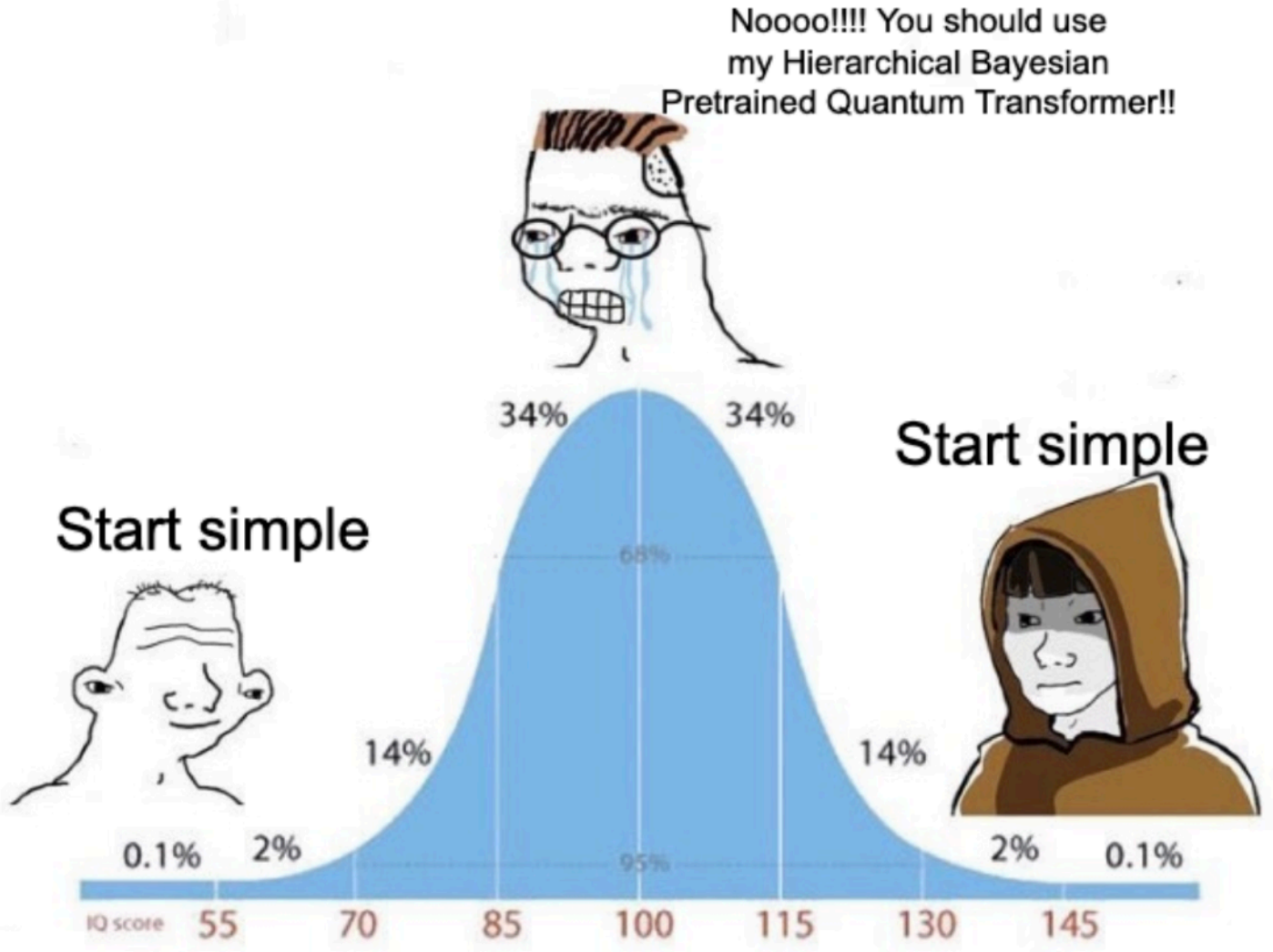
Machine Learning Best Practices



Miles Cranmer (Cambridge)

Good material from

- Andrej Karpathy [blog]
- Ian Goodfellow et al. [text]
- Josh Tobin [notes]
- Slav Ivanov [notes]
- Jeremy Howard [blog/notes]

Overview

- General neural network training recipe
- Small-scale experimentation, scaling, debugging
- Review Karpathy's “Recipe”
- Discuss experiment tracking; reproducibility

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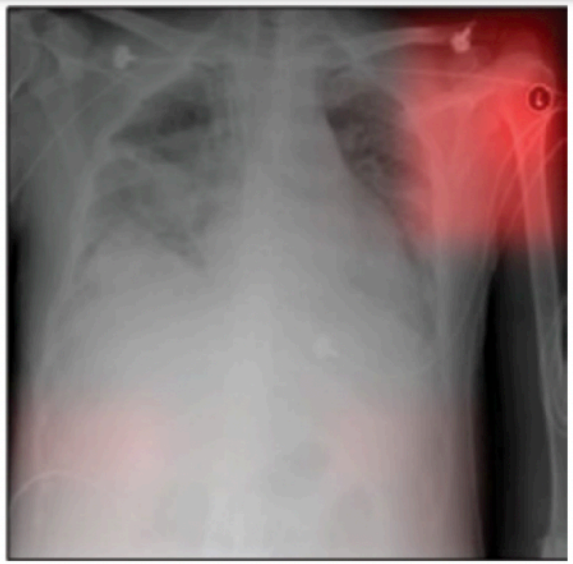

Zech 2018

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Problem	Fails on scans from new hospitals
Shortcut	Looks at hospital token, not lung

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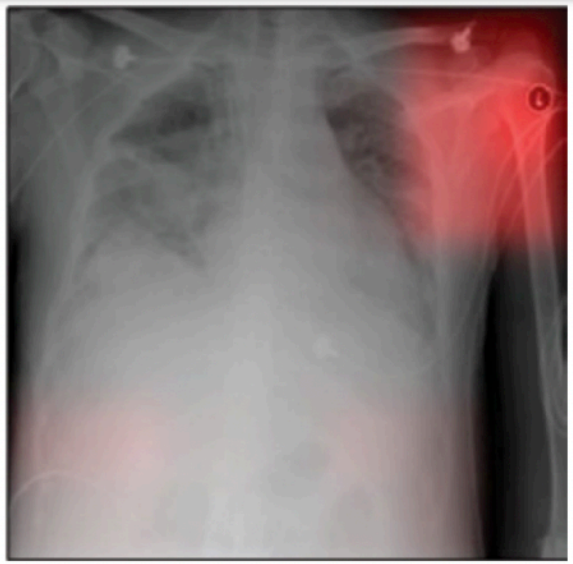

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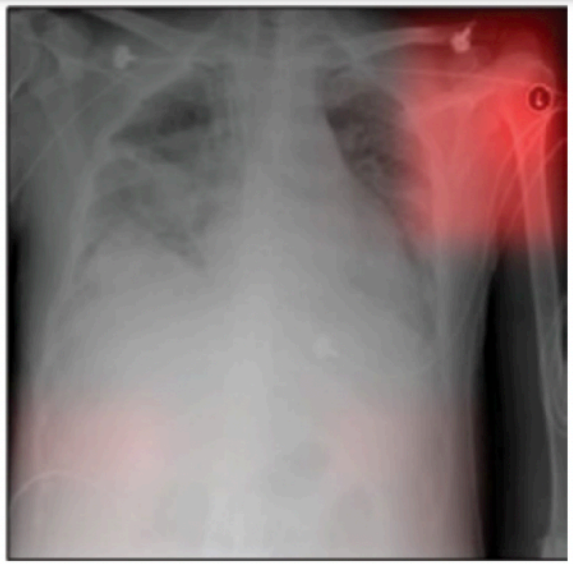

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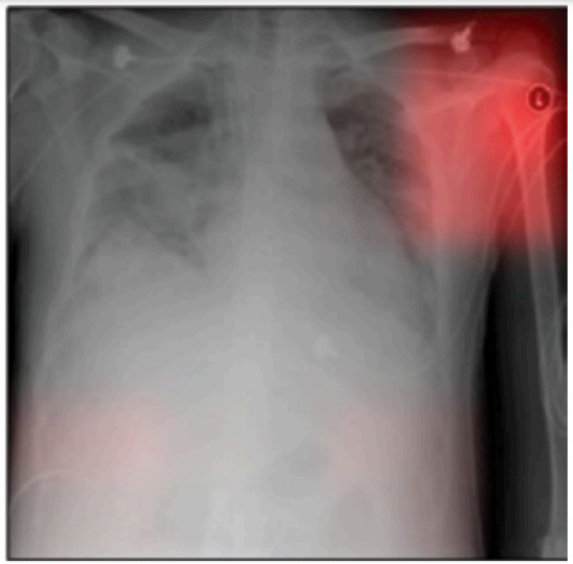

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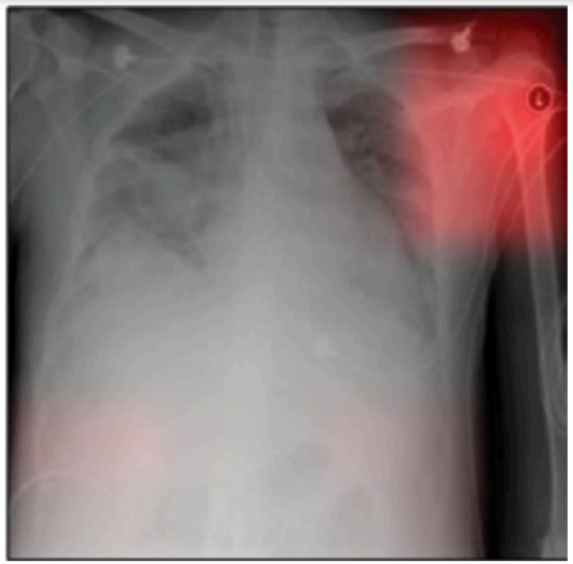

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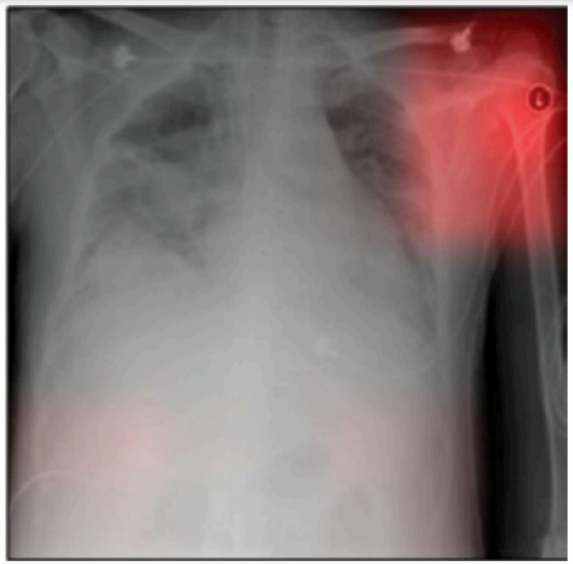

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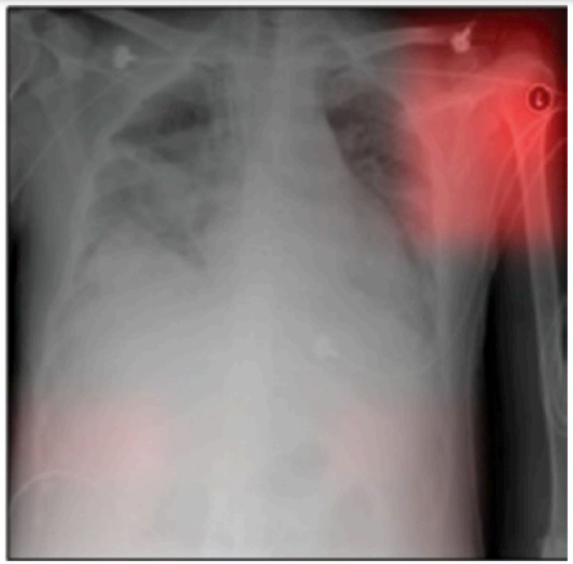

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- They often fail ***quietly***

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- Verify, verify, verify! Bugs in neural networks are much more sinister than bugs in regular software.

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6. Generally: do small-scale tuning; and only then do large-scale runs

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- ^Manual inspection reveals anomalies that will ***sabotage*** training! Very important to do this FIRST, rather than run around in circles fixing a bug only to realise it was the data all along!

2. Keep it simple; build an end-to-end training pipeline

- Set up an end-to-end training loop
- Start with a single linear model, or another “dumb" model
- Evaluate the training and validation loss, and ***confirm*** it is what you expect (should usually be better than random)
- Use this opportunity to create plotting/analysis scripts of trained models. You want to make these ***before*** you do any crazy ML, so you can verify they work

- You want to ***prove*** your code can learn something; and that your pipeline is correct

Check initial results

- Verify, by hand - does the loss start at the expected value (e.g., -log(1/num_classes))
- Does the model beat an ***input-independent*** baseline?
- Does the linear model train stably for at least a few epochs?

- Fix all issues before complicating the model!

3. Overfit on a small batch

- Overfit on ~1% of the dataset. (Now, use a slightly larger model).
- Focus on driving training loss down.
- This confirms no hidden bugs or capacity limitations.
- Once you can overfit, you know the pipeline's fundamentals are sound and ***all wires connect***

4. Increase model capacity

- Now, try to ***overfit the full training set***
- Use a larger model until you can do this (but don't complicate it yet)
- If you cannot overfit, there might be a problem!

Note: Inspect the data as it enters the model

- Even if you've thoroughly inspected your dataset, you might still have an issue at the preprocessing stage
- Solution: visualize the data ***as it enters the model***
- Right before it enters, you should add a hook that captures and logs the data - you can visualise it right there

5. Regularize

- After proving you can overfit, you want to improve generalization
- Techniques include weight decay, dropout, data augmentation, label smoothing, and early stopping.
- Gradually introduce each method, confirming your validation performance improves.
- Avoid adding too many new pieces at once.
- Monitor both training and validation losses carefully.

Augment dataset

- Data augmentation is often the strongest regularizer for images, text, or audio.
- Meaningful transformations (flips, crops, color jitter, synonyms) enlarge your dataset artificially.
- For physics datasets, there are often physically-motivated augmentations - these are very smart to use!
- Ensure they remain label-preserving. Overly aggressive augmentations can harm performance. Start simple (random flips or slight crops) and expand. Always check sample outputs to confirm correctness thoroughly.

6. Tune hyperparameters

- Tuning on small scale is very important
- Try to see the trends in hyper parameters, BEFORE moving to large-scale
- By staying at small scale first, you get a very quick prototype loop. You can quickly test new ideas
- There are some known scaling relations you can use for hyper parameters - such as