CS-453 Machine Learning

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Gradient Descent Variations

So far . . .

- Neural Networks are universal approximators.
- Backpropagation allows computation of derivatives in hidden layers.
- Gradient descent finds weights corresponding to local minimum of loss surface.
- In this lecture: alternative methods of finding local minima of loss surface.
  - First-order methods
    - Rprop
  - Second-order methods
    - Taylor series approximation
    - Newton's method
    - Quickprop
- Next lecture:
  - Momentum-based first-order methods

Gradient Descent in Higher Dimensions

- Let $\Delta \mathrm{w}^{\tau+1}$ denote the stepat time $\tau + 1$.

$$w^{\tau+1} = w^{\tau} + \Delta w^{\tau+1}$$

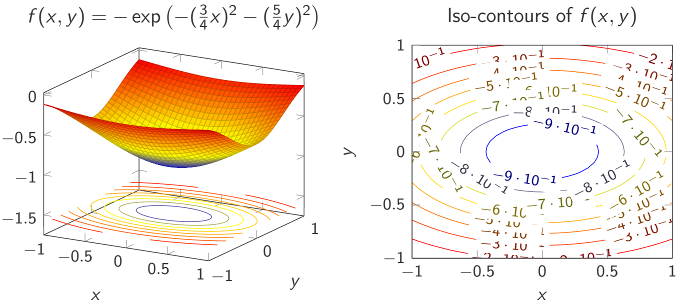
- For gradient descent

$$\Delta \mathrm{w}^{\tau+1} = -\eta \nabla_{\mathrm{w}}^{\tau} L$$

- For gradient descent in $1D$,

$$\Delta w^{\tau+1} = -\eta \left. \frac{dL}{dw} \right|_{\tau}$$

The only issue is determining learning rate η.



A function that changes faster in y-direction.

- In higher dimensions, if $\left|\frac{\partial L}{\partial w_i}\right| >> \left|\frac{\partial L}{\partial w_j}\right|$ then using the same η *can* result in overshooting in the direction of w_i and very slow convergence in the direction of w_j.
- Solution: separate learning rate η_i for each direction w_i.

Resilient Propagation (Rprop)

- In Rprop[1], each direction is handled independently.
- Increase learning rate for direction i if current derivative has same sign as previous derivative.
- Otherwise, you just overshot a minimum.
  - So go back to previous location.
  - Decrease learning rate for that direction.
  - Update parameter with this smaller step.

$$\eta_i = \begin{cases} \alpha\eta_i & \text{if } \left.\frac{\partial L}{\partial w_i}\right|_{\tau} * \left.\frac{\partial L}{\partial w_i}\right|_{\tau-1} > 0 \\ \beta\eta_i & \text{if } \left.\frac{\partial L}{\partial w_i}\right|_{\tau} * \left.\frac{\partial L}{\partial w_i}\right|_{\tau-1} < 0 \\ \eta_i & \text{otherwise} \end{cases}$$

- *Hyperparameters* should follow the constraint $\alpha > 1$ and $\beta < 1$.

[1] Riedmiller and Braun, 'A direct adaptive method for faster backpropagation learning: The RPROP algorithm'.

Resilient Propagation (Rprop)

- Typical values are $\alpha = 1.2$ and $\beta = 0.5$.
  - Increase learning rate slowly but decrease quickly when you overshoot.
- In practice, learning rates are bounded via η_{min} and η_{max}.

$$\eta_i = \begin{cases} \min(\alpha\eta_i, \eta_{\text{max}}) & \text{if } \left.\frac{\partial L}{\partial w_i}\right|_{\tau} * \left.\frac{\partial L}{\partial w_i}\right|_{\tau-1} > 0 \\ \max(\beta\eta_i, \eta_{\text{min}}) & \text{if } \left.\frac{\partial L}{\partial w_i}\right|_{\tau} * \left.\frac{\partial L}{\partial w_i}\right|_{\tau-1} < 0 \\ \eta_i & \text{otherwise} \end{cases}$$

- Rprop converges much faster than gradient descent.
- But it works well when derivatives are accumulated over large batches.

Taylor Series Approximation

- If values of a function $f(a)$ and its derivatives $f'(a), f''(a), \ldots$ are known at a value a, then we can approximate $f(x)$ for x close to a via the *Taylor series expansion*

$$f(x) \approx f(a) + (x-a)^1 \frac{f'(a)}{1!} + (x-a)^2 \frac{f''(a)}{2!} + (x-a)^3 \frac{f'''(a)}{3!} + O((x-a)^4)$$

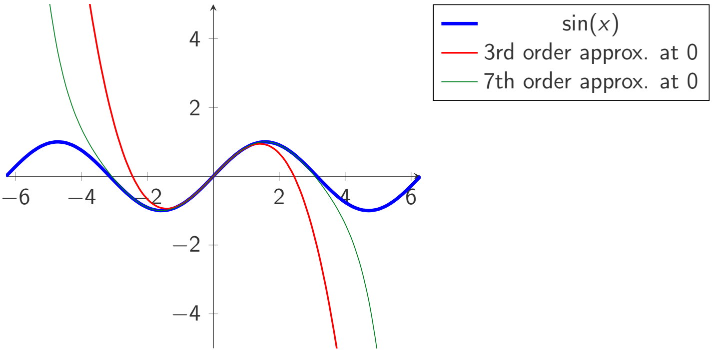
- Using $\Delta x = x - a$, Taylor series can be equivalently expressed as

$$\begin{aligned} f(a+\Delta x) &\approx f(a) + (\Delta x)^1 \frac{f'(a)}{1!} + (\Delta x)^2 \frac{f''(a)}{2!} + (\Delta x)^3 \frac{f'''(a)}{3!} + O((\Delta x)^4) \\ &= \sum_{n=0}^{\infty} \frac{1}{n!} f^n(a)(\Delta x)^n \end{aligned}$$

Taylor Series Approximation
Examples

- For x around $a = 0$
  - $\sin(x) \approx x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + \dots$
  - $e^x \approx 1 + \frac{x^1}{1!} + \frac{x^2}{2!} + \frac{x^3}{3!} + \frac{x^4}{4!} + \dots$

Taylor Series Approximation
Not very useful for x not close to a



The sine function (blue) is closely approximated around 0 by its Taylor polynomials. The 7th order approximation (green) is good for a full period centered at 0. However, it becomes poor for $|x - 0| > \pi$.

Taylor Series Approximation

- It is often convenient to use the first-order Taylor expansion

$$f(a+\Delta x) \approx f(a) + \Delta x f'(a)$$

or the second order Taylor expansion

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

- In d-dimensional input space

$$f(\mathrm{a}+\Delta \mathrm{x}) \approx f(\mathrm{a}) + \Delta \mathrm{x}^T \nabla f + \frac{1}{2}\Delta \mathrm{x}^T \mathrm{H} \Delta \mathrm{x}$$

where $\mathrm{H} \in \mathbb{R}^{d\times d}$ is the Hessian matrix composed from second derivatives.

$$\mathrm{H} = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1 \partial x_1} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_d} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_d} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_d \partial x_1} & \frac{\partial^2 f}{\partial x_d \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_d \partial x_d} \end{bmatrix}$$

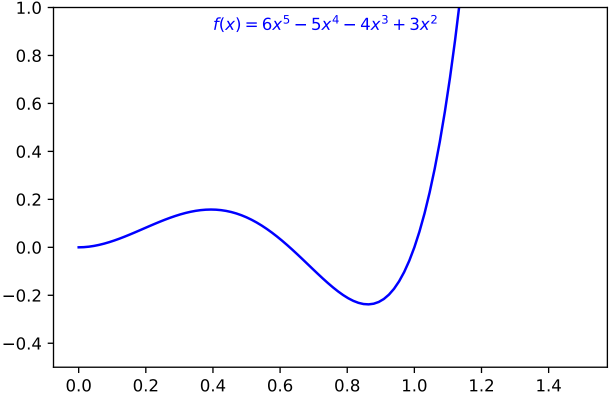
Newton's Method for finding stationary points

- Starting from a_0, we want to find a stationary point of f.
- Instead of actual function f, use a quadratic approximation (second-order Taylor expansion) of f at a_0.
- Find a step Δx such that $a_0 + \Delta x$ minimizes the quadratic approximation of f.

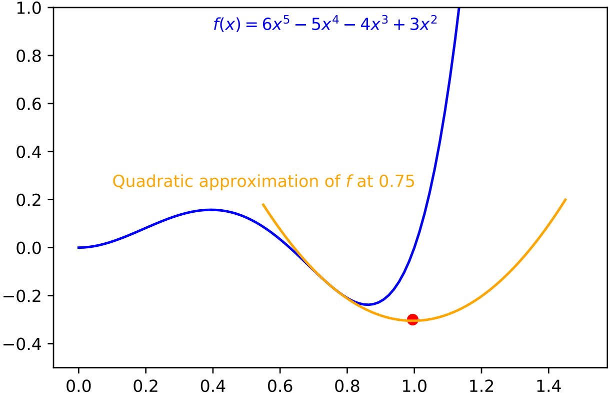
$$\begin{aligned} \frac{d}{d\Delta x}\left(f(a_0) + f'(a_0)\Delta x + \frac{1}{2}f''(a_0)(\Delta x)^2\right) &= 0 \\ f'(a_0) + f''(a_0)\Delta x &= 0 \\ \Delta x &= -\frac{f'(a_0)}{f''(a_0)} \end{aligned}$$

- Move to $a_1 = a_0 + \Delta x$ and repeat the process at a_1.
- Continue until convergence to a stationary point a_n.

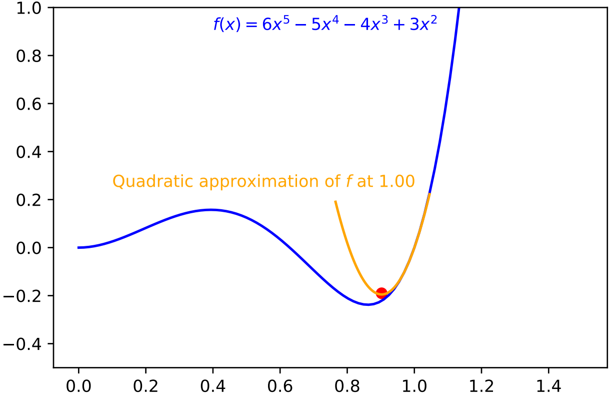
Newton's Method for finding stationary points



Newton's Method for finding stationary points



Newton's Method for finding stationary points



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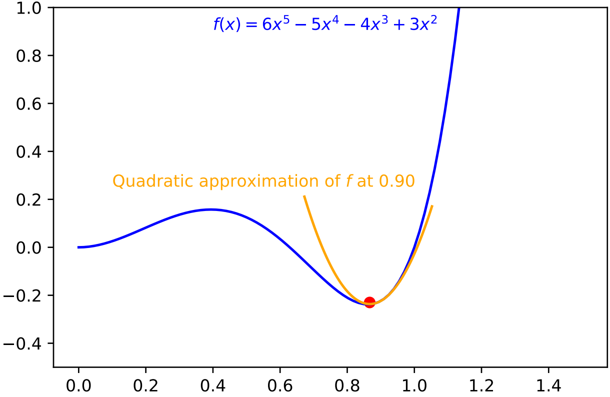
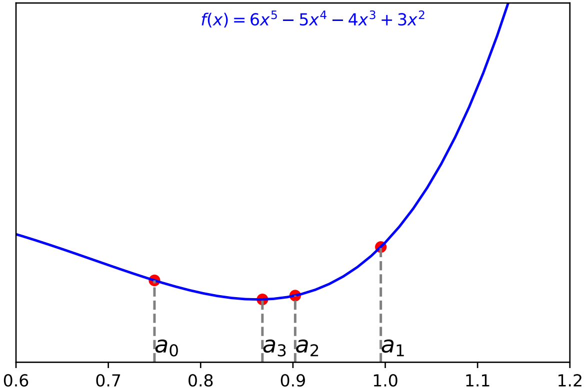


Newton's Method for finding stationary points



Newton's Method
Role of the 2nd-derivative

- For weights of a neural network, Newton's update corresponds to

$$w^{\tau+1} = w^{\tau} - \left(\frac{\partial^2 L}{\partial w^2}\right)^{-1} \frac{\partial L}{\partial w}$$

- In other words, gradient descent learning rate η corresponds to inverse of 2nd-derivative.
- Division by 2nd-derivative can also be viewed as normalising the gradient.
- In higher dimensions

$$\mathrm{w}^{\tau+1} = \mathrm{w}^{\tau} - \mathrm{H}^{-1}\nabla_{\mathrm{w}} L$$

  The inverse Hessian matrix normalises the gradient vector.

Newton's Method
Role of the 2nd-derivative

- Complete Hessian matrix is rarely used because of its size and computational cost of inverting it.
- Common assumption: diagonal Hessian matrix.

$$H = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1 \partial x_1} & 0 & \dots & 0 \\ 0 & \frac{\partial^2 f}{\partial x_2 \partial x_2} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \frac{\partial^2 f}{\partial x_d \partial x_d} \end{bmatrix}$$

- Inverse of diagonal matrix is cheap (reciprocal of entries on the diagonal).

Quickprop

- Decouple all directions.
- Perform Newton updates in each direction.

$$w_i^{\tau+1} = w_i^{\tau} - \left(\frac{\partial^2 L}{\partial w_i^2}\right)^{-1} \frac{\partial L}{\partial w_i}$$

- Approximate 2nd-derivative *numerically* by finite difference of 1st-derivatives.

$$\frac{\partial^2 L}{\partial w_i^2} \approx \frac{\left.\frac{\partial L}{\partial w_i}\right|_{\tau} - \left.\frac{\partial L}{\partial w_i}\right|_{\tau-1}}{\Delta w_i^{\tau-1}}$$

- Leads to very fast convergence.
- Some instability where loss is non-convex since everything is based on assumptions of convexity (quadratic approximation in Newton's method).

Fahlman, *An empirical study of learning speed in back-propagation networks*.

Summary

- For complex and non-convex loss functions of deep networks, vanilla gradient descent can get stuck in poor local minima and saddle points.
- It can also converge very slowly.
- Different directions require different learning rates.
- Adaptive learning rates are very important.
- Next lecture: momentum-based first-order methods.