

# Actionable Interpretability via Causal Hypergraphs: Unravelling Batch Size Effects in Deep Learning

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## Motivation

### Why does batch size affect generalisation?

Although batch size is widely known to affect convergence and generalisation, especially in graph/text models, existing explanations remain heuristic and non-interventionist.

### We address:

- Lack of causal understanding of batch-size effects.
- No modelling of higher-order (joint) training interactions.
- No bridge between interpretability and training-time control.

**Our solution:** **HGCNet**, a causal hypergraph framework that models batch dynamics structurally, enabling do-calculus-based training insights.

## HGCNet: Causal Hypergraph Framework

We treat batch size  $B$  as a root intervention acting via:

$$B \rightarrow N \rightarrow S \rightarrow C \rightarrow G$$

### Nodes:

- $N$ : Gradient noise
- $S$ : Sharpness (Hessian)
- $C$ : Complexity (e.g. norm, margin)
- $G$ : Generalisation (Test Acc.)

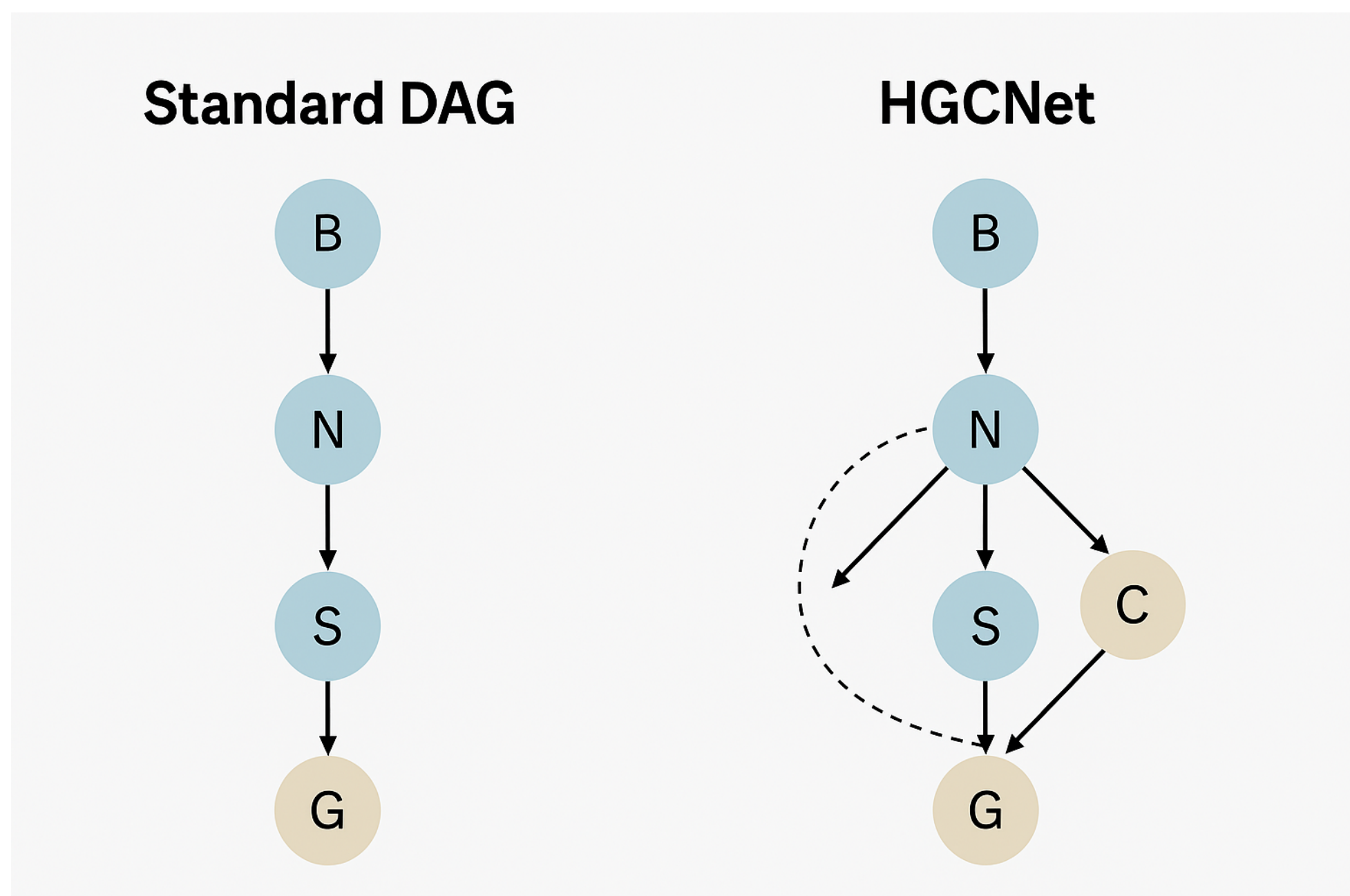


Figure 1. Causal Hypergraph Structure in HGCNet

**Hyperedge:**  $\{N, S\} \rightarrow C$  enables joint mediation.

**Implication:** Enables do-calculus estimation and training-time policy derivation via ATE curves.

## HGCNet Algorithm and Estimation

**Input:** Dataset  $D$ , batch sizes  $B \in \{16, 32, \dots, 512\}$

### Steps:

1. Estimate gradient variance  $N(B)$
2. Compute Hessian-based sharpness  $S$
3. Estimate complexity  $C = f(N, S)$
4. Measure generalisation  $G$
5. Fit structural equations, apply:

$$P(G \mid do(B = b)) = \sum_{N, S, C} P(G|C) P(C|N, S) P(S|N) P(N|B = b)$$

6. Derive ATE curves and counterfactual predictions.

## HGCNet Construction Details

We model the training process using a directed hypergraph: nodes are stochastic variables (e.g., gradient noise, sharpness), and hyperedges capture joint causal interactions. Key design:

- Edges like  $\{N, S\} \rightarrow C$  encode higher-order effects (e.g., joint influence of noise and sharpness on complexity).
- Conditional independence relations enable efficient ATE and do-calculus inference.
- Training-time policy can be derived by counterfactuals:  $do(B = b')$  reveals expected test performance.

This approach allows edge removal as a structured ablation tool, identifying dominant mediators.

## Theoretical Insights

We treat batch size  $B$  as a \*policy variable\*, inducing downstream effects via gradient noise and sharpness:

$$B \rightarrow N \rightarrow S \rightarrow C \rightarrow G$$

We leverage:

- \*Causal mediation analysis\* to identify how training-time variables influence generalisation.
- \*Do-calculus\* for counterfactual estimation of policies like batch size intervention.
- ATE (Average Treatment Effect) curves to formalise generalisation tradeoffs.

## Empirical Setup & Main Results

### Domains & Datasets:

- **Graphs:** Cora, CiteSeer
- **Text:** PubMed, Amazon Reviews

**Models:** GCN, GAT, PI-GNN, BERT, RoBERTa, HGCNet

### Measured Quantities:

- **Gradient Noise** (variance of updates)
- **Hessian Sharpness** (spectral norm)
- **Model Complexity** (norm, margin)
- **Generalisation Accuracy / Precision**

### Main Results (ATE Estimate):

Dataset	B=16	B=512	Gain
Cora	83.9%	80.5%	<b>+3.4%</b>
CiteSeer	79.1%	76.0%	<b>+3.1%</b>
PubMed	88.2%	85.1%	<b>+3.1%</b>
Amazon	92.4%	89.0%	<b>+3.4%</b>

Smaller batches causally improve generalisation.

### Causal Ablation (Edge Removal):

Ablation	Drop in Generalisation (G)
Remove Noise Node (N)	-3.4%
Remove Sharpness Node (S)	-2.8%
Remove $\{N, S\} \rightarrow C$ Edge	-2.0%
SAM-only Control	-1.5%

Gradient noise is the dominant causal mediator.

## Broader Impact

### Scientific Impact:

- Introduces the first causally grounded model for analysing batch size effects in training dynamics.
- Provides a foundation for causal benchmarking of generalisation-efficiency tradeoffs.

### Practical Relevance:

- Enables interpretable, theory-driven batch size selection policies.
- Reduces reliance on heuristic tuning, especially in resource-constrained or safety-critical domains.

### Future Applications:

- Can inform policy decisions in curriculum learning, fairness-aware training, and robust model deployment.
- Lays groundwork for causal training-time interventions in domains such as reinforcement learning and automated ML.

## References

Keskar, N.S., Mudigere, D., Nocedal, J., Smelyanskiy, M. and Tang, P.T.P., 2016. On large-batch training for deep learning: Generalization gap and sharp minima. arXiv preprint arXiv:1609.04836.  
 Pearl, J., 2009. Causality. Cambridge university press.  
 Peters, J., Janzing, D. and Schölkopf, B., 2017. Elements of causal inference: foundations and learning algorithms (p. 288). The MIT Press.

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