Gradient Descent

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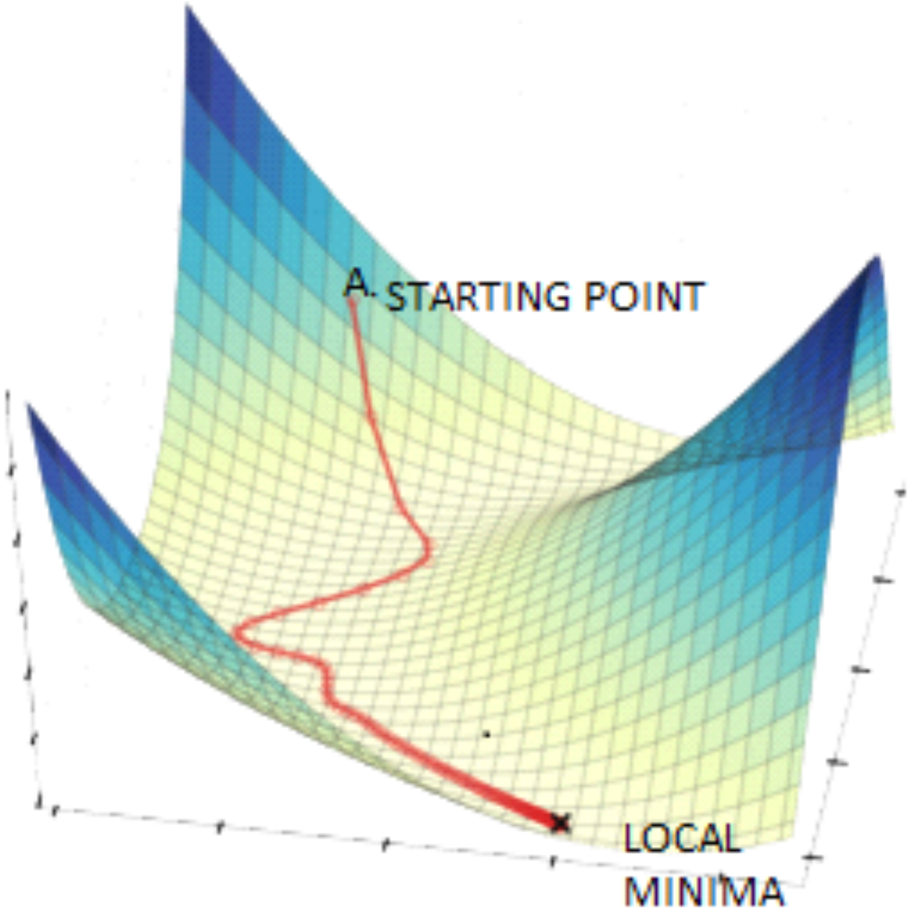
Most AI/ML optimizations must be **numerically** optimized

- One common algorithm is **<u>gradient descent</u>**
  - Primary algorithm for deep learning
  - Works in very high dimensions

- Other optimization algorithms
  - Expectation Maximization (alternating optimization)
  - Sampling-based optimization (MCMC/Gibb)
  - Greedy optimization (e.g., decision trees)

Gradient descent is like taking steps down the steepest descent into a valley



https://www.hackerearth.com/blog/developers/3-types-gradient-descent-algorithms-small-large-data-sets/

Vanilla **gradient descent (GD)** has simple form

- Objective (**Loss**) function denoted by $\mathcal{L}(\theta; \mathcal{D})$:

$$\arg\min_{\theta} \mathcal{L}(\theta; \mathcal{D})$$

1. Start at random parameter, e.g., $\theta^0 \sim \mathcal{N}(0,1)$

2. Iteratively update parameter via **negative gradient** of loss function (η_t is step size or

$$\theta^{t+1} = \theta^t - \eta_t \nabla_\theta \mathcal{L}(\theta^t)$$

- η_t is **learning rate** (or **step size**)

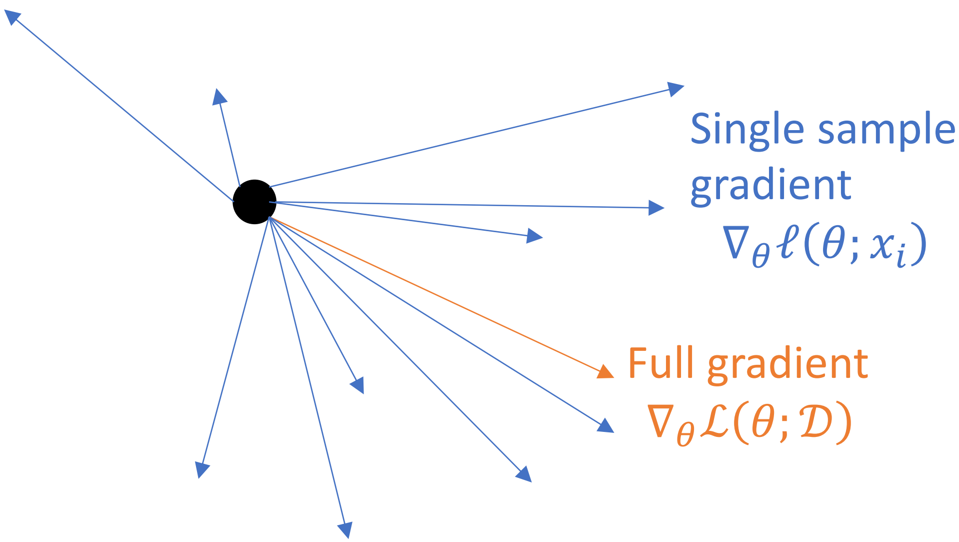
<u>Stochastic gradient descent (SGD)</u> merely uses one sample in the gradient calculation

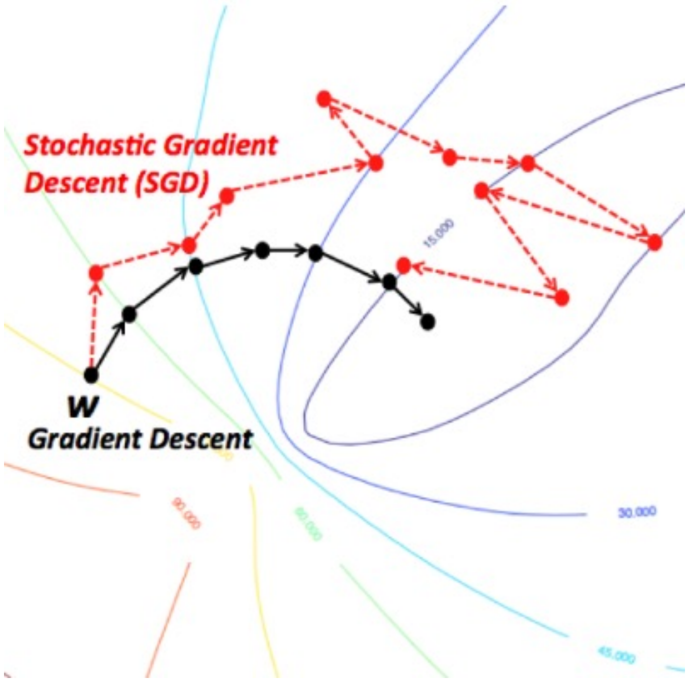
- The loss function can usually be split into a summation of losses $\ell(\theta; x_i)$ for each sample x_i: $\mathcal{L}(\theta; \mathcal{D}) = \frac{1}{n}\sum_{i=1}^{n} \ell(\theta; x_i)$
- SGD approximates the full gradient by the gradient of a *single* sample
  - $\nabla_\theta \mathcal{L}(\theta^t; \mathcal{D}) \approx \nabla_\theta \ell(\theta^t; x_i)$
  - Theoretically, $\mathbb{E}_i[\nabla_\theta \ell(\theta^t; x_i)] = \nabla_\theta \mathcal{L}(\theta^t; \mathcal{D})$
- Loop through all $x_i \in \mathcal{D}$

$$\theta^{t+1} = \theta^t - \eta_t \nabla_\theta \ell(\theta^t; x_i)$$

- One pass through dataset
  - GD: 1 large update with $O(n)$ cost
  - SGD: n smaller updates with $O(1)$ cost each

<u>Stochastic gradient descent (SGD)</u> merely uses one sample in the gradient calculation





Full gradient is average over single sample gradients. This is why it is “stochastic”.

https://golden.com/wiki/Stochastic_gradient_descent_(SGD)

Mini-batch SGD (or just SGD) uses a small batch of samples in the gradient calculation

- **Mini-batch SGD** approximates the full gradient by the gradient of a batch of samples
  - Sample mini-batch

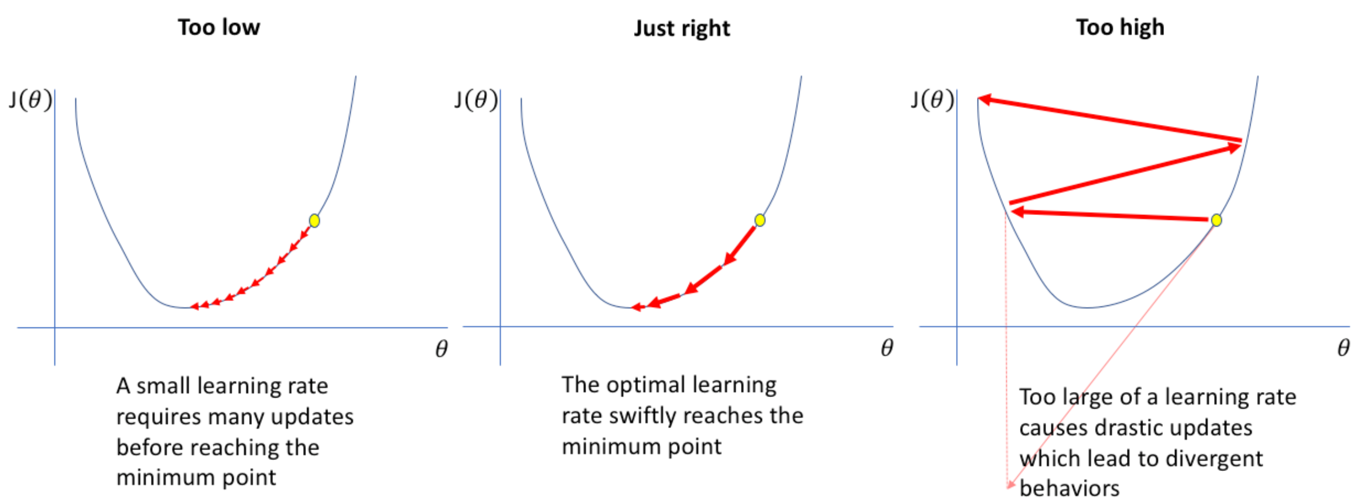
$$\theta^{t+1} = \theta^t - \eta_t \sum_{k=1}^{b} \frac{1}{b} \nabla_\theta \ell(\theta^t; x_k)$$

- One pass through dataset
  - GD: 1 large update
  - SGD: n smaller updates
  - Mini-batch SGD: $\frac{n}{b}$ medium-size updates

Gradient descent demo for simplified logistic regression

Learning rate / step size is critical for convergence and correctness of algorithm

- If learning rate is **too high**, the algorithm could diverge.
  - Diverge means to get farther away from the solution.
- If learning rate **too low**, the algorithm could take a very long time to converge.



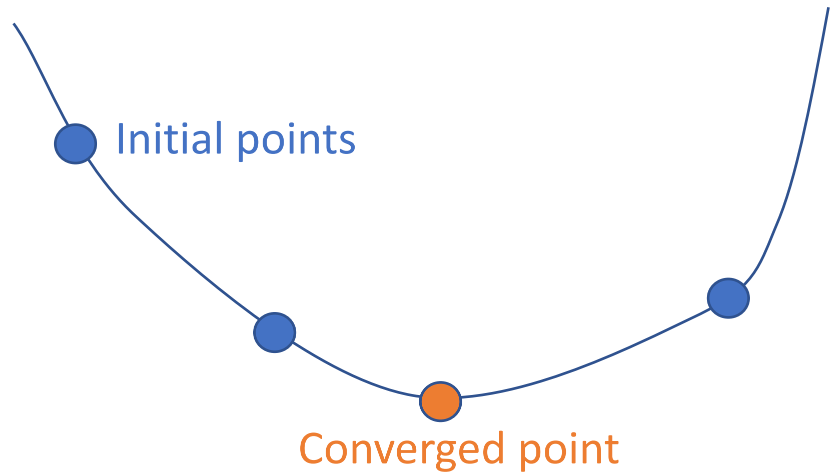
https://www.jeremyjordan.me/nn-learning-rate/

Adaptive learning rates may help **(but not always)**

- Decreasing step size, $\eta_t = \frac{1}{t}$
  - Intuition: Approaches 0 but can cover an infinite distance since $\lim_{a \to \infty} \sum_{t=1}^{a} \frac{1}{t} = \infty$
- ADAM – Adaptive Moment Estimation
- See https://pytorch.org/docs/stable/optim.html for more options

<u>Parameter initialization</u> can be important if non-convex or step size incorrect

- If convex function, initial parameter θ^0 **will not** affect final optimization result $\hat{\theta} = \underset{\theta}{\operatorname{argmin}}\, \mathcal{L}(\theta)$.
  - Yay! (Assuming appropriate step size.)



- If *non-convex*, starting position **<u>WILL</u>** affect final converged $\hat{\theta}$.
  - Sad day. (But sometimes it’s not too bad in practice.)