CHEM 116	February 13, 2018

Unit 4, Lecture 2

Numerical Methods and Statistics

Companion Reading

Bulmer Chapter 5

1 Expected Values

The expected value of a samlpe x is

$$\mathrm{E}\left[\,\mathrm{X}\,\right] = \sum_{\mathcal{Q}} \mathrm{P}(\mathrm{X} = \mathrm{x})\mathrm{x} \tag{1}$$

An expected value is analagous to a mean, except you don't add data points. You add the elements in your sample space, weighted by their probability. Be careful not to be confused: the expected value is not the most likely outcome. The most likely outcome is the x which maximizes $P(x)$, written as:

$$\underset{x}{\operatorname{argmax}}\, P(x) \tag{2}$$

Think of an expected value as a measure of the center point of the sample space.

1.1 Die Roll Example

Consider a fair die example, where d is an element in our sample space. Our sample space is one through six and the probability of a sample occuring is 1/6.

$$\mathrm{E}\left[\,\mathrm{D}\,\right] = \frac{1}{6} \times 1 + \frac{1}{6} \times 2 + \frac{1}{6} \times 3 \ldots$$

$$\mathrm{E}\left[\,\mathrm{D}\,\right] = \frac{1}{6} \times 21 = 3.5$$

Notice that the expected value is NOT an element of the sample space.

1.2 Unfair Die Example

Now consider our unfair die, where

$$P(D = d) = \frac{d}{21}$$

so for example, the probability of rolling a 4 is 4/21.

$$\mathrm{E}\left[\,\mathrm{D}\,\right] = \sum_{1,\ldots,6} \frac{\mathrm{d}}{21} \times \mathrm{d} = \frac{91}{21}$$

2 Expected Value of a Random Variable

To calculate the expected value of a random variable S, use:

$$\mathrm{E}\left[\mathrm{S}\right] = \sum_{\mathcal{Q}} \mathrm{P(X = x)S(x)} \tag{3}$$

Remember that the random variable S is defined by some $S(x)$ function, whose input is an element in the sample space and has an output of some real number.

2.1 Expected Value for Sum of 2 Dice

Consider the product sample space of two dice: $Q_2 = Q \otimes Q$, where Q is $1, \ldots, 6$. Example of elements of this sample space are rolling a 2 for the first die and a 4 for the second die: $(2, 4)$. There are 36 elements in the sample space and we'll take the probability of each to be equivalent. This gives:

$$P(X = x) = P(X = (x_1, x_2)) = \frac{1}{36}$$

Define S as our random variable representing the sum of the two dice.

$$S(x) = S(\,(x_1, x_2)\,) = x_1 + x_2$$

Now we can plug these into our expected value equation:

$$\mathrm{E}\left[\mathrm{S}\right] = \sum_{\mathrm{Q}} \mathrm{P(X = x)S(x)} = \sum_{(\mathrm{x_1,x_2}) \in \mathrm{Q_2}} \frac{1}{36}\mathrm{S((x_1, x_2))}$$

$$= \frac{1}{36} \times (1+1) + \frac{1}{36} \times (1+2) + \frac{1}{36} \times (1+3) + \ldots + \frac{1}{36} \times (6+6)$$

To calculate the answer, we need to sum all 36 possible dice rolls together. That turns out to be 252. So we have:

$$\mathrm{E}\left[\mathrm{S}\right] = \frac{252}{36} = 7$$

2.2 Expected Value for Sum of 2 Dice - Alternate

Another way to solve this problem is to DEFINE our sample space to be the possible sums. Then $Q = \{2, 3, \ldots, 12\}$. Our correponding probability is going to be the number of permutations to roll the sum divided by some normalizing constant. For example, the probability of rolling a 6 is 5 / Z, where Z is some constant to make sure our probabilities sum to 1. The 5 comes from the number of ways to roll a 6: $(1, 5), (2, 4), (3, 3), (4, 2), (5, 1)$. I'm calling these permutations because $(1, 5)$ and $(5, 1)$ are both counted. Now we to find Z:

$$Z = \underbrace{1}_{\text{permutations to roll a 2}} + \underbrace{2}_{\text{permutations to roll a 3}}, \ldots, \underbrace{1}_{\text{permutations to roll a 12}}$$

$$Z = \underbrace{1}_{2} + \underbrace{2}_{3} + \underbrace{3}_{4} + \underbrace{4}_{5} + \underbrace{5}_{6} + \underbrace{6}_{7} + \underbrace{5}_{8} + \underbrace{4}_{9} + \underbrace{3}_{10} + \underbrace{2}_{11} + \underbrace{1}_{12} = 36$$

where the underbraces indicate which dice roll sum each term corresponds to. Doing this work also reveals an equation for the probability:

$$P(S = s) = \frac{6 - |s - 7|}{36}$$

Finally, we are ready to utilize the expected value equation:

$$\begin{aligned}\mathrm{E}\left[\,\mathrm{S}\,\right] = \sum_{\mathcal{Q}} \mathrm{P}(\mathrm{S} = \mathrm{s})\mathrm{s} &= \sum_{2,\ldots,12} \frac{6 - |\mathrm{s} - 7|}{36} \times \mathrm{s} \\ &= \frac{1 \times 2}{36} + \frac{2 \times 3}{36} + \frac{3 \times 4}{36} + \ldots + \frac{1 \times 12}{36} \\ &= \frac{252}{36} = 7\end{aligned}$$

Thus we've arrived at the same answer.

2.3 Continuous Expected Value

$$\mathrm{E}\left[\,\mathrm{X}\,\right] = \int_{\mathcal{X}} \mathrm{xp}(\mathrm{x})\,\mathrm{dx} \tag{4}$$

2.4 Continuous Example

$$p'(x) \propto x,\ Q = [0, 5]$$

First, we must normalize it:

$$\int_0^5 x\,dx = \frac{25}{2}$$

$$p(x) = \frac{2x}{25}$$

$$\int_0^5 x \times \frac{2x}{25} = \frac{2 \times 125}{25 \times 3} = \frac{10}{3}$$

2.5 Conditional Expectation Value

$$\mathrm{E}\left(X \mid Y = y\right) = \sum_{\mathcal{X}} \mathrm{P}\left(X = x \mid Y = y\right) x \tag{5}$$

2.6 Die Roll Example

Our random variable X is the observation, and $Y = 0$ if the observation is odd and $Y = 1$ if the observation is even.

$$\mathrm{E}\left(X \mid Y = 0\right) = \frac{1}{3} \times 1 + \frac{1}{3} \times 3 + \frac{1}{3} \times 5 = 3$$

Expected value gives the center of a random variable or probability distribution.

3 Variance

Variance gives the average deviation from that center. To make sure variation above and below the center contributes, it is the expected squared distance from the expected value:

$$\mathrm{Var}(X) = \mathrm{E}\left[\,(\mathrm{E}\left[\,\mathrm{X}\,\right] - \mathrm{X})^2\,\right] = \mathrm{E}\left[\,\mathrm{X}^2\,\right] - \mathrm{E}\left[\,\mathrm{X}\,\right]^2 \tag{6}$$

3.1 Die Roll Example

We already know $\mathrm{E}\left[\,\mathrm{X}\,\right] = 21/6 = 3.5$. To find $\mathrm{E}\left[\,\mathrm{D}^2\,\right]$, we can use our random variable expectation equation. Take F to be our random variable deinfed by $F(x) = x^2$:

$$\mathrm{E}\left[\,\mathrm{D}^2\,\right] = \mathrm{E}\left[\,\mathrm{F}\,\right] = \sum_{\mathrm{Q}} \mathrm{P(x)x^2} =$$

$$= \frac{1}{6} \times 1^2 + \frac{1}{6} \times 2^2 + \frac{1}{6} \times 3^2 \dots$$

$$= \frac{91}{6}$$

$$\mathrm{Var}(D) = \frac{91}{6} - \frac{21^2}{6^2} = \frac{35}{12} = 2.92$$