TRENDy: Temporal Regression of Effective Nonlinear DYnamics

Matthew Ricci[1], Guy Pelc[2], Zoe Piran[2], Noa Moriel[2], Mor Nitzan[2,3,4]

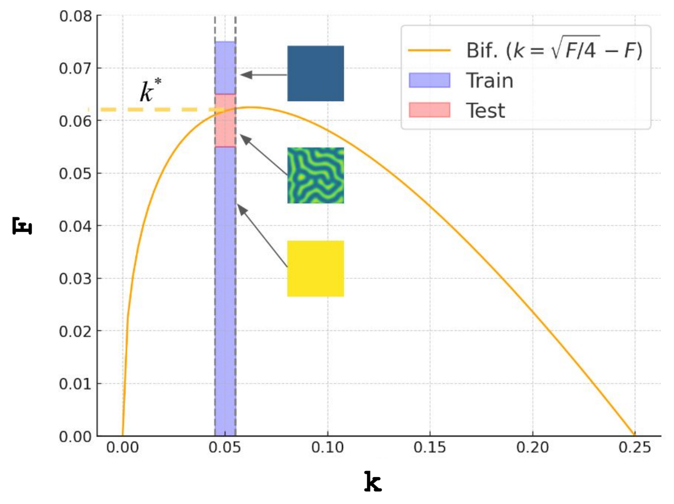
1. Institut Imagine (Paris), 2. School of Computer Science and Engineering (HUJI), 3. Racah Institute of Physics (HUJI), 4. Faculty of Medicine (HUJI)

Introduction

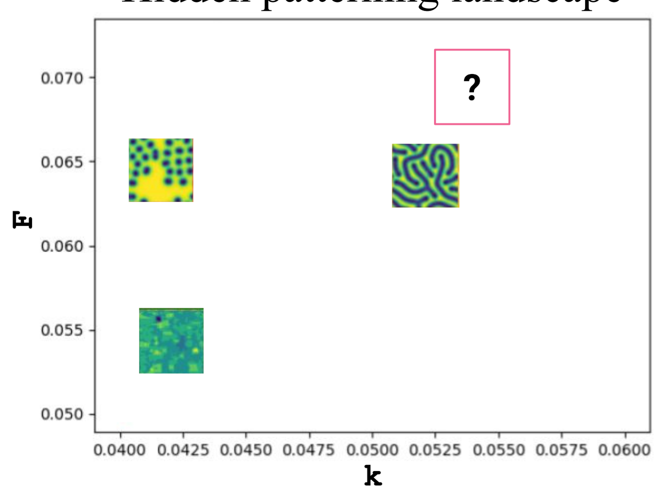
- Spatiotemporal dynamics can give rise to complex patterning processes in biology as a function of control parameters.
- Predicting how patterns will appear as a function of these parameters is challenging when governing equations are unknown and data is sparse and noisy.
- By training parametric neural ODEs on robust, multiscale features, **TRENDy** learns a reduced-order, predictive model of spatial patterning which outperforms competing methods in bifurcation prediction and long-term forecasting.

The problem

- Let $u_t = N[u;\theta] = d\nabla^2 u + f(u;\theta)$ be a partial differential equation (PDE) with a state $u \in H^2(\mathbb{R}^2)$ and a parameter vector θ. We call this a *reaction-diffusion equation*.
- If there are some θ for which an otherwise stable $u \equiv 0$ is destabilized whenever $d>0$, we call this a *Turing bifurcation*. It can lead to complex spatial patterns like spots, stripes, vermiculation and waves.
- For example, the Gray-Scott model[1] (below, left) transitions from homogeneity to a patterning regime as a function of two reaction parameters, F and k.



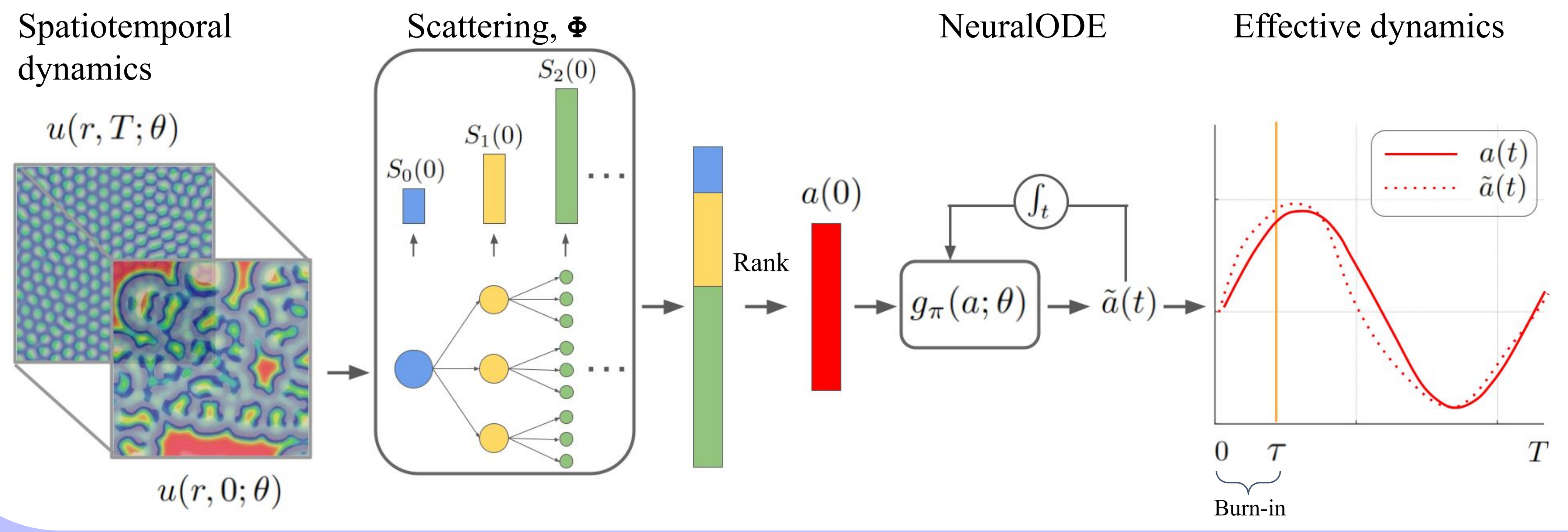
Hidden patterning landscape



- If governing equations are unknown and data sparse/noisy data (above, right), can we *fill in* the patterning landscape and predict how the system will behave in *new conditions*?

The TRENDy Framework

TRENDy uses multiscale features to build a reduced-order, *effective*[2] model of the dynamics: it learns to convert the complicated, hidden PDE to a simpler, interpretable ODE. It does this by representing the dynamics with multiscale scattering[3] (i.e. hierarchical Morlet wavelet) features, $a = \Phi[u]$, and then training a neural ODE, g_π, to predict how these features evolve in time as a function of the known control parameters, θ.



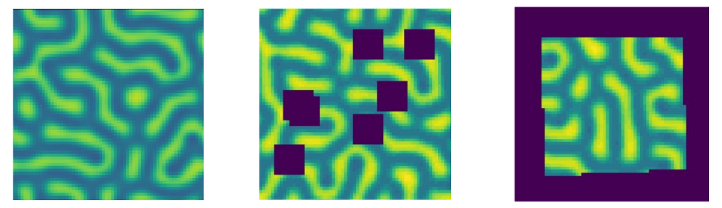
Train/Test. True effective dynamics $a(t)$ are used for training. The NODE is initialized on $a(0)$ and its estimate is regressed against ground truth. Only the top n scattering coefficients are used for training.

In the test phase, we only need the initial state $a(0) = \Phi[u](0)$ to predict the evolution of the system.

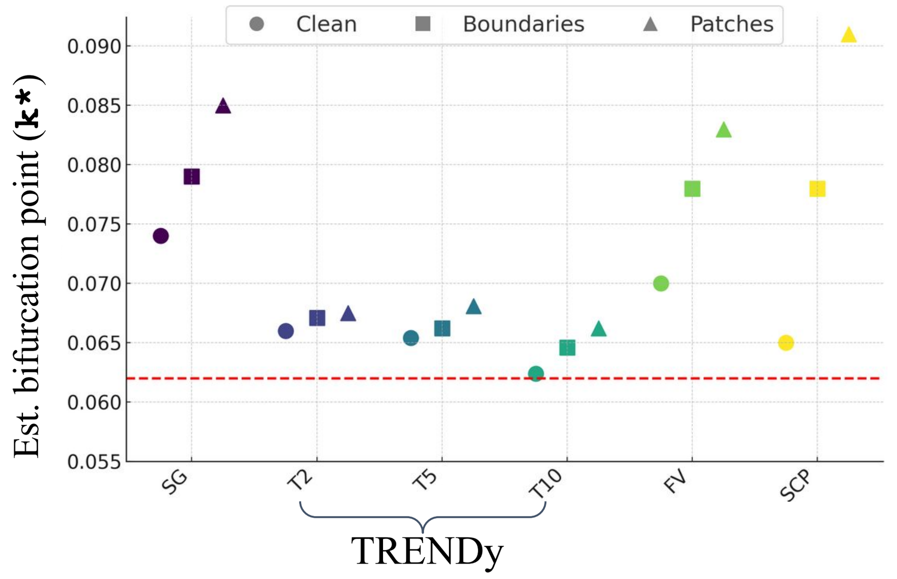
Revealing the Gray-Scott patterning landscape from noisy data

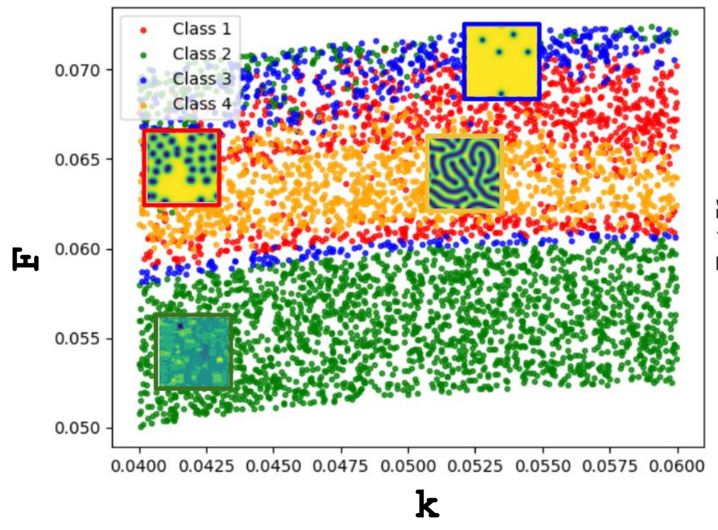
TRENDy was trained on the Gray-Scott model (Eq. 1), including in noisy conditions (left). Solutions were given GT labels with 4-way K-means. On test data, TRENDy outcompete benchmarks (middle) in predicting the transition to patterning (k^*). Further, a 4-way SVM on TRENDy's state closely predicted true pattern labels (right).

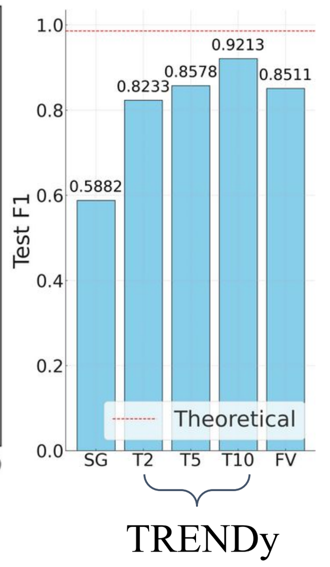
$$u_t = d_u \nabla^2 u - uv^2 + F(1-u)$$
$$v_t = d_v \nabla^2 v + uv^2 - (F+k)v \quad (1)$$



Clean Patches Boundaries



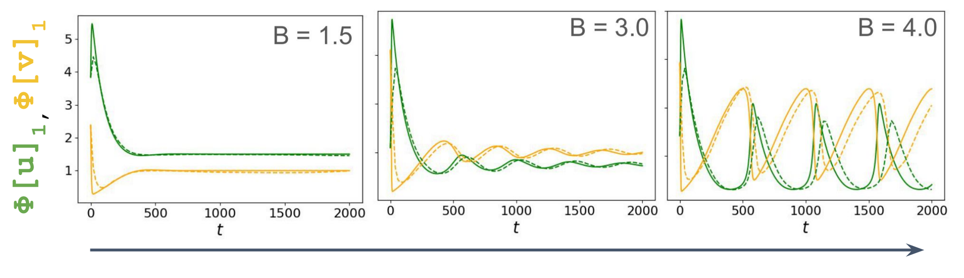




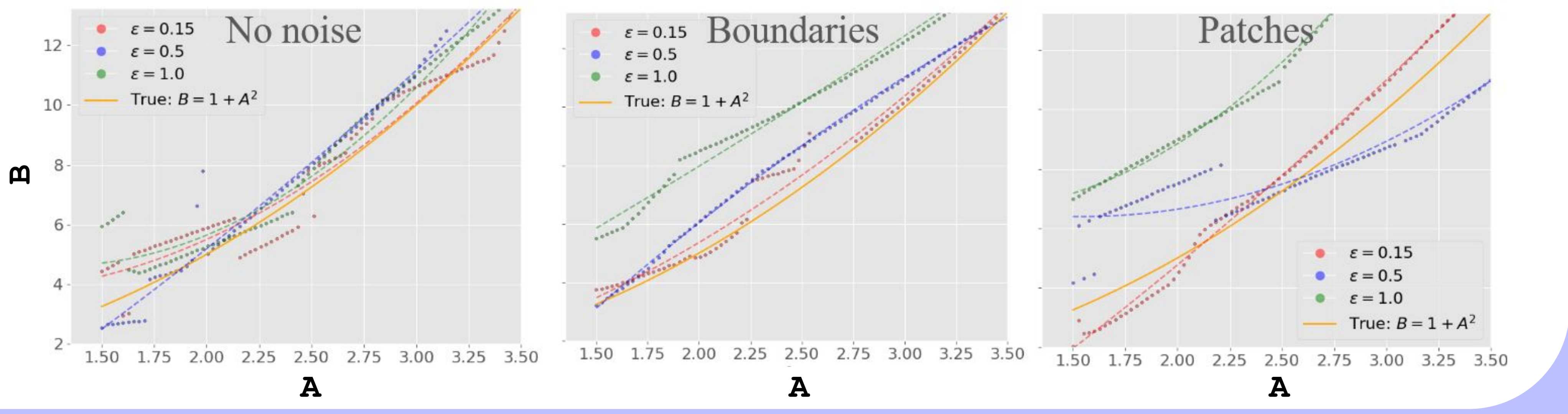
Predicting the transition to oscillations in the BZ reaction

TRENDy can also be used to predict the transition to oscillatory dynamics (left), as in the Belousov-Zhabotinsky reaction[4] (Eq. 2). We could also estimate the full bifurcation curve ($B=1+A^2$) across noise and hold-out conditions (ε = area left out around transition zone).

$$u_t = d_u \nabla^2 u + u^2 v - (B+1)u + A$$
$$v_t = d_v \nabla^2 v - u^2 v + Bu \quad (2)$$



Turing-Hopf bifurcation (—— GT, ---- Est.)

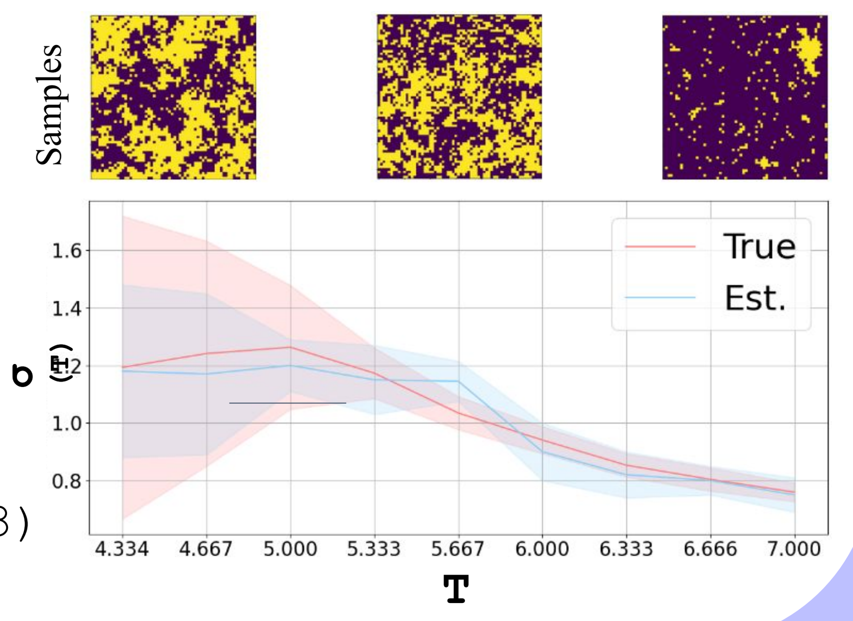


Predicting Ising scale correlation

The use of features with known structure (e.g. scale, orientation) means we can make interpretable predictions about dynamics. After training on the Ising model, we could predict the decrease in average spatial correlation between spins as a function of temperature, T, by measuring the expected scale (Eq. 3) on test data.

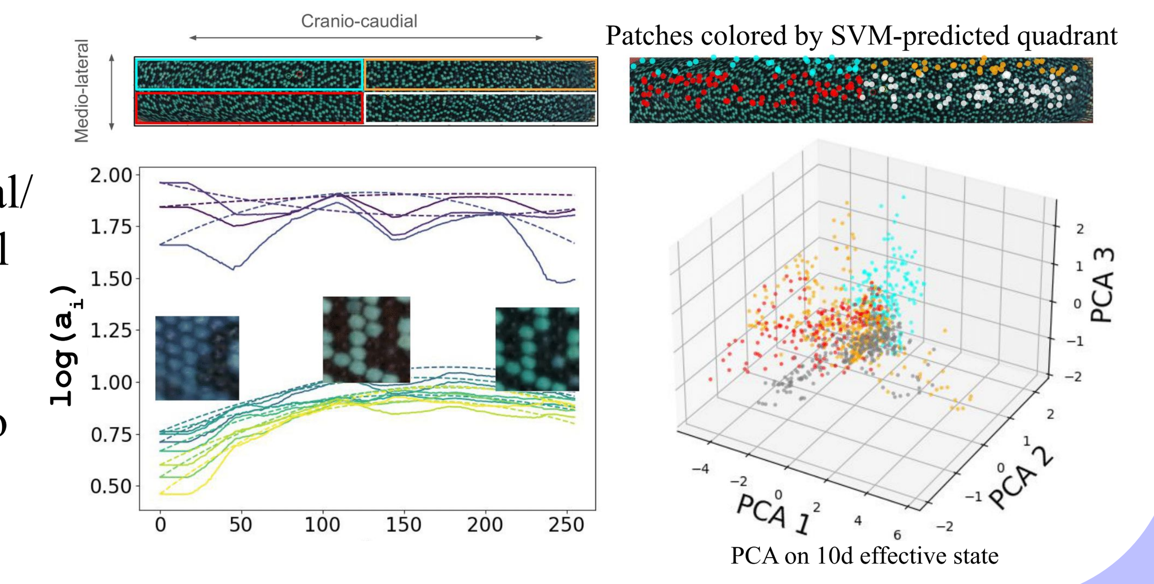
Interpreting structure. Scattering features were averaged across orientation, so that the effective states, a_j, measured only scales 2^j. Then, average scale as a function of temperature, T, was defined as

$$\sigma^{(T)} = 1/c \sum_j j\, a_j^{(T)}. \quad (3)$$



Linking patterning to anatomy in the ocellated lizard[5]

We fit TRENDy to high-resolution video patches of the developing scales of the ocellated lizard. On test data, we could predict the development of spatial features (left), and could classify (right) patch dynamics by their location in medio-lateral/craniocaudal coordinates, linking patterning to anatomy.



Conclusions

- Reduced-order "effective" dynamics can be fit with a parametric neural ODE, leading to a robust, interpretable model of bifurcation prediction and spatial patterning.
- TRENDy can be used to analyze synthetic and real biological datasets.
- Ongoing work integrates spatial transcriptomic data into forecasting.

References

1. Pearson, 1996
2. Vlachas et al., 2022
3. Mallat, 2011
4. Prigogine & Lefever, 1968
5. Fofonjka & Milinkovitch, 2021