Optimization

Week 4 Day 4

May 20th, 2021

Zain Hasan

Adapted from slides by Eric

Agenda

- Issues and challenges in ML
- Optimization
  - Gradient descent
  - Stochastic (and mini-batch) gradient descent
- Break
- Regularization
  - L1 (Lasso) regularization
  - L2 (Ridge) regularization
  - Elastic Net regularization

Issues and Challenges in ML

Machine Learning At Its Worst

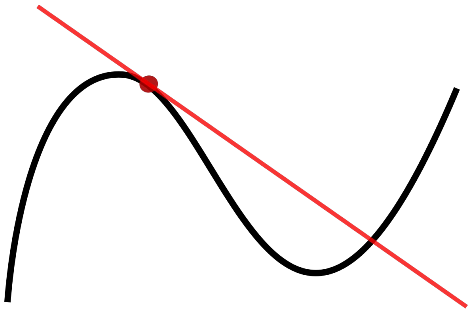
- Machine learning models fit the data we give them
- If the data is sexist, the model will be too. If the data is racist, the model will be too. Any **bias** in the data is a pattern that the model will learn
- Amazon trained a recruiting model that exhibited gender bias
- COMPAS predicted risk of repeating a crime and exhibited racial bias
- We want models to be fair and objective, so this is a big issue: ML Ethics
- The bias is not in the model; it is in the *data*
- Be wary of thinking of these models as “artificial intelligence”. **They don’t *think*, they find patterns in data**

Optimization: The Method Used to Train a Machine Learning Model

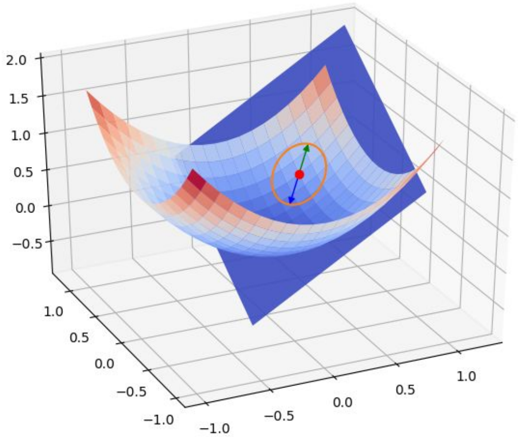
- What are we trying to optimize?

The Gradient: Multidimensional Derivative

Derivative for 1D
independent variable
(slope)



Derivative (gradient) for >1D
independent variable
(slope + steepest direction)

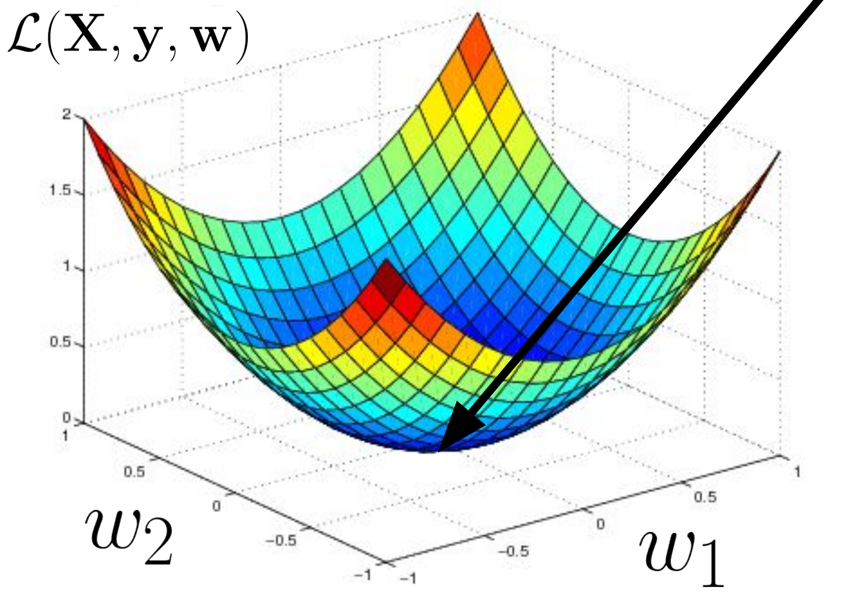


Derivative of function
with respect to a vector

$$\frac{\partial}{\partial \mathbf{v}} f(\mathbf{v}, ...) = \begin{bmatrix} \frac{\partial}{\partial v_1} f(\mathbf{v}, ...) \\ \frac{\partial}{\partial v_2} f(\mathbf{v}, ...) \\ \vdots \\ \frac{\partial}{\partial v_n} f(\mathbf{v}, ...) \end{bmatrix}$$

Interpretation: *f* would increase most if **v** moved in this direction

Motivation and Intuition: What are we optimizing?



Lowest loss (best performance)

$\rightarrow$ Optimal weight vector $\hat{\mathbf{w}}$

$\rightarrow$ Occurs when $\mathcal{L}$ is flat

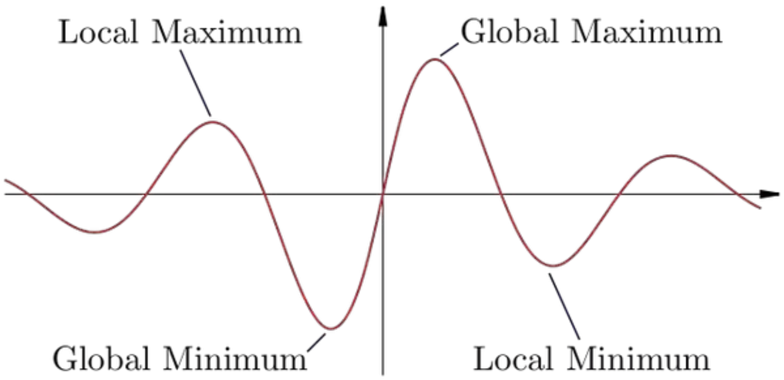
$\rightarrow$ $\mathcal{L}$ is flat when $\dfrac{\partial}{\partial \mathbf{w}} \mathcal{L}(\mathbf{X}, \mathbf{y}, \mathbf{w}) = 0$

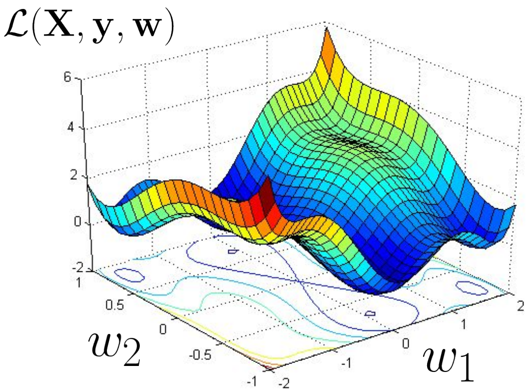
Just solve for $\hat{\mathrm{w}}$, right!?
For linear regression:

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

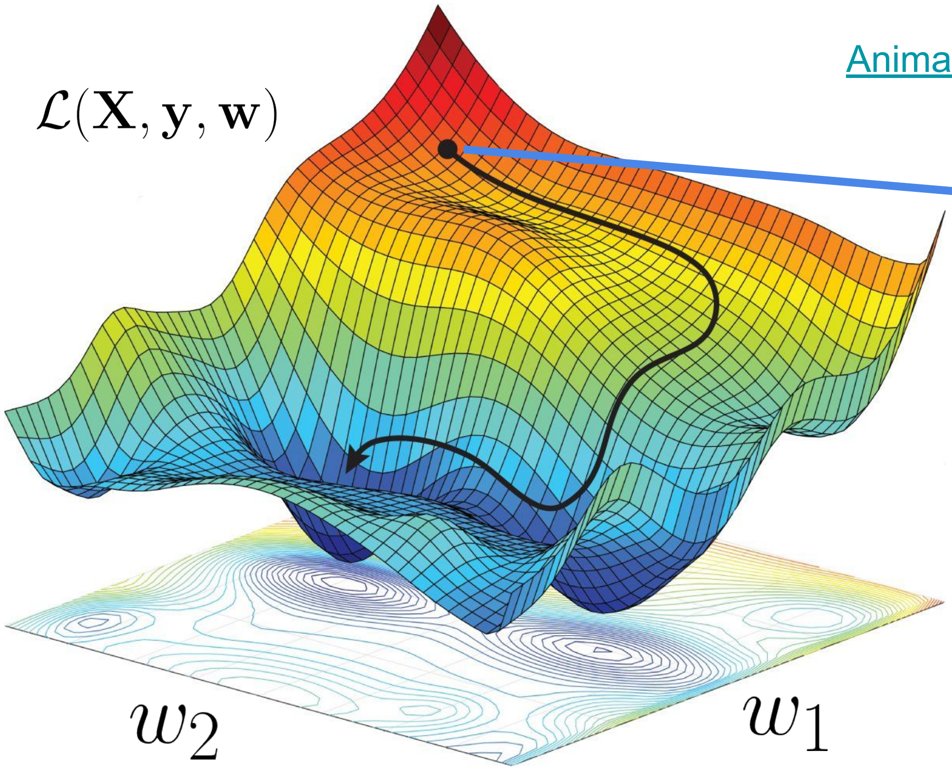
Motivation and intuition: It's hard to find good **w**'s?

- Sometimes, we can't solve for the **w** that makes the derivative (gradient) of the loss function 0 (e.g. deep neural network)
- Other times, there are multiple solutions where the gradient will be zero and the loss function is in a valley (i.e. loss function is not *convex*)





Gradient Descent: Going Downhill



[Animation (near the bottom)]

Gradient Descent

Loss function with respect to data, labels, and parameters

$$\mathcal{L}(\mathbf{X}, \mathbf{y}, \mathbf{w})$$

$$\frac{\partial}{\partial \mathbf{w}} \mathcal{L}(\mathbf{X}, \mathbf{y}, \mathbf{w})$$

Gradient: derivative of loss with respect to parameters

Example for **linear regression**

$$\hat{y}_i = \mathbf{w}\mathbf{x}_i$$

$$\mathcal{L}(\mathbf{X}, \mathbf{y}, \mathbf{w}) = \frac{1}{n} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

$$\mathcal{L}(\mathbf{X}, \mathbf{y}, \mathbf{w}) = \frac{1}{n} \sum_{i=1}^{n} (y_i - \mathbf{w}\mathbf{x}_i)^2$$

$$\frac{\partial}{\partial \mathbf{w}} \mathcal{L}(\mathbf{X}, \mathbf{y}, \mathbf{w}) = \frac{-2}{n} \sum_{i=1}^{n} \mathbf{x}_i (y_i - \mathbf{w}\mathbf{x}_i)$$

Gradient descent procedure

1) Initialize the parameters - w (e.g. randomly)
2) Compute the gradient of the loss function with respect to the parameters

   *The loss function would **increase** if we moved the parameters in the direction of this gradient*

3) Move the parameters in the **opposite** direction (direction of the **–** gradient) of the gradient so that the loss function would **decrease**

   *The parameters are now better because they result in a lower loss. **This is the goal of training***

4) Repeat (2) and (3) several times so that the loss gradually decreases

We can always use gradient descent to optimize a set of parameters, so long as the loss function is **differentiable** with respect to those parameters

Two Gradient descent decisions/hyperparameters

- How much do we move in the opposite direction of the gradient each update iteration? This is called the **learning rate**
  - Optimal setting depends on your model and the loss function
  - Don’t know the optimal value beforehand. Try different values, see which is best (grid search with cross-validation)
  - Doesn’t necessarily need to be a constant value (learning rate scheduling/decay)
- How many update iterations do we want to perform?
  - Can use a constant value. Number of times we update using the entire dataset is called the number of **epochs**
  - Can keep updating until loss stops decreasing/has plateaued (i.e. loss has **converged**)

Gradient descent algorithm

Algorithm: Gradient Descent

Initialize $\mathbf{w}$ (e.g. randomly)

for $epoch \in nEpochs$ **do**

$$\mathbf{w}_{grad} = \frac{\partial}{\partial \mathbf{w}} \mathcal{L}(\mathbf{X}, \mathbf{y}, \mathbf{w})$$

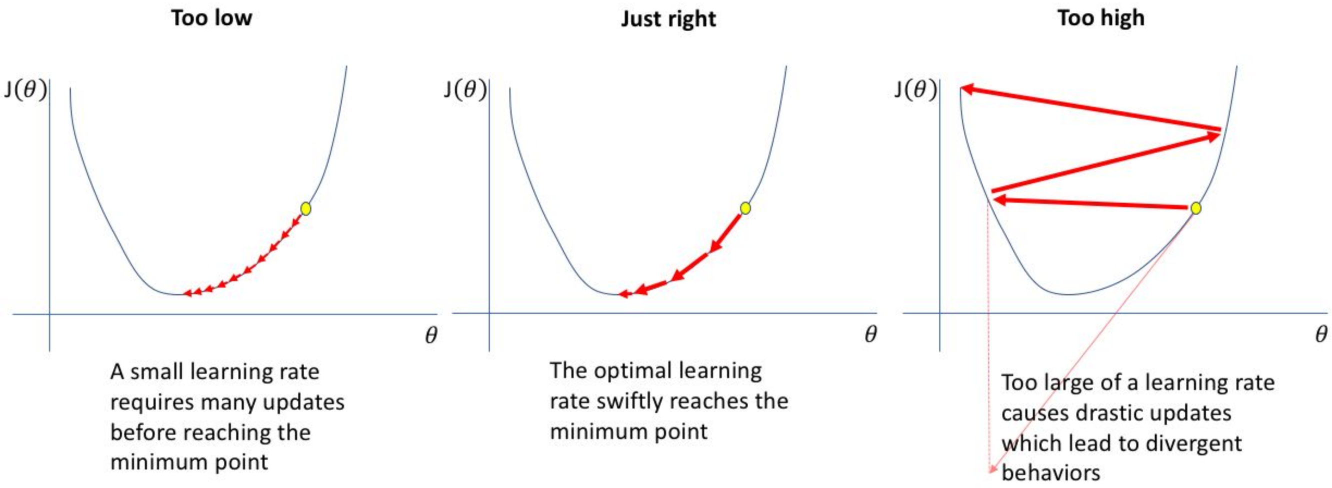
$$\mathbf{w} = \mathbf{w} - \alpha \mathbf{w}_{grad}$$

end

α denotes the Learning Rate

Effect of the **learning rate**

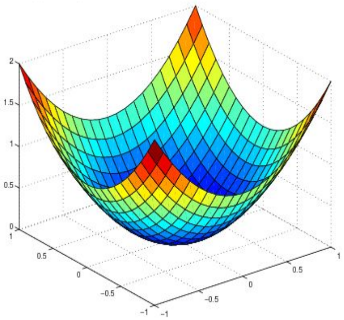
- Learning rate too large: end up missing the local minima (overshooting)
- Learning rate too small: learning takes too long (need more iterations/epochs)
- An Analogy: Think of this of this as a sticky marble rolling around in a bowl

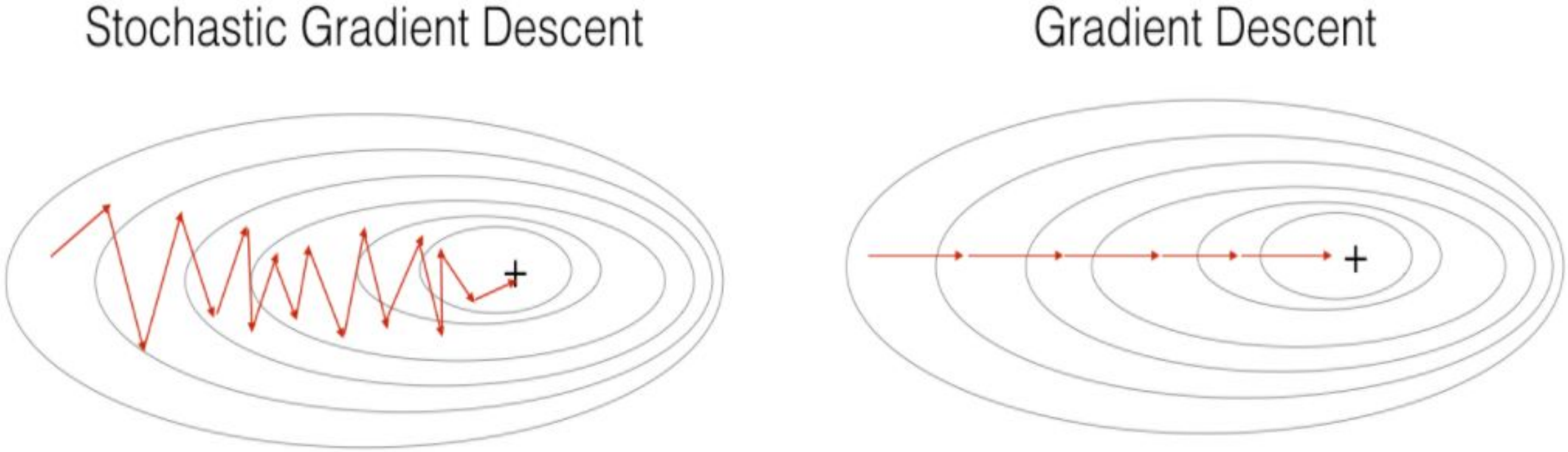


Stochastic Gradient Descent vs Gradient Descent
SGD vs GD

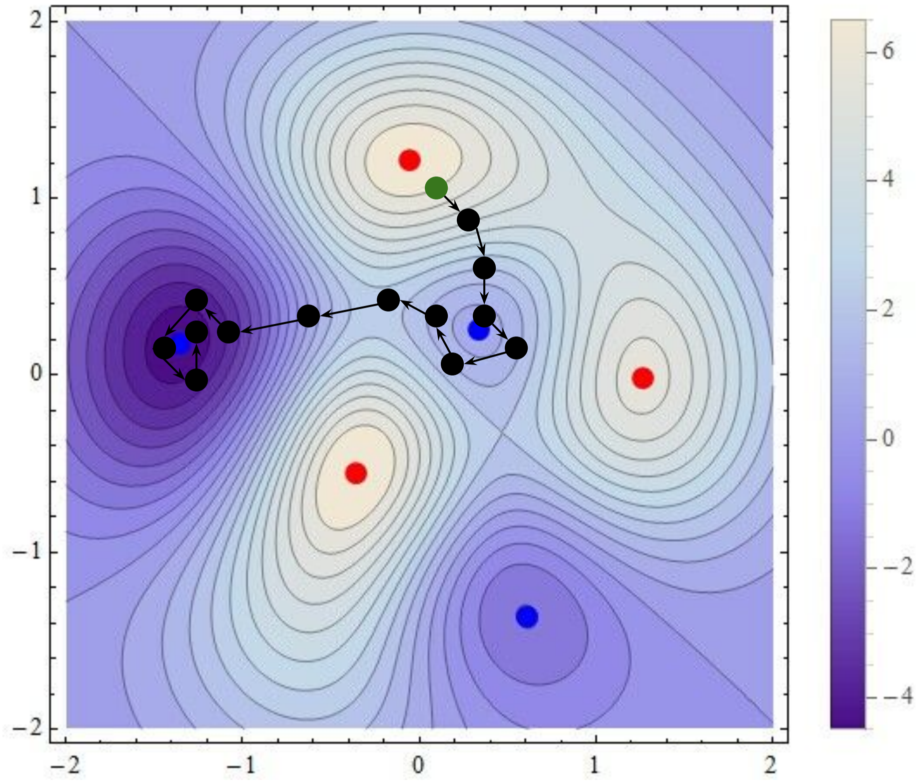
- Gradient descent can be computationally expensive and slow (uses the entire **X** dataset each weight update)
- **<u>Stochastic gradient descent</u>**: randomly select ***one*** **data point** (row in **X**) and updates **w** using its gradient
- Results in noisy approximate of the true (full dataset) gradient
- In practice, using noisy updates converges to better solutions that are closer to the *global minimum* (can escape bad local minima)

Stochastic gradient descent





Stochastic gradient descent: escaping bad minima



Stochastic gradient descent algorithm

Algorithm: Stochastic Gradient Descent

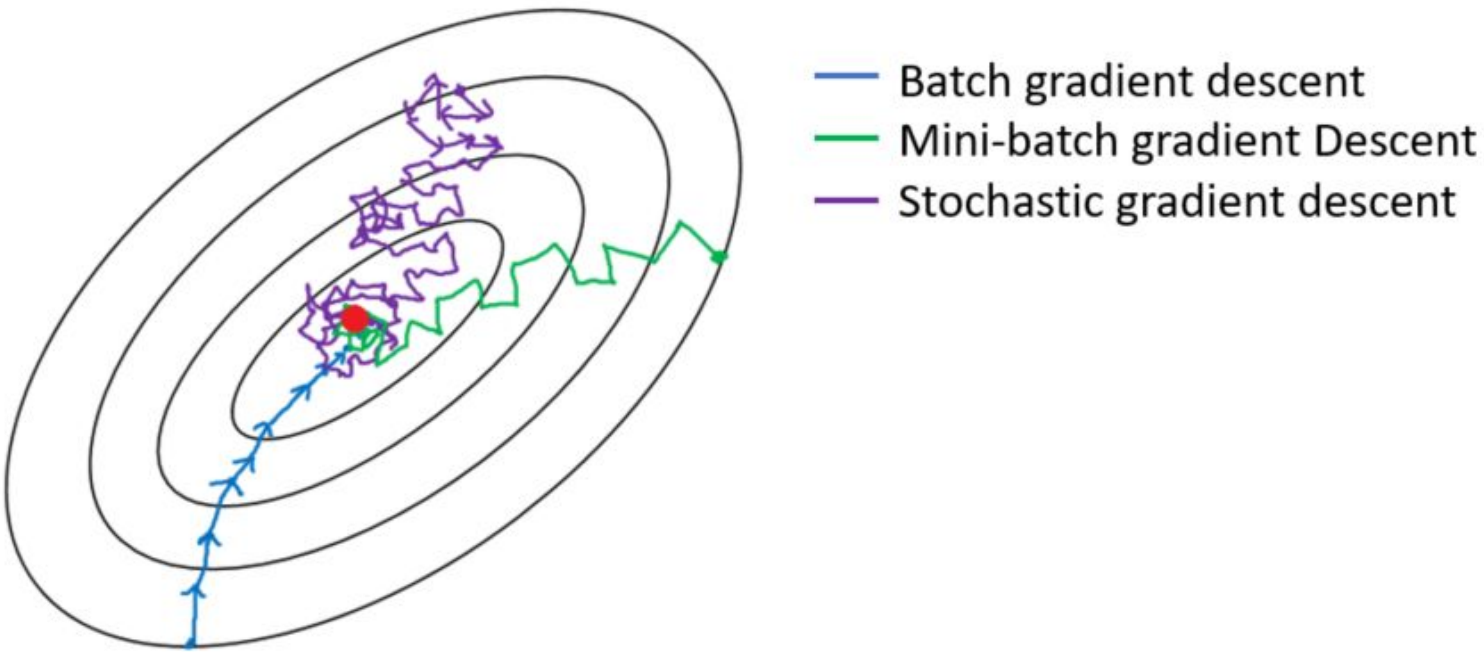
Initialize $\mathbf{w}$ (e.g. randomly)
for $epoch \in nEpochs$ **do**
  shuffle $\mathbf{X}$
  for $\mathbf{x}_i \in \mathbf{X}$ **do**
    $\mathbf{w}_{grad} = \frac{\partial}{\partial \mathbf{w}} \mathcal{L}(\mathbf{x}_i, y_i, \mathbf{w})$
    $\mathbf{w} = \mathbf{w} - \alpha \mathbf{w}_{grad}$
  end
end

α denotes the Learning Rate

Mini-batch gradient descent: Compromise b/w GD and SGD

- A bit of noise can help us find the optimal solution by escaping local minima
- Too much noise can slow training due to lack of sustained downhill progress
- Big matrix multiplications may make our computers run out of memory
- Small matrix multiplications may not make efficient use of parallel computing
- **We often want something in between**: estimate the gradient each iteration using some, but not all, of the data

Mini-batch gradient descent



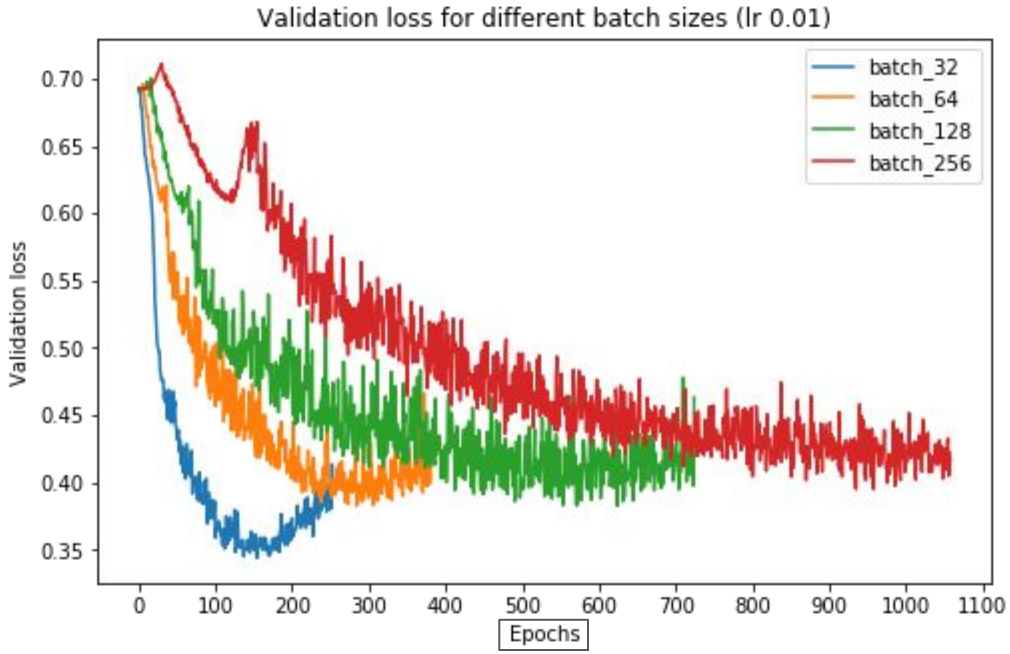
Mini-batch gradient descent algorithm

Algorithm: Mini-Batch Gradient Descent

Initialize $\mathbf{w}$ (e.g. randomly)
for $epoch \in nEpochs$ **do**
  shuffle $\mathbf{X}$
  for $\mathbf{X}_{i:i+BS} \in \mathbf{X}$, *with i increasing by BS at a time* **do**
    $\mathbf{w}_{grad} = \frac{\partial}{\partial \mathbf{w}} \mathcal{L}(\mathbf{X}_{i:i+BS}, \mathbf{y}_{i:i+BS}, \mathbf{w})$
    $\mathbf{w} = \mathbf{w} - \alpha \mathbf{w}_{grad}$
  end
end

α denotes the Learning Rate
BS denotes the Batch Size

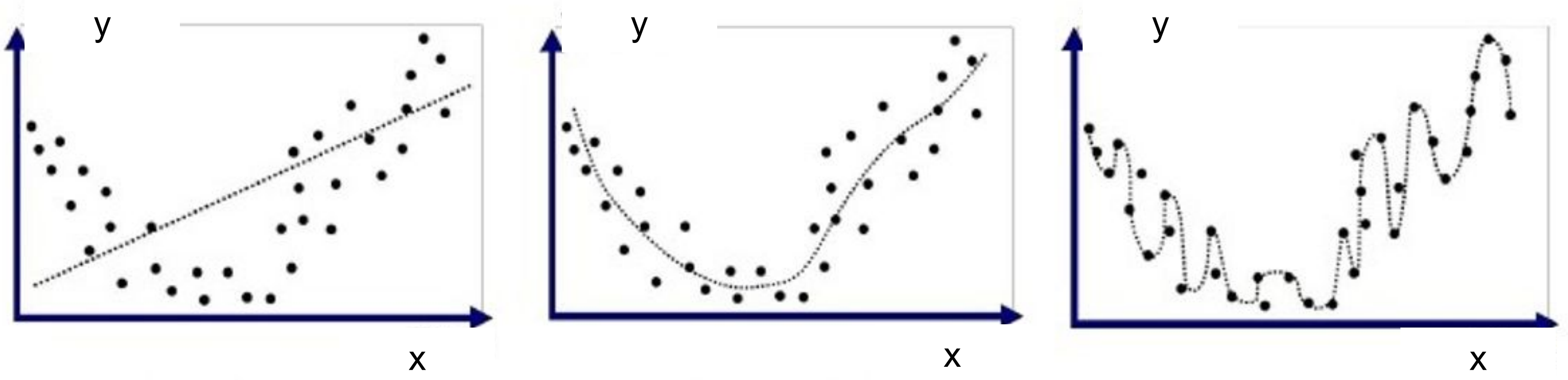
Effect of the batch size



Note: graph is for a deep neural network
(many local minima, noise is more important)

Regularization

Motivation

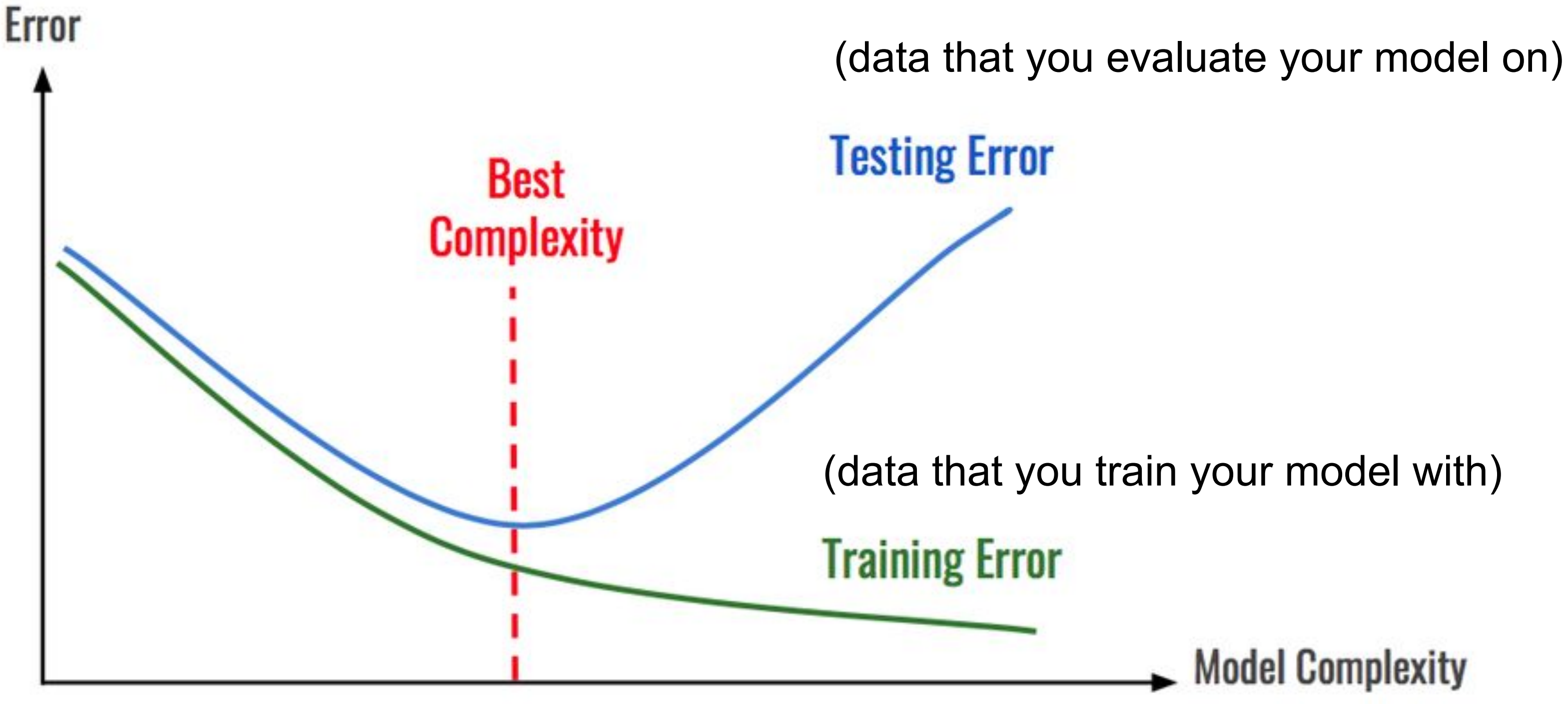


Underfitted   Good Fit/Robust   Overfitted

Motivation

- Data has two components components: *signal (pattern)* + *noise*
- Example: predicting house prices from # of bedrooms, area, age, etc.
    - Signal: degree to which these features influence the price
    - Noise: random variation, or variation due to unknown features
- **Goal of machine learning**: model the signal/pattern, ignore the noise
- When the model is fitting (trying to predict) the noise, we say that it is **overfitting**
- Overfitting is undesirable, because the **noise is random** and therefore won't be the same on new data seen out in the real world – won't Generalize

Detecting Overfitting



What is model complexity?

- The space of functions a model can learn (ie. Degree of a polynomial fit)
- Influenced by:
    - Model architecture (structure, type)
    - Model flexibility (e.g. number of parameters)
    - The particular solution we converge to (i.e. final parameters)
- Example for linear regression architecture: parameters come from weights connecting features to dependent variable
    - Complexity of linear regression models increases as the number of parameters increases
    - The number of parameters increases with the number of features you use (dimensionality)

Combating overfitting

- Option 1: use a less powerful model – low complexity
- Option 2: reduce the number of parameters
  - For linear regression, corresponds to reducing the number of features (dimensionality reduction or feature selection)
- Option 3: limit the parameter space (effectively reducing the space of possible functions the model can learn)
  - A common way of doing this is to use parameter **regularization**

Regularization

- Constrain the parameter space by adding an additional loss term on the model parameters
- With this *weight penalty*, parameters can no longer vary freely

$$\mathcal{L}(\mathbf{X}, \mathbf{y}, \mathbf{w}) = \underbrace{V(\mathbf{X}, \mathbf{y}, \mathbf{w})}_{\text{prediction error}} \quad + \quad \lambda \quad \underbrace{R(\mathbf{w})}_{\text{weight penalty}}$$

Where $\lambda \geq 0$

Ridge regression

- Uses an *L2 penalty* (penalizes weights based on their *squared sum*)
- In practice:
  - Prevents overfitting when there is a lot of correlation between the features
  - Model has reduced variance (more consistent model for small variations in the data)
  - Irrelevant features get small weights, instead of being used by the model to fit noise

$$\begin{aligned}\mathcal{L}(\mathbf{X}, \mathbf{y}, \mathbf{w}) &= V(\mathbf{X}, \mathbf{y}, \mathbf{w}) \quad + \quad \lambda \quad \mathbf{w}^T\mathbf{w} \\ &= V(\mathbf{X}, \mathbf{y}, \mathbf{w}) \quad + \quad \lambda \quad \sum_{i=0}^{n} w_i^2\end{aligned}$$

Lasso regression

- Uses an *L1 penalty* (penalizes weights based on their *absolute value sum*)
- In practice:
  - Prevents overfitting when there is a lot of correlation between the features
  - Model has reduced variance (more consistent model for small variations in the data)

$$
\begin{aligned}
\mathcal{L}(\mathbf{X}, \mathbf{y}, \mathbf{w}) &= V(\mathbf{X}, \mathbf{y}, \mathbf{w}) \quad + \quad \lambda \quad |\mathbf{w}| \\
&= V(\mathbf{X}, \mathbf{y}, \mathbf{w}) \quad + \quad \lambda \quad \sum_{i=0}^{n} |w_i|
\end{aligned}
$$

Elastic net regression

- Generally, we care about getting the best performance on the test set. We don’t care if we do it using L1 or L2 regularization
- Elastic net uses both, each with their own λ

Picking λ

- If λ is too small, we can overfit (model too complex)
- If λ is too large, we can underfit (model ignores prediction error)
- Like all other hyperparameters, the simplest way to pick it is to try a lot of values and see which works best (grid search with cross-validation)

$$\begin{aligned}\mathcal{L}(\mathbf{X},\mathbf{y},\mathbf{w}) &= V(\mathbf{X},\mathbf{y},\mathbf{w}) \quad + \quad \lambda \quad \mathbf{w}^T\mathbf{w} \\ &= V(\mathbf{X},\mathbf{y},\mathbf{w}) \quad + \quad \lambda \quad \sum_{i=0}^{n} w_i^2\end{aligned}$$