## Chapter 4: Unconstrained Optimization

- Unconstrained optimization problem $\min _{x} F(x)$ or $\max _{x} F(x)$
- Constrained optimization problem

$$
\begin{array}{ll}
\min _{x} F(x) \text { or } \max _{x} F(x) \\
\text { subject to } & g(x)=0 \\
\text { and/or } & h(x)<0 \text { or } h(x)>0
\end{array}
$$

Example: minimize the outer area of a cylinder subject to a fixed volume. Objective function

$$
F(x)=2 \pi r^{2}+2 \pi r h, x=\left[\begin{array}{l}
r \\
h
\end{array}\right]
$$

Constraint: $2 \pi r^{2} h=V$


Outline:

- Part I: one-dimensional unconstrained optimization
- Analytical method
- Newton's method
- Golden-section search method
- Part II: multidimensional unconstrained optimization
- Analytical method
- Gradient method - steepest ascent (descent) method
- Newton's method


## PART I: One-Dimensional Unconstrained Optimization Techniques

## 1 Analytical approach (1-D)

$\min _{x} F(x)$ or $\max _{x} F(x)$

- Let $F^{\prime}(x)=0$ and find $x=x^{*}$.
- If $F^{\prime \prime}\left(x^{*}\right)>0, F\left(x^{*}\right)=\min _{x} F(x), x^{*}$ is a local minimum of $F(x)$;
- If $F^{\prime \prime}\left(x^{*}\right)<0, F\left(x^{*}\right)=\max _{x} F(x), x^{*}$ is a local maximum of $F(x)$;
- If $F^{\prime \prime}\left(x^{*}\right)=0, x^{*}$ is a critical point of $F(x)$

Example 1: $F(x)=x^{2}, F^{\prime}(x)=2 x=0, x^{*}=0 . F^{\prime \prime}\left(x^{*}\right)=2>0$. Therefore, $F(0)=\min _{x} F(x)$
Example 2: $F(x)=x^{3}, F^{\prime}(x)=3 x^{2}=0, x^{*}=0 . F^{\prime \prime}\left(x^{*}\right)=0$. $x^{*}$ is not a local minimum nor a local maximum.
Example 3: $F(x)=x^{4}, F^{\prime}(x)=4 x^{3}=0, x^{*}=0 . F^{\prime \prime}\left(x^{*}\right)=0$.
In example $2, F^{\prime}(x)>0$ when $x<x^{*}$ and $F^{\prime}(x)>0$ when $x>x^{*}$.
In example $3, x^{*}$ is a local minimum of $F(x) . F^{\prime}(x)<0$ when $x<x^{*}$ and $F^{\prime}(x)>0$ when $x>x^{*}$.


Figure 1: Example of constrained optimization problem

## 2 Newton's Method

$\min _{x} F(x)$ or $\max _{x} F(x)$
Use $x_{k}$ to denote the current solution.

$$
\begin{aligned}
F\left(x_{k}+p\right) & =F\left(x_{k}\right)+p F^{\prime}\left(x_{k}\right)+\frac{p^{2}}{2} F^{\prime \prime}\left(x_{k}\right)+\ldots \\
& \approx F\left(x_{k}\right)+p F^{\prime}\left(x_{k}\right)+\frac{p^{2}}{2} F^{\prime \prime}\left(x_{k}\right)
\end{aligned}
$$

$$
\begin{aligned}
F\left(x^{*}\right) & =\min _{x} F(x) \approx \min _{p} F\left(x_{k}+p\right) \\
& \approx \min _{p}\left[F\left(x_{k}\right)+p F^{\prime}\left(x_{k}\right)+\frac{p^{2}}{2} F^{\prime \prime}\left(x_{k}\right)\right]
\end{aligned}
$$

Let

$$
\frac{\partial F(x)}{\partial p}=F^{\prime}\left(x_{k}\right)+p F^{\prime \prime}\left(x_{k}\right)=0
$$

we have

$$
p=-\frac{F^{\prime}\left(x_{k}\right)}{F^{\prime \prime}\left(x_{k}\right)}
$$

Newton's iteration

$$
x_{k+1}=x_{k}+p=x_{k}-\frac{F^{\prime}\left(x_{k}\right)}{F^{\prime \prime}\left(x_{k}\right)}
$$

Example: find the maximum value of $f(x)=2 \sin x-\frac{x^{2}}{10}$ with an initial guess of $x_{0}=2.5$.
Solution:

$$
f^{\prime}(x)=2 \cos x-\frac{2 x}{10}=2 \cos x-\frac{x}{5}
$$

$$
\begin{gathered}
f^{\prime \prime}(x)=-2 \sin x-\frac{1}{5} \\
x_{i+1}=x_{i}-\frac{2 \cos x_{i}-\frac{x_{i}}{5}}{-2 \sin x_{i}-\frac{1}{5}}
\end{gathered}
$$

$$
x_{0}=2.5, x_{1}=0.995, x_{2}=1.469
$$

Comments:

- Same as N.-R. method for solving $F^{\prime}(x)=0$.
- Quadratic convergence, $\left|x_{k+1}-x^{*}\right| \leq \beta\left|x_{k}-x^{*}\right|^{2}$
- May diverge
- Requires both first and second derivatives
- Solution can be either local minimum or maximum


## 3 Golden-section search for optimization in 1-D

$\max _{x} F(x)\left(\min _{x} F(x)\right.$ is equivalent to $\left.\max _{x}-F(x)\right)$
Assume: only 1 peak value ( $x^{*}$ ) in $\left(x_{l}, x_{u}\right)$
Steps:

1. Select $x_{l}<x_{u}$
2. Select 2 intermediate values, $x_{1}$ and $x_{2}$ so that $x_{1}=x_{l}+d, x_{2}=x_{u}-d$, and $x_{1}>x_{2}$.
3. Evaluate $F\left(x_{1}\right)$ and $F\left(x_{2}\right)$ and update the search range

- If $F\left(x_{1}\right)<F\left(x_{2}\right)$, then $x^{*}<x_{1}$. Update $x_{l}=x_{l}$ and $x_{u}=x_{1}$.
- If $F\left(x_{1}\right)>F\left(x_{2}\right)$, then $x^{*}>x_{2}$. Update $x_{l}=x_{2}$ and $x_{u}=x_{u}$.
- If $F\left(x_{1}\right)=F\left(x_{2}\right)$, then $x_{2}<x^{*}<x_{1}$. Update $x_{l}=x_{2}$ and $x_{u}=x_{1}$.

4. Estimate
$x^{*}=x_{1}$ if $F\left(x_{1}\right)>F\left(x_{2}\right)$, and
$x^{*}=x_{2}$ if $F\left(x_{1}\right)<F\left(x_{2}\right)$


Figure 2: Golden search: updating search range

- Calculate $\epsilon_{a}$. If $\epsilon_{a}<\epsilon_{\text {threshold }}$, end.

$$
\epsilon_{a}=\left|\frac{x_{\mathrm{new}}-x_{\mathrm{old}}}{x_{\mathrm{new}}}\right| \times 100 \%
$$

## The choice of $d$

- Any values can be used as long as $x_{1}>x_{2}$.
- If $d$ is selected appropriately, the number of function evaluations can be minimized.


Figure 3: Golden search: the choice of $d$
$d_{0}=l_{1}, d_{1}=l_{2}=l_{0}-d_{0}=l_{0}-l_{1}$. Therefore, $l_{0}=l_{1}+l_{2}$.
$\frac{l_{0}}{d_{0}}=\frac{l_{1}}{d_{1}}$. Then $\frac{l_{0}}{l_{1}}=\frac{l_{1}}{l_{2}}$.
$l_{1}^{2}=l_{0} l_{2}=\left(l_{1}+l_{2}\right) l_{2}$. Then $1=\left(\frac{l_{2}}{l_{1}}\right)^{2}+\frac{l_{2}}{l_{1}}$.

Define $r=\frac{d_{0}}{l_{0}}=\frac{d_{1}}{l_{1}}=\frac{l_{2}}{l_{1}}$. Then $r^{2}+r-1=0$, and $r=\frac{\sqrt{5}-1}{2} \approx 0.618$ $d=r\left(x_{u}-x_{l}\right) \approx 0.618\left(x_{u}-x_{l}\right)$ is referred to as the golden value.

## Relative error

$$
\epsilon_{a}=\left|\frac{x_{\mathrm{new}}-x_{\mathrm{old}}}{x_{\mathrm{new}}}\right| \times 100 \%
$$

Consider $F\left(x_{2}\right)<F\left(x_{1}\right)$. That is, $x_{l}=x_{2}$, and $x_{u}=x_{u}$.
For case (a), $x^{*}>x_{2}$ and $x^{*}$ closer to $x_{2}$.

$$
\begin{aligned}
\Delta x & \leq x_{1}-x_{2}=\left(x_{l}+d\right)-\left(x_{u}-d\right) \\
& =\left(x_{l}-x_{u}\right)+2 d=\left(x_{l}-x_{u}\right)+2 r\left(x_{u}-x_{l}\right) \\
& =(2 r-1)\left(x_{u}-x_{l}\right) \approx 0.236\left(x_{u}-x_{l}\right)
\end{aligned}
$$

For case (b), $x^{*}>x_{2}$ and $x^{*}$ closer to $x_{u}$.

$$
\begin{aligned}
\Delta x & \leq x_{u}-x_{1} \\
& =x_{u}-\left(x_{l}+d\right)=x_{u}-x_{l}-d \\
& =\left(x_{u}-x_{l}\right)-r\left(x_{u}-x_{l}\right)=(1-r)\left(x_{u}-x_{l}\right) \\
& \approx 0.382\left(x_{u}-x_{l}\right)
\end{aligned}
$$

Therefore, the maximum absolute error is $(1-r)\left(x_{u}-x_{l}\right) \approx 0.382\left(x_{u}-x_{l}\right)$.

$$
\begin{aligned}
\epsilon_{a} & \leq\left|\frac{\Delta x}{x^{*}}\right| \times 100 \% \\
& \leq \frac{(1-r)\left(x_{u}-x_{l}\right)}{\left|x^{*}\right|} \times 100 \% \\
& =\frac{0.382\left(x_{u}-x_{l}\right)}{\left|x^{*}\right|} \times 100 \%
\end{aligned}
$$

Example: Find the maximum of $f(x)=2 \sin x-\frac{x^{2}}{10}$ with $x_{l}=0$ and $x_{u}=4$ as the starting search range.
Solution:
Iteration 1: $x_{l}=0, x_{u}=4, d=\frac{\sqrt{5}-1}{2}\left(x_{u}-x_{l}\right)=2.472, x_{1}=x_{l}+d=2.472$, $x_{2}=x_{u}-d=1.528 . f\left(x_{1}\right)=0.63, f\left(x_{2}\right)=1.765$.
Since $f\left(x_{2}\right)>f\left(x_{1}\right), x^{*}=x_{2}=1.528, x_{l}=x_{l}=0$ and $x_{u}=x_{1}=2.472$.
Iteration 2: $x_{l}=0, x_{u}=2.472, d=\frac{\sqrt{5}-1}{2}\left(x_{u}-x_{l}\right)=1.528, x_{1}=x_{l}+d=1.528$, $x_{2}=x_{u}-d=0.944 . f\left(x_{1}\right)=1.765, f\left(x_{2}\right)=1.531$. Since $f\left(x_{1}\right)>f\left(x_{2}\right), x^{*}=x_{1}=1.528, x_{l}=x_{2}=0.944$ and $x_{u}=x_{u}=2.472$.

Multidimensional Unconstrained Optimization

## 4 Analytical Method

- Definitions:
- If $f(x, y)<f(a, b)$ for all $(x, y)$ near $(a, b), f(a, b)$ is a local maximum;
- If $f(x, y)>f(a, b)$ for all $(x, y)$ near $(a, b), f(a, b)$ is a local minimum.
- If $f(x, y)$ has a local maximum or minimum at $(a, b)$, and the first order partial derivatives of $f(x, y)$ exist at $(a, b)$, then

$$
\left.\frac{\partial f}{\partial x}\right|_{(a, b)}=0, \text { and }\left.\frac{\partial f}{\partial y}\right|_{(a, b)}=0
$$

- If

$$
\left.\frac{\partial f}{\partial x}\right|_{(a, b)}=0 \text { and }\left.\frac{\partial f}{\partial y}\right|_{(a, b)}=0
$$

then $(a, b)$ is a critical point or stationary point of $f(x, y)$.

- If

$$
\left.\frac{\partial f}{\partial x}\right|_{(a, b)}=0 \text { and }\left.\frac{\partial f}{\partial y}\right|_{(a, b)}=0
$$

and the second order partial derivatives of $f(x, y)$ are continuous, then

- When $|H|>0$ and $\left.\frac{\partial^{2} f}{\partial x^{2}}\right|_{(a, b)}<0, f(a, b)$ is a local maximum of $f(x, y)$.
- When $|H|>0$ and $\left.\frac{\partial^{2} f}{\partial x^{2}}\right|_{(a, b)}>0, f(a, b)$ is a local minimum of $f(x, y)$.
- When $|H|<0, f(a, b)$ is a saddle point.

Hessian of $f(x, y)$ :

$$
H=\left[\begin{array}{ll}
\frac{\partial^{2} f}{\partial x^{2}} & \frac{\partial^{2} f}{\partial x \partial y} \\
\frac{\partial^{2} f}{\partial y \partial x} & \frac{\partial^{2} f}{\partial y^{2}}
\end{array}\right]
$$

- $|H|=\frac{\partial^{2} f}{\partial x^{2}} \cdot \frac{\partial^{2} f}{\partial y^{2}}-\frac{\partial^{2} f}{\partial x \partial y} \cdot \frac{\partial^{2} f}{\partial y \partial x}$
- When $\frac{\partial^{2} f}{\partial x \partial y}$ is continuous, $\frac{\partial^{2} f}{\partial x \partial y}=\frac{\partial^{2} f}{\partial y \partial x}$.
- When $|H|>0, \frac{\partial^{2} f}{\partial x^{2}} \cdot \frac{\partial^{2} f}{\partial y^{2}}>0$.

Example (saddle point): $f(x, y)=x^{2}-y^{2}$.
$\frac{\partial f}{\partial x}=2 x, \frac{\partial f}{\partial y}=-2 y$.
Let $\frac{\partial f}{\partial x}=0$, then $x^{*}=0$. Let $\frac{\partial f}{\partial y}=0$, then $y^{*}=0$.

Therefore, $(0,0)$ is a critical point.
$\frac{\partial^{2} f}{\partial x^{2}}=\frac{\partial}{\partial x}(2 x)=2, \frac{\partial^{2} f}{\partial y^{2}}=\frac{\partial}{\partial y}(-2 y)=-2$
$\frac{\partial^{2} f}{\partial x \partial y}=\frac{\partial}{\partial x}(-2 y)=0, \frac{\partial^{2} f}{\partial y \partial x}=\frac{\partial}{\partial y}(2 x)=0$
$|H|=\frac{\partial^{2} f}{\partial x^{2}} \cdot \frac{\partial^{2} f}{\partial y^{2}}-\frac{\partial^{2} f}{\partial x \partial y} \cdot \frac{\partial^{2} f}{\partial y \partial x}=-4<0$
Therefore, $\left(x^{*}, y^{*}\right)=(0,0)$ is a saddle maximum.
Example: $f(x, y)=2 x y+2 x-x^{2}-2 y^{2}$, find the optimum of $f(x, y)$.
Solution:
$\frac{\partial f}{\partial x}=2 y+2-2 x, \frac{\partial f}{\partial y}=2 x-4 y$.
Let $\frac{\partial f}{\partial x}=0,-2 x+2 y=-2$.
Let $\frac{\partial f}{\partial y}=0,2 x-4 y=0$.
Then $x^{*}=2$ and $y^{*}=1$, i.e., $(2,1)$ is a critical point.
$\frac{\partial^{2} f}{\partial x^{2}}=\frac{\partial}{\partial x}(2 y+2-2 x)=-2$
$\frac{\partial^{2} f}{\partial y^{2}}=\frac{\partial}{\partial y}(2 x-4 y)=-4$
$\frac{\partial^{2} f}{\partial x \partial y}=\frac{\partial}{\partial x}(2 x-4 y)=2$, or


Figure 4: Saddle point

$$
\begin{aligned}
& \frac{\partial^{2} f}{\partial y \partial x}=\frac{\partial}{\partial y}(2 y+2-2 x)=2 \\
& |H|=\frac{\partial^{2} f}{\partial x^{2}} \cdot \frac{\partial^{2} f}{\partial y^{2}}-\frac{\partial^{2} f}{\partial x \partial y} \cdot \frac{\partial^{2} f}{\partial y \partial x}=(-2) \times(-4)-2^{2}=4>0 \\
& \frac{\partial^{2} f}{\partial x^{2}}<0 .\left(x^{*}, y^{*}\right)=(2,1) \text { is a local maximum. }
\end{aligned}
$$

## 5 Steepest Ascent (Descent) Method

Idea: starting from an initial point, find the function maximum (minimum) along the steepest direction so that shortest searching time is required.
Steepest direction: directional derivative is maximum in that direction - gradient direction.
Directional derivative

$$
D_{h} f(x, y)=\frac{\partial f}{\partial x} \cdot \cos \theta+\frac{\partial f}{\partial y} \cdot \sin \theta=\left\langle\left[\frac{\partial f}{\partial x} \frac{\partial f}{\partial y}\right]^{\prime} \cdot\left[\begin{array}{cc}
\cos \theta & \sin \theta
\end{array}\right]^{\prime}\right\rangle
$$

$\langle\cdot\rangle$ : inner product
Gradient

When $\left[\begin{array}{ll}\frac{\partial f}{\partial x} & \frac{\partial f}{\partial y}\end{array}\right]^{\prime}$ is in the same direction as $\left[\begin{array}{ccc}\cos \theta & \sin \theta\end{array}\right]^{\prime}$, the directional derivative is maximized. This direction is called gradient of $f(x, y)$.
The gradient of a 2-D function is represented as $\nabla f(x, y)=\frac{\partial f}{\partial x} \vec{i}+\frac{\partial f}{\partial y} \vec{j}$, or $\left[\frac{\partial f}{\partial x} \quad \frac{\partial f}{\partial y}\right]^{\prime}$. The gradient of an $n$-D function is represented as $\nabla f(\vec{X})=\left[\begin{array}{llll}\frac{\partial f}{\partial x_{1}} & \frac{\partial f}{\partial x_{2}} & \ldots & \frac{\partial f}{\partial x_{n}}\end{array}\right]^{\prime}$, where $\vec{X}=\left[\begin{array}{llll}x_{1} & x_{2} & \ldots & x_{n}\end{array}\right]^{\prime}$
Example: $f(x, y)=x y^{2}$. Use the gradient to evaluate the path of steepest ascent at $(2,2)$.
Solution:
$\frac{\partial f}{\partial x}=y^{2}, \frac{\partial f}{\partial y}=2 x y$.
$\left.\frac{\partial f}{\partial x}\right|_{(2,2)}=2^{2}=4,\left.\frac{\partial f}{\partial y}\right|_{(2,2)}=2 \times 2 \times 2=8$
Gradient: $\nabla f(x, y)=\frac{\partial f}{\partial x} \vec{i}+\frac{\partial f}{\partial y} \vec{j}=4 \vec{i}+8 \vec{j}$
$\theta=\tan ^{-1} \frac{8}{4}=1.107$, or $63.4^{\circ}$.
$\cos \theta=\frac{4}{\sqrt{4^{2}+8^{2}}}, \sin \theta=\frac{8}{\sqrt{4^{2}+8^{2}}}$.
Directional derivative at $(2,2): \frac{\partial f}{\partial x} \cdot \cos \theta+\frac{\partial f}{\partial y} \cdot \sin \theta=4 \cos \theta+8 \sin \theta=8.944$

If $\theta^{\prime} \neq \theta$, for example, $\theta^{\prime}=0.5325$, then

$$
\left.D_{h^{\prime}} f\right|_{(2,2)}=\frac{\partial f}{\partial x} \cdot \cos \theta^{\prime}+\frac{\partial f}{\partial y} \cdot \sin \theta^{\prime}=4 \cos \theta^{\prime}+8 \sin \theta^{\prime}=7.608<8.944
$$

Steepest ascent method
Ideally:

- Start from $\left(x_{0}, y_{0}\right)$. Evaluate gradient at $\left(x_{0}, y_{0}\right)$.
- Walk for a tiny distance along the gradient direction till $\left(x_{1}, y_{1}\right)$.
- Reevaluate gradient at $\left(x_{1}, y_{1}\right)$ and repeat the process.

Pros: always keep steepest direction and walk shortest distance Cons: not practical due to continuous reevaluation of the gradient.

Practically:

- Start from $\left(x_{0}, y_{0}\right)$.
- Evaluate gradient $(h)$ at $\left(x_{0}, y_{0}\right)$.
- Evaluate $f(x, y)$ in direction $h$.
- Find the maximum function value in this direction at $\left(x_{1}, y_{1}\right)$.
- Repeat the process until $\left(x_{i+1}, y_{i+1}\right)$ is close enough to $\left(x_{i}, y_{i}\right)$.

Find $\vec{X}_{i+1}$ from $\vec{X}_{i}$
For a 2-D function, evaluate $f(x, y)$ in direction $h$ :

$$
g(\alpha)=f\left(x_{i}+\left.\frac{\partial f}{\partial x}\right|_{\left(x_{i}, y_{i}\right)} \cdot \alpha, y_{i}+\left.\frac{\partial f}{\partial y}\right|_{\left(x_{i}, y_{i}\right)} \cdot \alpha\right)
$$

where $\alpha$ is the coordinate in $h$-axis.
For an $n$-D function $f(\vec{X})$,

$$
g(\alpha)=f\left(\vec{X}+\left.\nabla f\right|_{\left(\vec{X}_{i}\right)} \cdot \alpha\right)
$$

Let $g^{\prime}(\alpha)=0$ and find the solution $\alpha=\alpha^{*}$.
Update $x_{i+1}=x_{i}+\left.\frac{\partial f}{\partial x}\right|_{\left(x_{i}, y_{i}\right)} \cdot \alpha^{*}, y_{i+1}=y_{i}+\left.\frac{\partial f}{\partial y}\right|_{\left(x_{i}, y_{i}\right)} \cdot \alpha^{*}$.


Figure 5: Illustration of steepest ascent


Figure 6: Relationship between an arbitrary direction $h$ and $x$ and $y$ coordinates

Example: $f(x, y)=2 x y+2 x-x^{2}-2 y^{2},\left(x_{0}, y_{0}\right)=(-1,1)$.

First iteration:

$$
\begin{aligned}
& x_{0}=-1, y_{0}=1 \\
& \begin{aligned}
&\left.\frac{\partial f}{\partial x}\right|_{(-1,1)}=2 y+2-\left.2 x\right|_{(-1,1)}=6,\left.\frac{\partial f}{\partial y}\right|_{(-1,1)}=2 x-\left.4 y\right|_{(-1,1)}=-6 \\
& \begin{aligned}
\nabla f & =6 \vec{i}-6 \vec{j}
\end{aligned} \\
& \begin{aligned}
g(\alpha) & =f\left(x_{0}+\left.\frac{\partial f}{\partial x}\right|_{\left(x_{0}, y_{0}\right)} \cdot \alpha, y_{0}+\left.\frac{\partial f}{\partial y}\right|_{\left(x_{0}, y_{0}\right)} \cdot \alpha\right) \\
& =f(-1+6 \alpha, 1-6 \alpha) \\
& =2 \times(-1+6 \alpha) \cdot(1-6 \alpha)+2(-1+6 \alpha)-(-1+6 \alpha)^{2}-2(1-6 \alpha)^{2} \\
& =-180 \alpha^{2}+72 \alpha-7
\end{aligned} \\
& g^{\prime}(\alpha)=-360 \alpha+72=0, \alpha^{*}=0.2 .
\end{aligned}
\end{aligned}
$$

Second iteration:
$x_{1}=x_{0}+\left.\frac{\partial f}{\partial x}\right|_{\left(x_{0}, y_{0}\right)} \cdot \alpha^{*}=-1+6 \times 0.2=0.2, y_{1}=y_{0}+\left.\frac{\partial f}{\partial y}\right|_{\left(x_{0}, y_{0}\right)} \cdot \alpha^{*}=1-6 \times 0.2=$ $-0.2$
$\left.\frac{\partial f}{\partial x}\right|_{(0.2,-0.2)}=2 y+2-\left.2 x\right|_{(0.2,-0.2)}=2 \times(-0.2)+2-2 \times 0.2=1.2$,
$\left.\frac{\partial f}{\partial y}\right|_{(0.2,-0.2)}=2 x-\left.4 y\right|_{(0.2,-0.2)}=2 \times 0.2-4 \times(-0.2)=1.2$

$$
\begin{aligned}
& \nabla f=1.2 \vec{i}+1.2 \vec{j} \\
& \qquad \begin{aligned}
\nabla(\alpha)= & f\left(x_{1}+\left.\frac{\partial f}{\partial x}\right|_{\left(x_{1}, y_{1}\right)} \cdot \alpha, y_{1}+\left.\frac{\partial f}{\partial y}\right|_{\left(x_{1}, y_{1}\right)} \cdot \alpha\right) \\
= & f(0.2+1.2 \alpha,-0.2+1.2 \alpha) \\
= & 2 \times(0.2+1.2 \alpha) \cdot(-0.2+1.2 \alpha)+2(0.2+1.2 \alpha) \\
& -(0.2+1.2 \alpha)^{2}-2(-0.2+1.2 \alpha)^{2} \\
= & -1.44 \alpha^{2}+2.88 \alpha+0.2 \\
g^{\prime}(\alpha)=-2.88 \alpha+ & 2.88=0, \alpha^{*}=1
\end{aligned}
\end{aligned}
$$

Third iteration:
$x_{2}=x_{1}+\left.\frac{\partial f}{\partial x}\right|_{\left(x_{1}, y_{1}\right)} \cdot \alpha^{*}=0.2+1.2 \times 1=1.4, y_{2}=y_{1}+\left.\frac{\partial f}{\partial y}\right|_{\left(x_{1}, y_{1}\right)} \cdot \alpha^{*}=$ $-0.2+1.2 \times 1=1$
$\left(x^{*}, y^{*}\right)=(2,1)$

## 6 Newton's Method

Extend the Newton's method for 1-D case to multidimensional case.
Given $f(\vec{X})$, approximate $f(\vec{X})$ by a second order Taylor series at $\vec{X}=\vec{X}_{i}$ :

$$
f(\vec{X}) \approx f\left(\vec{X}_{i}\right)+\nabla f^{\prime}\left(\vec{X}_{i}\right)\left(\vec{X}-\vec{X}_{i}\right)+\frac{1}{2}\left(\vec{X}-\vec{X}_{i}\right)^{\prime} H_{i}\left(\vec{X}-\vec{X}_{i}\right)
$$

where $H_{i}$ is the Hessian matrix

$$
H=\left[\begin{array}{llll}
\frac{\partial^{2} f}{\partial x_{1}^{2}} & \frac{\partial^{2} f}{\partial x_{1} \partial x_{2}} & \cdots & \frac{\partial^{2} f}{\partial x_{1} \partial x_{n}} \\
\frac{\partial^{2} f}{\partial x_{2} \partial x_{1}} & \frac{\partial^{2} f}{\partial x_{2}^{2}} & \cdots & \frac{\partial^{2} f}{\partial x_{2} \partial x_{n}} \\
& \cdots & & \\
\frac{\partial^{2} f}{\partial x_{n} \partial x_{1}} & \frac{\partial^{2} f}{\partial x_{n} \partial x_{2}} & \cdots & \frac{\partial^{2} f}{\partial x_{n}^{2}}
\end{array}\right]
$$

At the maximum (or minimum) point, $\frac{\partial f(\vec{X})}{\partial x_{j}}=0$ for all $j=1,2, \ldots, n$, or $\nabla f=\overrightarrow{0}$. Then

$$
\nabla f\left(\vec{X}_{i}\right)+H_{i}\left(\vec{X}-\vec{X}_{i}\right)=0
$$

If $H_{i}$ is non-singular,

$$
\vec{X}=\vec{X}_{i}-H_{i}^{-1} \nabla f\left(\vec{X}_{i}\right)
$$

Iteration: $\vec{X}_{i+1}=\vec{X}_{i}-H_{i}^{-1} \nabla f\left(\vec{X}_{i}\right)$
Example: $f(\vec{X})=0.5 x_{1}^{2}+2.5 x_{2}^{2}$
$\nabla f(\vec{X})=\left[\begin{array}{l}x_{1} \\ 5 x_{2}\end{array}\right]$

$$
\begin{gathered}
H=\left[\begin{array}{ll}
\frac{\partial^{2} f}{\partial x^{2}} & \frac{\partial^{2} f}{\partial x \partial y} \\
\frac{\partial^{2} f}{\partial y \partial x} & \frac{\partial^{2} f}{\partial y^{2}}
\end{array}\right]=\left[\begin{array}{ll}
1 & 0 \\
0 & 5
\end{array}\right] \\
\vec{X}_{0}=\left[\begin{array}{l}
5 \\
1
\end{array}\right], \vec{X}_{1}=\vec{X}_{0}-H^{-1} \nabla f\left(\vec{X}_{0}\right)=\left[\begin{array}{l}
5 \\
1
\end{array}\right]-\left[\begin{array}{ll}
1 & 0 \\
0 & \frac{1}{5}
\end{array}\right]\left[\begin{array}{l}
5 \\
5
\end{array}\right]=\left[\begin{array}{l}
0 \\
0
\end{array}\right]
\end{gathered}
$$

Comments: Newton's method

- Converges quadratically near the optimum
- Sensitive to initial point
- Requires matrix inversion
- Requires first and second order derivatives

