Topic 5: Gradient methods

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Updates by Toryn Schafer 2024-09-10

Before we start

- Please accept the **GradientMethodsExamples** link that gives you access to Github with some starter code: Click this link for starter code
- **Star** the repository for easy access later
- Clone the repository to your local computer
- Initiate an R project in Rstudio

There will also be some algebra, so you may want to have pen/pencil and notebook ready.

Gradient methods: steepest (gradient) descent

- Choose a step size $\alpha > 0$ (more on this later, sometimes called **learning rate** or **learning step**)
- Start with an initial guess x_0
- At each iteration t, compute $x_{t+1} = x_t - \alpha \nabla f(x_t)$
- Continue until some **convergence criterion** is met
  i.e. $f(x_{t+1}) \approx f(x_t)$

Steepest descent - intution

Want to find solution x^* such that

$$\nabla f(x^*) = 0.$$

For $\alpha > 0$, at solution

$$\alpha \nabla f(x^*) = x^* - x^*.$$

Steepest descent update rewritten

$$\alpha \nabla f(x_t) = x_t - x_{t+1}.$$

Steepest descent - intution

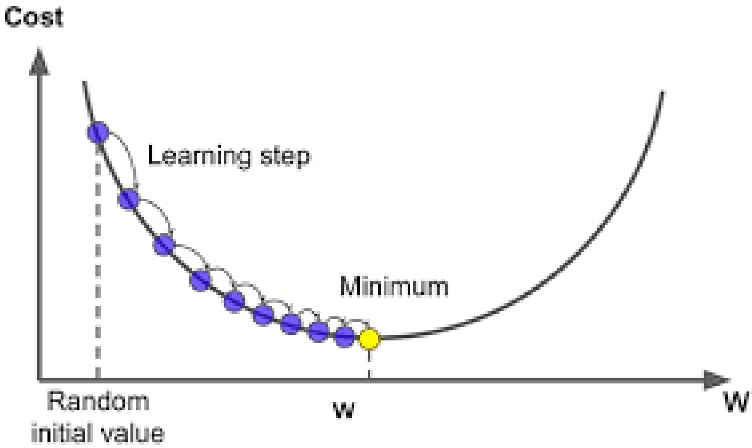


Figure 1: Illustration of steepest descent

Steepest descent

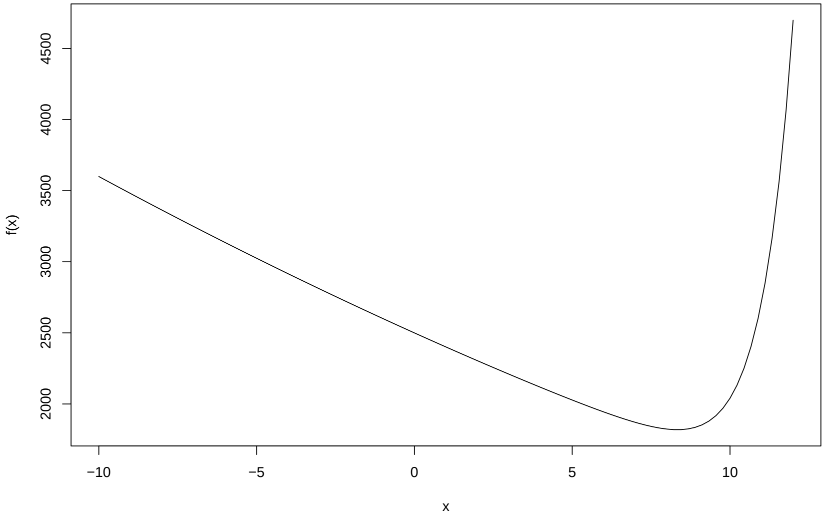
- Choose a step size $\alpha > 0$ (more on this later, sometimes called **learning rate** or **learning step**)
- Start with an initial guess x_0
- At each iteration t, compute $x_{t+1} = x_t - \alpha \nabla f(x_t)$
- Continue until some **convergence criterion** is met
  i.e. $f(x_{t+1}) \approx f(x_t)$

This attempts to find solution to

$$\nabla f(x) = 0.$$

Steepest descent - example

$$f(x) = (x - 50)^2 + e^x/50$$



Steepest descent - implementation

- For simplicity, focus on one-dimensional case first
- Open **SteepestDescent.R** and follow the instructions to implement steepest descent
- If you go ahead, **Example1.R** has the code that lets you play with function $f(x)$ and optimization with different α values

Steepest descent - example

$$f(x) = (x-50)^2 + e^x/50, \quad f'(x) = 2x - 100 + e^x/50 = 0$$

The choice of step size is very important!!

- **Too small** α - very small difference between updates, larger number of iterations
- **Too large** α - oscillations, may not converge

Use **Example1.R** to check different values of α on the given function. How may you monitor the convergence?

Steepest descent in practice

- Very simple
- Only requires the first derivative
- Used in many machine learning methods, i.e. in neural nets (with additional stochastic updates)

Newton's method

Recall we want to find solution x^* to

$$\nabla f(x) = 0.$$

By Taylor expansion

$$\nabla f(x^*) = \nabla f(x) + \nabla^2 f(x)(x^* - x) + \text{higher order terms.}$$

Since $\nabla f(x^*) = 0$, must have $\nabla f(x) + \nabla^2 f(x)(x^* - x) \approx 0$, leading to

$$x^* \approx x - \{\nabla^2 f(x)\}^{-1} \nabla f(x).$$

One dimensional case update

$$x_{t+1} = x_t - \frac{f'(x_t)}{f''(x_t)}$$

Newton's method vs Steepest descent (one - dimensional)

- Steepest descent

$$x_{t+1} = x_t - \alpha f'(x_t)$$

- Newton's method: Steepest descent with $\alpha = 1/f''(x_t)$ (**changes with t**)

$$x_{t+1} = x_t - \frac{f'(x_t)}{f''(x_t)}$$

Newton's method - illustration

- The closer is x_0 to the optimal value x^*, the faster is the convergence

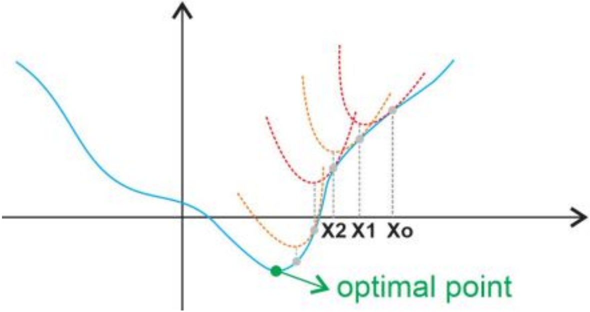


Figure 2: Illustration of Newton's method, taken from Ardian Umam blog

Newton's method - example

$$f(x) = (x-50)^2 + e^x/50, \quad f'(x) = 2x - 100 + e^x/50 = 0$$

$$f''(x) = 2 + e^x/50$$

Implement Newton's method in **NewtonsMethod.R**, and then test it on function f following **Example1.R**

Recall

Convex optimization problem:

$$\text{minimize}_x f(x), \quad f - \text{convex function.}$$

To find global optimum, need to solve optimality conditions

$$\nabla f(x) = 0.$$

Discussed R built-in solvers, steepest descent algorithm and Newton's method.

In general, these algorithms aim to find any solution to the above, so may be applied with nonconvex problems as well.

Next: Application in the context of binary logistic regression.

Binary logistic regression

n samples (x_i, y_i), $x_i \in \mathbb{R}^p$, $y_i \in \{0, 1\}$ (two classes, similar to discriminant analysis, but different coding)

$$P(y_i = 1|x_i) := p(x_i), \quad P(y_i = 0|x_i) = 1 - p(x_i).$$

In logistic regression, we assume

$$\log \frac{p(x_i)}{1 - p(x_i)} = \beta_0 + \beta_1 x_{i,1} + \cdots + \beta_p x_{i,p} = \beta_0 + \beta^\top x_i = \beta^\top x_i,$$

where the last equality holds if we add a column of 1s to matrix $X \in \mathbb{R}^{n \times p}$

Binary logistic regression

$$P(y_i = 1|x_i) := p(x_i), \quad P(y_i = 0|x_i) = 1 - p(x_i).$$

The class membership y_i is dependent on covariates $x_i \in \mathbb{R}^p$ via some unknown function $p(x_i) : \mathbb{R}^p \to [0, 1]$.

$$\log \frac{p(x_i)}{1 - p(x_i)} = \beta^\top x_i.$$

In binary logistic regression, we make an assumption that this function has a specific form:

$$p(x_i; \beta) = \frac{e^{x_i^\top \beta}}{1 + e^{x_i^\top \beta}}.$$

$p(x_i; \beta)$ emphasizes that β **is the only unknown component of this function**

Binary logistic regression

In binary logistic regression, we make an assumption that

$$P(y_i = 1|x_i) = p(x_i; \beta) = \frac{e^{x_i^\top \beta}}{1 + e^{x_i^\top \beta}}.$$

If we know β, we can calculate these probabilities for any new observation x and determine class assignment based on the largest probability

How do we find β? Use maximum likelihood

Binary logistic regression

$$\log \frac{p(x_i)}{1 - p(x_i)} = \beta^\top x_i \quad \text{leads to} \quad p(x_i; \beta) = \frac{e^{x_i^\top \beta}}{1 + e^{x_i^\top \beta}}$$

Similarly

$$1 - p(x_i; \beta) = \frac{1}{1 + e^{x_i^\top \beta}}.$$

For the ith sample with (x_i, y_i), the log-likelihood becomes

$$l_i(\beta | x_i, y_i) = (1 - y_i) \log\{1 - p(x_i; \beta)\} + y_i \log p(x_i; \beta).$$

Why?

Joint likelihood for logistic regression

$$l_i(\beta|x_i, y_i) = (1 - y_i)\log\{1 - p(x_i;\beta)\} + y_i \log p(x_i;\beta).$$

Expression for probabilities

$$p(x_i;\beta) = \frac{e^{x_i^\top \beta}}{1 + e^{x_i^\top \beta}}, \quad 1 - p(x_i;\beta) = \frac{1}{1 + e^{x_i^\top \beta}}.$$

For n independent samples,

$$\begin{aligned} l(\beta|X, Y) &= \sum_{i=1}^{n} l_i(\beta|x_i, y_i) = \text{some algebra} && (1) \\ &= \sum_{i=1}^{n} \{y_i x_i^\top \beta - \log(1 + e^{x_i^\top \beta})\} && (2) \end{aligned}$$

Some algebra

Recall $\log \frac{p(x_i)}{1-p(x_i)} = \beta^\top x_i$.

$$
\begin{aligned}
& l(\beta|X, Y) && (3)\\
&= \sum_{i=1}^{n} l_i(\beta|x_i, y_i) && (4)\\
&= \sum_{i=1}^{n} [(1 - y_i)\log\{1 - p(x_i; \beta)\} + y_i \log p(x_i; \beta)] && (5)\\
&= \sum_{i=1}^{n} [y_i \log(p(x_i; \beta)/(1 - p(x_i; \beta)) + \log\{1 - p(x_i; \beta)\}] && (6)\\
&= \sum_{i=1}^{n} [y_i x_i^\top \beta - \log(1 + e^{x_i^\top \beta})] && (7)
\end{aligned}
$$

Maximum likelihood estimation

In binary logistic regression, we make an assumption that

$$P(y_i = 1|x_i) = p(x_i; \beta) = \frac{e^{x_i^\top \beta}}{1 + e^{x_i^\top \beta}}.$$

We want to estimate the unknown β by solving

$$\hat{\beta} = \arg\min_{\beta} \underbrace{\sum_{i=1}^{n} \{-y_i x_i^\top \beta + \log(1 + e^{x_i^\top \beta})\}}_{f(\beta)}.$$

Go to **FunctionsBinaryLogistic.R** and fill in the function **logistic_objective** to calculate the objective value $f(\beta)$ for given matrix X, vector y and vector β.

Maximum likelihood estimation

We want to find

$$\hat{\beta} = \arg\min_{\beta} \sum_{i=1}^{n} \{-y_i x_i^\top \beta + \log(1 + e^{x_i^\top \beta})\}.$$

Is this a convex optimization problem?

Yes, because

- $-y_i x_i^\top \beta$ is linear in β, hence convex
- $f(x) = \log(1 + e^x)$ is convex because

$$f'(x) = \frac{e^x}{1 + e^x}, \quad f''(x) = \frac{e^x}{1 + e^x} - \frac{e^{2x}}{(1 + e^x)^2} = \frac{e^x}{(1 + e^x)^2} > 0.$$

- $\log(1 + e^{x_i^\top \beta}) = f(x_i^\top \beta)$ - convex function of linear combination

Maximum likelihood estimation - gradient calculation

We want to find

$$\hat{\beta} = \arg\min_{\beta} \underbrace{\sum_{i=1}^{n} \{-y_i x_i^{\top} \beta + \log(1 + e^{x_i^{\top} \beta})\}}_{f(\beta)}.$$

This is a convex optimization problem. Need gradient (for both steepest descent and Newton), and Hessian matrix (for Newton). One can check (**exercise**) that

$$\frac{\partial f(\beta)}{\partial \beta_j} = \sum_{i=1}^{n} x_{ij} \{-y_i + p(x_i; \beta)\} = -X_j^{\top} \{y - P(X; \beta)\},$$

where X_j is the jth column of matrix X, and $P(X; \beta) \in \mathbb{R}^n$ is a vector with elements $p(x_i; \beta)$.

Maximum likelihood estimation - gradient calculation

$$\frac{\partial f(\beta)}{\partial \beta_j} = \sum_{i=1}^{n} x_{ij}\{-y_i + p(x_i;\beta)\} = X_j^\top\{P(X;\beta) - y\},$$

Compactly

$$\nabla f(\beta) = X^\top\{P(X;\beta) - y\}.$$

$P(X;\beta) \in \mathbb{R}^n$ is a vector with elements $p(x_i;\beta)$, where

$$p(x_i;\beta) = \frac{e^{x_i^\top \beta}}{1 + e^{x_i^\top \beta}}.$$

Go to **FunctionsBinaryLogistic.R** and fill in the function **logistic_gradient** to calculate gradient value $\nabla f(\beta)$ for a given matrix X, vector y and vector β.

Steepest descent for binary logisitc regression

Possible solution for calculating $P(X;\beta)$

```
Xb = X %*% beta
pbeta = exp(Xb)
pbeta = pbeta / (1 + pbeta)
```

Possible solutions for calculating $f(\beta)$

```
Xb = X %*% beta
pbeta = exp(Xb)
# pbeta is only numerator still
obj1 = sum(-y * Xb + log(1 + pbeta))
pbeta = pbeta / (1 + pbeta)
# original objective formula
obj2 = sum(y * log(pbeta) + (1 - y) * log(1 - pbeta))
```

Steepest descent for binary logisitc regression

Can use steepest descent update

$$\beta_{t+1} = \beta_t - \alpha \nabla f(\beta_t).$$

- Use **Example2.R** to apply steepest descent using the functions you created, pass X and y as ... arguments to SteepestDescentVec
- Note that both objective function calculation and gradient calculation rely on similar terms. In **FunctionsBinaryLogistic.R**, write customized solver **SteepestDescentBinLogistic**

Steepest descent example

- Compare customized solver and original solver in terms of solutions agreement and speed
- Try the two settings in **Example2.R** to see the effect of the learning rate and the starting point on convergence

Hessian calculation

We want to find

$$\widehat{\beta} = \arg\min_{\beta} \sum_{i=1}^{n} \{-y_i x_i^{\top}\beta + \log(1 + e^{x_i^{\top}\beta})\}.$$

Recall

$$\nabla l(\beta) = X^{\top}\left\{P(X;\beta) - Y\right\}$$

$$\frac{\partial l(\beta)}{\partial \beta_j} = \sum_{i=1}^{n} x_{ij}\{p(x_i;\beta) - y_i\}$$

Want to calculate

$$\frac{\partial^2 l(\beta)}{\partial \beta_j \beta_l} = \sum_{i=1}^{n} x_{ij} \frac{\partial}{\partial \beta_l} p(x_i;\beta)$$

Hessian calculation continued

Want to calculate

$$\frac{\partial^2 l(\beta)}{\partial\beta_j\beta_l} = \sum_{i=1}^{n} x_{ij} \frac{\partial}{\partial\beta_l} p(x_i;\beta)$$

Recall

$$p(x_i;\beta) = \frac{e^{x_i^\top \beta}}{1 + e^{x_i^\top \beta}}$$

Try to derive Hessian on your own.

Hessian calculation: it can be shown (algebra + calculus)

Recall

$$p(x_i;\beta) = \frac{e^{x_i^\top \beta}}{1 + e^{x_i^\top \beta}}$$

$$\frac{\partial}{\partial \beta_l} p(x_i;\beta) = x_{il} p(x_i;\beta) - x_{il} p(x_i;\beta)^2 = x_{il} p(x_i;\beta)\{1 - p(x_i;\beta)\}$$

$$\frac{\partial^2 l(\beta)}{\partial \beta_j \beta_l} = \sum_{i=1}^{n} x_{ij} x_{il} p(x_i;\beta)\{1 - p(x_i;\beta)\}$$

Hessian calculation continued

We got

$$\frac{\partial^2 l(\beta)}{\partial \beta_j \beta_l} = \sum_{i=1}^{n} x_{ij} x_{il} p(x_i; \beta)\{1 - p(x_i; \beta)\}$$

This can be simplied in matrix notation for Hessian (staring + algebra)

$$\nabla^2 l(\beta) = X^\top W X$$

where W is n times n diagonal matrix with elements

$$w_i = p(x_i; \beta)\{1 - p(x_i; \beta)\}$$

Newton's method for binary logistic regression

Recall Newton's method for minimizing f over x

$$x_{t+1} = x_t - \{\nabla^2 f(x_t)\}^{-1} \nabla f(x_t).$$

In our case

$$\nabla l(\beta) = X^\top \{P(X;\beta) - Y\}; \quad \nabla^2 l(\beta) = X^\top W X.$$

Therefore

$$\beta_{t+1} = \beta_t - (X^\top W X)^{-1} X^\top \{P(X;\beta) - Y\}.$$

Recall that W is n times n diagonal matrix with elements

$$w_i = p(x_i;\beta)\{1 - p(x_i;\beta)\}$$

Newton's method for binary logistic regression

$$\beta_{t+1} = \beta_t - (X^\top WX)^{-1}X^\top \left\{P(X;\beta) - Y\right\}.$$

Recall that W is n times n diagonal matrix with elements

$$w_i = p(x_i;\beta)\{1 - p(x_i;\beta)\}$$

- Use **FunctionsBinaryLogistic.R**, and write customized solver **NewtonBinLogistic**
- Continue **Example2.R** but this time use Newton's method

Newton's method for binary logistic regression

Hint for calculation of $X^\top DX$ when D is a diagonal matrix.

Let $n = 2$, then

$$DX = \begin{pmatrix} d_1 & 0 \\ 0 & d_2 \end{pmatrix} \begin{pmatrix} x_1^\top \\ x_2^\top \end{pmatrix} = \begin{pmatrix} d_1 x_1^\top \\ d_2 x_2^\top \end{pmatrix}.$$

```r
X = matrix(1, 2, 3) # 2 by 3 matrix of 1s
d = c(2, 0.5)
X * d
```

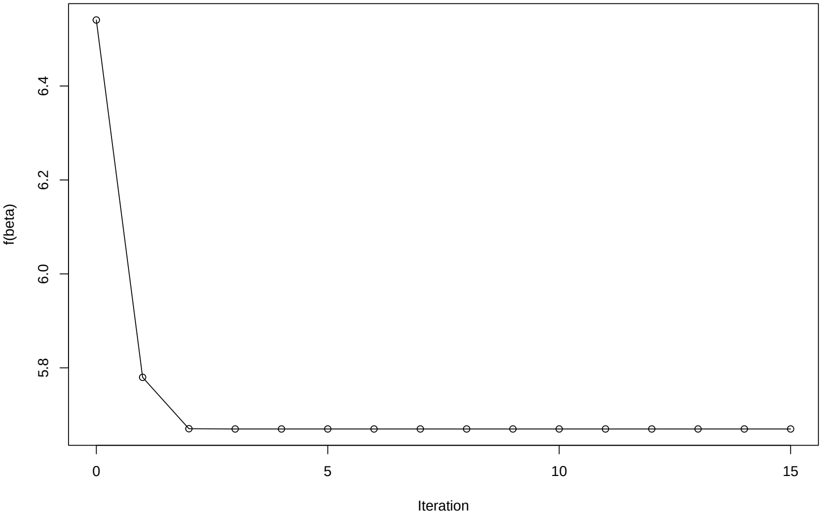
```
##      [,1] [,2] [,3]
## [1,]  2.0  2.0  2.0
## [2,]  0.5  0.5  0.5
```

Newton's method for binary logistic

```r
beta_init = c(0, 0.2) # initial starting value
nIter = 15 # number of iterations
out_Newton1 <- NewtonBinLogistic(X = X, y = y,
                    beta_init = beta_init, nIter = nIter)
```

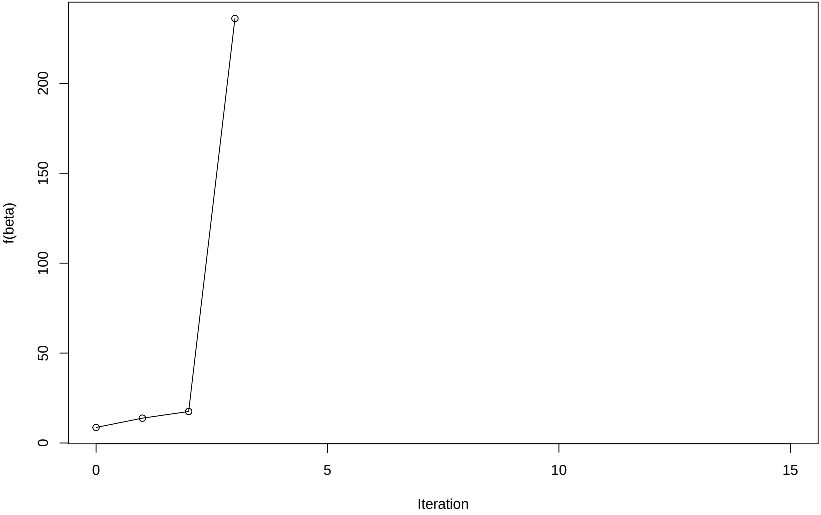
Newton's method example

$\beta_{\text{init}} = (0\ 0.2)$. Much faster convergence compared to **steepest descent**.



Newton's method example

$\beta_{\text{init}} = (0.33\ 0.33)$. Bad starting point can lead to no convergence.



Newton's method - effect of the starting point

Good starting point: - faster convergence than steepest descent

Bad starting point: - may fail to converge

How can you monitor convergence?

Newton's method - practical issues

- The update may be too agressive - lead to divergence for some starting points

Solution: adjust the magnitude of each step

- The inverse $(X^\top WX)^{-1}$ may not exist, especially for large datasets

Solution: add regularization

Newton's method - step adjustment

Recall

$$\beta_{t+1} = \beta_t - (X^\top W X)^{-1} X^\top \{P(X;\beta) - Y\}$$

Introduce **learning rate** $\eta > 0$, often $\eta = 0.01$ (similar to step size in steepest descent)

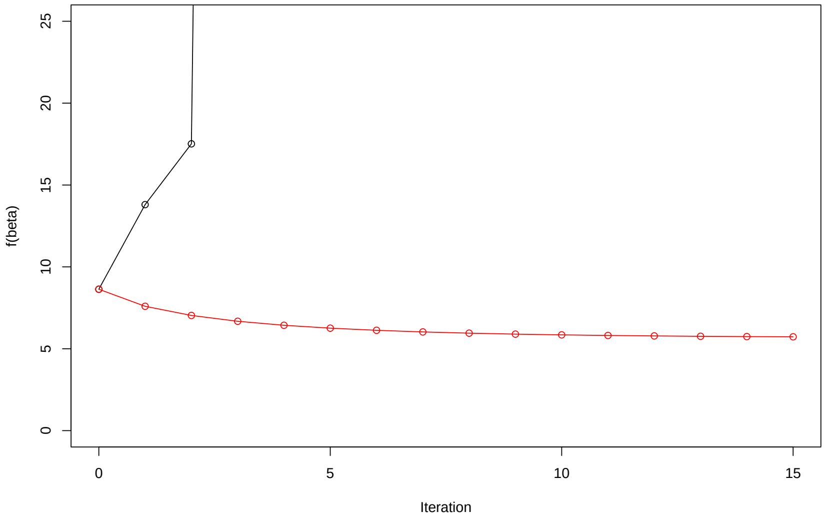
$$\beta_{t+1} = \beta_t - \eta (X^\top W X)^{-1} X^\top \{P(X;\beta) - Y\}$$

Helps the convergence by taking smaller steps.

This is called **Damped Newton's Method** (damping the step size using η)

Newton's method with smaller steps

Red - new steps, Black - old steps. Same $\beta_{\text{init}} = (0.33\ 0.33)$



Logistic regression - regularization

Addition of **ridge** penalty to the objective function

For $\lambda \geq 0$, want to solve

$$\hat{\beta} = \arg\min_{\beta} \sum_{i=1}^{n} \{-y_i {x_i}^\top \beta + \log(1 + e^{{x_i}^\top \beta})\} + \frac{\lambda}{2} \sum_{j=1}^{p} \beta_j^2.$$

Helps avoid issues when $X^\top W X$ is not invertible.

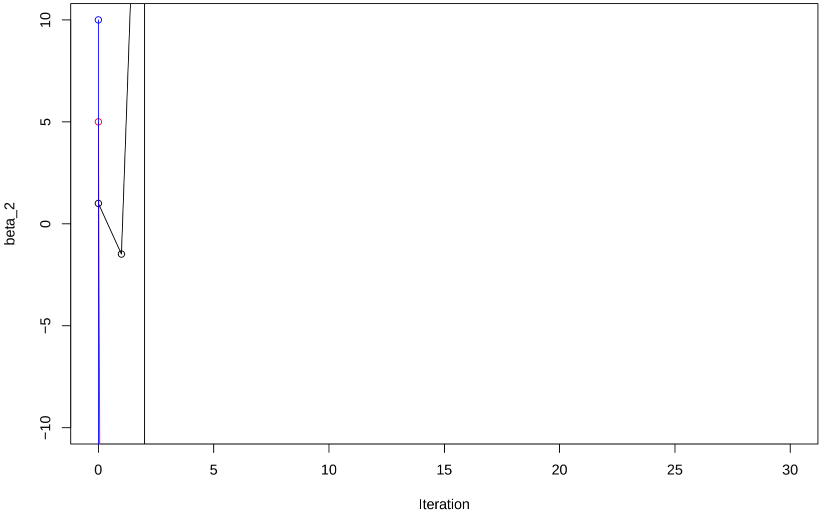
A new update is (**check**)

$$\beta_{t+1} = \beta_t - \eta (X^\top W X + \lambda I)^{-1} [X^\top \{P(X; \beta) - Y\} + \lambda \beta_t]$$

$X^\top W X + \lambda I$ is non-singular when $\lambda > 0$.

No regularization ($\lambda = 0$, $\eta = 0.1$)

Here $\beta_{\text{init}} = (0, 1)$ (black), $\beta_{\text{init}} = (0, 5)$ (red) and $\beta_{\text{init}} = (0, 10)$ (blue)



Some regularization ($\lambda = 1$, $\eta = 0.1$)

Here $\beta_{\text{init}} = (0, 1)$ (black), $\beta_{\text{init}} = (0, 5)$ (red) and $\beta_{\text{init}} = (0, 10)$ (blue)