Multi-D optimization problem

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Lecture 14

Find \( \vec{x} \) that minimize \( E(\vec{x}) \) 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

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

Solution with Matlab built in Multi-D minimization - \textit{fminsearch}

\[
[x, fval] = \text{fminsearch}(\text{fun}, x0)
\]

fun handle to the multi-variable function

x0 initial 'guess' (vector)

x optimum position vector

fval value of the function at the optimum

Example

\[
\text{function ret=fsample_sinc(v)}
\]

\[
x=v(1); \quad y=v(2);
\]

\[
r=\sqrt{x^2+y^2};
\]

\[
\text{ret} = \frac{-\sin(r)}{r};
\]

end

x0vec=[0.5, 0.5];

[xResVec, zopt] = fminsearch(@fsample_sinc, x0vec)

xResVec = [0.2852e-4, 0.1043e-4]

zopt = -1.0000
It is easy to miss global minimum

Example

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

Example

```matlab
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

\[ F(x, y, z) = 2x^2 + 2y^2 + z^2 + 2xy + 1 - 2y + 2xz \]

Minimum is \([x, y, z]=[-1, 1, 1]\)

Sample problem 2: Potential well

Consider a 1D potential well with the following potential

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

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 \( k = \sqrt{2m(U_0 - E)} \) and \( \alpha = \sqrt{2mU_0} \)

We know that \( \psi \) function must be continuous and differentiable

\[ \psi_0(L) = \psi_{out}(L) \\
\psi'_0(L) = \psi'_{out}(L) \]

Suppose that we somehow know \( k \). What are the values for \( \alpha \) and \( B \)?
Sample problem 2: Potential well (cont)

Instead of solving system of linear equations
\[ \Psi_{\text{in}}(L) = \Psi_{\text{out}}(L) \]
\[ \Psi'_{\text{in}}(L) = \Psi'_{\text{out}}(L) \]

Let's construct merit function:
\[ M(\alpha, B) = (\Psi_{\text{in}}(L) - \Psi_{\text{out}}(L))^2 + (\Psi'_{\text{in}}(L) - \Psi'_{\text{out}}(L))^2 \]

\[ k = 5.1416; L = 1; \]
\[ v_0 = fminsearch(...@merit_psi, [.11,1]) \]
\[ v_0 = 2.3531 -9.5640 \]

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 \( \theta_1 \), \( \theta_2 \), and \( \theta_3 \).

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

For the following initial conditions:
\[ m_1 = 2; m_2 = 2; \]
\[ L_1 = 3; L_2 = 2; L_3 = 3; \]
\[ L_{\text{tot}} = 4; H_{\text{tot}} = 0; \]

The answer should be close to \( \theta_1 = -1.231; \theta_2 = 0; \theta_3 = 1.231 \).

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