Deep Learning

04 Gradient Descent

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Loss/Risk

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    - Regression: $l(f, (x, y)) = (f(x) - y)^2$
    - Classification: $l(f, (x, y)) = \mathbf{1}(f(x) \neq y)$
    - 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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2. $f^* = \underset{f \in \mathcal{F}}{\operatorname{argmin}} R(f)$
3. This is unknown. However, if the training data $\mathcal{D} = \{z_1, \ldots, z_N\}$ is i.i.d. we can estimate the risk empirically (known as empirical risk),

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

Optimization

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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

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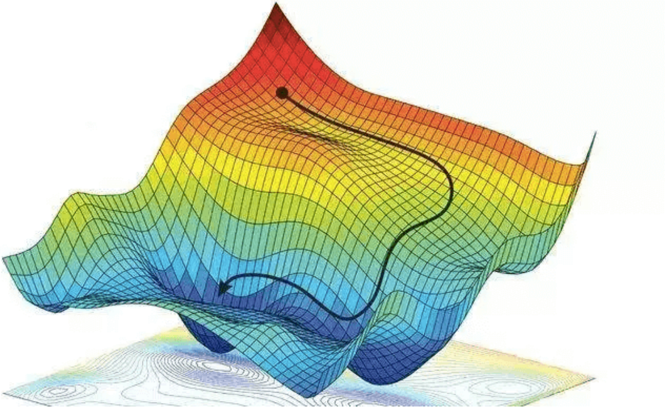
    - Closed form solution (e.g. linear regression)
    - Ad-hoc recipes (e.g. Perceptron, K-NN classifier)
    - What if the loss function can't be minimized analytically?

Loss surface



Source: Medium

Not-so-intelligent idea!

- Probe random directions

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- `Probe random directions`
- `Progress if you find a useful direction`

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- Repeat

Not-so-intelligent idea!

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

A better looking one: Follow the slope!

- Sense the slope around the feet

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- This is Gradient Descent!

Derivative and Gradient

- In 1D, derivative of a function gives the slope

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

gradient is the mapping

$$\begin{aligned} \nabla f : & \mathcal{R}^D \to \mathcal{R}^D \\ & x \to \left(\frac{\partial f}{\partial x_1}, \ldots, \frac{\partial f}{\partial x_D} \right) \end{aligned}$$

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- ∇f vector gives the direction and rate of fastest increase for f.

Gradient Descent

$$
\begin{aligned}
\mathcal{L}(w + \eta u) &= \mathcal{L}(w) + \eta u^T \nabla_w \mathcal{L}(w) + \frac{\eta^2}{2!} u^T \nabla^2 \mathcal{L}(w) u + \ldots \\
&\approx \mathcal{L}(w) + \eta u^T \nabla_w \mathcal{L}(w)
\end{aligned}
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- For $\mathcal{L}(w + \eta u)$ to be lesser than $\mathcal{L}(w)$, $u^T \nabla_w \mathcal{L}(w) < 0$

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

Gradient Descent

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

Gradient Descent

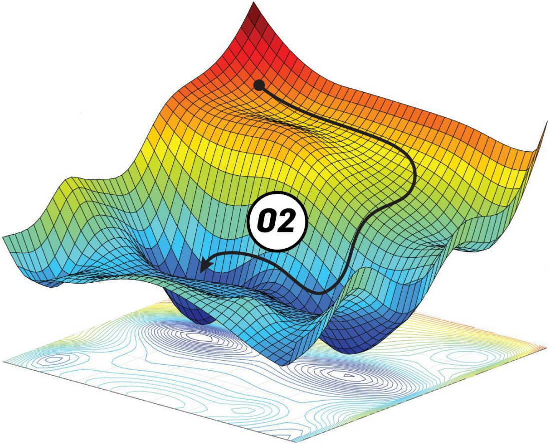

Figure credits:Ahmed Fawzy Gad

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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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- 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)
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$$\text{for } i \text{ in range(nb\_epochs):}$$
$$\nabla L_w = \text{evaluate\_gradient}(L, \mathcal{D}, w)$$
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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

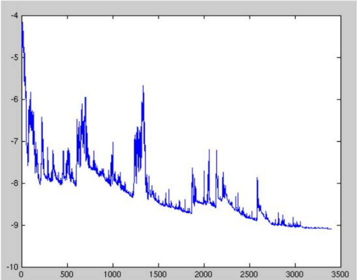

Figure credits: Wikipedia

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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($\mathcal{D}$)
  for $x_i \in \mathcal{D}$:
    ∇L_w = evaluate_gradient(L, x_i, w)
    $w = w - \eta * \nabla L_w$

Mini-batch Gradient Descent

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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($\mathcal{D}$)
  for batch in get_batches($\mathcal{D}$, batch_size = 128):
   ∇L_w = evaluate_gradient(L, batch, w)
    $w = w - \eta * \nabla L_w$

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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