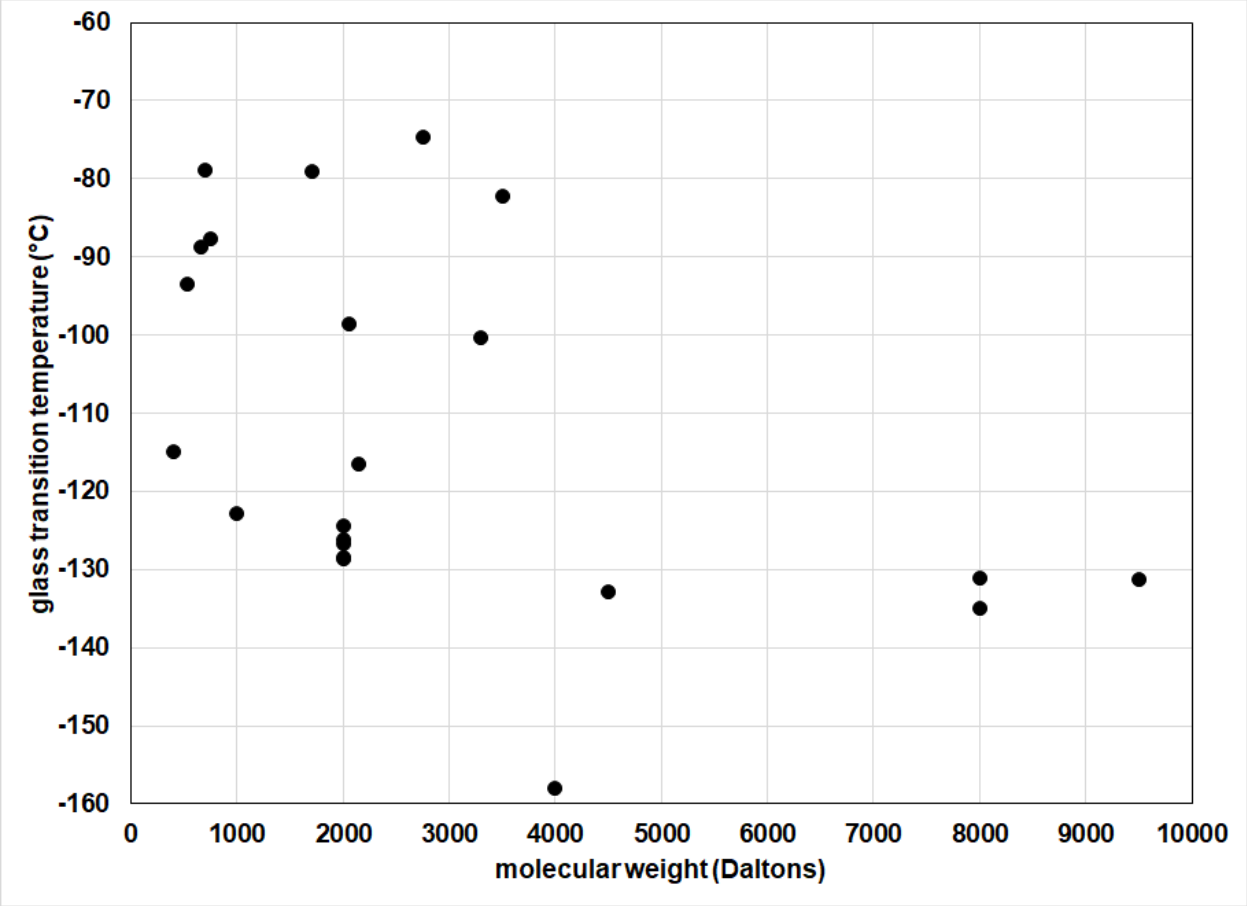
Exam I Solutions
Administered: Monday, September 14, 2026
24 points

For each problem part: 0 points if not attempted or no work shown,
1 point for partial credit, if work is shown,
2 points for correct numerical value of solution

Problem 1. (12 points)

Consider the relationship between molecular weight and glass transition temperature for the following **22** polymers plotted below. The data in this plot is available electronically on the course website in a spreadsheet file.



Answer the following questions for the materials in this table.

(a) Determine the mean molecular weight.
(b) Determine the mean glass transition temperature.
(c) Determine the standard deviation of the molecular weight.
(d) Determine the standard deviation of the glass transition temperature.
(e) Determine the correlation coefficient between the glass transition temperature and the molecular weight.
(f) What is the physical significance of your answer to part (e)?

Data taken from Katritzky, A.R. et al, "Prediction of Polymer Glass Transition Temperatures Using a General Quantitative Structure-Property Relationship Treatment", *J. Chem. Inf. Comput. Sci*. **36** 1996 pp. 879-884.

Solution:
(a) Determine the mean molecular weight.

$$\mu_{MW} = \frac{\sum_{i=1}^{n} MW_i}{n} = 2886 \text{ Da}$$

The mean molecular weight of these materials is 2886 Da.

(b) Determine the mean glass transition temperature.

$$\mu_{Tg} = \frac{\sum_{i=1}^{n} Tg_i}{n} = -111.8 \text{ °C}$$

The mean glass transition temperature of these materials is −111.8 °C.

(c) Determine the standard deviation of the molecular weight.

$$\sigma_{MW}^2 = E\left[MW^2\right] - E[MW]^2 = 14537482.14 - (2885.772727)^2 = 6209797.903 \text{ Da}^2$$
$$\sigma_{MW} = \sqrt{\sigma_{MW}^2} = 2491.946609 \text{ Da}$$

The standard deviation of the molecular weight is 2491 Da.

(d) Determine the standard deviation of the glass transition temperature.

$$\sigma_{Tg}^2 = E\left[Tg^2\right] - E[Tg]^2 = 13021.745 - (-111.8318182)^2 = 515.3894421 \text{ °C}^2$$

$$\sigma_{Tg} = \sqrt{\sigma_{Tg}^2} = 22.70219025 \text{ °C}$$

The standard deviation of the glass transition temperature is 22.7 °C.

(e) Determine the correlation coefficient between the glass transition temperature and the molecular weight.

First we determine the covariance.

$$\sigma_{MW \cdot Tg} = E[MW \cdot Tg] - E[MW]E[Tg] = -349189.0682 - 2885.77 \cdot -111.8318182 = -26467.85723 \text{ Da°C}$$

With the covariance in hand, we can determine the correlation coefficient.

$$\rho_{MW \cdot Tg} = \frac{\sigma_{MW \cdot Tg}}{\sigma_{MW} \cdot \sigma_{Tg}} = \frac{-26467.8}{2491.9 \cdot 22.7} = -0.468$$

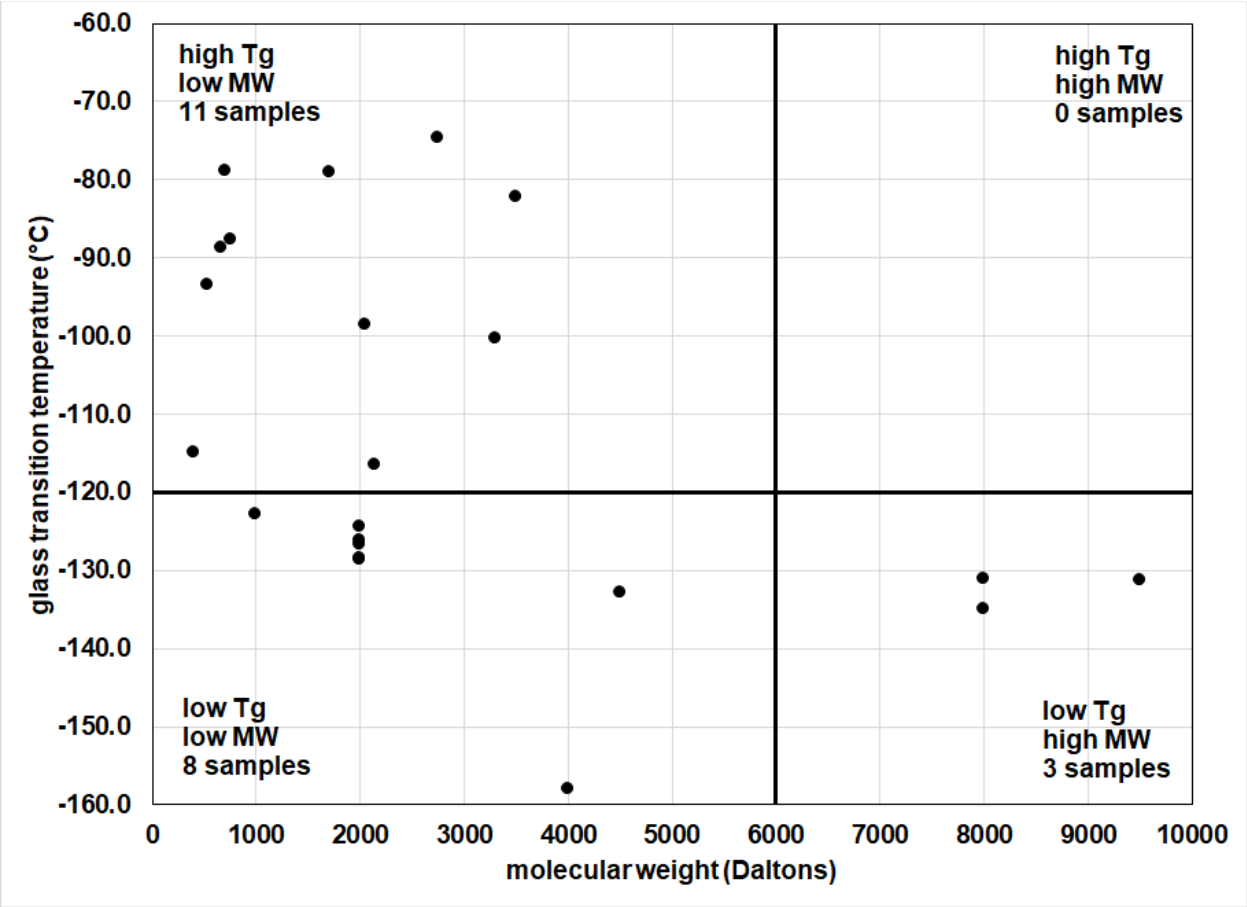
The correlation coefficient between the glass transition temperature and the molecular weight is -0.47.

(f) What is the physical significance of your answer to part (e)?

The value of the correlation coefficient is negative. Therefore, there is a negative correlation between glass transition temperature and molecular weight. An increase in the molecular weight statistically corresponds to a decrease in glass transition temperature. In class we said that in general a reliably strong correlation should have a correlation coefficient with an absolute value greater than 0.8. This correlation coefficient of -0.47 is not in that range. It is a negative correlation but not a strong one, for this collection of relatively small polymers. You can see the extent of the deviation from the correlation in the plot.

Problem 2. (12 points)

Consider the **22** materials in the plot below. We are evaluating these materials in terms of glass transition temperature and molecular weight. We have created a definition of low and high glass transition temperature and low and high molecular weight as indicated by the horizontal and vertical lines in the plot.



Using this information, answer the following questions.

(a) Draw a Venn Diagram of the sample space for this data.
(b) What is the probability that a material has low molecular weight and low glass transition temperature?
(c) What is the probability that a material has low glass transition temperature?
(d) What is the probability that a material has low molecular weight given that it has low glass transition temperature.
(e) What is the probability that a material has high glass transition temperature given that it has low molecular weight?
(f) Given this classification, prove that glass transition temperature and molecular weight are not independent of each other.

Solution:
There are a total of 22 materials.
From the plot we see:

$$P(MW_{lo} \cap Tg_{lo}) = \frac{8}{22}$$
$$P(MW_{hi} \cap Tg_{lo}) = \frac{3}{22}$$

$P(MW_{lo} \cap Tg_{hi}) = \frac{11}{22}$
$P(MW_{hi} \cap Tg_{hi}) = \frac{0}{22}$

(a) Draw a Venn Diagram of the sample space for this experiment.

$MW_{lo} \cap Tg_{hi}$	$MW_{hi} \cap Tg_{hi}$
$MW_{lo} \cap Tg_{lo}$	$MW_{hi} \cap Tg_{lo}$

(b) What is the probability that a material has low molecular weight and low glass transition temperature?
From the data given,

$$P(MW_{lo} \cap Tg_{lo}) = \frac{8}{22} = \frac{4}{11}$$

The probability that a material has low molecular weight and low glass transition temperature is $\frac{4}{11}$.

(c) What is the probability that a material has low glass transition temperature?

Consider the union probability rule.

$$P(Tg_{lo}) = P(MW_{lo} \cap Tg_{lo}) + P(MW_{hi} \cap Tg_{lo}) - P[(MW_{hi} \cap Tg_{lo}) \cap (MW_{lo} \cap Tg_{lo})]$$

$$= \frac{8}{22} + \frac{3}{22} - 0 = \frac{11}{22} = \frac{1}{2}$$

The probability that a material has a low glass transition temperature can be computed from the union rule. The intersection of low molecular weight and high molecular weight is zero by definition of the categorization of these materials. The probability that a material has a low glass transition temperature is $\frac{1}{2}$.

(d) What is the probability that a material has low molecular weight given that it has low glass transition temperature.

Consider the conditional probability rule.

$$P(MW_{lo}|Tg_{lo}) = \frac{P(MW_{lo} \cap Tg_{lo})}{P(Tg_{lo})} = \frac{\frac{4}{11}}{\frac{1}{2}} = \frac{8}{11}$$

The probability that a material has low glass transition temperature given that it has low molecular weight is $\frac{8}{11}$.

(e) What is the probability that a material has high glass transition temperature given that it has low molecular weight?

There are two equivalent ways to work this problem.
First, consider the conditional probability rule.

$$P(Tg_{hi}|MW_{lo}) = \frac{P(Tg_{hi} \cap MW_{lo})}{P(MW_{lo})}$$

We can determine the denominator as

$$P(MW_{lo}) = P(MW_{lo} \cap Tg_{lo}) + P(MW_{lo} \cap Tg_{hi}) - P[(MW_{lo} \cap Tg_{lo}) \cap (MW_{lo} \cap Tg_{hi})]$$

$$= \frac{8}{22} + \frac{11}{22} - 0 = \frac{19}{22}$$

$$P(Tg_{hi}|MW_{lo}) = \frac{P(Tg_{hi} \cap MW_{lo})}{P(MW_{lo})} = \frac{\frac{11}{22}}{\frac{19}{22}} = \frac{11}{19}$$

The probability that a material has high glass transition temperature given that it has low molecular weight is $\frac{11}{19}$.

(f) Given this classification, prove that glass transition temperature and molecular weight are not independent of each other.

There are a variety of ways to prove this.

If A & B are independent, then $P(A|B) = P(A)$ or $P(B|A) = P(B)$.

So for example, we can show that glass transition temperature and molecular weight are not independent of each other through either of the following statements.

$$P(MW_{lo}|Tg_{lo}) = \frac{8}{11} \neq P(MW_{lo}) = \frac{19}{22}$$

$$P(Tg_{hi}|MW_{lo}) = \frac{11}{19} \neq P(Tg_{hi}) = \frac{1}{2}$$

Since these statements are not equalities, we know that the variables are not independent of each other.