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Intro to Radiotherapy Computer Dose Algorithms

MATLAB Student Course

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Exercise I: Variables and Functions

Write a MATLAB function to calculate and return the linear stopping power S (MeV/cm) of a proton with any kinetic energy E (MeV) stopping in a graphite absorber. Use the Bethe-Bloch equation given below.

If you have time, include a logic test so the function will return `-1` if the relativistic particle velocity β is less than 0.1 (indicating the calculation is not valid). Compare your calculations for proton $E = 10$, 100, 500, and 1000 MeV with the NIST PSTAR program results (see web address below).

Bethe-Bloch Equation (Leo 1994, without shell and density effect corrections)

$$S = 2\pi N_a r_e^2 m_e c^2 \rho \frac{Z}{A}\frac{z^2}{\beta^2}\left[\ln(\frac{2m_e c^2\gamma^2\beta^2 W_{\max}}{I^2}) - 2\beta^2\right],$$

where

$$\begin{aligned}
N_a &= \text{Avogadro's number} = 6.022 \times 10^{23}\ \text{mol}^{-1},\\
r_e &= \text{classical electron radius} = 2.817 \times 10^{-13}\ \text{cm},\\
m_e &= \text{rest mass of electron} = 0.511\ \text{MeV/c}^2,\\
c &= \text{speed of light},\\
\rho &= \text{density of absorber (graphite)} = 1.7\ \text{g/cm}^3,\\
Z &= \text{atomic number of absorber (graphite)} = 6,\\
A &= \text{atomic mass of absorber (graphite)} = 12.01\ \text{u},\\
z &= \text{charge of incident particle (proton)} = 1,\\
\beta &= \text{velocity of incident particle } (\nu/c) = \sqrt{1-(m_o c^2/(E+m_o c^2))^2},\\
m_o &= \text{rest mass of incident particle (proton)} = 938.272\ \text{MeV/c}^2,\\
\gamma &= (E+m_o c^2)/(m_o c^2),\\
W_{\max} &= \text{maximum energy transfer in a single collision (see following)},\\
I &= \text{mean excitation potential of absorber (carbon)} = 78.0\ \text{eV},
\end{aligned}$$

and

$$W_{\max} = \frac{2m_e c^2 \eta^2}{1 + 2s\sqrt{(1+\eta^2)} + s^2},$$

and

$$\begin{aligned} \eta &= \beta\gamma, \\ s &= m_e/M, \\ M &= \text{incident particle mass (proton)} = 938.272\ \text{MeV/c}^2. \end{aligned}$$

References

- Leo, W. R., 1994. Techniques for Nuclear and Particle Physics Experiments, 2nd ed., Springer-Verlag. Page 24.

- `http://physics.nist.gov/PhysRefData/Star/Text/PSTAR.html`

Exercise II: Conditional Statements and Visualization

1. Plot the linear stopping power $S(E)$ of a proton stopping in graphite as a function of energy from E = 0 to 1000 MeV with 1 MeV increments. Use a `for` loop and store E and $S(E)$ in 1D arrays. *Note: If you have implemented the logic test in Exercise 1, you should see on your plot where the proton velocity is below the accurate range of the Bethe-Bloch equation. If you have not implemented this, just plot E from 10 to 1000 MeV.*

2. Plot linear stopping power as a function of depth in a graphite slab for a 500 MeV proton. You should see a Bragg peak distribution. Use a `while` loop to iterate over 0.01 cm depth resolution (ΔZ) until the proton energy drops below 10 MeV. Subtract energy loss per step from the proton in each iteration ($\Delta E = S(E)\Delta Z$).

Exercise III: Monte Carlo Radiation Transport Simulations

1. Write a Monte Carlo function to return a randomly-sampled distance t_i (cm) to first interaction for a 100 keV photon incident (normal) on a uniform slab of aluminum. Use the MATLAB pseudo-random number generator `rand` to produce a number ρ_i between 0 and 1. The cumulative probability distribution

$$F(t) = 1 - \exp(-\mu t)$$

gives the probability (ranging from 0 to 1) that a photon has interacted by distance t in the aluminum slab. The randomly-sampled distance to interaction t_i can be calculated using a randomly generated number ρ_i (from 0 to 1) and inverting the cumulative probability distribution

$$t_i = F^{-1}(\rho_i) = -\ln(1-\rho_i)/\mu,$$

where

$$\mu = \text{probability interaction per unit thickness (100 keV, Al)} = 0.462 \text{ cm}^{-1}.$$

2. Write a Monte Carlo code to randomly sample the Compton scatter angle Θ_i of a photon scattering in aluminum using the Klein-Nishina equation for the differential scattering cross section $\partial\sigma/\partial\Omega$ (Knoll 2000). Implement this as a MATLAB function that accepts photon kinetic energy E (MeV) and atomic number Z of the scattering material and returns both the random scatter angle Θ_i (radians) and the corresponding energy lost ΔE_i (MeV) during the interaction. Recall the Compton scatter equations

$$f(\Theta) = \frac{\partial\sigma}{\partial\Omega} = Zr_o^2\left(\frac{1}{1+\alpha(1-\cos\Theta)}\right)^2\left(\frac{1+\cos^2\Theta}{2}\right)\left(1+\frac{\alpha^2(1-\cos\Theta)^2}{(1+\cos^2\Theta)[1+\alpha(1-\cos\Theta)]}\right)$$

where

$$\begin{aligned} Z &= \text{atomic number}, \\ r_o &= \text{classical electron radius} = 2.817 \times 10^{-13} \text{ cm}, \\ \alpha &= E/(m_o c^2), \end{aligned}$$

and

$$E' = \frac{E}{1+(E/m_o c^2)(1-\cos\Theta)}.$$

Instead of the cumulative probability function inversion method used in part 1, use the Rejection Method (Schultis and Faw 2000) which does not require integration or inversion. It will be necessary to first determine the maximum value M of the Klein-Nishina cross section $\partial\sigma/\partial\Omega$ on the interval from 0 to π. Once you have determined M for the given photon energy and scattering material (Z), use the following rejection method.

(a) Generate a random number ρ_i between 0 and 1.

(b) Let $\Theta_i = a + \rho_i(b-a)$, with $a = 0$ and $b = \pi$.

(c) Generate a second random number ρ_j.

(d) If $\rho_j M \leq f(\Theta_i)$, accept Θ_i, otherwise reject Θ_i and return to step 1.

3. Using your functions, for 1000 histories of 100 keV photons in aluminum, tally (1) distance to first interaction (in cm), and (2) the angle of Compton scatter (in radians). Ignore competing

interactions such as photoelectric absorption in this implementation. Create histograms to display your data. If you have time, generate a polar plot of the scatter angles.

References

- Schultis, J. K. and Faw, R. E., 2000. Radiation Shielding, American Nuclear Society. Page 408-30.
- Metcalfe, P., Kron, T., and Hoban, P., 2007. The Physics of Radiotherapy X-rays and Electrons, Medical Physics Publishing. Page 619-50.

Recommended Monte Carlo Codes

- MCNPX, `http://mcnpx.lanl.gov`
- EGSnrc, `http://irs.inms.nrc.ca/software/egsnrc`
- Geant4, `http://www.geant4.org/geant4`

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Introduction to Radiotherapy Computer Dose Algorithms

Intro to Monte Carlo Method

Objective

- Calculate an accurate dose to a patient in a radiation field

- Difficulties
  - Patient is heterogeneous material w/ irregular geometry
  - Radiation fields often contain mixed particle types w/ wide range of energies & often produce 2° particles and/or activate matter

Ideal dose calculation

- Accounts for heterogeneous patient composition
- Considers all radiation particles and all possible physical interactions

This field of study is Radiation Transport Theory

Possible approaches

1) Make gross approximations to simplify calculations
   - e.g., patient is a sphere of water and we only consider energy loss of 1° radiation type
   - Advantages: Fast, easy to implement, dose calculation possible in seconds

Deterministic Approach

2) Assemble a very large differential equation to describe all possible physical interactions for the particle spectrum and patient anatomy
   - Linearized Boltzmann Transport Equation
   - Typically, so many variables are needed to accurately describe the radiation field (and patient anatomy) that the differential equations are almost impossible to solve
   - Uncharged particles (photons & neutrons) work fairly well, charged particles harder to solve

Possible approaches (continued)

3) Stochastic Approach

Monte Carlo Method

- Assemble a very long list of all possible physical interactions for all particle types and all geometries & materials (of the patient)
- Don't write 1 large equation to describe everything
- Instead, focus on having very accurate equations for individual interactions and probabilities of interaction
- Stochastically simulate the (random) behavior of a single particle as it traverses matter
  - track length b/w interactions
  - probabilities of different interaction types
  - energy loss & direction changes
  - Use self-contained (highly accurate) equations to model each step

(e.g. energy loss in a voxel)

- Repeat simulations for large numbers of particles and look at average behavior

Monte Carlo Overview

- Define initial conditions
  - particle types ($p, e^-, n, \gamma \ldots$)
  - energy distributions
  - direction
- Define geometry and materials radiation will interact with (e.g., patient)
  - Any coordinate system may be used, pick simplest
- Define physics interaction types
  - Analytical models
  - Measured cross-section libraries
- Define tallies
  - Points or volumes at which to record properties of the radiation field (e.g. energy deposition, 2° neutron fluence, ...)
  - Tallies may be single volumes, or meshes, concentric rings, etc..
  - Use symmetry to your advantage (increased volume $\Rightarrow$ increased counts $\Rightarrow$ better statistics)
- Simulate histories of incident particles
  - track 2° particles also
  - repeat until statistics are good

Typical flowchart to calculate 1 history

1) Select an incident particle type, kinetic energy, and direction (randomly sample this from distribution if you have a mixed particle field)

2) Determine geometry & materials the particle will interact with (ρ, Z, A, mixtures . . .)

3) Calculate distance to 1st interaction
   - Generate a pseudo random number
   - Randomly sample the probability distribution that a particle reaches depth w/out interaction

     (e.g., $f(x) = e^{-\mu x}$)

     $\mu \equiv$ total linear attenuation coefficient

4) Determine type of 1st interaction
   - If competing interactions, randomly sample the probability of each interaction type

5) Calculate effect of interaction
   - ΔE, change in direction (again, randomly sample these angular distributions & energy loss)
   - If any 2° particles are generated, store particle type, kinetic energy, & direction & calculate histories for these (at a later time)

6) If interactions occur within the bounds of a tally, record the interaction data

Typical flowchart to calculate 1 history (continued)

7) Repeat process (distance to next interaction + interaction type) until kinetic energy of initial particle is entirely lost (or falls below a threshold at which the remaining range or dosimetric effect is negligible)

8) Repeat process for all 2° particles generated along the way

END Calculate 1 history

Uncertainties

- Events such as energy deposition in a tally voxels are often random + follow Poisson statistics

$$\therefore \quad \sigma \propto \frac{1}{\sqrt{N}}$$

- Typically must quadruple the number of histories to reduce uncertainty by a factor of 2

and hence computation time

Random Numbers

- ideally have random access to an infinite set of numbers b/w 0 & 1
- Practically, a very large repository of random integers will work
  - for integers from 1 to N, divide by N
- Also, sequentially generated pseudorandom numbers are most practical approach (& works well if you have a good pseudorandom # generator)
- MATLAB and other software packages typically have pseudorandom number generators
  - these are most likely inadequate for Monte Carlo dose calculations
- If you are serious about writing your own Monte Carlo code, read up on mathematical methods to produce pseudorandom numbers

(Today, we will just use MATLAB's rand function) for example

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Stochastic Sampling Method: Invert Cumulative Distribution Function

Background

- Consider a probability Density Function (PDF), $\underline{\underline{f(x)}}$ where $f(x)$ is limited to a range from a to b
- The probability that x lies b/w a & b is written

$$P\{a < x < b\} = \int_a^b f(x)\, dx$$

- Related to the PDF, a cumulative probability distribution (CPD) $\rightarrow \underline{\underline{F(x)}}$ is written

$$F(x) = \int_a^x f(x')\, dx'$$

and the probability that a randomly selected value of x is less than x_1 is given by $F(x_1)$

Method

1) Normalize $f(x)$ so that $F(a) = \emptyset$ & $F(b) = 1$
   (equivalently $P\{a < x < b\} = 1$)
2) Select a number ρ_i randomly b/w 0 & 1
3) Invert CPD, $F(x_i) = \rho_i \implies \boxed{x_i = F^{-1}(\rho_i)}$
   to solve a randomly sampled x_i

Stochastic Sampling Method: Invert CPD - Example

e.g., To compute distance to 1st interaction

- The PDF that a particle reaches a depth t in a material without interaction is

$$f(t) = \mu e^{-\mu t}$$

- The corresponding CPD gives the probability that a random interaction ~~depth~~ will occur at a depth less than t

$$F(t) = 1 - e^{-\mu t} \left(= \int_{\emptyset}^{t} \mu e^{-\mu t'} dt' \right)$$

- Here the limits of interaction depth would be $\emptyset$ & $+\infty$

$$\underbrace{F(t=\emptyset) = \emptyset \quad \& \quad F(t \Rightarrow \infty) = 1}$$

Good, this means we can use a random number ρ_i b/w $\emptyset$ & 1

- Invert the CPD to find the depth of a random interaction (t_i) for a given random # ρ_i

$$\boxed{t_i = F^{-1}(\rho_i) = -\ln(1-\rho_i)/\mu}$$

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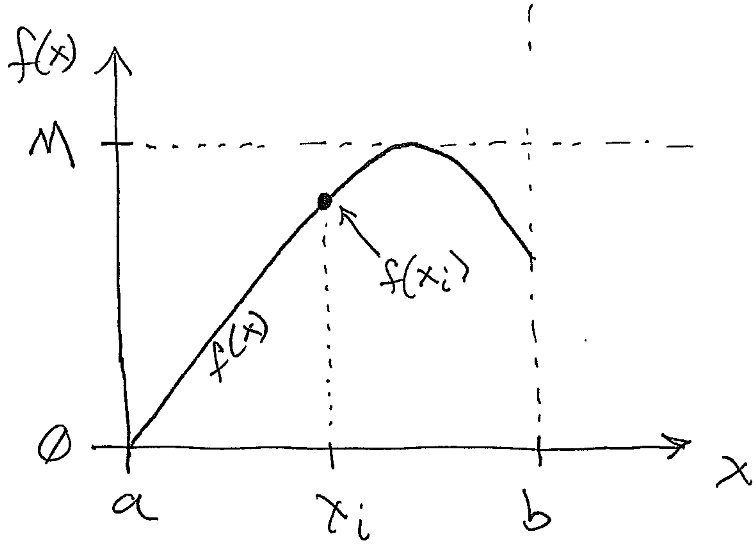
Stochastic Sampling Method: Rejection Method

- Use when PDF $f(x)$ cannot be integrated analytically <u>or</u> if $F^{-1}(\rho_i)$ is difficult to determine analytically

e.g.,



Rejection Method

1) Generate a random number $\underline{\rho_i}$ b/w 0 + 1

2) Let $x_i = a + \rho_i(b-a)$ [not done yet, haven't used PDF yet]

   a = lower band of x to sample
   b = upper band of x

3) Select another random number ρ_j

4) If $\rho_j M \le f(x_i)$, accept x_i, otherwise reject x_i and return to step $\underline{1}$

Optimization overview

Iterations of minimization

1) evaluate objective function

$$\chi^2(\vec{N})$$

2) Calculate search direction

$$-\nabla \chi^2(\vec{N})$$

3) perform a line search along search direction to find 1-D minimum of $\chi^2(\vec{N})$

4) Repeat until $\chi^2(\vec{N})$ converges to minimum

$\boxed{\text{crude pencil beam dose algorithm}}$

N pencil beams

$$D(x,y,z) = \sum_{i=1}^{N} f N_i \, g(z) \, f(x,y,z)$$

depth in water

$f \equiv$ particle number to dose conversion factor

$N_i \equiv$ number of particles in the ith pencil beam

$g(z) \equiv$ central axis depth dose (broad beam)

$f(x,y,z) \equiv$ off axis term

e.g.,

$$f(x,y,z) = e^{\frac{-(x^2+y^2)}{2\,\sigma(z)^2}}$$

Gaussian $\sigma(z)$ comes from Multiple Coulomb Scattering

Objective function

$$\boxed{\chi^2(\vec{N}) = \sum_{k \in \text{target}} W_T\left(D_{\text{prescribed}} - D_k(\vec{N})\right)^2 + \sum_{k \in OAR} W_{OAR}\left(D_k(\vec{N})\right)^2}$$

organ at risk

Assumes any dose in OAR is bad

$W \equiv$ weights for target coverage vs. OAR sparing

Derivative of objective function W.R.T. N_i for all pencil beams i gives the

Search direction for 1 iteration of minimization.

$$\boxed{-\nabla \chi^2(\vec{N})}$$

Line Search

(Golden Search in One Dimension
Press et al. 2007, Numerical Recipes, 3rd. ed.)

$F \equiv$ objective function

$\vec{N} \equiv$ vector of particle numbers for each pencil beam

Use $F(\vec{N}) \Rightarrow$ evaluation of objective function

$+$ $\nabla F(\vec{N}) \Rightarrow$ gradient of objective function

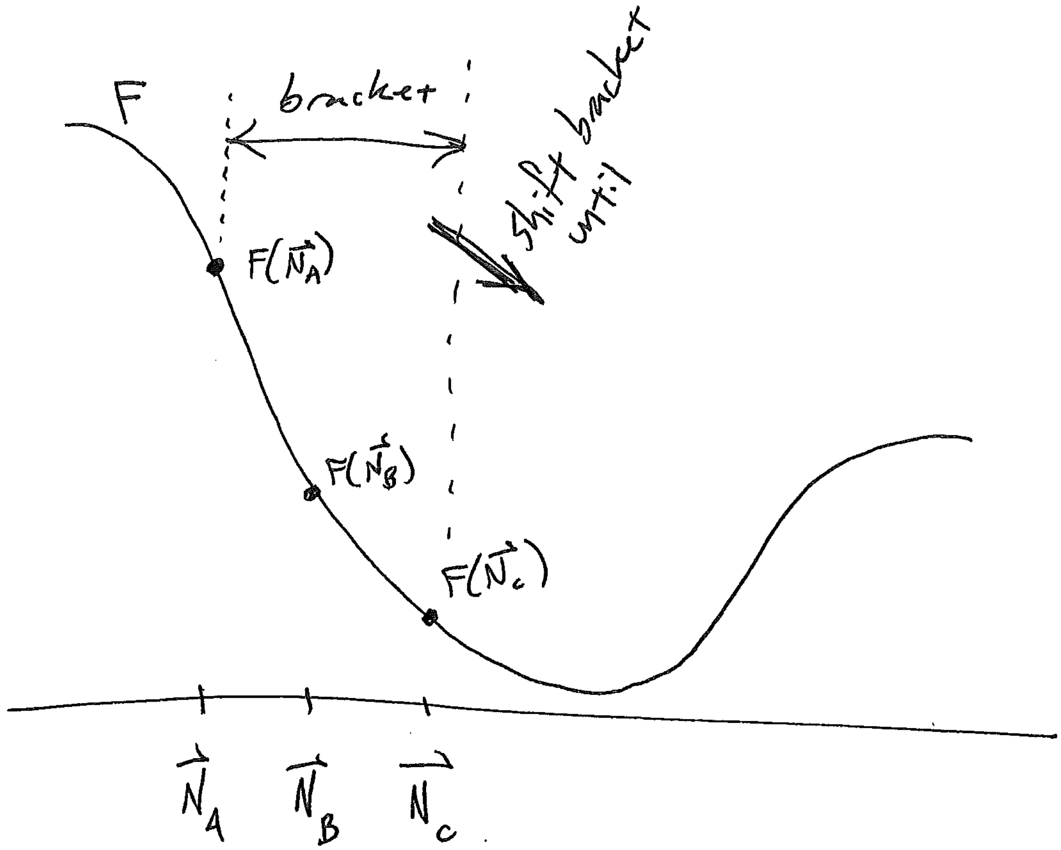
(derivatives W.R.T. particle numbers for each pencil beam)

1) Evaluate $F(\vec{N}_A)$ at first particle numbers $\vec{N}_A$

2) Step $$\vec{N}_B = \vec{N}_A - \underbrace{\Delta n}_{\text{Stepsize}} \underbrace{\nabla F(\vec{N}_A)}_{\text{vector of derivatives of } F \text{ with respect to } N_i}$$

3) Evaluate $F(\vec{N}_B)$

4) Initial $F(\vec{N}_c) = \vec{N}_A - 2\,\Delta n \nabla F(\vec{N}_A)$



5) $a \equiv$ amplifier, for golden search

$a = 1.61$ (golden ratio)

6) while $F(\vec{N}_c)$ is decreasing, advance bracket A, B, C

e.g., while $F(\vec{N}_c) <= F(\vec{N}_B)$

$$\vec{N}_A = \vec{N}_B$$

$$\vec{N}_B = \vec{N}_c$$

$$\vec{N}_c = \vec{N}_B - (\Delta n)(a) \overbrace{\nabla F(\vec{N}_A)}^{\text{search direction vector}}$$

Calc $F(\vec{N}_c)$

end $\quad a = a \times a$

7) After while loop stops,
Now, $F(\vec{N}_B)$ is at a minimum of $F(\vec{N})$

with particle numbers $\underline{\underline{\vec{N}_B}}$