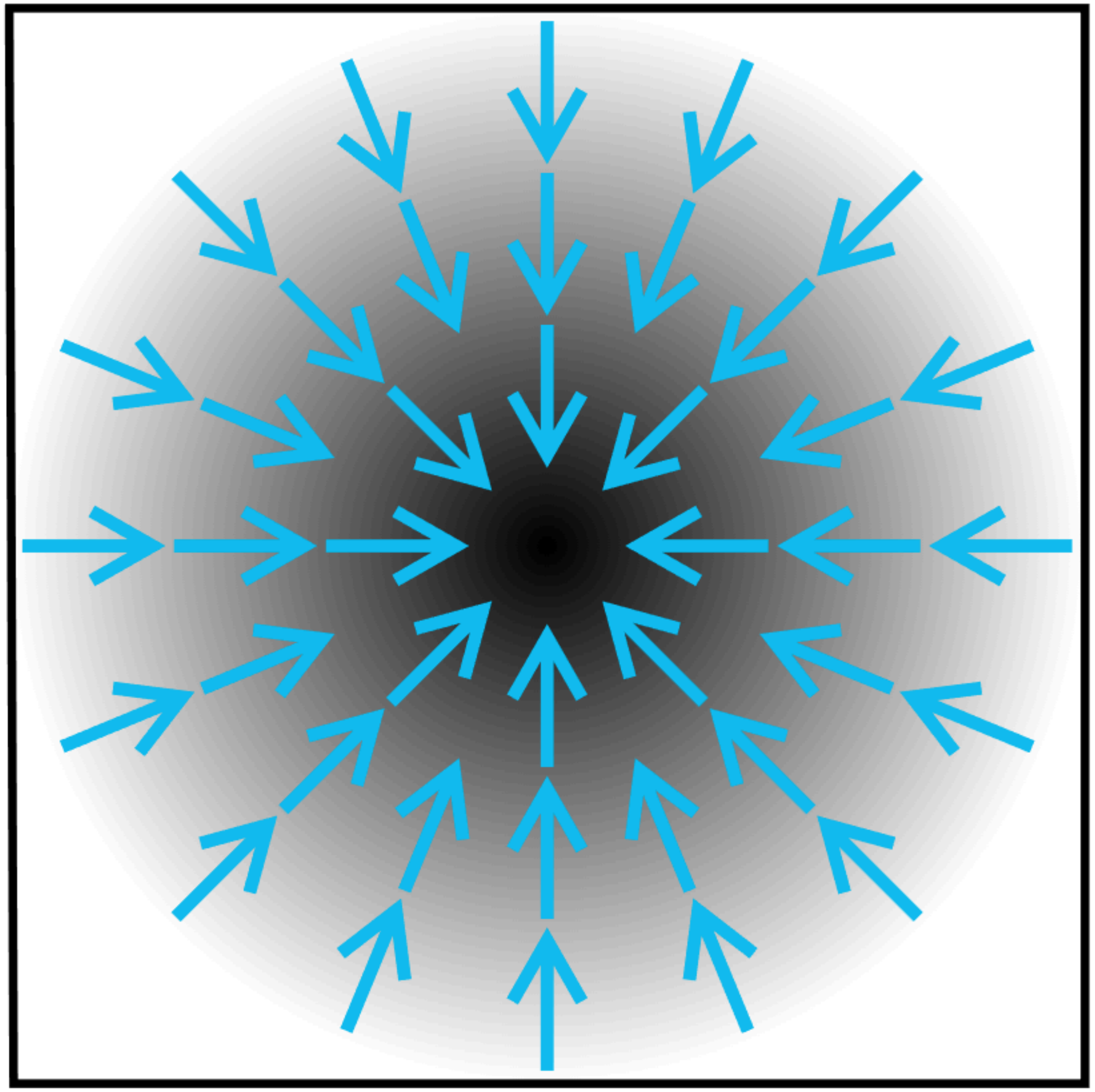

Logistic Regression: Loss Function and Gradient Descent

Leandro L. Minku

Outline

- Logistic regression optimisation problem
  - What problem needs to be solved to learn a logistic regression model?
  - Maximum likelihood estimation.
- Solving the logistic regression optimisation problem
  - Gradient descent.

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How to Learn $\mathbf{w}$?

$$\text{logit}(p_1) = \mathbf{w}^T\mathbf{x} \quad \begin{cases} \mathbf{w}^T\mathbf{x} \geq 0 \rightarrow \text{class 1} \\ \mathbf{w}^T\mathbf{x} < 0 \rightarrow \text{class 0} \end{cases}$$

$$p_1 = \frac{e^{(\mathbf{w}^T\mathbf{x})}}{1 + e^{(\mathbf{w}^T\mathbf{x})}}$$

$$p_0 = 1 - p_1$$

- Given a training set (drawn i.i.d. from the true underlying distribution):

$$\mathcal{T} = \{(\mathbf{x}^{(1)}, y^{(1)}), (\mathbf{x}^{(2)}, y^{(2)}), \cdots, (\mathbf{x}^{(N)}, y^{(N)})\}$$

- Maximum likelihood estimation for supervised learning

Principle: the most reasonable values for $\mathbf{w}$ are the ones for which the "probability" of the observed examples is largest.

1. How likely would we get the output y for the input $\mathbf{x}$ for our training examples if the target distribution is really $\{p_1 = p(1 \mid \mathbf{x}, \mathbf{w}), p_0 = p(0 \mid \mathbf{x}, \mathbf{w})\}$?

2. Find the value $\mathbf{w}$ that maximises this quantity.

Likelihood

How likely would we get the output y for the input $\mathbf{x}$ for our training examples if the target distribution is really $\{p_1 = p(1 \mid \mathbf{x}, \mathbf{w}), p_0 = p(0 \mid \mathbf{x}, \mathbf{w})\}$?

$$\mathcal{T} = \{(\mathbf{x}^{(1)}, y^{(1)}), (\mathbf{x}^{(2)}, y^{(2)}), \cdots, (\mathbf{x}^{(N)}, y^{(N)})\}$$

For each example $(\mathbf{x}^{(i)}, y^{(i)}) \in \mathcal{T}$,
this is captured as $p_{y^{(i)}} = p(y^{(i)} \mid \mathbf{x}^{(i)}, \mathbf{w})$, where $y^{(i)} \in \{0, 1\}$

conditional likelihood

As examples are drawn i.i.d., jointly we have $\prod_{i=1}^{N} p_{y^{(i)}}$.

joint conditional likelihood

Probability vs likelihood: the term probability is usually used when we assume the model's parameters are reliable. The term likelihood is usually used when we're trying to determine whether the parameters in a model are good given the data.

Notation

$$\prod_{i=1}^{N} p_{y^{(i)}} = \prod_{i=1}^{N} p(y^{(i)} \mid \mathbf{x}^{(i)}, \mathbf{w}) = p(\mathbf{y} \mid \mathbf{X}, \mathbf{w}) = \mathscr{L}(\mathbf{w})$$

$$\mathscr{T} = \{(\mathbf{x}^{(1)}, y^{(1)}), (\mathbf{x}^{(2)}, y^{(2)}), \cdots, (\mathbf{x}^{(N)}, y^{(N)})\}$$

Design matrix: $\mathbf{X} = \begin{pmatrix} x_1^{(1)}, x_2^{(1)}, & \cdots, & x_d^{(1)} \\ x_1^{(2)}, x_2^{(2)}, & \cdots, & x_d^{(2)} \\ \vdots \quad \vdots & \ddots & \vdots \\ x_1^{(N)}, x_2^{(N)}, & \cdots, & x_d^{(N)} \end{pmatrix}$

Vector of outputs: $\mathbf{y} = \begin{pmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(N)} \end{pmatrix}$

Maximum Likelihood Estimation

$$\prod_{i=1}^{N} p_{y^{(i)}} = \prod_{i=1}^{N} p(y^{(i)} \mid \mathbf{x}^{(i)}, \mathbf{w}) = p(\mathbf{y} \mid \mathbf{X}, \mathbf{w}) = \mathscr{L}(\mathbf{w})$$

$$\mathscr{T} = \{(\mathbf{x}^{(1)}, y^{(1)}), (\mathbf{x}^{(2)}, y^{(2)}), \cdots, (\mathbf{x}^{(N)}, y^{(N)})\}$$

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Vector of outputs: $\mathbf{y} = \begin{pmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(N)} \end{pmatrix}$

Problem: find $\mathbf{w}$ that maximises the likelihood: $\underset{\mathbf{w}}{\operatorname{argmax}} \, \mathscr{L}(\mathbf{w})$

Log-Likelihood

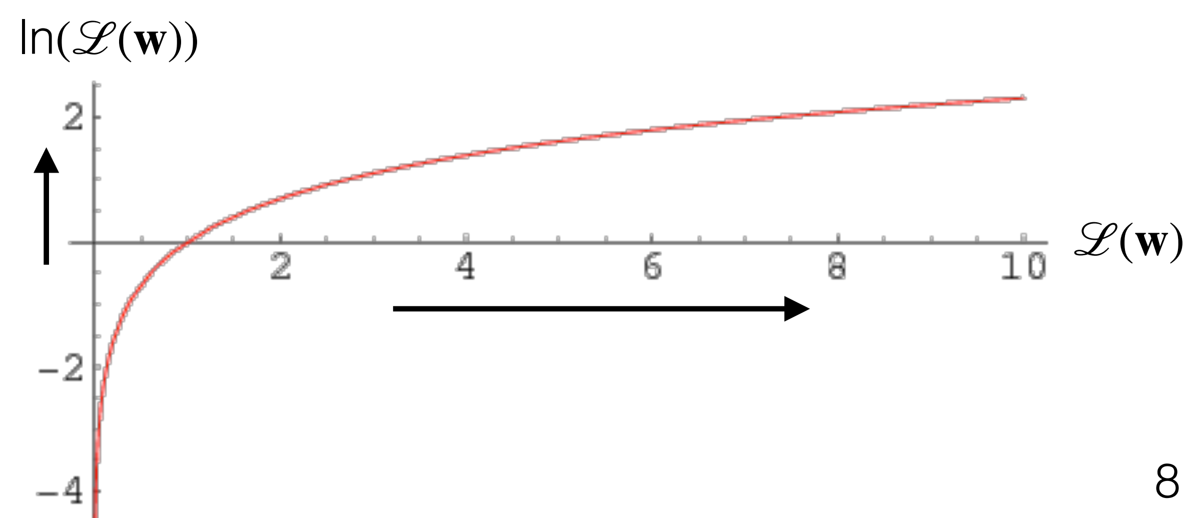
Problem: find $\mathbf{w}$ that maximises the likelihood, $\underset{\mathbf{w}}{\operatorname{argmax}}\, \mathscr{L}(\mathbf{w})$

The products in $\mathscr{L}(\mathbf{w}) = \prod_{i=1}^{N} p_{y^{(i)}}$ can be numerically unstable.

Equivalent to: find $\mathbf{w}$ that maximises the log-likelihood, $\underset{\mathbf{w}}{\operatorname{argmax}}\, \ln(\mathscr{L}(\mathbf{w}))$

$$\ln(\mathscr{L}(\mathbf{w})) = \ln \prod_{i=1}^{N} p_{y^{(i)}} = \sum_{i=1}^{N} \ln\, p_{y^{(i)}}$$

Product rule



Loss Function

Problem: find $\mathbf{w}$ that maximises the log-likelihood, $\underset{\mathbf{w}}{\operatorname{argmax}} \ln(\mathscr{L}(\mathbf{w}))$

$$\ln(\mathscr{L}(\mathbf{w})) = \sum_{i=1}^{N} \ln p_{y^{(i)}}$$

Equivalent to: find $\mathbf{w}$ that minimises the loss, $\underset{\mathbf{w}}{\operatorname{argmin}} E(\mathbf{w})$

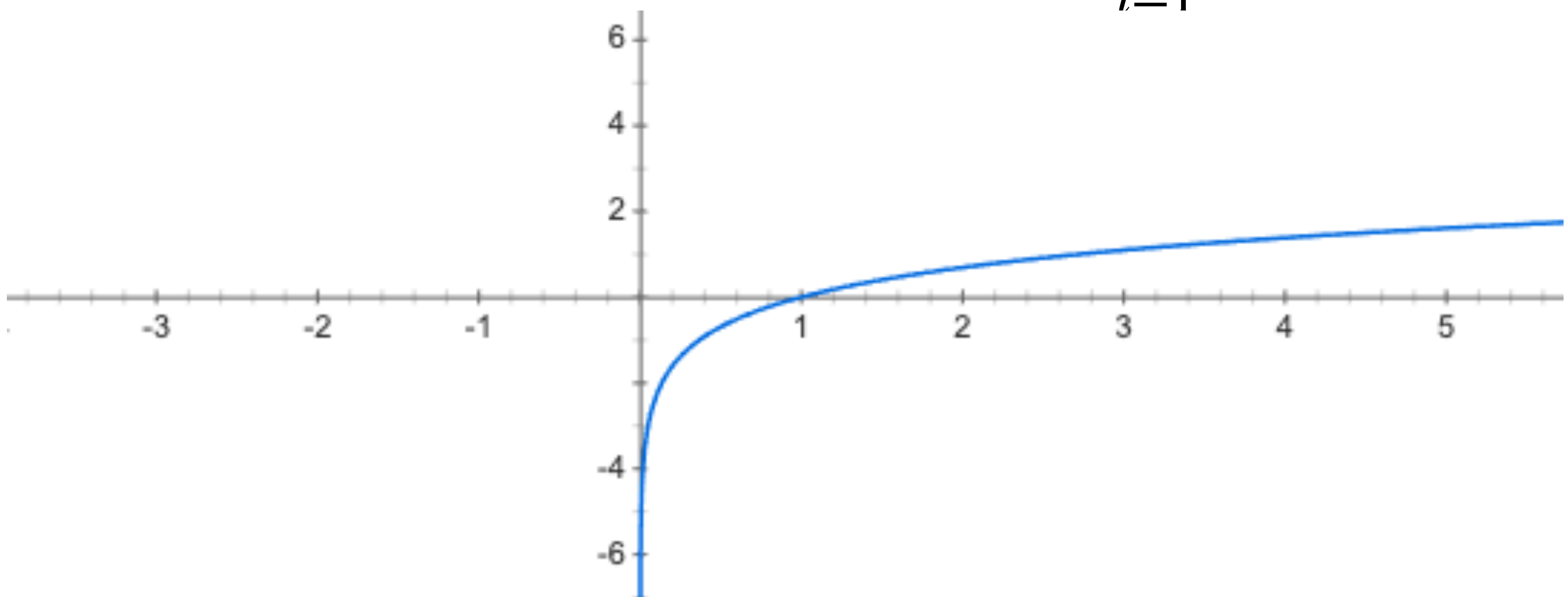
$$E(\mathbf{w}) = -\ln(\mathscr{L}(\mathbf{w})) = -\sum_{i=1}^{N} \ln p_{y^{(i)}}$$

Understanding the Loss

Learning $\mathbf{w}$ can be achieved by finding the $\mathbf{w}$ that minimises $E(\mathbf{w})$, calculated based on the training set.

$$\underset{\mathbf{w}}{\operatorname{argmin}}\, E(\mathbf{w})$$

$$E(\mathbf{w}) = -\ln(\mathscr{L}(\mathbf{w})) = -\sum_{i=1}^{N} \ln p_{y^{(i)}}$$



Understanding the Loss

Learning $\mathbf{w}$ can be achieved by finding the $\mathbf{w}$ that minimises $E(\mathbf{w})$, calculated based on the training set.

$$\underset{\mathbf{w}}{\operatorname{argmin}}\, E(\mathbf{w})$$

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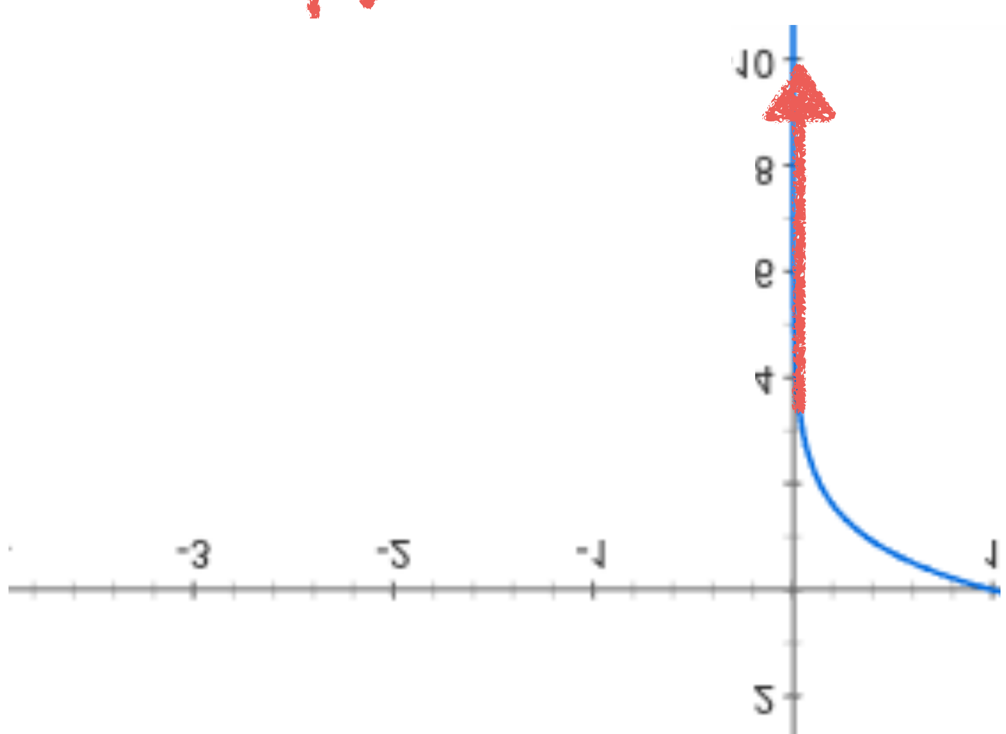


Assume $(\mathbf{x}^{(i)}, y^{(i)} = 1)$

$$p_1 = 0.99 \rightarrow -0.01 \rightarrow +0.01$$

$$p_1 = 0.5 \rightarrow -0.69 \rightarrow +0.69$$

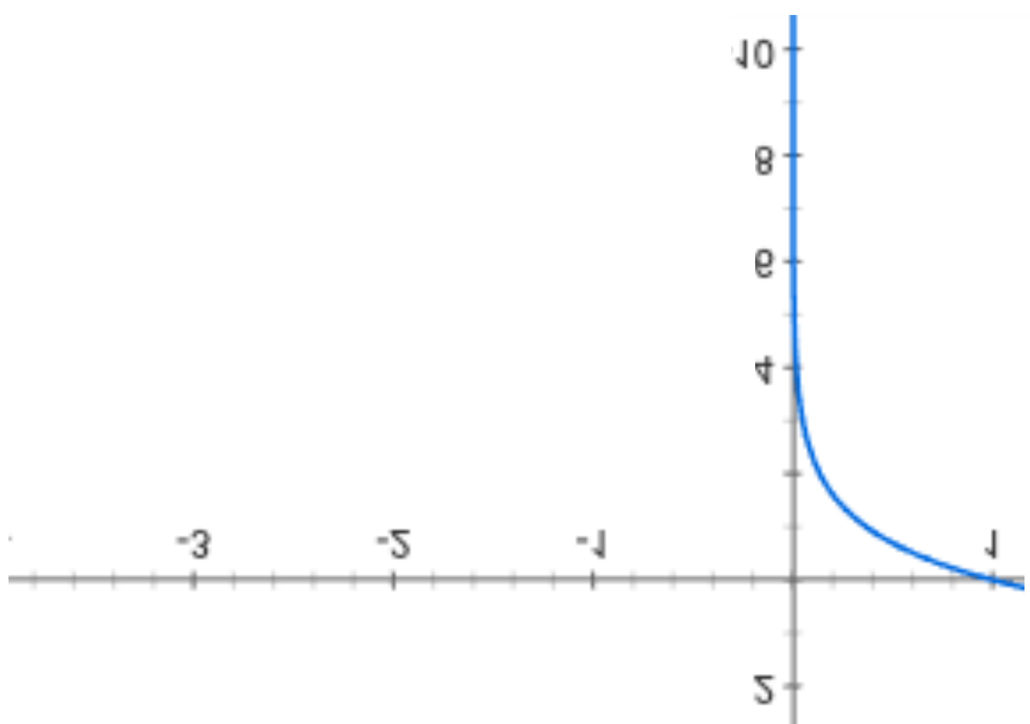
$$p_1 = 0.01 \rightarrow -4.6 \rightarrow +4.6$$

Understanding the Loss

Learning $\mathbf{w}$ can be achieved by finding the $\mathbf{w}$ that minimises $E(\mathbf{w})$, calculated based on the training set.

$$\underset{\mathbf{w}}{\operatorname{argmin}}\, E(\mathbf{w})$$

$$E(\mathbf{w}) = -\ln(\mathscr{L}(\mathbf{w})) = -\sum_{i=1}^{N} \ln p_{y^{(i)}}$$



For examples of class 1, we sum $-\ln p_1$.

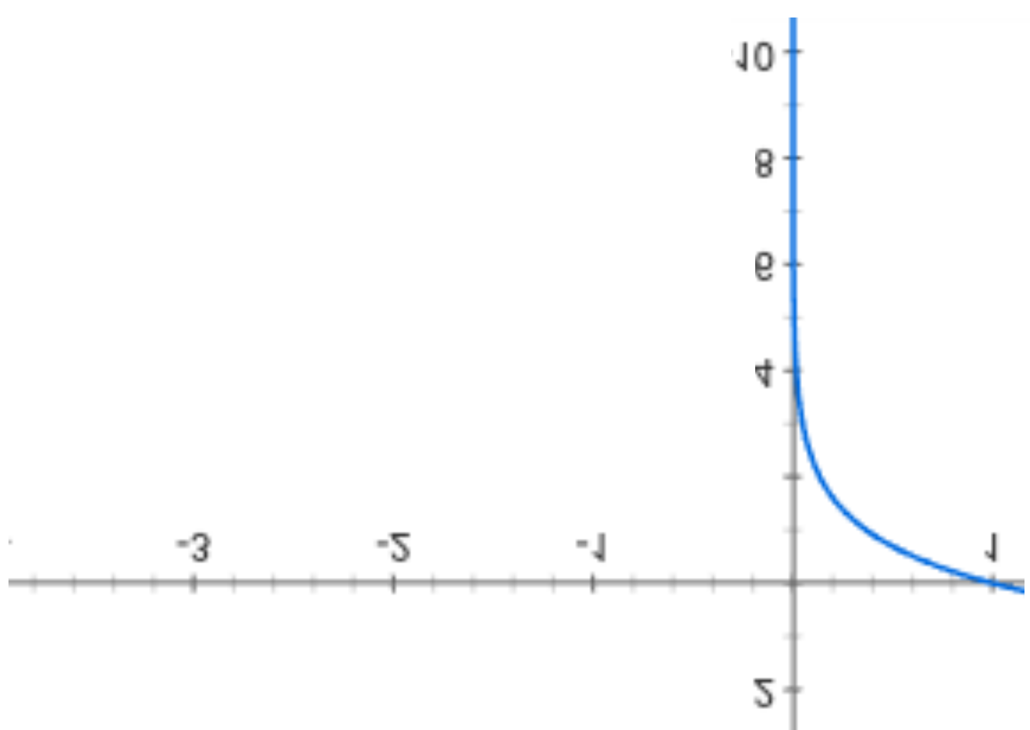
The closer p_1 is to 1, the smaller the value that we sum to $E(\mathbf{w})$, and so the loss is smaller.

Understanding the Loss

Learning $\mathbf{w}$ can be achieved by finding the $\mathbf{w}$ that minimises $E(\mathbf{w})$, calculated based on the training set.

$$\underset{\mathbf{w}}{\operatorname{argmin}}\, E(\mathbf{w})$$

$$E(\mathbf{w}) = -\ln(\mathscr{L}(\mathbf{w})) = -\sum_{i=1}^{N} \ln p_{y^{(i)}}$$



For examples of class 1, we sum $-\ln\, p_1$.

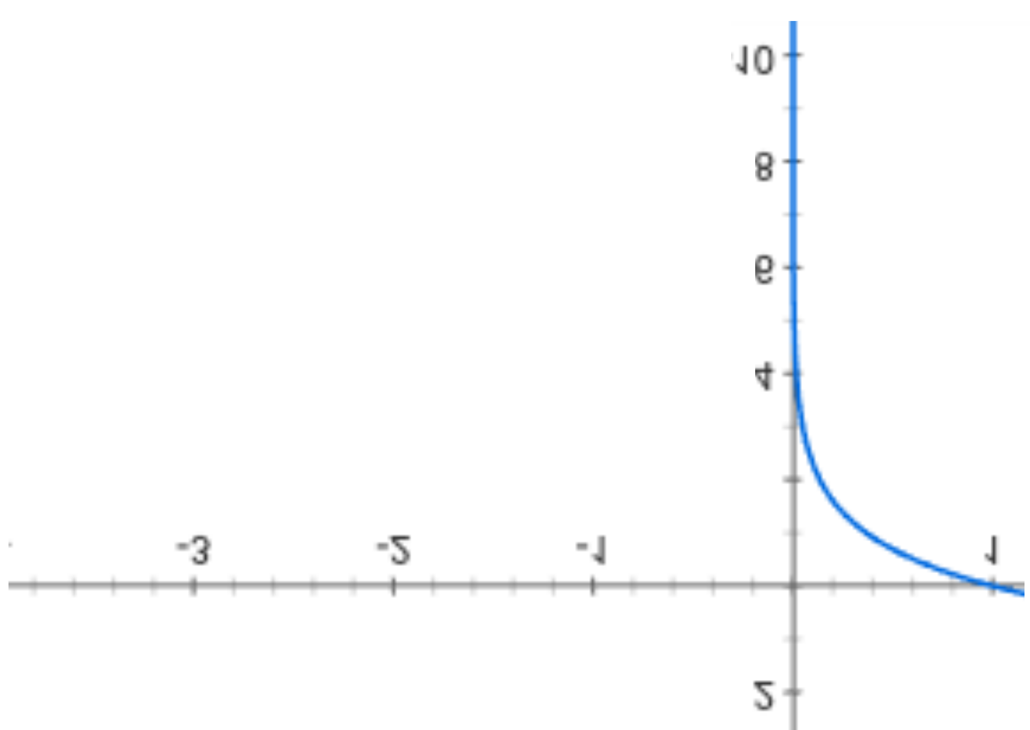
The closer p_1 is to 0, the larger the value that we sum to $E(\mathbf{w})$, and we strongly penalise being too close to 0.

Understanding the Loss

Learning $\mathbf{w}$ can be achieved by finding the $\mathbf{w}$ that minimises $E(\mathbf{w})$, calculated based on the training set.

$$\underset{\mathbf{w}}{\operatorname{argmin}}\, E(\mathbf{w})$$

$$E(\mathbf{w}) = -\ln(\mathscr{L}(\mathbf{w})) = -\sum_{i=1}^{N} \ln p_{y^{(i)}}$$



A similar idea holds for examples of class 1, based on p_0.

Cross Entropy Loss

$$E(\mathbf{w}) = -\ln(\mathscr{L}(\mathbf{w})) = -\sum_{i=1}^{N} \ln p_{y^{(i)}}$$

equivalent to:

$$E(\mathbf{w}) = -\sum_{i=1}^{N} y^{(i)} \ln p(1 \mid \mathbf{x}^{(i)}, \mathbf{w}) + (1 - y^{(i)}) \ln (1 - p(1 \mid \mathbf{x}^{(i)}, \mathbf{w}))$$

Cross-entropy is a measure of dissimilarity between two probability distributions.

Here, it is used to measure the dissimilarity between the true (target) distribution $P(y \mid \mathbf{x})$ and learned distribution $p(y \mid \mathbf{x}, \mathbf{w})$, estimated based on the training examples.

Summary So Far

$$\text{logit}(p_1) = \mathbf{w}^T\mathbf{x} \quad \begin{cases} \mathbf{w}^T\mathbf{x} \geq 0 \rightarrow \text{class } 1 \\ \mathbf{w}^T\mathbf{x} < 0 \rightarrow \text{class } 0 \end{cases}$$

$$g(\mathbf{x}) = p_1 = p(1 \mid \mathbf{x}, \mathbf{w}) \quad \begin{cases} p_1 \geq 0.5 \rightarrow \text{class } 1 \\ p_1 < 0.5 \rightarrow \text{class } 0 \end{cases}$$

Optimisation problem: $\underset{\mathbf{w}}{\text{argmin}}\, E(\mathbf{w})$

$$E(\mathbf{w}) = -\sum_{i=1}^{N} y^{(i)} \ln p(1 \mid \mathbf{x}^{(i)}, \mathbf{w}) + (1 - y^{(i)}) \ln (1 - p(1 \mid \mathbf{x}^{(i)}, \mathbf{w}))$$

How to solve this optimisation problem?

Outline

- Logistic regression optimisation problem
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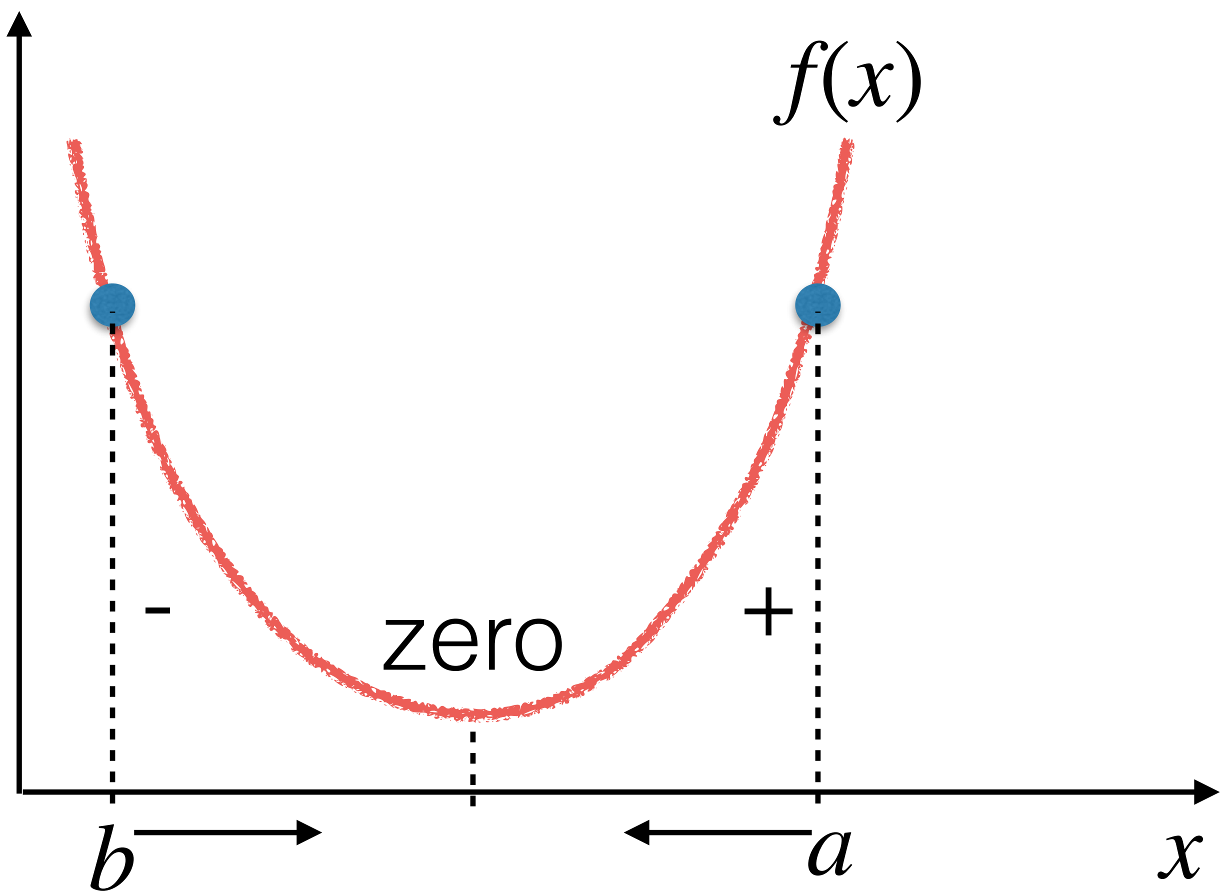
- Solving the logistic regression optimisation problem
  - Gradient descent.

General Idea of Gradient Descent

Gradient descent adjusts $\mathbf{w}$ iteratively in the direction that leads to the biggest decrease (steepest descent) in $E(\mathbf{w})$.

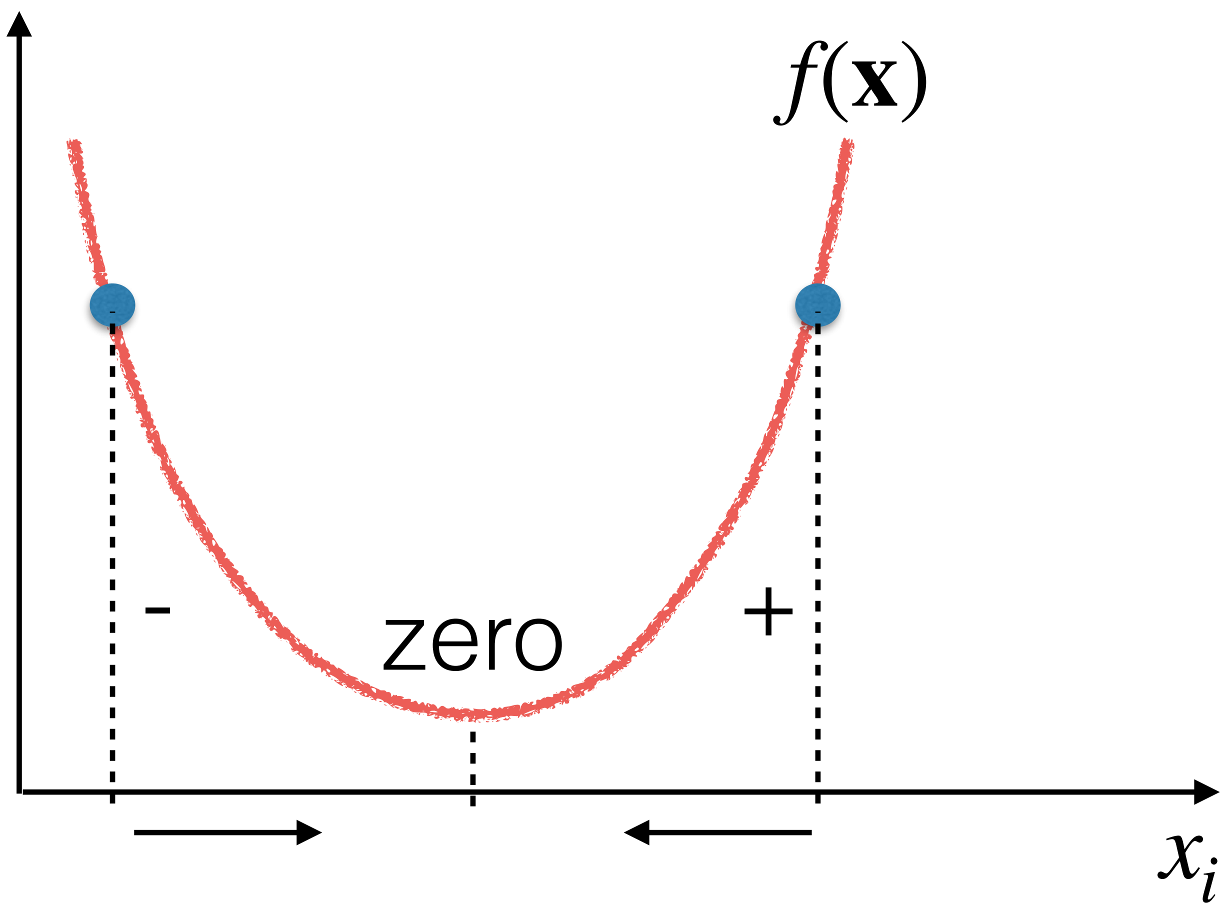
Some Relevant Properties of Derivatives



$$x = x - \eta \frac{df}{dx}$$ where $\eta > 0$

This can be used to search for the minimum of a function!

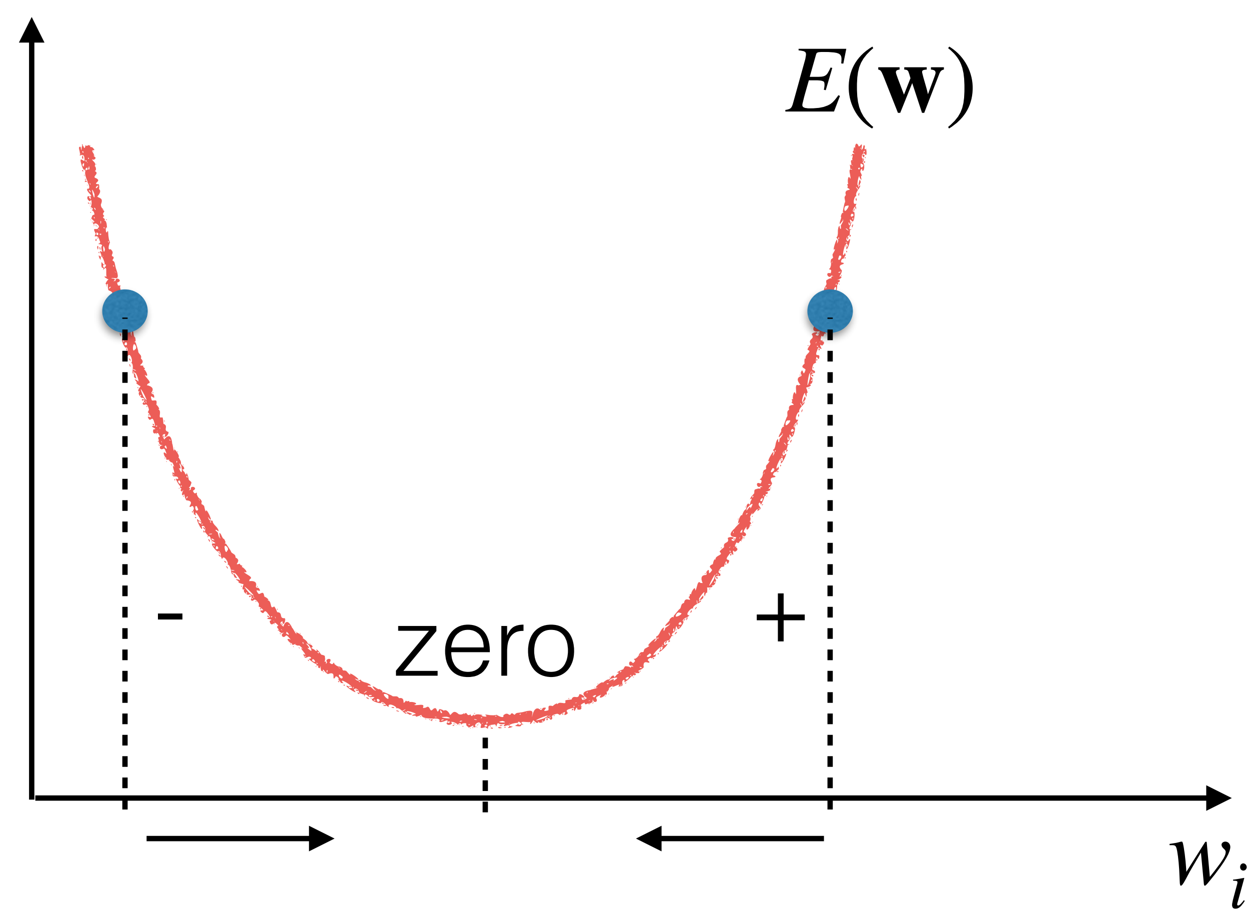
Some Relevant Properties of (Partial) Derivatives



This can be used to search for the minimum of a function!

$$x_i = x_i - \eta \frac{\partial f}{\partial x_i} \quad \text{where } \eta > 0$$

Some Relevant Properties of (Partial) Derivatives



$$w_i = w_i - \eta \frac{\partial E}{\partial w_i} \text{ where } \eta > 0$$

This can be used to search for the weights $\mathbf{w}$ that minimise our cross-entropy loss $E(\mathbf{w})$!

Note: The function drawn here is just for illustration purposes. The cross-entropy for logistic regression is not a quadratic function.

Adjusting $\mathbf{w}$ In The Direction that Reduces $E(\mathbf{w})$

$$w_0 = w_0 - \eta \frac{\partial E}{\partial w_0} \qquad w_1 = w_1 - \eta \frac{\partial E}{\partial w_1} \qquad \cdots \qquad w_d = w_d - \eta \frac{\partial E}{\partial w_d}$$

$$\begin{pmatrix} w_0 \\ w_1 \\ \vdots \\ w_d \end{pmatrix} = \begin{pmatrix} w_0 \\ w_1 \\ \vdots \\ w_d \end{pmatrix} - \eta \begin{pmatrix} \frac{\partial E}{\partial w_0} \\ \frac{\partial E}{\partial w_1} \\ \vdots \\ \frac{\partial E}{\partial w_d} \end{pmatrix}$$

$$\mathbf{w} = \mathbf{w} - \eta \nabla E(\mathbf{w})$$ "gradient"

Gradient Descent (Batch Version)

Initialise $\mathbf{w}$ with zeroes or random values near zero.

Repeat for a given number of iterations or until $\nabla E(\mathbf{w})$ is a vector of zeroes:

$$\mathbf{w} = \mathbf{w} - \eta \nabla E(\mathbf{w})$$ where $\eta > 0$ is the learning rate.

Applying Gradient Descent (Batch Version) To Logistic Regression

Initialise $\mathbf{w}$ with zeroes or random values near zero.

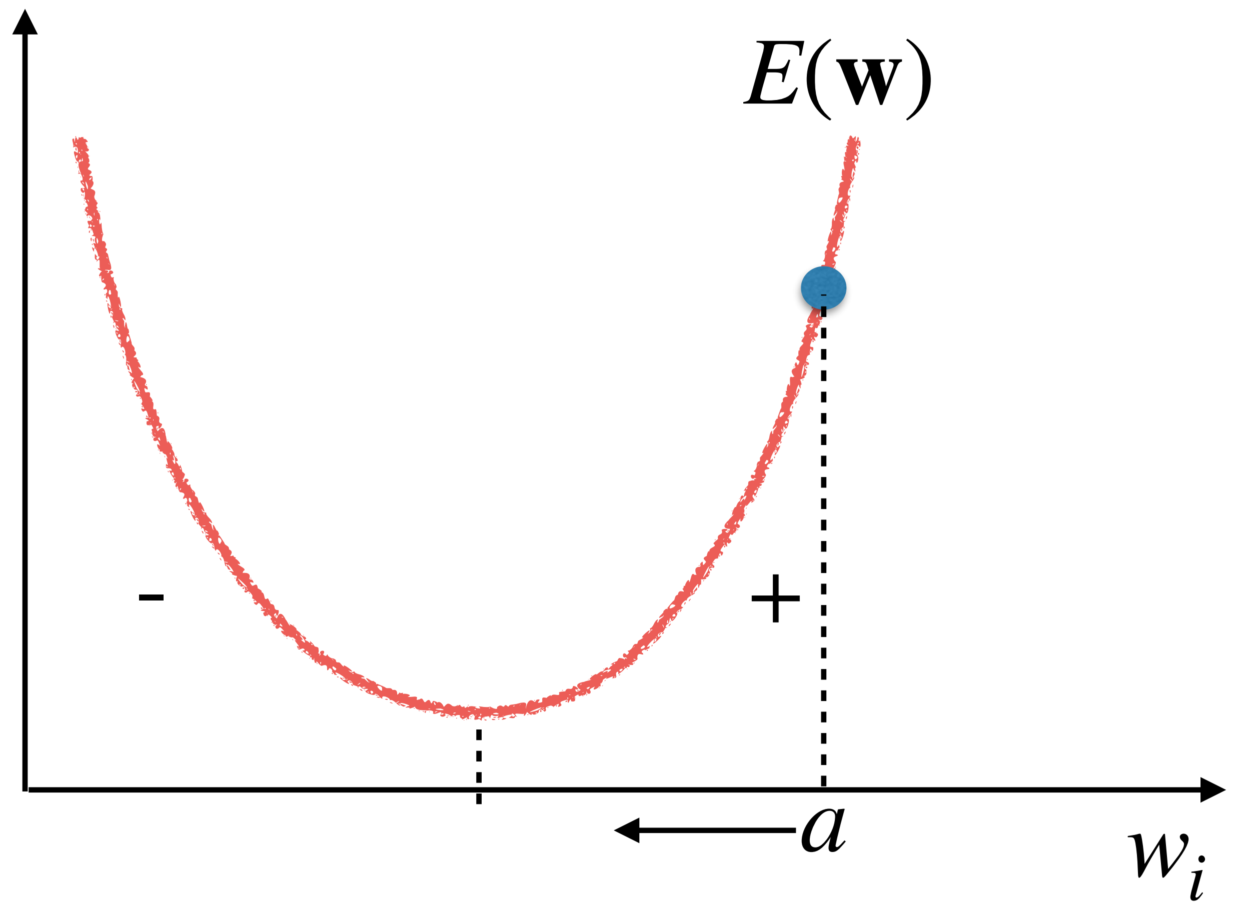
Repeat for a given number of iterations or until $\nabla E(\mathbf{w})$ is a vector of zeroes:

$$\mathbf{w} = \mathbf{w} - \eta \nabla E(\mathbf{w})$$ where $\eta > 0$ is the learning rate.

$$E(\mathbf{w}) = -\sum_{i=1}^{N} y^{(i)} \ln p(1 \mid \mathbf{x}^{(i)}, \mathbf{w}) + (1 - y^{(i)}) \ln (1 - p(1 \mid \mathbf{x}^{(i)}, \mathbf{w}))$$

$$\nabla E(\mathbf{w}) = \sum_{i=1}^{N} (p(1 \mid \mathbf{x}^{(i)}, \mathbf{w}) - y^{(i)})\ \mathbf{x}^{(i)}$$

Steepest Descent



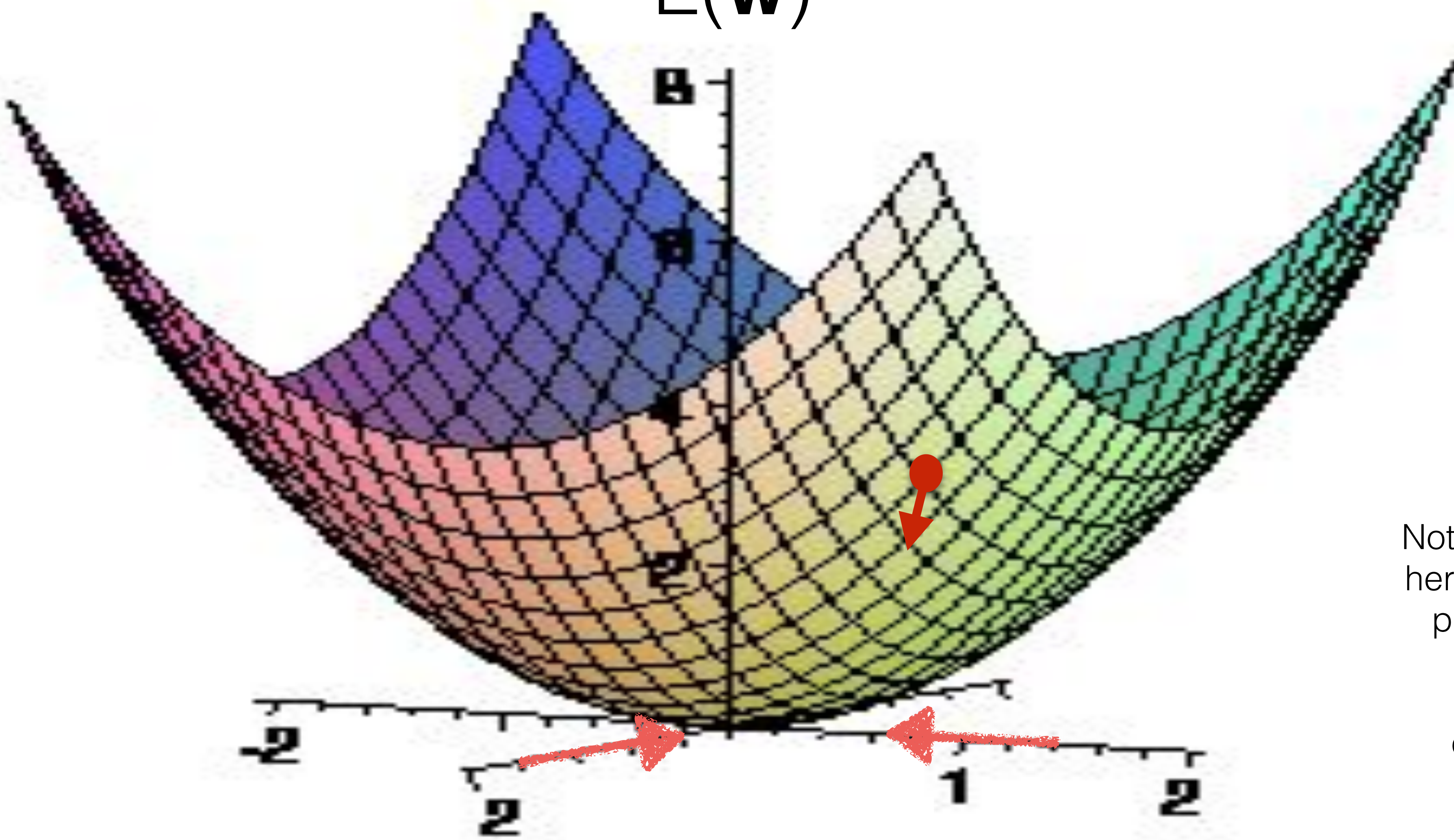
Note: The function drawn here is just for illustration purposes. The cross-entropy for logistic regression is not a quadratic function.

$$\mathbf{w} = \mathbf{w} - \eta \nabla E(\mathbf{w})$$

Changes coefficients $\mathbf{w}$ in the direction of the **steepest** descent, i.e., the direction that causes the largest reduction in $E(\mathbf{w})$.

Steepest Descent

E($\mathbf{w}$)

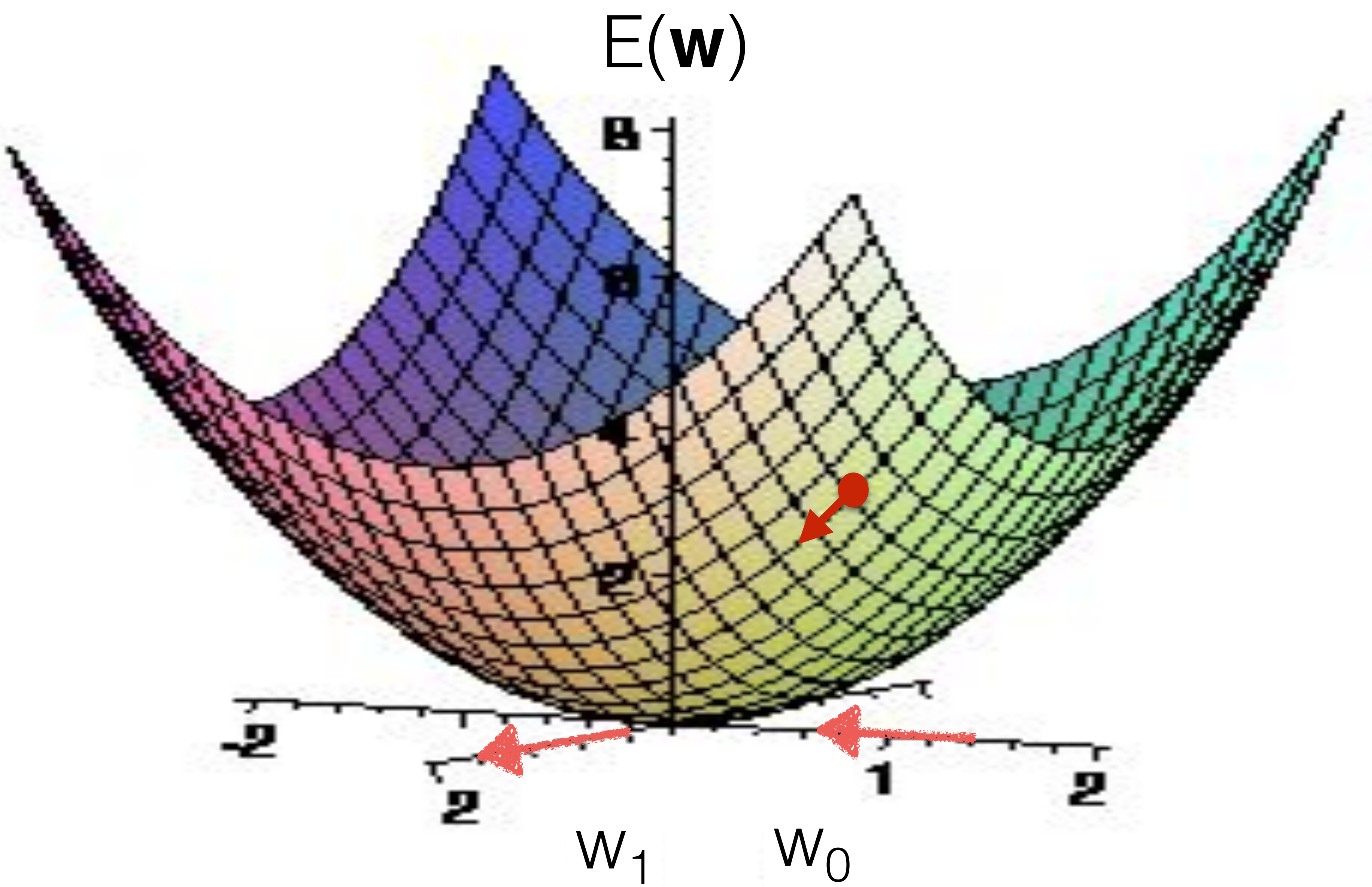


w_1 w_0

Note: The function drawn here is just for illustration purposes. The cross-entropy for logistic regression is not a quadratic function.

Changes coefficients $\mathbf{w}$ in the direction of the **steepest** descent, i.e., the direction that causes the largest reduction in $E(\mathbf{w})$.

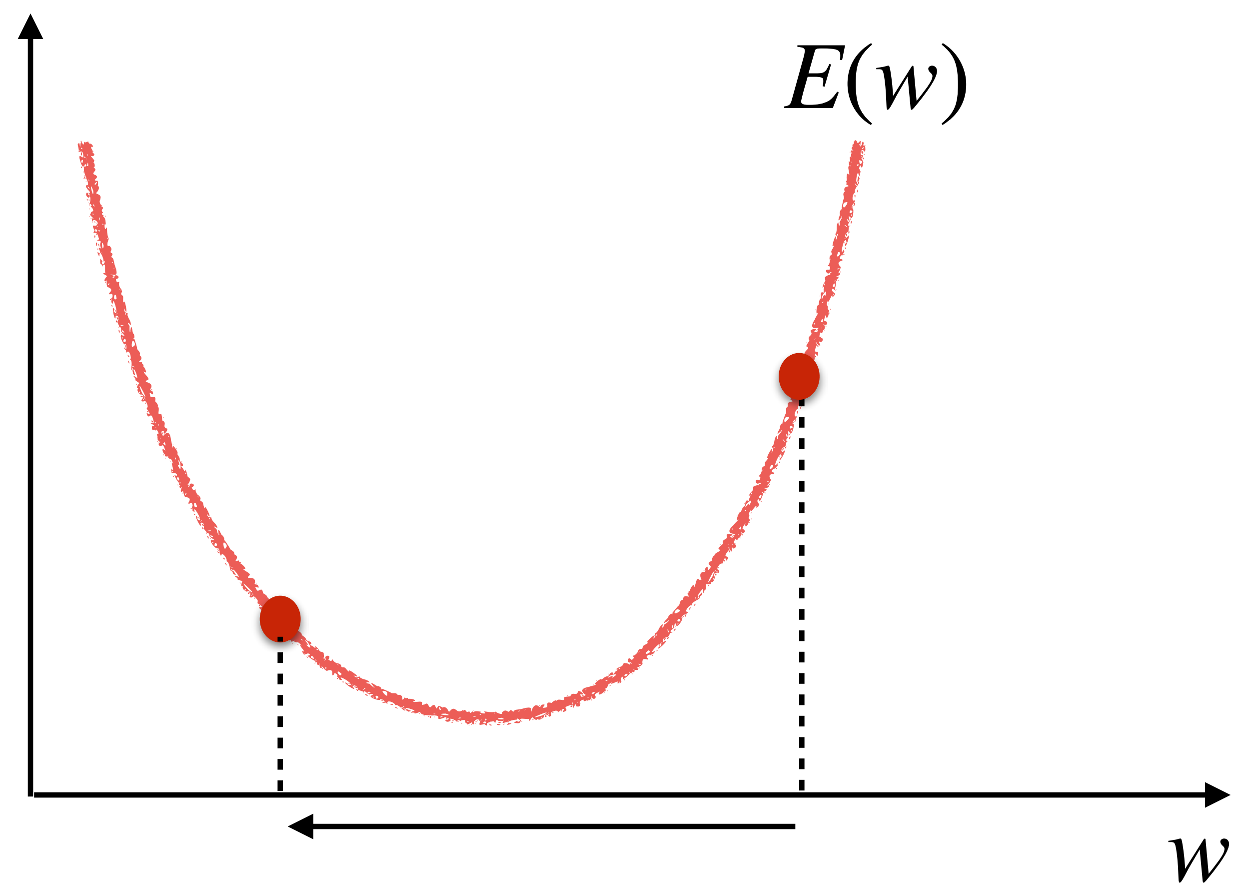
Steepest Descent



Changes coefficients $\mathbf{w}$ in the direction of the **steepest** descent, i.e., the direction that causes the largest reduction in $E(\mathbf{w})$.

The Effect of the Hyperparameter η

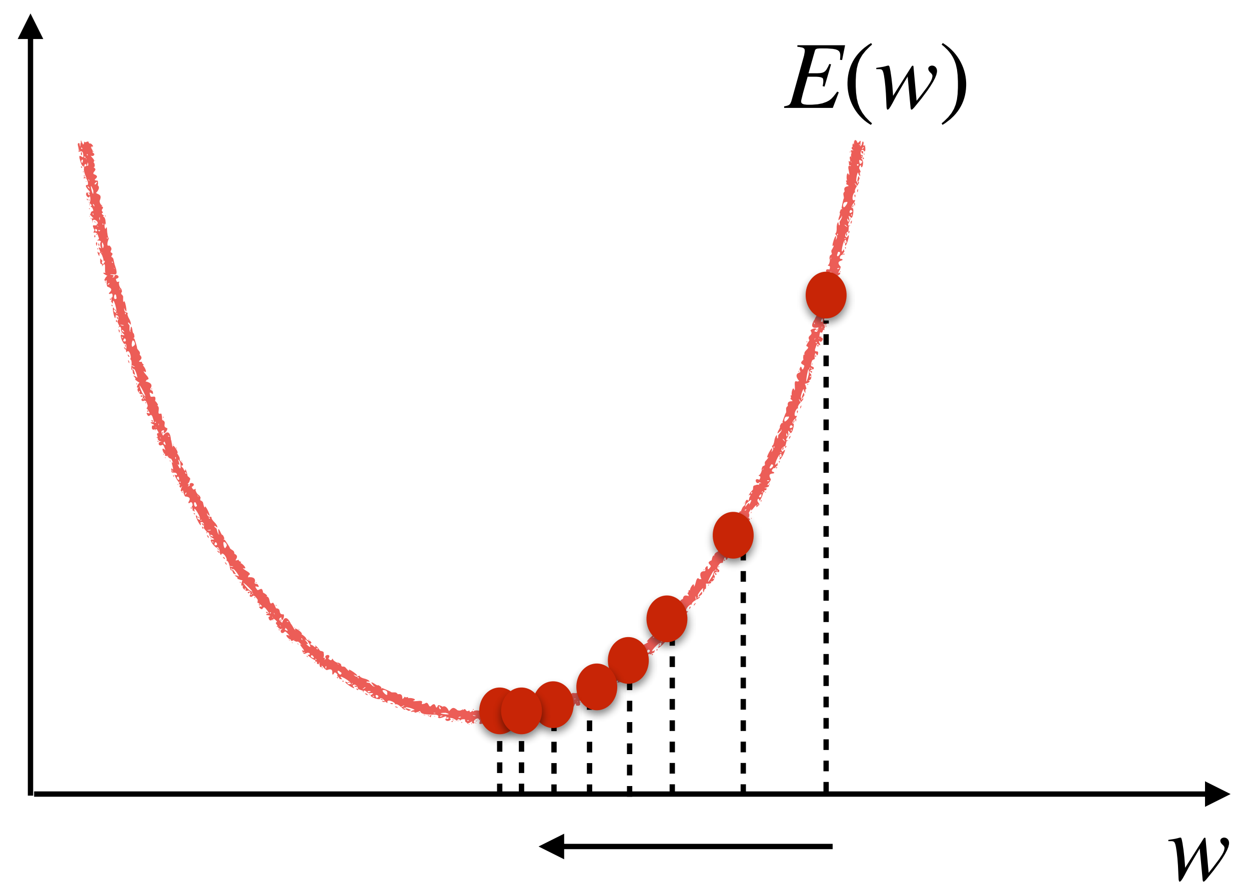
$$\mathbf{w} = \mathbf{w} - \eta \nabla E$$



Too large values of η may result in jumping across the optimum, lacking stability.

The Effect of η

$$\mathbf{w} = \mathbf{w} - \eta \nabla E$$

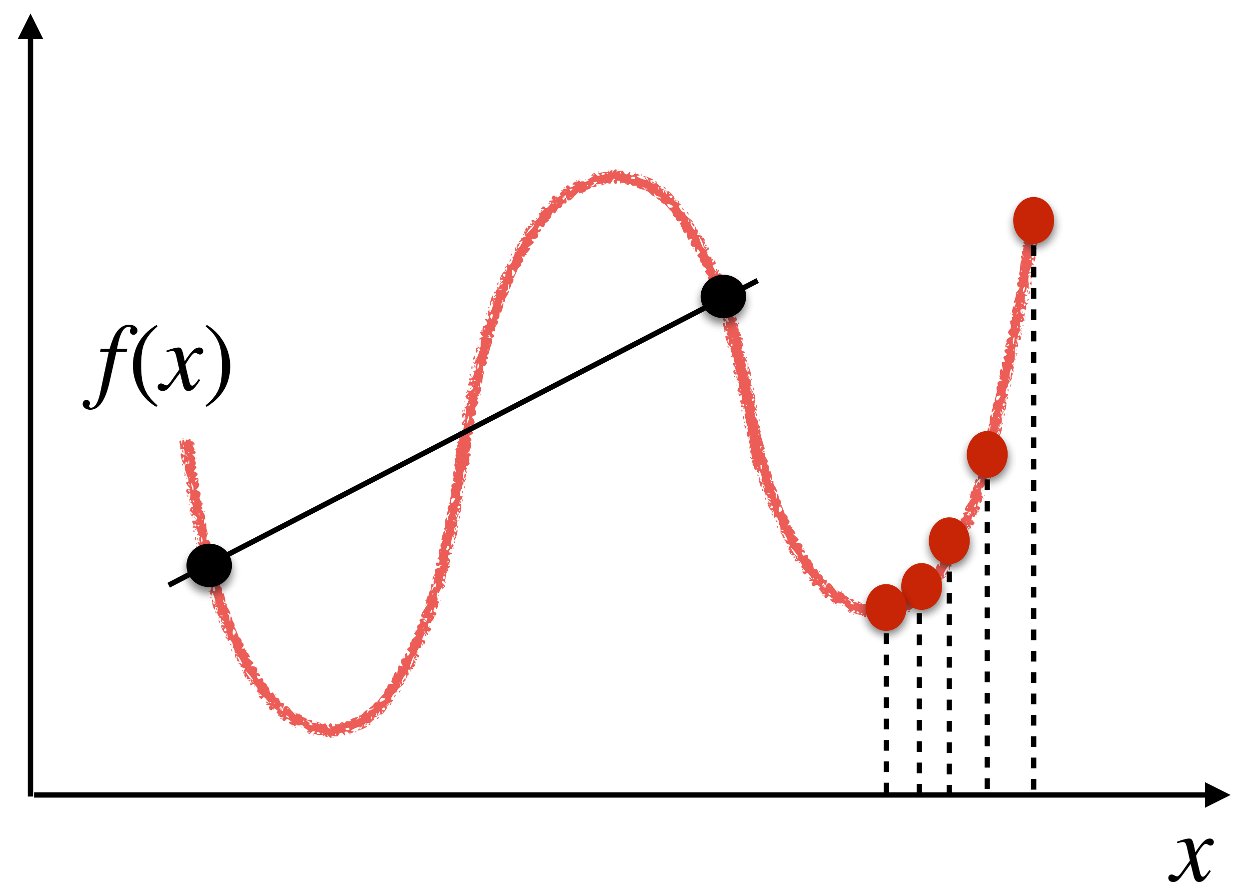


Too small values of η may result in longer time to converge to the optimum.

A Note on Local Minima

Gradient descent is a general purpose optimisation algorithm.

But is likely to get stuck in local minima.



For logistic regression using cross-entropy loss, this is not a problem, as its $E(\mathbf{w})$ is strictly convex with respect to $\mathbf{w}$, having a single unique minimum.

Summary

- We can use maximum likelihood estimation to formulate the optimisation problem to be solved for learning a logistic regression model.
- Maximum likelihood estimation is about finding the parameters (coefficients $\mathbf{w}$) that maximise the likelihood of the observed training examples.
- Finding the coefficients $\mathbf{w}$ that maximise the likelihood is equivalent to finding the coefficients $\mathbf{w}$ that minimise the cross-entropy loss.
- We can use Gradient Descent to find good values for $\mathbf{w}$.
- Gradient descent iteratively updates the coefficients $\mathbf{w}$ in the direction of the the steepest descent of $E(\mathbf{w})$, which is the opposite direction of the gradient.
- Next: is Gradient Descent the best optimisation algorithm for us to use?