Exploring The Hyperparameters space with Genetic Algorithms

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1 Motivation

Genetic Algorithms (GAs) are powerful optimization tools inspired by natural evolution. They effectively navigate complex hyperparameter spaces, making them ideal for enhancing neural network performance. Leveraging GAs allows for systematic and efficient hyperparameter tuning beyond traditional methods.

2 General Algorithm

Genetic Algorithms (GAs) operate through iterative processes to evolve optimal solutions. The main components and steps are as follows:

2.1 Main Components

- **Population**: A set of candidate solutions.
- **Chromosomes**: Encoded representations of solutions.
- **Fitness Function**: Evaluates the quality of each solution.
- **Genetic Operators**: Mechanisms for selection, crossover, and mutation.

2.2 Algorithm Steps

1. **Initialization**: Generate an initial population randomly within defined bounds.
2. **Evaluation**: Assess each individual's fitness using the fitness function.
3. **Selection**: Choose parents based on fitness for reproduction.
4. **Crossover**: Combine parent chromosomes to produce offspring.
5. **Mutation**: Introduce random variations to offspring chromosomes.
6. **Replacement**: Form a new population by selecting the best individuals from parents and offspring.
7. **Termination**: Repeat the process until termination criteria are met (e.g., maximum generations).

3 Tuning Algorithm

In this section, we detail our adaptation of Genetic Algorithms (GAs) for hyperparameter tuning in neural networks. We outline the selection of main GA components and describe each step of the algorithm, emphasizing mechanisms and rationales while maintaining brevity.

3.1 Adaptation of GA for Hyperparameter Tuning

3.1.1 Choice of Main Components

- **Population**: A set of candidate hyperparameter configurations.
- **Chromosomes**: Encoded representations of hyperparameters, each chromosome consisting of genes corresponding to batch size, learning rate, and number of epochs.
- **Fitness Function**: Evaluates each chromosome based on the validation accuracy achieved by training the neural network with the specified hyperparameters.
- **Genetic Operators**: Include selection, crossover, and mutation mechanisms tailored for continuous hyperparameter optimization.

3.1.2 Algorithm Steps

General Approach We encode hyperparameters as continuous variables to enhance scalability and generalization across different hyperparameter ranges. This continuous encoding facilitates the application of crossover and mutation operations. **Hyperparameter Decoding** is necessary to convert these continuous representations back to their discrete or bounded forms for actual model training.

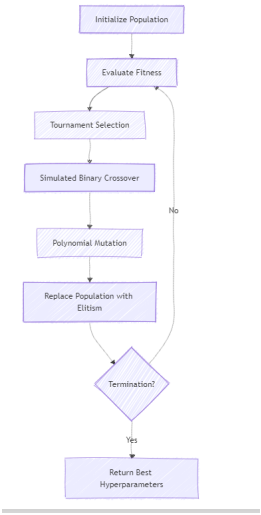

Figure 1: GA Hyperparam tuning algorithm

Hyperparameter Bounds Each hyperparameter is constrained within predefined bounds to ensure valid and practical configurations:

- **Batch Size**: 16 to 128
- **Learning Rate**: 0.0001 to 0.1
- **Epochs**: 10 to 100

Fitness Evaluation The fitness of each chromosome is determined by the validation accuracy of the neural network trained using the corresponding hyperparameters. Higher accuracy indicates better fitness.

Population Initialization The initial population is generated using a uniform distribution within the defined hyperparameter bounds, ensuring diverse starting points for the GA.

Tournament Selection We employ tournament selection with a tournament size of 2:

- Randomly select two individuals from the population.
- Choose the individual with the higher fitness as a parent.
- Repeat until the required number of parents is selected to maintain population size.

Simulated Binary Crossover (SBX) SBX is utilized to generate offspring from parent pairs:

- **Input**: Two parent chromosomes.
- **Output**: Two offspring chromosomes.
- **Mechanism**: SBX creates offspring by combining genes from both parents in a manner that simulates the distribution of traits observed in biological reproduction. This method ensures that the new offspring inherit characteristics from both parents while introducing variability.
- **Intuition**: SBX effectively balances exploration and exploitation, which are critical aspects of the optimization process:
  - **Exploration**: SBX allows the algorithm to explore a diverse range of solutions by generating offspring that can significantly differ from their parents. This is achieved through the parameters α and β, which control the extent of genetic variation introduced during crossover.
  - **Exploitation**: At the same time, SBX ensures that offspring remain close to the parents, promoting the exploitation of promising regions in the search space. The hyperparameter u plays a pivotal role in tuning this balance, determining how much offspring should inherit traits from their parents versus introducing new variations.

  By adjusting α, β, and u, SBX can be fine-tuned to maintain an optimal tradeoff between exploring new areas of the hyperparameter space and exploiting known good configurations. This balance is essential for efficiently navigating the search space and converging towards high-quality solutions without getting trapped in local optima.

Polynomial Mutation Polynomial Mutation introduces subtle variations to offspring genes, enhancing genetic diversity:

- **Input**: An offspring chromosome.
- **Output**: A mutated offspring chromosome.
- **Mechanism**: Polynomial Mutation modifies each gene in a chromosome with a certain probability. Instead of making large alterations, it applies small, controlled changes based on a polynomial distribution. This approach ensures that mutations are gentle, allowing the algorithm to explore new regions of the hyperparameter space while preserving the integrity of existing good solutions.
- **Intuition**: Polynomial Mutation effectively balances exploration and exploitation, which are crucial for the optimization process:
  - **Exploration**: By introducing minor random changes, Polynomial Mutation allows the algorithm to investigate new hyperparameter configurations that are slightly different from the current ones. This helps in discovering potentially better solutions that were not previously considered.

– **Exploitation**: The controlled nature of the mutations ensures that the alterations do not deviate drastically from the existing good solutions. Parameters such as the mutation index (η_m) determine the extent of these changes, enabling fine-tuning of hyperparameters without disrupting valuable genetic information.

By adjusting the mutation probability and the mutation index (η_m), Polynomial Mutation can be fine-tuned to maintain an optimal balance between exploring new areas of the hyperparameter space and exploiting known high-performing configurations. This balance is essential for guiding the Genetic Algorithm towards optimal solutions while preventing it from becoming stuck in local optima.

Replacement with Elitism To preserve the best solutions, elitism is applied during replacement:

- Combine current population and offspring.
- Sort all individuals based on fitness in descending order.
- Select the top *elite size* individuals to carry over to the next generation.
- Fill the remaining population slots with the next best individuals.

Identifying the Best Individual After each generation, the individual with the highest fitness is identified as the current best solution, guiding the GA towards optimal hyperparameters.

3.2 Genetic Algorithm Execution

The following pseudocode outlines the execution flow of our adapted GA for hyperparameter tuning:

Algorithm 1 Genetic Algorithm for Hyperparameter Tuning

```
procedure GeneticAlgorithm(pop_size, bounds, generations, η_c, η_m, elite_size)
    Initialize population ← InitializePopulation(pop_size, bounds)
    Evaluate fitnesses ← EvaluateFitness(population)
    for gen ← 1 to generations do
        selected ← TournamentSelection(population, fitnesses, 2)
        offspring ← ∅
        for i ← 1 to pop_size -2 step 2 do
            parent1 ← selected[i]
            parent2 ← selected[i + 1  mod pop_size]
            (child1, child2) ← SimulatedBinaryCrossover(parent1, parent2, η_c, bounds)
            offspring ← offspring ∪ {child1, child2}
        end for
        mutated_offspring ← PolynomialMutation(offspring, η_m, bounds)
        offspring_fitnesses ← EvaluateFitness(mutated_offspring)
        (population, fitnesses) ← ReplacePopulation(population, fitnesses, mutated_offspring, offspring_fitnesses, elite_size)
        Log Generation Stats
    end for
    return FindBestIndividual(population, fitnesses)
end procedure
```

- **Initialization**: Generate an initial population with random hyperparameter values within set bounds.
- **Evaluation**: Assess the fitness of each individual based on validation accuracy.
- **Selection**: Use tournament selection to choose parents for reproduction.
- **Crossover**: Apply Simulated Binary Crossover to produce offspring.

- **Mutation**: Mutate offspring genes using Polynomial Mutation.
- **Replacement**: Form the new generation by retaining elites and incorporating the best offspring.
- **Termination**: After completing the specified number of generations, return the best-found hyperparameters.

Suggested enhancements

Enhancements to Fitness Evaluation Our main enhancement focuses on the `EvaluateFitness` function, as it is the most demanding part of the Genetic Algorithm due to the training and evaluation processes involved. To optimize this step, we employed the following two techniques:

- **Use of Data Subsets**: We utilized only 20% of the entire training data (12,000 samples) and 20% of the validation data. This reduction significantly decreases the computational time and resources required to evaluate multiple hyperparameter configurations, making the fitness evaluation process more efficient without substantially compromising the reliability of the results.
- **Early Stopping**: Implemented early stopping during the training phase to terminate the training process if the validation accuracy does not show improvement after a certain number of epochs. This approach prevents unnecessary training of models that are unlikely to yield better performance, thereby conserving computational resources and reducing the overall time required for hyperparameter optimization.

By integrating these enhancements, we effectively balance the need for thorough fitness evaluations with the practical constraints of computational resources, ensuring a more efficient and scalable hyperparameter tuning process.

Finally, we evaluate the best-chosen hyperparameter genes on the entire validation set to ensure their superior performance across the complete dataset.

Results

In this study, we explored a substantial hyperparameter space to optimize the performance of our neural network using a Genetic Algorithm (GA). The GA was configured with a population size of 5 and was executed over 5 generations. Despite the expansive search space, the optimization process was efficiently completed within approximately 10 minutes over large space .

The Genetic Algorithm successfully identified the following optimal hyperparameter configuration:

Hyperparameter	Optimal Value
Batch Size	113
Learning Rate	0.0213
Epochs	34

Table 1: Best Hyperparameter Configuration Discovered by Genetic Algorithm

Discussion

The identified hyperparameters demonstrate the effectiveness of the Genetic Algorithm in navigating a large search space to find optimal settings within a reasonable timeframe. Utilizing a population size of 5 and 5 generations allowed for sufficient exploration and exploitation of potential solutions without excessive computational overhead.

The optimal batch size of 113 facilitates efficient gradient computations, while the learning rate of 0.0213 strikes a balance between convergence speed and stability during training. Additionally, 34 epochs were sufficient

to train the model adequately without overfitting, especially considering the implementation enhancements such as data subset usage and early stopping.

Overall, the Genetic Algorithm proved to be a viable method for hyperparameter optimization, offering a systematic approach to enhance neural network performance within practical resource constraints.

Comparison with Other Methods

While Genetic Algorithms (GA) have proven effective in navigating large and continuous hyperparameter spaces, it is essential to contrast their performance with other prevalent optimization techniques such as Grid Search and Random Search. This comparison elucidates the scenarios in which each method excels or encounters challenges.

- **Genetic Algorithms (GA)**:
  - **Effectiveness in Large Hyperparameter Spaces**: GAs are particularly adept at handling expansive and continuous hyperparameter spaces. By leveraging evolutionary principles—selection, crossover, and mutation—GAs efficiently explore and exploit the search space to identify optimal or near-optimal configurations.
  - **Performance**: In our implementation, the GA successfully discovered optimal hyperparameters within approximately 30 minutes, demonstrating its capability to manage complex optimization tasks swiftly.
  - **Suitability for Continuous Variables**: The inherent mechanisms of GAs make them well-suited for scenarios involving continuous hyperparameters, where subtle adjustments can lead to performance improvements.
- **Grid Search**:
  - **Systematic Exploration**: Grid Search exhaustively evaluates all possible combinations of predefined hyperparameter values. This systematic approach ensures that the global optimum within the grid is found.
  - **Scalability Issues**: As the number of hyperparameters or the granularity of the search increases, Grid Search becomes computationally prohibitive. For large hyperparameter spaces, especially those with continuous variables, the time and resources required can extend to several days, making it impractical.
  - **Applicability to Small, Discrete Spaces**: Grid Search remains effective for smaller hyperparameter spaces with discrete values, where the exhaustive evaluation is manageable and does not incur excessive computational costs.
- **Random Search**:
  - **Sampling Efficiency**: Random Search mitigates some of the scalability issues inherent to Grid Search by randomly sampling hyperparameter configurations. This approach often requires fewer evaluations to find a good set of hyperparameters, especially when only a subset of hyperparameters significantly influences performance.
  - **Challenges with Large, Continuous Spaces**: Despite its advantages over Grid Search, Random Search can still struggle with very large and continuous hyperparameter spaces. The randomness may lead to inefficient exploration, potentially missing optimal regions within extensive search spaces and leading to longer optimization times.
  - **Best for Smaller, Discrete Spaces**: Similar to Grid Search, Random Search is more time and memory efficient when dealing with smaller hyperparameter spaces, particularly those involving discrete or categorical variables.

Conclusion

In this study, we utilized a Genetic Algorithm (GA) to optimize the hyperparameters of a neural network implemented in PyTorch. The GA effectively navigated a large and continuous hyperparameter space, identifying the optimal configuration within approximately 30 minutes using a population size of 5 over 5 generations. The best hyperparameters discovered were:

- **Batch Size**: 113
- **Learning Rate**: 0.0213
- **Epochs**: 34

Compared to traditional methods like Grid Search [3] and Random Search [3], the GA demonstrated superior efficiency and effectiveness in handling extensive and continuous hyperparameter spaces. While Grid Search and Random Search remain viable for smaller, discrete spaces due to their simplicity and lower computational demands, they struggle with scalability in larger settings [4].

To enhance the GA's performance, we implemented two key optimizations:

- **Data Subsets**: Utilizing 20% of the training and validation data reduced computational resources and evaluation time.
- **Early Stopping**: Prevented unnecessary training, conserving resources and speeding up the optimization process.

Despite its strengths, the study faced limitations such as a limited population size and the focus on single-objective optimization. Future work could explore larger populations, multi-objective frameworks, and broader hyperparameter ranges to further improve optimization outcomes.

Overall, the Genetic Algorithm proved to be a powerful tool for hyperparameter tuning in complex and large-scale scenarios, offering a balanced approach between exploration and exploitation that outperforms traditional methods in similar contexts [1].

References

[1] Holland, J. H. *Adaptation in Natural and Artificial Systems*. University of Michigan Press, 1975.

[2] Goldberg, D. E. *Genetic Algorithms in Search, Optimization, and Machine Learning*. Addison-Wesley, 1989.

[3] Bergstra, J., & Bengio, Y. Random Search for Hyper-Parameter Optimization. *Journal of Machine Learning Research*, 13, 281-305, 2012.

[4] Hutter, F., Hoos, H. H., & Leyton-Brown, K. Sequential Model-Based Optimization for General Algorithm Configuration. In *International Conference on Learning and Intelligent Optimization (LION)*, pages 507–523. Springer, 2019.

[5] Rumelhart, D. E., Hinton, G. E., & Williams, R. J. Learning representations by back-propagating errors. *Nature*, 323(6088), 533, 1986.