DSC 140A

Probabilistic Modeling & Machine Learning

Lecture 4 | Part 1

Introduction

Empirical Risk Minimization (ERM)

- Step 1: choose a **hypothesis class**
  - We've chosen linear predictors.
- Step 2: choose a **loss function**
- Step 3: find H minimizing **empirical risk**

Gradient Descent

- But sometimes we **can't** solve for $\vec{w}$ **directly**.
  - It's too costly.
  - There's no closed-form solution.

- **Idea:** use **gradient descent** to iteratively minimize risk.

Gradient Descent

- Starting from an initial guess $\vec{w}^{(0)}$, iteratively update:

$$\vec{w}^{(t+1)} = \vec{w}^{(t)} - \eta \frac{dR}{d\vec{w}}(\vec{w}^{(t)})$$

Today

We'll address two modifications to gradient descent.

1. Can be **expensive** to compute the exact gradient.
   - Especially when we have a large data set.
   - **Solution:** **stochastic gradient descent**.

2. Doesn't work as-is if risk is **not differentiable**.
   - Such as with the absolute loss.
   - **Solution:** **subgradient descent**.

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Lecture 4 | Part 2

Motivation: Large Scale Learning

Example

- Suppose you're doing **least squares linear regression** on a medium-to-large data set.
- Say, $n = 200{,}000$ examples, $d = 5{,}000$ features.
- Encoded as 64 bit floats, X is 8 GB.
  - Fits in your laptop's memory, but barely.
- **Example:** predict sentiment from text.

Attempt 0: Normal Equations

- You start by solving the normal equations:

```
np.linalg.solve(X.T @ X, X.T @ y)
```

design matrix

- **Time:** 30.7 seconds.
- **Mean Squared Error:** 7.2×10^{-7}.
- Can we speed this up?

Attempt 1: Gradient Descent

- Recall[1] that the gradient of the MSE is:

$$\frac{dR}{d\vec{w}}(\vec{w}) = \frac{2}{n}\sum_{i=1}^{n}\left(\text{Aug}(\vec{x}^{(i)})\cdot\vec{w} - y_i\right)\text{Aug}(\vec{x}^{(i)})$$

$$= \frac{1}{n}\left(2X^TX\vec{w} - 2X^T\vec{y}\right)$$

- You code up a function:[2]

```
def gradient(w):
    n = len(y)
    return (2/n) * X.T @ (X @ w - y)
```

[1] From Lecture 02, where we derived this.

[2] There's a good and a bad way to do this.

Attempt 1: Gradient Descent

- You plug this into `gradient_descent` from last lecture, run it, and...
- **Time:** **8.6 seconds** total
  - 14 iterations
  - ≈ 0.6 seconds per iteration
- **Mean Squared Error:** 9.4×10^{-7}.

Trivia: why is it faster?

- **Solving normal equations** takes $\Theta(nd^2 + d^3)$ time.
  - $\Theta(nd^2)$ time to compute $X^T X$.
  - $\Theta(d^3)$ time to solve the system.
- **Gradient descent** takes $\Theta(nd)$ time per iteration.
  - $\Theta(nd)$ time to compute $X\vec{w}$.
  - $\Theta(nd)$ time to compute $X^T(X\vec{w} - \vec{y})$.

More is different...

- What if you had a **really big** data set?
- Say, n = 10,000,000 examples, d = 5,000 features.
- Encoded as 64 bit floats, X is **400 GB**.
  - Doesn't fit in your laptop's memory!
  - Barely fits on your hard drive.

Approach 0: Normal Equations

- You can try solving the normal equations:

```
np.linalg.solve(X.T @ X, X.T @ y)
```

- One of three things will happen:
  1. You will receive an **out of memory** error.
  2. The process will be killed (or your OS will freeze).
  3. It will run, but take a **very long time**.

Approach 1: Gradient Descent

- We can't store the data in memory all at once.
- But we can **still** compute the **gradient**, $\frac{dR}{d\vec{w}}$.
  - Read a little bit of data at once.
  - Or, distribute the computation to several machines.
- eg. Computing gradient involves a loop over data:

$$\frac{dR}{d\vec{w}}(\vec{w}) = \frac{2}{n}\sum_{i=1}^{n}\left(\text{Aug}(\vec{x}^{(i)}) \cdot \vec{w} - y_i\right)\text{Aug}(\vec{x}^{(i)})$$

Problem

$$\frac{dR}{d\vec{w}}(\vec{w}) = \frac{2}{n}\sum_{i=1}^{n}\left(\text{Aug}(\vec{x}^{(i)}) \cdot \vec{w} - y_i\right)\text{Aug}(\vec{x}^{(i)})$$

- In machine learning, the number of training points n can be **very large**.
- Computing the gradient can be **expensive** when n is large.
  - So each step of gradient descent is **expensive**.

Idea

- Don’t worry about computing the **exact** gradient.
- An **approximation** will do.

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Lecture 4 | Part 3

Stochastic Gradient Descent

Gradient Descent for Minimizing Risk

- In ML, we often want to minimize a **risk function**:

$$R(\vec{w}) = \frac{1}{n}\sum_{i=1}^{n} \ell(H(\vec{x}^{(i)}; \vec{w}), y_i)$$

Observation

- The gradient of the risk is the average of the gradient of the losses:

$$\frac{d}{d\vec{w}}R(\vec{w}) = \frac{1}{n}\sum_{i=1}^{n}\frac{d}{d\vec{w}}\ell(H(\vec{x}^{(i)};\vec{w}), y_i)$$

- The averaging is over **all training points**.
- This can take a long time when n is large.[3]

[3] Trivia: this usually takes $\Theta(nd)$ time.

Idea

- The (full) gradient of the risk uses all of the training data:

$$\frac{d}{d\vec{w}} R(\vec{w}) = \frac{1}{n} \sum_{i=1}^{n} \frac{d}{d\vec{w}} \ell(H(\vec{x}^{(i)}; \vec{w}), y_i)$$

- **Idea:** instead of using all n training points, randomly choose a smaller set, B:

"cardinality of B"
⇒ # of things in B

$$\frac{d}{d\vec{w}} R(\vec{w}) \approx \frac{1}{|B|} \sum_{i \in B} \frac{d}{d\vec{w}} \ell(H(\vec{x}^{(i)}; \vec{w}), y_i)$$

Stochastic Gradient

- The smaller set B is called a **mini-batch**.
- We now compute a **stochastic gradient**:

$$\frac{d}{d\vec{w}} R(\vec{w}) \approx \frac{1}{|B|} \sum_{i \in B} \frac{d}{d\vec{w}} \ell(H(\vec{x}^{(i)}; \vec{w}), y_i)$$

- "Stochastic," because it is a random.

Stochastic Gradient

$$\frac{d}{d\vec{w}} R(\vec{w}) \approx \frac{1}{|B|} \sum_{i \in B} \frac{d}{d\vec{w}} \ell(H(\vec{x}^{(i)}; \vec{w}), y_i)$$

- The stochastic gradient is an **approximation** of the full gradient.
- When $|B| \ll n$, it is **much faster** to compute.
- But the approximation is **noisy**.

Stochastic Gradient Descent for ERM

To minimize empirical risk $R(\vec{w})$:

- Pick starting weights $\vec{w}^{(0)}$, learning rate $\eta > 0$, batch size m.
- Until convergence, repeat:
  - **Randomly sample** a batch B of m training data points.
  - **Compute stochastic gradient:**

$$\vec{g} = \frac{1}{|B|} \sum_{i \in B} \frac{d}{d\vec{w}} \ell(H(\vec{x}^{(i)}; \vec{w}), y_i)$$

  - **Update:** $\vec{w}^{(t+1)} = \vec{w}^{(t)} - \eta \vec{g}$
- When converged, return $\vec{w}^{(t)}$.

Note

- A **new batch** should be randomly sampled on each iteration!
- This way, the entire training set is used over time.
- Size of batch should be **small** compared to n.
  - Think: $m = 64$, $m = 32$, or even $m = 1$.

Example: Linear Least Squares

- We can use SGD to perform linear least squares regression.
- Need to compute the gradient of the square loss:

$$\ell_{\text{sq}}(H(\vec{x}^{(i)}; \vec{w}), y_i) = \left(\text{Aug}(\vec{x}^{(i)}) \cdot \vec{w} - y_i\right)^2$$

Exercise

What is the gradient of the square loss of a linear predictor? That is, what is $\frac{d}{d\vec{w}}\left(\text{Aug}(\vec{x}^{(i)}) \cdot \vec{w} - y_i\right)^2$?

$\frac{d}{d\vec{w}}\left(\vec{x}^{(i)} \cdot \vec{w} - y_i\right)^2 = 2\left(\vec{x}^{(i)} \cdot \vec{w} - y_i\right)\vec{x}^{(i)}$

Example: Linear Least Squares

- The gradient of the square loss of a linear predictor is:

$$
\begin{aligned}
\frac{d}{d\vec{w}}\ell_{\text{sq}}(H(\vec{x}^{(i)}; \vec{w}), y_i)
&= \frac{d}{d\vec{w}}\left(\text{Aug}(\vec{x}^{(i)}) \cdot \vec{w} - y_i\right)^2 \\
&= 2\left(\text{Aug}(\vec{x}^{(i)}) \cdot \vec{w} - y_i\right) \frac{d}{d\vec{w}}\left(\text{Aug}(\vec{x}^{(i)}) \cdot \vec{w} - y_i\right) \\
&= 2\left(\text{Aug}(\vec{x}^{(i)}) \cdot \vec{w} - y_i\right) \text{Aug}(\vec{x}^{(i)})
\end{aligned}
$$

Example: Linear Least Squares

- Therefore, on each step we compute the stochastic gradient:

$$\vec{g} = \frac{2}{m} \sum_{i \in B} \left(\text{Aug}(\vec{x}^{(i)}) \cdot \vec{w} - y_i \right) \text{Aug}(\vec{x}^{(i)})$$

- The update rule is:

$$\vec{w}^{(t+1)} = \vec{w}^{(t)} - \eta \vec{g}$$

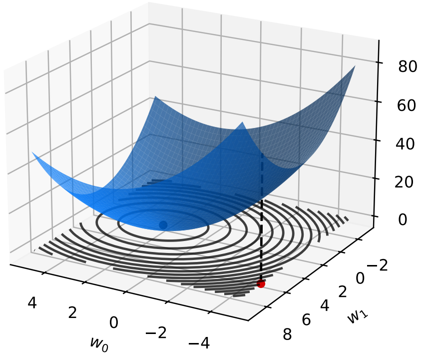
Example: Linear Least Squares

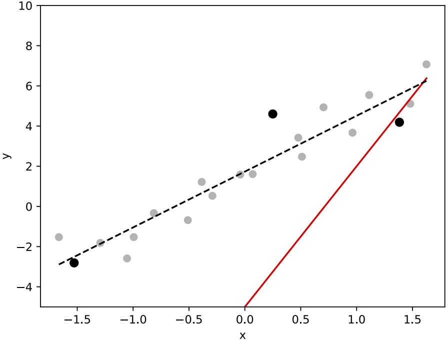
- We can write in matrix-vector form, too:
  - Let X_B be the design matrix using only the examples in batch B.
  - Let y_B be the corresponding vector of labels.

- Then:

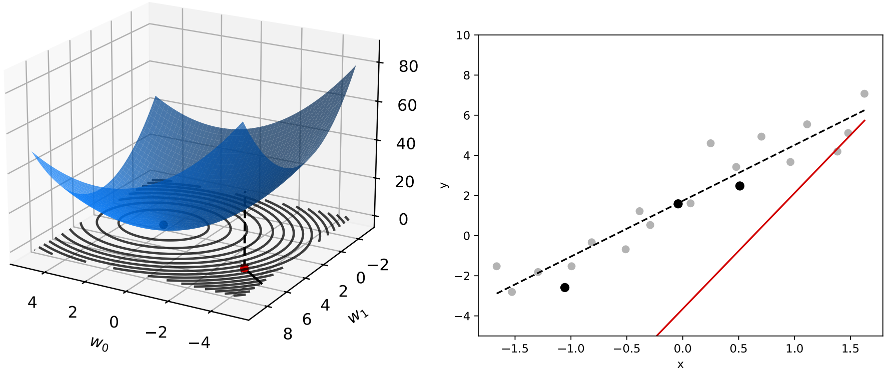
$$\vec{g} = \frac{2}{m} X_B^T (X_B \vec{w} - y_B)$$

Example: SGD





Example: SGD



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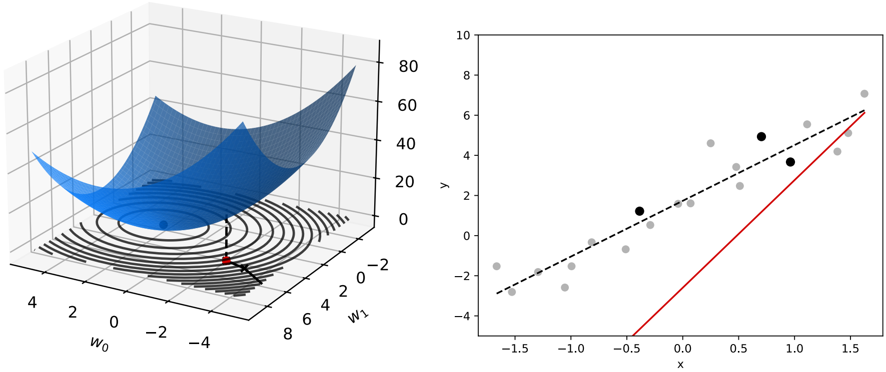

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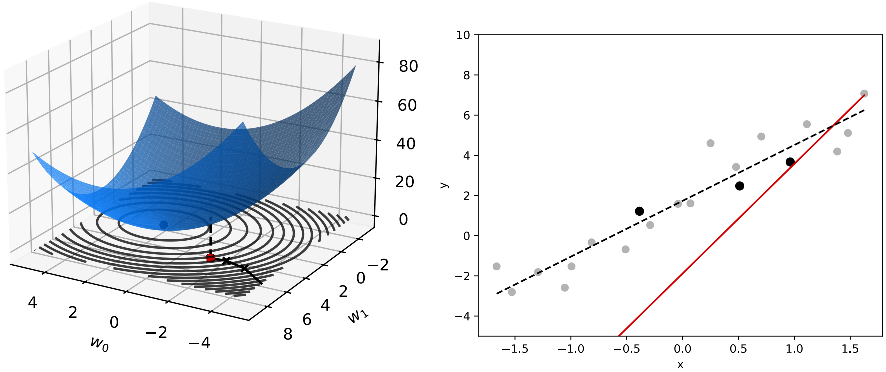

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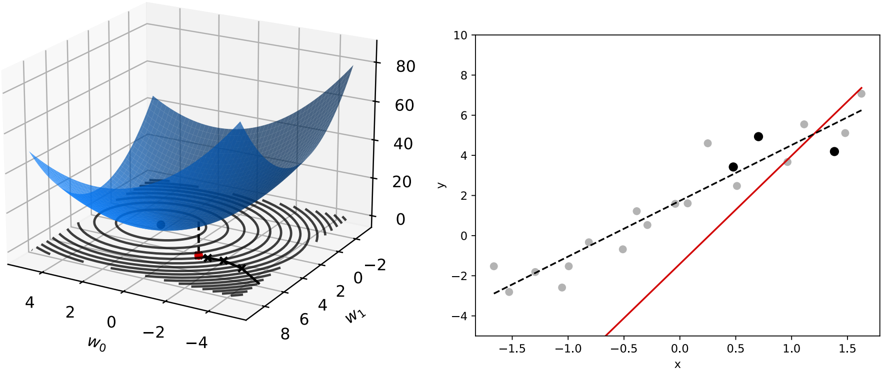

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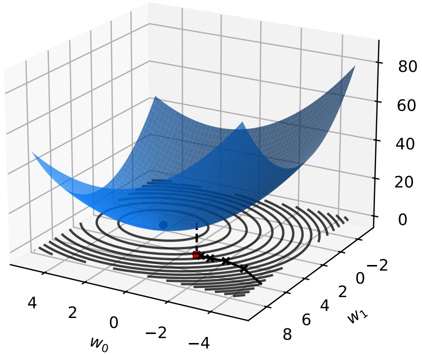

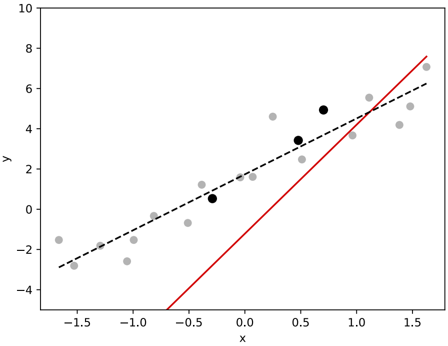

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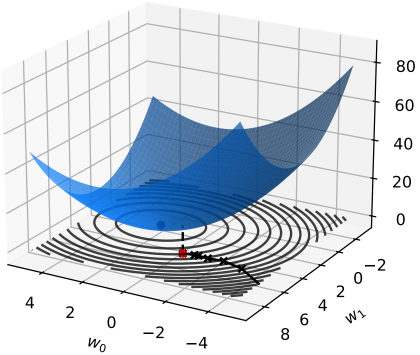

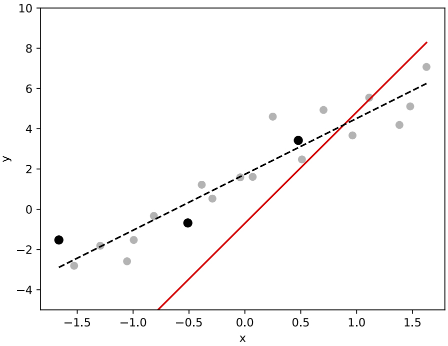

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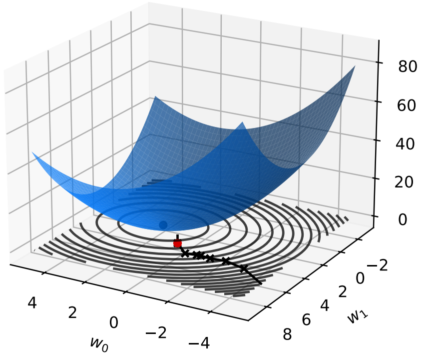

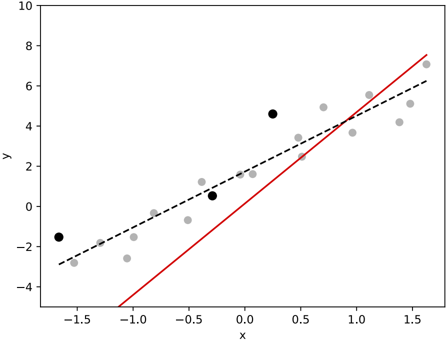

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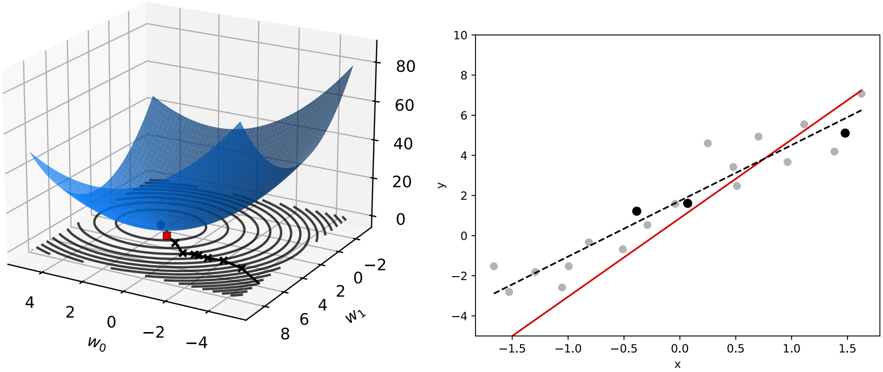

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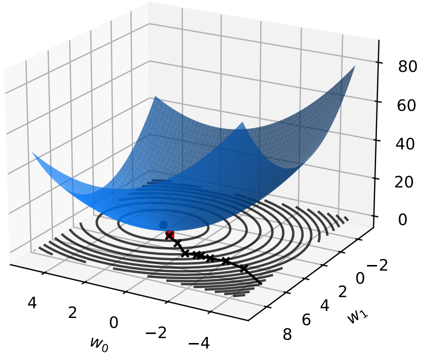

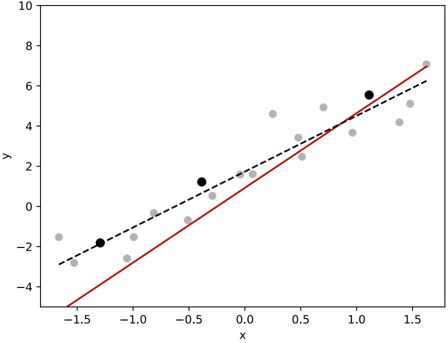

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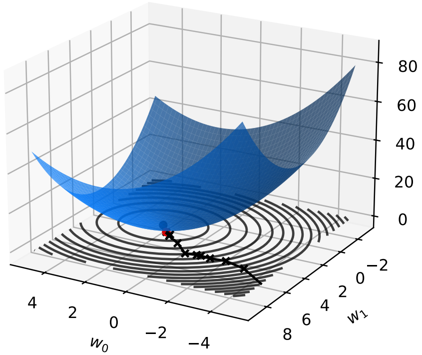

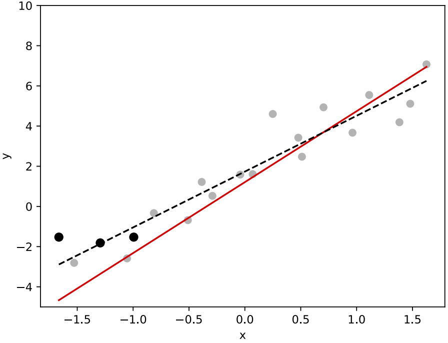

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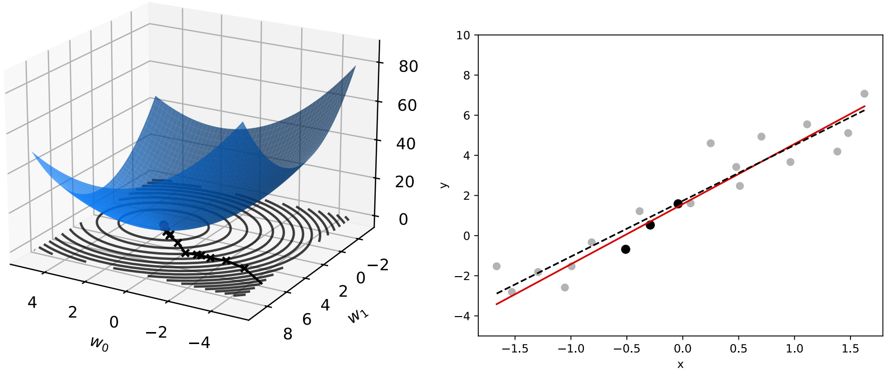

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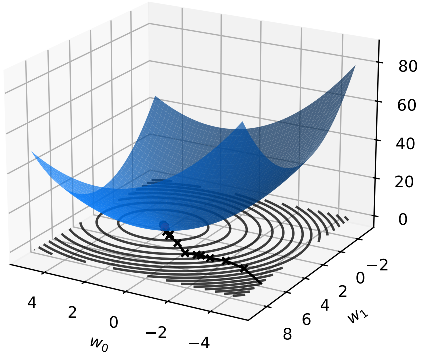

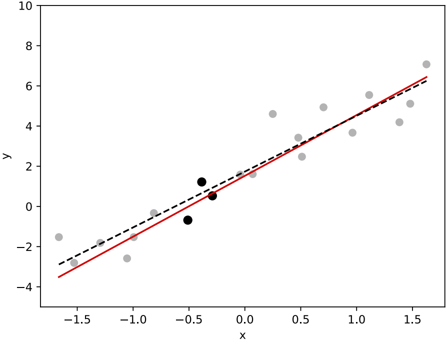

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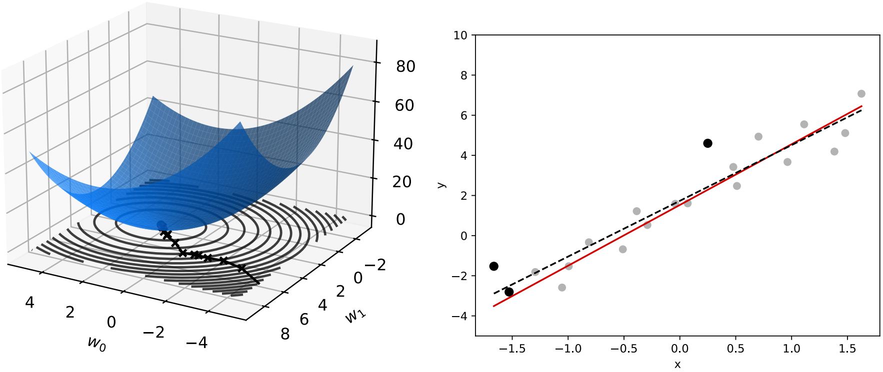

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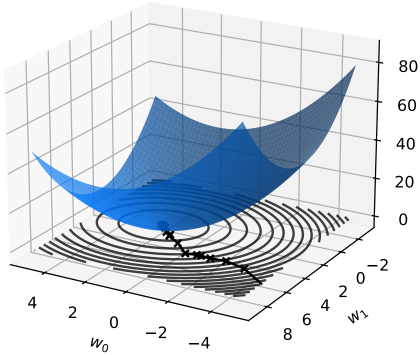
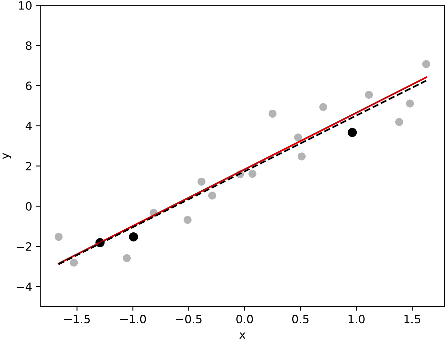
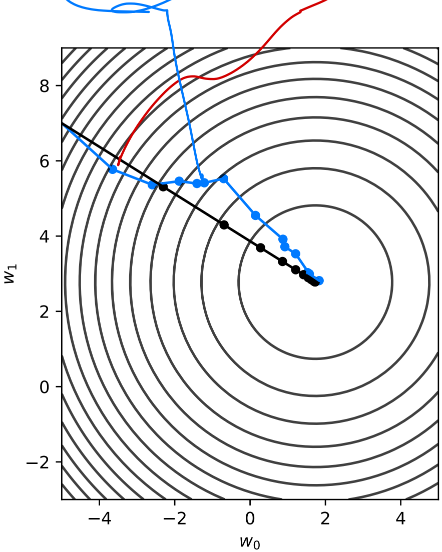




SGD vs. GD



Tradeoffs

- In each step of GD, move in the “best” direction.
  - But **slowly!**
- In each step of SGD, move in a “good” direction.
  - But **quickly!**
- SGD may take more steps to converge, but can be faster overall.

Example

- Suppose you're doing **least squares regression** on a medium-to-large data set.
- Say, $n = 200{,}000$ examples, $d = 5{,}000$ features.
- Encoded as 64 bit floats, X is 8 GB.
  - Fits in your laptop's memory, but barely.
- **Example:** predict sentiment from text.

We saw...

- Solving the normal equations took **30.7 seconds**.
- Gradient descent took **8.6 seconds**.
  - 14 iterations, ≈ 0.6 seconds per iteration.
- Stochastic gradient descent takes **3 seconds**.
  - Batch size $m = 16$.
  - 13,900 iterations, ≈ 0.0002 seconds per iteration.

Aside: Terminology

- Some people say "stochastic gradient descent" only when batch size is 1.
- They say "mini-batch gradient descent" for larger batch sizes.
- **In this class**: we'll use "SGD" for any batch size, as long as it's chosen randomly.

Aside: A Popular Variant

- One variant of SGD uses **epochs**.
- During each epoch, we:
  - Randomly shuffle the training data.
  - Partition the training data into n/m mini-batches.
  - Perform one step for each mini-batch.

Usefulness of SGD

- SGD **enables** learning on **massive** data sets.
  - Billions of training examples, or more.

- Useful even when exact solutions available.
  - E.g., least squares regression / classification.