Security and Fairness of Deep Learning

Second-Order Optimization Methods

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Key insight

Leverage second-order derivatives (gradient) in addition to first-order derivatives to converge faster to minima

Newton's method for convex functions

- Iterative update of model parameters like gradient descent

- Key update step

$$x^{k+1} = x^k - H(x^k)^{-1} \nabla f(x^k)$$

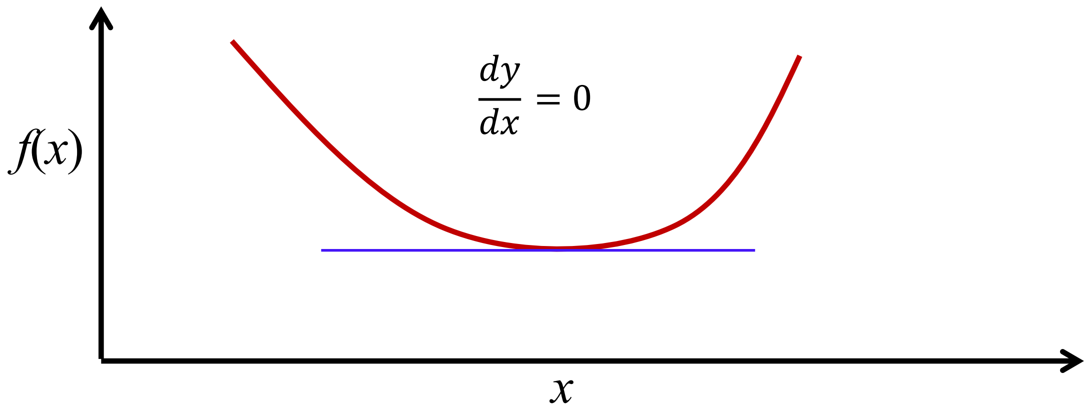
- Compare with gradient descent

$$x^{k+1} = x^k - \eta^k \nabla f(x^k)$$

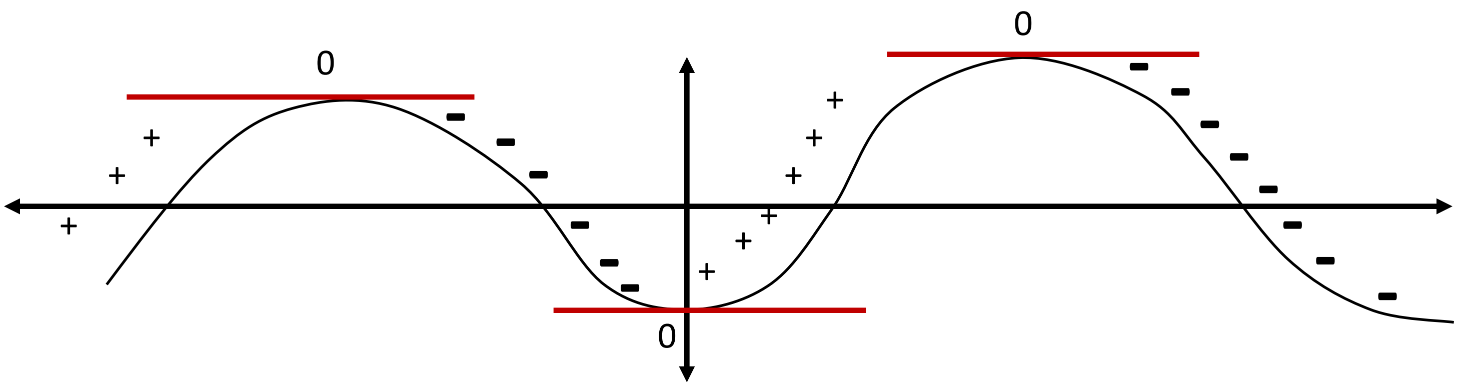
In two steps

- Function of single variable
- Function of multiple variables

Derivative at minima

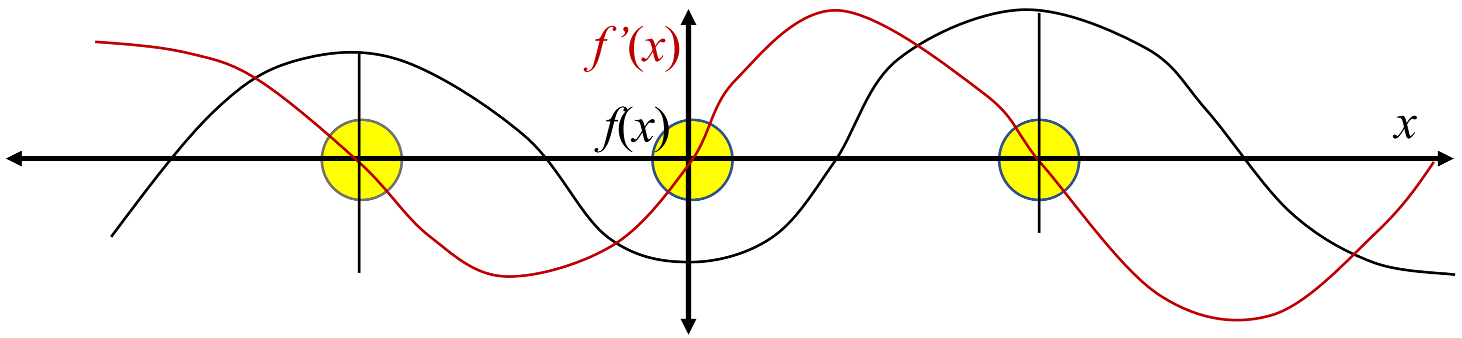


Turning Points



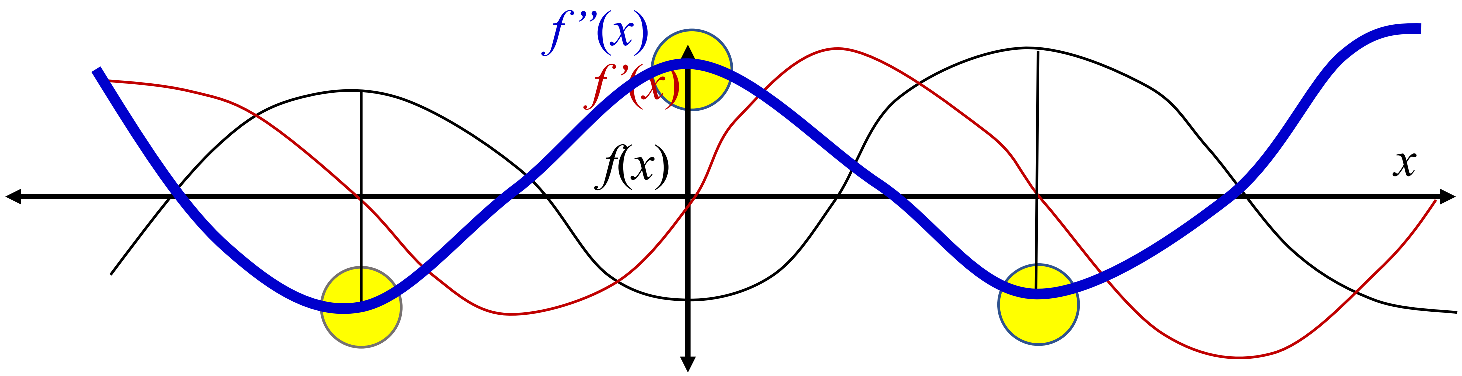
- Both *maxima* and *minima* have zero derivative
- Both are turning points

Derivatives of a curve



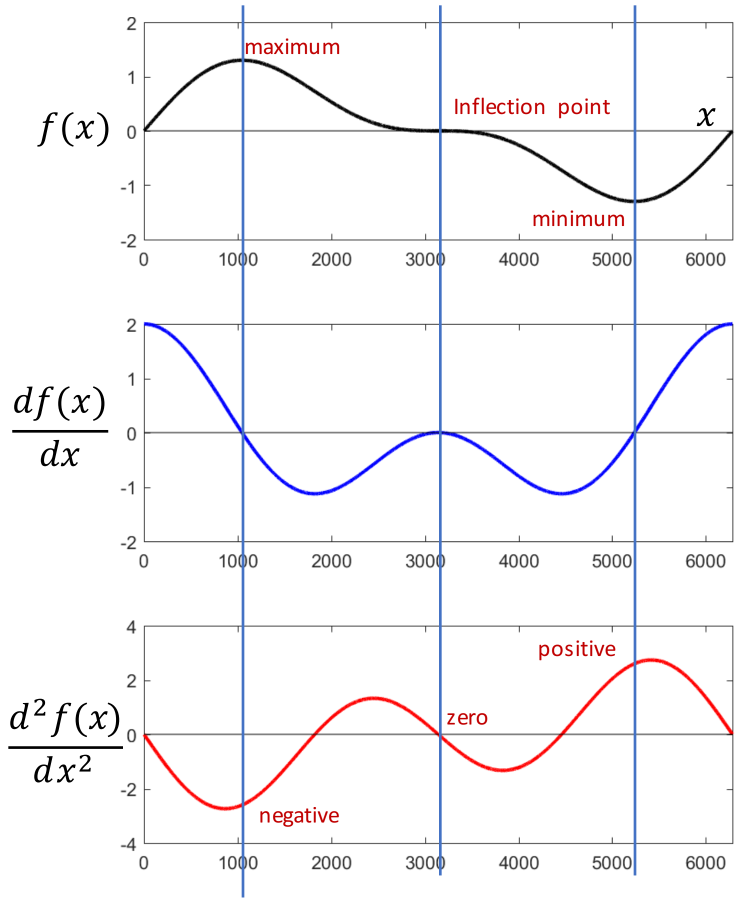
- Both *maxima* and *minima* are turning points
- Both *maxima* and *minima* have zero derivative

Derivative of the derivative of the curve



- The *second derivative f''*(*x*) is –ve at maxima and +ve at minima

Summary



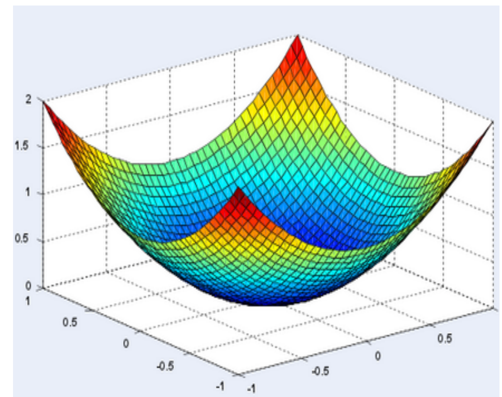
- All locations with zero derivative are *critical* points
- The *second* derivative is
  - ≥ 0 at minima
  - ≤ 0 at maxima
  - Zero at inflection points

In two steps

- Function of single variable
- Function of multiple variables

Gradient of function with multi-variate inputs

- Consider $f(X) = f(x_1, x_2, \dots, x_n)$
- $\nabla f(X) = \begin{bmatrix} \frac{\partial f(X)}{\partial x_1} & \frac{\partial f(X)}{\partial x_2} & \cdots & \frac{\partial f(X)}{\partial x_n} \end{bmatrix}$



Note: Scalar function of multiple variables

The Hessian

- The Hessian of a function $f(x_1, x_2, \dots, x_n)$

$$\nabla^2 f(x_1,\dots,x_n) := \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & . \; . & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & . \; . & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ . & . & . \; . & . \\ . & . & . \; . & . \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & . \; . & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix}$$

Unconstrained minimization of multivariate function

1. Solve for the X where the gradient equation equals to zero

$$\nabla f(X) = 0$$

2. Compute the Hessian Matrix $\nabla^2 f(X)$ at the candidate solution and verify that
   - Hessian is positive definite (eigenvalues positive) -> to identify local minima
   - Hessian is negative definite (eigenvalues negative) -> to identify local maxima

Catch

- Closed form solutions not always available

- Instead use an iterative refinement approach
  - (Stochastic) gradient descent makes use of first-order derivatives (gradient)
  - Can we do better with second-order derivatives (Hessian)?

Newton's method for convex functions

- Iterative update of model parameters like gradient descent

- Key update step

$$x^{k+1} = x^k - H(x^k)^{-1} \nabla f(x^k)$$

- Compare with gradient descent

$$x^{k+1} = x^k - \eta^k \nabla f(x^k)$$

Taylor series

The Taylor series of a function $f(x)$ that is infinitely differentiable at the point a is the power series

$$f(a) + \frac{f'(a)}{1!}(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \frac{f'''(a)}{3!}(x-a)^3 + \cdots.$$

Taylor series second-order approximation

The Taylor series second-order approximation of a function $f\,(x)$ that is infinitely differentiable at the point a is

$$f(a) + f'(a)(x-a) + \frac{1}{2} f''(a)(x-a)^2$$

Local minimum of Taylor series second-order approximation

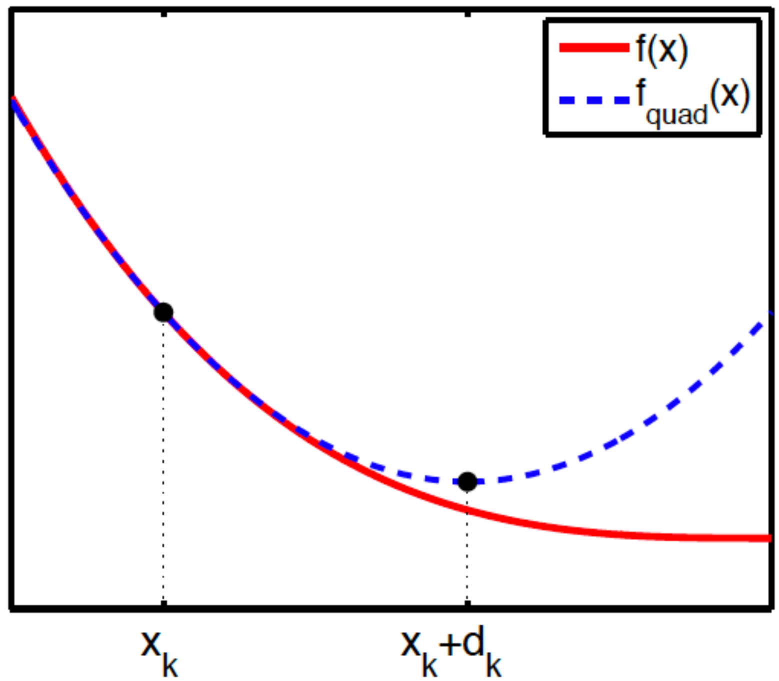
$$f(a) + f'(a)(x-a) + \frac{1}{2}f''(a)(x-a)^2$$

$$x_m = a - \frac{1}{f''(a)}f'(a) \ if \, f''(a) > 0$$

Newton's method approach

Take step to local minima of second-order Taylor approximation of loss function

Example



Murphy, Machine Learning, Fig 8.4

Taylor series second-order approximation for multivariate function

$$f(a) + \bigtriangledown f(a)(x-a) + \frac{1}{2} \bigtriangledown f^2(a)(x-a)^2$$

$$f(x^k) + \bigtriangledown f(x^k) + \frac{1}{2} H(x^k)(x-x^k)^2$$

Deriving update rule

Local minima of this function

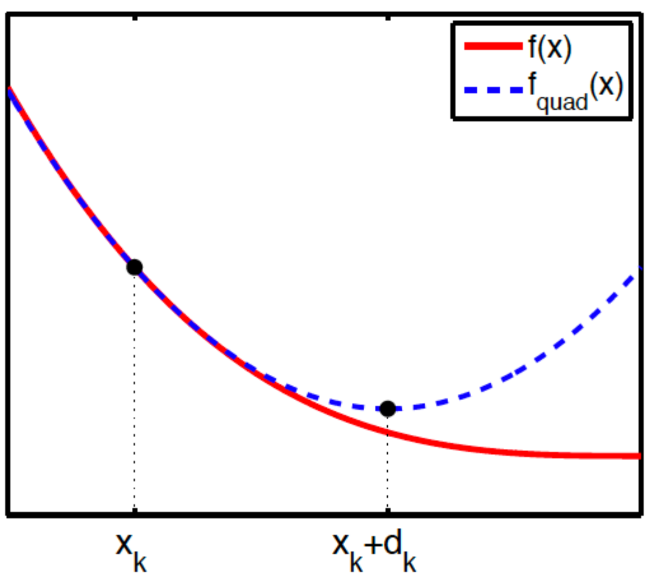
$$f(x^k) + \bigtriangledown f(x^k) + \frac{1}{2} H(x^k)(x - x^k)^2$$

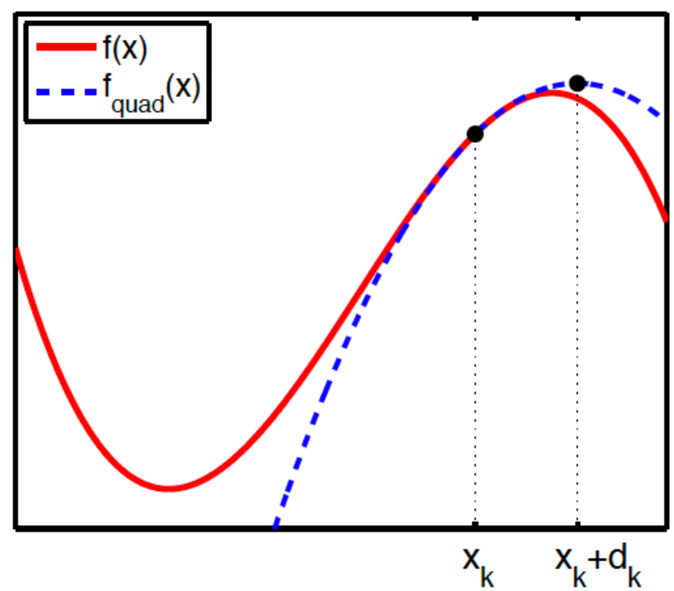
is

$$x = x^k - H(x^k)^{-1} \bigtriangledown f(x^k)$$

Weakness of Newton's method (1)

- Appropriate when function is strictly convex
  - Hessian always positive definite





Murphy, Machine Learning, Fig 8.4

Weakness of Newton's method (2)

- Computing inverse Hessian explicitly is too expensive
  - O(k^3) if there are k model parameters: inverting a k x k matrix

Quasi-Newton methods address weakness

- Iteratively build up approximation to the Hessian
- Popular method for training deep networks
  - Limited memory BFGS (L-BFGS)
  - Will discuss in a later lecture

Acknowledgment

Based in part on material from CMU 11-785

Example

- Minimize

$$f(x_1, x_2, x_3) = (x_1)^2 + x_1(1 - x_2) - (x_2)^2 - x_2 x_3 + (x_3)^2 + x_3$$

- Gradient

$$\nabla f = \begin{bmatrix} 2x_1 + 1 - x_2 \\ -x_1 + 2x_2 - x_3 \\ -x_2 + 2x_3 + 1 \end{bmatrix}^T$$

Example

- Set the gradient to null

$$\nabla f = 0 \Rightarrow \begin{bmatrix} 2x_1 + 1 - x_2 \\ -x_1 + 2x_2 - x_3 \\ -x_2 + 2x_3 + 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

- Solving the 3 equations system with 3 unknowns

$$x = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} -1 \\ -1 \\ -1 \end{bmatrix}$$

Example

- Compute the Hessian matrix $\nabla^2 f = \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix}$
- Evaluate the eigenvalues of the Hessian matrix

$$\lambda_1 = 3.414, \quad \lambda_2 = 0.586, \quad \lambda_3 = 2$$

- All the eigenvalues are positive => the Hessian matrix is positive definite
- This point is a minimum $x = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} -1 \\ -1 \\ -1 \end{bmatrix}$