GRADIENT DESCENT

LECTURE 4
SECTION 2
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INSTITUTE FOR APPLIED
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MAXIMIZING THE LIKELIHOOD OF LOGISTIC REGRESSION

MAXIMUM LIKELIHOOD ESTIMATOR:

Given a data set $D = \{(x^{(1)}, y^{(1)}), \dots, (x^{(N)}, y^{(N)})\}$, with $x^{(n)} \in \mathbb{R}^D$ and $y^{(n)} = 0, 1$, the likelihood of D under a Logistic Regression model with linear boundary is:

$$\mathcal{L}(w) = \prod_{n=1}^{N} \sigma(f_w(x^{(n)}))^{y^{(n)}} (1 - \sigma(f_w(x^{(n)})))^{1-y^{(n)}}$$

where the decision boundary is $f_w(x) = w^T x = 0$.

Fitting the model means finding the maximum likelihood estimator of w:

$$w_{MLE} = \arg\max_w \mathcal{L}(w)$$

This is equivalent to maximizing the log-likelihood:

$$\begin{aligned}
\arg\max_w \mathcal{L}(w) = \arg\max_w \ell(w) &= \arg\max_w \log \prod_{n=1}^{N} \sigma(f_w(x^{(n)}))^{y^{(n)}} (1 - \sigma(f_w(x^{(n)})))^{1-y^{(n)}} \\
&= \arg\max_w \sum_{n=1}^{N} y^{(n)} \log \frac{1}{1+e^{-w^T x^{(n)}}} + (1-y^{(n)}) \log \frac{1}{1+e^{-(1-w^T x^{(n)})}} \\
&= \arg\max_w \sum_{n=1}^{N} -y^{(n)} \log(1+e^{-w^T x^{(n)}}) - (1-y^{(n)}) \log(1+e^{-(1-w^T x^{(n)})})
\end{aligned}$$

We compute the stationary points of the gradient with respect to w:

$$\nabla_w \ell(w) = \sum_{n=1}^{N} \left(y^{(n)} - \frac{1}{1+e^{-w^T x^{(n)}}}\right) x^{(n)} = 0$$

But we can't analytically solve this equation!

ITERATIVE OPTIMIZATION

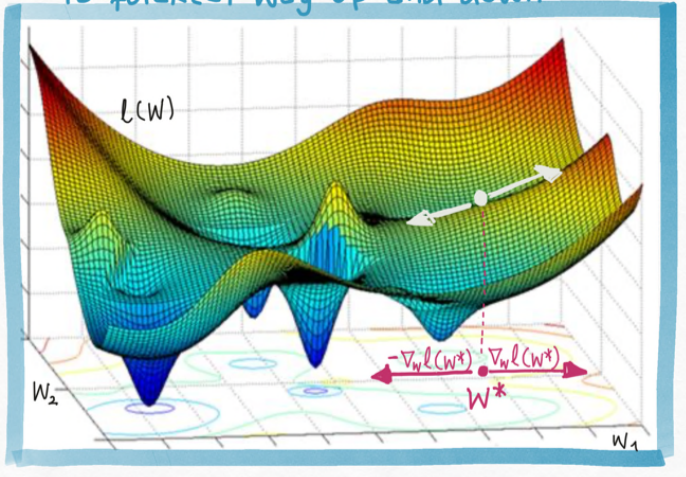
GRADIENT DESCENT:

When we can't analytically solve for the stationary points of the gradient, we can still exploit the information in the gradient.

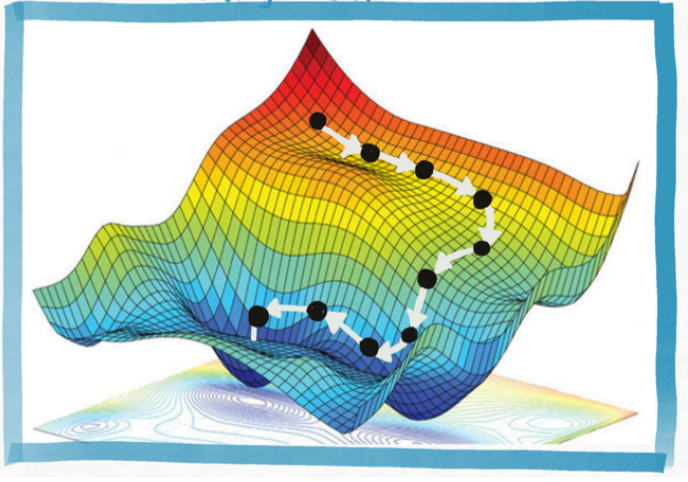
The gradient $\nabla_w \ell(w^*)$ at a point w^* is the direction of the steepest increase.
The negative gradient $-\nabla_w \ell(w^*)$ is the direction of the steepest decrease.

By following the negative gradient we can eventually find a valley (lowest point. By following the gradient we can eventually find a peak (highest point). This method is called Gradient Descent (or Gradient Ascent if going up).

Gradient and Negative Gradients Point to quickest way up and down



Following the negative gradient step by step leads all the way down



THE GRADIENT DESCENT ALGORITHM:

Our intuition about using the gradient to minimize $\ell(w)$ step-by-step can be formalized by an algorithm:

Gradient Descent Algorithm:

0. start at any point $w^{(0)}$
1. Repeat until stopping condition is met:
   A. Compute the gradient at the current point $w^{(n)}$:
   $$\nabla_w \ell(w^{(n)})$$
   B. Take a step in the negative gradient direction:
   $$w^{(n+1)} = w^{(n)} - \eta \cdot \nabla_w \ell(w^{(n)})$$

The constant η is called the learning rate and is a hyperparameter that we must choose before hand. η controls the size of the step we take in the negative gradient direction.

The stopping condition typically limits the total number of iterations, or terminates when the update to $w^{(n)}$ is suffciently small, i.e.

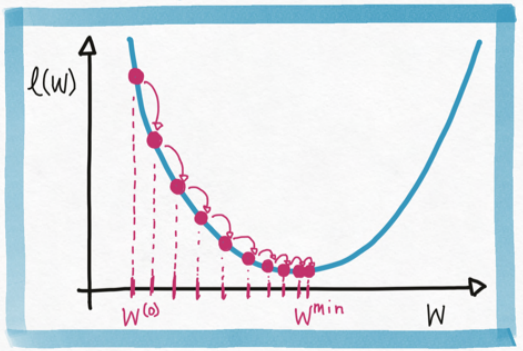
$$\|w^{(n+1)} - w^{(n)}\|_2 < \varepsilon$$

REASONING ABOUT GRADIENT DESCENT

DIAGNOSING GRADIENT DESCENT:

Our choice of the learning rate has a significant impact on the performance of gradient descent.

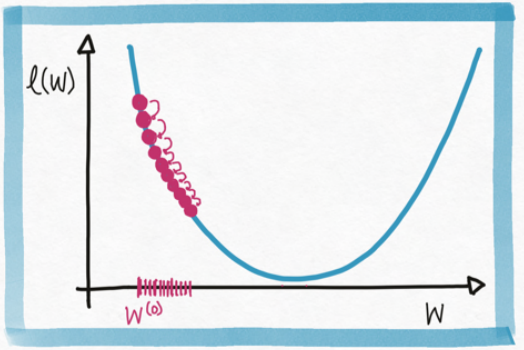
Learning Rate Appropriate



When η is appropriate, the algorithm will eventually find the bottom of a valley, where the gradient is zero.

We say the algorithm converges

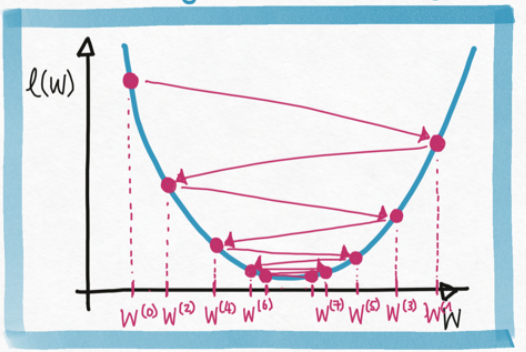
Learning Rate Too Small



When η is too small, the algorithm makes very little progress.

The convergence is too slow.

Learning Rate Too Large



When η is too large, the algorithm may overshoot the optimum value and oscillate.

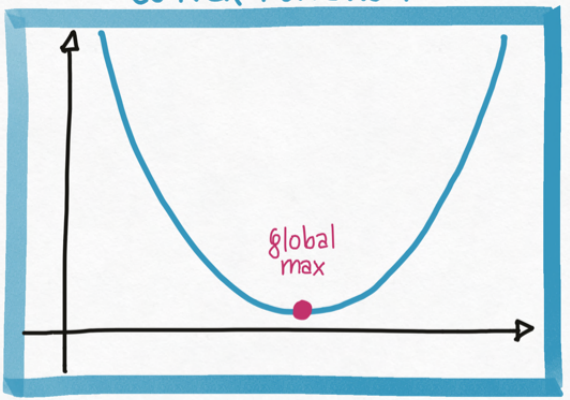
We may fail to converge.

LOCAL VS GLOBAL OPTIMA:

If we choose η correctly, then gradient descent will converge to a stationary point. But will this point be a global minima?

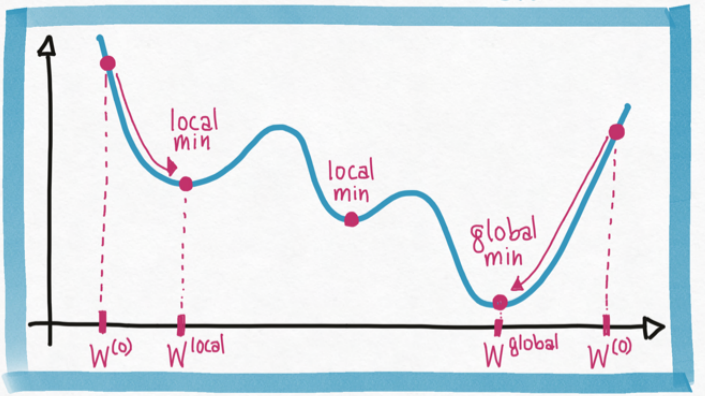
If the function we are optimizing is convex then the stationary point will be a global minimum.

Convex Function



Hessian (2nd Derivative) positive semi-definite everywhere.
Every stationary point of the gradient is a global min.

Non-Convex Function



Hessian (2nd Derivative) not positive semi-definite everywhere.
Some stationary points are local minima but not global optima.

MAXIMIZING LIKELIHOOD OF LOGISTIC REGRESSION

INFERENCE FOR LOGISTIC REGRESSION:

Model

Given a data set $D = \{(x^{(1)}, y^{(1)}), \ldots, (x^{(N)}, y^{(N)})\}$, with $x^{(n)} \in \mathbb{R}^D$ and $y^{(n)} = 0, 1$, the likelihood of D under a Logistic Regression model with linear boundary is:

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where the decision boundary is $f_w(x) = w^T x = 0$.

Inference

Fitting the model means finding the maximum likelihood estimator of w:

$$w_{MLE} = \arg\max_w \mathcal{L}(w)$$

This is equivalent to minimizing the negative log-likelihood:

$$w_{MLE} = \arg\min_w -\log \mathcal{L}(w) = \arg\min_w -\ell(w)$$

We minimize $-\ell(w)$ by gradient descent.

Finally, we show that $-\ell(w)$ is convex, so the stationary point found by gradient descent is a global minimum: w_{MLE}.