0.3291642 0.3291642 0.3291642 0.3291642
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