MRC/CSO Social and Public Health Sciences Unit




Convolutional Neural Networks for Cellular Automata Classification

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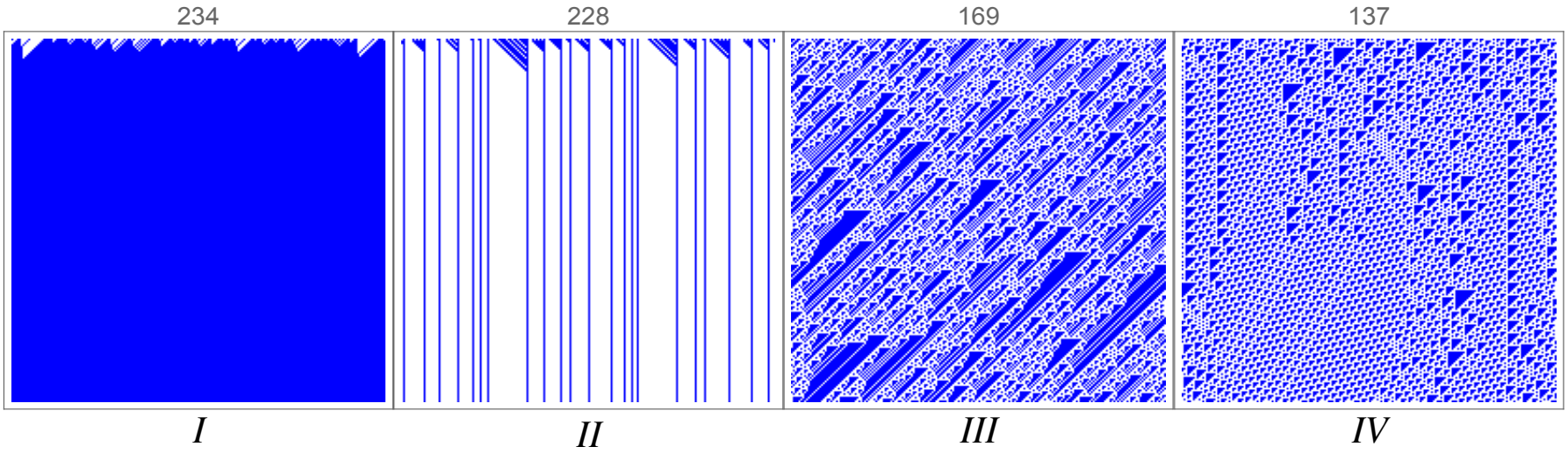
ALife 2019

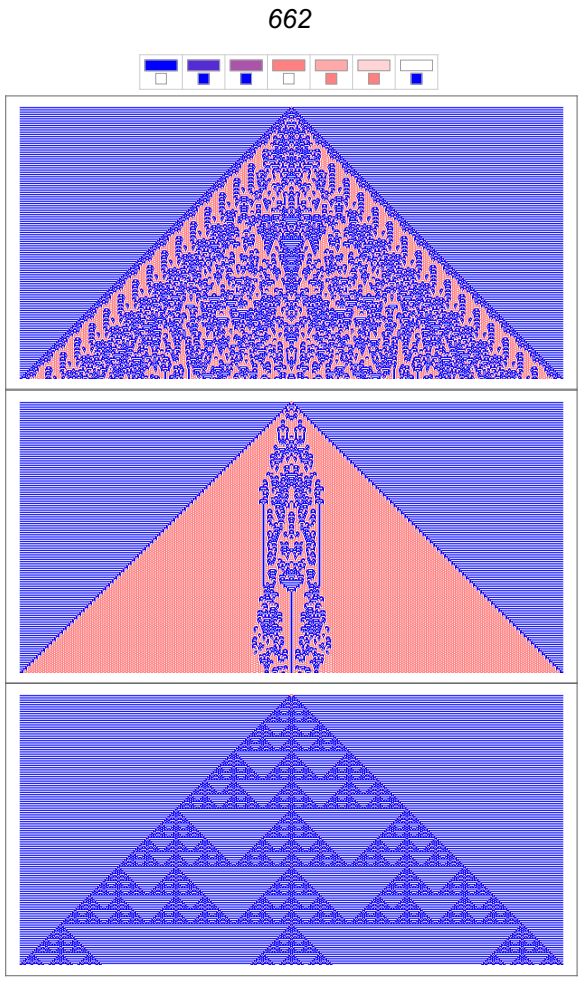
30 July 2019

Motivations



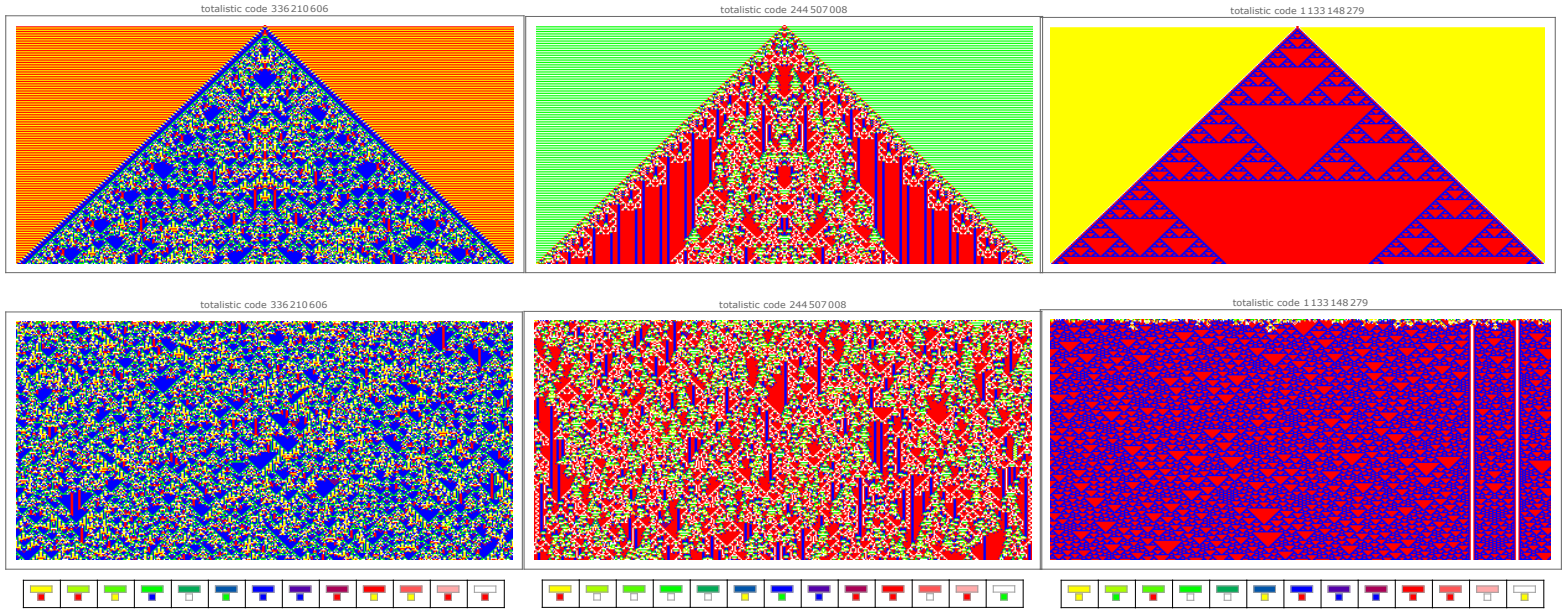
- Stephen Wolfram (1984) proposed a four-way classification of cellular automaton behaviour:
  - Class I: converge to a homogeneous state
  - Class II: generate periodic or stable structures
  - Class III: generate chaotic, aperiodic patterns
  - Class IV: complex localised structures

Motivations



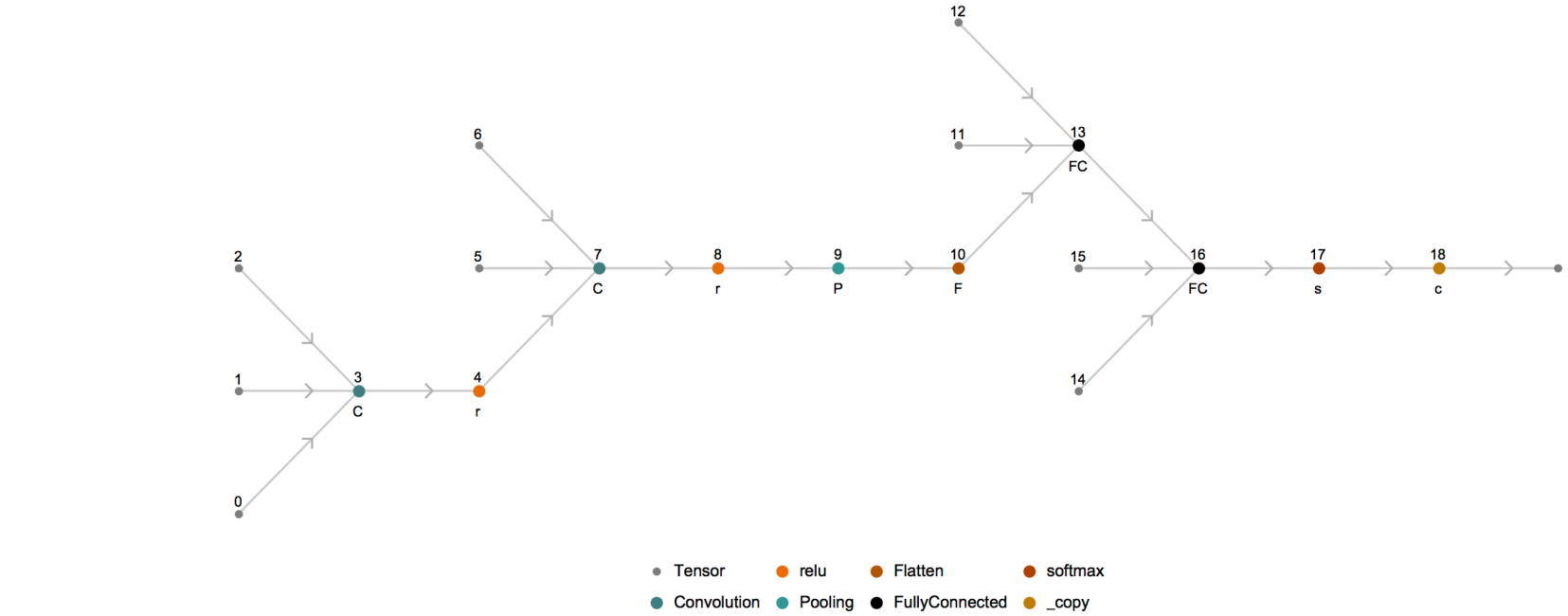
- Wolfram's classification scheme has spawned much discussion
- The definition is qualitative – can we better define what makes a CA Class IV?
- Some CAs show behaviours from multiple classes depending on initial conditions
- Classifying a CA is ultimately an undecidable problem (Culik and Yu, 1988)

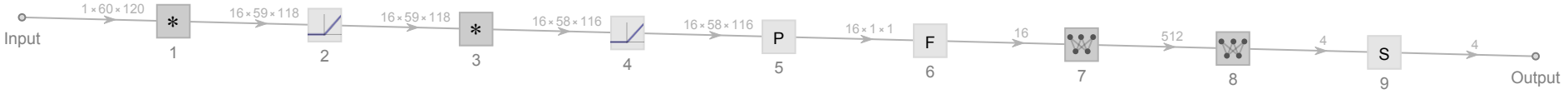
Research Questions



- Can a deep convolutional neural net (DCNN) learn to classify CA rules based only on images of CA output?
- Can the DCNN generalise to complex rule spaces, where distinguishing persistent structures becomes more difficult?

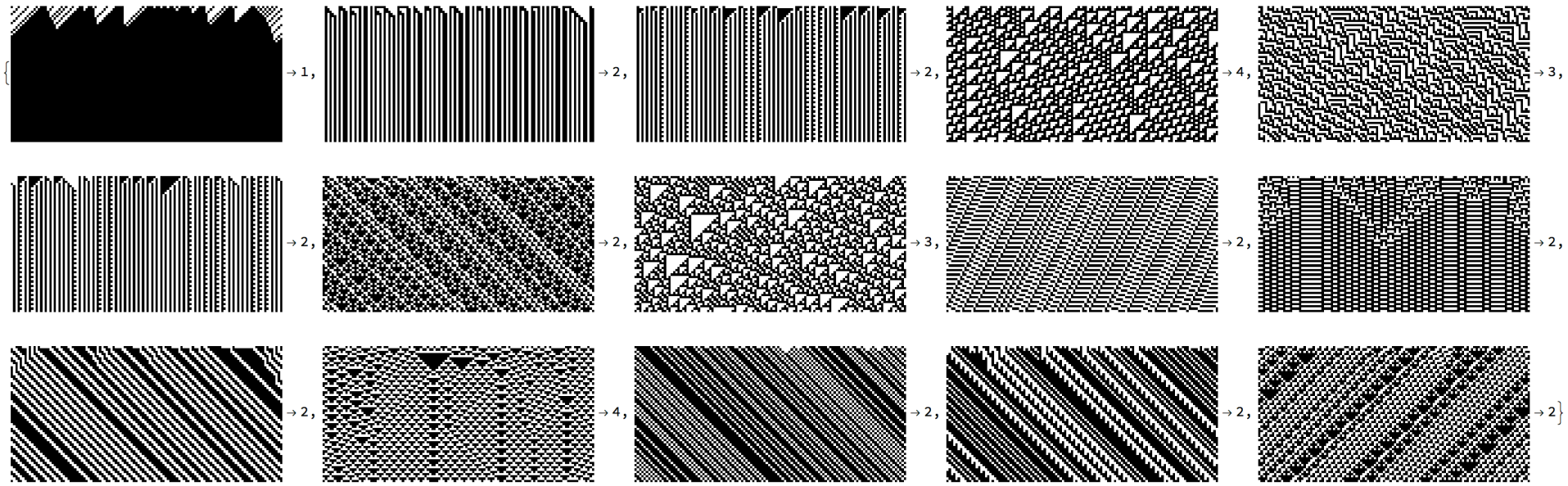
Network Structure (Network I/II)





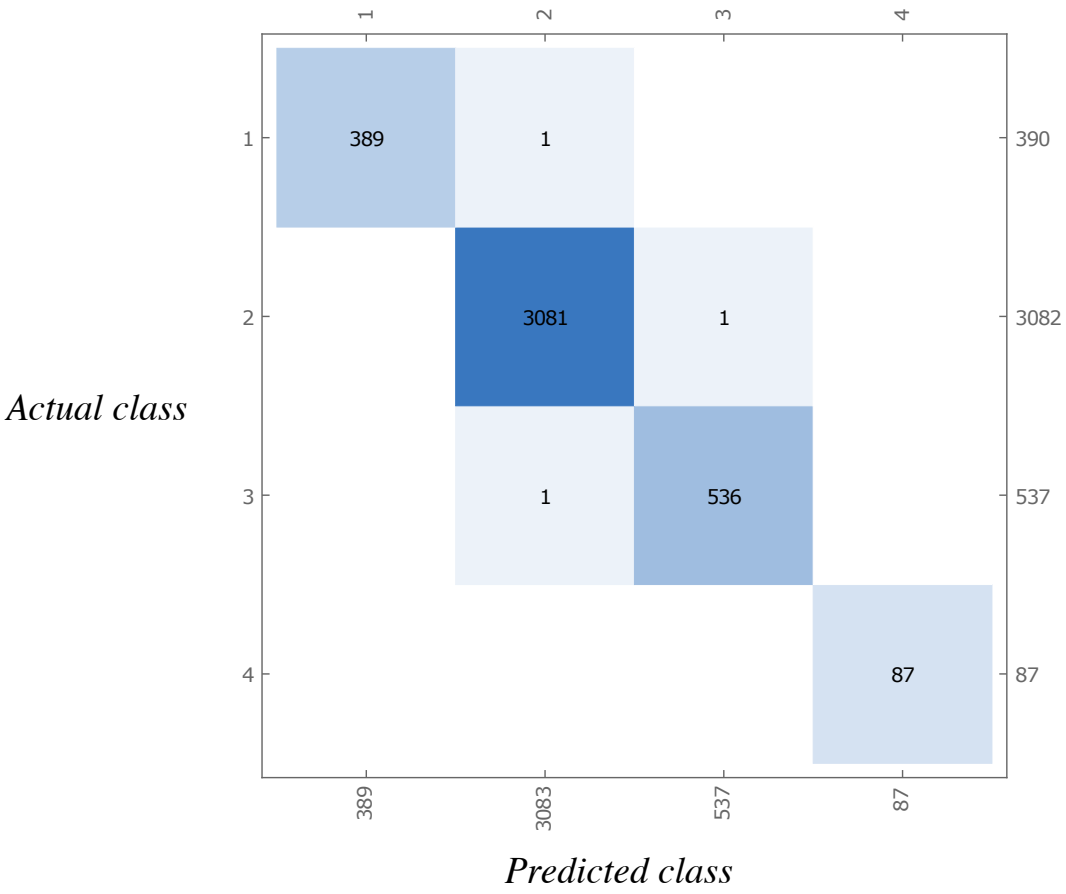
- Nine-layer CNN with two convolutional layers
- 512-node fully-connected layer
- 4-node SoftMax layer outputs Wolfram classification

Training Data: Elementary Cellular Automata (ECA)



- 120 x 60 pixel images of ECA rules with random initial conditions
- Each image tagged with Wolfram class of the given rule
- 32,768 training images used

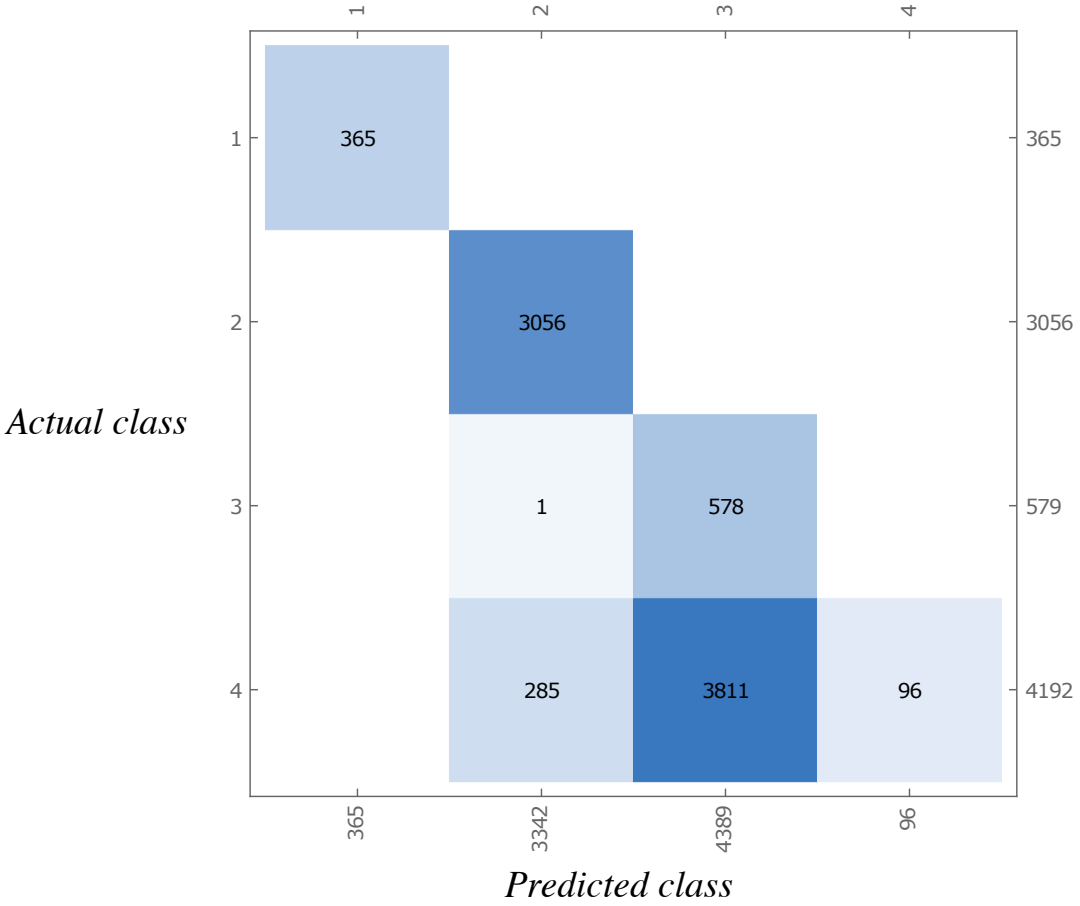
Results: Confusion Matrix (Network I, grayscale ECAs)



ECAs only:

- Accuracy: 99.93%
- Precision by class:
  - 1: 100%, 2: 99.94%, 3: 99.81%, 4: 100%

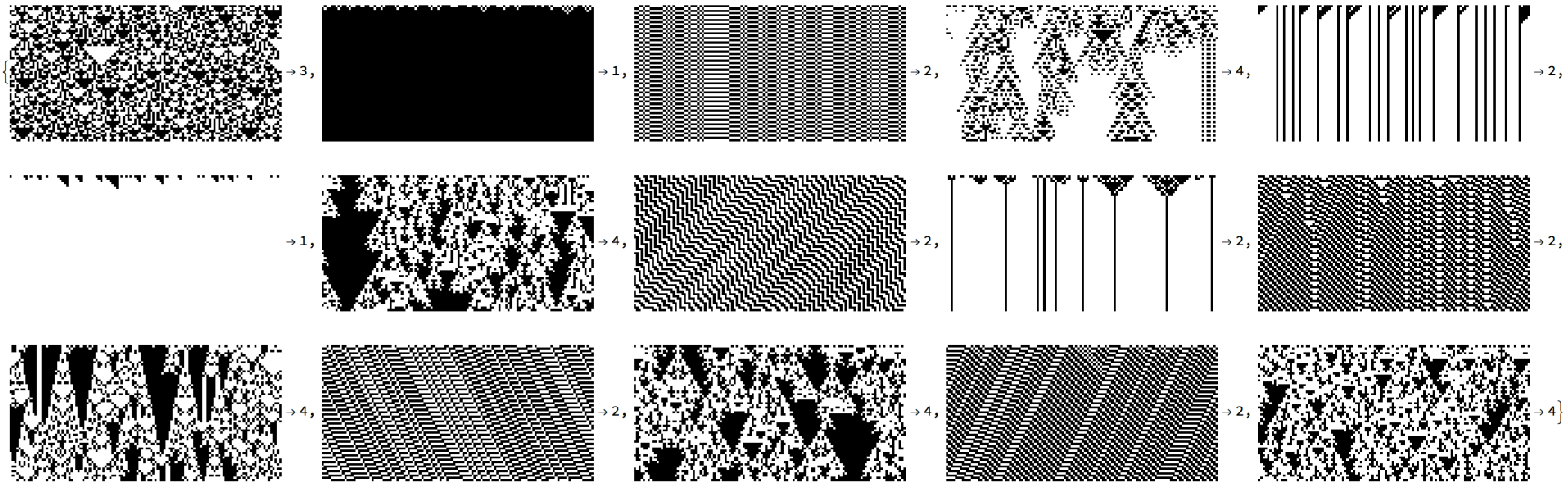
Results: Confusion Matrix (Network I, grayscale ECAs)



ECAs and 3-colour totalistic CAs:

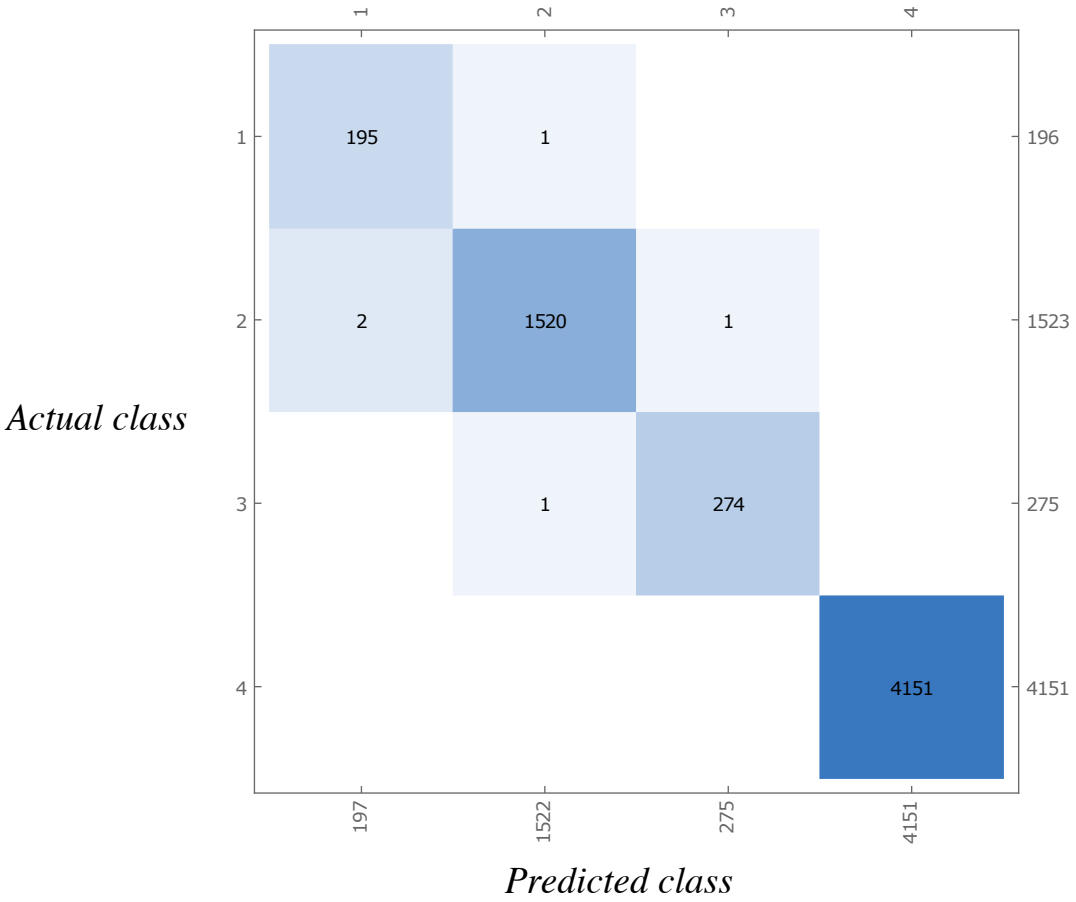
- Accuracy: 49.98%
- Precision by class:
  - 1: 100%, 2: 91.44%, **3: 13.17%,** 4: 100%

Training Data II: ECAs + Totalistic 2, 3 and 4 Colour Rules



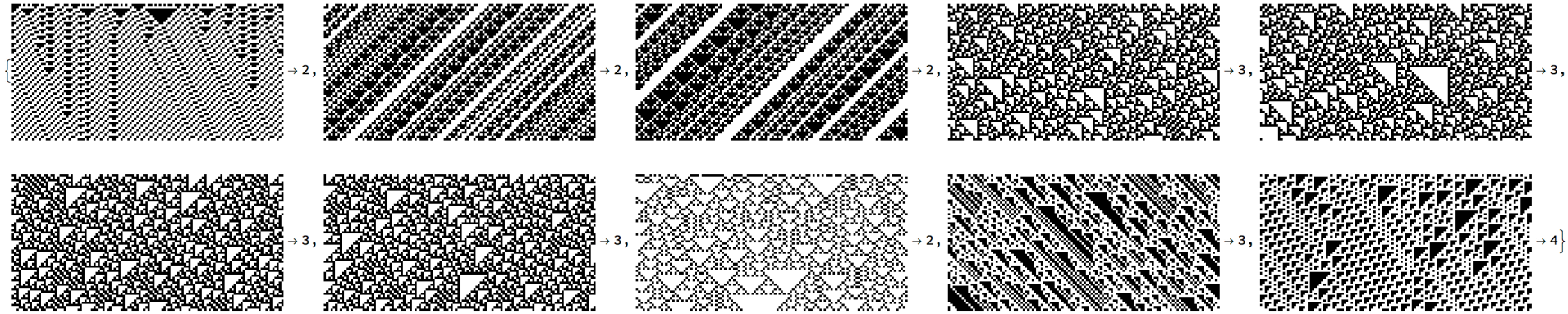
- 120 x 60 pixel images of ECA rules and totalistic CA rules with 2, 3 and 4 colours
- 16,384 ECA training images, 8,192 totalistic images

Results: Confusion Matrix (Network II, grayscale)

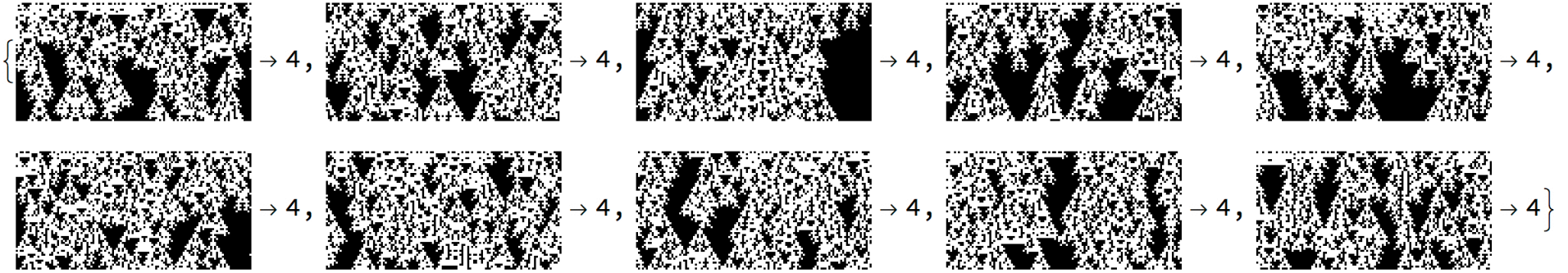


- Accuracy: 99.92%
- Precision by class:
  - 1: 99.0%, 2: 99.87%, **3: 99.64%,** 4: 100%

Results: Image Entropies (Network II, grayscale)

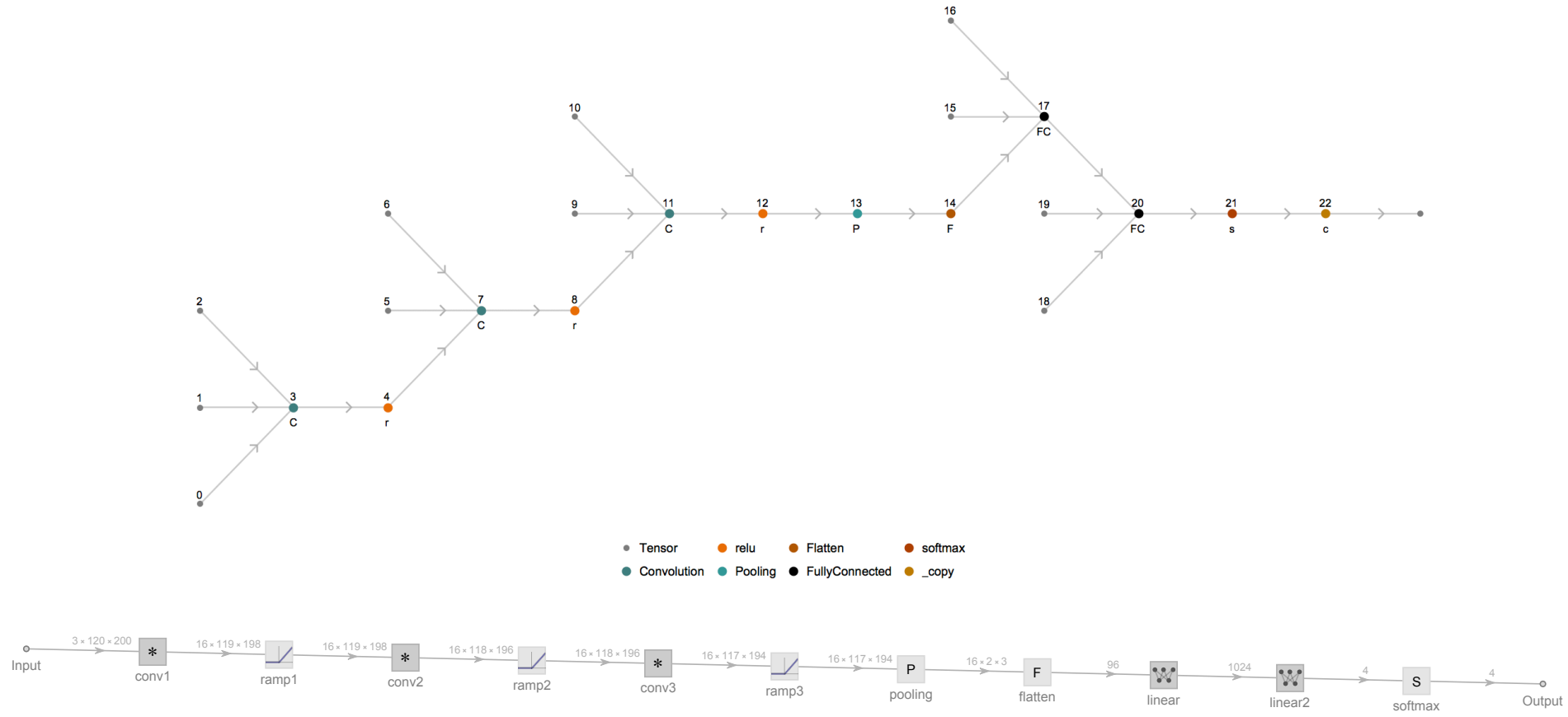


Highest Entropy



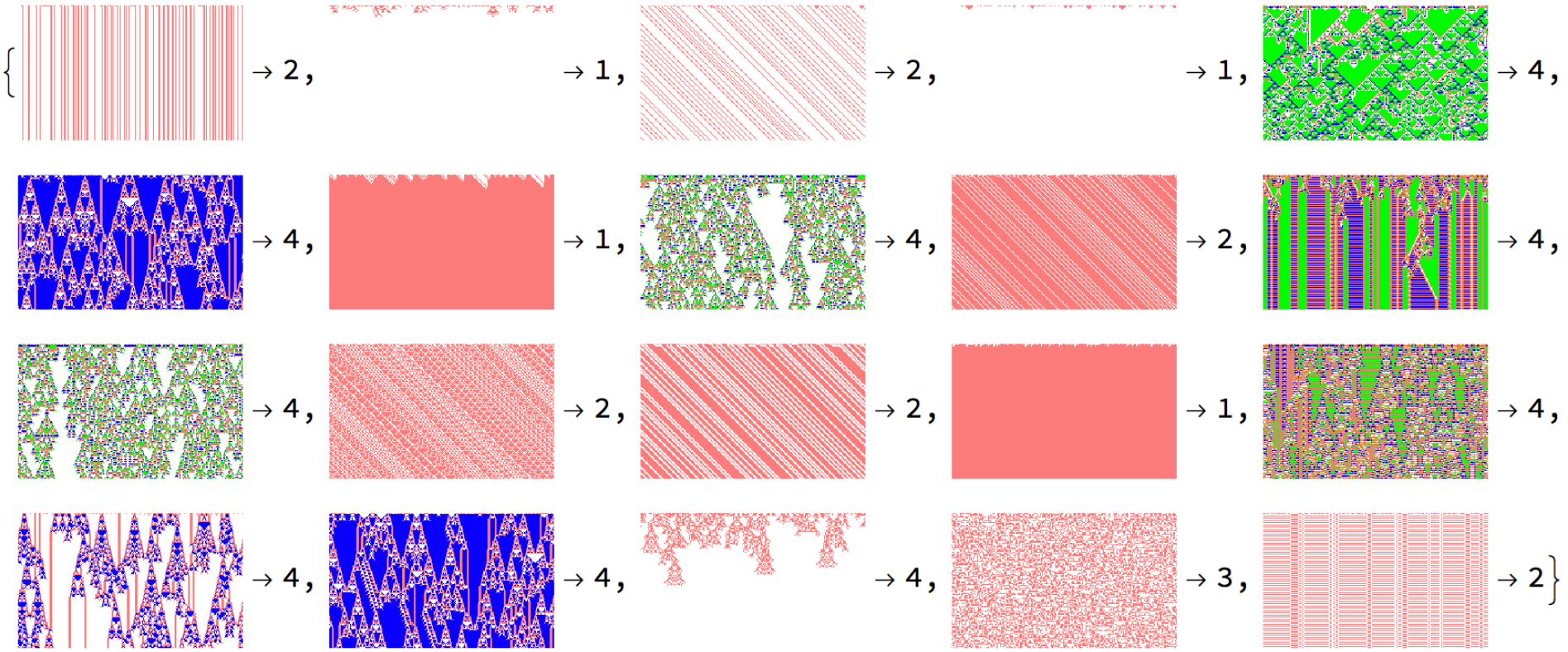
Lowest Entropy

Network Structure (Network VI/VII)



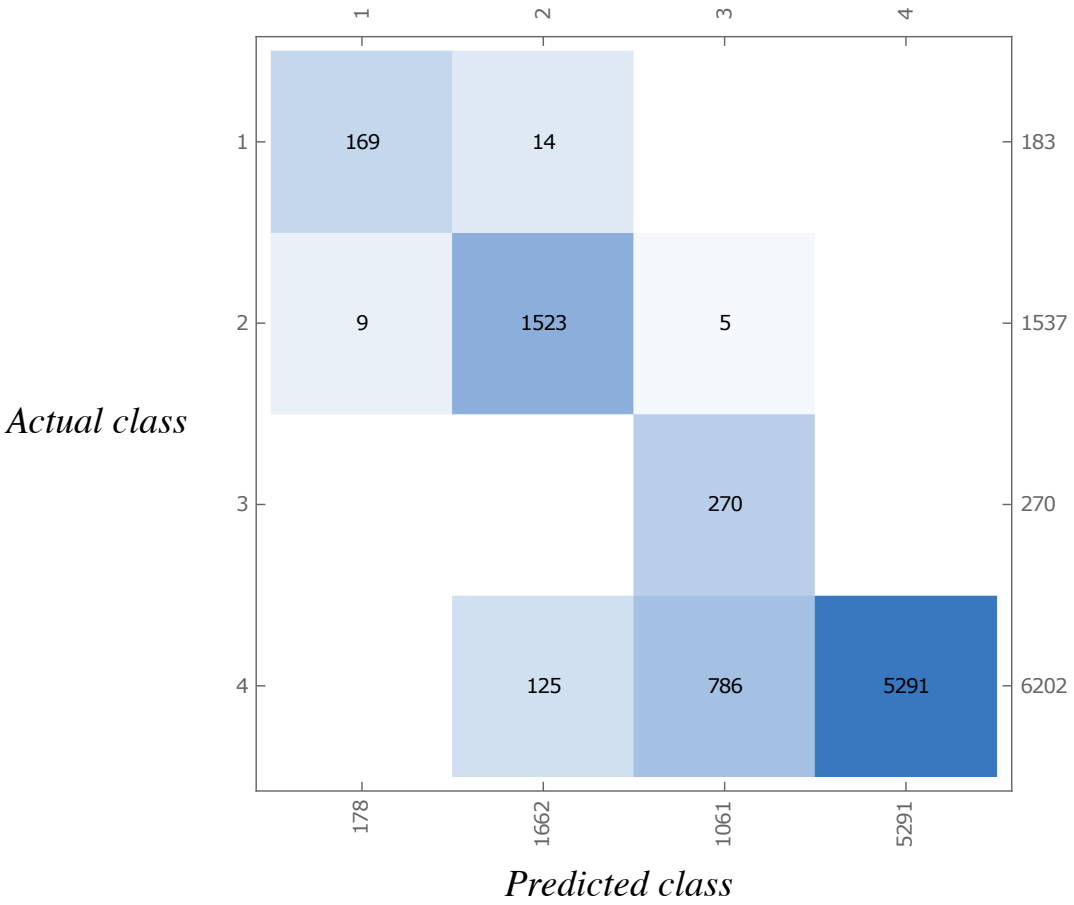
- Eleven-layer CNN with three convolutional layers
- 1,024-node fully-connected layer
- 4-node SoftMax layer outputs Wolfram classification

Training Data VI: ECAs + Totalistic 2, 3, 4 and 5 Colour Rules



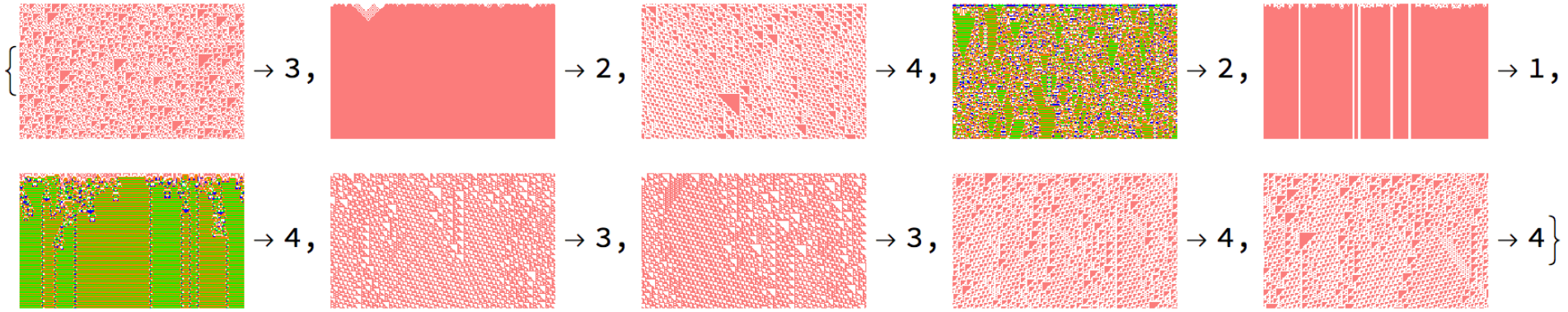
- 200 x 120 pixel colour images of ECA rules and totalistic CA rules with 2, 3, 4 and 5 colours
- 24,576 total training images

Results: Confusion Matrix (Network VI, colour)

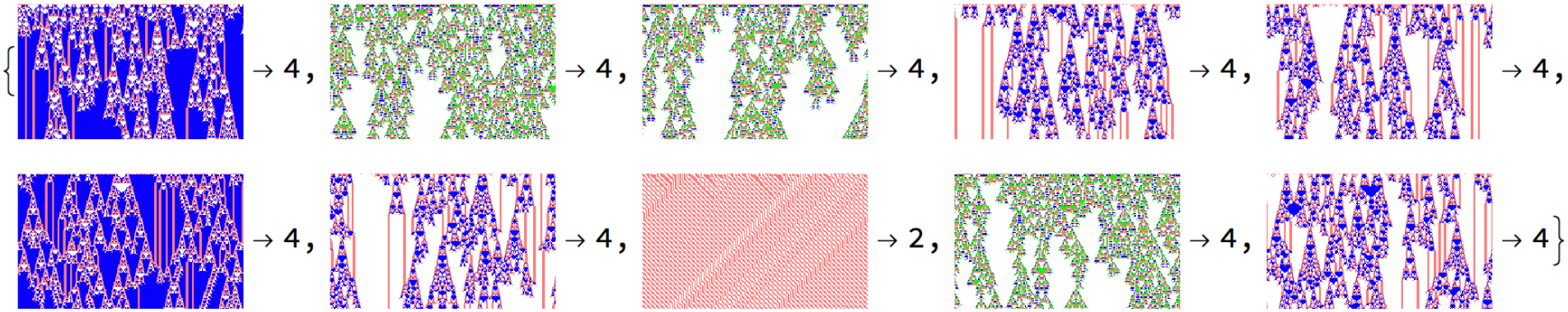


- Accuracy: 88.5%
- By class:
  - 1: 94.9%, 2: 91.6%, **3: 25.4%**, 4: 100%

Results: Image Entropies (Network VI, colour)

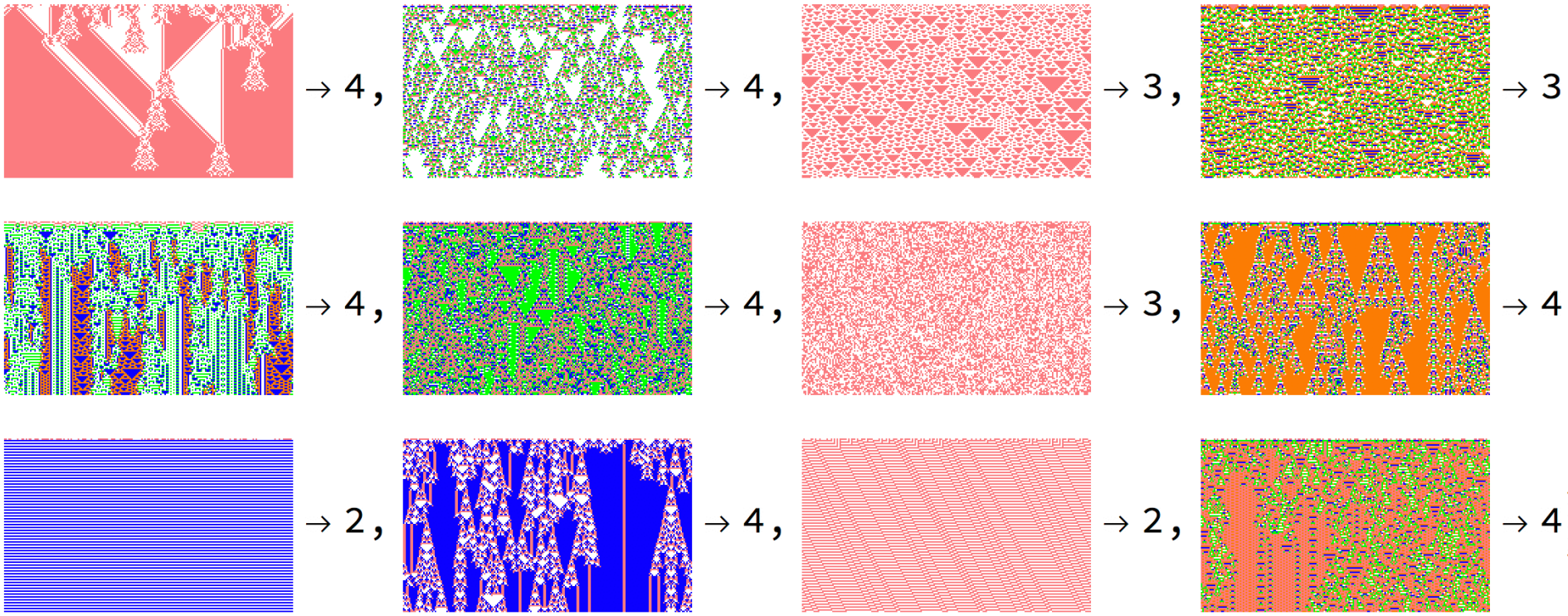


Highest Entropy



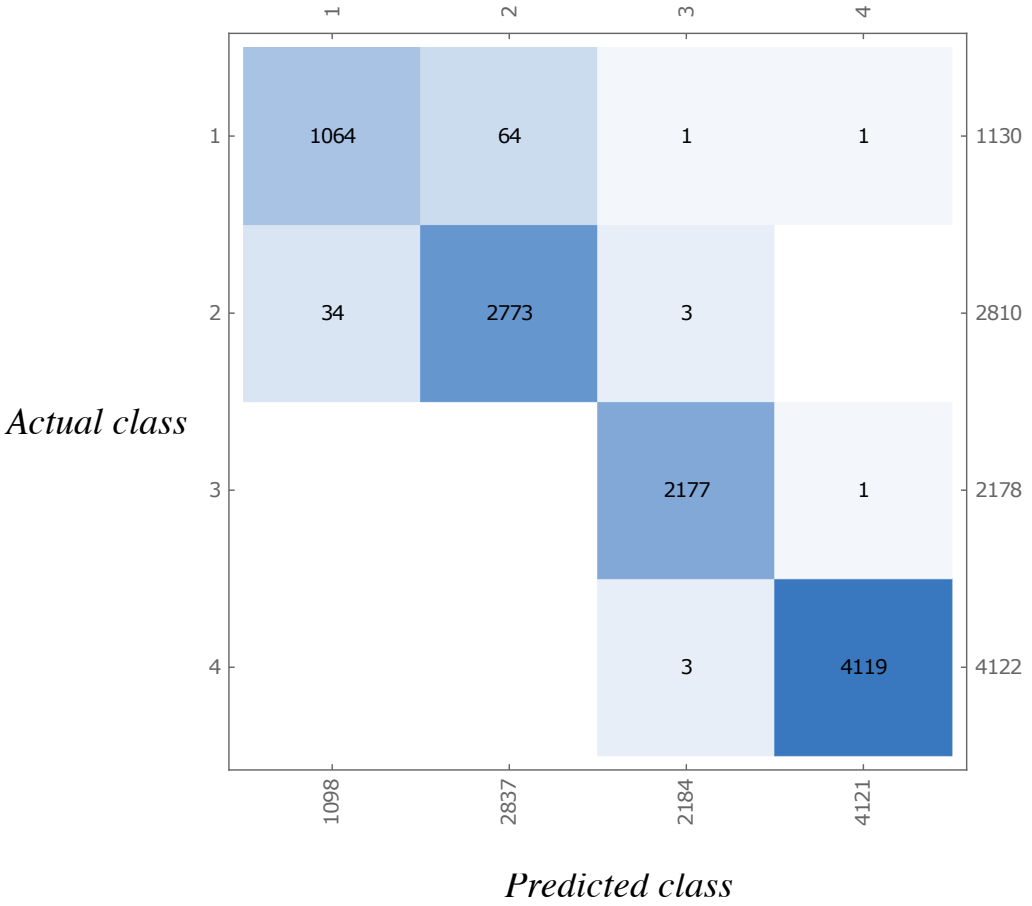
Lowest Entropy

Training Data VII: ECAs + Totalistic 2, 3 ,4 and 5 Colour Rules



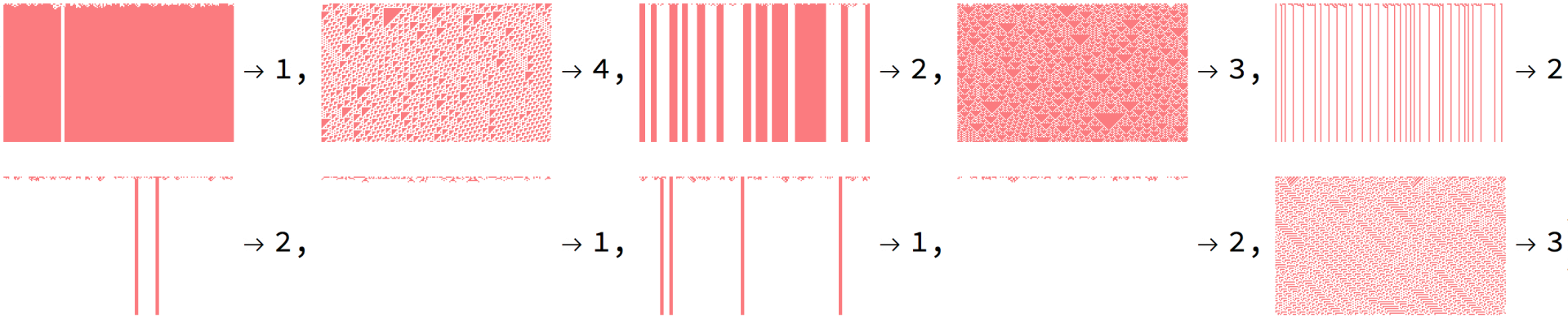
- 200 x 120 pixel colour images of ECA rules and totalistic CA rules with 2, 3, 4 and 5 colours
- Additional Class III images
- 38,912 total training images

Results: Confusion Matrix (Network VII, colour)

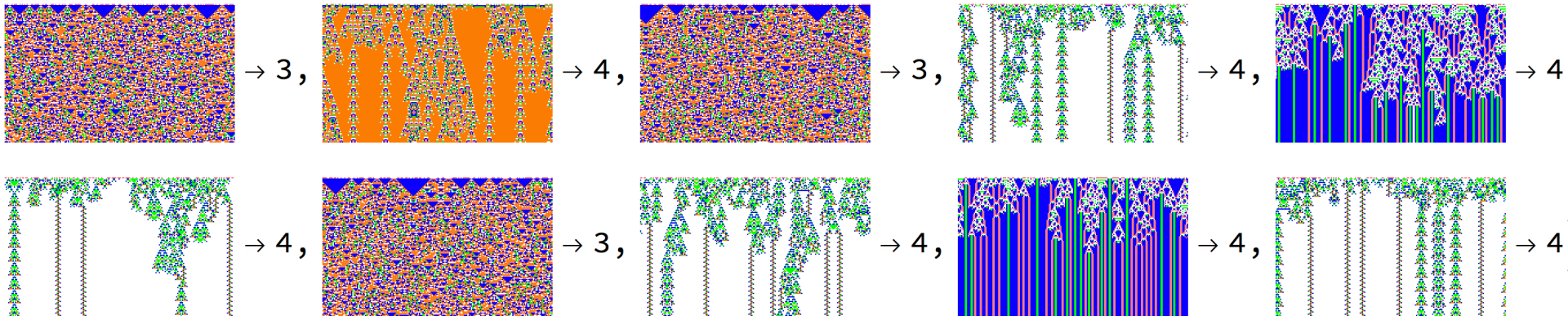


- Accuracy: 98.95%
- By class:
  - 1: 96.9%, 2: 97.74%, **3: 99.68%**, 4: 99.95%

Results: Image Entropies (Network VII, colour)

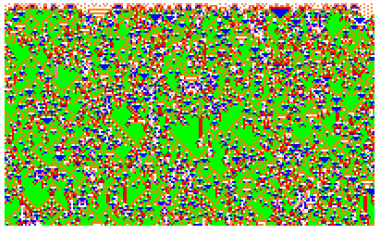
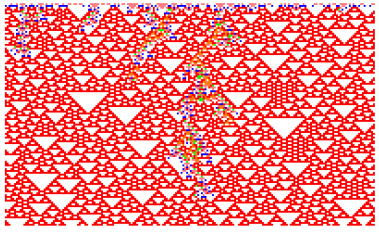


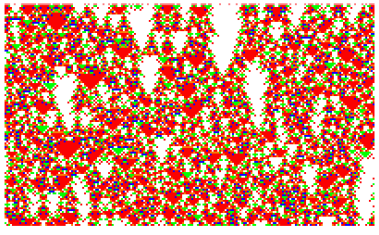
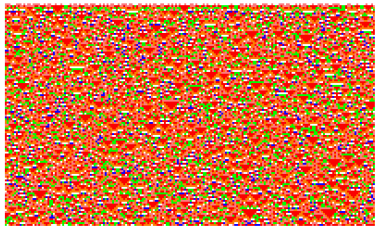
Highest Entropy

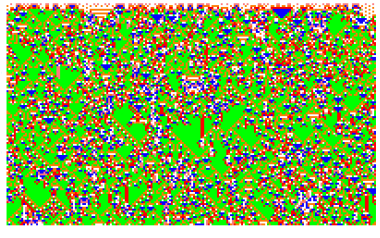
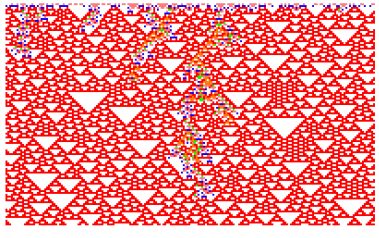


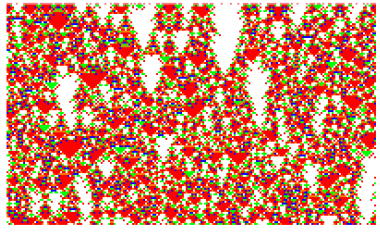
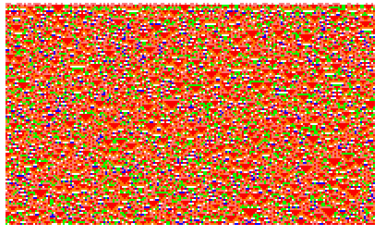
Lowest Entropy

Results: Comparing VI/VII on new 6-colour CAs

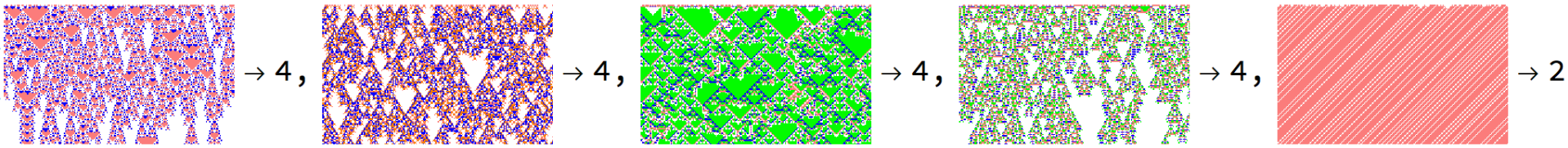

→ {4 → 0.9355458021},

→ {3 → 0.8451589346}


→ {4 → 0.6793112159},

→ {4 → 0.9979349375}


→ {3 → 0.9946493506},

→ {3 → 0.9977535605}


→ {3 → 0.9999990463},

→ {3 → 0.9999983311}

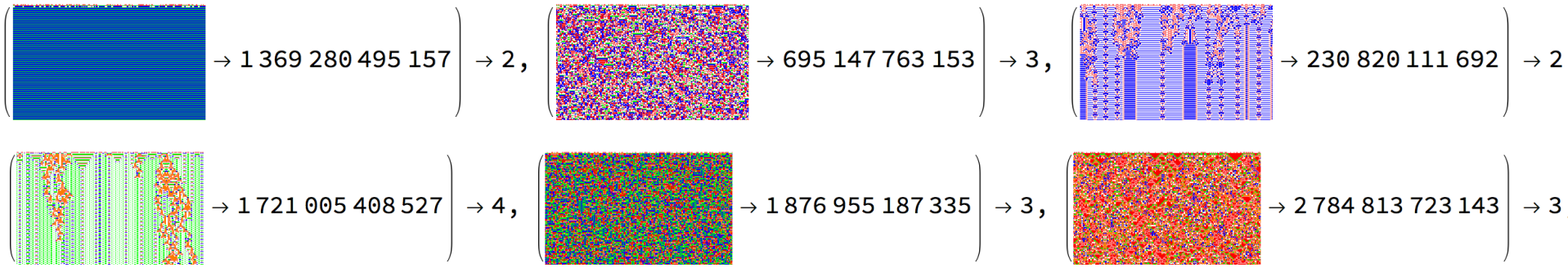
Conclusions



- CNNs are capable of classifying 2 - 5 colour CAs into the four Wolfram classes
- Despite the simple network architecture, it learns quickly and can classify accurately
- **However:**
  - Generalisation is very difficult
  - Can still classify Classes 1/2 in unseen rule spaces, but differentiating between 3 and 4 remains difficult
- Additional convolutional layers is not sufficient to solve this issue
- Need more/better data

Complete Mathematica code + nets available here: https://github.com/thorsilver/Neural-Networks-for-CA-Classification

Future Work



- Improve the network's performance by:
  - Experimenting with different architectures specialised for image recognition
  - Larger input datasets
  - Larger images (substantially increases training time)
- Longer-term:
  - Unsupervised learning
  - Extension to 2D CAs?
  - Can we use DCNNs to help us identify/classify complex behaviour in other contexts – i.e., simulations?

PHASE

POPULATION HEALTH AGENT-BASED SIMULATION NETWORK

- Build and support multi-disciplinary research teams focused on addressing population health challenges
- Support methodological innovation
- Co-develop research programmes between ABM specialists and users
- Provide evidence to enable change within complex systems to prevent non-communicable diseases

Get in touch: info@phasenetwork.org

Website coming soon: www.phasenetwork.org

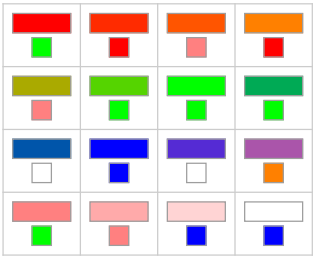
UKPRP
Prevention Research Partnership
Joint action for a healthier, fairer future

Laika Silverman

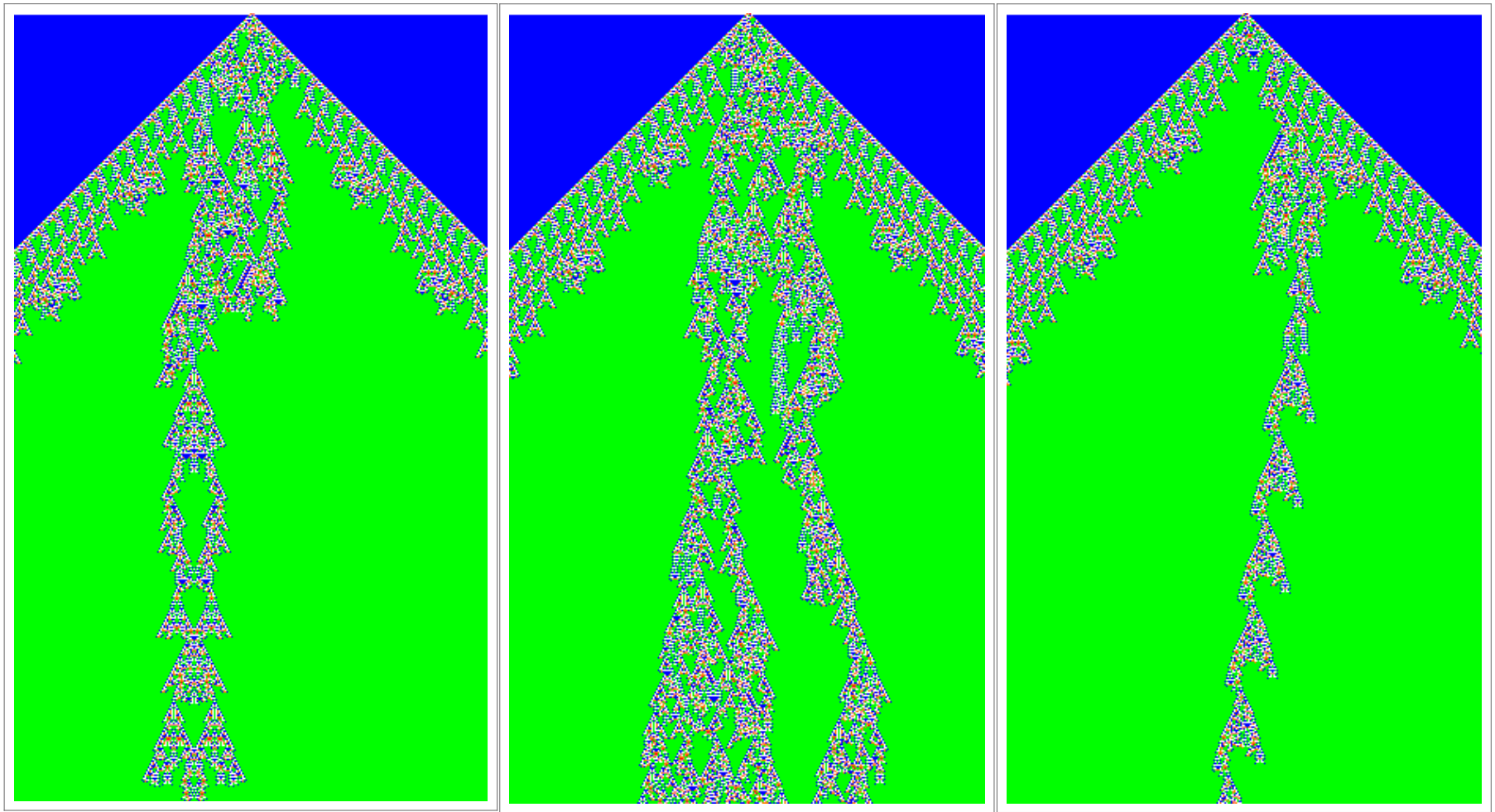
Thanks for listening!

SECRET BONUS SLIDES

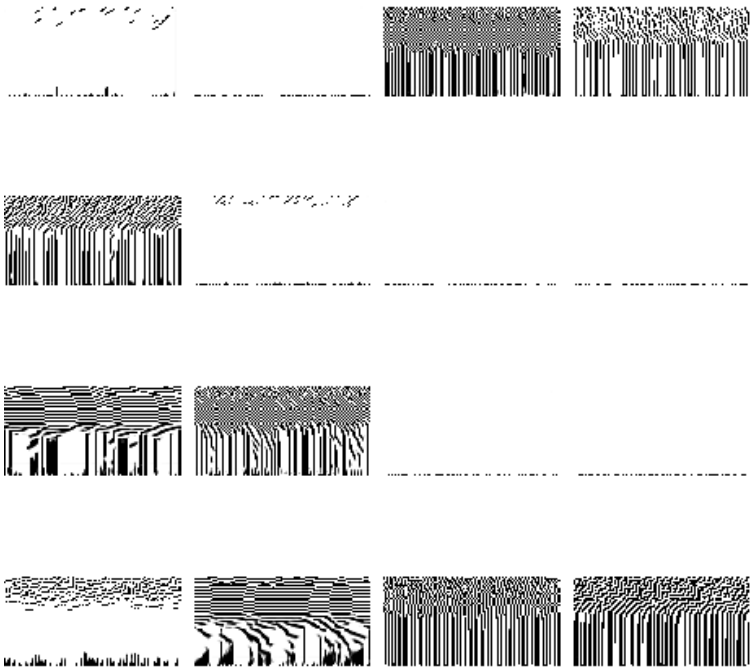
Favourite Rule Found by DCNN



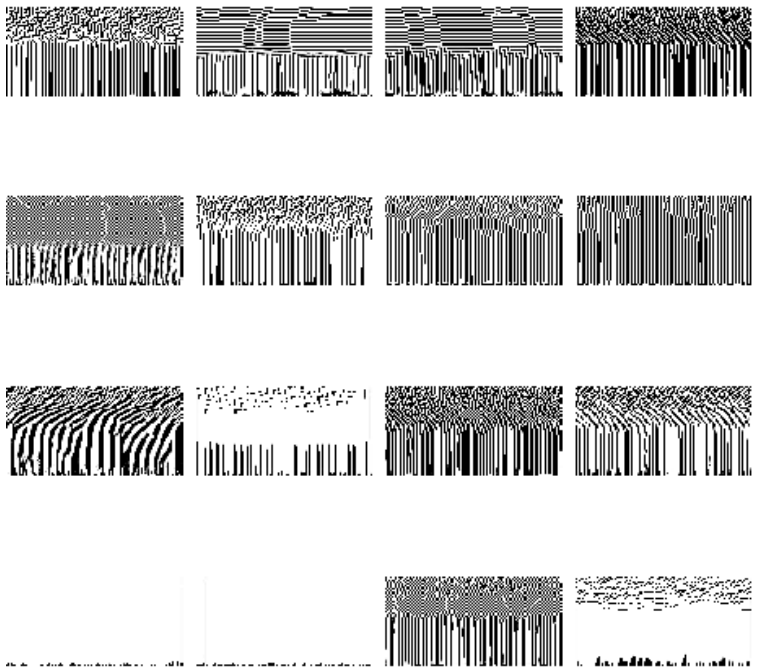
6-Colour Totalistic Rule 1826899946618



Network II: Visualising network feature detectors



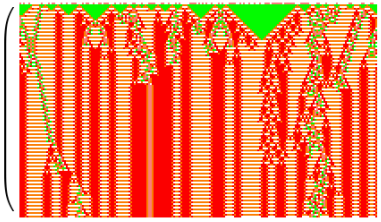
Convolutional Layer 1



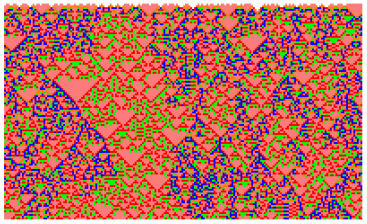
Convolutional Layer 2

- Using Google's *Deep Dream* algorithm to generate images that maximise activity in selected neurons
- Enables visualisation of what each neuron most responds to

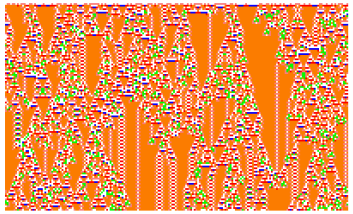
Results: Testing on new CA rules (k=5) (Network VI, colour)



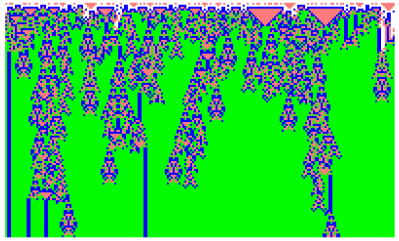
→ 2 743 020 733 306 → {2 → 0.01243278477, 4 → 0.9860057831}



→ 1 661 403 844 932 → {2 → 0.09809479862, 3 → 0.8950021267}

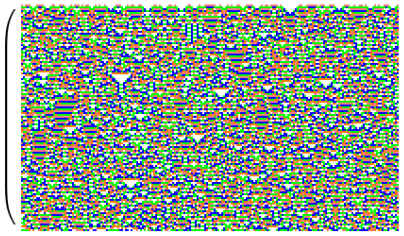


→ 1 941 732 867 200 → {3 → 0.00005406229684, 4 → 0.9999457598}

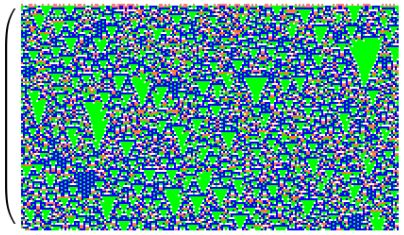


→ 319 713 877 → {3 → 0.1868763715, 4 → 0.8131222129}

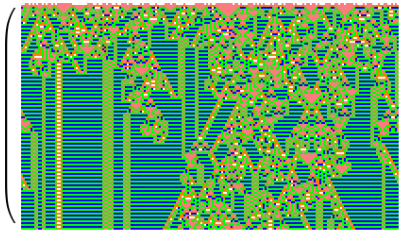
Results: Testing on new CA rules (k=5) (Network VII, colour)



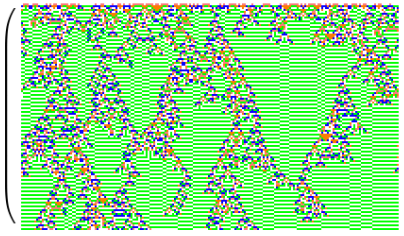
→ 60 914 090 → {4 → 0.008076984435, 3 → 0.9919230342},



→ 416 227 792 → {4 → 0.2091663182, 3 → 0.7908337116},

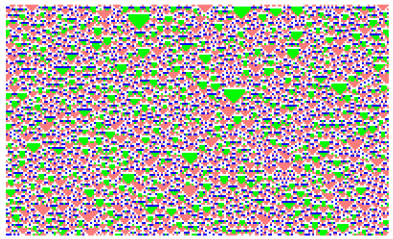


→ 44 277 671 → {3 → 0.1086276472, 4 → 0.8912305832},

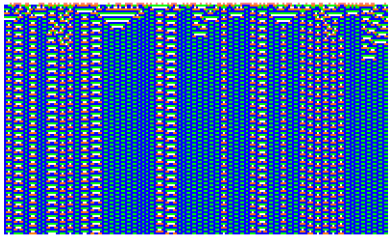


→ 1 123 916 113 → {3 → 0.352267921, 4 → 0.6477320194},

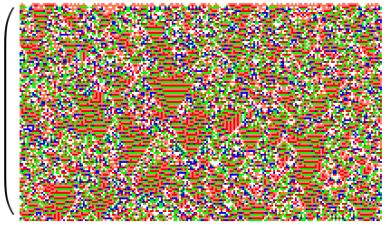
Results: Testing on new CA rules (k=6) (Network VI, colour)



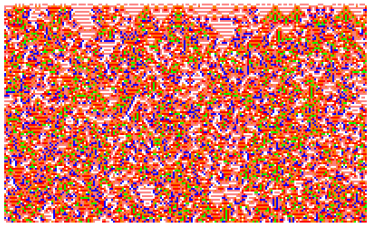
→ 1 188 797 638 → {4 → 0.4440203607, 3 → 0.5559796095}



→ 655 296 617 → {3 → 0.06664989889, 4 → 0.9333165288}

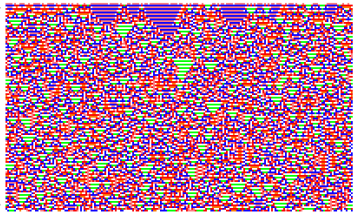


→ 1 613 375 044 836 → {3 → 0.2211419493, 4 → 0.7788577676}

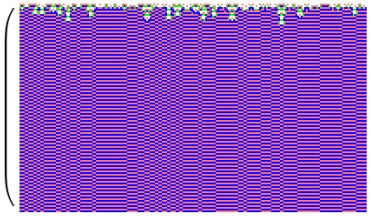


→ 1 931 468 347 465 → {4 → 0.4315021932, 3 → 0.5608764291}

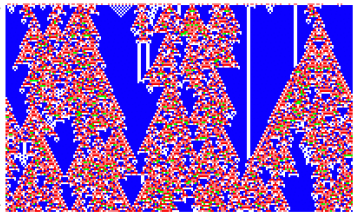
Results: Testing on new CA rules (k=6) (Network VII, colour)



→ 2 298 811 569 801 → {4 → 0.03871776909, 3 → 0.9612821937},



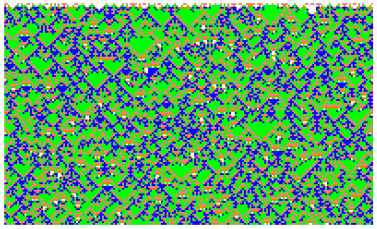
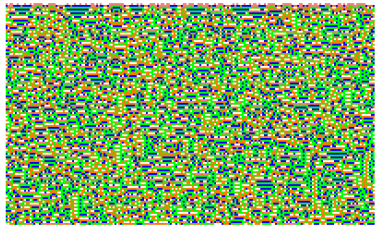
→ 1 843 311 712 861 → {3 → 0.2481572926, 2 → 0.7497182488},

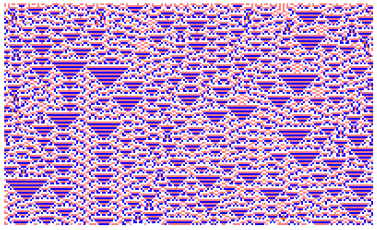


→ 277 609 027 910 → $\{3 \to 2.535965905 \times 10^{-6}, 4 \to 0.9999974966\}$

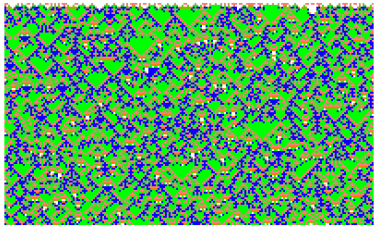
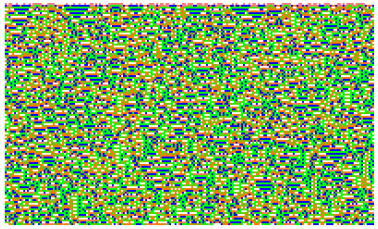
→ 2 413 949 709 384 → {3 → 0.0000825846073, 4 → 0.9999135733}

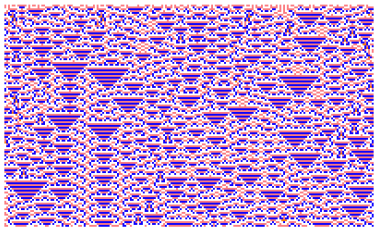
Results: Comparing VI/VII on new 5-colour CAs


→ {3 → 0.9854582548},

→ {3 → 0.9841322899}


→ {4 → 0.9820075631},

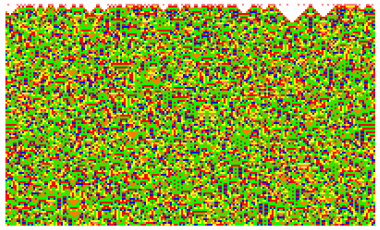
→ {1 → 0.9905155897}

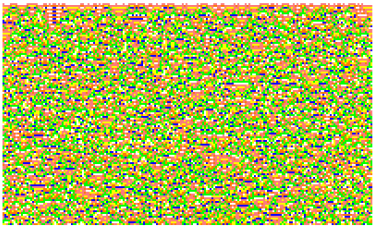

→ {4 → 0.9998366833},

→ {3 → 1.},

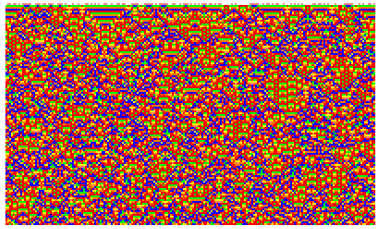

→ {3 → 0.9941664934},

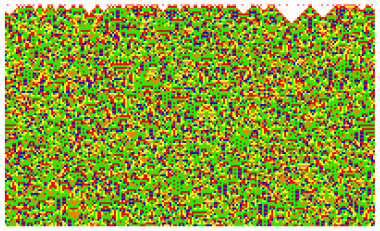
→ {1 → 0.9571000934}

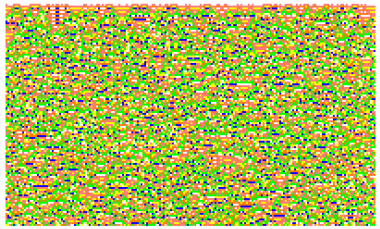
Results: Comparing VI/VII on new 7-colour CAs

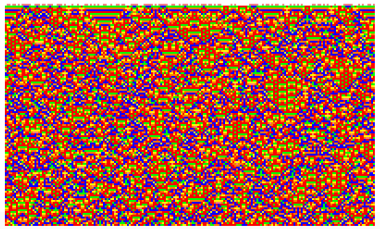




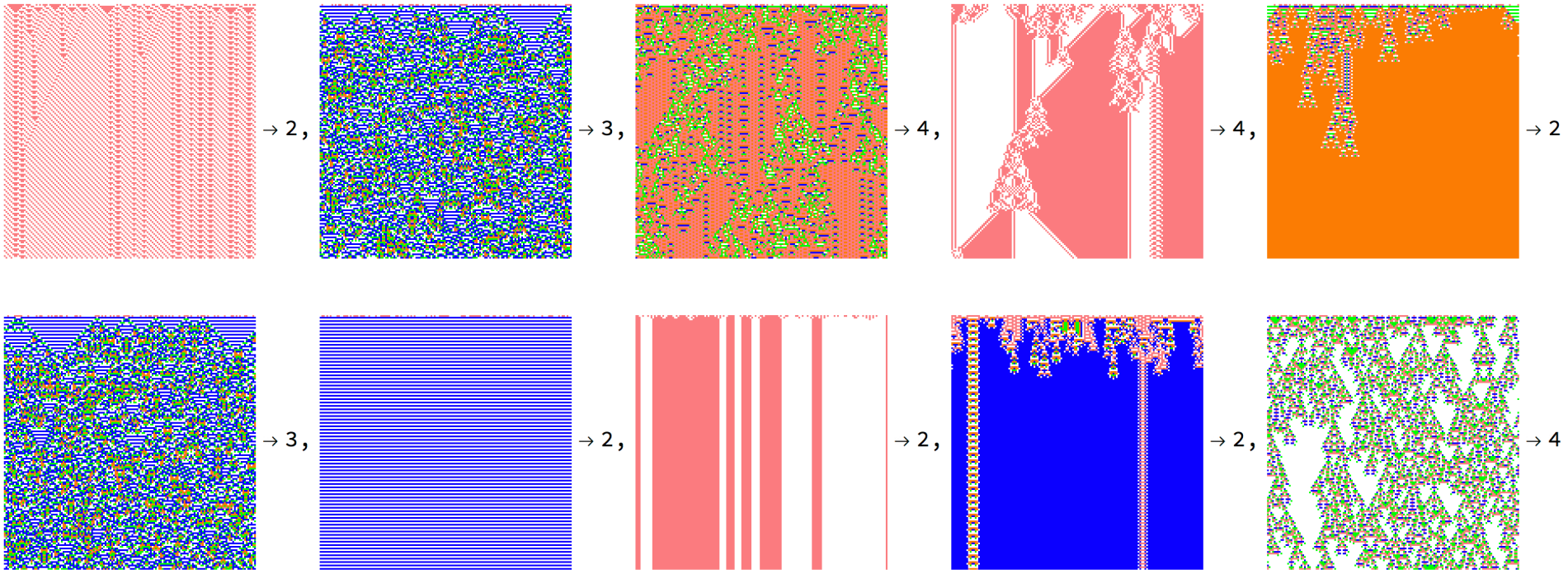






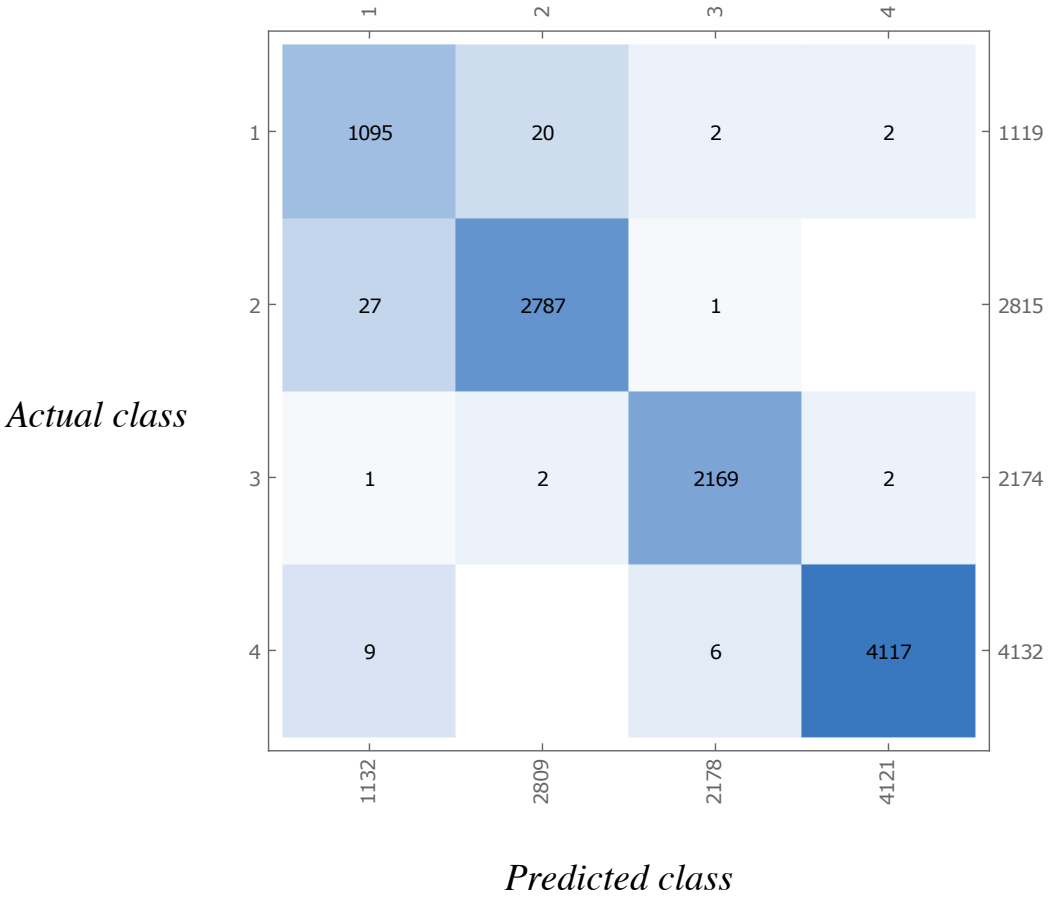


Training Data VIII: ECAs + Totalistic 2, 3, 4 and 5 Colour Rules



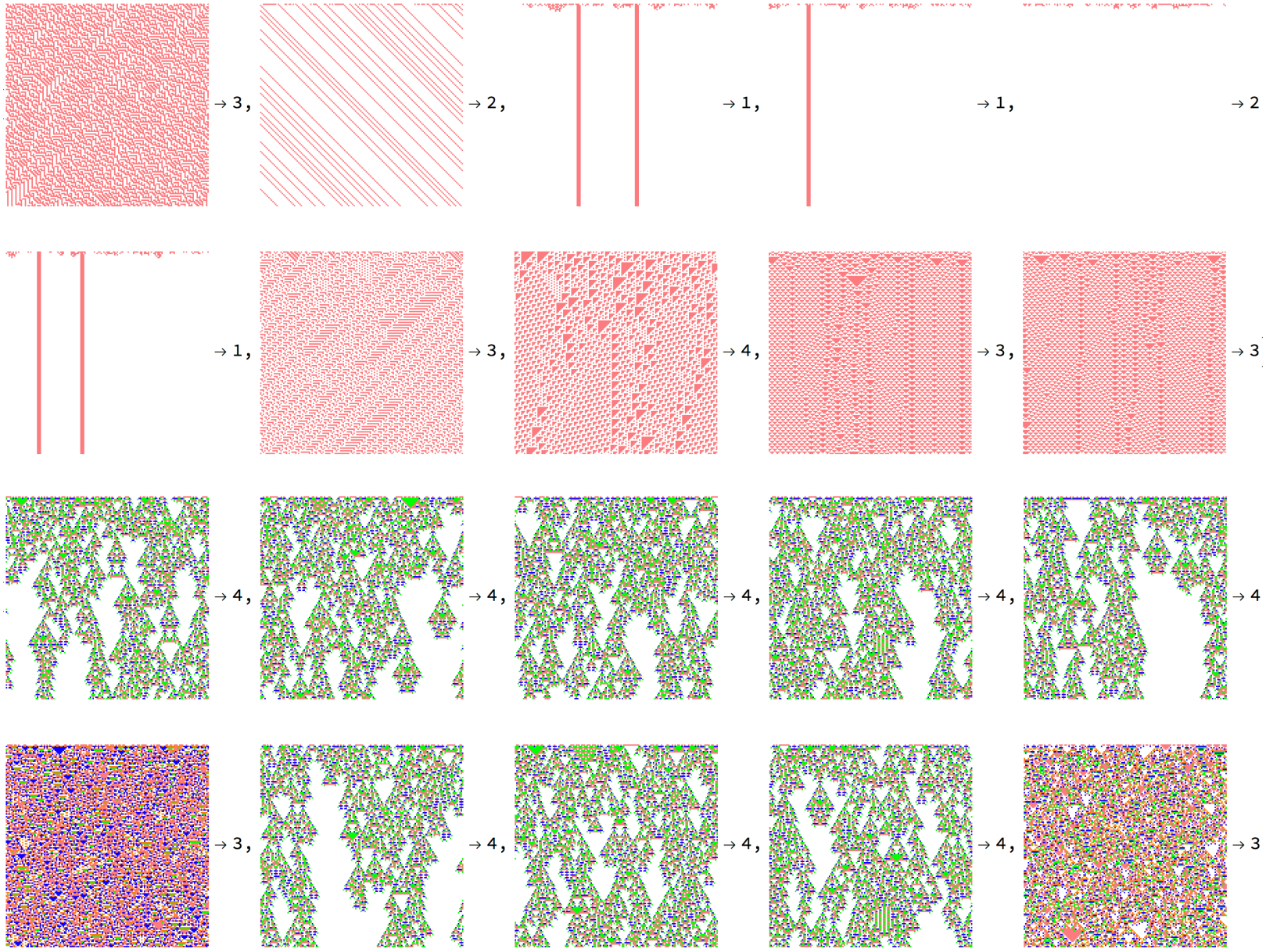
- 150 x 150 pixel colour images of ECA rules and totalistic CA rules with 2, 3, 4 and 5 colours
- Testing whether longer CA evolutions produce better results
- 38,912 total training images

Results: Confusion Matrix (Network VIII, colour)



- Accuracy: 99.30%
- By class:
  - 1: 96.73%, 2: 99.22%, **3: 99.59%**, **4: 99.90%**

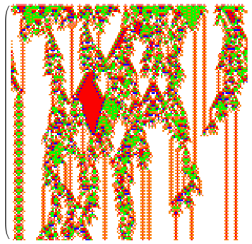
Results: Image Entropies (Network VIII, colour)



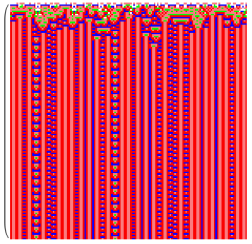
Highest Entropy

Lowest Entropy

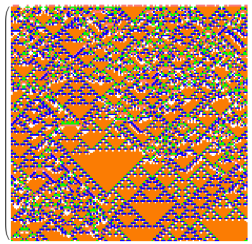
Results: Testing on new CA rules (k=6) (Network VIII, colour)



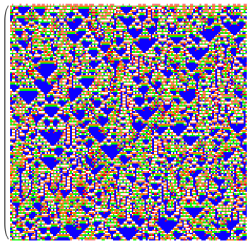
→ 2 389 241 801 724 | → {3 → 0.3430433571, 4 → 0.6569566131},



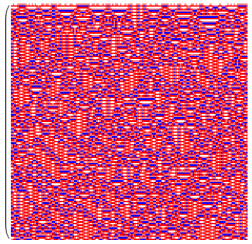
→ 946 778 045 702 | → {4 → 0.001319971867, 2 → 0.9986792207},



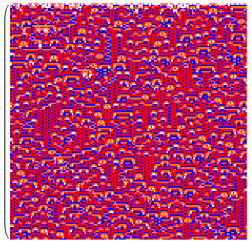
→ 1 864 250 050 050 | → {3 → 0.4850532413, 4 → 0.5149310827},



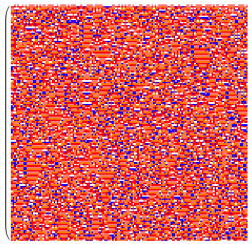
→ 712 191 474 379 | → {4 → 0.00001838360913, 3 → 0.9999816418}



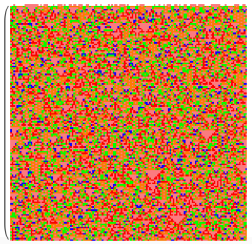
→ 41 902 188 403 | → {4 → 0.0007199073443, 3 → 0.9992794394},



→ 1 031 607 472 117 | → $\{4 \to 1.250594739 \times 10^{-8}, 3 \to 1.\}$,

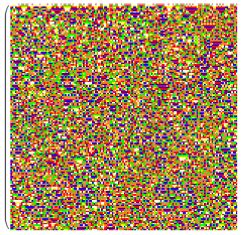


→ 585 874 950 116 | → $\{4 \to 7.003355222 \times 10^{-6}, 3 \to 0.9999927282\}$

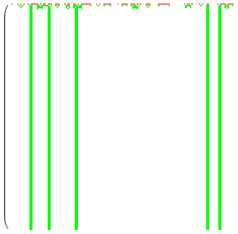


→ 2 027 177 136 526 | → {4 → 0.0005097757094, 3 → 0.9994902611}

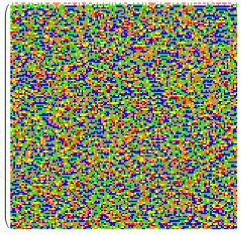
Results: Testing on new CA rules (k=7) (Network VIII, colour)



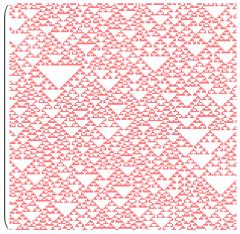
→ 308 913 505 773 326 → {4 → 0.02208719589, 3 → 0.9779127836},



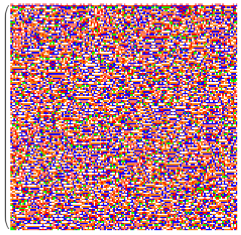
→ 555 706 238 130 239 → {1 → 0.0001219267724, 2 → 0.9998633862},



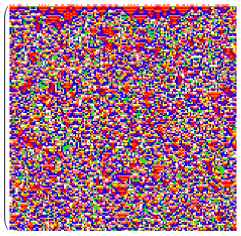
→ 6 026 519 161 847 641 → {4 → 0.0209327098, 3 → 0.979067266},



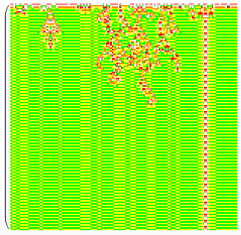
→ 10 071 225 612 238 266 → {4 → 0.4851866663, 3 → 0.5138067007},



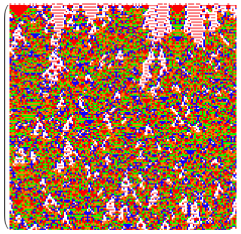
→ 8 855 980 036 396 763 → {4 → 0.0002560535504, 3 → 0.9997439981},



→ 7 466 826 532 023 477 → {4 → 0.07160818577, 3 → 0.9283918738},

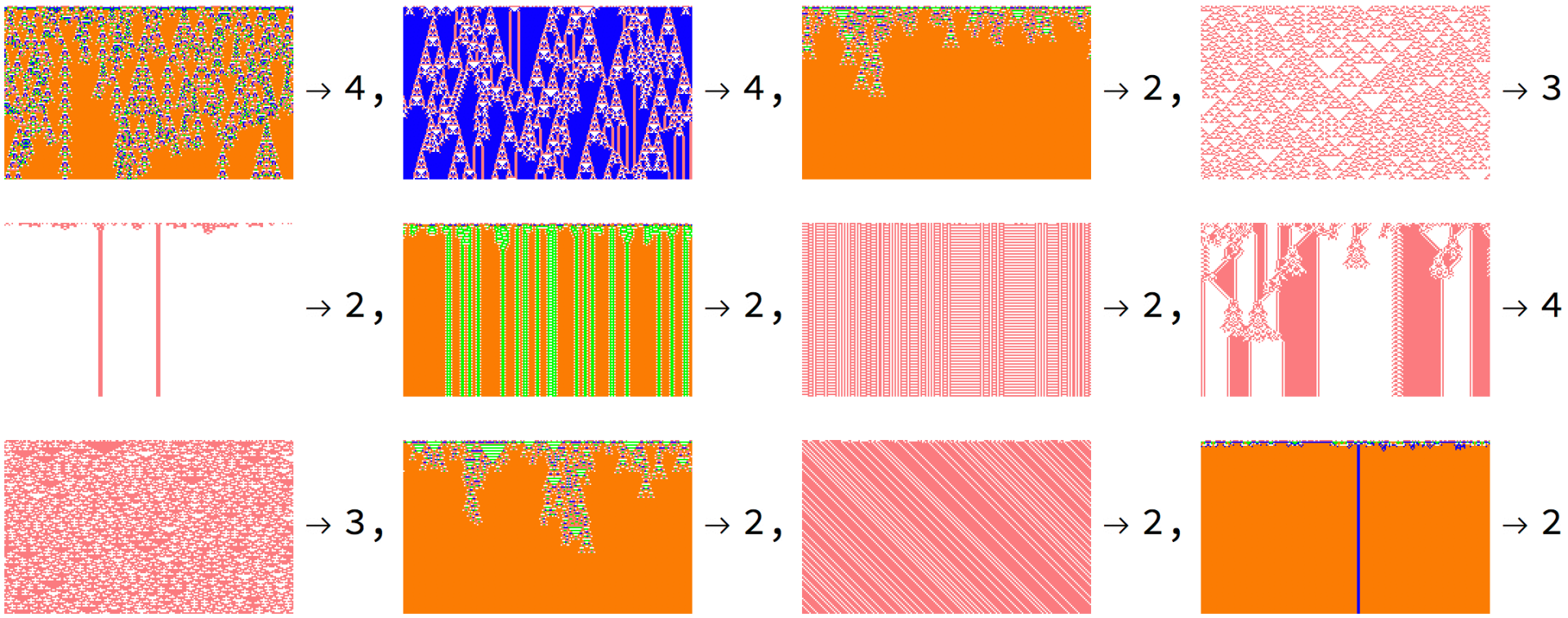


→ 6 096 341 557 178 898 → $\{4 \to 1.694715053 \times 10^{-7}, 2 \to 0.9999998808\}$



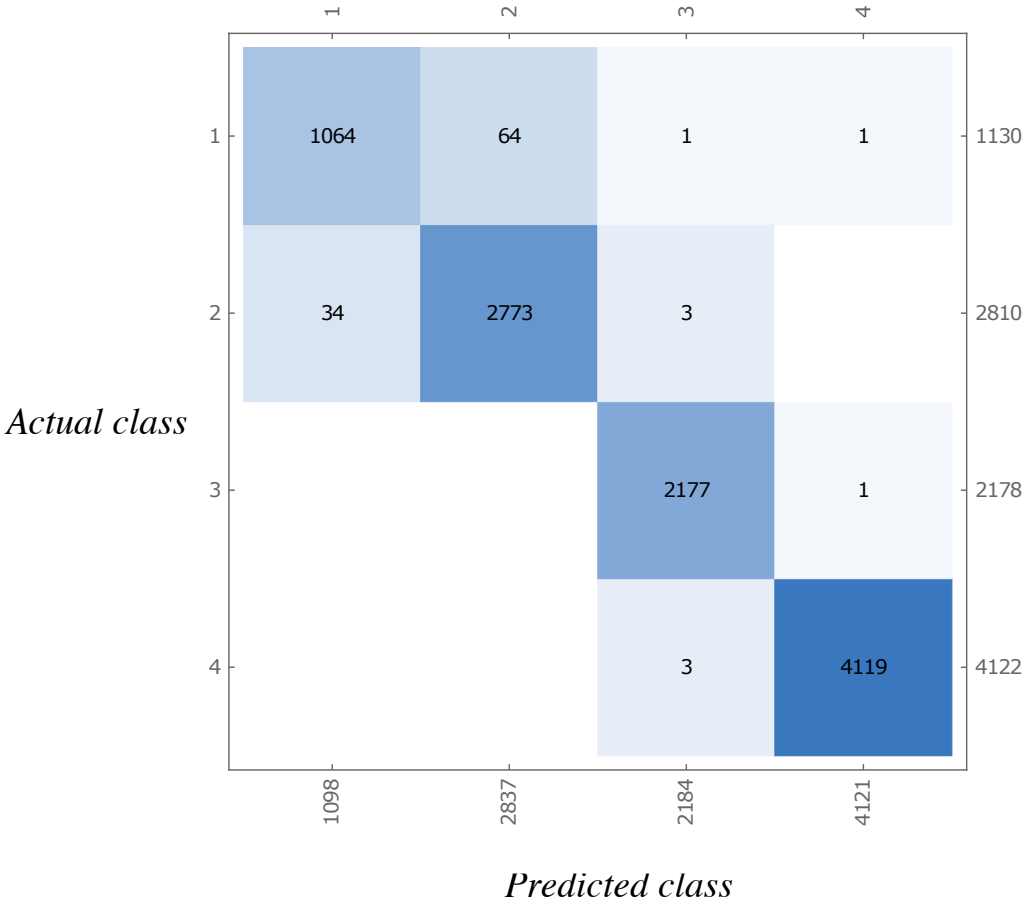
→ 2 751 312 505 446 359 → {4 → 0.001107691438, 3 → 0.9988923669}

Training Data IX: ECAs + Totalistic 2, 3, 4 and 5 Colour Rules



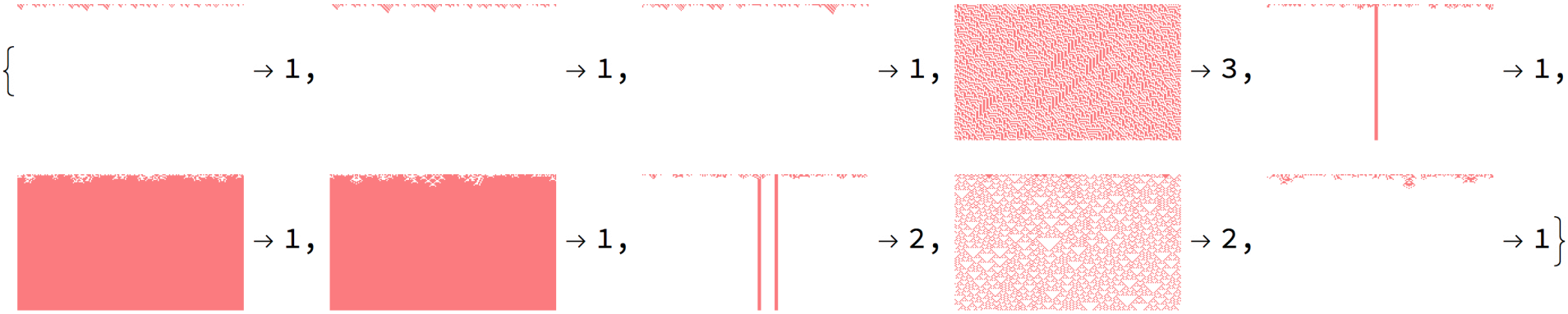
- 200 x 120 pixel colour images of ECA rules and totalistic CA rules with 2, 3, 4 and 5 colours
- Two larger convolutional layers (32 x 2 x 3)
- 38,912 total training images

Results: Confusion Matrix (Network IX, colour)

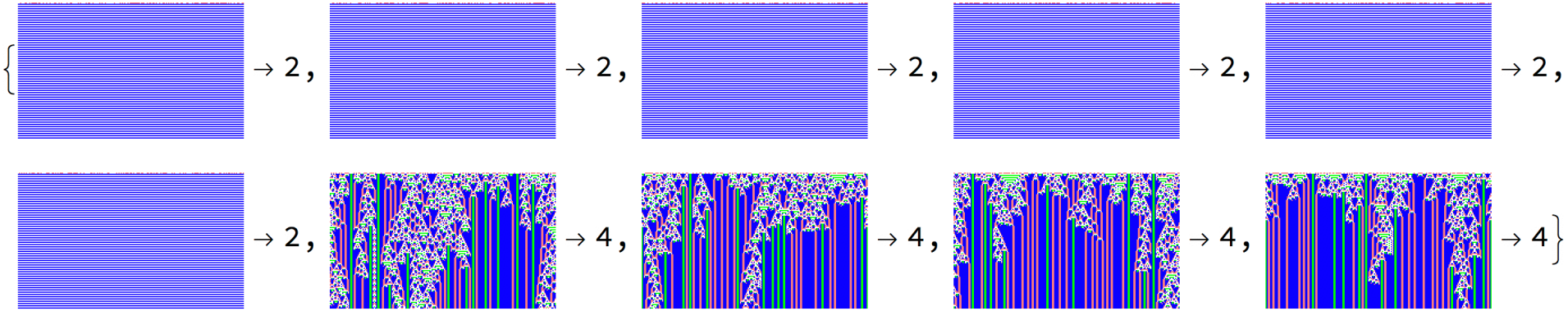


- Accuracy: 98.84%
- By class:
  - 1: 98.84%, 2: 99.91%, **3: 98.27%**, **4: 99.95%**

Results: Image Entropies (Network IX, colour)

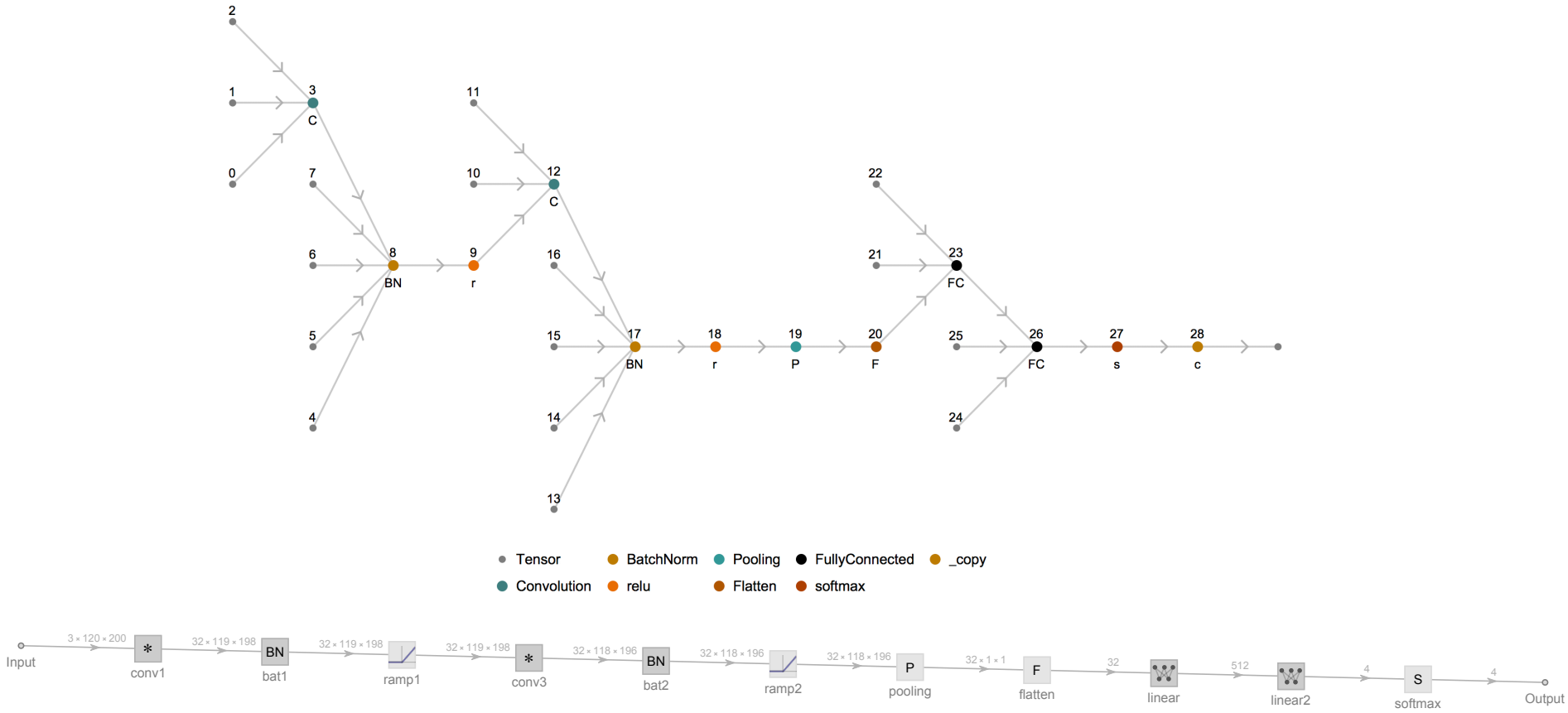


Highest Entropy



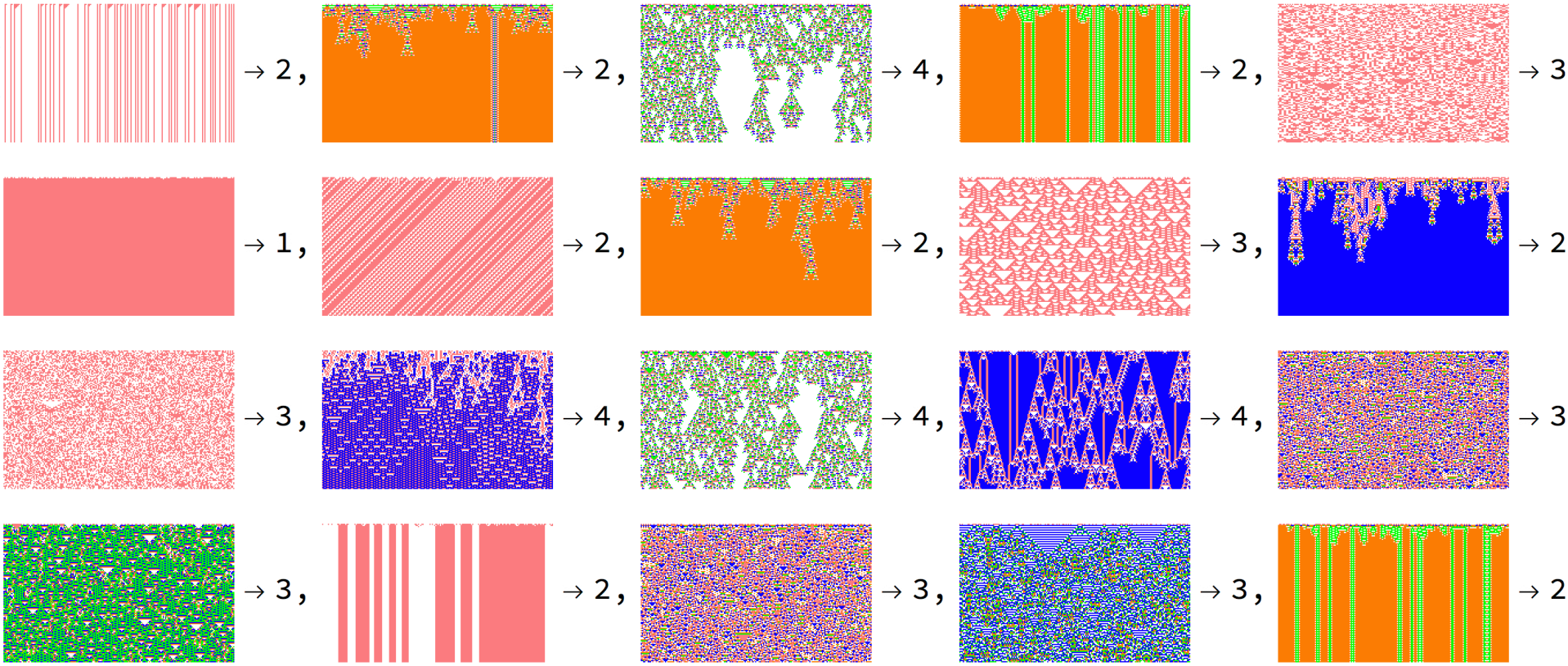
Lowest Entropy

Network Structure (Network X)



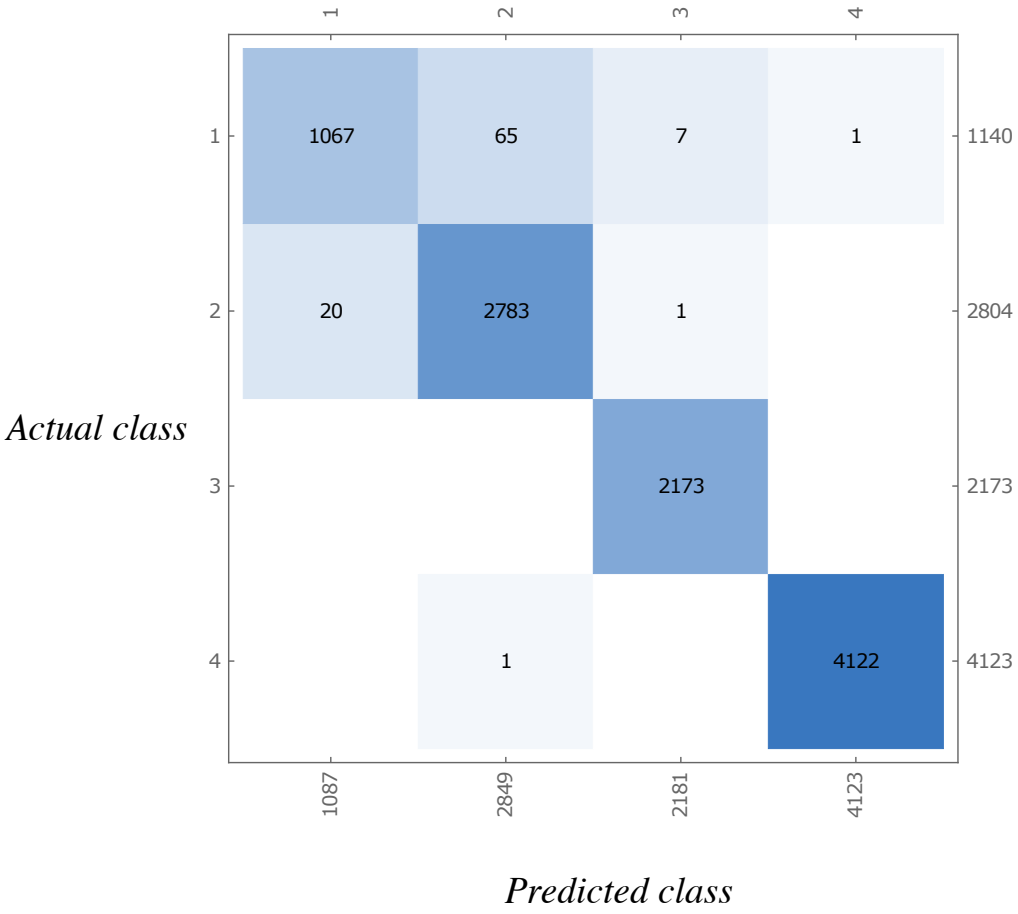
- Eleven-layer CNN with two convolutional layers
- Batch Normalization Layers
- 512-node fully-connected layer
- 4-node SoftMax layer outputs Wolfram classification

Training Data X: ECAs + Totalistic 2, 3, 4 and 5 Colour Rules



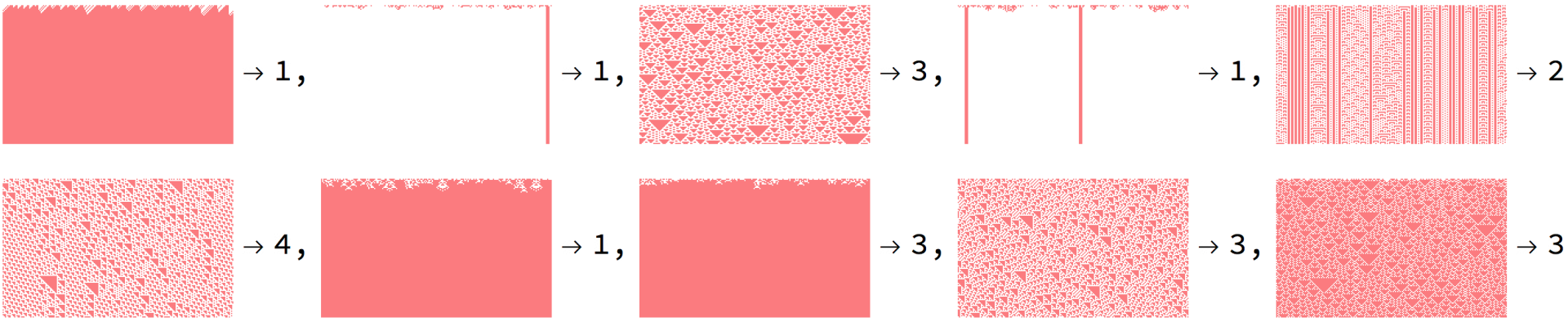
- 200 x 120 pixel colour images of ECA rules and totalistic CA rules with 2, 3, 4 and 5 colours
- 16,384 total training images

Results: Confusion Matrix (Network X, BatchNorm)

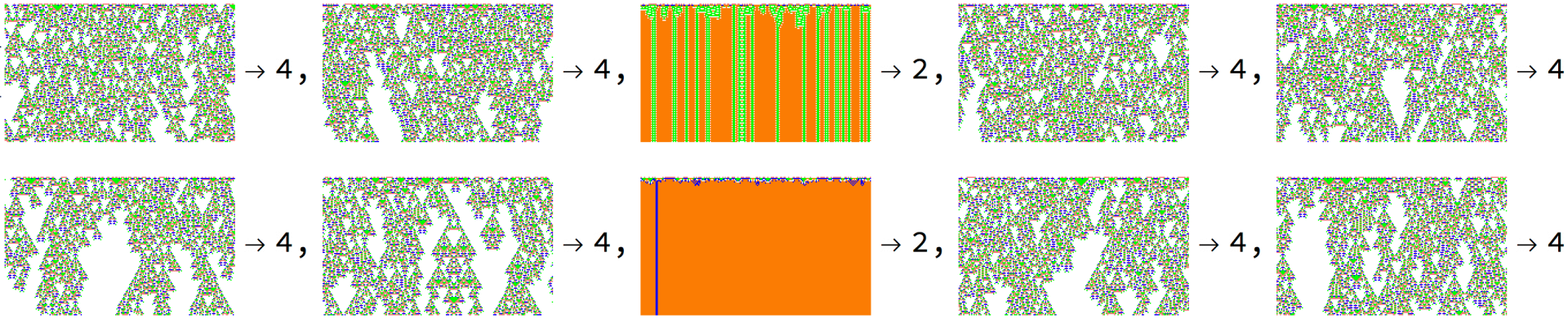


- Accuracy: 99.07%
- By class:
  - 1: 98.16%, 2: 97.68%, **3: 99.63%**, **4: 99.98%**

Results: Image Entropies (Network X, BatchNorm)

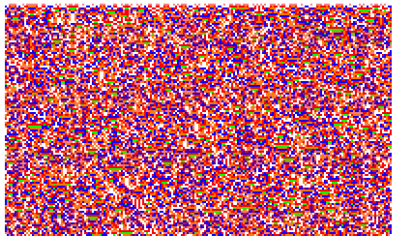


Highest Entropy

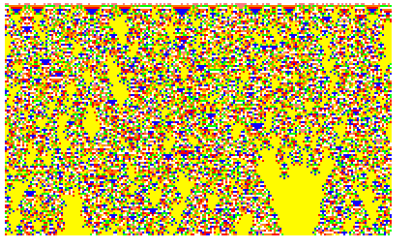


Lowest Entropy

Testing Network X on 7-colour totalistic CAs

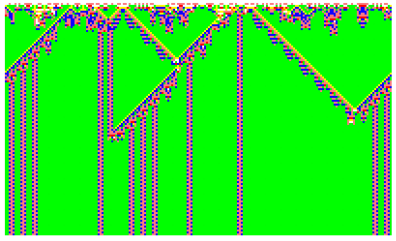


→ 8 823 913 694 494 635 → {3 → 0.9942973256},



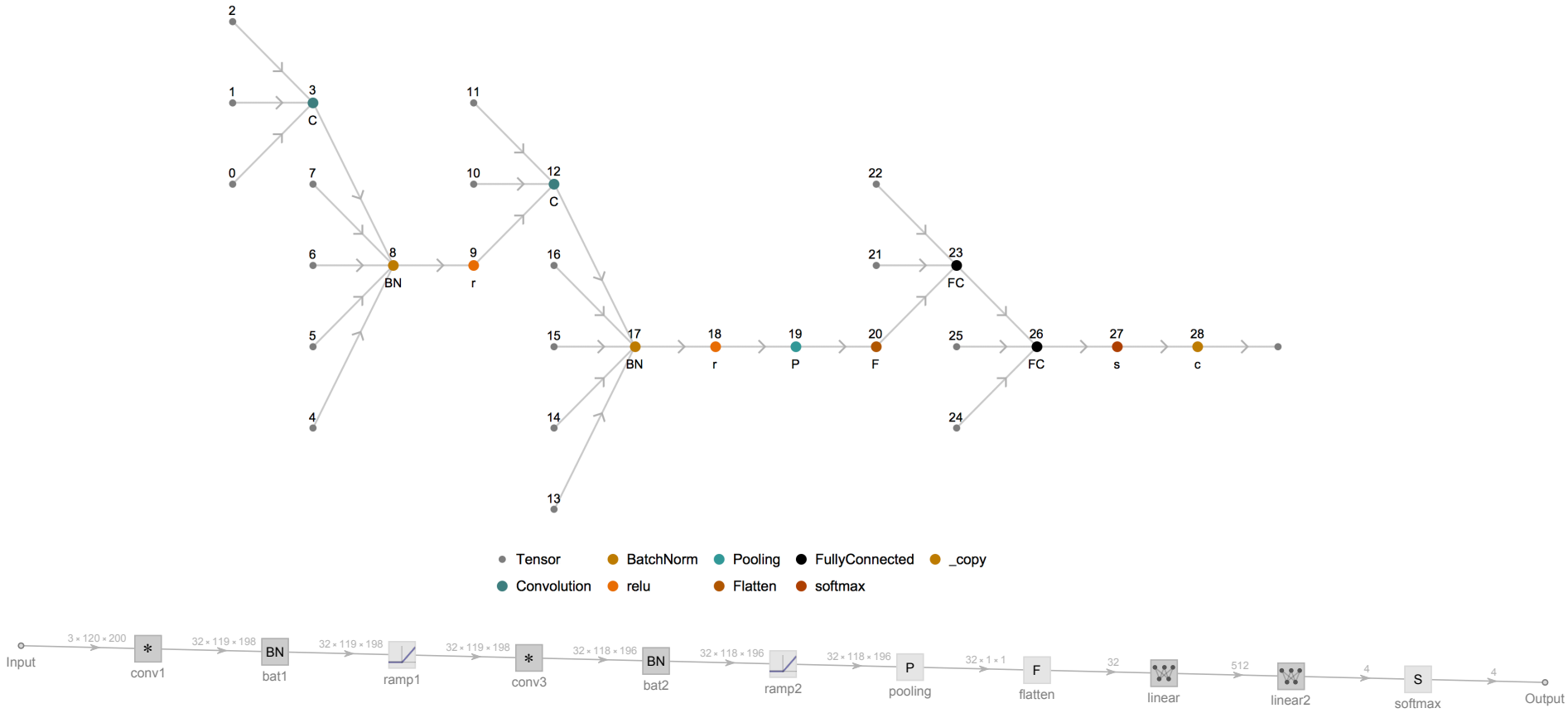
→ 11 279 996 571 927 052 → {4 → 0.6158138514}

→ 9 401 097 035 811 122 → {3 → 0.9915812612},



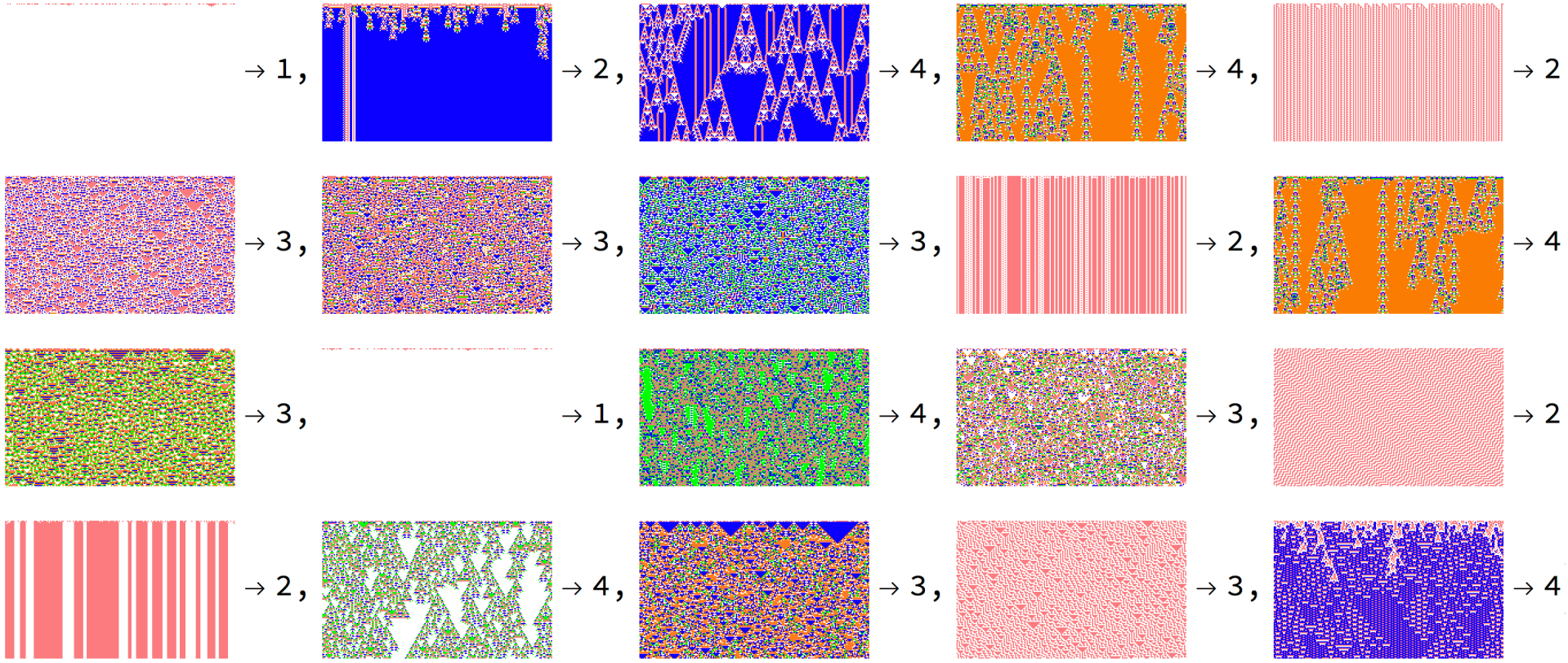
→ 3 631 971 980 939 595 → {4 → 0.6878272891},

Network Structure (Network XII)



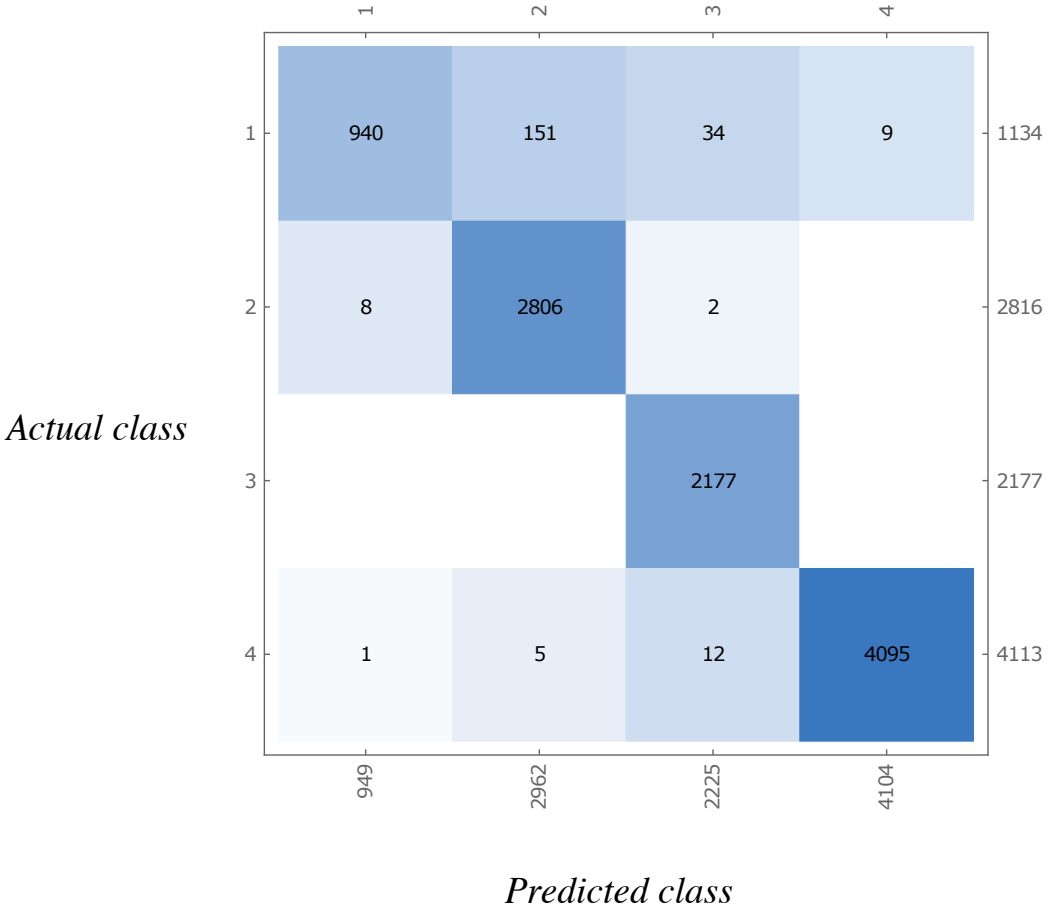
- Eleven-layer CNN with two convolutional layers
- Batch Normalization, dropout (linear layer only)
- 512-node fully-connected layer
- 4-node SoftMax layer outputs Wolfram classification

Training Data XII: ECAs + Totalistic 2, 3, 4 and 5 Colour Rules



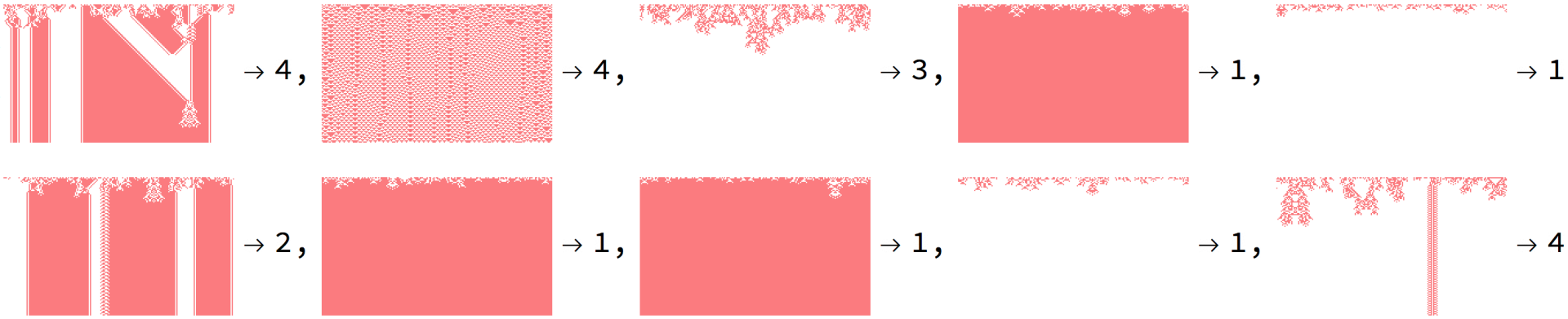
- 200 x 120 pixel colour images of ECA rules and totalistic CA rules with 2, 3, 4 and 5 colours
- 26,624 total training images

Results: Confusion Matrix (Network XII, BatchNorm/dropout)

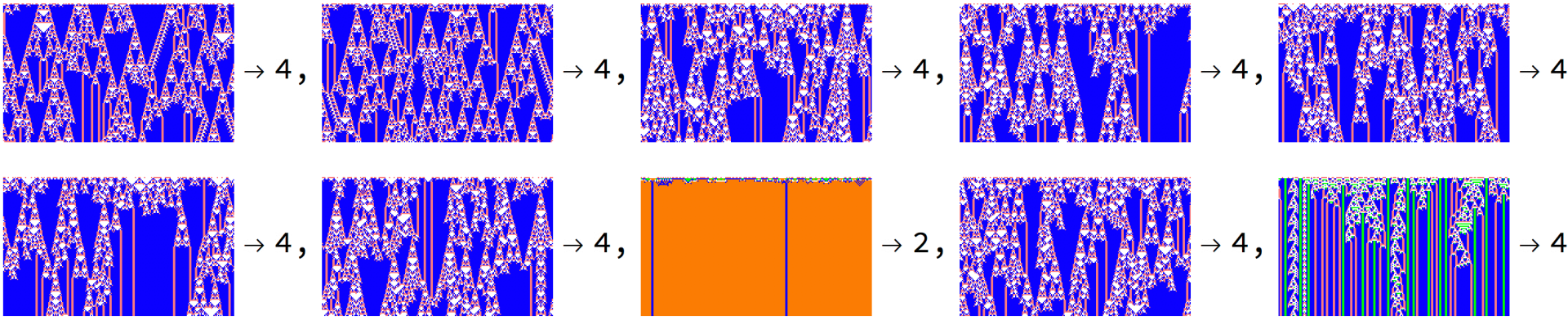


- Accuracy: 97.83%
- By class:
  - 1: 99.05%, 2: 94.73%, **3: 97.84%**, **4: 99.78%**

Results: Image Entropies (Network X, BatchNorm)

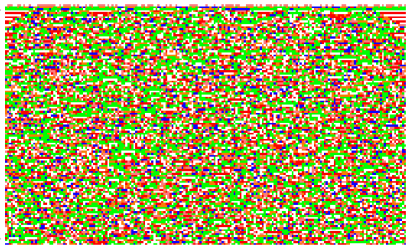


Highest Entropy

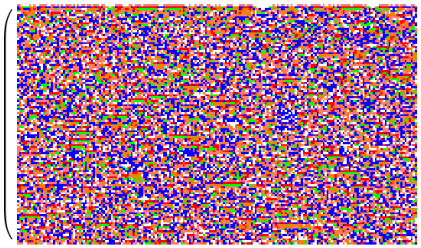


Lowest Entropy

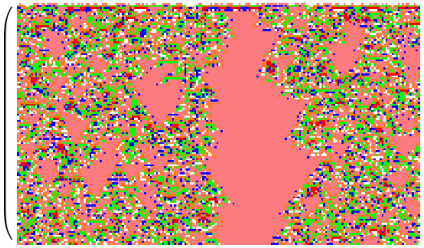
Testing Network XII on 6 colour, range 2 totalistic CAs



→ 27 148 559 305 859 136 233 → {4 → 0.04718473181, 3 → 0.9528138041}



→ 109 406 220 086 847 849 858 → {4 → 0.08999076486, 3 → 0.8959928751



→ 26 205 502 254 809 163 684 → {3 → 0.4052188694, 4 → 0.5943811536},

→ 86 427 159 345 288 879 260 → {3 → 0.06899219006, 4 → 0.9309860468}