CS 230, Quiz 4

Solutions

You will have 15 minutes to complete this quiz. This quiz contains 2 problems of equal value; **only the highest-scoring question will contribute to your grade**. Choose carefully.

Problem 1 (4 points)

The Lennard-Jones potential is simple model describing the interaction between two molecules. With this model, two molecules have potential energy ϕ given by

$$\phi(r) = 4\epsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right),$$

where ϵ and σ are constants and $r = \|\mathbf{x}_1 - \mathbf{x}_2\|$ is the distance between two molecules at locations $\mathbf{x}_1$ and $\mathbf{x}_2$. Find the force $\mathbf{f}_1$ felt by the molecule at $\mathbf{x}_1$ as a result of this interaction.

$$
\begin{aligned}
r &= \|\mathbf{x}_1 - \mathbf{x}_2\| \\
\frac{\partial r}{\partial \mathbf{x}_1} &= \frac{\mathbf{x}_1 - \mathbf{x}_2}{\|\mathbf{x}_1 - \mathbf{x}_2\|} \\
\phi(r) &= 4\epsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right) \\
\phi(r) &= 4\epsilon\left(\frac{\sigma^{12}}{r^{12}} - \frac{\sigma^{6}}{r^{6}}\right) \\
\phi'(r) &= 4\epsilon\left(-12\frac{\sigma^{12}}{r^{13}} + 6\frac{\sigma^{6}}{r^{7}}\right) \\
V(\mathbf{x}_1, \mathbf{x}_2) &= \phi(r) \\
\mathbf{f}_1 = -\frac{\partial}{\partial \mathbf{x}_1} V(\mathbf{x}_1, \mathbf{x}_2) &= -\frac{\partial}{\partial \mathbf{x}_1}\phi(r) \\
&= -\phi'(r)\frac{\partial r}{\partial \mathbf{x}_1} \\
&= -4\epsilon\left(-12\frac{\sigma^{12}}{r^{13}} + 6\frac{\sigma^{6}}{r^{7}}\right)\frac{\mathbf{x}_1 - \mathbf{x}_2}{\|\mathbf{x}_1 - \mathbf{x}_2\|} \\
&= \frac{24\epsilon}{r}\left(2\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right)\frac{\mathbf{x}_1 - \mathbf{x}_2}{\|\mathbf{x}_1 - \mathbf{x}_2\|}
\end{aligned}
$$

Problem 2 (4 points)

In class, we saw a few schemes for solving the differential equation $x' = f(x)$, where the function $f(x)$ is given. One of these was the midpoint rule, which is *implicit*. We analyzed the stability by considering the differential equation $x' = -\lambda x$ with $\lambda > 0$, where we found $x^{n+1} = Ax^n$ for some number A that depended on λ and Δt. We then concluded that the method would be stable if $|A| < 1$. There is also an *explicit* midpoint rule, which is given by the rule

$$x^{n+1} = x^n + \Delta t f\left(x^n + \frac{\Delta t}{2} f(x^n)\right).$$

(a) If we apply this scheme to $x' = -\lambda x$, show that $x^{n+1} = Ax^n$ for some number A; find A (it should depend on λ and Δt). (b) What restrictions are required of Δt so that $|A| < 1$?

$$\begin{aligned}
x^{n+1} &= x^n + \Delta t f\left(x^n + \frac{\Delta t}{2} f(x^n)\right) \\
x^{n+1} &= x^n + \Delta t(-\lambda)\left(x^n + \frac{\Delta t}{2}(-\lambda)x^n\right) \\
x^{n+1} &= x^n - \Delta t\lambda\left(x^n - \frac{\Delta t}{2}\lambda x^n\right) \\
x^{n+1} &= x^n - \Delta t\lambda x^n + \frac{\Delta t^2}{2}\lambda^2 x^n \\
x^{n+1} &= \left(1 - (\Delta t\lambda) + \frac{1}{2}(\Delta t\lambda)^2\right)x^n \\
A &= 1 - (\Delta t\lambda) + \frac{1}{2}(\Delta t\lambda)^2 \\
-1 &< 1 - (\Delta t\lambda) + \frac{1}{2}(\Delta t\lambda)^2 < 1 \\
-2 &< 2 - 2(\Delta t\lambda) + (\Delta t\lambda)^2 < 2 \\
-3 &< 1 - 2(\Delta t\lambda) + (\Delta t\lambda)^2 < 1 \\
-3 &< (\Delta t\lambda - 1)^2 < 1
\end{aligned}$$

The first inequality is trivial. The second inequality implies

$$\begin{aligned}
-1 < \Delta t\lambda - 1 < 1 \\
0 < \Delta t\lambda < 2 \\
0 < \Delta t < \frac{2}{\lambda}
\end{aligned}$$