Population Based Training of Neural Networks (PBT)

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Presentation Structure

- Overview of PBT
- Problem context
- Solution proposed
- Comparison with existing work
- Conclusion and discussion

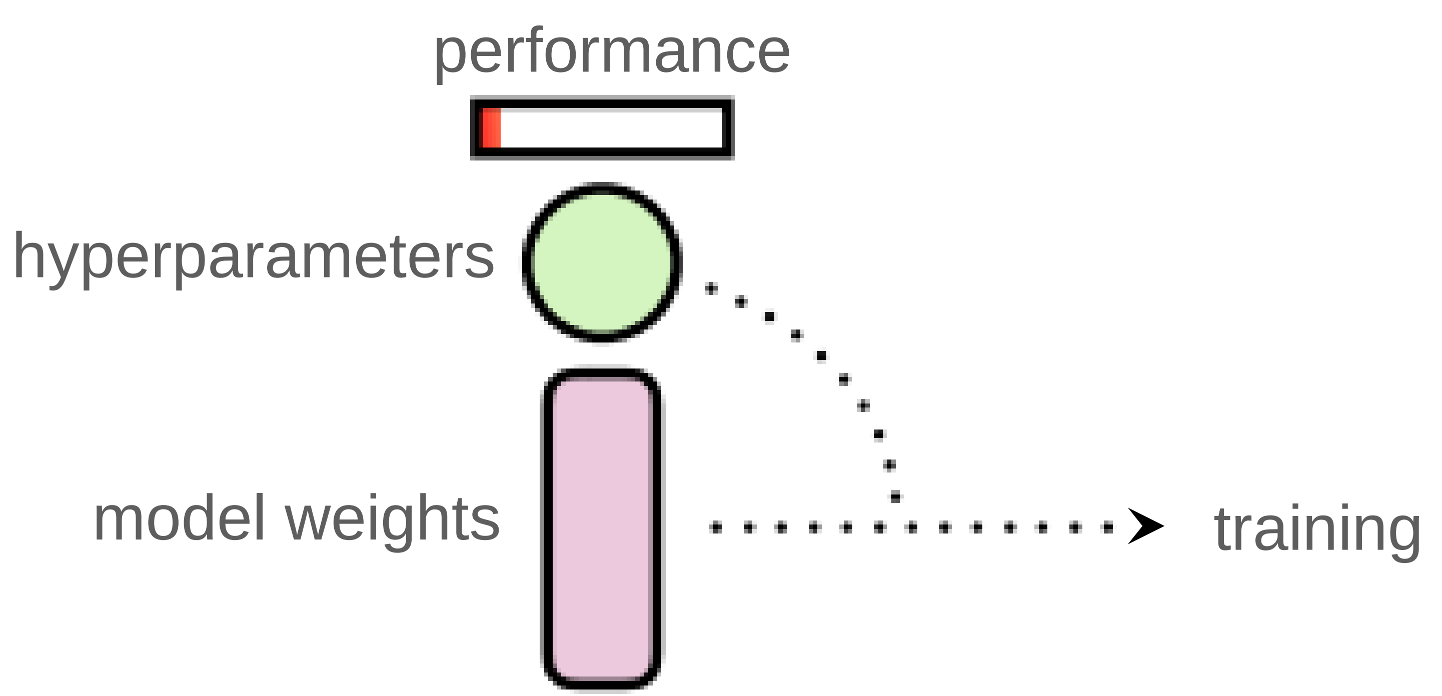
Overview of PBT

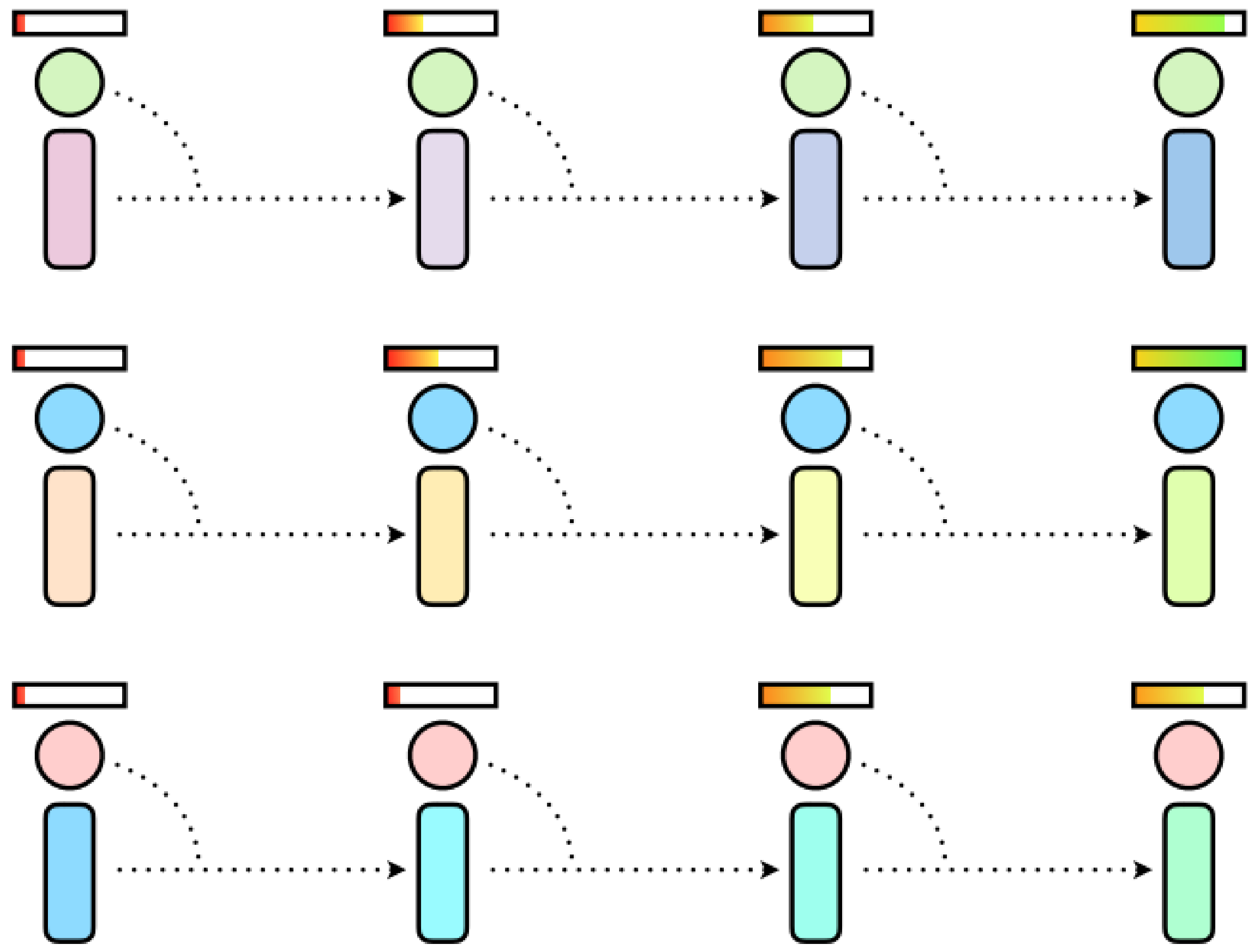
- Algorithm for optimisation of neural network hyperparameters
- Naturally inspired approach based on metal annealing – note PBT is <u>not</u> a genetic algorithm!
- Dynamically assigns computational resources to most promising solutions
- Uses exploration + exploitation mechanism
- Hybridisation of parallel and sequential methods

Problem Context

Parallel optimisation

- E.g. grid search. Allows multiple models to be evaluated with little manual intervention
- Can cover the full solution space reasonably effectively
- Scope for significant speedup IF we assume hyperparameters independent from one another – not always wise…
- Assumes uniform prior over hyperparameters
- Often time exploring poor areas





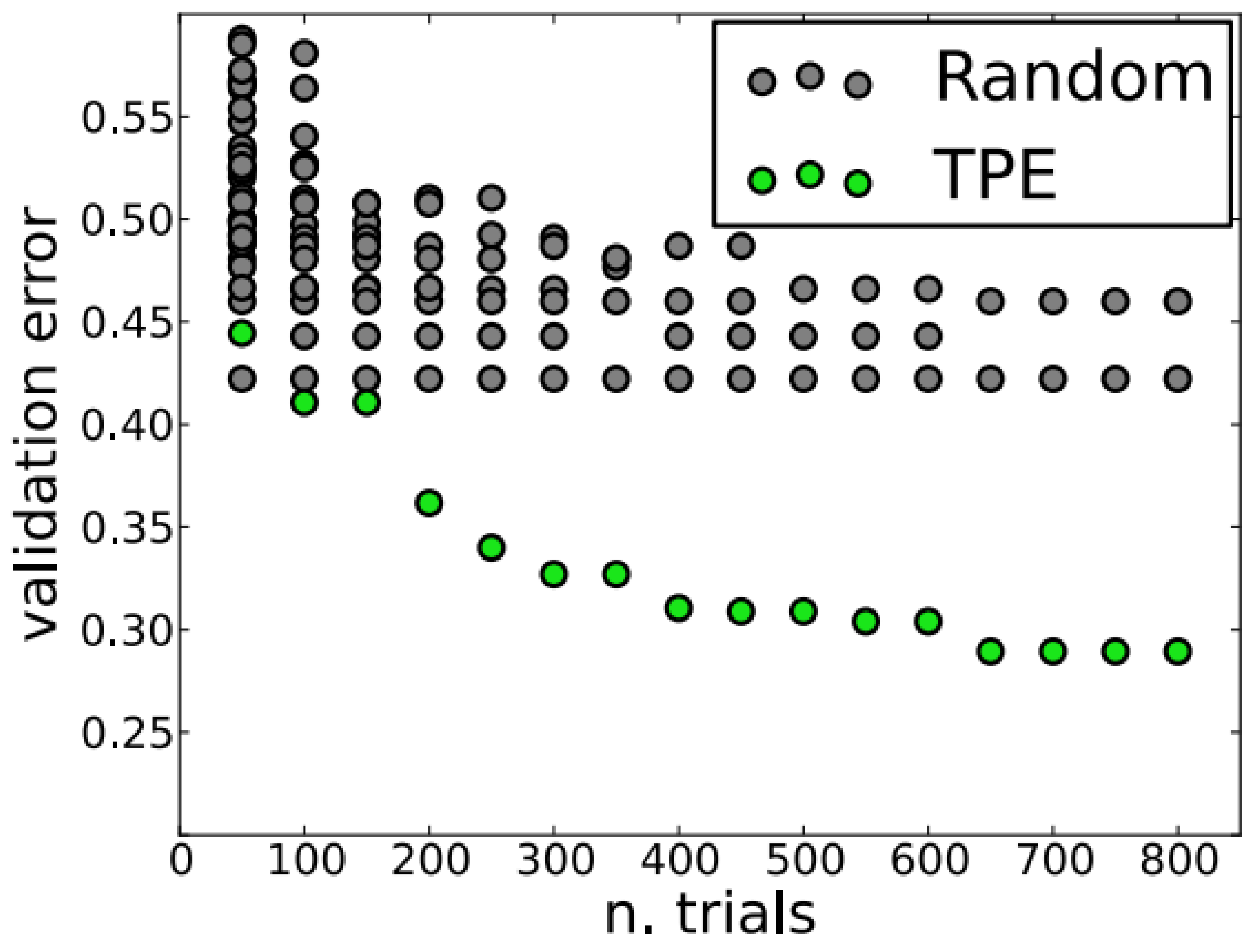
Problem context

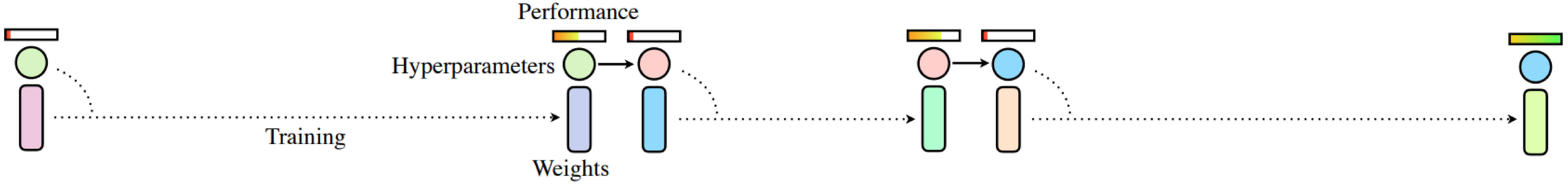
Sequential optimisation

$$p(h|y) = \frac{p(h) \times p(y|h)}{p(y)}$$

- Example: hand-tuning after each run
- Example: Bayesian optimisation
- We choose (sample) hyperparameters based on a priori assumptions, as well as what we learn from running the network each time – minimises evaluations

random vs tree parzen estimators





Problem context

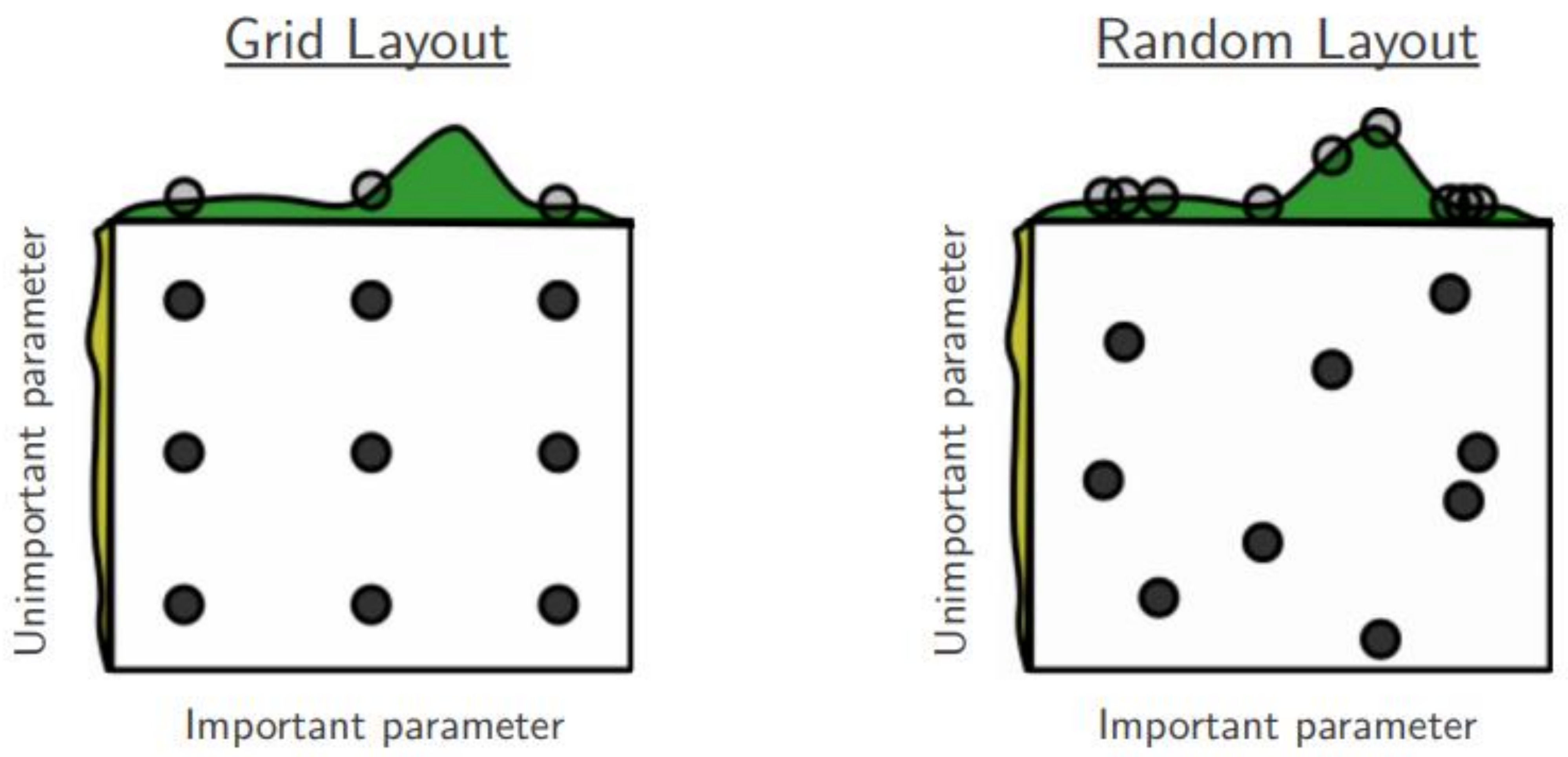
The “unreasonable success” of random search

- Random search generally much faster than grid search (more likely to modify important parameters – most hyperparameters have little effect on outcome)

- BUT still sampling from a uniform prior

- No ‘honing in’ on optimal solutions

- How to combine computational benefits of parallelisation, but still leverage knowledge gained from each (expensive) solution evaluation?



Solution proposed

Population based training

- Randomly initialise population of candidate solutions
- Evaluate solutions asynchronously for *a while* (# evaluations? Threshold?)
- When a solution is ‘ready’, use knowledge from population to decide whether to persist, or tack off and try a more promising alternative
- Important: no need for global synchronisation. Just copy more promising solution (+ some noise) and start from there

Solution proposed

Proposed algorithm

Algorithm 1 Population Based Training (PBT)

procedure TRAIN($\mathcal{P}$) ▷ initial population $\mathcal{P}$
  for $(\theta, h, p, t) \in \mathcal{P}$ (asynchronously in parallel) **do**
    while not end of training **do**
      $\theta \leftarrow \mathtt{step}(\theta | h)$ ▷ one step of optimisation using hyperparameters h
      $p \leftarrow \mathtt{eval}(\theta)$ ▷ current model evaluation
      if $\mathtt{ready}(p, t, \mathcal{P})$ **then**
        $h', \theta' \leftarrow \mathtt{exploit}(h, \theta, p, \mathcal{P})$ ▷ use the rest of population to find better solution
        if $\theta \neq \theta'$ **then**
          $h, \theta \leftarrow \mathtt{explore}(h', \theta', \mathcal{P})$ ▷ produce new hyperparameters h
          $p \leftarrow \mathtt{eval}(\theta)$ ▷ new model evaluation
        end if
      end if
      update $\mathcal{P}$ with new $(\theta, h, p, t + 1)$ ▷ update population
    end while
  end for
  return θ with the highest p in $\mathcal{P}$
end procedure

Solution proposed

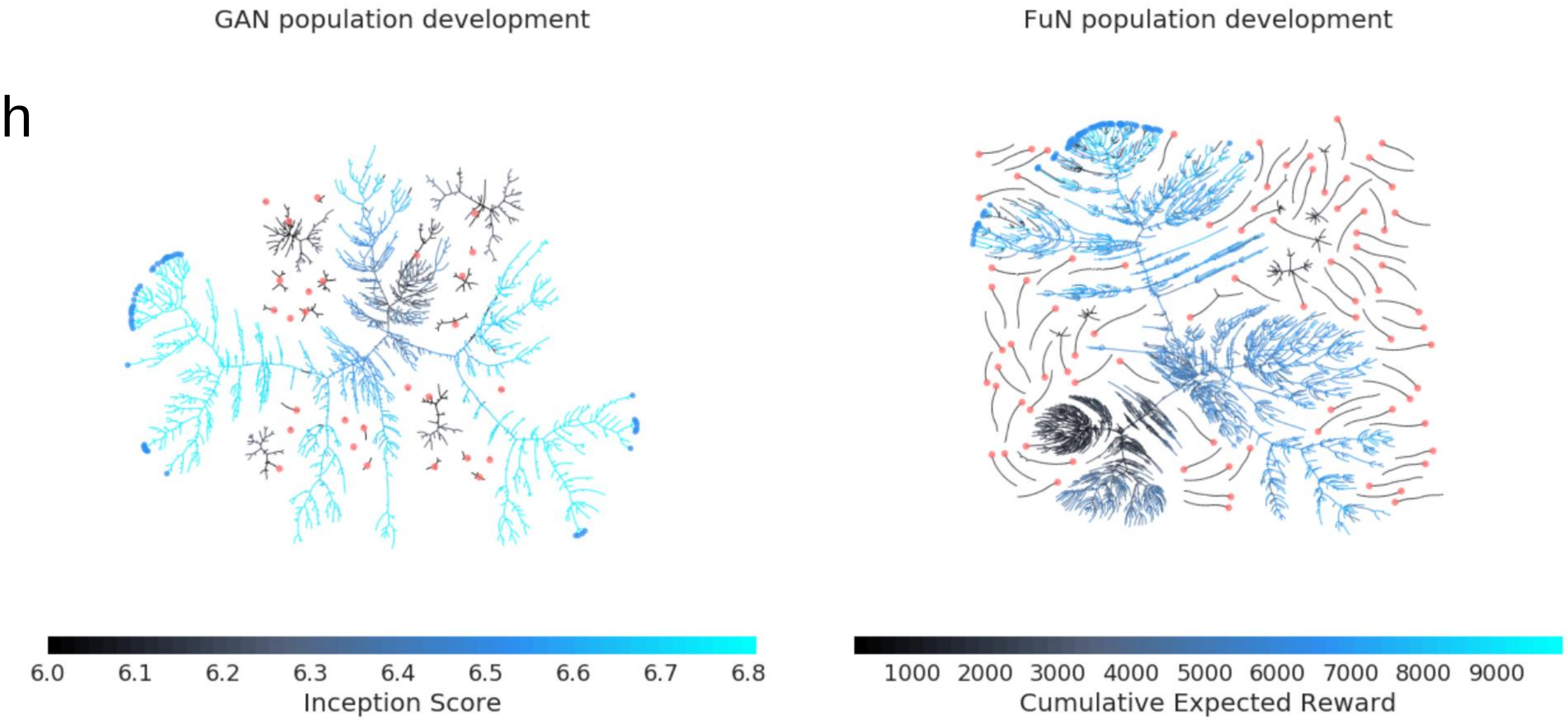
Exploit and explore

- Similar to cloning and mutation genetic operators – but note no recombination
- Typical exploitation: tournament selection, truncation, elitist. May copy entire alternative, or just hyperparameters, omitting model weights
- Explore: can be gradient-based, re-sampling from original prior, or adding random noise/perturbations
- Actual implementation simply applies a multiplier of either 1.2 or 0.8 to hyperparameters (mild perturbations) or 2.0/0.5 (aggressive)

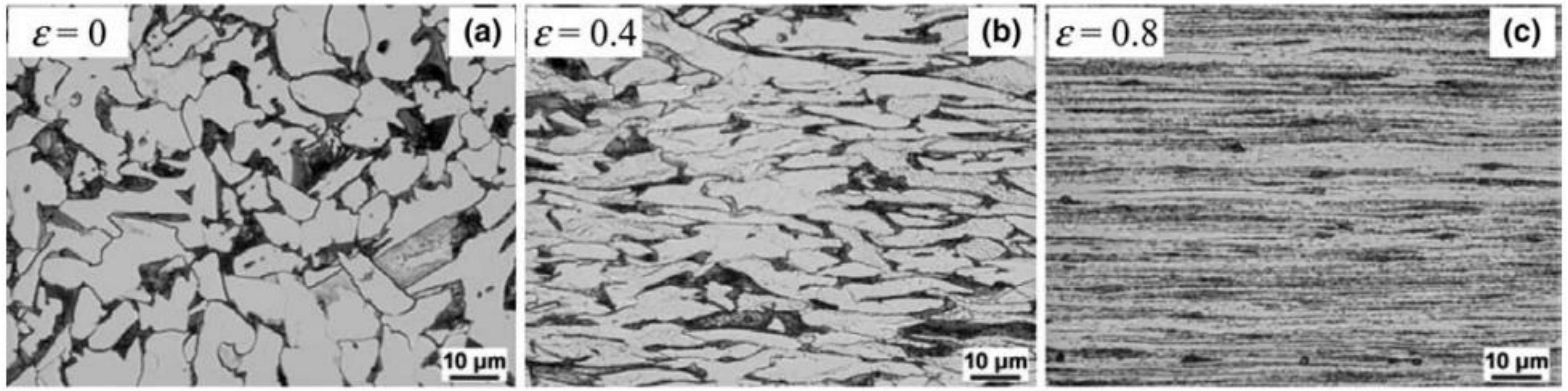
Solution proposed

Output interpretation

- Solutions are not retrained from scratch – model weights are copied over
- So output is not a fixed set of optimal hyperparameters, but actually an adaptive schedule



changing optical microstructure of steel during deformation (work hardening)



Solution proposed

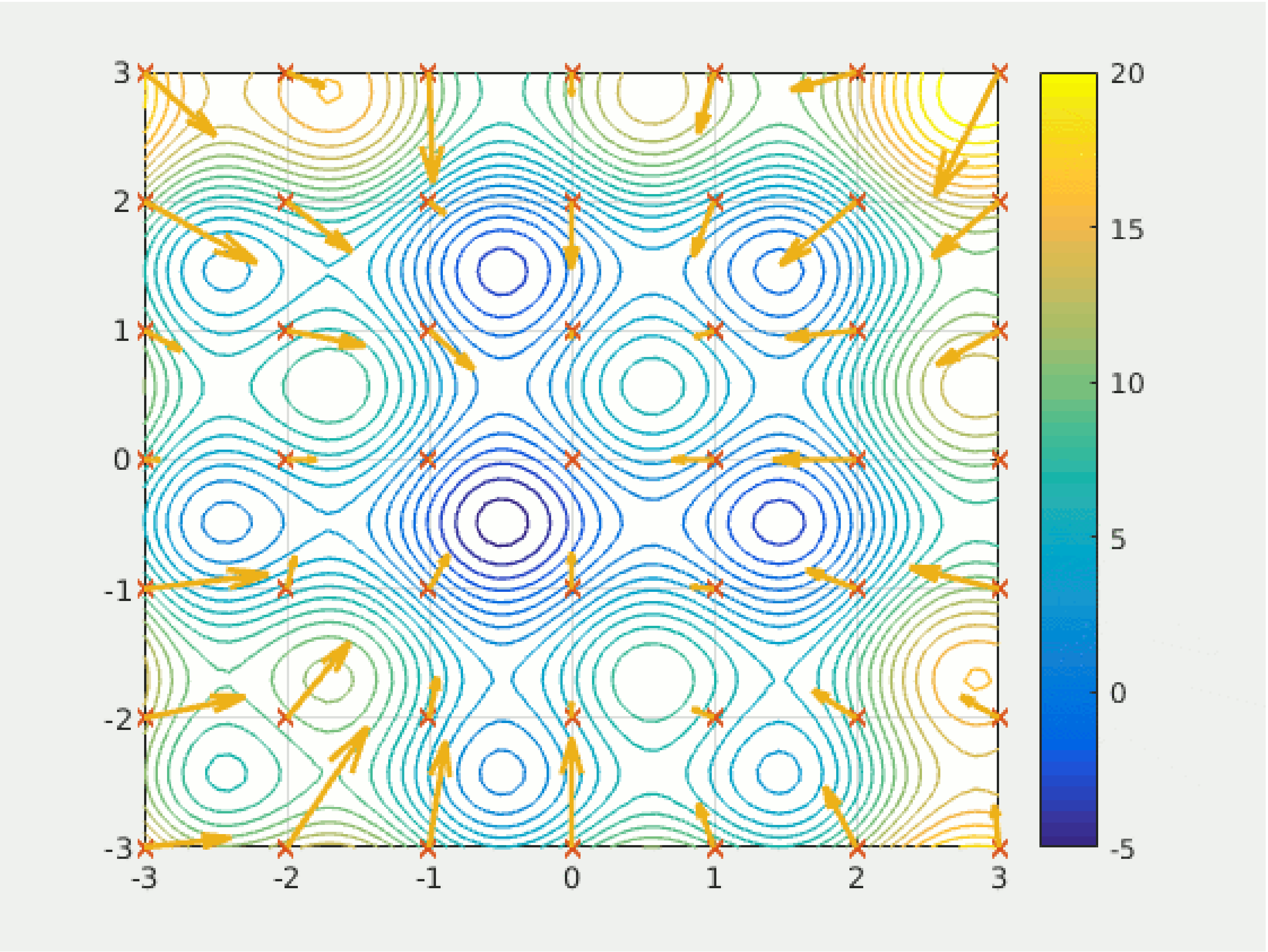
Annealing analogy

- PBT more akin to metal annealing than genetic algorithms
- When working metal, grains becomes brittle and needle-like, dislocations (abrupt changes in structure) introduced in stressed positions
- Heating to gentle glow breaks atomic bonds, relaxes molecular structure, dislocations fall away to stress-free positions
- Slow cooling results in gradual recrystallisation, atoms set in place but remain softer, malleable. <u>Slower cooling = better grain growth</u>
- Simulated annealing: aims to replicate this with hyperparameters (or weights…); over time, become less tolerant of poor solutions

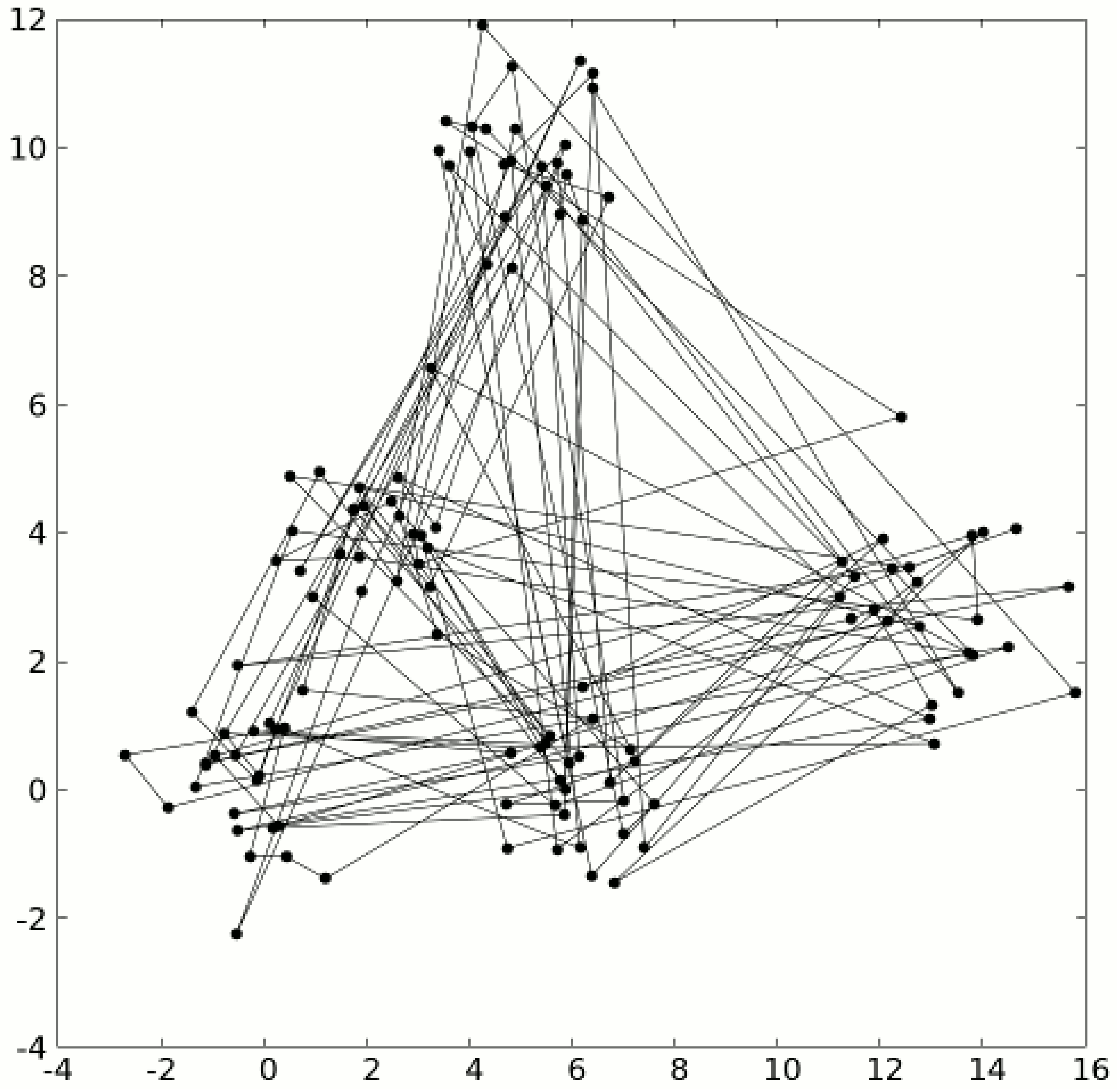
Existing work

- Particle swarm optimisation uses knowledge from population, but keeps individuals separate, i.e. no branching
- Simulated annealing, is itself its own optimisation technique
- Obvious parallels with REGAL, but more different than at first glance
- Practical Bayesian optimisation of ML algorithms (Snoek, Lerochelle, Adams, 2012) approach from other direction, starting with a Gaussian Process, then parallelising it

particle swarm optimisation



simulated annealing



Concluding thoughts

- No constant set of hyperparameters output, so really more ‘model optimisation’ than hyperparameter optimisation. Hyperparameters optimised just like weights, only with lower frequency updates
- Not wholly convinced by the decision to perturb parameters by 1.2/0.8 multiplier rather than adding random noise. (May be to keep better track of annealing schedule, though questionable benefit. As likely for sake of simplicity)

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