Gradient Descent

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Introduction

We've seen a variety of modeling algorithms that can be divided into two paradigms:

1. Data-dependent models, such as decision trees or KNN, where the model structure is directly shaped by the training data without any fixed functional form
2. Parametric models, such as linear/logistic regression, where the model has a pre-defined functional form, and the parameters of that form (weights) are learned from the data

Data-dependent models typically rely upon their own specialized optimization algorithms, but parametric models can be optimized by **gradient descent**.

Cost Functions

- When we talk about a model "learning" from the training data, what we really mean is that it alters its parameters to achieve a lower error rate, which is measured by a **cost function**
  - Cost functions quantify how well a model's predictions align with actual outcomes
- The two cost functions we'll focus on are:
  - **Squared-error** - $\text{Cost} = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$
    - We'll use this for numeric outcomes
  - **Cross-entropy** - $\text{Cost} = -\sum_{i=1}^{n}\left(y_i \cdot log(\hat{y}_i) + (1 - y_i) \cdot log(1 - \hat{y}_i)\right)$
    - We'll use this for categorical outcomes

Linear Regression and Squared-error

Recall that linear regression represents the outcome as a linear combination of predictive features:

$$Y = w_o + w_1 X_1 + w_2 X_2 + \ldots + w_p X_p + error$$

This model can be expressed using matrix notation:

$$\mathbf{y} = \mathbf{X}\mathbf{w} + \mathbf{error}$$

For a given set of weight estimates, $\widehat{\mathbf{w}}$, we can define the cost:

$$Cost = \frac{1}{n}(\mathbf{y} - \mathbf{X}\hat{\mathbf{w}})^T(\mathbf{y} - \mathbf{X}\hat{\mathbf{w}})$$

This value measures the effectiveness of $\widehat{\mathbf{w}}$

Linear Regression and Squared-error

As you might be expecting, we generally want the *best possible* set of weights, or the set that minimizes the cost function. We can use calculus to perform this minimization, but first let's rearrange a few terms:

$$\begin{aligned} Cost &= \frac{1}{n}(\mathbf{y} - \mathbf{X}\hat{\mathbf{w}})^T(\mathbf{y} - \mathbf{X}\hat{\mathbf{w}}) \\ &= \frac{1}{n}\mathbf{y}^T\mathbf{y} + \frac{1}{n}(-2\mathbf{y}^T\mathbf{X}\hat{\mathbf{w}} + (\mathbf{X}\hat{\mathbf{w}})^T\mathbf{X}\hat{\mathbf{w}}) \\ &= \frac{1}{n}\mathbf{y}^T\mathbf{y} + \frac{-2}{n}\mathbf{y}^T\mathbf{X}\hat{\mathbf{w}} + \frac{1}{n}\hat{\mathbf{w}}^T\mathbf{X}^T\mathbf{X}\hat{\mathbf{w}} \end{aligned}$$

For linear regression, we can differentiate with respect to $\widehat{\mathbf{w}}$, set the resulting expression equal to zero, then solve for a closed form solution of: $\hat{\mathbf{w}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$

Gradient Descent

- The derivative is the slope of a function at a particular location, so we can use the gradient to gradually move towards the minimum of any (convex) cost function
  - The **gradient descent algorithm** works to minimize the cost function using sequential updates:

$$\hat{\mathbf{w}}^{(j)} = \hat{\mathbf{w}}^{(j-1)} - \alpha \frac{\partial \text{Cost}}{\partial \mathbf{w}}\left(\hat{\mathbf{w}}^{(j-1)}\right)$$

- α is a tuning parameter that controls the *learning rate*, or how quickly to update the weight vector at each iteration
  - A small α requires many iterations for the algorithm to converge (reach the minimum)
  - A large α can overshoot the minimum, which can also cause convergence issues

Gradient Descent for Linear Regression

Recall our rearranged cost function is:

$$Cost = \frac{1}{n}\mathbf{y}^T\mathbf{y} + \frac{1}{n}(-2\mathbf{y}^T\mathbf{X}\hat{\mathbf{w}} + \hat{\mathbf{w}}^T\mathbf{X}^T\mathbf{X}\hat{\mathbf{w}})$$

Thus, after applying some matrix calculus shortcuts the gradient is:

$$Gradient = \frac{-2}{n}\mathbf{X}^T(\mathbf{y} - \mathbf{X}\hat{\mathbf{w}})$$

So, our gradient descent update scheme is:

$$\hat{\mathbf{w}}^{(j)} = \hat{\mathbf{w}}^{(j-1)} - \alpha \cdot \left(\frac{-2}{n}\mathbf{X}^T(\mathbf{y} - \mathbf{X}\hat{\mathbf{w}}^{(j-1)})\right)$$

Simple Example

As an illustration, consider a very simple special case of linear regression involving no bias term (intercept) and a single weight parameter where data are generated via:

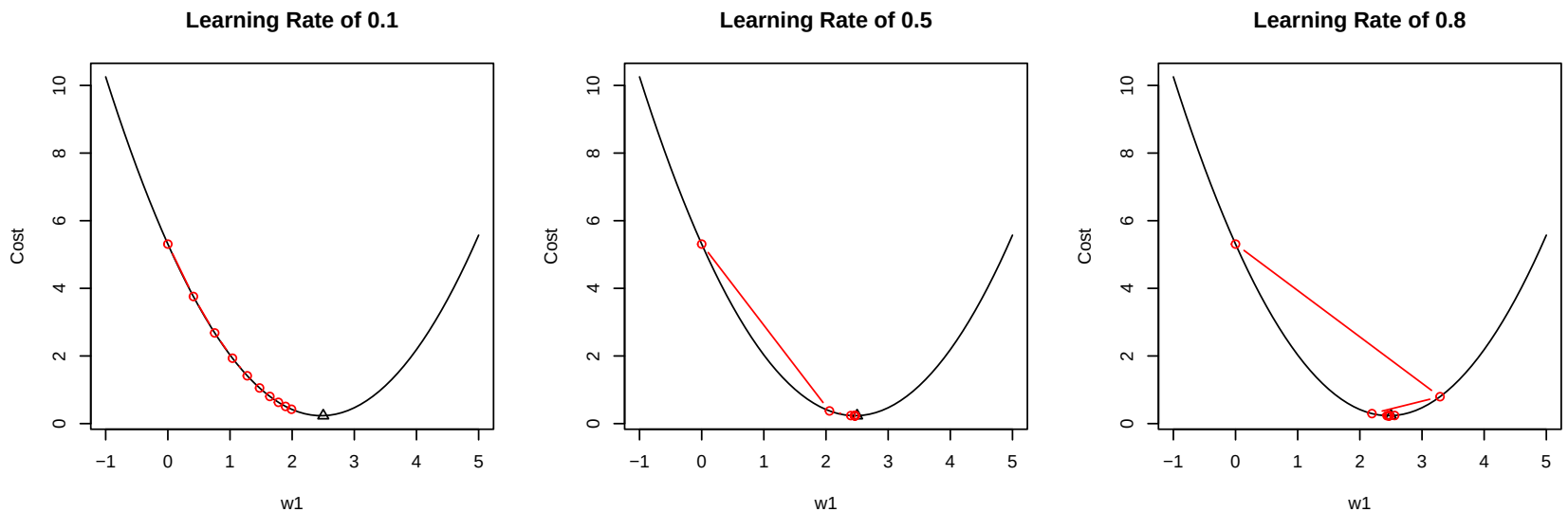
$$Y = 2.5X_1 + error$$

For this model, the squared error cost function is:

$$Cost = \frac{1}{n}(\mathbf{y} - \mathbf{x}_1^T \hat{w}_1)^T(\mathbf{y} - \mathbf{x}_1^T \hat{w}_1)$$

Simple Example (cont.)

The graphs below illustrate 10 iterations of gradient descent for our simple example (starting at $w_1^{(0)} = 0$):



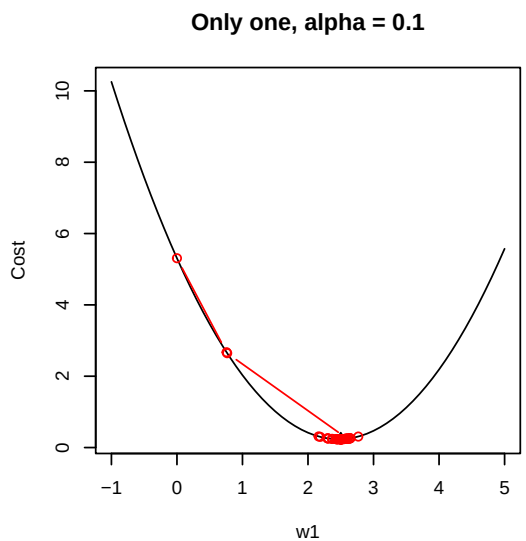
Gradient descent typically stops when the next update uses weight changes that are below a small, predefined threshold.

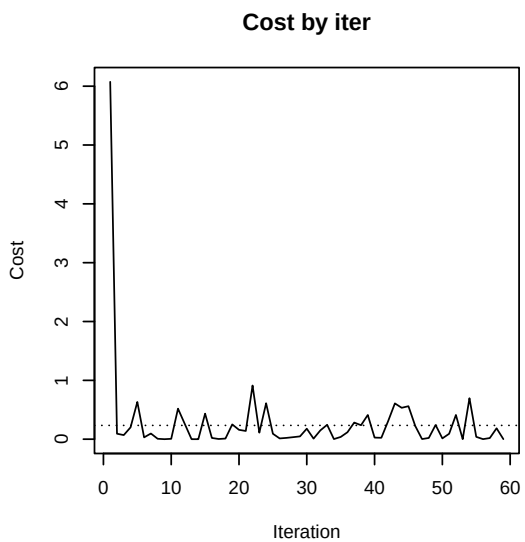
Stochastic Gradient Descent

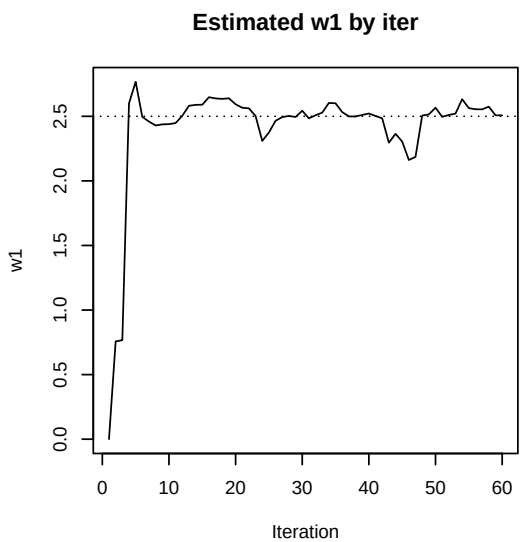
- In our simple example, computing the gradient at each iteration required two vector-product calculations: $\mathbf{y}^T\mathbf{x}_1$ and $\mathbf{x}_1^T\mathbf{x}_1$
  - Fortunately, these can both be computed ahead of time (rather than at each iteration) which makes algorithm very computationally efficient
- For other models, the parameter vector is involved in vector-product calculations within the gradient, so these vector-product calculations must be redone at each iteration
  - In big-data settings, this computational challenge (among others) has led to the popularity of **stochastic gradient descent**

Stochastic Gradient Descent

Stochastic Gradient Descent uses the same framework as gradient descent (updating parameters using the gradient to improve the cost function) but it does so using only one training sample at a time:



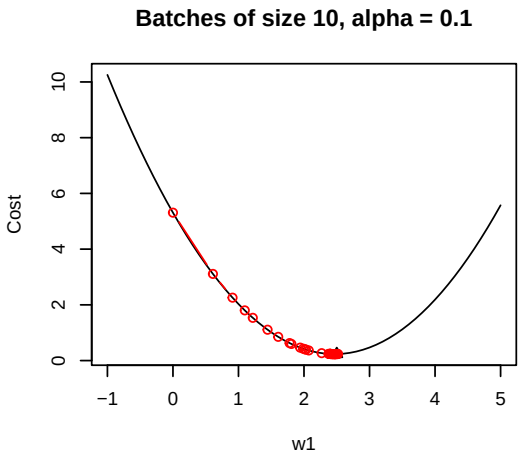


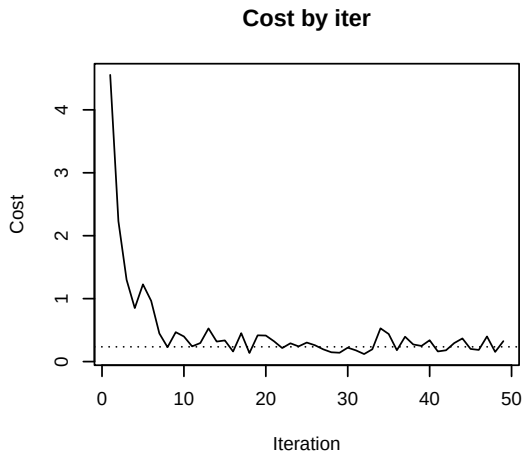


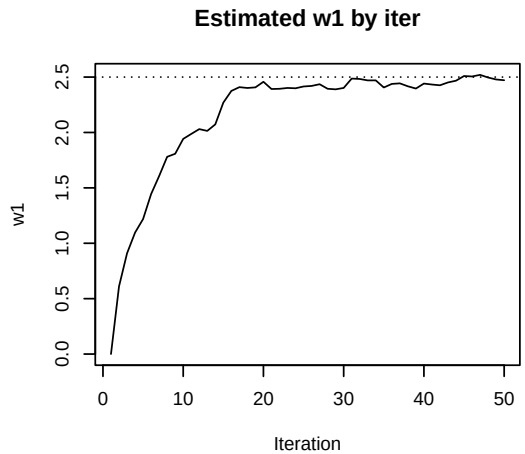
Mini-Batch Gradient Descent

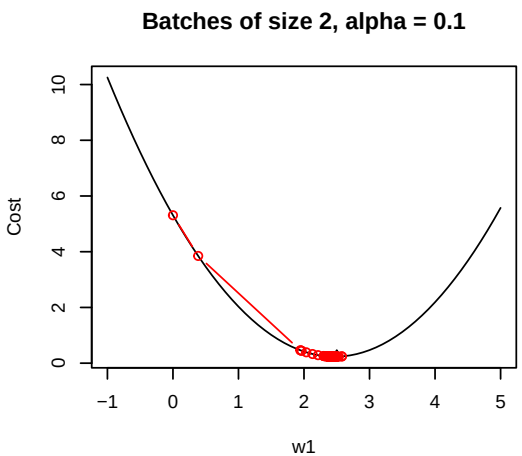
- Stochastic gradient descent has an added benefit of allowing the optimization to avoid getting trapped at local minima
  - However, the convergence is noisy and the algorithm is difficult to parallelize when the number of training samples is large
- **Mini-batch gradient descent** divides the data into batches and performs each update using a batch of data rather than the entire thing (or only one observation)
  - This is less noisy and more parallelizable than stochastic gradient descent, while still introducing enough randomness to help overcome local minima

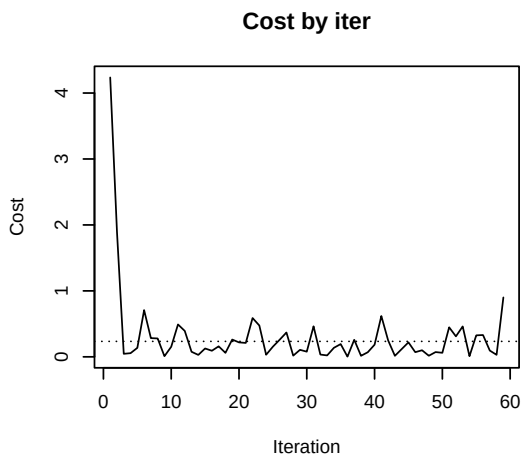
Mini-Batch Gradient Descent

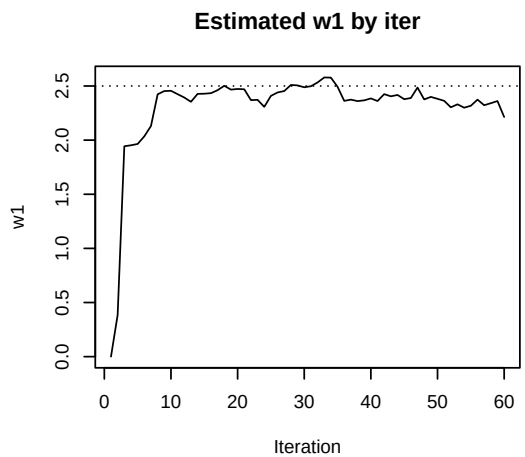












What to Know for the Next Quiz

- Understand the fundamental ideas behind cost functions and gradient descent
  - The cost function measures how accurate predictions are
  - The derivative (gradient) of the cost function evaluated at a particular set of weights is a slope, which indicates how to update the weights in order to reduce the cost
- Understand the role of the learning rate in gradient descent
- Be familiar with the advantages and reasons to use stochastic or mini-batch gradient descent