Topic 2: Logistic Regression

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2.1 Introduction

Arguably the simplest task that we can teach a computer is to distinguish between two classes. For example:

1. Does this image contain a dog or a cat?
2. Is this person healthy or diabetic?
3. Would this individual survive a disaster?

Logistic regression is one of the most elemental yet powerful techniques for this purpose. The main idea is to compute the *likelihood* that a sample (e.g., a person) belongs to each class, based on its information and the information of previous (training) samples, and then choose the most likely class.

2.2 Setup

Suppose you want to determine whether your girlfriend/boyfriend is cheating on you, based on certain information (features) about her/him, like age, gender, height, weight, etc. Let $\mathbf{x}_i \in \mathbb{R}^d$ denote the vector containing this information, which looks like this:

$$\mathbf{x}_i = \begin{bmatrix} age \\ gender \\ height \\ weight \\ \vdots \end{bmatrix}.$$

Here d denotes the number of features. Similarly, let y be the random variable indicating whether s/he is not cheating on you: $y = 1$ means s/he is, $y = 0$ means s/he isn't. Hence we can rephrase our goal as determining whether $y = 0$ or $y = 1$ based on $\mathbf{x}$. Mathematically, we want to find a function f such that

$$y \;=\; f(\mathbf{x}).$$

Perhaps the most natural way to achieve this is to let f be of the form:

$$f(\mathbf{x}) \;=\; \begin{cases} 0 & \text{if } \mathbb{P}(y=0|\mathbf{x}) > \mathbb{P}(y=1|\mathbf{x}) \\ 1 & \text{otherwise.} \end{cases} \tag{2.1}$$

In words, (2.1) is simply saying: decide $y = 0$ if the probability of y being 0 (based on $\mathbf{x}$) is larger than the probability of y being 1, and decide $y = 1$ otherwise. We can rewrite this as follows:

$$\mathbb{P}(y = 1|\mathbf{x}) \underset{f(\mathbf{x})=0}{\overset{f(\mathbf{x})=1}{\gtrless}} \mathbb{P}(y = 0|\mathbf{x}),$$

or equivalently, as:

$$\frac{\mathbb{P}(y = 1|\mathbf{x})}{\mathbb{P}(y = 0|\mathbf{x})} \underset{f(\mathbf{x})=0}{\overset{f(\mathbf{x})=1}{\gtrless}} 1.$$

The term on the left is often known as the *odds*. If we know the odds, we know whether $\mathbb{P}(y = 1|\mathbf{x})$ or $\mathbb{P}(y = 0|\mathbf{x})$ is more likely, and we can decide accordingly. Hence, our goal is to determining what are the odds, based on $\mathbf{x}$. Arguably, the simplest, most natural approach is to model the odds as a linear combination of the entries in $\mathbf{x}$, i.e.,

$$\frac{\mathbb{P}(y = 1|\mathbf{x})}{\mathbb{P}(y = 0|\mathbf{x})} \;=\; \boldsymbol{\beta}^{\mathsf{T}}\mathbf{x}, \tag{2.2}$$

where $\boldsymbol{\beta} \in \mathbb{R}^{\mathrm{d}}$ contains the *coefficients* of the linear combination of $\mathbf{x}$. Notice that $\boldsymbol{\beta}^{\mathsf{T}}$ is just the compact (grown up) way to write $\beta_1\mathrm{x}_1 + \beta_2\mathrm{x}_2 + \cdots + \beta_{\mathrm{d}}\mathrm{x}_{\mathrm{d}}$. The problem with (2.2) is that $\frac{\mathbb{P}(y=1|\mathbf{x})}{\mathbb{P}(y=0|\mathbf{x})} \geq 0$, while $\boldsymbol{\beta}^{\mathsf{T}}\mathbf{x} \in \mathbb{R}$. To avoid this discrepancy, rather than (2.2), logistic regression simply applies a log function on the odds, to obtain:

$$\log\left(\frac{\mathbb{P}(y = 1|\mathbf{x})}{\mathbb{P}(y = 0|\mathbf{x})}\right) \;=\; \boldsymbol{\beta}^{\mathsf{T}}\mathbf{x}. \tag{2.3}$$

The term on the left is often known as *log-odds*. It is from this idea that logistic regression obtains its name. Notice that in (2.3), both the log-odds and $\boldsymbol{\beta}^{\mathsf{T}}\mathbf{x}$ are real numbers, so there is no longer any discrepancy. Letting $\mathrm{p} := \mathbb{P}(y = 1|\mathbf{x})$ we can rewrite (2.3) as

$$\frac{\mathrm{p}}{1-\mathrm{p}} \;=\; e^{\boldsymbol{\beta}^{\mathsf{T}}\mathbf{x}},$$

and solving for p we have:

$$\begin{aligned}
\mathrm{p} &= (1-\mathrm{p})e^{\boldsymbol{\beta}^{\mathsf{T}}\mathbf{x}} \\
\mathrm{p} &= e^{\boldsymbol{\beta}^{\mathsf{T}}\mathbf{x}} - \mathrm{p}(e^{\boldsymbol{\beta}^{\mathsf{T}}\mathbf{x}}) \\
\mathrm{p}(1+e^{\boldsymbol{\beta}^{\mathsf{T}}\mathbf{x}}) &= e^{\boldsymbol{\beta}^{\mathsf{T}}\mathbf{x}} \\
\mathrm{p} &= \frac{e^{\boldsymbol{\beta}^{\mathsf{T}}\mathbf{x}}}{1+e^{\boldsymbol{\beta}^{\mathsf{T}}\mathbf{x}}},
\end{aligned}$$

which we can further simplify to:

$$\mathrm{p} \;=\; \frac{\frac{e^{\boldsymbol{\beta}^{\mathsf{T}}\mathbf{x}}}{e^{\boldsymbol{\beta}^{\mathsf{T}}\mathbf{x}}}}{\frac{1+e^{\boldsymbol{\beta}^{\mathsf{T}}\mathbf{x}}}{e^{\boldsymbol{\beta}^{\mathsf{T}}\mathbf{x}}}} \;=\; \frac{1}{\frac{1}{e^{\boldsymbol{\beta}^{\mathsf{T}}\mathbf{x}}} + \frac{e^{\boldsymbol{\beta}^{\mathsf{T}}\mathbf{x}}}{e^{\boldsymbol{\beta}^{\mathsf{T}}\mathbf{x}}}} \;=\; \frac{1}{\frac{1}{e^{\boldsymbol{\beta}^{\mathsf{T}}\mathbf{x}}} + 1} \;=\; \frac{1}{1+e^{-\boldsymbol{\beta}^{\mathsf{T}}\mathbf{x}}}.$$

To summarize, logistic regression is modeling $\mathbb{P}(y = 1|\mathbf{x})$ as $\frac{1}{1+e^{-\boldsymbol{\beta}^{\mathsf{T}}\mathbf{x}}}$. Hence, we can rewrite our decision function as:

$$\frac{1}{1+e^{-\boldsymbol{\beta}^{\mathsf{T}}\mathbf{x}}} \underset{f(\mathbf{x})=0}{\overset{f(\mathbf{x})=1}{\gtrless}} 1-\frac{1}{1+e^{-\boldsymbol{\beta}^{\mathsf{T}}\mathbf{x}}}, \tag{2.4}$$

which intuitively says: if $\mathbb{P}(y=1|\mathbf{x})$ is larger than $\mathbb{P}(y=0|\mathbf{x})$ (or equivalently, larger than $1/2$), then we conclude that $y=1$, and otherwise we conclude that $y=0$.

This means that if you want to know whether your girlfriend/boyfriend is cheating on you, all you have to do is plug her/his feature vector $\mathbf{x}$ in (2.4), and decide accordingly. The catch here is that (2.4) depends on $\boldsymbol{\beta}$, which you do not know a priori. So, which $\boldsymbol{\beta}$ should you use? The answer is: you have to infer/learn it.

2.3 Inferring/Learning β

Logistic regression uses (2.4) to decide whether $y=0$ or $y=1$. However, our function f in (2.4) depends on $\boldsymbol{\beta}$, which is unknown a priori. To estimate/learn $\boldsymbol{\beta}$ we use *training* data, meaning a collection of pairs $(\mathbf{x}_1, \mathrm{y}_1), (\mathbf{x}_2, \mathrm{y}_2), \ldots, (\mathbf{x}_\mathrm{n}, \mathrm{y}_\mathrm{n})$ containing features $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_\mathrm{n}$ and their corresponding variables of interest $\mathrm{y}_1, \mathrm{y}_2, \ldots, \mathrm{y}_\mathrm{n}$. In our example, this would mean features about n people and their information about whether they are cheating or not.

In words, our goal is to find the parameter $\boldsymbol{\beta}$ that best explains our training samples. More precisely, we want to find the parameter $\boldsymbol{\beta}$ that maximizes the *likelihood* of our sample. Intuitively, this likelihood is the chance that our observed samples are correctly predicted by f (which depends on $\boldsymbol{\beta}$), i.e., the probability that $\mathrm{y}_\mathrm{i} = f(\mathbf{x}_\mathrm{i})$, for every $\mathrm{i} = 1, \ldots, \mathrm{n}$.

2.4 Likelihood

Recall that a probability distribution $\mathbb{P}(x = \mathrm{x}|\theta)$ determines the probability that a random variable x takes a certain value x, given some parameter θ. For example, if $x \sim \mathit{Bernoulli}(\mathrm{p})$, then the probability that x takes the value 1 is p. In this case p is the parameter θ.

Similarly, the likelihood $\mathbb{L}(\theta|x = \mathrm{x})$ determines the probability that a parameter θ was the one that generated a sample x.

Example 2.1. Suppose we know x is distributed i.i.d. $\mathit{Bernoulli}(\mathrm{p})$, and we observe $\mathrm{x} = 1$. Then the likelihood of parameter p given sample $\mathrm{x} = 1$ is:

$$\mathbb{L}(\mathrm{p}|\mathrm{x}=1) \;=\; \mathbb{P}(x|\mathrm{p})\Big|_{x=1} \;=\; \mathrm{p}.$$

$\mathbb{P}(x|\theta)$ and $\mathbb{L}(\theta|\mathrm{x})$ may *look* the same. The difference is that $\mathbb{P}(x|\theta)$ is a function where x is the variable, and θ is fixed. In contrast, $\mathbb{L}(\theta|\mathrm{x})$ is a function where θ is the variable, and x is fixed. In other words, we use $\mathbb{P}(x|\theta)$ when we have not observed x, but we know θ; we use $\mathbb{L}(\theta|\mathrm{x})$ when we have already observed x, and we want to know the likelihood that a certain parameter θ that generated it. This is why we use of x (as opposed to x), to denote that data is already observed.

Example 2.2. Suppose $x \sim \mathcal{N}(\mu, 1)$. Then

$$\mathbb{P}(x|\mu) \;=\; \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}(x-\mu)^2}.$$

Notice that with probability, μ is known, and x is the variable. In contrast, with the likelihood, x is known, and μ is the variable:

$$\mathbb{L}(\mu|\mathrm{x}) \;=\; \mathbb{P}(x|\mu)\Big|_{x=\mathrm{x}} \;=\; \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}(\mathrm{x}-\mu)^2}$$

Example 2.3. Suppose $x_1, \ldots, x_6$ are distributed i.i.d. *Bernoulli*(1/4). Then the probability that $\mathrm{x}_1 = \mathrm{x}_2 = \mathrm{x}_3 = 1$, and $\mathrm{x}_4 = \mathrm{x}_5 = \mathrm{x}_6 = 0$ is:

$$\begin{aligned}\mathbb{P}(x_1 = x_2 = x_3 = 1, x_4 = x_5 = x_6 = 0|\mathrm{p}) \;&=\; \prod_{\mathrm{i}=1}^{3} \mathbb{P}(x_\mathrm{i} = 1|\mathrm{p}) \cdot \prod_{\mathrm{i}=4}^{6} \mathbb{P}(x_\mathrm{i} = 0|\mathrm{p}) \\ &=\; \mathrm{p}^3(1-\mathrm{p})^3 \;=\; (1/4)^3\,(3/4)^3.\end{aligned}$$

Instead, suppose that we observe $\mathrm{x}_1 = \mathrm{x}_2 = \mathrm{x}_3 = 1$, and $\mathrm{x}_4 = \mathrm{x}_5 = \mathrm{x}_6 = 0$. Then the likelihood of p under this sample is:

$$\mathbb{L}(\mathrm{p}|\mathrm{x}_1, \ldots, \mathrm{x}_6) \;=\; \prod_{\mathrm{i}=1}^{6} \mathbb{P}(x_\mathrm{i}|\mathrm{p})\Big|_{x_\mathrm{i}=\mathrm{x}_\mathrm{i}} \;=\; \prod_{\mathrm{i}=1}^{3} \mathbb{P}(x_\mathrm{i}|\mathrm{p})\Big|_{x_\mathrm{i}=1} \cdot \prod_{\mathrm{i}=4}^{6} \mathbb{P}(x_\mathrm{i}|\mathrm{p})\Big|_{x_\mathrm{i}=0} \;=\; \mathrm{p}^3(1-\mathrm{p})^3.$$

Based on this sample, which would be your best guess at the value of p? Is this the same value that maximizes $\mathbb{L}(\mathrm{p}|\mathrm{x}_1, \ldots, \mathrm{x}_6)$?

2.5 Maximum Likelihood

Back to logistic regression, we can model our training data $\mathrm{y}_1, \ldots, \mathrm{y}_\mathrm{n}$ as i.i.d. realizations of a *Bernoulli*(p) random variable, where $\mathrm{p} = \frac{1}{1+e^{-\boldsymbol{\beta}^\mathsf{T}\mathbf{x}}}$. A little thought shows that the likelihood of a *Bernoulli*(p) random variable can be written as:

$$\mathbb{L}(\mathrm{p}|\mathrm{y}) \;=\; \mathrm{p}^\mathrm{y}(1-\mathrm{p})^{1-\mathrm{y}}.$$

Make sure you understand why this is true. By independence, the likelihood of our training sample is:

$$\mathbb{L}(\mathrm{p}|\mathrm{y}_1, \ldots, \mathrm{y}_\mathrm{n}) \;=\; \prod_{\mathrm{i}=1}^{\mathrm{n}} \mathbb{L}(\mathrm{p}|\mathrm{y}_\mathrm{i}) \;=\; \prod_{\mathrm{i}=1}^{\mathrm{n}} \mathrm{p}^{\mathrm{y}_\mathrm{i}}(1-\mathrm{p})^{1-\mathrm{y}_\mathrm{i}}.$$

Since p is in turn a function of the unknown parameter $\boldsymbol{\beta}$ and the known data $\mathbf{x}_1, \ldots, \mathbf{x}_\mathrm{n}$, we can rewrite this as

$$\mathbb{L}(\boldsymbol{\beta}|\mathrm{y}_1, \ldots, \mathrm{y}_\mathrm{n}, \mathbf{x}_1, \ldots, \mathbf{x}_\mathrm{n}) \;=\; \prod_{\mathrm{i}=1}^{\mathrm{n}} \left(\frac{1}{1+e^{-\boldsymbol{\beta}^\mathsf{T}\mathbf{x}}}\right)^{\mathrm{y}_\mathrm{i}} \left(1 - \frac{1}{1+e^{-\boldsymbol{\beta}^\mathsf{T}\mathbf{x}}}\right)^{1-\mathrm{y}_\mathrm{i}}. \tag{2.5}$$

To ease our notation we will use $\mathbb{L}(\boldsymbol{\beta}|\mathbf{Y}, \mathbf{X})$ as shorthand for $\mathbb{L}(\boldsymbol{\beta}|\mathrm{y}_1, \ldots, \mathrm{y}_\mathrm{n}, \mathbf{x}_1, \ldots, \mathbf{x}_\mathrm{n})$. Our goal is to find the $\boldsymbol{\beta}$ that maximizes this likelihood. Maximizing products as in (2.5) can be difficult (as you know from the chain rule of derivatives), so to simplify this maximization, we will use a common trick: apply log, so

that products transform into sums, which are easily maximized (because of the linearity of derivatives: the derivative of a sum is the sum of derivatives). We know we can do this because $\mathbb{L}$ is positive (so we can apply log), and log is monotonically increasing, implying that

$$\underset{\boldsymbol{\beta}\in\mathbb{R}^{\mathrm{d}}}{\arg\min}\ \mathbb{L}(\boldsymbol{\beta}|\mathbf{Y},\mathbf{X}) \ = \ \underset{\boldsymbol{\beta}\in\mathbb{R}^{\mathrm{d}}}{\arg\min}\ \log\left[\mathbb{L}(\boldsymbol{\beta}|\mathbf{Y},\mathbf{X})\right].$$

So instead of maximizing the likelihood directly, we can equivalently maximize the so-called log-likelihood:

$$\begin{aligned}
\ell(\boldsymbol{\beta}|\mathbf{Y},\mathbf{X}) \ &:= \ \log\left[\mathbb{L}(\boldsymbol{\beta}|\mathbf{Y},\mathbf{X})\right] && (2.6)\\
&= \ \log\left[\prod_{\mathrm{i}=1}^{\mathrm{n}}\left(\frac{1}{1+e^{-\boldsymbol{\beta}^{\mathsf{T}}\mathbf{x}}}\right)^{\mathrm{y_i}}\left(1-\frac{1}{1+e^{-\boldsymbol{\beta}^{\mathsf{T}}\mathbf{x}}}\right)^{1-\mathrm{y_i}}\right] && (2.7)\\
&= \ \sum_{\mathrm{i}=1}^{\mathrm{n}}\log\left[\left(\frac{1}{1+e^{-\boldsymbol{\beta}^{\mathsf{T}}\mathbf{x}}}\right)^{\mathrm{y_i}}\left(1-\frac{1}{1+e^{-\boldsymbol{\beta}^{\mathsf{T}}\mathbf{x}}}\right)^{1-\mathrm{y_i}}\right] && (2.8)\\
&= \ \sum_{\mathrm{i}=1}^{\mathrm{n}}\mathrm{y_i}\log\left(\frac{1}{1+e^{-\boldsymbol{\beta}^{\mathsf{T}}\mathbf{x}}}\right)+(1-\mathrm{y_i})\log\left(1-\frac{1}{1+e^{-\boldsymbol{\beta}^{\mathsf{T}}\mathbf{x}}}\right), && (2.9)
\end{aligned}$$

which is easier to maximize than (2.5) because it contains a sum, rather than a product. Sadly, (2.6) is still complex enough that it cannot be maximized with our calculus 101 recipe (take derivative, set to zero, and solve for the optimizer), so instead we will use gradient ascent.

2.6 Gradient Ascent

One often wants to find the *maximizer* of a function $g(\beta)$, that is, the value $\beta^\star$ such that $g(\beta^\star)\geq g(\beta)$ for every β in the domain of g. If g is concave and *simple* enough, $\beta^\star$ can be determined using our elemental calculus recipe:

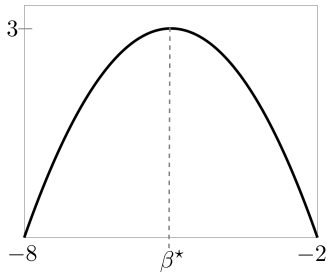
1. Take derivative of $g(\beta)$
2. Set derivative to zero, and solve for the maximizer.

Example 2.4. Consider $g(\beta)=3-(\beta+5)^2$. We can follow our recipe to find its maximizer:

1. The derivative of g is given by $\nabla g(\beta)=-2(\beta+5)$.
2. Setting the derivative to zero and solving for β we obtain:

$$\begin{aligned}
-2(\beta+5) \ &= \ 0\\
\beta \ &= \ -5.
\end{aligned}$$

Since g is concave (can you show this?), we conclude that its maximizer is $\beta^\star=-5$, as depicted below:



Some functions, however, are either not concave, or too complex that we cannot solve for β in step 2. For example, the gradient of (2.6) is:

$$\nabla \ell(\boldsymbol{\beta}|\mathbf{Y},\mathbf{X}) \;=\; \sum_{\mathrm{i}=1}^{\mathrm{N}} \left(\mathrm{y_i} - \frac{1}{1+e^{-\boldsymbol{\beta}^{\mathsf{T}}\mathbf{x}_\mathrm{i}}} \right) \mathbf{x}_\mathrm{i}. \tag{2.10}$$

If we set this to zero, can you solve for $\boldsymbol{\beta}$?

For cases where our calculus 101 recipe does not work, we use *optimization*, which is the field of mathematics that deals with finding maximums (and minimums). In particular, we will use one of the most elemental tools of optimization: gradient ascent.

The setting is is this: you have a function $g(\beta)$. You want to find its maximum. You cannot solve for it directly using the derivative trick, so what can you do? You can *test* the value of g for different values of β. For example, you can test $g(0)$, then maybe $g(1)$, then maybe $g(-1)$, then maybe $g(1.5)$, and so on, until you find the maximizer. Of course, depending on the domain of g, there could be infinitely many options, so testing them all would be infeasible.

As the name suggests, the main idea of gradient ascent is to test some initial value β_0 (for example 0), and iteratively use the gradient (another name for derivative) to determine which value of β to test next, such that the each new value β_{t+1} produces a higher value for g, until we find the maximum. The main intuition is that the gradient $\nabla g(\beta)$ tells us the slope of g at β. If this slope is positive, then we know that g is increasing, and we should try a larger value of β, say $\beta_{t+1} = \beta_t + \eta$, where η is often referred to as *step-size*. If the slope is negative, then we know that g is decreasing, and we should try a smaller value of β, say $\beta_{t+1} = \beta_t - \eta$ (see Figure 2.1 to build some intuition).

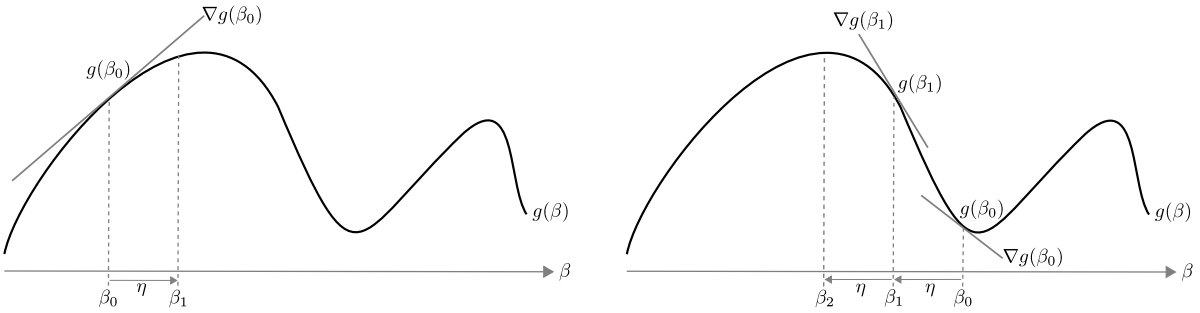


Figure 2.1: Start at some point β_0. If the gradient is positive (left figure), try a larger value of β, say $\beta_1 = \beta_0 + \eta$. If the gradient is negative (right figure), try a smaller value of β, say $\beta_1 = \beta_0 + \eta$. Repeat this until convergence.

The same insight extends to multivariable functions. If g is a function of a vector $\boldsymbol{\beta} \in \mathbb{R}^\mathrm{d}$, then $\nabla g(\boldsymbol{\beta}) \in \mathbb{R}^\mathrm{d}$

gives the slope of g in each of the d coordinates of β. Based on this insight, gradient ascent can be summarized as follows:

Algorithm 1: Gradient Ascent

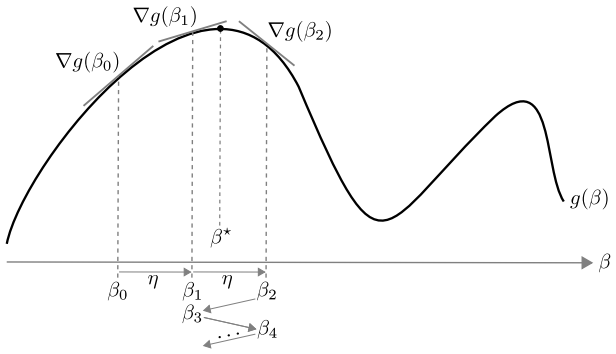
Input: Function g, step-size parameter $\eta > 0$.
Initialize $\boldsymbol{\beta}_0$. For example, $\boldsymbol{\beta}_0 = \mathbf{0}$.
Repeat until convergence: $\boldsymbol{\beta}_{t+1} = \boldsymbol{\beta}_t + \eta \nabla g(\boldsymbol{\beta}_t)$.
Output: $\boldsymbol{\beta}^\star = \boldsymbol{\beta}_t$.

2.6.1 Step-size η

The keen reader will be wondering, what if we move too far? In our example of Figure 2.1, we could run into an infinite loop, where

$$\begin{aligned} \beta_1 &= \beta_3 = \beta_5 = \beta_7 = \cdots \\ \beta_2 &= \beta_4 = \beta_6 = \beta_8 = \cdots, \end{aligned}$$

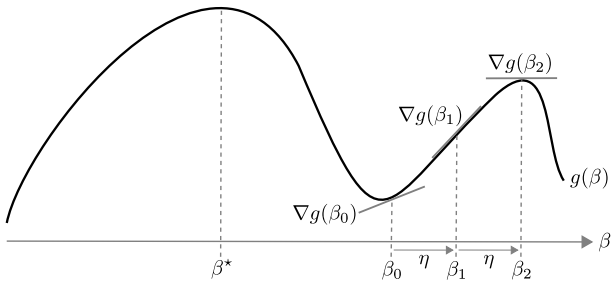
without ever achieving $\beta^\star$, as depicted below:



How would you solve this?

2.6.2 Initialization

The keen reader will also be wondering: what if we start at the wrong place, as depicted below:



In cases like these we could run into a so-called local maximum, that is, a point that is larger than all other points in its vicinity, but not necessarily the maximum over the whole domain of g. In the figure above, β_2 is a local maximizer.

How would you solve this?

2.7 Maximizing Likelihood for Logistic Regression

Equipped with gradient ascent, we can go back to logistic regression to find the parameter $\boldsymbol{\beta}$ that maximizes the likelihood. All we need to do is use gradient ascent to find:

$$\boldsymbol{\beta}^\star \;=\; \underset{\boldsymbol{\beta}\in\mathbb{R}^{\mathrm{d}}}{\arg\max}\; \mathbb{L}(\boldsymbol{\beta}|\mathbf{Y},\mathbf{X}).$$

Once we have found $\boldsymbol{\beta}^\star$, we can determine whether $y = 0$ or $y = 1$ for a new sample with features $\mathbf{x}$, by simply using (2.4), with $\boldsymbol{\beta}^\star$ instead of $\boldsymbol{\beta}$.