Numerical Methods

Multidimensional Gradient Methods in Optimization- Theory

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Multidimensional Gradient Methods - Overview

- Use information from the derivatives of the optimization function to guide the search
- Finds solutions quicker compared with direct search methods
- A good initial estimate of the solution is required
- The objective function needs to be differentiable

Gradients

- The *gradient* is a vector operator denoted by ∇ (referred to as "del")
- When applied to a function , it represents the functions directional derivatives
- The gradient is the special case where the direction of the gradient is the direction of most or the *steepest ascent/descent*
- The gradient is calculated by

$$\nabla f = \frac{\partial f}{\partial x}\mathrm{i} + \frac{\partial f}{\partial y}\mathrm{j}$$

Gradients-Example

Calculate the gradient to determine the direction of the steepest slope at point (2, 1) for the function

$$f(x, y) = x^2 y^2$$

Solution: To calculate the gradient we would need to calculate

$$\frac{\partial f}{\partial x} = 2xy^2 = 2(2)(1)^2 = 4 \qquad \frac{\partial f}{\partial y} = 2x^2 y = 2(2)^2(1) = 8$$

which are used to determine the gradient at point (2,1) as

$$\nabla f = 4\mathrm{i} + 8\mathrm{j}$$

Hessians

- The *Hessian* matrix or just the *Hessian* is the Jacobian matrix of second-order partial derivatives of a function.
- The determinant of the Hessian matrix is also referred to as the Hessian.
- For a two dimensional function the Hessian matrix is simply

$$H = \begin{bmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x \partial y} \\ \frac{\partial^2 f}{\partial y \partial x} & \frac{\partial^2 f}{\partial y^2} \end{bmatrix}$$

Hessians cont.

The determinant of the Hessian matrix denoted by $\left|H\right|$ can have three cases:

1. If $\left|H\right| > 0$ and $\partial^2 f / \partial^2 x^2 > 0$ then $f\left(x, y\right)$ has a local minimum.
2. If $\left|H\right| > 0$ and $\partial^2 f / \partial^2 x^2 < 0$ then $f\left(x, y\right)$ has a local maximum.
3. If $\left|H\right| < 0$ then $f\left(x, y\right)$ has a saddle point.

Hessians-Example

Calculate the hessian matrix at point (2, 1) for the function $f(x,y)=x^2y^2$

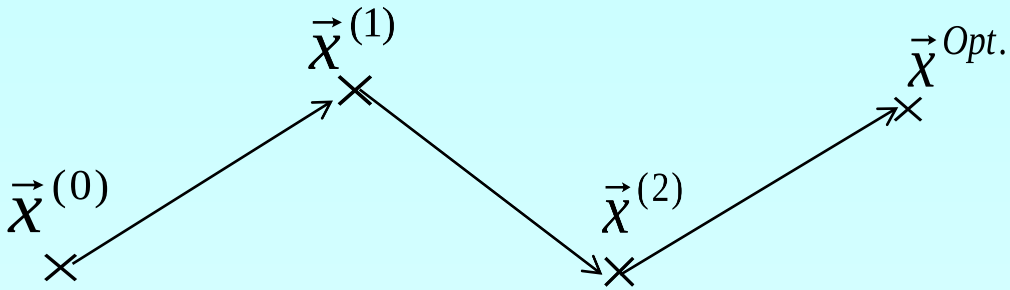
Solution: To calculate the Hessian matrix; the partial derivatives must be evaluated as

$$\frac{\partial^2 f}{\partial^2 x^2}=2y^2=2(1)^2=2 \qquad \frac{\partial^2 f}{\partial y^2}=2x^2=2(2)^2=8 \qquad \frac{\partial^2 f}{\partial x\partial y}=\frac{\partial^2 f}{\partial y\partial x}=4xy=4(2)(1)=8$$

resulting in the Hessian matrix

$$H=\begin{bmatrix}\frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x\partial y}\\ \frac{\partial^2 f}{\partial y\partial x} & \frac{\partial^2 f}{\partial y^2}\end{bmatrix}=\begin{bmatrix}2 & 8\\ 8 & 8\end{bmatrix}$$

Steepest Ascent/Descent Method



- **Step** Starts from an initial guessed point $\vec{x}^{(i=0)}$ and looks for a local optimal solution along a gradient.
- **Step2** The gradient at the initial solution is calculated(or finding the direction to travel),compute $\nabla \vec{f}_{\min} = \frac{\partial f_{\min}}{\partial x_k} = [\frac{\partial f_{\min}}{\partial x_1}, \frac{\partial f_{\min}}{\partial x_2}, ..., \frac{\partial f_{\min}}{\partial x_k}, ...]$.

Steepest Ascent/Descent Method

- **Step3** Find the step size "h" along the Calculated (gradient) direction (using Golden Section Method or Analytical Method).
- **Step4**:A new solution is found at the local optimum along the gradient ,compute

$$\vec{x}^{i+1} = \vec{x}^{(i)} + h\vec{\nabla} f_{\min}\Big|_{\vec{x}_{(i)}}$$

- **Step5**: If "converge",such as $\nabla\vec{f}_{x^{i+1}} \leq (\varepsilon_{tol} = 10^{-5})$ then stop. Else, return to step 2 (using the newly computed point $\vec{x}^{(i+1)}$).

THE END

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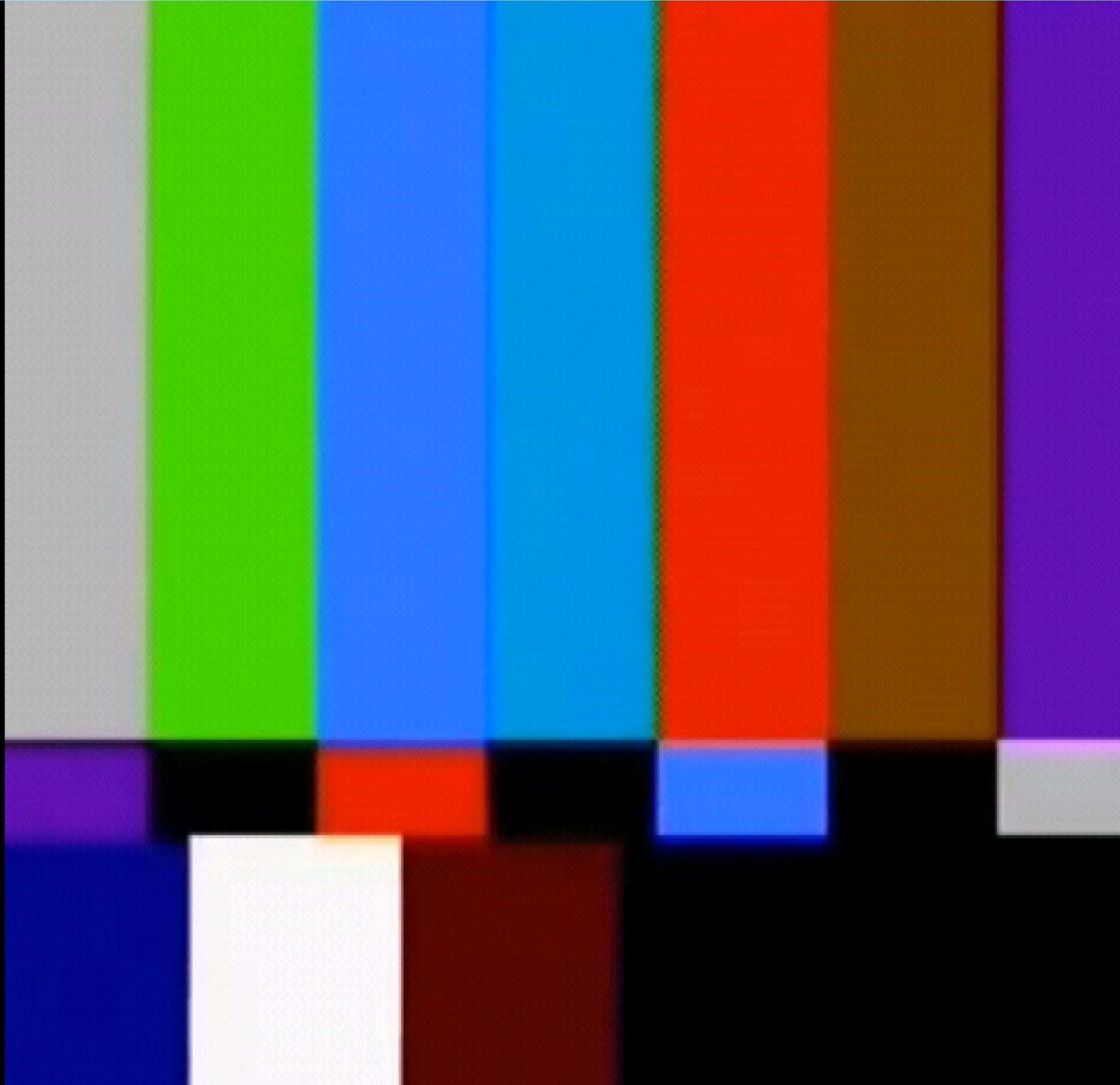

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Example

Determine the minimum of the function

$$f(x, y) = x^2 + y^2 + 2x + 4$$

Use the poin $\vec{x}^{(0)} = \begin{Bmatrix} x^{(0)} \\ y^{(0)} \end{Bmatrix} =$ (2, 1) as the initial estimate of the optimal solution.

Solution

Iteration 1: To calculate the gradient; the partial derivatives must be evaluated as

Recalled that $f(x, y) = x^2 + y^2 + 2x + 4$

$$\frac{\partial f}{\partial x} = 2x + 2 = 2(2) + 2 = 6 \qquad \frac{\partial f}{\partial y} = 2y = 2(1) = 2$$

$$\nabla f = 6\mathrm{i} + 2\mathrm{j}$$

$$\vec{x}^{(i+1)} = \vec{x}^{(i)} + h\nabla\vec{f}$$

$$\vec{x}^{(i+1)} = \begin{Bmatrix} 2 \\ 1 \end{Bmatrix} + h\begin{Bmatrix} 6 \\ 2 \end{Bmatrix} = \begin{Bmatrix} 2 + 6h \\ 1 + 2h \end{Bmatrix}$$

Solution

Now the function $f(x, y)$ can be expressed along the direction of gradient as

$$f(\vec{x}^{\,i+1}) = (2+6h)^2 + (1+2h)^2 + 2(2+6h) + 4 \equiv g(h)$$

$$g(h) = 40h^2 + 40h + 13$$

To get $g_{\min}$,we set $\dfrac{dg}{dh} = 0 = 80h + 40 \Rightarrow h^* = -0.5$

Solution Cont.

Iteration 1 continued:

This is a simple function and it is easy to determine $h^* = -0.50$ by taking the first derivative and solving for its roots.

This means that traveling a step size of $h = -0.5$ along the gradient reaches a minimum value for the function in this direction. These values are substituted back to calculate a new value for x and y as follows:

$$x = 2 + 6(-0.5) = -1$$

$$y = 1 + 2(-0.5) = 0$$

Note that $f(2,1) = 13$ $f(-1,0) = 3.0$

Solution Cont.

Iteration 2: The new initial point is $(-1, 0)$ .We calculate the gradient at this point as

$$\frac{\partial f}{\partial x} = 2x + 2 = 2(-1) + 2 = 0$$

$$\frac{\partial f}{\partial y} = 2y = 2(0) = 0$$

$$\nabla f = (0)\,\hat{\mathrm{i}} + (0)\,\hat{\mathrm{j}}$$

Solution Cont.

This indicates that the current location is a local optimum along this gradient and no improvement can be gained by moving in any direction. The minimum of the function is at point (-1,0),and $f_{\min} = (-1)^2 + (0)^2 + 2(-1) + 4 = 3$.

THE END

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