Gradient Descent

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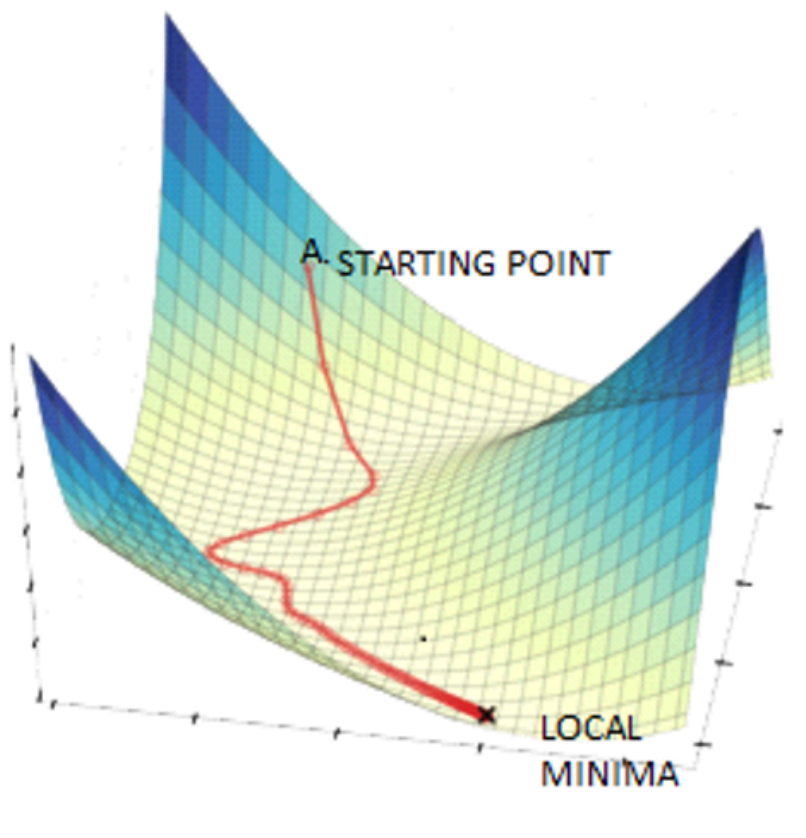
Most AI/ML Optimizations Must Be **Numerically** Optimized

- One common algorithm is **gradient descent**
  - 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 $\mathcal{L}(\theta; \mathcal{D})$:

$$\underset{\theta}{\operatorname{argmin}}\, \mathcal{L}(\theta; \mathcal{D})$$

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 learning rate)

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

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

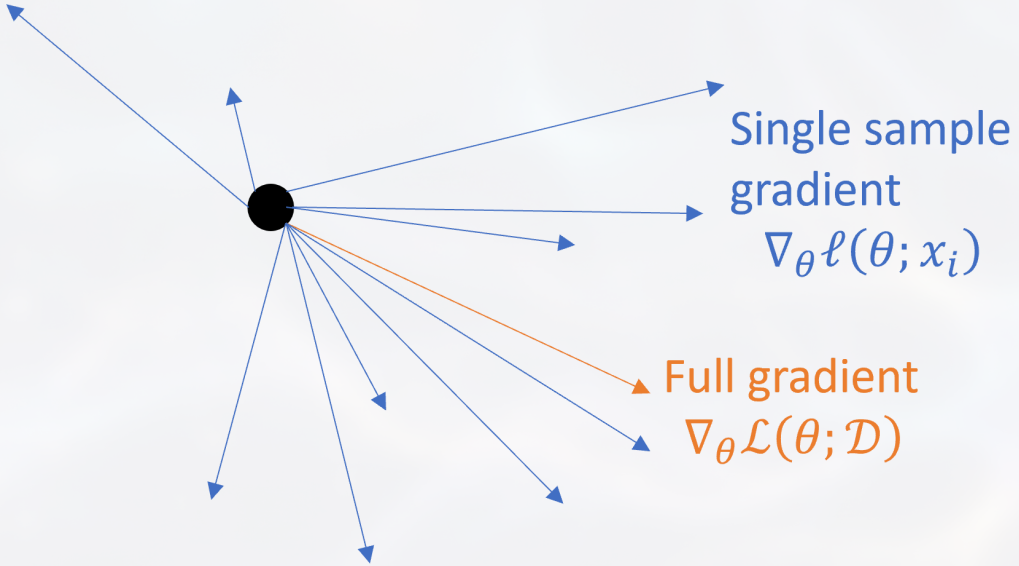
Stochastic Gradient Descent (SGD) Merely Uses One Sample in the Gradient Calculation

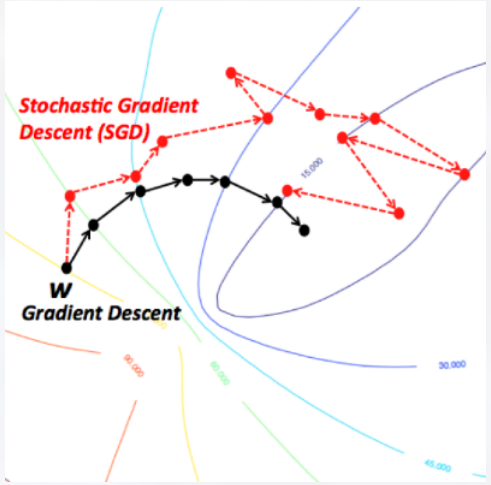
- The loss function can usually be split into a summation of losses $l(\theta; x_i)$ for each sample x_i:
  - $\mathcal{L}(\theta; \mathcal{D}) = \frac{1}{n} \sum_{i=1}^{n} l(\theta; x_i)$
- SGD approximates the full gradient by the gradient of a single sample
  - $\nabla_\theta \mathcal{L}(\theta^t;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

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

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

Stochastic Gradient Descent (SGD) 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

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

- 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

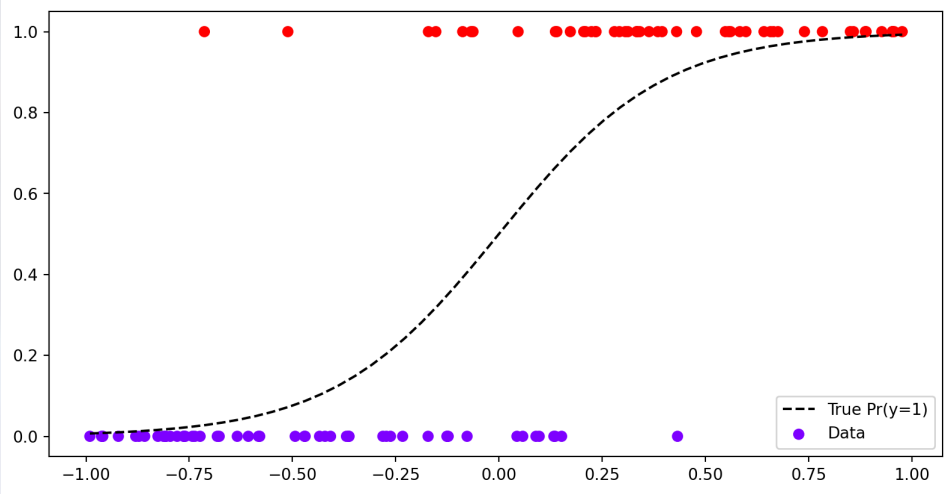
Create Simple Logistic Data and Plot True Model

```python
import numpy as np
import scipy.stats
import matplotlib.pyplot as plt

# Create simple logistic data
rng = np.random.RandomState(0)
n_samples = 100
x = 2*(rng.rand(n_samples)-0.5)

theta_true = 5
# Very simplified logistic regression model with only 1 param
def model(x, theta):
    return 1 / (1 + np.exp(-x.dot(theta)))
y = (rng.rand(*x.shape) <= model(x, theta_true)).astype(float
print(y.shape)
# Plot data
xq = np.linspace(np.min(x), np.max(x))
plt.plot(xq, model(xq, theta_true), '--k', label='True Pr(y=1
plt.scatter(x, y, c=y, cmap='rainbow', label='Data')
plt.legend()
```

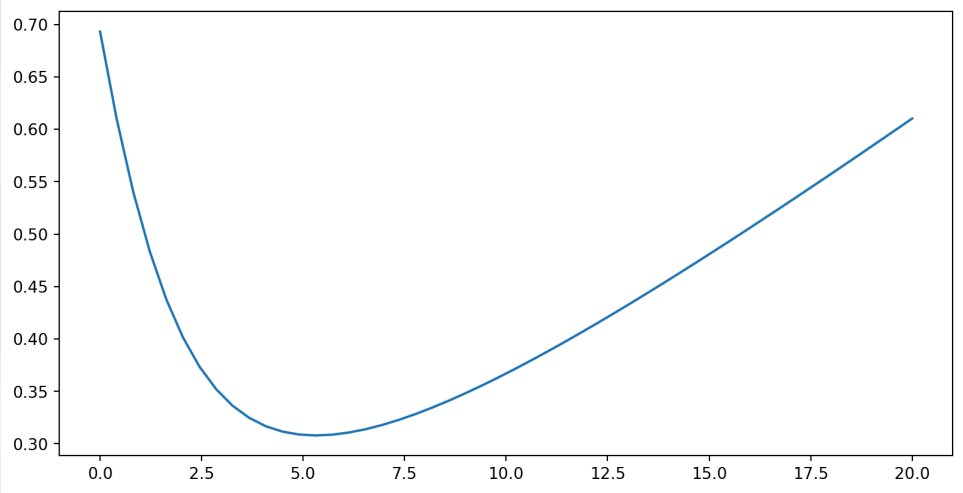
```
(100,)
```



Define the Logistic Loss (Negative Log-Likelihood)

```
def objective(x, y, theta):
    prob = model(x, theta)
    return -np.mean(y * np.log(prob) + (1-y) * np.log(1 - pro

theta_arr = np.linspace(0, 20)
obj_arr = [objective(x, y, theta) for theta in theta_arr]
plt.plot(theta_arr, obj_arr)
```

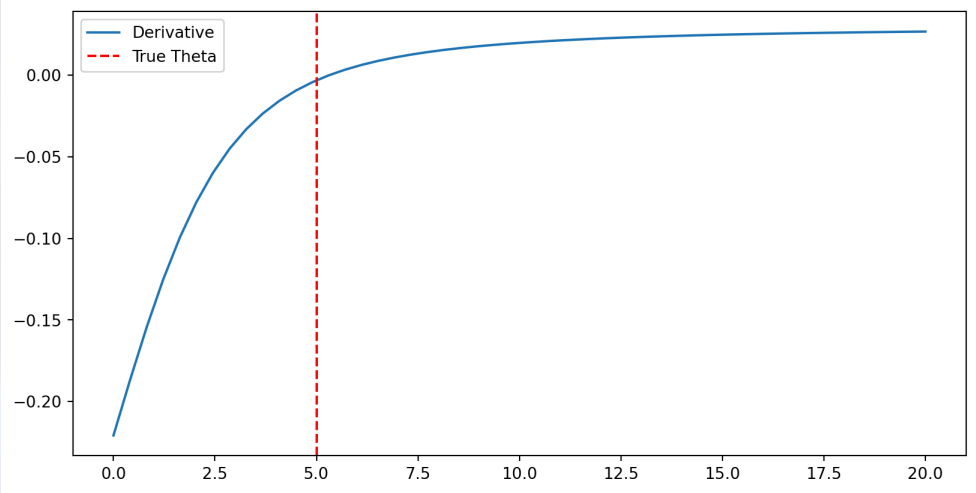


NOTE: Because of randomness, empirical estimate will not exactly match true model. (e.g., this has a minimum closer to 5.3 or so

Explicitly compute (by hand) the gradient of the function

```python
def grad_objective(x, y, theta):
    #See https://web.stanford.edu/~jurafsky/slp3/5.pdf
    return np.mean((model(x, theta) - y) * x)

grad_arr = [grad_objective(x, y, theta) for theta in theta_ar
plt.plot(theta_arr, grad_arr, label='Derivative')
plt.axvline(5, linestyle='--', color='r', label='True Theta')
plt.legend()
```



Gradient Descent with various step sizes

```python
# Gradient descent parameters
max_iter = 5
step_size = 10
sgd = False
if sgd: max_iter *= 10 # Increase number of iterations for SG
rng = np.random.RandomState(0)

# Initialization
theta_hat = 10.2 # An arbitrary starting value
theta_hat_arr = [theta_hat]
obj_hat_arr = [objective(x, y, theta_hat)]

# Gradient descent iterations
for it in range(max_iter):
    if sgd:
        # Select random data point
        rand_idx = rng.randint(len(y))
        xg, yg = x[rand_idx:rand_idx+1], y[rand_idx:rand_idx+
    else:
        # Use all data points in gradient calculation
        xg, yg = x, y
    grad = grad_objective(xg, yg, theta_hat)
    theta_hat = theta_hat - step_size * grad

    # Save estimates for visualization
    theta_hat_arr.append(theta_hat)
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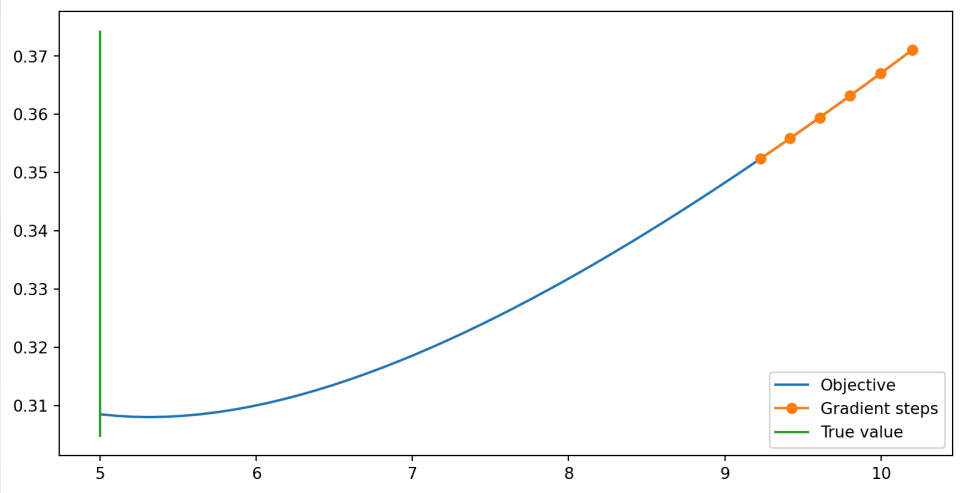

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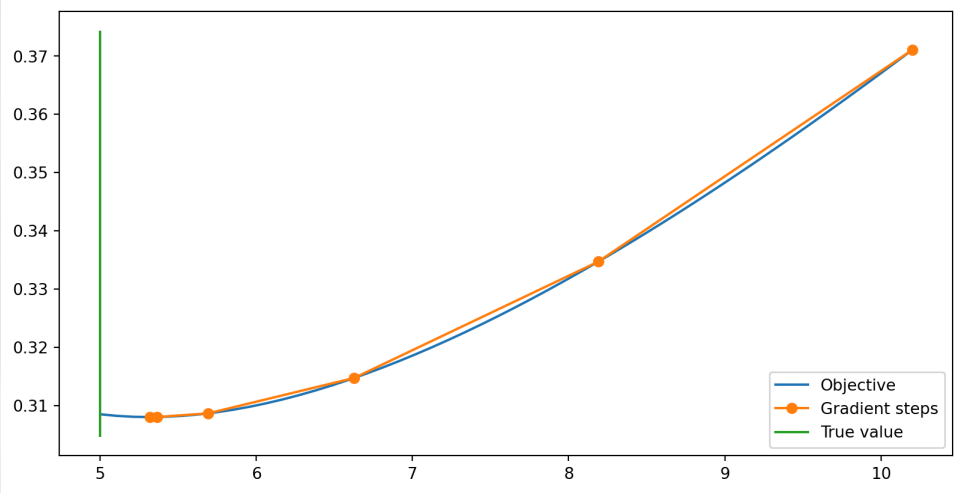

Gradient Descent with various step sizes

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# Gradient descent parameters
max_iter = 5
step_size = 300
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if sgd: max_iter *= 10 # Increase number of iterations for SG
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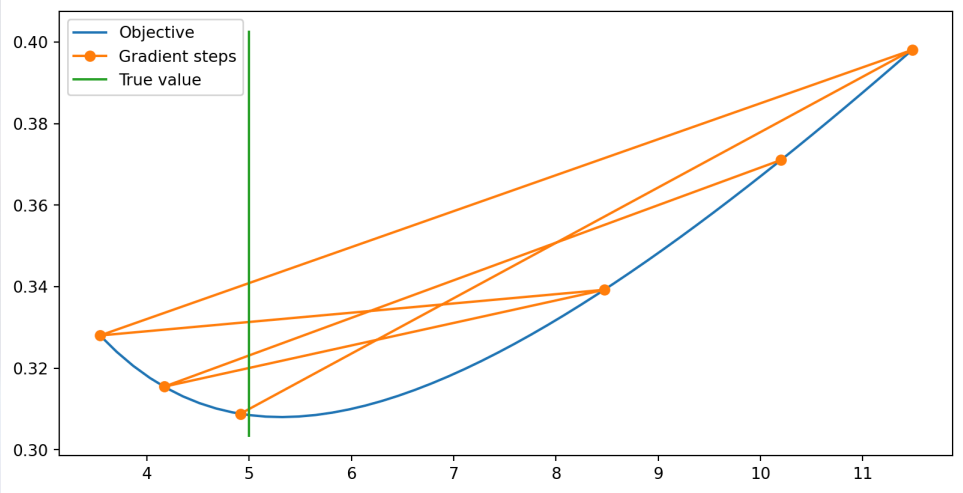

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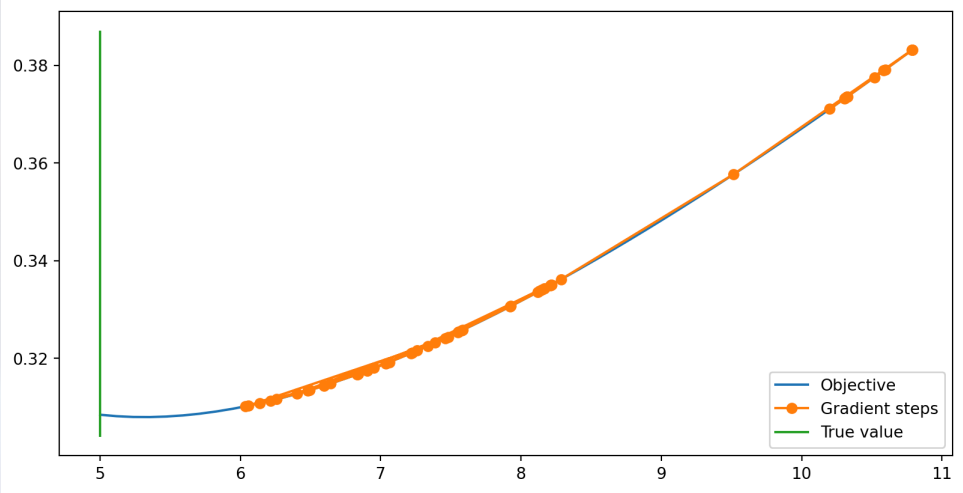

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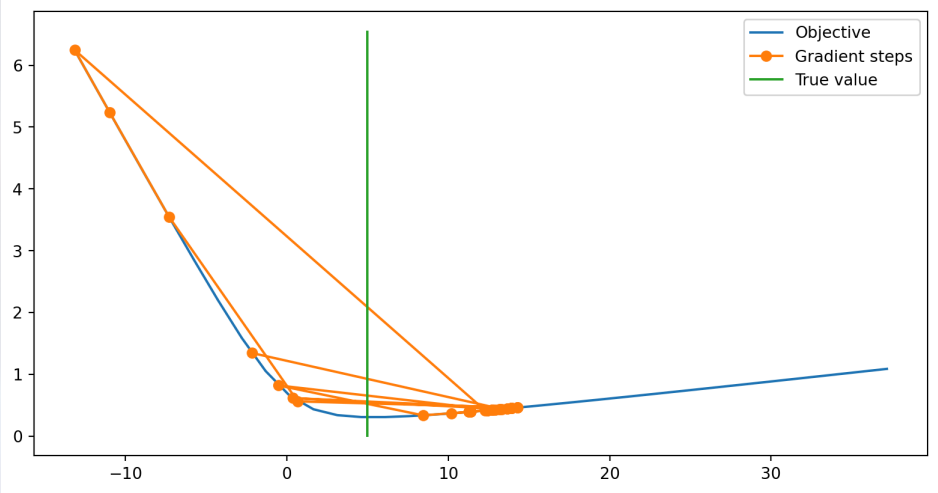

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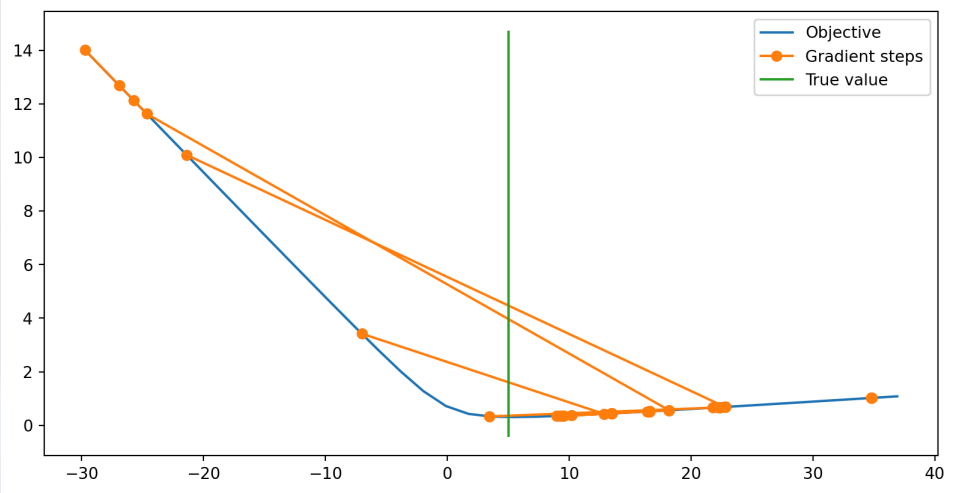
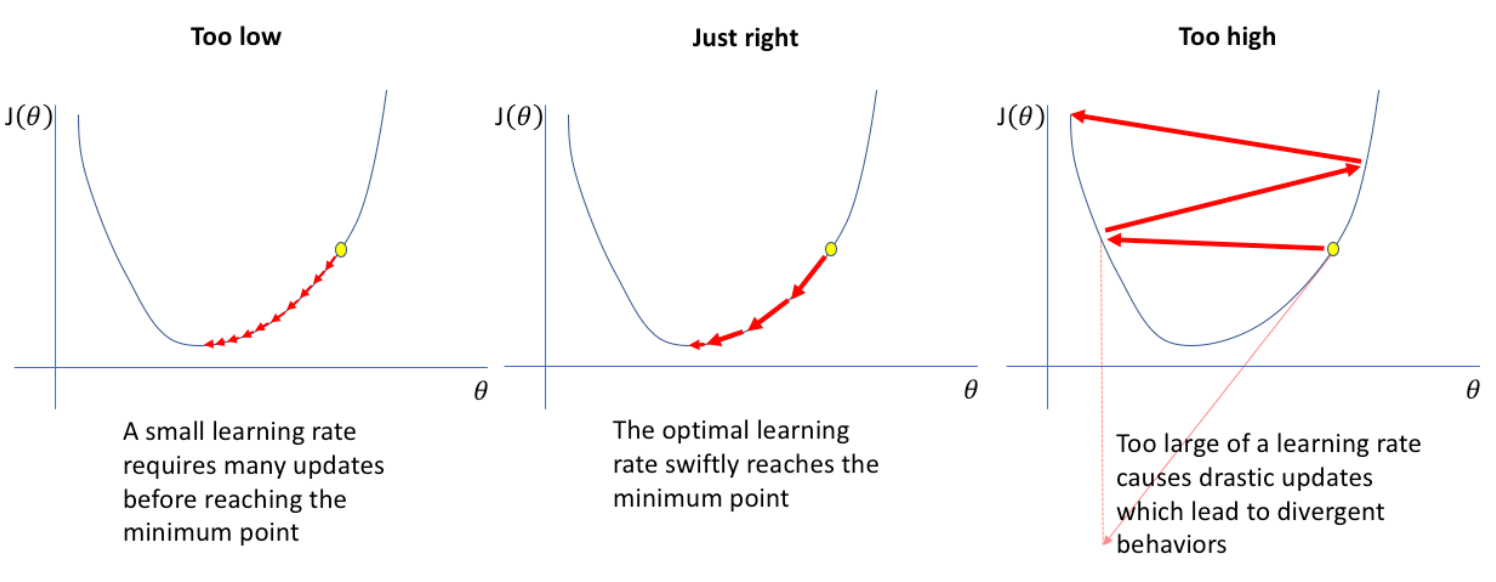


Learning Rate / Step Size Is Critical for Convergence and Correctness of Algorithm

- 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.



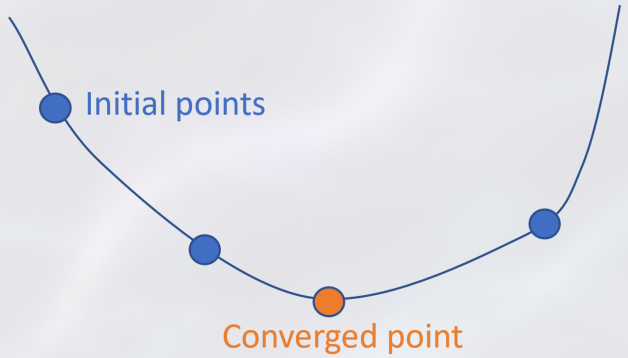
https://www.jeremyjordan.me/nn-learning-rate/

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

Parameter Initialization Can Be Important if Non-Convex or Step Size Incorrect

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



- If non-convex, starting position **WILL** affect final converged θ.
  - Sad day. (But sometimes it's not too bad in practice.)