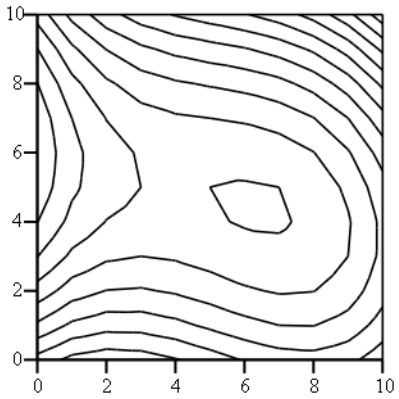
An illustration of using Mathcad to make a contour plot.

$i := 0 .. 10$ $\quad j := 0 .. 10$

$x_i := -5 + i$ $\quad y_j := -5 + j$

$E(x, y) := 0.25x^3 + x \cdot y - x + y + 2y^2$

$C_{i,j} := E(x_i, y_j)$



C

$xo := 1$ $\quad yo := 0$ $\quad Minimize(E, xo, yo) = \begin{pmatrix} 1.468 \\ -0.617 \end{pmatrix}$

To generate a contour plot, you need to set up a two dimensional array (matrix).

The contour plot can provide estimates of locations of minima and maxima that can be used with the minimize and maximize functions.

Stationary points on potential energy surface .

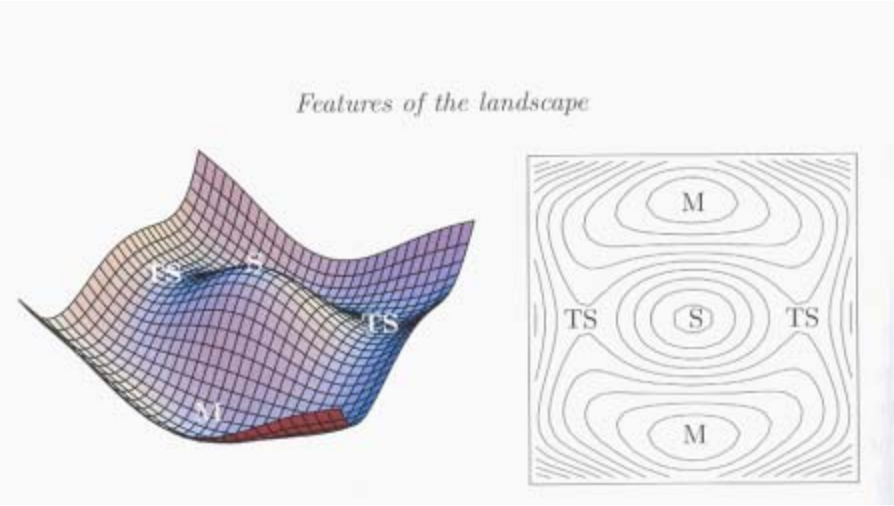
$\frac{d}{dx_i} E$ *=0, wrt all* x_i.

minima: *all second derivates are positive (positive curvature)*

transition state *(first order saddle point) : one negative curvature direction*

reaction pathway: *min1 -> TS -> min2*

thus it is of interest to find the different minima, the TS's, and the pathways that connect them.



"c:\ken\junk\wales_contour_scaled.bmp"

Potential energy surface for a two-dimensional system, i.e., E(x,y) [from Wales]

Contour map of PES; M = minimum, TS =1st order saddle point, S = 2nd order saddle point

Programs like Mathcad have lots of built-in functions but In some cases it may be better to use your own programs (or programs/algorithms from web-based libraries).

This is illustrated by use of the Newton Raphson algorithm for finding minima.

Programs like Mathcad have lots of built-in functions but In some cases it may be better