Deep Learning

04 Gradient Descent

Dr. Konda Reddy Mopuri
Dept. of Artificial Intelligence
IIT Hyderabad
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Loss/Risk

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భారతీయ సాంకేతిక విజ్ఞాన సంస్థ హైదరాబాద్
भारतीय प्रौद्योगिकी संस्थान हैदराबाद
Indian Institute of Technology Hyderabad

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    - Density estimation: $l(q, z) = -log(q(z))$

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6. Loss may have additional terms (from prior knowledge)

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3. This is unknown. However, if the training data $\mathcal{D} = \{z_1, \dots, z_N\}$ is i.i.d. we can estimate the risk empirically (known as empirical risk),

   $\hat{R}(f;\mathcal{D}) = \hat{\mathbb{E}}_{\mathcal{D}}(l(f,z)) = \frac{1}{N}\sum_{i=1}^{N} l(f, z_n)$

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$$w^* = \underset{w}{\operatorname{argmin}} \, L(w)$$

Optimization

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- General and vast, but we will discuss within our context

Optimization

- Finding the parameters that minimize the training loss

$$W^*, \mathbf{b}^* = \underset{W,\mathbf{b}}{\operatorname{argmin}} \mathcal{L}(f(\cdot; W, \mathbf{b}); \mathcal{D})$$

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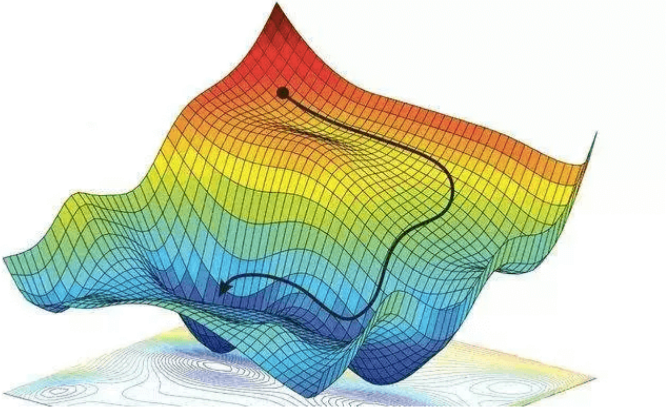
  - Closed form solution (e.g. linear regression)
  - Ad-hoc recipes (e.g. Perceptron, K-NN classifier)
  - What if the loss function can't be minimized analytically?

Loss surface



Source: Medium

Not-so-intelligent idea!

- Probe random directions

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- Progress if you find a useful direction

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Not-so-intelligent idea!

- Probe random directions
- Progress if you find a useful direction
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- Very ineffective!

A better looking one: Follow the slope!

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- This is Gradient Descent!

Derivative and Gradient

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$$\frac{\partial f}{\partial x} = \lim_{\delta \to 0} \frac{f(x+\delta) - f(x)}{h}$$

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- $\Delta f = \frac{\partial f}{\partial x} \Delta x$

Derivative and Gradient

- In higher dimensions, given a function

$$f : \mathcal{R}^D \rightarrow \mathcal{R}$$

gradient is the mapping

$$\nabla f : \mathcal{R}^D \rightarrow \mathcal{R}^D$$
$$x \rightarrow \left(\frac{\partial f}{\partial x_1}, \ldots, \frac{\partial f}{\partial x_D} \right)$$

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- $\Delta f = \nabla f \cdot \Delta x$ (dot product!)

Gradient Descent

$$\mathcal{L}(w+u) = \mathcal{L}(w) + \nabla_w \mathcal{L}(w) \cdot u + \frac{1}{2!} u^T \nabla^2 \mathcal{L}(w) u + \dots$$
$$\approx \mathcal{L}(w) + \nabla_w \mathcal{L}(w) \cdot u$$

- For $\mathcal{L}(w+u)$ to be lesser than $\mathcal{L}(w)$, we need $\nabla_w \mathcal{L}(w) \cdot u < 0$

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- For $\mathcal{L}(w+u)$ to be lesser than $\mathcal{L}(w)$, we need $\nabla_w \mathcal{L}(w) \cdot u < 0$
- The difference would be least if u is in the opposite direction to $\nabla_w \mathcal{L}(w)$, the gradient

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- Gradient points uphill $\rightarrow$ negative of gradient points downhill

Gradient Descent

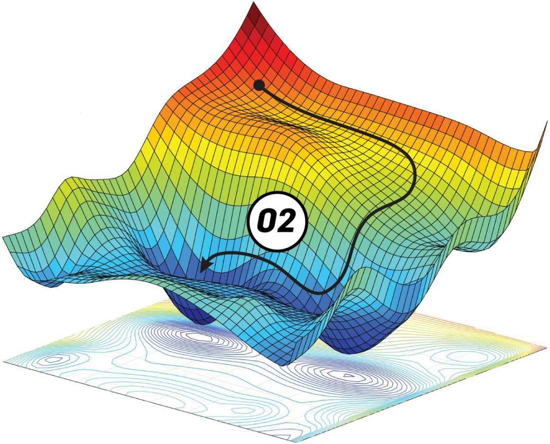

Figure credits:Ahmed Fawzy Gad

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2. Repeatedly modify it via updating in small steps
3. At each step, modify in the direction that produces steepest descent along the error surface

How to compute the gradient?

- Numerically, for each component of w using the derivative formula

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- Slow and approximate!

How to compute the gradient?

- Analytically, using calculus for computing the derivatives

$$L_i = \sum_{j \neq y_i} max\{0, s_j - s_{y_i} + 1\}$$

$$L = \frac{1}{N} \sum_i L_i + \sum_k w_k^2$$

$$s = f(x, W)$$

$$\nabla L_{iw}?$$

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$$\nabla L_{iw}?$$

- Analytic way is fast, exact, but error-prone!

Batch Gradient Descent

for i in range(nb_epochs):
  ∇L_w = evaluate_gradient(L, $\mathcal{D}$, w)
  w = w - η * ∇L_w

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1. Guaranteed to converge to global minima in case of convex functions, and to a local minima in case of non-convex functions

Stochastic Gradient Descent (SGD)

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Stochastic Gradient Descent (SGD)

1. Performs updates parameters for each training example
   $w = w - \eta \nabla_w \mathcal{L}(w, x^i, y^i)$
2. In case of large datasets, Batch GD computes redundant gradients for similar examples for each parameter update
3. SGD does away with redundancy and generally faster and can be used to learn online

Stochastic Gradient Descent (SGD)

1. However, frequent updates with a high variance cause the objective function to fluctuate heavily

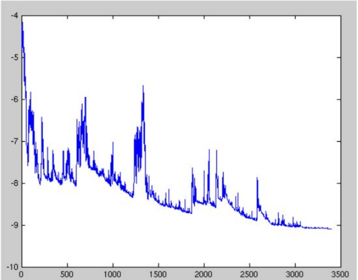

Figure credits: Wikipedia

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1. SGD's fluctuations enable it to jump to new and potentially better local minima
2. This complicates the convergence, as it overshoots
3. However, if the learning rate is slowly decreased, we can show similar convergence to Batch GD

Stochastic Gradient Descent (SGD)

```
for i in range(nb_epochs):
  np.random.shuffle(𝒟)
  for x_i ∈ 𝒟:
    ∇L_w = evaluate_gradient(L, x_i, w)
    w = w − η ∗ ∇L_w
```

Mini-batch Gradient Descent

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   - Can make use of highly optimized matrix optimizations
3. Common mini-batch sizes vary from 32 to 1024, depending on the application
4. This is the algorithm of choice while training DNNs (also, incorrectly referred to as SGD in general)

Mini-batch Gradient Descent

```
for i in range(nb_epochs):
  np.random.shuffle(𝒟)
  for batch in get_batches(𝒟, batch_size = 128):
   ∇L_w = evaluate_gradient(L, batch, w)
    w = w − η * ∇L_w
```

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   - However, these schedules are defined in advance and hence unable to adapt to the task at hand
2. Same learning rate applies to all the parameters
3. Avoiding numerous sub-optimal local minima