Hawes ①

Lecture #23 - Multidimensional Green's Functions and Probability

I. Green's Functions in Multiple Dimensions

A. Basic Properties

1. Many properties carry over from the 1D case.

2. Definition: $\boxed{\mathcal{L}\, G(\underset{\sim}{r}, \underset{\sim}{r}') = \delta(\underset{\sim}{r} - \underset{\sim}{r}')}$

 a. Here $\delta(\underset{\sim}{r} - \underset{\sim}{r}') = \delta(x - x')\,\delta(y - y')\,\delta(z - z')$

3. Hermitian 2nd-order PDE:

$$\mathcal{L}\,\psi(\underset{\sim}{r}) = \nabla \cdot \left[p(\underset{\sim}{r})\,\nabla\psi(\underset{\sim}{r})\right] + q(\underset{\sim}{r})\,\psi(\underset{\sim}{r}) = f(\underset{\sim}{r})$$

4. Solution to $\mathcal{L}\,\psi(\underset{\sim}{r}) = f(\underset{\sim}{r})$:

$$\psi(\underset{\sim}{r}) = \int G(\underset{\sim}{r}, \underset{\sim}{r}')\, f(\underset{\sim}{r}')\, d^3\underset{\sim}{r}'$$

NOTE: $\underset{\sim}{r}$ is held constant
$\underset{\sim}{r}'$ is variable of integration.

5. If $\mathcal{L}\,\psi(\underset{\sim}{r}) = \lambda\,\psi(\underset{\sim}{r})$ defines a Hermitian eigenvalue problem with eigenfunctions $\phi_n(\underset{\sim}{r})$ and eigenvalues λ_n, then

 a. Symmetric: $G(\underset{\sim}{r}, \underset{\sim}{r}') = G^*(\underset{\sim}{r}', \underset{\sim}{r})$

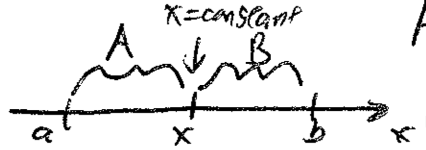
 b. Eigenfunction Expansion: $G(\underset{\sim}{r}, \underset{\sim}{r}') = \sum_n \dfrac{\phi_n^*(\underset{\sim}{r}')\,\phi_n(\underset{\sim}{r})}{\lambda_n}$

6. a. $G(\underset{\sim}{r}, \underset{\sim}{r}')$ is continuous and differentiable at all points $\underset{\sim}{r} \neq \underset{\sim}{r}'$.

 b. $G(\underset{\sim}{r}, \underset{\sim}{r}')$ has singularities in first derivatives so that second-order operator $\mathcal{L}$ generates the necessary delta function ((2) above).

I. (Continued)

B. Differences from 1D Case



1. Division into intervals $a<x'<x$, $x<x'<b$

a. In the multi-dimensional case, one may not simply divide in to two intervals!

2. Specific forms of solution (such as solution for constant A) do not apply!

3. Ex: 3D Laplacian

a. Obtain Green's Function for convenient BC's.

b. Then, add solution to homogeneous equation $\mathcal{L}\psi(\mathbf{r})=0$ to satisfy required BC's.

c. $(\nabla')^2 G(\mathbf{r},\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}')$ where $\lim_{\mathbf{r}'\to\infty} G(\mathbf{r},\mathbf{r}')=0.$

operates on r' variable!

d. NOTE: i) BCs are spherically symmetric and at an infinite distance from both $\mathbf{r}$ and $\mathbf{r}'$

ii) We may make simplifying assumption $G(\mathbf{r},\mathbf{r}')$ is a function only of $\delta r = |\mathbf{r}-\mathbf{r}'|$

iii) Then we can divide region along 1D variable δr.

e. Following this strategy, we may obtain

$$\boxed{G(\mathbf{r},\mathbf{r}') = -\frac{1}{4\pi}\frac{1}{|\mathbf{r}-\mathbf{r}'|}}$$ Fundamental Green's Function of Laplace's Equation in 3D

f. May add a suitable solution to $\nabla^2\psi=0$ (homogeneous eq.) to convert BCs from 0 at $\mathbf{r}'=\infty$ to satisfy whatever BC's are needed.

II. Probability

A. Basic Concepts and Definitions

1. Random Event: Practically impossible to predict from initial state
   ⇒ Includes when we have incomplete information about initial state.
   Ex: Gas in a box: i. We do not know individual particle positions and velocities, but only average quantities such as pressure, temp.

2. Key Concept: Average properties of many similar events are predictable

3. Probability quantifies our level of ignorance!

4. Statistics connects observations on a small data sample to inferences about probable content of entire population

5. Def: Sample space: All possible mutually exclusive outcomes of an experiment.
   a. Mutually exclusive means if one event did occur, others did not.
   Ex: Flip a coin: If heads, then it cannot be tails.

6. Def: a. Trial: A single instance that produces an outcome.
   b. Event: Unique, equally likely occurrence
   c. Outcome: Events that satisfy some particular criterion.

7. Def: Experimental Probability

$$\boxed{P(x_i) \equiv \frac{\text{Number of times event } x_i \text{ occurs}}{\text{Total number of trials}}}$$

8. Def: Theoretical Probability

$$\boxed{P(x_i) \equiv \frac{\text{Number of outcomes } x_i}{\text{Total number of all possible events}}}$$

II. A. (Continued)

9. Experimental definition is appropriate when:
   a. Total number of possible <u>events</u> is not well defined
   b. Cannot identify <u>equally likely</u> outcomes.

10. <u>Example</u>: <u>Two coin tosses</u>: Theoretical Probability
   a. <u>Outcome</u>: Number of heads:
      i) Possible values x_0, x_1, x_2 for 0, 1, or 2 heads
   b. Possible Events:

	Trial	Toss 1	Toss 2	Outcome
Four possible events $N_{tot}=4$	Result	H	H	x_2
		H	T	x_1
		T	H	x_1
		T	T	x_0

   c. <u>Theoretical Probability</u> $P(x_0) = \frac{1}{4}$, $P(x_1) = \frac{2}{4} = \frac{1}{2}$, $P(x_2) = \frac{1}{4}$

11. <u>Example</u>: Grains of Sand: Experimental Probability
   a. Consider two piles of sand with same number of grains:
      one pile has <u>black grains</u>, other has <u>white grains</u>
   b. Mix both piles together thoroughly
   c. Counting all grains of sand is <u>impractical</u>
   d. Choosing a small sample, the probability of choosing a black grain is near $\frac{1}{2}$
   e. With a larger sample, the probability will get closer to $\frac{1}{2}$

12. <u>Axioms</u>
   a. $\xrightarrow{\text{impossibility}} 0 \leq P \leq 1$ ✓certainty
   b. Probabilities for mutually exclusive events add.
      <u>Ex</u>: One head from two coin tosses: $P = \frac{1}{2}$ where $P_1 = \frac{1}{4}$ for (T, H) & $P_2 = \frac{1}{4}$ for (H, T)

II. A. (Continued)

13. Or vs. "Exclusive Or"

a. In probability, "A or B" means A, B, or "both A and B".
b. Exclusive or (xor) means A or B but "not both A and B"

14. Example: Drawing Cards

a. What is probability for drawing a club or a jack?
b. NOTE: These events are not mutually exclusive, since there is a jack of clubs.
c. Deck of playing cards: 52 card's total → N_{tot}
4 suits of 13 cards each
d. Each card is equally likely to be drawn.
e. A: drawing a club: 13 events ← BUT → this include jack of clubs
B: drawing a jack: 4 events
f. Thus:

Theoretical Prob: $P = \underbrace{\frac{12}{52}}_{\text{clubs without jack}} + \underbrace{\frac{4}{52}}_{\text{all jacks}} = \frac{16}{52} = \boxed{\frac{4}{13} = P}$

B. Sets, Unions, Intersections

1. Consider a sample space S

2. Def: Subset, $\subset$

a. $A \subset S$ if all events in A are also in S.

3. Equality of A and B if $A \subset B$ and $B \subset A$

4. Def: Union, $\cup$

a. $A \cup B$ is all points in A, B, or both A and B.

5. Def: Intersection, $\cap$

a. $A \cap B$ is all points in both A & B.

II. B. (Continued)

6. If A and B have no common points, $A \cap B = \emptyset$ ← Empty Set.

7. Subtraction: $A - (A \cap B)$

a. All points in A are also in B.

8. Addition Rule for Probabilities

a. $P(A)$ is probability of event A from full sample S.

b. $0 \le P(A) \le 1$

c. $P(S) = 1$ Probability of entire sample space.

d. $\boxed{P(A \cup B) = P(A) + P(B) - P(A \cap B)}$ Subtract double-counted points.

e. If $A \cap B = \emptyset$ (Mutually exclusive outcomes), then

$$P(A \cup B) = P(A) + P(B)$$

9. Conditional Probability $P(B|A)$

a. Def: Probability that B occurs, given that A has already occurred.

b. Def: Ordered Events $P(A, B)$

Probability that A occurs, then B occurs.

c. $$\boxed{P(A, B) = \underbrace{P(A)}_{\text{Probability of A}} P(B|A)}$$

← Probability of B after A has occurred.

d. Thus $$\boxed{P(B|A) = \frac{P(A, B)}{P(A)}}$$

10. Example: Conditional Probability

a. Consider a box of 10 identical ~~red~~ & 20 identical blue pens.

b. What is $P(R, B)$? (Drawing red pen, then drawing blue pen).

II B. 10. (Continued) Hawes ⑦

c. NOTE: Pens are not replaced after they are drawn;

d.

$$P(R,B) = \left(\frac{10}{30}\right)\cdot\left(\frac{20}{29}\right) = \boxed{\frac{20}{87}}$$

10 red, 20 blue, 30 total, 29 total

$P(A)$ $P(B|A)$

11 a. If A and B are independent, then $P(B|A) = P(B)$

b. Thus $P(A,B) = P(A)\,P(B)$

c. This would be the case if we replace pens after each drawing.

d. For A and B independent, we may write

$$P(B|A) = \frac{P(A\cap B)}{P(A)} \quad \text{where } P(A\cap B) = P(A)\,P(B)$$

12. Bayes Theorem: $P(A|B)\,P(B) = P(B|A)\,P(A)$

C. Counting Permutations (Ordered) and Combinations (Unordered)

1. Permutations: (Order Matters)

a. How many ways can we arrange (permute) n different letters?

$$\underline{n}\cdot\underline{n-1}\cdot\underline{n-2}\cdot\ldots\underline{2}\cdot\underline{1} = \boxed{n!}$$

b. How many (ordered) ways can we seat n people in k chairs? $(n > k)$

$$\underline{n}\cdot\underline{(n-1)}\cdot\underline{(n-2)}\ldots\underline{(n-k+2)}\cdot\underline{(n-k+1)} = \boxed{\frac{n!}{(n-k)!}}$$

Seat# 1 2 3 ... k-1 k

2. Combinations: (Order does not matter)

a. How many ways can you choose k particles from n distinguishable particles?

b. NOTE: for the same k particles, there are k! possible permutations.

I. C2 (Continued)

c. Thus divide by possible permutations $\boxed{\frac{n!}{(n-k)!\,k!}}$

d. <u>Symbol</u>: $\binom{n}{k}$ "n choose k" $\boxed{\binom{n}{k} = \frac{n!}{(n-k)!\,k!}}$

e. This is the <u>binomial coefficient</u>.

3. <u>Classical vs. Quantum Statistics</u> (n particles, k possible states)

a. <u>Maxwell-Boltzmann Statistics</u>: Distinguishable particles

i. Total possibilities $\boxed{k^n}$

b. <u>Bose-Einstein Statistics</u>: Indistinguishable Particles

i. Wave function symmetric under particle interchange

ii. Total possibilities: $\boxed{\binom{n+k-1}{n} = \binom{n+k-1}{k-1}}$

c. <u>Fermi-Dirac Statistics</u>: Indistinguishable Particles

i. Wave function reverses sign under particle interchange.

ii. Total Possibilities $\boxed{\binom{k}{n}}$

iii. <u>NOTE</u>: Probability is zero if $n > k$ (more particles than states).
since maximum one particle per state.