1

(a) To find the minimum of a 1-d function, we can do an iterative update

$$x^{(t+1)} = x^{(t)} - r f'(x^{(t)})$$

where r is a learning rate and $f'(t)$ is the derivative of the function, $f(x)$ we are minimising. Supposing that

$$f(x) = \frac{c}{2}(x - x^*)^2$$

where $c > 0$. Write down a recursion formula for $x^{(t+1)}$ and $x^{(t)}$. [2 marks]

$$\begin{aligned} x^{(t+1)} &= x^{(t)} - cr(x^{(t)} - x^*) \\ &= (1 - cr)x^{(t)} + crx^*. \end{aligned}$$

(b) Show by induction that $x^{(t)} = F(t) = x^* + (x^{(0)} - x^*)(1 - cr)^t$ is a solution to the recursion relation. Hence find a condition on the value of r to ensure convergence. [5 marks]

In the base case, if we take $t = 0$ then

$$\begin{aligned} F(0) &= x^* + (x^{(0)} - x^*)(1 - cr)^0 \\ &= x^* + (x^{(0)} - x^*) = x^{(0)}. \end{aligned}$$

Thus the formula is true for $t = 0$. Assuming the formula is true for $x^{(t)}$ then substituting this into the recursion relation

$$\begin{aligned} x^{(t+1)} &= (1 - cr)F(t) + crx^* \\ &= (1 - cr)\left(x^* + (x^{(0)} - x^*)(1 - cr)^t\right) + crx^* \\ &= x^* + (x^{(0)} - x^*)(1 - cr)^{(t+1)} = F(t + 1). \end{aligned}$$

Thus, we shown that assuming $x^{(t)} = F(t)$ then $x^{(t+1)} = F(t + 1)$, but as it is true for $t = 0$ the formula will be true for all non-negative integers.

The condition for convergence is that $0 < cr < 2$. Assuming $c > 0$ then $0 < r < 2/c$.

(c) Now consider the case when $\boldsymbol{x} \in \mathbb{R}^n$. We assume that

$$g(\boldsymbol{x}) = \frac{1}{2}(\boldsymbol{x} - \boldsymbol{x}^*)^\mathsf{T}\mathbf{Q}(\boldsymbol{x} - \boldsymbol{x}^*)$$

Answers

Copyright 2023© University of Southampton

where **Q** is a symmetric, positive-definite matrix. The Hessian, **H**, of $g(\boldsymbol{x})$ is a matrix with components

$$H_{ij} = \frac{\partial^2 g(\boldsymbol{x})}{\partial x_i \partial x_j}.$$

By writing out $g(\boldsymbol{x})$ as a double sum over the components compute the Hessian [2 marks]

$$H_{ij} = \frac{\partial^2}{\partial x_i \partial x_j} \frac{1}{2} \sum_{k\ell} (x_k - x_k^*) Q_{k\ell} (x_\ell - x_\ell^*) = Q_{ij}$$

(d) Gradient descent in $\mathbb{R}^n$ is given by

$$\boldsymbol{x}^{(t+1)} = \boldsymbol{x}^{(t)} - r \boldsymbol{\nabla} g(\boldsymbol{x}).$$

Using the definition of $g(\boldsymbol{x})$ write down a recursion relation between $\boldsymbol{x}^{(t+1)}$ and $\boldsymbol{x}^{(t)}$. [2 marks]

$$\boldsymbol{x}^{(t+1)} = \boldsymbol{x}^{(t)} - r \mathbf{Q} (\boldsymbol{x}^t - \boldsymbol{x}^*)$$

(e) Defining $\boldsymbol{\Delta}^{(t)} = (\boldsymbol{x}^{(t)} - \boldsymbol{x}^*)$ obtain a recursion relation between $\boldsymbol{\Delta}^{(t+1)}$ and $\boldsymbol{\Delta}^{(t)}$. (This is easy if you subtract $\boldsymbol{x}^*$ from both sides of the recursion equation for $\boldsymbol{x}^{(t+1)}$.) [2 marks]

$$\boldsymbol{\Delta}^{(t+1)} = (\mathbf{I} - r\mathbf{Q}) \boldsymbol{\Delta}^{(t)}.$$

(f) Using the eigenvalue decomposition $\mathbf{Q} = \mathbf{V}\boldsymbol{\Lambda}\mathbf{V}^\mathsf{T}$ and defining $\boldsymbol{z}^{(t)} = \mathbf{V}^\mathsf{T} \boldsymbol{\Delta}^t$ write out a recursion relation between $\boldsymbol{z}^{(t+1)}$ and $\boldsymbol{z}^{(t)}$. (This is helped by multiplying the recursion relation on the left by $\mathbf{V}^\mathsf{T}$ and using the fact that $\mathbf{V}$ is an orthogonal matrix.) [3 marks]

$$\boldsymbol{z}^{(t+1)} = (\mathbf{I} - r\boldsymbol{\Lambda}) \boldsymbol{z}^t$$

(g) Solve the recursion relation to obtain a formula for $\boldsymbol{x}^{(t)}$ in terms of the initial state $\boldsymbol{x}^{(0)}$. Express this formula for the i^{th} component of $\boldsymbol{x}^{(t)}$ and hence find a condition on the learning rate r to ensure convergence. [4 marks]

The solution to the recursion equation is trivially.

$$\boldsymbol{z}^{(t)} = (\mathbf{I} - r\boldsymbol{\Lambda})^t \boldsymbol{z}^{(0)}.$$

Answers

As Λ is diagonal

$$z_i^{(t)} = (1 - r\lambda_i)^t z_i^{(0)}.$$

Thus the condition for $z_i^{(t)}$ to converge is that $0 < r\lambda_i < 2$. For all $z^{(t)}$ to converge we require $0 < r < 2/\lambda_{max}$.

End of question 1

2

(a) Consider the non-quadratic minimum at x^* given by

$$f(x) = \frac{c}{2}(x - x^*)^2 + \frac{d}{6}(x - x^*)^3$$

where we use Newton's method

$$x^{(t+1)} = x^{(t)} - \frac{f'(x^{(t)})}{f''(x^{(t)})}.$$

by computing the derivatives and expanding for small $x^{(t)} - x^*$ show that $x^{(t+1)} - x^* = O\left(\left(x^{(t)} - x^*\right)^2\right)$.

(To do this we need to expand a term with the structure

$$\frac{r + s\epsilon}{u + v\epsilon}.$$

Note that we can use the geometric series expansion to write

$$\frac{1}{u + v\epsilon} = \frac{1}{u}\frac{1}{1 + \frac{v}{u}\epsilon} = \frac{1}{u}\left(1 - \frac{v}{u}\epsilon + \left(\frac{v}{u}\epsilon\right)^2 - \cdots\right)$$

which is convergent provided $|\frac{v}{u}\epsilon| < 1$.) [5 marks]

Using

$$f'(x) = c(x - x^*) + \frac{d}{2}(x - x^*)^2 \qquad f''(x) = c + d(x - x^*)$$

so that

$$x^{(t+1)} = x^{(t)} - \frac{c\left(x^{(t)} - x^*\right) + \frac{d}{2}\left(x^{(t)} - x^*\right)^2}{c + d\left(x^{(t)} - x^*\right)}$$

Subtracting x^* from both sides of this equation and writing $\epsilon^{(n)} = x^{(t)} - x^*$.

Copyright 2023© University of Southampton

Answers

We find

$$\begin{aligned}
\epsilon^{(t+1)} &= \epsilon^{(t)} - \frac{c\epsilon^{(t)} + \frac{d}{2}\left(\epsilon^{(t)}\right)^2}{c + d\epsilon^{(t)}} \\
&= \epsilon^{(t)} - \left(c\epsilon^{(t)} + \frac{d}{2}\left(\epsilon^{(t)}\right)^2\right)\frac{1}{c}\left(1 - \frac{d}{c}\epsilon^{(t)} + \frac{d^2}{c^2}\left(\epsilon^{(t)}\right)^2 + \cdots\right) \\
&= \frac{d}{2c}\left(\epsilon^{(t)}\right)^2 + O\left(\left(\epsilon^{(t)}\right)^3\right) = O\left(\left(\epsilon^{(t)}\right)^2\right)
\end{aligned}$$

that is $x^{(t+1)} - x^* = O\left(\left(x^{(t)} - x^*\right)^2\right)$**.**

(b) Consider the function

$$h(x) = -x\log(x)$$

defined for $0 < x \leq 1$. By computing $h'(x)$ and setting $h'(x) = 0$ compute the value of x^* that maximises $h(x)$. [2 marks]

$$h'(x) = -\log(x) - 1$$

Thus $h'(x) = 0$ **has a solution at** $x^* = \mathrm{e}^{-1}$**.**

(c) Compute $h''(x)$ and thus compute the Newton update function

$$n(x) = x - \frac{h'(x)}{h''(x)}$$

(the answer is rather surprising and in no way general). [3 marks]

$h''(x) = \frac{-1}{t}$ **so that**

$$n(x) = x - x\,(x\log(x) + 1) = -x\log(x).$$

It is a coincident that $n(x) = h(x)$**.**

(d) On the axes given below plot $x^{(t)}$ for $t = 0,1,2,\ldots,10$, starting from $x^{(0)} = 0.5$ where we use the gradient ascent updates

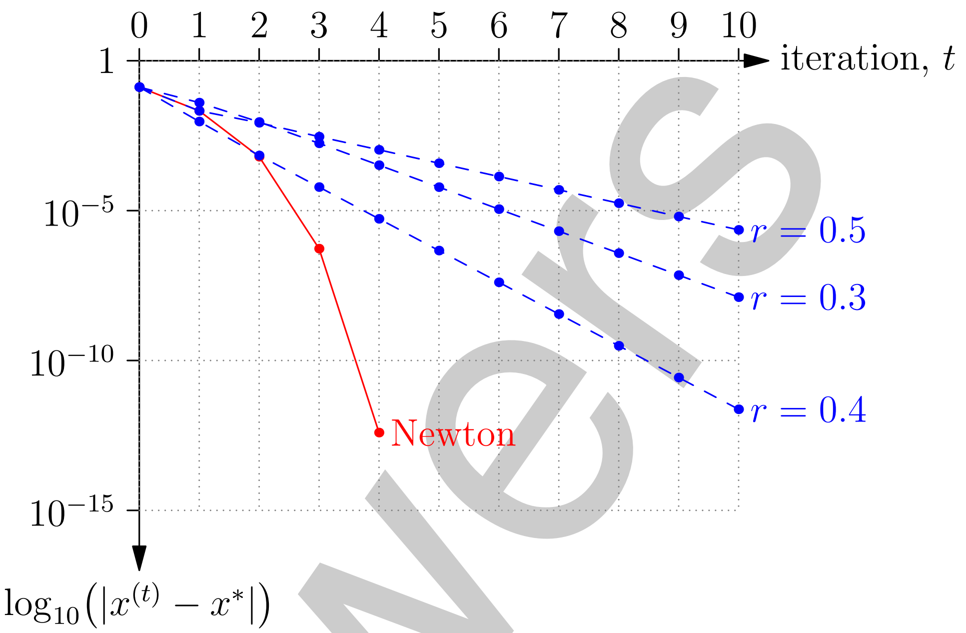
$$x^{(t+1)} = x^{(t)} + r\,h'(x^t)$$

for $r = \{0.3,0.4,0.5\}$ (that is you should plot three curves).

Also plot $x^{(t)}$ where $x^{(t+1)} = n(x^{(t)})$ (that is using Newton's update formula) for $t = 0,1,2,3$ and 4—note that to machine precision $x^{(5)} = x^*$. [10 marks]

Copyright 2023© University of Southampton

Answers



End of question 2

3

(a) Show that for $p_i > 0$ the function

$$h(\boldsymbol{p}) = -\sum_i p_i \log(p_i)$$

is strongly convex-down. Hint: show that the Hessian matrix is negative-definite. [3 marks]

We note that the Hessian H has entries

$$H_{ij} = \frac{\partial^2 h(\boldsymbol{p})}{\partial p_i \partial p_j} = 0 \qquad\qquad H_{ii} = \frac{\partial^2 h(\boldsymbol{p})}{\partial p_i^2} = -\frac{1}{p_i}$$

Thus the Hessian is a diagonal matrix with $H_{ii} = -1/p_i < 0$ (since $p_i > 0$). The eigenvalues of a diagonal matrix are equal to the diagonal elements so that $\lambda_i < 0$ for all i. This is a necessary and sufficient condition for H to be negative-definite and hence $h(\boldsymbol{p})$ is strongly convex-down.

(b) Write down the Lagrangian, $\mathcal{L}$, for the problem of maximising $h(\boldsymbol{p})$ subject to the constraints

$$\sum_i p_i = 1 \qquad\qquad \sum_i p_i E_i = U.$$

Then explain why there is a unique solution to this constrained optimisation problem.

[2 marks]

TURN OVER

Copyright 2023© University of Southampton

Answers

The Lagrangian is given by

$$\mathcal{L} = h(\boldsymbol{p}) - \alpha\left(\sum_i p_i - 1\right) - \beta\left(\sum_i p_i E_i - U\right).$$

The problem has a unique solution because the Lagrangian is strongly convex-down. This follows because $h(\boldsymbol{p})$ is strongly convex-down and the constraints are linear (both convex-up and convex-down). The sum of a strongly convex function and another convex functions is strongly convex.

(c) By setting $\partial\mathcal{L}/\partial p_i = 0$ find the value of p_i that maximises $\mathcal{L}$ in terms of E_i and the Lagrange multipliers. Use the constraint $\sum_i p_i = 1$ to eliminate the Lagrange multiplier that enforces this constraint. [5 marks]

We note that

$$\frac{\partial h(\boldsymbol{p})}{\partial p_i} = -\log(p_i) - 1 - \alpha - \beta E_i$$

so that

$$p_i = \mathrm{e}^{-\alpha-1-\beta E_i}$$

Using the constraint $\sum_i p_i = 1$ then

$$\sum_i \mathrm{e}^{-\alpha-1-\beta E_i} = 1$$

Dividing through by this we find

$$p_i = \frac{\mathrm{e}^{-\beta E_i}}{\sum_j \mathrm{e}^{-\beta E_j}}.$$

This is the famous Boltzmann distribution.

End of question 3

END OF PAPER

Answers