

Kimi's Performance on Homework 6

Interwoven Transcript and Evaluation

1 Problem 2: Graph Dynamics and GNN Concepts

1.1 (a) Output of the j -th Node at Layer k

Kimi's Response:

We index layers $k = 0, 1, \dots$, nodes i, j , channels c .
Initial input $X^{(0)} = I$.
Update: $X^{(k+1)} = A X^{(k)}$.
Thus $X^{(k)} = A^k$.
The output of node j at layer k is row j of A^k .

Evaluation: Fully correct.

1.2 (b) Counting Walks Using A^k

Kimi's Response:

Prove $(A^k)_{\{j,i\}} = L_k(i,j)$.
Base: $A^0 = I$.
Inductive step uses $(A^{(k+1)})_{\{j,i\}} = \sum_l A_{\{j,l\}} (A^k)_{\{l,i\}}$
 $= \sum_{\{l \in V(j)\}} L_k(i,l) = L_{\{k+1\}}(i,j)$.

Evaluation: Fully correct.

1.3 (c) Update Function

Kimi's Response:

Matrix update: $H^{(k+1)} = A H^{(k)}$.
Node update: $h_j^{(k+1)} = \sum_{\{i \in V(j)\}} h_i^{(k)}$.

Evaluation: Fully correct.

1.4 (d) Max Aggregation Interpretation

Kimi's Response:

Using max means $x_j^{(k+1)}[c] = \max_{\{i \in V(j)\}} x_i^{(k)}[c]$.

This acts like Boolean OR. Output is 1 iff a length-k path from c to j exists.

Evaluation: Fully correct.

1.5 (e)(i) Representing Molecules as Graphs

Kimi's Response (Excerpt):

Nodes contain detailed atomic features (electronegativity, hybridization, ring membership, charges...). Edges contain bond order, conjugation, Wiberg bond index, etc. Global contains molecule type and other global properties.

Evaluation: Correct idea but significantly over-engineered for homework expectations.

1.6 (e)(ii) Using Outputs to Predict First Broken Bond

Kimi's Response:

Use per-edge logits: $s_{uv} = \text{MLP}([h_u; h_v; h_{uv}; h_G])$.

Softmax over all edges plus one "no-bond-break" class.

Evaluation: Fully correct.

1.7 (e)(iii) Encoding Node Representations

Kimi's Response (Excerpt):

Learned atomic embedding + physical features + positional encodings + MLP.

Evaluation: Conceptually correct, but much more complex than expected. Homework expects to use learned element embedding.

2 Problem 3: Graph Neural Networks

2.1 (a) Validity of Update Rules

Kimi's Response:

- (i) Valid.
- (ii) Invalid.
- (iii) Valid.

Evaluation: Fully correct.

2.2 (b) Training Loss

Kimi's Response:

Loss = $-(1/3) [\log(b) + \log(c) + \log(1 - e)]$.

Evaluation: Fully correct.

2.3 (c)(i) Design Patterns

Kimi's Response:

Residual connection present. No batch normalization.

Evaluation: Fully correct.

2.4 (c)(ii) Dimensions of W_1

Kimi's Response:

W_1 is $d \times k$.

Evaluation: Fully correct.

2.5 (c)(iii) Expanded Update Rules for Nodes 2 and 3

Kimi's Response (Incorrect):

Neighbors for node 2: {1,3}

Neighbors for node 3: {1,2,4}

(Uses these to expand update rules.)

Evaluation: Incorrect. Kimi used the wrong neighbor sets.

2.6 (g) Missing Node Features

Kimi's Response (Excerpt):

Uses mask vectors, learnable unknown token, auxiliary reconstruction loss, variational treatment, etc.

Evaluation: Conceptually fine, but far more complex than expected. Homework expects: - Use a "missing" token or mean fill; - Train with random masking augmentation.

2.7 (h) GraphNet Architecture

Kimi's Response:

- (i) Params unchanged; computation doubles in sparse case or $\times 4$ in dense.
- (ii) Weights live in update MLPs.
- (iii) Directed edges handled by treating incoming/outgoing edges differently.

Evaluation: Fully correct.