

Multi-D optimization problem

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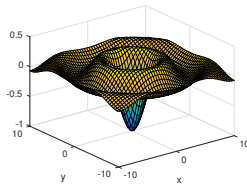
The College of William & Mary



Lecture 16

Notes

Multi-D optimization



Find \vec{x} that minimizes $E(\vec{x})$ subject to $g(\vec{x}) = 0, h(\vec{x}) \leq 0$

\vec{x} design variables

$E(\vec{x})$ merit or objective or fitness or energy function

$g(\vec{x})$ and $h(\vec{x})$ constrains

It is easy to see that the maximization problem is the same as minimization once $E(\vec{x}) \rightarrow -E(\vec{x})$.

Notes

Solution with Matlab built in Multi-D minimization - fminsearch

```
[x, fval] = fminsearch(fun, x0)
```

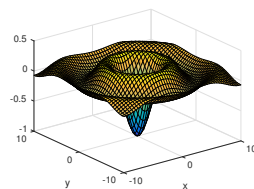
- fun handle to the multi-variable function
- x0 initial 'guess' (vector)
- x optimum position vector
- fval value of the function at the optimum

Notes

fminsearch - usage example

Example

```
function ret=fsample_sinc(v)
x=v(1); y=v(2);
r=sqrt(x^2+y^2);
ret= -sin(r)/r;
end
```



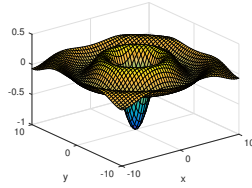
```
x0vec=[0.5, 0.5];
[xResVec,zopt]=fminsearch(@fsample_sinc, x0vec)
xResVec = [0.2852e-4, 0.1043e-4]
zopt = -1.0000
```

Notes

It is easy to miss global minimum

Example

```
function ret=fsample_sinc(v)
x=v(1); y=v(2);
r=sqrt(x^2+y^2);
ret= -sin(r)/r;
end
```



Example

```
x0vec=[5, 5];
[xResVec,zopt]=fminsearch(@fsample_sinc, x0vec)
xResVec = [ 5.6560  5.2621 ]
zopt = -0.1284
```

Sample problem 1

Find the minimum of the function

$$F(x, y, z) = 2x^2 + y^2 + 2z^2 + 2xy + 1 - 2z + 2xz$$

Notes

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Sample problem 1

Find the minimum of the function

$$F(x, y, z) = 2x^2 + y^2 + 2z^2 + 2xy + 1 - 2z + 2xz$$

$$F(x, y, z) = (x + y)^2 + (x + z)^2 + (z - 1)^2$$

Minimum is $[x, y, z] = [-1, 1, 1]$

Notes

Sample problem 2: Potential well

Consider a 1D potential well with the following potential

$$U(x) = \begin{cases} \infty & : x < 0 \\ 0 & : x \leq L \\ U_0 & : x > L \end{cases}$$

The wave function for this problem

$$\Psi(x) = \begin{cases} 0 & : x < 0 \\ \sin(kx) & : x \leq L \\ Be^{-\alpha x} & : x > L \end{cases}$$

Quantum Mechanics requires that $k = \frac{\sqrt{2m(E-U_0)}}{\hbar}$ and $\alpha = \frac{\sqrt{2m(U_0-E)}}{\hbar}$

We know that Ψ function must be continuous and differentiable

$$\begin{aligned} \Psi_{in}(L) &= \Psi_{out}(L) \\ \Psi'_{in}(L) &= \Psi'_{out}(L) \end{aligned}$$

Suppose that we somehow know k . What are the values for α and B ?

Notes

Sample problem 2: Potential well (cont)

Instead of solving the system of linear equations

$$\begin{aligned}\Psi_{in}(L) &= \Psi_{out}(L) \\ \Psi'_{in}(L) &= \Psi'_{out}(L)\end{aligned}$$

Let's construct merit function

$$M(\alpha, B) = (\Psi_{in}(L) - \Psi_{out}(L))^2 + (\Psi'_{in}(L) - \Psi'_{out}(L))^2$$

Notes

Sample problem 2: Potential well (cont)

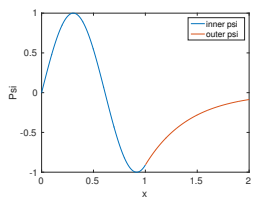
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$$M(\alpha, B) = (\Psi_{in}(L) - \Psi_{out}(L))^2 + (\Psi'_{in}(L) - \Psi'_{out}(L))^2$$

```
k=2+pi; L=1;
merit=@(v) merit_psi(v, k, L);
v0=fminsearch(...
    @merit, [.11,1])
v0 = 2.3531 -9.5640
% alpha B
```



Notes

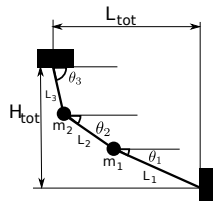
Sample problem 3: hanging weights

Consider masses m_1 and m_2 suspended by strings with length L_1 , L_2 , and L_3 . Find the angles θ_1 , θ_2 , and θ_3 .

We need to minimize potential energy subject to the length constraints. See merit function in the file 'EconstrainedSuspendedWeights.m'

For the following initial conditions

```
m1=2; m2=2;
L1=3; L2=2; L3=3;
Ltot=4; Htot=0;
```



Notes

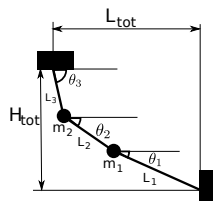
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The answer should be close to $\theta_1 = -1.231$; $\theta_2 = 0$; $\theta_3 = 1.231$;

```
theta = fminsearch (@EconstrainedSuspendedWeights,
    [-1,0,-1], optimset('TolX',1e-6))
theta = -1.2321 -0.0044 1.2311
```

Notes
