Lecture 12: Regularization

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Today's Topics

- Convergence of gradient descent
- Regularization

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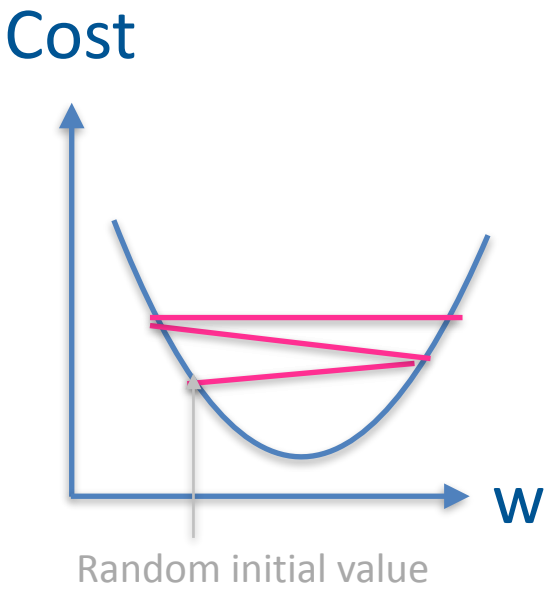
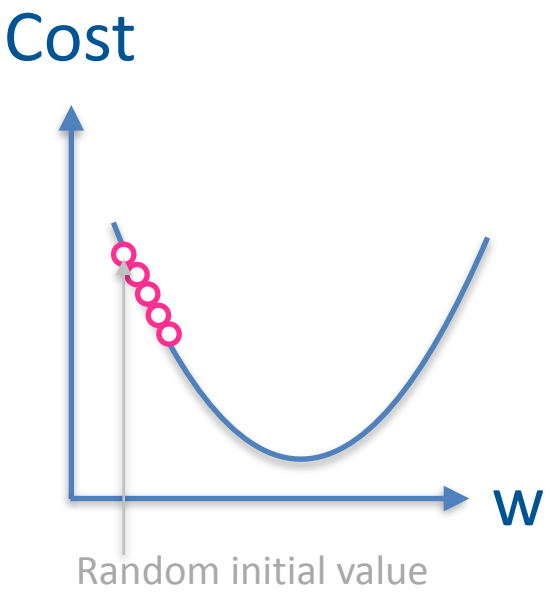
Gradient Descent

CONVERGENCE

Impact of learning rate



Learning rate too large



Learning rate too small

Impact of learning rate

- Stop after fixed number of iterations
- Stop once prediction error is less than threshold
- Stop when validation loss stops changing

Feature normalization

- Important to normalize features when using gradient descent (otherwise takes longer to converge)

- Normalization: all features should have a similar scale

LMS Regression

REGULARIZATION

Generalization

- Prediction functions that work on the training data might not work on other data

- Minimizing the training error is a reasonable thing to do, but it's possible to minimize it "too well"

- **Overfitting:** your function matches the training data well but is not learning general rules that will work for new data

Regularization

- Modify learning algorithm to favor “simpler” prediction rules to avoid overfitting

- Most commonly, regularization refers to modifying the loss function to **penalize** certain values of the weights you are learning. Specifically, penalize weights that are large.

Regularization

- How do we define whether weights are large?

$$d(\mathbf{w}, \mathbf{0}) = \sqrt{\sum_{i=1}^{k} (w_i)^2} = ||\mathbf{w}||$$

Note that bias term w_0 is not regularized

- This is called the L2 norm of $\mathbf{w}$
  - A norm is a measure of a vector's length
  - Also called the Euclidean norm

Regularization

- New goal for minimization

$$L(\mathbf{w}) + \lambda ||\mathbf{w}||^2$$

Square to eliminate square root: easier to work with mathematically

This is whatever loss function we are using

By minimizing this we prefer solutions where $\mathbf{w}$ is closer to $\mathbf{0}$

λ is a hyperparameter that adjusts trade-off between low training loss and having low weights

Regularization

- Regularization helps the computational problem because gradient descent won't try to make some feature weights grow larger and larger

- At some point, the penalty of having too large $||w||^2$ will outweigh whatever gain you would make in your loss function.

Regularization

- This also helps with generalization because it won't give large weight to features unless there is sufficient evidence that they are useful

- The usefulness of a feature toward improving the loss has to outweigh the cost of having large feature weights

Regularization

- More generally

$$L(\mathbf{w}) + \lambda R(\mathbf{w})$$

This is called the regularization term or regularizer or penalty. The squared L2 norm is one kind of penalty, but there are others

λ is called the regularization strength.

Other common names for λ: *alpha* in sklearn, *C* in many algorithms. Usually C actually refers to the inverse regularization strength, 1/λ. Figure out which one your implementation is using (whether this will increase or decrease regularization)

L2 Regularization

- When the regularizer is the squared L2 norm $||\mathbf{w}||^2$, this is called L2 regularization.
- This is the most common type of regularization
- When used with linear regression, this is called Ridge regression
- Logistic regression implementations usually use L2 regularization by default
- L2 regularization can be added to other algorithms like perceptron (or any gradient descent algorithm)

L2 Regularization

- The function $R(\mathbf{w}) = ||\mathbf{w}||^2$ is convex, so if it is added to a convex loss function, the combined function will still be convex.

L1 Regularization

- Another common regularizer is the L1 norm:

$$||\mathbf{w}||_1 = \sum_{j=1}^{k} |w_j|$$

- When used with linear regression, this is called Lasso

- Often results in many weights being exactly 0 (while L2 just makes them small but nonzero)

L1+L1 Regularization

- L2 and L1 regularization can be combined

$$R(\mathbf{w}) = \lambda_2 ||\mathbf{w}||^2 + \lambda_1 ||\mathbf{w}||_1$$

- Also called ElasticNet
- Can work better than either type alone
- Can adjust hyperparameters to control which of the two penalties is more important
- Once training is done, remove regularization term to measure model performance

Feature normalization

- The scale of the feature values matters when using regularization

- If one feature has values between [0, 1] and another between [0, 10000], the learned weights might be on very different scales – but whatever weights are "naturally" larger are going to get penalized more by the regularizer.

- Feature normalization or standardization refers to converting the values to a standard range.

Bias vs. variance

- Remember: the goal of machine learning is to learn a function that can correctly predict all data it might hypothetically encounter in the world

- We don't have access to all possible data, so we approximate this by doing well on the training data

- The training data is a sample of true data

Bias vs. variance

- When you estimate a parameter from a sample, the estimate is biased if the expected value of the parameter is different from the true value.

- The expected value of the parameter is the theoretical average value of all the different parameters you would get from different samples.

- Example: random sampling (e.g. in a poll) is unbiased because if you repeated the sampling over and over, on average your answer would be correct (even though each individual sample might give a wrong answer).

Bias vs. variance

- Regularization adds a bias because it systematically pushes your estimates in a certain direction (weights close to 0)

- If the true weight for a feature should actually be large, you will consistently make a mistake by underestimating it, so on average your estimate will be wrong (therefore biased).

Bias vs. variance

- The variance of an estimate refers to how much the estimate will vary from sample to sample.

- If you consistently get the same parameter estimate regardless of what training sample you use, this parameter has low variance.

Bias vs. variance

- Bias and variance both contribute to the error of your classifier.

- Variance is error due to randomness in how your training data was selected.

- Bias is error due to something systematic, not random.

Bias vs. variance

High bias

- Will learn similar functions even if given different training examples
- Prone to underfitting

High variance

- The learned function depends a lot on the specific data used to train
- Prone to overfitting

Some amount of bias is needed to avoid overfitting. Too much bias is bad, but too much variance is usually worse.