CSDS 440: Machine Learning

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Office hours T, Th 11:15-11:45 or by appointment

Multivariate functions

$$\min_{x_1,\ldots,x_m} f(x_1,\ldots,x_m)$$

$$J = \left(\frac{\partial f}{\partial x_i} \right) = 0$$

Jacobian is zero

$$H = \left(\frac{\partial^2 f}{\partial x_i \partial x_j} \right) > 0$$

Hessian is "positive definite"

Example

$$f(x,y,z) = x^5y^4 - z^6y^3 + x^4z^3$$

$$\nabla f = \begin{bmatrix} 5x^4y^4 + 4x^3z^3 & 4x^5y^3 - 3z^6y^2 & -6z^5y^3 + 3x^4z^2 \end{bmatrix} = 0$$

????

Observation

- In general, analytically solving for the zeros of the Jacobian is computationally (sometimes algebraically!) infeasible

- Alternative: switch to an *iterative* method

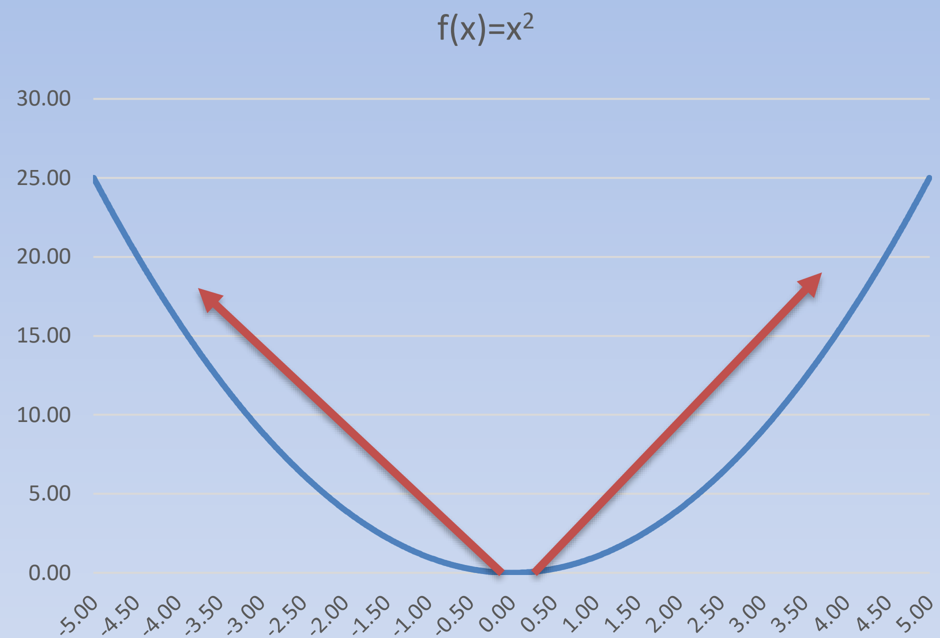
Iterative Optimization (One variable)

- *Initialize* the solution candidate with a *random guess* x
- Until we find the maximum or minimum ("convergence") loop:
  1. Choose a *direction* d
  2. Choose a *stepsize* λ
  3. Move the current guess by λ in the d direction ($x \leftarrow x + \lambda d$)
  4. Check: are we at a minimum/maximum?
     - By evaluating $\frac{df}{dx} = 0$ at the current guess, and ensuring $\frac{d^2f}{dx^2} \geq 0$ (if minimum) or $\frac{d^2f}{dx^2} \leq 0$ (if maximum)
     - In a computer, always check $\left|\frac{df}{dx}\right| \leq tolerance$ (a small quantity such as 1e-6)

Different optimization algorithms will do these steps differently

The derivative as a vector

“take a step in the derivative direction”



At each point, the derivative can be **viewed as (the slope of) a vector** pointing in the direction of *fastest increase* of the function value

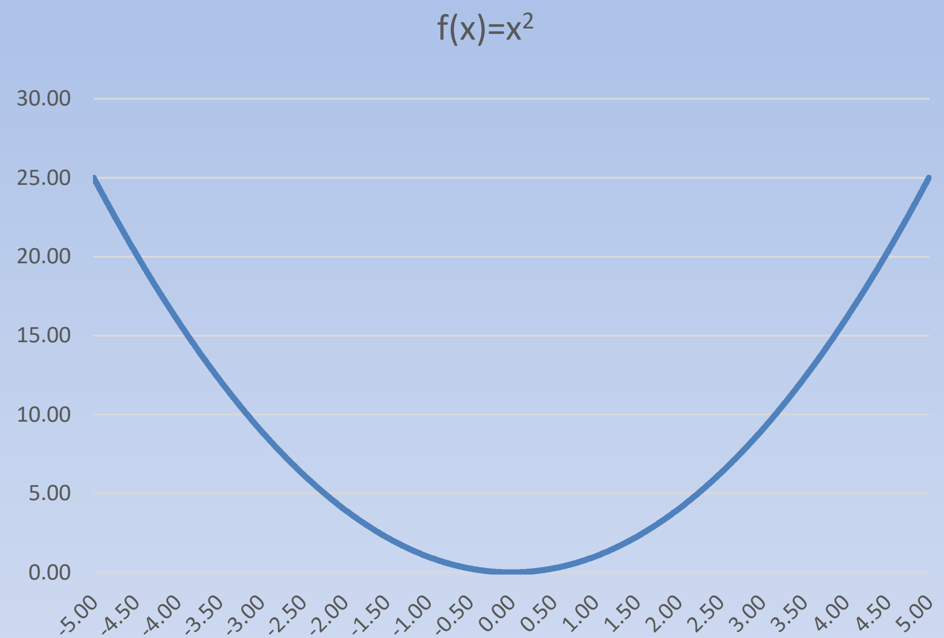
- Suppose $x=-1$, $f(x)=1$. Then $f'(x)=-2$. Let $y=x+f'(x)=-3$. $f(y)=9$.
- Suppose $x=1$, $f(x)=1$. $f'(x)=2$. $y=x+f'(x)=3$. $f(y)=9$.

Gradient Ascent/Descent

- From the current x, move in the gradient direction (for maximization) or negative gradient direction (for minimization)

$$x_{new} = x_{old} - \underbrace{\lambda}_{\text{Stepsize}} \left.\frac{df}{dx}\right|_{x_{old}}$$

Example



- Set stepsize=0.25, tolerance=0.02
- Start with $x_0=-0.4$, $f(x)=0.16$, $f'(x)=-0.8$.
- $x_1=x_0-(0.25)(-0.8)=-0.4+0.2=-0.2$.
- $f(x_1)=0.04$. $f'(x_1)=-0.4$. (not converged)
- $x_2=x_1-(0.25)(-0.4)=-0.2+0.1=-0.1$.
- $f(x_2)=0.01$. $f'(x_2)=-0.2$. (not converged)
- $x_3=x_2-(0.25)(-0.2)=-0.1+0.05=-0.05$.
- $f(x_3)=0.0025$. $f'(x_3)=-0.1$. (not converged)
- $x_4=x_3-(0.25)(-0.1)=-0.05+0.025=-0.025$.
- $f(x_4)=6.25\text{e-}3$. $f'(x_4)=-0.05$. (not converged)
- $x_5=x_4-(0.25)(-0.05)=-0.025+0.0125=-0.0125$.
- $f(x_5)=1.56\text{e-}3$. $f'(x_5)=-0.025$. (not converged)
- $x_6=x_5-(0.25)(-0.025)=-0.0125+0.00625=-0.00625$.
- $f(x_6)=3.9\text{e-}4$. $f'(x_6)=-0.015$. (converged)

Observations:
1. Stepsize and oscillations
2. Rate of convergence
3. Choice of starting point and solution found

Example

$$g'(x) = 4x^3 + 21x^2 + 10x - 17$$

$$g'(x) = 0 \text{ for } x = -4.5, -1.4, 0.7$$

$$g''(x) = 12x^2 + 42x + 10$$

$$= 64, -25.28, 45.28$$

Newton-Raphson Method

- From the current $\mathbf{x}$, take a Newton step:

$$f(\mathbf{x}_{old}+u)=f(\mathbf{x}_{old})+u^T\nabla f_{\mathbf{x}_{old}}(\mathbf{x})+\frac{1}{2}u^T\nabla^2 f_{\mathbf{x}_{old}}(\mathbf{x})u=g(u)$$

Set $\dfrac{\partial g}{\partial u}=0$, then

$$\nabla f_{\mathbf{x}_{old}}(\mathbf{x})+\nabla^2 f_{\mathbf{x}_{old}}(\mathbf{x})u=0$$

and

$$u=\underline{-\left[\nabla^2 f_{\mathbf{x}_{old}}(\mathbf{x})\right]^{-1}\nabla f_{\mathbf{x}_{old}}(\mathbf{x})}$$

Newton Step

$$\mathbf{x}_{new}=\mathbf{x}_{old}-\left[\nabla^2 f_{\mathbf{x}_{old}}(\mathbf{x})\right]^{-1}\nabla f_{\mathbf{x}_{old}}(\mathbf{x})$$

Properties of the NR method

- Fast convergence close to solution

- Not guaranteed to converge if started far from solution, may cycle or diverge in this case

Quasi-Newton methods

- Often, constructing the Hessian for a multivariate function is computationally difficult, because it takes $O(n^2)$ space and time and has to be done over and over

- So a number of methods exist that approximate the Hessian by using the Jacobian at nearby points

Random Restarts

- The solution we get from Gradient Ascent/Descent depends on the initialization

- One way to make it less dependent is to use *random restarts*
  - Run multiple gradient descents with *different, random initializations* and keep the best overall solution
  - Can be done in parallel