

ICASSP '25 notes and interesting posters

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1 Montag Vormittag

1.1 Tutorial: Generative AI and Model Optimization

Problem: (compute) cost, current foundation models not sustainable Solutions:

1.1.1 Sparsity

→ scalability, less overfitting, interpretability, adaptive ways to introduce sparsity

- post training: optimal brain damage (OBD)/ optimal brain surgery (OBS)
 - dropout by contribution to error, scale by Hessian \mathcal{H} contribution
- training:
 - L1-loss: Convex optim.; no free lunch: initial model very large!, more eqs.
 - exhaustive: very expensive
 - greedy/evolutionary solutions: StOMP, GOMP based on L0-norm, but very effective
- pre-training
 - SET
 - randomly initial init → evolutionary
- architectural: grow and shrink networks...

Problem: doesn't really work with LMs (empirical study), but well for other networks (esp. low-weight dropout)

1.1.2 Compression

- filter: storage compression
- low rank factorization (\neq LoRA), during train time not fine-tuning
- knowledge distillation

2 Dienstag Nachmittag

2.1 Talk: Underwater Communications

- Problem: very slow comm underwater, ≈ 10 kHz range
- Towards moving target, Doppler correction using active SP correction, very manual work

Comment: interesting manual process, tedious work to sample

3 Mittwoch Nachmittag

3.1 Talk: AI+SP

Comment: not great, just some basics on diffusion/transformers, a little bit of SP in NNs - not exciting

4 Donnerstag Vormittag

4.1 Talk: Multiomics

- Genomics: DNA understanding
- Transcriptomics: DNA- \rightarrow RNA understanding
- Proteomics: RNA- \rightarrow Protein structures
- Knowledge graphs: how do these systems influence each other
- Flow:
 - identify DNA mutation that triggers illness
 - find possible RNA mechanism
 - find good fitting small ring structure
 - \rightarrow check for side effects in knowledge graph! (certain protein effects unwanted)
 - \rightarrow then test \rightarrow animal tests, reduce through ML!
- Graph diffusion for drug discovery: noise schedule for diffusion essential, i.e. cosine-square schedule
 - diffuse graphs from atoms & edges as adjacency matrix
 - what is noise: discrete noise: each atom is discrete state \implies graph structure undergoes state transition change
 - naive: uniform structure, not really chemically sensible - conditional probabilities \implies not uniform but marginal distribution of molecules in training (just logical!), same for edge (with deletion!)
 - one step further: consider carbon rings, restriction based on maximum bonds of atom (free radicals)
 - SMILE-file, QED: Quantitative Estimate of Drug likeness (from RDKit)
 - Existing methods: Time-consuming, progress slow, very few good molecules
 - Their work: jointly perturb rings+nodes
 - other approaches: motives as super-node with rings, difficulty: ring attachments - only $\approx 1\%$ improvement!
 - novelty however high, one molecule of them even patented!
- Knowledge graphs:
 - GNN link prediction
 - none of the existing benchmarks include features!
 - maybe talk to author!

Comment: focused on drug discovery using diffusion, not much on multiomics...