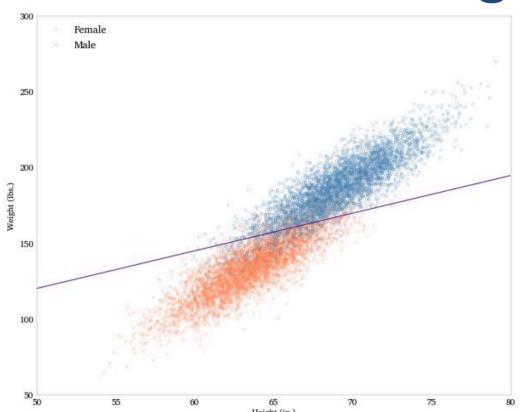
#### Minimizing Functions of Multiple Variables

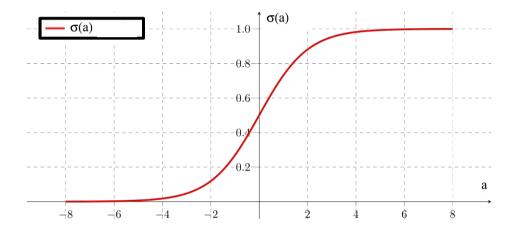
Pascal Fua IC-CVLab



## Reminder: Logistic Regression



$$y(\mathbf{x}; \tilde{\mathbf{w}}) = \sigma(\tilde{\mathbf{w}} \cdot \tilde{\mathbf{x}})$$
$$= \frac{1}{1 + \exp(-\tilde{\mathbf{w}} \cdot \tilde{\mathbf{x}})}$$



Given a **training** set  $\{(\mathbf{x}_n, t_n)_{1 \le n \le N}\}$  minimize

$$E(\tilde{\mathbf{w}}) = -\sum_{n} (t_n \ln y(\mathbf{x}_n) + (1 - t_n) \ln(1 - y(\mathbf{x}_n)))$$

with respect to  $\tilde{\mathbf{w}}$ .



# Reminder: Maximizing the Margin

$$\mathbf{w}^* = \min_{(\mathbf{w}, \{\xi_{\mathbf{n}}\})} \frac{1}{2} ||\mathbf{w}^2|| + C \sum_{n=1}^{N} \xi_n,$$
  
subject to  $\forall n, \quad t_n \cdot (\tilde{\mathbf{w}} \cdot \mathbf{x}_n) \ge 1 - \xi_n \text{ and } \xi_n \ge 0.$ 

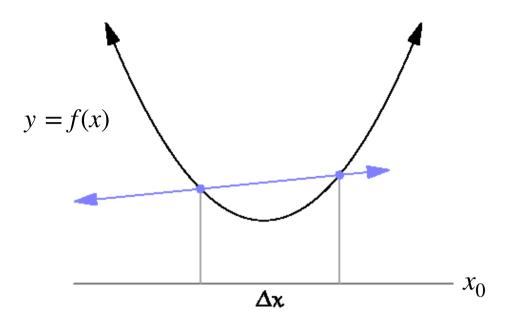
- C is constant that controls how costly constraint violations are.
- The problem is still convex.

- How do you minimize a function of several variables?
- Why does it matter that the problem is convex?

—> Let's talk about that today.



#### Derivative of a 1-Variable Function



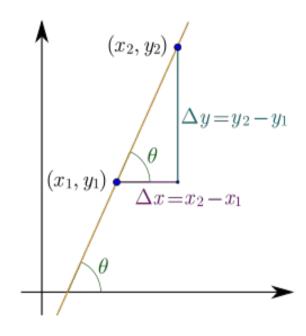
- The derivative of a function y = f(x) of a single variable x is the rate at which y changes as x changes. = pendiente
- It is measured for an infinitesimal change in x, starting from a point  $x_0$ , and written as

$$f'(x_0) = \frac{dy}{dx} = \lim_{\Delta x \to 0} \frac{f(x_0 + \Delta x) - f(x_0)}{\Delta x}$$



 $\rightarrow$  The derivative is the slope of the tangent at  $x_0$ .

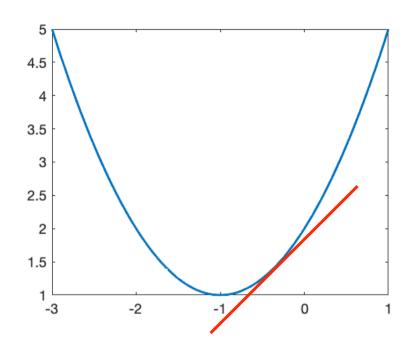
#### **Derivative of a Linear Function**



- The tangent to the function is the function itself: The slope is constant.
- For example, y = 2x 1 and  $\frac{dy}{dx} = 2$ .



#### **Derivative of a Non-Linear Function**



- The tangent (in red) to the function varies with x and so does the slope.
- For example,  $y = x^2 + 2x + 2$  and  $\frac{dy}{dx} = 2x + 2$ .



### **Evolution of the Tangent**

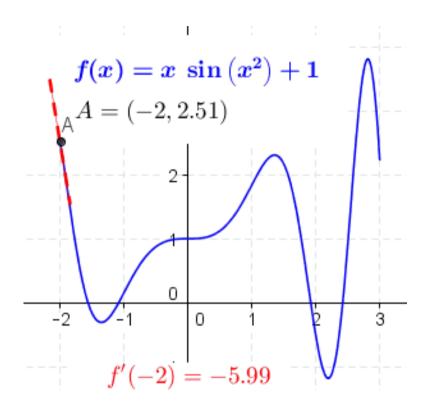
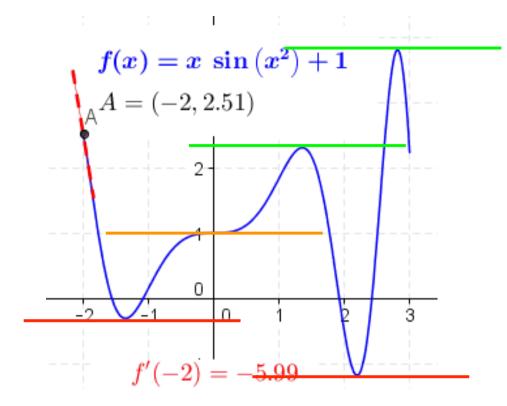


Figure from Wikipedia

$$y = x \sin(x^2) + 1$$
$$\frac{dy}{dx} = \sin(x^2) + 2x^2 \cos(x^2)$$



#### **First and Second Derivatives**



$$y = x\sin(x^2) + 1$$

$$\frac{dy}{dx} = \sin(x^2) + 2x^2 \cos(x^2)$$

$$\frac{d^2y}{dx^2} = 6x\cos(x^2) - 4x^3\sin(x^2)$$

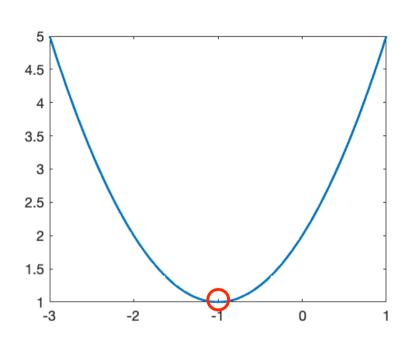
$$\frac{dy}{dx} = 0$$
 and  $\frac{d^2y}{dx^2} > 0$ : Minimum

$$\frac{dy}{dx} = 0$$
 and  $\frac{d^2y}{dx^2} < 0$ : Maximum

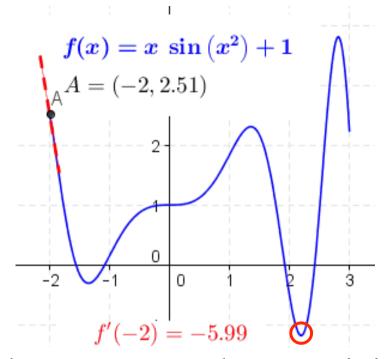
$$\frac{dy}{dx} = 0$$
 and  $\frac{d^2y}{dx^2} = 0$ : Saddle



#### Convex vs Non-Convex



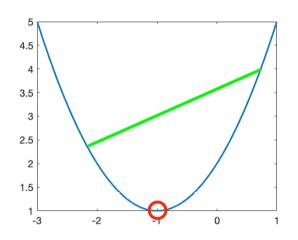
- There is only one minimum.
- The second derivative is  $\geq 0$ .



- There are several **local** minima.
- There is one global minimum.

—> Non-convex functions are much more difficult to minimize than convex ones.





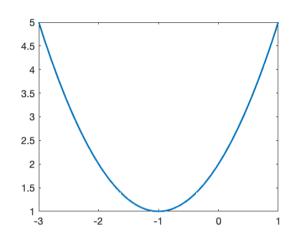
The line segment between any two points on the curve lies above the curve.

$$\frac{df(x^*)}{dx} = 0$$

For some simple functions this can be done in closed form, that is, by solving an equation.

#### Minimizing a Simple Convex Function

$$f(x) = x^2 + 2x + 2$$
$$\frac{df(x)}{dx} = 2x + 2$$

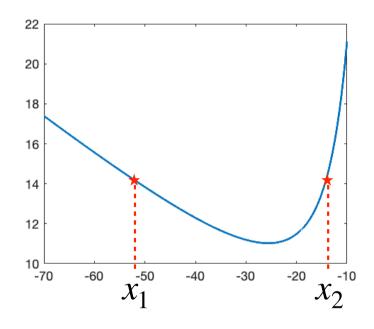


$$\frac{df(x^*)}{dx} = 0 \Leftrightarrow 2x^* + 2 = 0$$
$$\Leftrightarrow 2x^* = -2$$
$$\Leftrightarrow x^* = -1$$

#### Minimizing a Generic Convex Function

When the minimum cannot be found in closed-form, we use the derivative:

At  $x_1$ , the slope is negative. Hence, one should move in the positive direction  $(\Delta x > 0)$  to go towards the minimum



At  $x_2$ , the slope is positive. Hence, one should move in the negative direction ( $\Delta x < 0$ ) to go towards the minimum

—> One should move in the direction opposite to the derivative for minimization



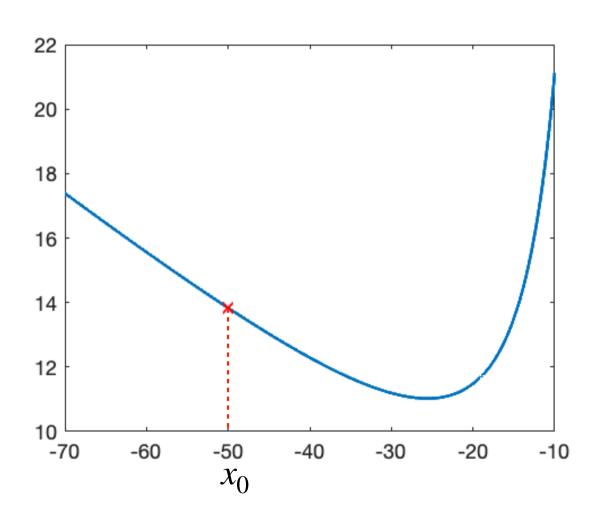
#### Simplest algorithm:

- 1. Initialize  $x_0$  (e.g., randomly)
- 2. While not converged

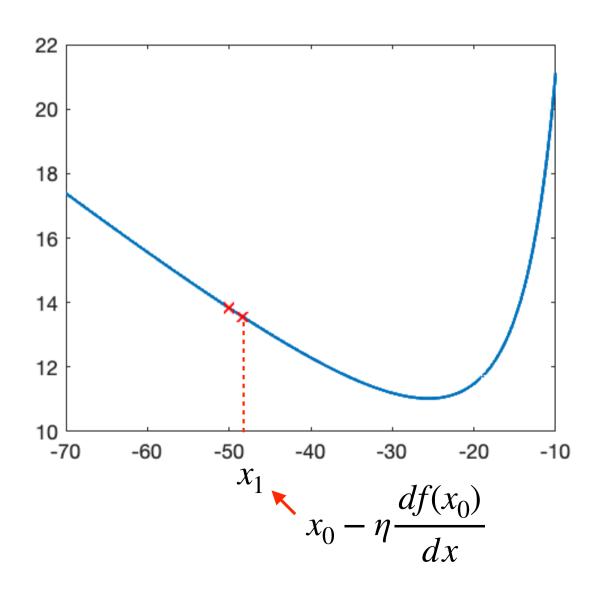
2.1. Update 
$$x_k \leftarrow x_{k-1} - \eta \frac{df(x_{k-1})}{dx}$$

- $\eta$  defines the step size of each iteration.
- In ML, it is often referred to as the *learning rate*.

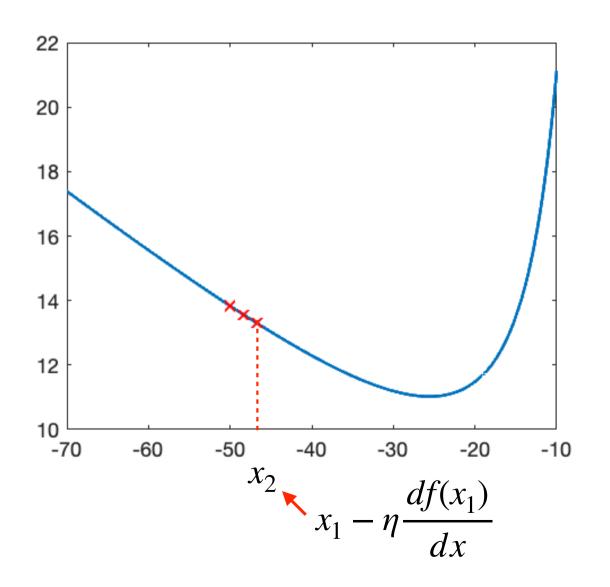




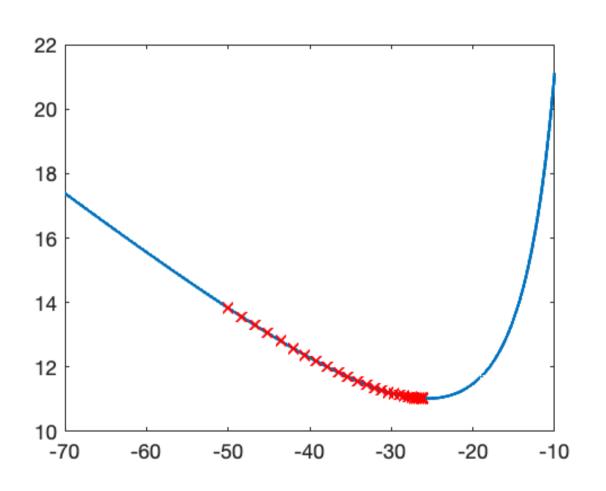








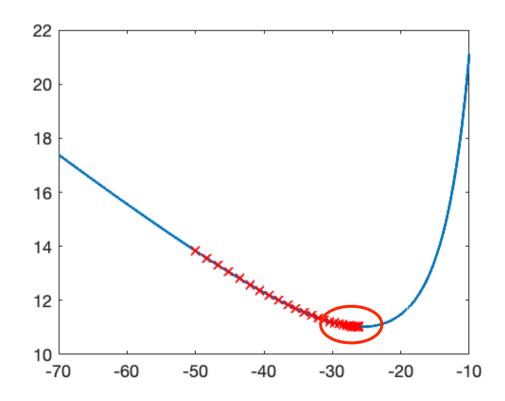






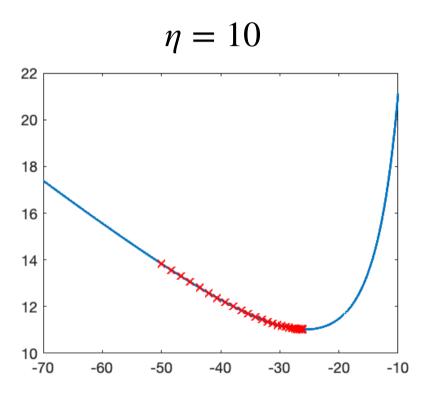
Potential stopping Criteria:

- Change in function value less than threshold:  $|f(x_{i-1}) f(x_i)| < \delta$ .
- Change in parameter value less than threshold:  $|x_{i-1} x_i| < \delta$ .
- Maximum number of iterations reached without a guarantee to have reached the minimum.

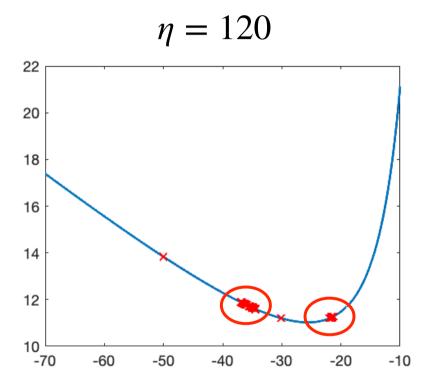




### Influence of the Step Size



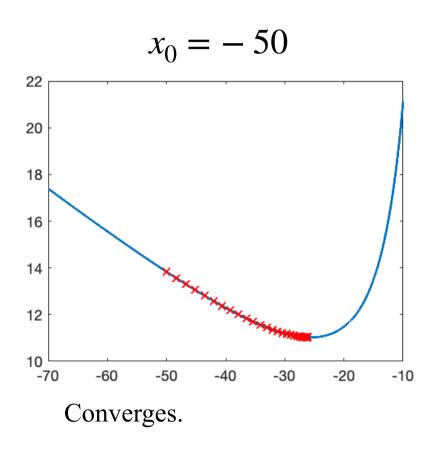
The steps are of the appropriate size for convergence.

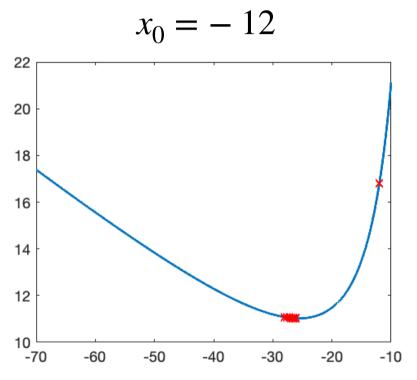


The steps are too large and the algorithm starts jumping between these two points.



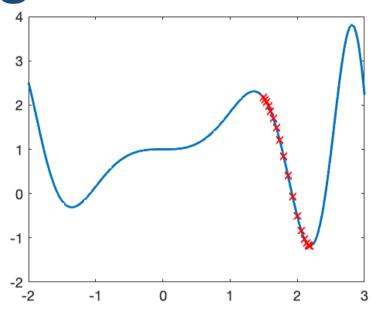
### Influence of the Starting Point



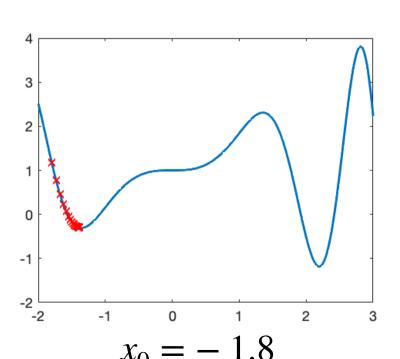


Converges to the same place, but faster.

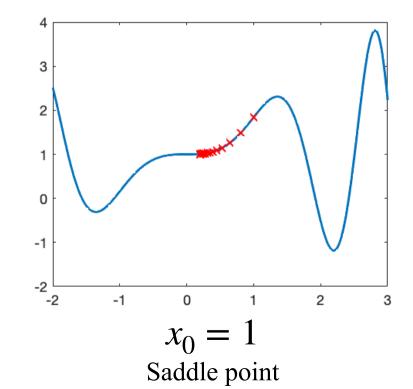




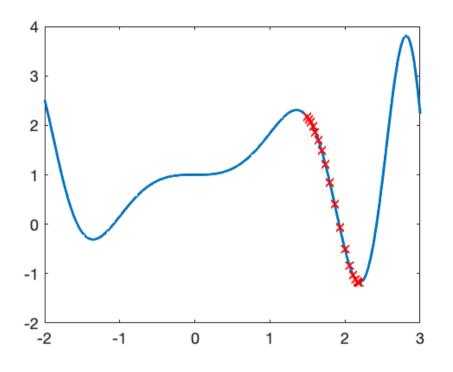
$$x_0 = 1.5$$
 Global minimum



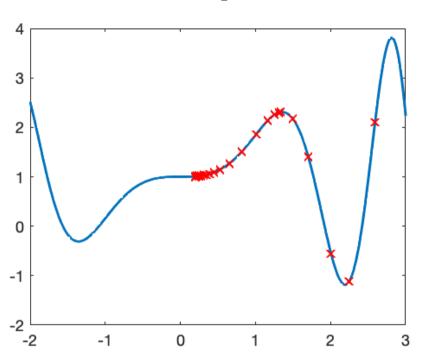
Local minimum



$$\eta = 0.01, \ x_0 = 1.5$$
Global minimum



$$\eta = 0.1, \ x_0 = 1.5$$
Saddle point



—> No guarantees when the function is not convex!



### **Functions of Multiple Variables**

Multivariate function:

$$f: R^D \to R$$
$$y = f(\mathbf{x}) = f(x_1, ..., x_D)$$

Partial derivative:

$$\frac{\delta y}{\delta x_d} = \lim_{\Delta x \to 0} \frac{f(\dots, x_d + \Delta x, \dots) - f(\dots, x_d, \dots)}{\Delta x}$$

Gradient vector:

$$\nabla f = \left[\frac{\delta f}{\delta x_1}, \dots, \frac{\delta f}{\delta x_D}\right]$$



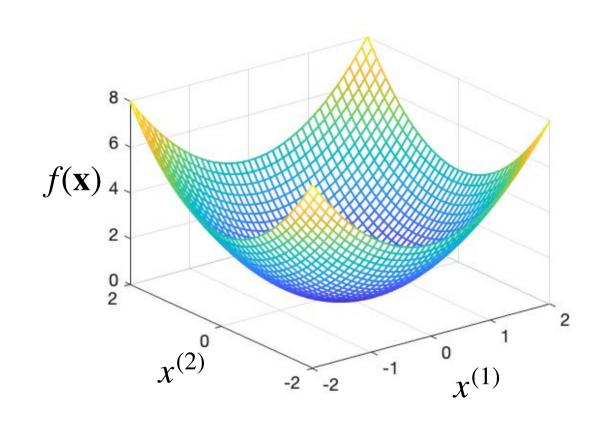
#### **Quadratic Function**

$$f(\mathbf{x}) = x_1^2 + x_2^2$$

$$\frac{\partial f}{\partial x_1} = 2x_1$$

$$\frac{\partial f}{\partial x_1} = 2x_1$$
$$\frac{\partial f}{\partial x_2} = 2x_2$$

$$\nabla f(\mathbf{x}) = \begin{bmatrix} 2x_1 \\ 2x_2 \end{bmatrix} \in \mathbb{R}^2$$



The color also represents the value of  $f(\mathbf{x})$ 



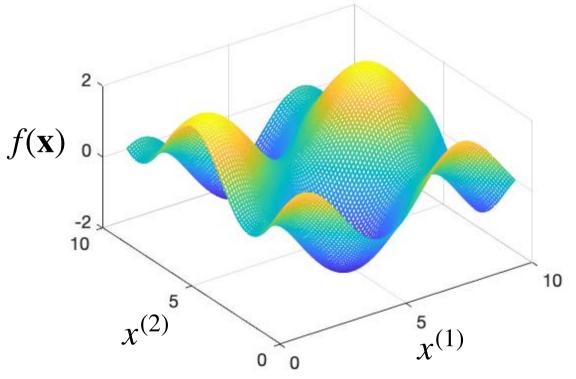
#### **Sinusoidal Function**

$$f(\mathbf{x}) = \sin x_1 + \cos x_2$$

$$\frac{\partial f}{\partial x_1} = \cos(x_1)$$

$$\frac{\partial f}{\partial x_2} = -\sin(x_2)$$

$$\nabla f(\mathbf{x}) = \begin{bmatrix} \cos(x_1) \\ -\sin(x_2) \end{bmatrix} \in \mathbb{R}^2$$



The color also represents the value of  $f(\mathbf{x})$ 



#### **Gradient in 4 Dimensions**

$$f(\mathbf{x}) = x_1^2 x_2^2 + x_1 x_2 x_3 + x_3 x_4 + 2x_4 + 1$$

$$\frac{\partial f}{\partial x_1} = 2x_1 x_2^2 + x_2 x_3$$

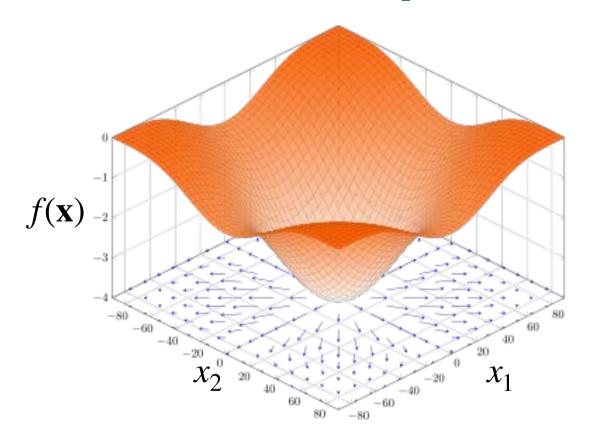
$$\frac{\partial f}{\partial x_2} = 2x_2x_1^2 + x_1x_3$$

$$\frac{\partial f}{\partial x_3} = x_1 x_2 + x_4$$

$$\frac{\partial f}{\partial x_4} = x_3 + 2$$

$$\nabla f(\mathbf{x}) = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \\ \frac{\partial f}{\partial x_3} \\ \frac{\partial f}{\partial x_4} \end{bmatrix} \in \mathbb{R}^4$$

### **Gradient Properties**



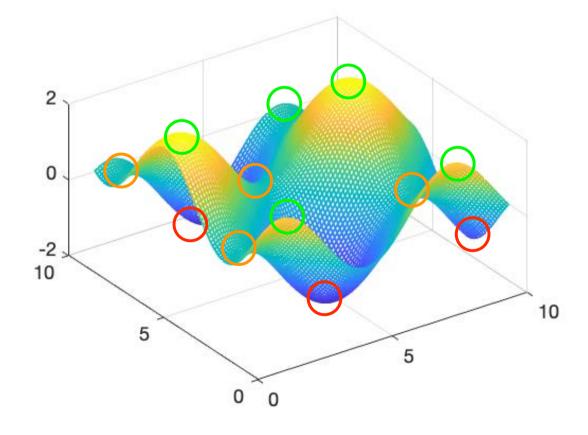
- The gradient at a point x indicates the direction of greatest increase of the function at x.
- Its magnitude is the rate of increase in that direction.



### **Gradient Properties**

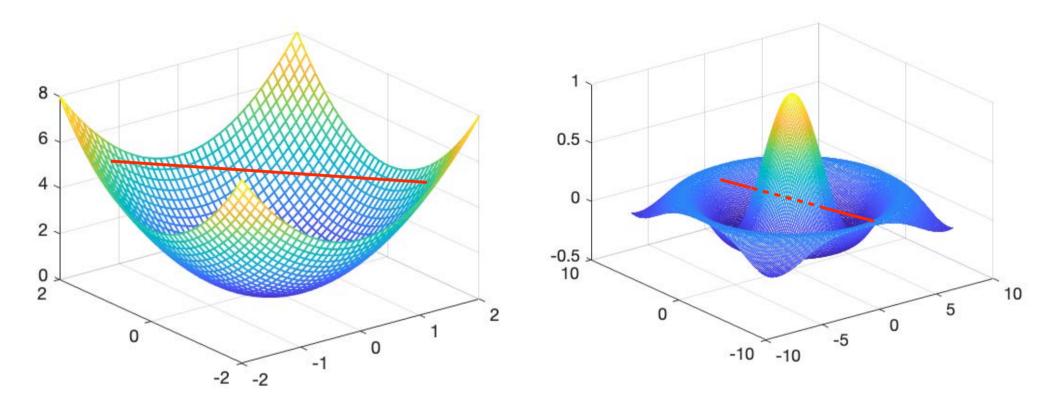
The gradient vanishes (becomes a zero vector) at the stationary points of the function:

- Minima,
- Maxima,
- Saddle points.





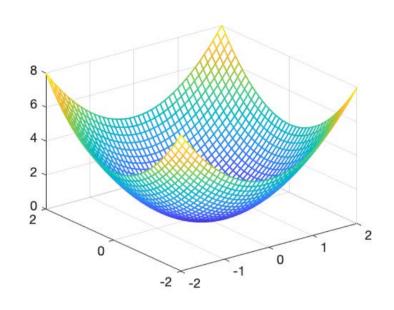
#### Convex vs Non-Convex



Convex: The line segment between any two points on the function lies above the function

Non-convex: At least one line segment between two points lies in part below the function.





$$\nabla f(\mathbf{x}^*) = \mathbf{0}$$

- Because the gradient is a vector, this yields a system of equations.
- It can still be solved in closed form for some functions.



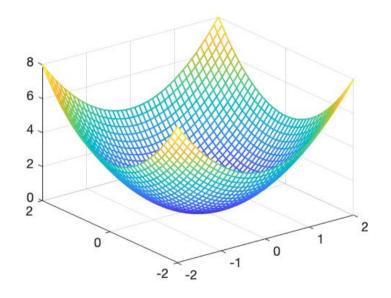
#### Minimizing a Simple Convex Function

$$f(\mathbf{x}) = x_1^2 + x_2^2$$

$$\frac{\partial f}{\partial x_1} = 2x_1 \qquad \frac{\partial f}{\partial x_2} = 2x_2$$

$$\nabla f(\mathbf{x}) = 0 \Leftrightarrow \begin{cases} 2x_1 = 0\\ 2x_2 = 0 \end{cases}$$

$$\Leftrightarrow x_1 = x_2 = 0$$



# Revisiting K means

$$\min_{\{\mu_k\},\{r_i^k\}} \sum_{i=1}^{N} \sum_{k=1}^{K} r_i^k ||\mathbf{x}_i - \mu_k||^2$$
 such that  $r_i^k \in \{0,1\}, \ \forall i, k$  
$$\sum_{k=1}^{K} r_i^k = 1, \ \forall i$$

—> We will derive the solution by alternating between the two types of variables.

# Revisiting K means

$$\min_{\{r_i^k\}} \sum_{i=1}^N \sum_{k=1}^K r_i^k ||\mathbf{x}_i - \mu_k||^2$$
 such that 
$$r_i^k \in \{0,1\}, \ \forall i,k$$
 
$$\sum_{k=1}^K r_i^k = 1, \ \forall i$$

- Because of the constraints, for each sample, only one  $r_i^k$  can be 1.
- We take it to be the one corresponding to the nearest center:

$$r_i^k = \begin{cases} 1, & \text{if } k = \underset{j}{\operatorname{argmin}} \|\mathbf{x}_i - \mu_j\|^2 \\ 0, & \text{otherwise} \end{cases}$$

# Revisiting K means

$$\min_{\{\mu_k\}} \sum_{i=1}^{N} \sum_{k=1}^{K} r_i^k ||\mathbf{x}_i - \mu_k||^2$$

• This can be done by zeroing out the gradient for each center:

$$\frac{\partial R}{\partial \mu_k} = 2 \sum_{i=1}^{N} r_i^k(\mathbf{x}_i - \mu_k) = 0$$

This yields:

$$\mu_k = \frac{\sum_{i=1}^N r_i^k \mathbf{x}_i}{\sum_{i=1}^N r_i^k}$$

This corresponds to the mean of the samples assigned to cluster k.

### **Back to Logistic Regression**

- Replace the step function by a smooth function  $\sigma$ .
- The prediction becomes  $y(\mathbf{x}; \tilde{\mathbf{w}}) = \sigma(\tilde{\mathbf{w}} \cdot \tilde{\mathbf{x}})$ .
- Given the training set  $\{(\mathbf{x}_n, t_n)_{1 \leq n \leq N}\}$  where  $t_n \in \{0, 1\}$ , minimize the cross-entropy

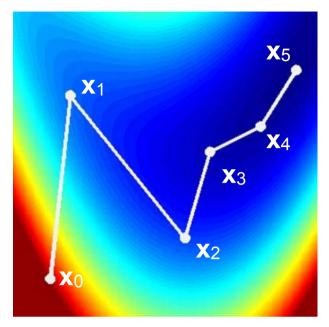
$$E(\tilde{\mathbf{w}}) = -\sum_{n} \{t_n \ln y_n + (1 - t_n) \ln(1 - y_n)\}$$
$$y_n = y(\mathbf{x}_n; \tilde{\mathbf{w}})$$

with respect to  $\tilde{\mathbf{w}}$ .

E is convex but cannot be minimized in closed form!



#### **Gradient Descent**



#### Simplest algorithm:

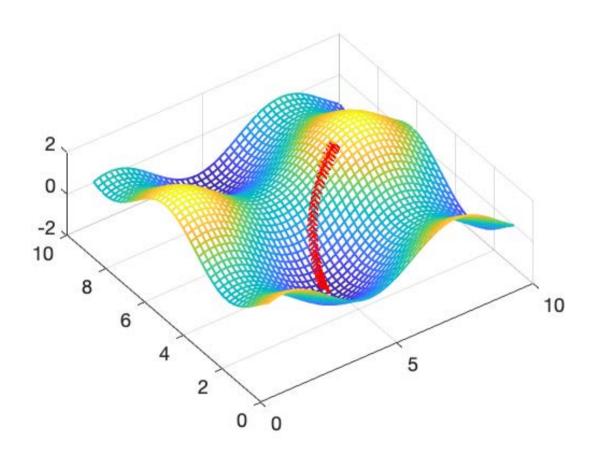
- 1. Initialize  $\mathbf{x}_0$  (e.g., randomly)
- 2. While not converged

2.1. Update 
$$\mathbf{x}_k \leftarrow \mathbf{x}_{k-1} - \eta \nabla f$$

- $\eta$  defines the step size of each iteration.
- In ML, it is often referred to as the *learning rate*.

The gradient replaces the derivative.

# Minimizing a Non-convex Function



$$f(\mathbf{x}) = \sin x_1 + \cos x_2$$

$$\nabla f(\mathbf{x}) = \begin{bmatrix} \cos(x_1) \\ -\sin(x_2) \end{bmatrix} \in \mathbb{R}^2$$

#### Stopping criteria:

- Thresholding the change in function value.
- Thresholding the change in parameters, i.e.  $\|\mathbf{x}_{k-1} \mathbf{x}_k\| < \delta$ .



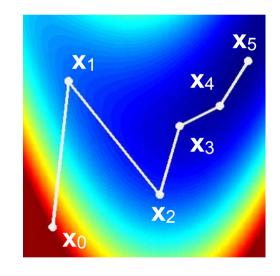
#### **Theoretical Justification**

Steepest gradient descent:

$$\mathbf{x}_k \leftarrow \mathbf{x}_{k-1} - \eta \, \nabla f$$

First order Taylor expansion:

$$f(\mathbf{x} + \mathbf{dx}) \approx f(\mathbf{x}) + \nabla f(\mathbf{x})^T \mathbf{dx}$$
$$f(\mathbf{x} - \eta \nabla f(\mathbf{x})) \approx f(\mathbf{x}) - \eta \|\nabla f(\mathbf{x})\|^2 < f(\mathbf{x})$$

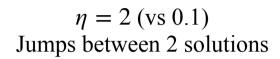


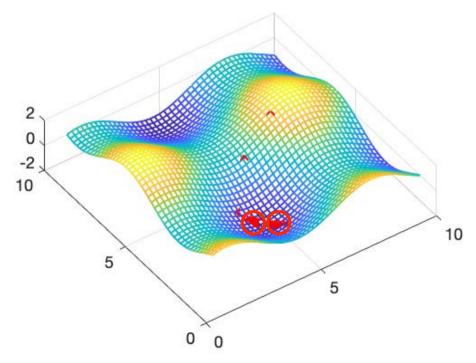
#### Issues:

- Justification but no guarantee
- How do we choose choose  $\eta$ ?
- Many iterations in long and narrow valleys.

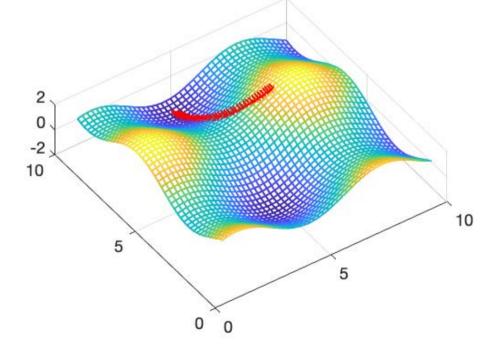


# **Trouble Spots**





$$\mathbf{x}_0 = \begin{bmatrix} 7 \\ 6.5 \end{bmatrix} \text{ (vs } \begin{bmatrix} 7 \\ 6 \end{bmatrix} \text{)}$$





# Learning Rate $\mathbf{x} - \eta_2 \nabla f$ $\mathbf{x} - \eta_1 \nabla f$

#### η too large:

- The first order approximation stops being valid.
- f can increase instead of decrease.

#### η too small:

Convergence rate will be very slow.

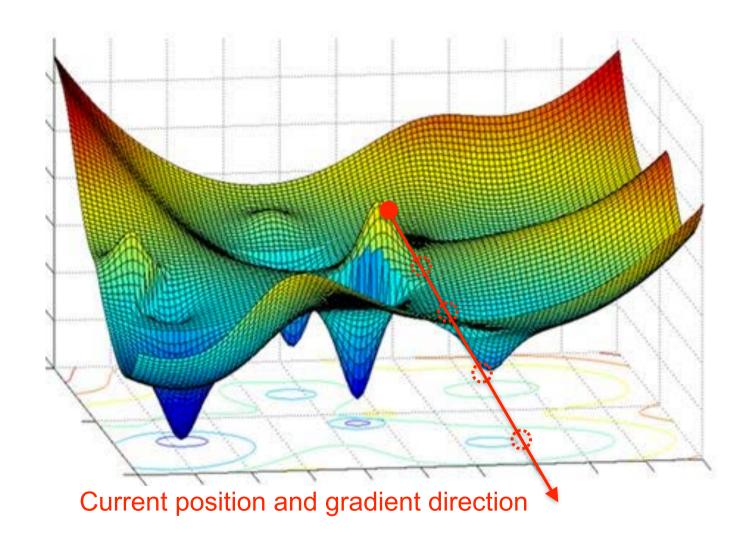
#### Partial solution:

probamos puntos en la linea del gradiente hasta encontrar el min

 Instead of using a fixed learning rate perform a line search in the direction of the gradient.



#### **Line Search**



- Search along the gradient direction for a minimum.
- This is a 1D search and therefore doable.

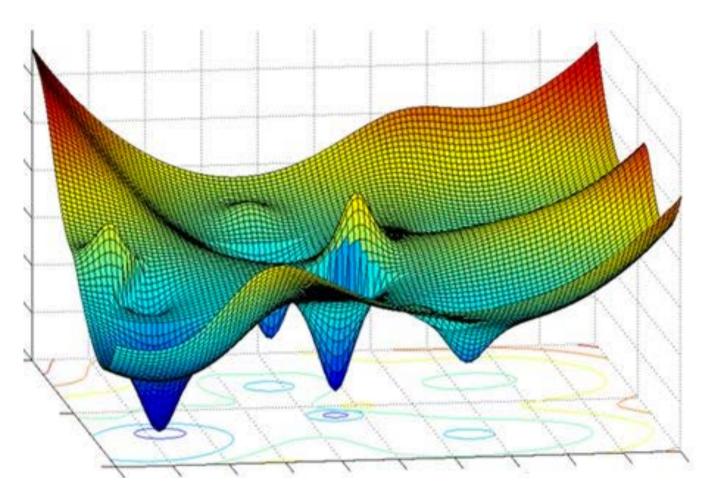


## **Python Implementation**

```
def steepestGrad(objF,x0,nIt=100,eps=1e-6,step=1.0):
  for i in range(nIt):
     y0,g0=objF(x0)
                                                     # Compute the value of objF and its gradient.
     x1=x0-step*g0
                                                     # Take a step in the direction of the gradient.
     y1,=objF(x1)
                                                     # Compute the new value of objF.
     while(y1>y0):
                                                      # Check that the function value has decreased.
        if(np.allclose(x0,x1,eps)):
                                                     # Stopping condition.
          return x0
        step=step/2.0
                                                     # Reduce the step size.
       x1 = x0-step*g0
                                                     # Try again.
       y1, =objF(x1)
     x0,y0=lineSearch(objF,x0,y0,x1,y1,params) \# \arg \min \lambda \mathbf{x}_0 + (1-\lambda)\mathbf{x}_1
  return x0
                                                                        y0
                                                                       y<sub>1</sub>
```



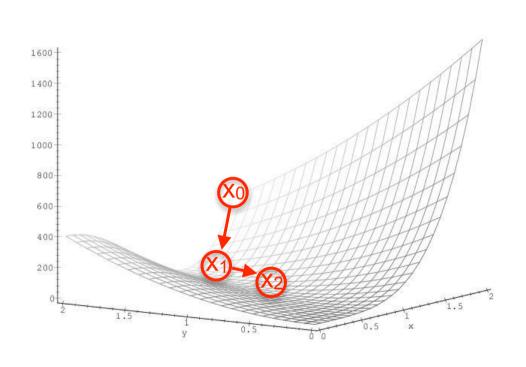
#### **Local Minima**

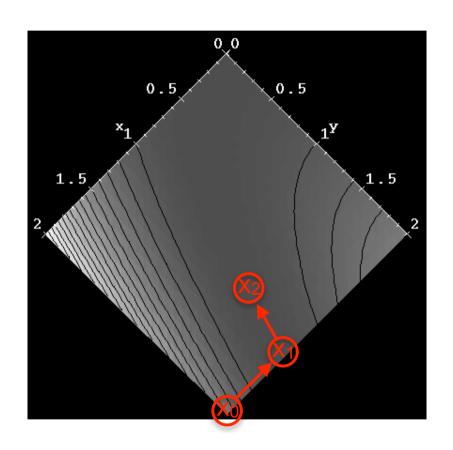


The result depends critically on the starting point and is very likely to be closest local minimum, which is not usually the global one.



### Zig-Zagging towards the Solution





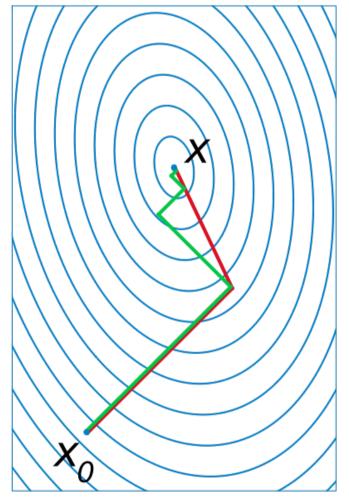
- Successive line searches tend to be perpendicular to each other.
- They would be if we found a true local minimum each time.



# **Conjugate Gradient**

Take the search direction to be a weighted average of the gradient vector and the previous search directions:

- 1. Start at  $\mathbf{x}_0$ .
- 2.  $\mathbf{g}_0 = \nabla F(\mathbf{x}_0)$ .
- 3. For k from 0 to n-1:
  - (a) Find  $\alpha_k$  that minimizes  $f(\mathbf{x}_k + \alpha_k \mathbf{g}_k)$ .
  - (b)  $\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k \mathbf{g}_k$ .
  - (c)  $\beta_k = \frac{\|\nabla f(\mathbf{x}_{k+1})\|^2}{\|\nabla f(\mathbf{x}_k)\|^2}$ .
  - (d)  $\mathbf{g}_{k+1} = -\nabla f(\mathbf{x}_{k+1}) + \beta_k \mathbf{g}_k$ .
- 4.  $\mathbf{x}_0 = \mathbf{x}_n$  and go to step 2 until convergence.







# **Python Implementation**

```
def conjugateGrad(objF,x0,nIt=100,eps=1e-10,step=1.0):
    y0,g0=objF(x0)
    h0 = -g0
                                                   # g: Function gradient.
    g0 = h0
                                                  # h: Conjugate direction.
    for i in range(1,nIt):
       10=np.linalg.norm(h0)
       if(10<eps):
          print('Gradient has vanished.')
          break
       x1 = x0 + (step/l0) * h0
       y1, =objF(x1)
       while(y1>y0):
                                                    # Check that the function value has decreased
         if(np.allclose(x0,x1,eps)):
                                                    # Stopping condition.
            return x0
         step=step/2.0
         x1 = x0 + (step/np.linalg.norm(h0))*h0
         y1, =objF(x1,False)
       x1,y1=lineSearch(objF,x0,y0,x1,y1)
       y1,g1=objF(x1)
                                                    # Recompute value and gradient.
       g1 = -g1
       h1=g1
       if((i\%n)>0):
                                                    # Compute conjugate direction but reset every n iterations.
          gamma=np.dot((g1-g0),g1)/np.dot(g0,g0) # Modified Polak Ribiere, i.e. only if gamma > 0.
         if(gamma>0):
            h1=g1+gamma*h0
       # Switch variables
       g0=g1
       h0=h1
       x0=x1
```



y0=y1

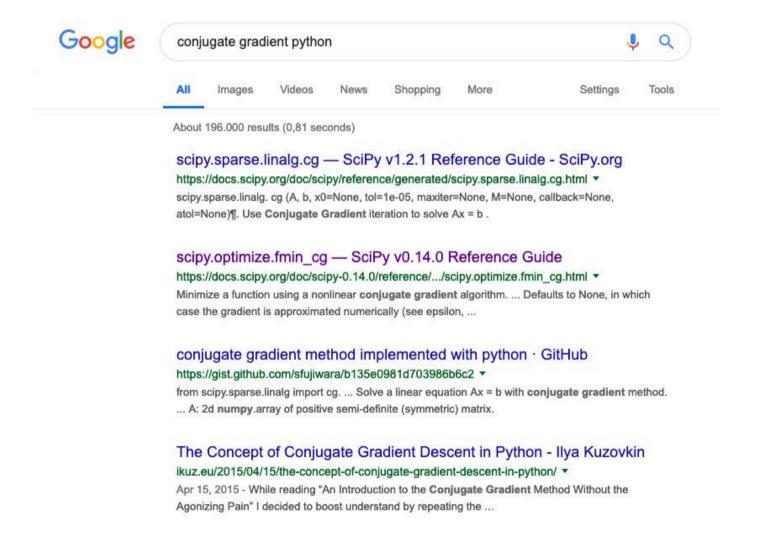


#### In Real Life (1)

```
import scipy
def f(x):
  ..... # return the value of the function.
def g(x):
  ..... # return the gradient of the function.
x0= .... # starting point.
x1 = scipy.optimize.fmin cg(f,x0,fprime=g,epsilon=eps,maxiter=nIt)
```



## In Real Life (2)







#### **Second Order Methods**

Second order Taylor expansion:

$$f(\mathbf{x} + \mathbf{dx}) \approx f(\mathbf{x}) + \nabla f(\mathbf{x})^T \mathbf{dx} + \frac{1}{2} \mathbf{dx}^T H(\mathbf{x}) \mathbf{dx}$$
$$\nabla f(\mathbf{x} + \mathbf{dx}) \approx \nabla f(\mathbf{x}) + H(\mathbf{x}) \mathbf{dx}$$

Newton method:

Solve 
$$H(\mathbf{x})\mathbf{dx} = -\nabla f(\mathbf{x})$$
  

$$\Rightarrow \mathbf{dx} = -H(\mathbf{x})^{-1}\nabla f(\mathbf{x})$$

$$\nabla f(\mathbf{x} + \mathbf{dx}) \approx 0$$

$$f(\mathbf{x} + \mathbf{dx})) \approx f(\mathbf{x}) - \nabla f(\mathbf{x})^T H(\mathbf{x})^{-1} \nabla f(\mathbf{x})$$

$$+ \frac{1}{2} \nabla f(\mathbf{x})^T H(\mathbf{x})^{-1} H(\mathbf{x}) H(\mathbf{x})^{-1} \nabla f(\mathbf{x})$$

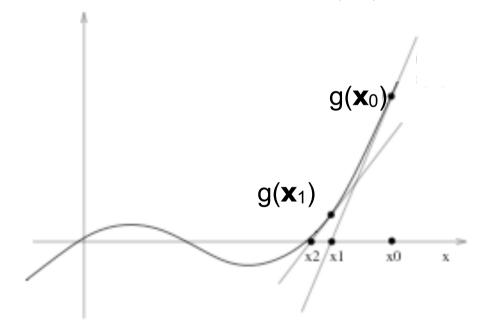
$$\approx f(\mathbf{x}) - \frac{1}{2} \nabla f(\mathbf{x})^T H(\mathbf{x})^{-1} \nabla f(\mathbf{x})$$



#### **Optional**

#### **Newton in 1D**

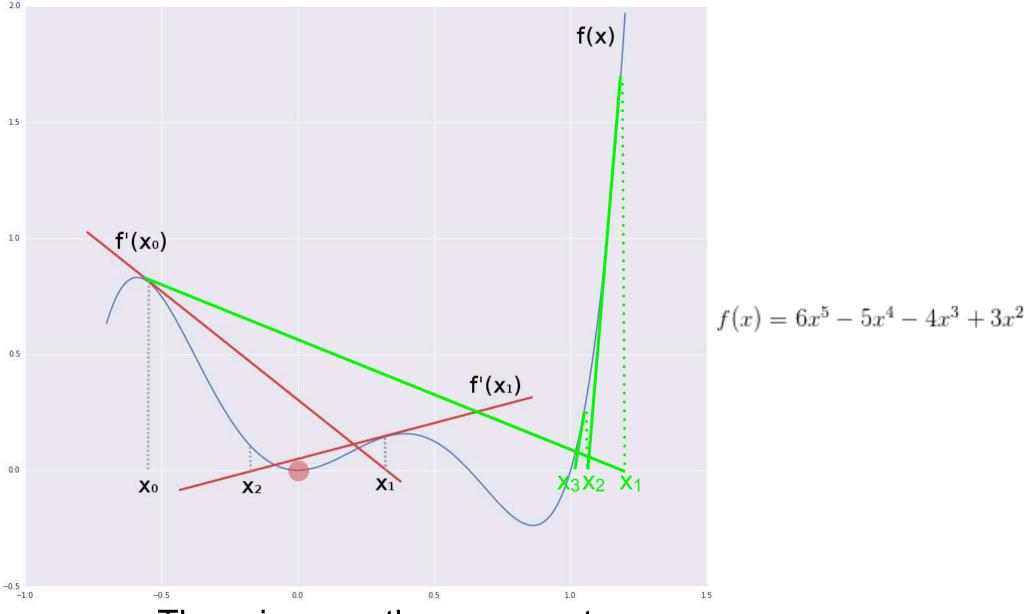
$$0 = g(x + dx) = g(x) + g'(x)dx$$
$$dx = -\frac{g(x)}{g'(x)}$$



$$x \leftarrow x - \frac{g(x)}{g'(x)}$$



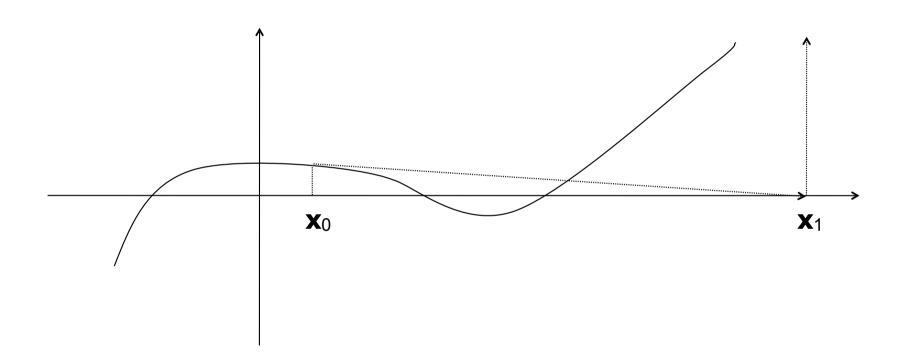
# Finding the Root of a Polynomial



- There is more than one root.
- The one you find depends on the starting point.



### **Potential Instability**



• Individual steps can be very large, leading to instability.



# **Damped Newton**

Second order Taylor expansion:

$$f(\mathbf{x} + \mathbf{dx}) \approx f(\mathbf{x}) + \nabla f(\mathbf{x})^T \mathbf{dx} + \frac{1}{2} \mathbf{dx}^T H(\mathbf{x}) \mathbf{dx}$$
$$\nabla f(\mathbf{x} + \mathbf{dx}) \approx \nabla f(\mathbf{x}) + H(\mathbf{x}) \mathbf{dx}$$

Introduce a damping term:

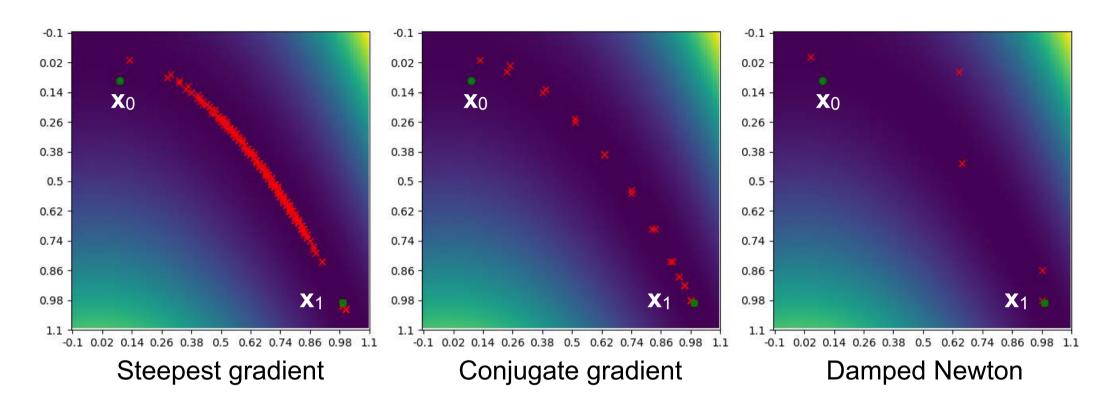
$$\mathbf{x} \leftarrow \mathbf{x} + \mathbf{dx} \text{ with } \begin{cases} & \text{Regular Newton Method: } H(\mathbf{x}) \mathbf{dx} = -\nabla f(\mathbf{x}) \\ & \text{Damped Newton: } (H(\mathbf{x}) + \lambda \mathbf{I}) \mathbf{dx} = -\nabla f(\mathbf{x}) \end{cases}$$

- $\lambda = 0$ : Regular Newton
- $\lambda >> 0$ : Gradient descent



**Optional** 

#### **Qualitative Result**



Damped Newton converges much faster!





## **Python Implementation**

```
def dampedNewton(objF,x,nIt=10,lbda=None):
  for i in range(nIt):
    f,g,H=objF(x)
                                     # Evaluate f, its gradient, and its Hessian.
    x = linSolve(H,g,lbda=lbda)
                                     # Solve (H + \lambda I) x = g
  return x
def linSolve(A,b,lbda=None):
  if(lbda is not None):
       A=A+lbda*np.eye(A.shape[0]) #A < A + \lambda I
                            # Solve A x = b
   x=np.linalg.solve(A,b)
  return(x)
```





# **Optimization in Short**

- Convex functions have a global minimum.
- It can be found using either 1st or 2nd order methods. The latter is usually faster but requires computing second derivatives.
- Non-convex functions can be optimized in a similar manner but this will usually yield a local minimum.

