ECE 595 (Numerical Simulations) - Quiz 1 Solution

Friday, March 22, 2013

1. Provide 3 examples of numerical problems in class **P**.

- CONNECTED: the set of all connected graphs
- TRIANGLEFREE: the set of all graphs without a triangle
- BIPARTITE: the set of all bipartite (distinct) graphs
- TREE: the set of all trees

2. Provide 3 examples of numerical problems in class **NP**.

- Independent set
- Traveling salesman
- Linear programming
- Composite numbers
- Prime factorization

3. Provide 2 examples of **NP** problems that can be solved in **P** time.

- Connectivity: breadth-first search
- Composite numbers
- Linear programming

4. Is Gauss-Jordan elimination more stable with or without pivoting, and why?

With pivoting. Otherwise, one may have nearly zero values in diagonal elements, which go into the denominator of the solutions.

5. What is the significance of Crout's algorithm?

Allows one to perform an LU decomposition in place, which can assist with processes such as matrix inversion.

6. What is the fastest and simplest numerical algorithm to find the largest eigenvalue of a generalized square matrix?

The power method.

7. Name three reasonable strategies for diagonalizing a generalized square matrix.

- Jacobi transformation
- QR/QL factorization methods
- Householder transformation

8. How quickly can the Newton-Raphson method converge on a root with a sufficiently good guess?

In the best case, in one step; more generally, quadratically convergent (increasing accuracy one significant figure per step).

9. Does Brent's method always converge in 1D, and why?

For root-finding, it does, because it combines the speed of fitting with the reliability of bracketing.

10. Is optimization faster for convex or non-convex problems, and why?

Convex optimization is faster because one can be guaranteed to have only a single solution, and can employ fast algorithms such as Newton's method to find the zeros of the derivative.

11. How can a Laplacian operator be represented as a matrix? Please indicate the basis used.

In the real-space representation in 1D:

$$\nabla^2 = \frac{1}{h^2}\begin{pmatrix} -2 & 1 & 0 & 0 & \cdots \\ 1 & -2 & 1 & 0 & \cdots \\ 0 & 1 & -2 & 1 & \ddots \\ \vdots & \vdots & \ddots & \ddots & \ddots \end{pmatrix} \tag{1}$$

12. What theorem allows us to use discrete Fourier transforms much like the continuous versions?

The sampling theorem.

13. What are three reasonable methods to identify resonant frequencies in discrete time data?

- Fourier transforms
- Fast-fourier transforms
- Filter diagonalization

14. With the beam propagation method: when is it appropriate to drop the second-order derivative in the z-direction?

When propagation in the z-direction is fairly uniform (i.e., no wide-angle branches).

15. Give two examples of finite element shape functions in 1D.

- Lagrange functions
- Quadratic function

16. What are two physical effects that allow one to tune the performance of optical devices?

- Electro-optic effect (Pockels or Kerr)
- Liquid-crystal electrostatic tuning

17. Why would one use the Scharfetter-Gummel scheme to solve for current transport?

Debye screening causes exponential decay of electrostatic charge, making the Brillouin function a better fit than a linear function for the electrostatic potential.

18. How do you construct reciprocal lattice vectors in 3D?

$$V = \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3) \tag{2}$$
$$\vec{b}_1 = \frac{2\pi}{V}(\vec{a}_2 \times \vec{a}_3) \tag{3}$$
$$\vec{b}_2 = \frac{2\pi}{V}(\vec{a}_3 \times \vec{a}_1) \tag{4}$$
$$\vec{b}_3 = \frac{2\pi}{V}(\vec{a}_1 \times \vec{a}_2) \tag{5}$$
$$G = m\vec{b}_1 + p\vec{b}_2 + q\vec{b}_3 \tag{6}$$

19. What is the tight-binding method?

The tight-binding method solves bandstructures with a linear combination of atomic orbitals, such that

$$\psi_{\vec{k}}(\vec{r}) = \frac{1}{\sqrt{N}} \sum_j e^{i\vec{k}\cdot\vec{r}_j} \phi(\vec{r} - \vec{r}_j) \tag{7}$$

20. What do LDA and GGA represent in density functional theory?

- LDA = local density approximation
- GGA = generalized gradient approximation