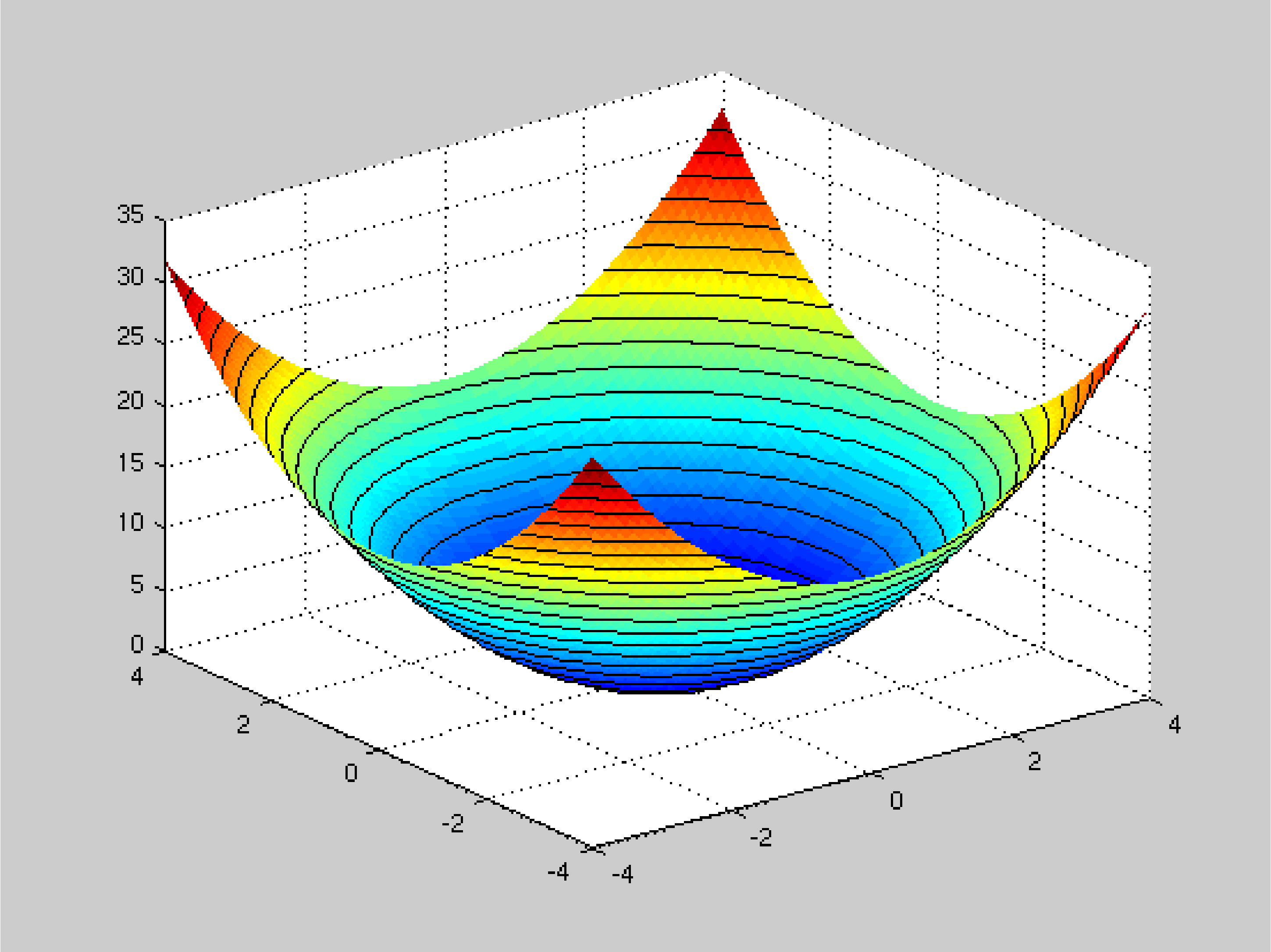
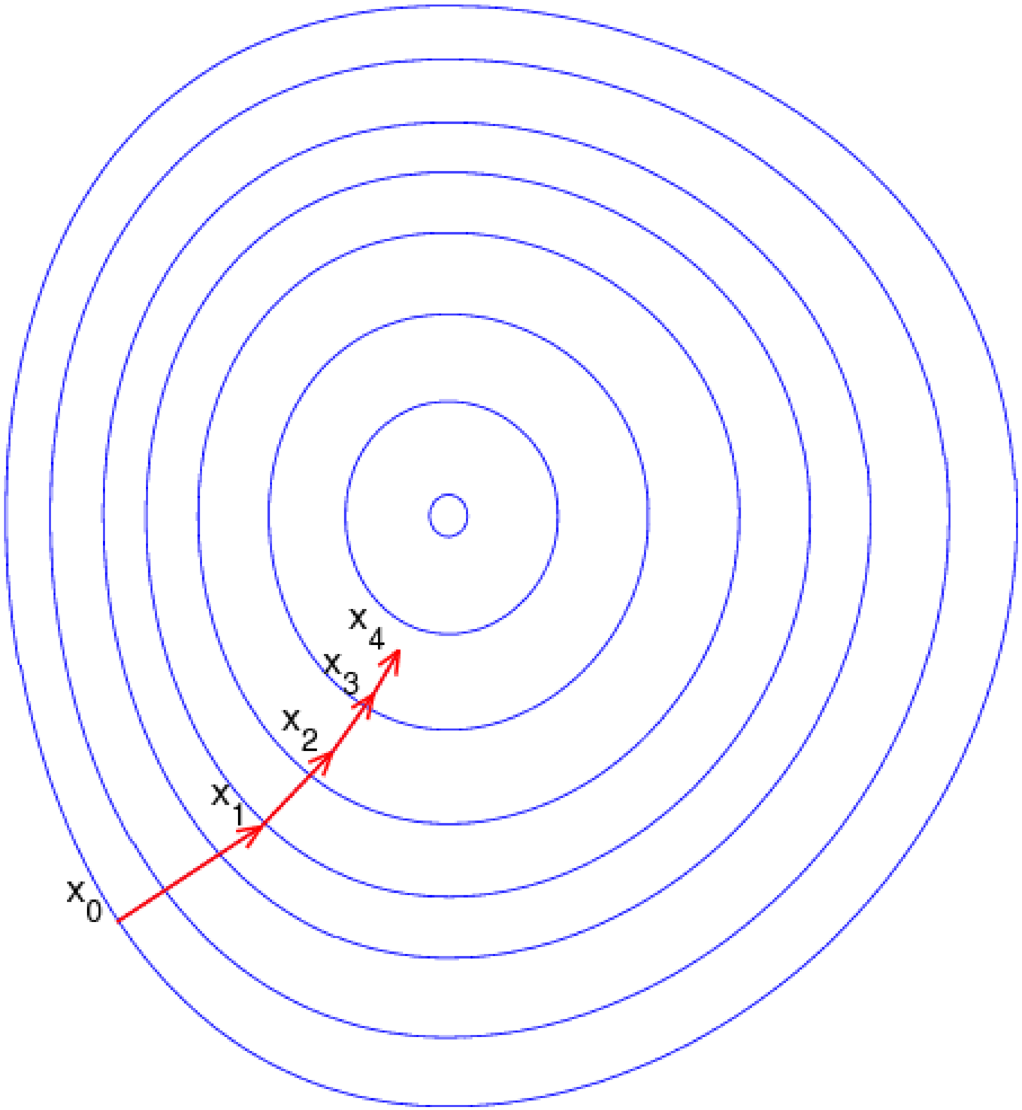
Computational Intelligence

Gradient Descent and Newton's Methods

Assume the following 2D Function



Contour plot



Gradient descent: head downhill

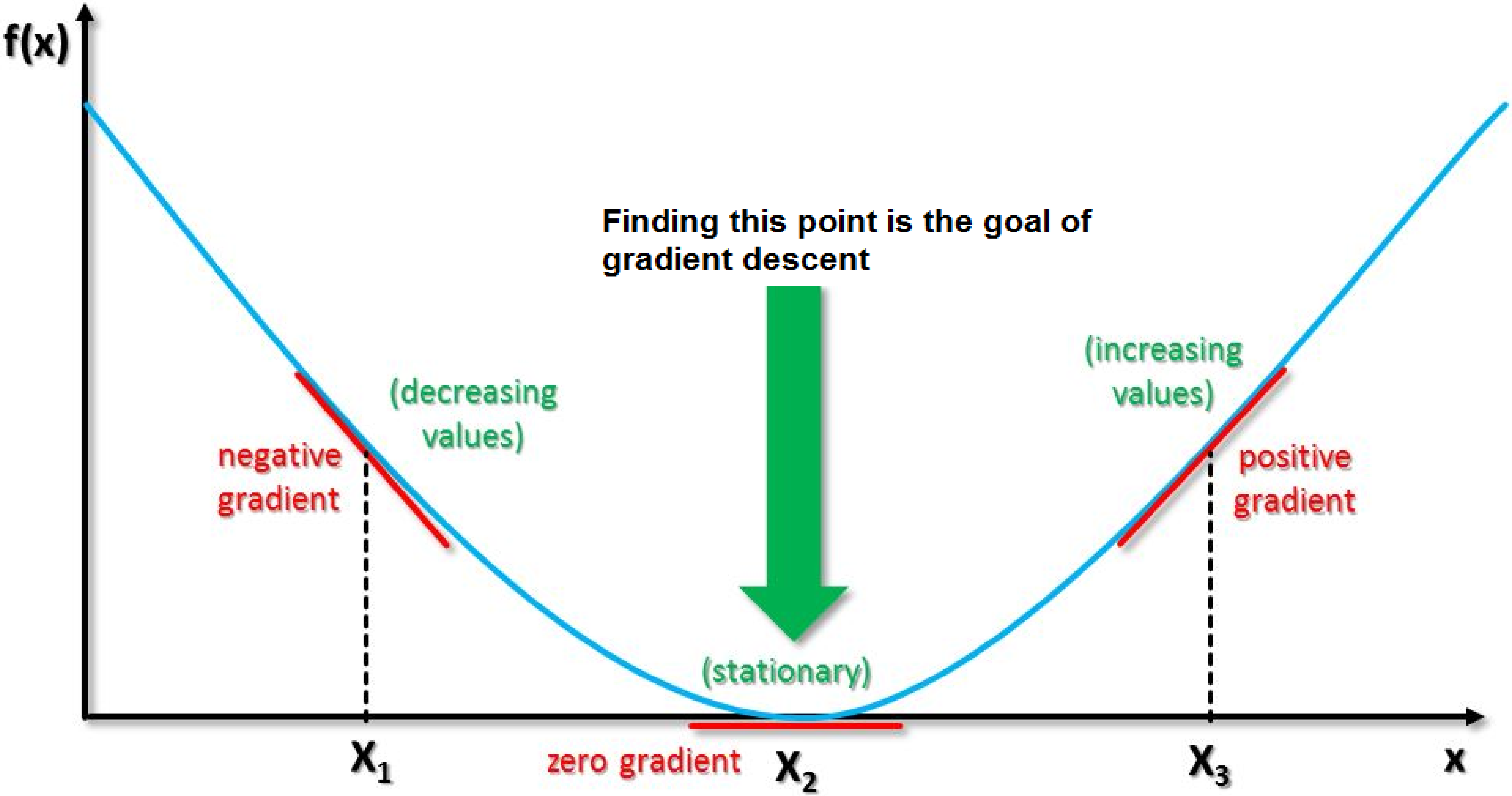
http://en.wikipedia.org/wiki/Gradient_descent

The Gradient Descent

**We select moving in the gradient direction such that:-

$$f(X_0) \geq f(X_1) \geq f(X_2) \dots \geq f(X_{n-1}) \geq f(X_n)$$

The Gradient Descent Algorithm



The Gradient Descent Algorithm

Step 0: $Select\ X_0 \in R^n,\ Set\ \alpha, and\ i = 0$

Step 1: Compute $\nabla f(X_i)$

Step 2: if $||\nabla f(X_i)|| < \varepsilon, Stop$
Otherwise Go To Step 3

Step 3: Compute $X_{i+1} = X_i - \alpha \nabla f(X_i)$

Step 4: Update i=i+1

Step 5: Go To Step 1

Computing the Gradient

$$f : R^n \to R$$

$$\nabla f(x_1, \ldots, x_n) := \left(\frac{\partial f}{\partial x_1}, \ldots, \quad \frac{\partial f}{\partial x_n} \right)$$

Step Size Selection (α)

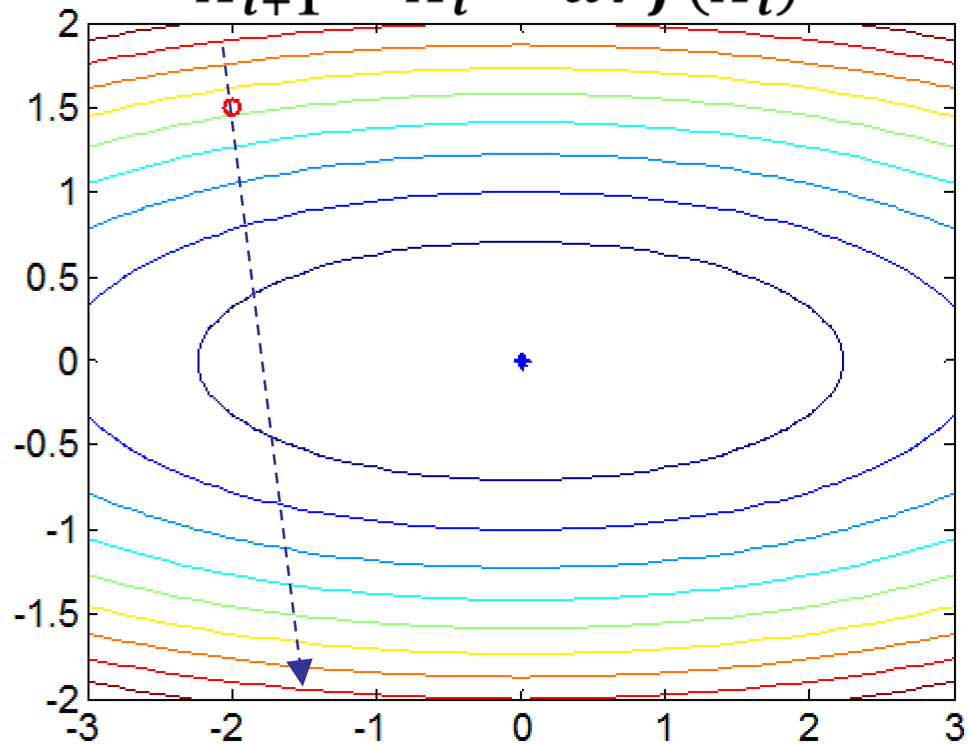
How should we select the step size?

- α too small: convergence takes long time
- α too large: overshoot minimum

Line minimization:

$$\alpha = \arg\min_{\alpha} f(X_i - \alpha \nabla f(X_i))$$

$$X_{i+1} = X_i - \alpha \nabla f(X_i)$$



The Steepest Gradient Descent Algorithm (Line Search)

Step 0: $Select\ X_0 \in R^n,\ Set\ \alpha, and\ i = 0$

Step 1: Compute $\nabla f(X_i)$

Step 2: if $||\nabla f(X_i)|| < \varepsilon, Stop$
Otherwise Go To Step 3

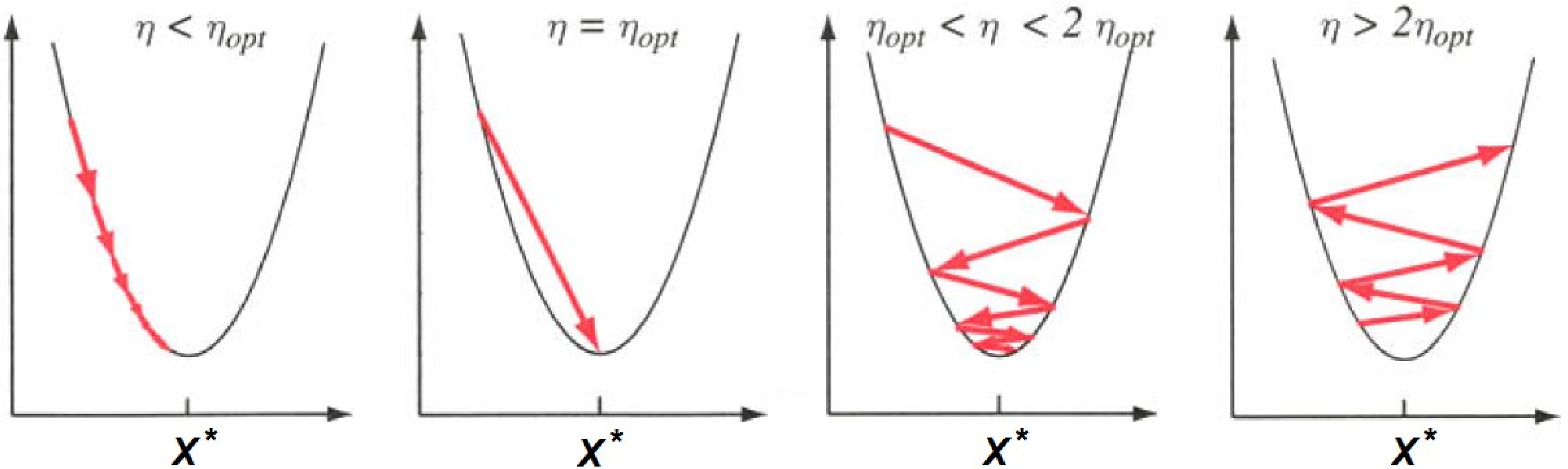
Step 3: Update $\alpha^* = \underset{\alpha}{\operatorname{argmin}} f(X_i - \alpha \nabla f(X_i))$

Step 4: Compute $X_{i+1} = X_i - \alpha^* \nabla f(X_i)$

Step 5: Update i=i+1

Step 6: Go To Step 1

The Steepest Gradient Descent Algorithm



Gradient descent in a one-dimensional quadratic criterion with different learning rates. If $\eta < \eta_{opt}$, convergence is assured, but training can be needlessly slow. If $\eta = \eta_{opt}$, a single learning step suffices to find the error minimum. If $\eta_{opt} < \eta < 2\eta_{opt}$, the system will oscillate but nevertheless converge, but training is needlessly slow. If $\eta > 2\eta_{opt}$, the system diverges.

The Hessian Matrix

Specifically, suppose $f: \mathbb{R}^n \to \mathbb{R}$ is a function taking as input a vector $\mathbf{x} \in \mathbb{R}^n$ and outputting a scalar $f(\mathbf{x}) \in \mathbb{R}$; if all second partial derivatives of f exist and are continuous over the domain of the function, then the Hessian matrix $\mathbf{H}$ of f is a square $n \times n$ matrix, usually defined and arranged as follows:

$$\mathbf{H} = \begin{bmatrix} \dfrac{\partial^2 f}{\partial x_1^2} & \dfrac{\partial^2 f}{\partial x_1\,\partial x_2} & \cdots & \dfrac{\partial^2 f}{\partial x_1\,\partial x_n} \\[2.2ex] \dfrac{\partial^2 f}{\partial x_2\,\partial x_1} & \dfrac{\partial^2 f}{\partial x_2^2} & \cdots & \dfrac{\partial^2 f}{\partial x_2\,\partial x_n} \\[2.2ex] \vdots & \vdots & \ddots & \vdots \\[2.2ex] \dfrac{\partial^2 f}{\partial x_n\,\partial x_1} & \dfrac{\partial^2 f}{\partial x_n\,\partial x_2} & \cdots & \dfrac{\partial^2 f}{\partial x_n^2} \end{bmatrix}.$$

or, by stating an equation for the coefficients using indices i and j:

$$\mathbf{H}_{i,j} = \frac{\partial^2 f}{\partial x_i \partial x_j}.$$

The determinant of the above matrix is also sometimes referred to as the Hessian.

Step Size Automatic Selection: The Newton-Raphson Algorithm

Step 0: $Select\ X_0 \in R^n,\ and\ i = 0$

Step 1: Compute $\nabla f(X_i)\ and\ H$

Step 2: if $||\nabla f(X_i)|| < \varepsilon, Stop$
Otherwise Go To Step 3

Step 3: Compute $\alpha = H^{-1}$

Step 4: Compute $X_{i+1} = X_i - \alpha \nabla f(X_i)$

Step 5: Update i=i+1

Step 6: Go To Step 1

Ex1: Gradient Descent

$\alpha = 0.1$

$f(x)=x^4 - x^3 + x^2 - x+1$ $df/dx=4x^3 - 3x^3 + 2x - 1$

	Xn	f(Xn)	df/dx
1	1	1	2
2	0.8000	0.7376	0.7280
3	0.7272	0.6967	0.4062
4	0.6866	0.6834	0.2536
5	0.6612	0.6781	0.1672
6	0.6445	0.6757	0.1137
7	0.6331	0.6746	0.0789
8	0.6252	0.6741	0.0554
9	0.6197	0.6738	0.0393
10	0.6158	0.6737	0.0280
11	0.6130	0.6736	0.0200
12	0.6110	0.6736	0.0144
13	0.6095	0.6736	0.0103
14	0.6085	0.6736	0.0074
15	0.6078	0.6736	0.0054
16	0.6072	0.6736	0.0039
17	0.6068	0.6736	0.0028
18	0.6066	0.6736	0.0020
19	0.6064	0.6736	0.0015
20	0.6062	0.6736	0.0011
21	0.6061	0.6736	7.6266e-04

Ex2: Newton Raphson

$f(x)=x^4 - x^3 + x^2 - x+1$

$df/dx=4x^3 - 3x^3 + 2x - 1$

$d^2f/dx^2=12x^2 - 9x^2 + 2$

X	f(X)	df/dx	d2f/dx2
10	9091	3719	1142
6.7434	1.8010e+03	1.1027e+03	507.2260
4.5695	357.8926	327.1530	225.1489
3.1165	71.6578	97.1690	99.8496
2.1433	14.7075	28.8891	44.2657
1.4907	3.3569	8.5650	19.7216
1.0564	1.1260	2.4805	9.0532
0.7824	0.7255	0.6441	4.6514
0.6439	0.6756	0.1119	3.1121
0.6080	0.6736	0.0059	2.7876
0.6058	0.6736	1.9371e-05	2.7694
0.6058	0.6736	2.0890e-10	2.7694
0.6058	0.6736	-1.1102e-16	2.7694
0.6058	0.6736	-1.1102e-16	2.7694
0.6058	0.6736	-1.1102e-16	2.7694

Ex3: Line Search
$X_0=(1,1)^T$

$f(x,y) = x^4+xy+y^2$

$f_x = 4x^3+y$

$f_y = x+2y$

	fx	fy	α	x	y
1	5	3	0.2721	-0.3606	0.1836
2	-0.0040	0.0066	1.0032	-0.3566	0.1770
3	-0.0045	-0.0027	0.3955	-0.3549	0.1780
4	-7.2371e-04	0.0012	1.0128	-0.3541	0.1768
5	-8.3974e-04	-5.0392e-04	0.3972	-0.3538	0.1770
6	-1.3802e-04	2.3000e-04	1.0146	-0.3537	0.1768
7	-1.6110e-04	-9.6683e-05	0.3976	-0.3536	0.1768
8	-2.6553e-05	4.4238e-05	1.0151	-0.3536	0.1768
9	-3.1020e-05	-1.8622e-05	0.3976	-0.3536	0.1768
10	-5.1118e-06	8.5225e-06	1.0148	-0.3536	0.1768

Ex4: Newton Raphson $X_0=(-2,-2)^T$

$f(x,y) = x^4+xy+y^2$

$f_x = 4x^3+y$

$f_y = x+2y$

x	y	f(x,y)	fx	fy	fxx	fxy	fyx	fyy
-1.3474	0.6737	2.8418	-9.1104	6.6613e-16	21.7848	1	1	2
-0.9193	0.4597	0.5031	-2.6484	-1.1102e-16	10.1424	1	1	2
-0.6447	0.3223	0.0688	-0.7494	0	4.9873	1	1	2
-0.4777	0.2388	-0.0050	-0.1971	0	2.7381	1	1	2
-0.3896	0.1948	-0.0149	-0.0417	0	1.8214	1	1	2
-0.3580	0.1790	-0.0156	-0.0045	0	1.5380	1	1	2
-0.3536	0.1768	-0.0156	-8.1783e-05	0	1.5007	1	1	2
-0.3536	0.1768	-0.0156	-2.8342e-08	0	1.5000	1	1	2
-0.3536	0.1768	-0.0156	-3.4139e-15	0	1.5000	1	1	2
-0.3536	0.1768	-0.0156	-2.7756e-17	0	1.5000	1	1	2