Phytomorphic Surrogate Neural Network for Synthetic Maize L-system Parameter Optimization

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INTRODUCTION

The Problem:
Optimizing plant architecture is a key challenge in computational biology, especially for creating models that accurately reflect real biological structures.
Traditional methods for tuning L-system parameters are limited:
- High-dimensional complexity
- Non-differentiable simulation processes
- Slow and computationally expensive searches

The Approach:
- We propose a neural network-based method for efficient, gradient-based optimization of L-system plant models.
- This technique leverages artificial intelligence to automate plant modeling and image-matching.
- By combining structural realism with modern AI, the method produces biologically meaningful, realistic plant architectures.

DISCUSSION

Phytomorphic Surrogate Model:
- Enables direct, gradient-based optimization of plant parameters within the L-system framework.
- Embeds plant structure into the optimization process, maintaining biological plausibility and preventing unrealistic parameter values.
- Produces synthetic plants that closely resemble real specimens by optimizing parameters over meaningful morphological differences.

Benchmark Models:
- Treat parameter optimization as a simple mapping from parameters to cost, without structural awareness.
- Frequently exploit the boundaries of parameter ranges, resulting in unrealistic or degenerate plant models.

Parameter Optimization Performance:
- The phytomorphic surrogate supports efficient and interpretable parameter exploration, discovering plausible sets that yield biologically valid plant architectures.
- Benchmark models and phytomorphic model achieve similar prediction accuracies, with the batch-trained benchmark performing best.

Key Advantage:
- By combining structural modeling and gradient-based optimization, the phytomorphic surrogate achieves both reliable cost prediction and biologically meaningful parameter optimization.

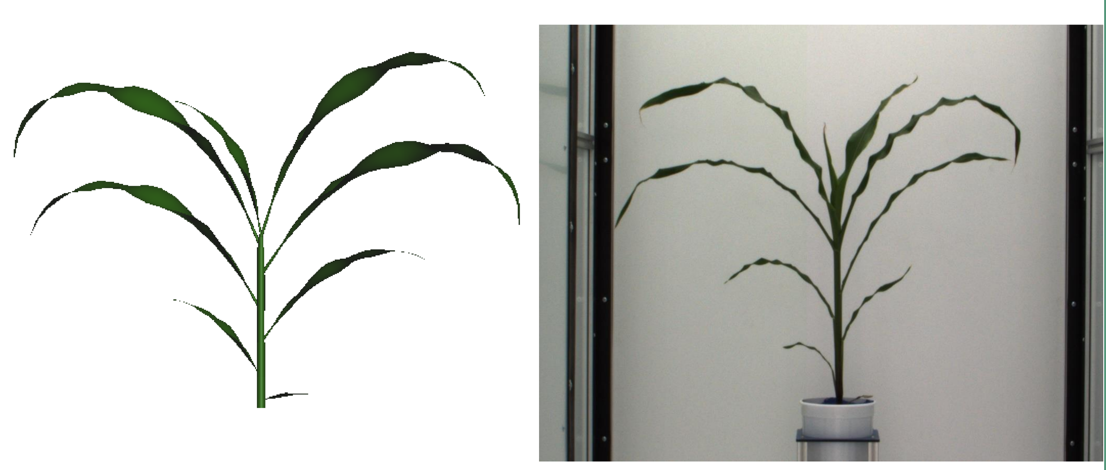
METHODS

Optimization Problem:
We seek to identify the optimal set of 13 L-system parameters that allow synthetic maize plant images to closely match real plant images. This high-dimensional optimization task requires fine-tuning structural, geometric, and angular features to minimize differences between simulated and real plant morphology.

Key Steps in the Optimization Pipeline:
- **Parameter Search:**
  - Adjust 13 L-system parameters affecting plant structure, geometry, and angles.
- **Synthetic Plant Generation:**
  - Use the L-system model to generate plants by varying these parameters.
- **Image Rendering:**
  - Render each synthetic plant as a standardized 2D image for comparison.
- **Similarity Evaluation:**
  - Compare synthetic images to real maize plant images.
  - Use a similarity metric to quantify how well the simulated plant matches the real specimen.

Goal:
The objective is to discover parameter sets that yield synthetic plants with morphology and appearance closely resembling real maize specimens.

Visual Example:
Below, a synthetic plant image (left) and a real plant image (right) illustrate the image matching goal central to this study.



Neural Network Approach:
Optimizing L-system plant parameters for image matching requires a gradient-based method. However, standard L-system generation is not differentiable, so it cannot be used directly with gradient descent techniques.
To solve this, we developed a spatially-aware neural network surrogate. This model approximates both plant generation and similarity measurement in a way that supports differentiation.
- The surrogate takes parameter vectors and learns to predict the cost (image similarity) between simulated and real plants.
- By making the optimization pipeline differentiable, the model enables efficient gradient-based searching for parameter sets that best match real plant images.

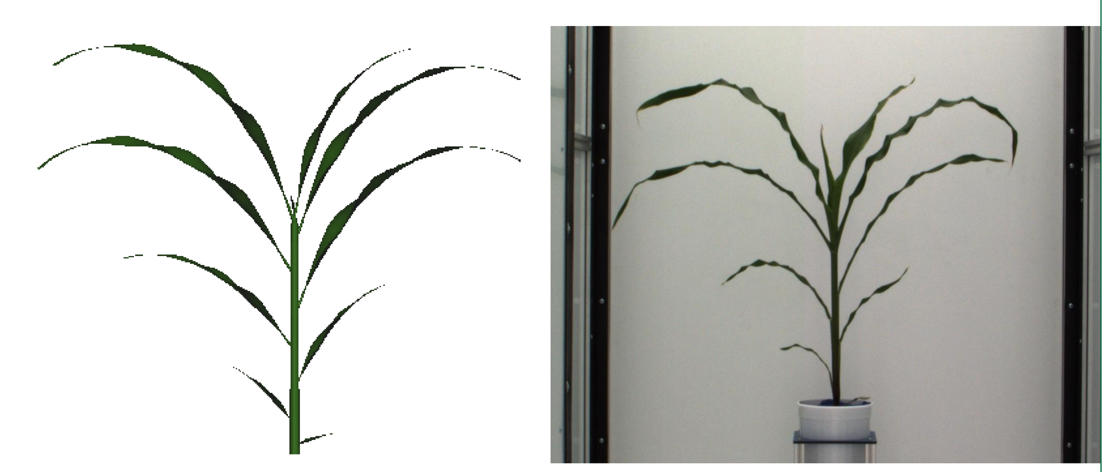
RESULTS

Parameter Optimization Performance
We evaluated our spatially-aware neural network surrogate against benchmark optimization models for fitting L-system parameters.

Benchmark Models:
- Produced unrealistic parameter sets due to boundary artifacts.
- Failed to generate plant models that resemble real specimens.

Phytomorphic Surrogate:
- Supports robust, gradient-based optimization.
- Consistently yields synthetic plants that closely match real maize plants.

Visual Example:
A synthetic plant image optimized by the phytomorphic surrogate (left) is shown next to a real plant image (right) to illustrate the accuracy of our approach.



Surrogate Model Cost Prediction
Each model's ability to predict image similarity ("cost") between synthetic and real plant was evaluated, after being trained with 480,000 samples each. Below are the results taken from the last 4,800 training samples:

Evaluation Metrics	Benchmark1 (Batch)	Benchmark2 (Online)	Phytomorph
Acc <1%	74.3%	67.4%	71.8%
Acc <5%	99.7%	99.7%	99.7%
Acc <10%	100%	100%	100%
Mean Relative Error	0.0077	0.0088	0.0081
Median Relative Error	0.0054	0.0066	0.0057
R^2 Score	0.9911	0.9887	0.9896
Convergence Stability	0.000223	0.000162	0.000254

CONCLUSION

- The phytomorphic surrogate neural network robustly optimizes L-system plant model parameters, outperforming benchmark models that suffer from boundary exploitation.
- Structural and morphological information is integrated directly into the surrogate and optimization process.
- Efficient gradient-based parameter discovery is achieved, with solutions maintaining close fidelity to real plant phenotypes.
- The approach eliminates the need for direct image generation during optimization.
- Synthetic plant structures produced by this method consistently match real specimens, advancing surrogate-driven phenotyping for complex biological systems.

REFERENCES/ACKNOWLEDGEMENTS

References:
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