Lyapunov Exponents for Diversity in Differentiable Games

Conference on Autonomous and Multi-agent Systems (AAMAS) 2022

arXiv link

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February 7^{th}, 2022

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- We generalize Ridge Rider [2] to differentiable games, providing a method which finds bifurcations and branches the optimization process across them: animation
- How do we find bifurcations? With Lyapunov exponent based objectives: animation

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- Why do we want to find different solutions? For example...
- In image classification, some generalize better than others - ex., shape vs. texture solutions.
- In differentiable games, some solutions have much higher social welfare – ex., cooperating vs. battling.
- But, what is a differentiable game?

Background: Differentiable Games

- Differentiable games generalize single-objective minimization:

$$\boldsymbol{\theta}_A^* \in \arg\min_{\boldsymbol{\theta}_A} \mathcal{L}_A(\boldsymbol{\theta}_A, \boldsymbol{\theta}_B^*),$$
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- Today's example: The Iterated Prisoner's Dilemma. A infinitely repeated version of the Prisoner's dilemma, where agents choose to cooperate or defect each round.
- Notable solutions: Defect-defect (DD) where agents always defect, and tit-for-tat (TT) which repeats what the opponent did last round allowing for higher welfare via cooperation.

Hyperparameter Optimization as a Differentiable Game

- Hyperparameter optimization and many meta-learning problems can be formulated as a differentiable game.

$$\boldsymbol{\lambda}^* \in \arg\min_{\boldsymbol{\lambda}} \mathcal{L}_V(\boldsymbol{\lambda}, \mathbf{w}^*(\boldsymbol{\lambda})),$$
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- I have various papers on this - some slides with connections at the end.

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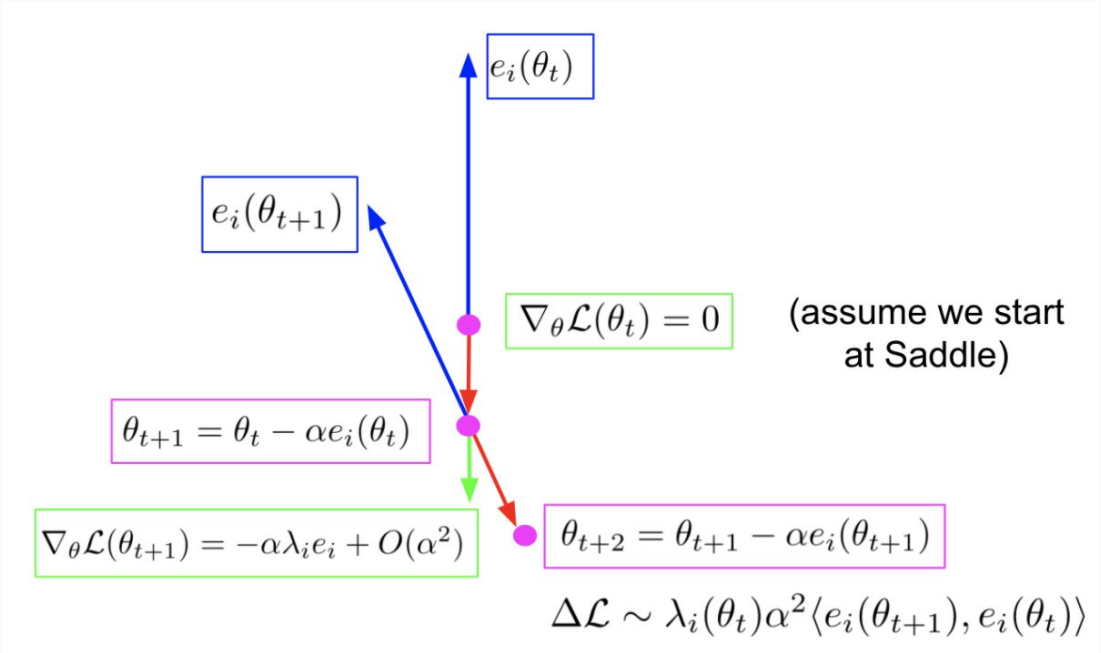

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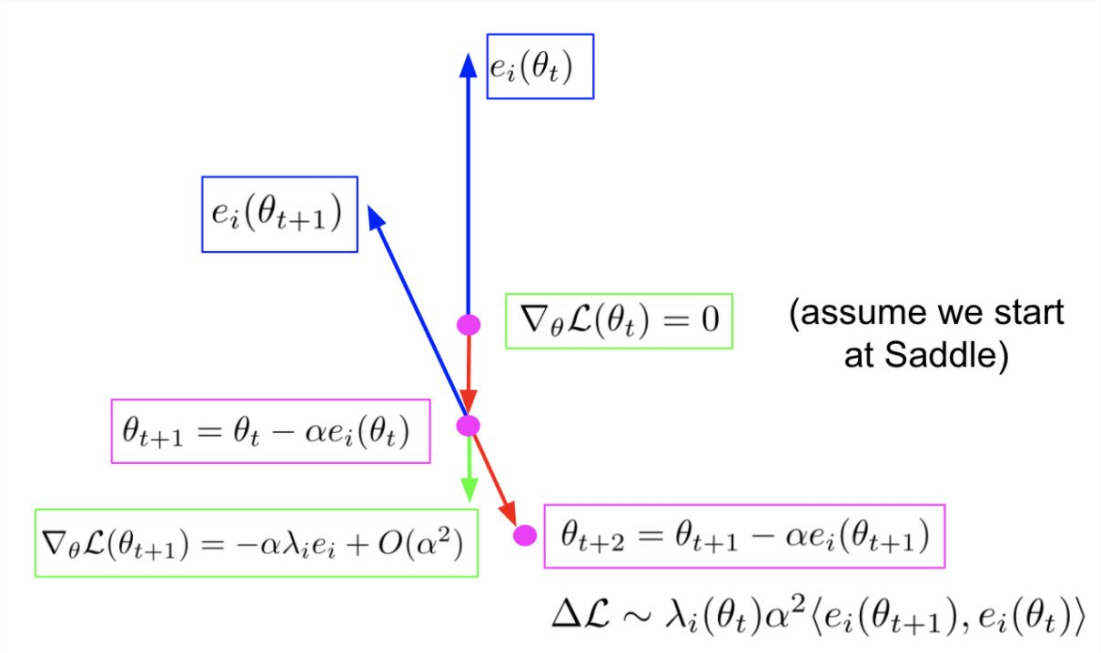

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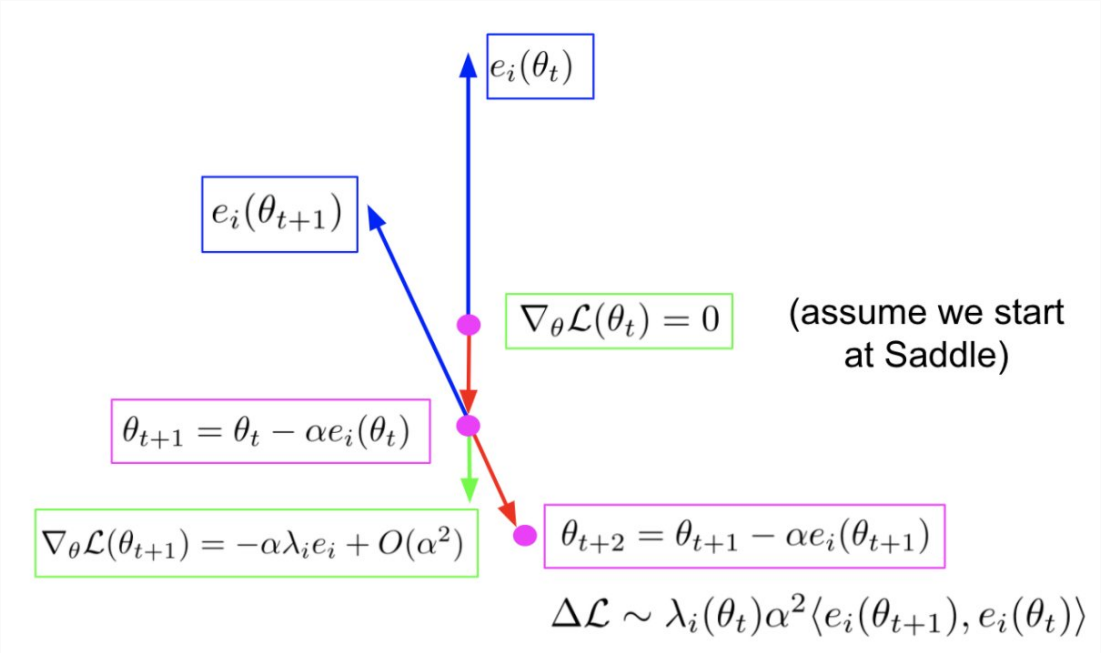

- Ridge rider (RR) [2] finds diverse solutions in single-objective optimization by branching optimization at saddle points.
- Optimization is branched by following/"riding" the most negative eigenvectors of the Hessian.
- Notable uses: Zero-shot learning, out-of-distribution generalization

RR for Differentiable Games?

- But, what if we wanted to use Ridge Rider to find multiple solutions in multi-agent setups like the Iterated Prisoner's Dilemma (IPD)?
- In differentiable games, there's no single Hessian with eigenvectors to follow. Ridge Rider is not defined!
- Generalizations of the Hessian's for games – i.e., the *Game Hessian* – may have complex EVals from lack of symmetry.

$$\overbrace{\hat{\mathcal{H}}}^{\text{Game Hessian}} = \begin{bmatrix} \text{Player } A \text{ Hessian} \nabla^2_{\theta_A} \mathcal{L}_A & \nabla_{\theta_A} \nabla_{\theta_B} \mathcal{L}_A \\ \nabla_{\theta_B} \nabla_{\theta_A} \mathcal{L}_B{}^\top & \text{Player } B \text{ Hessian} \nabla^2_{\theta_B} \mathcal{L}_B \end{bmatrix}$$

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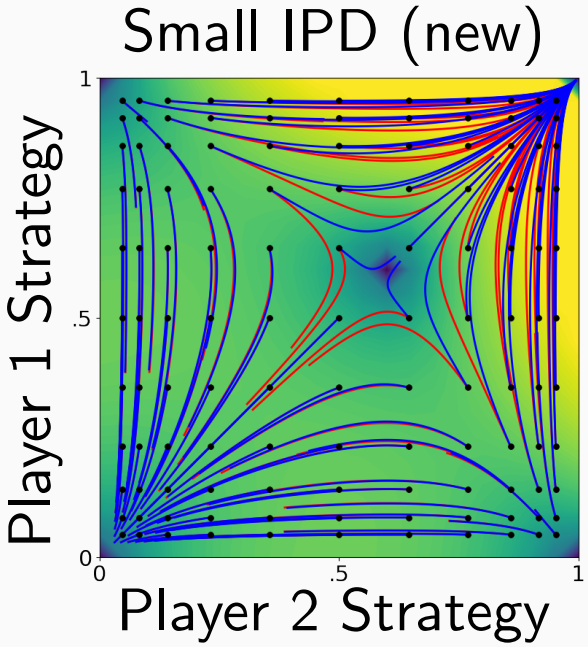
- Following the simultaneous gradient for differentiable games can form a non-conservative vector field. No single loss for vector-field to be gradient of!
- In non-conservative fields, many more bifurcation types.
- Now, let's look at toys to illustrate the difference:

Illustrative Toy Problems

Following the gradient in red, LOLA [1] in blue



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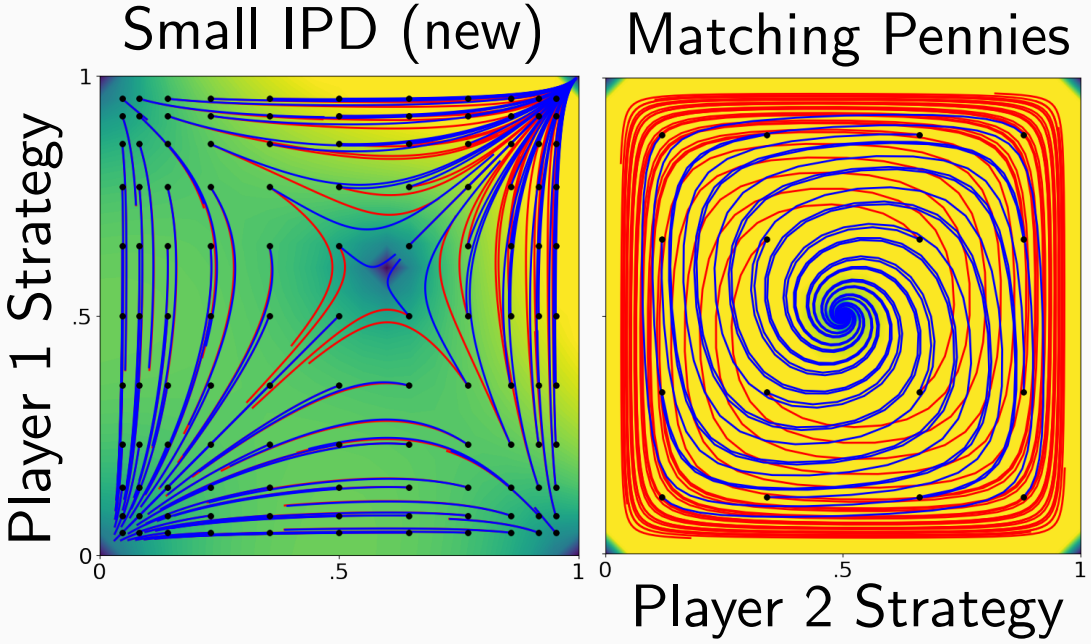

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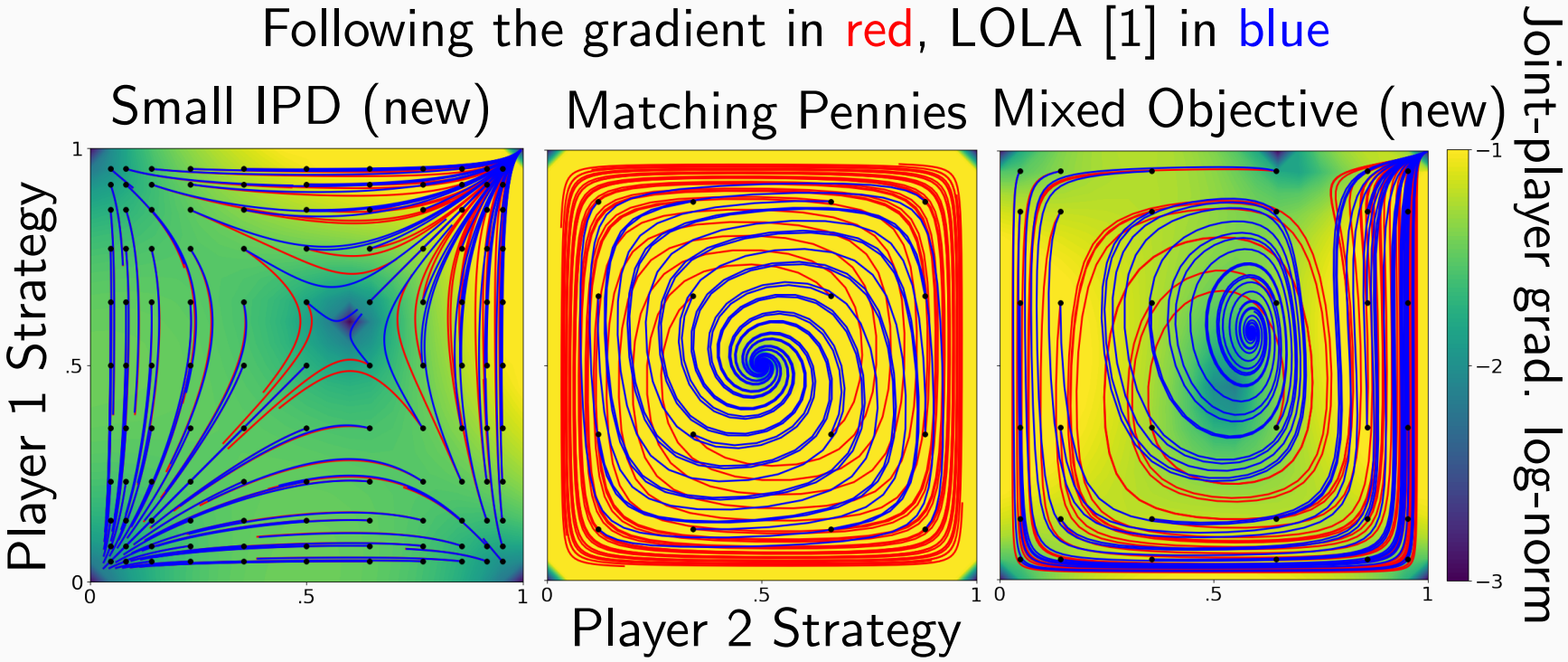
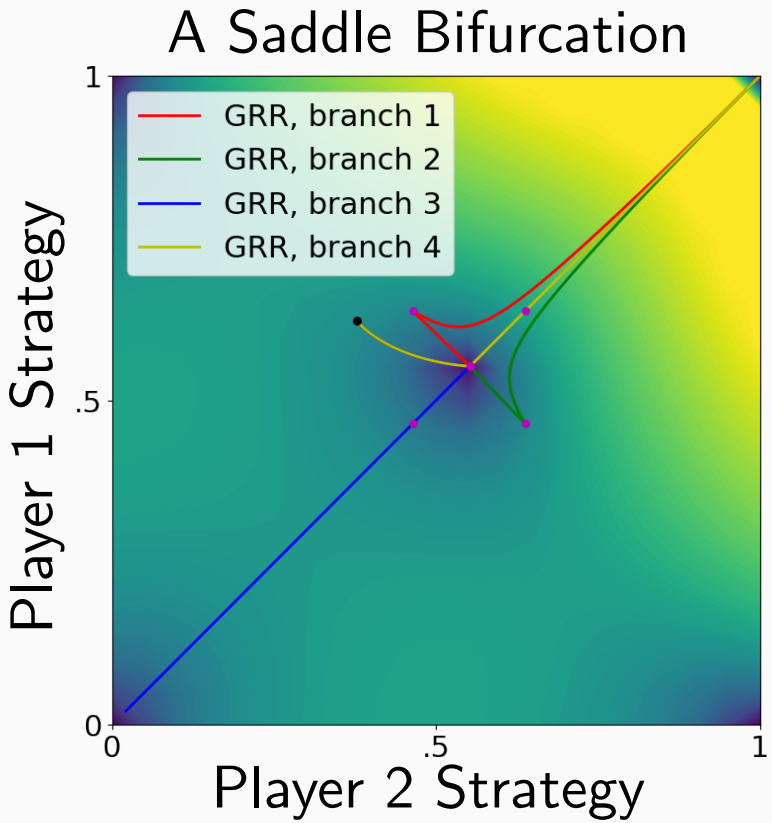


- Small IPD is a 2 param. Iterated Prisoner's Dilemma with TT and DD solutions, but only real EVals.
- Matching Pennies is a 2 param. rock-paper-scissors with imaginary EVals, but only 1 solution.
- Mixing these gives a 2 param. problem like the full IPD with multiple solutions, complex EVals, and a Hopf bifurcation.

Showing the Bifurcations



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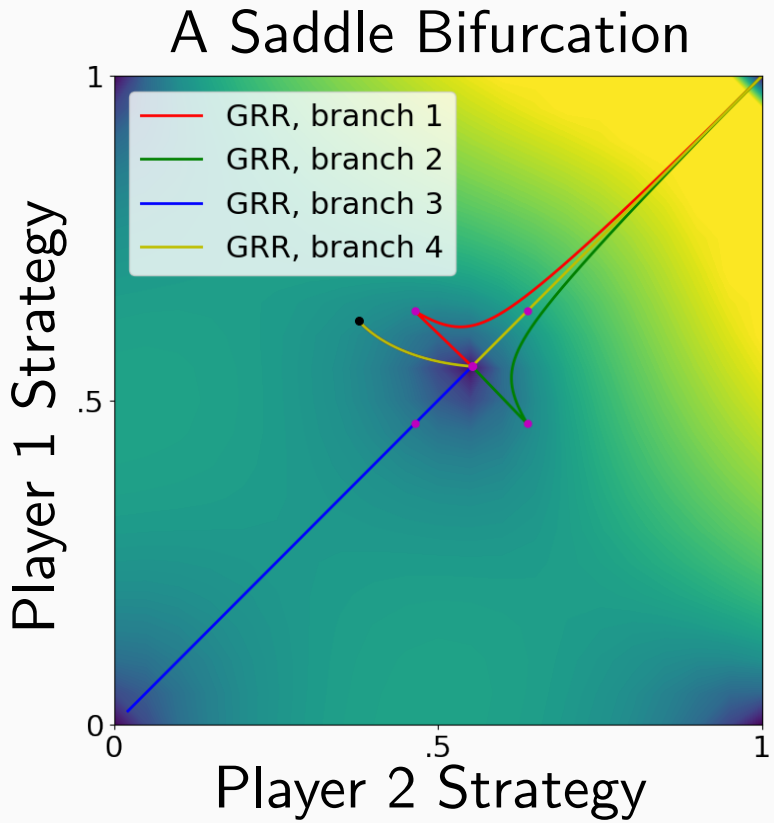

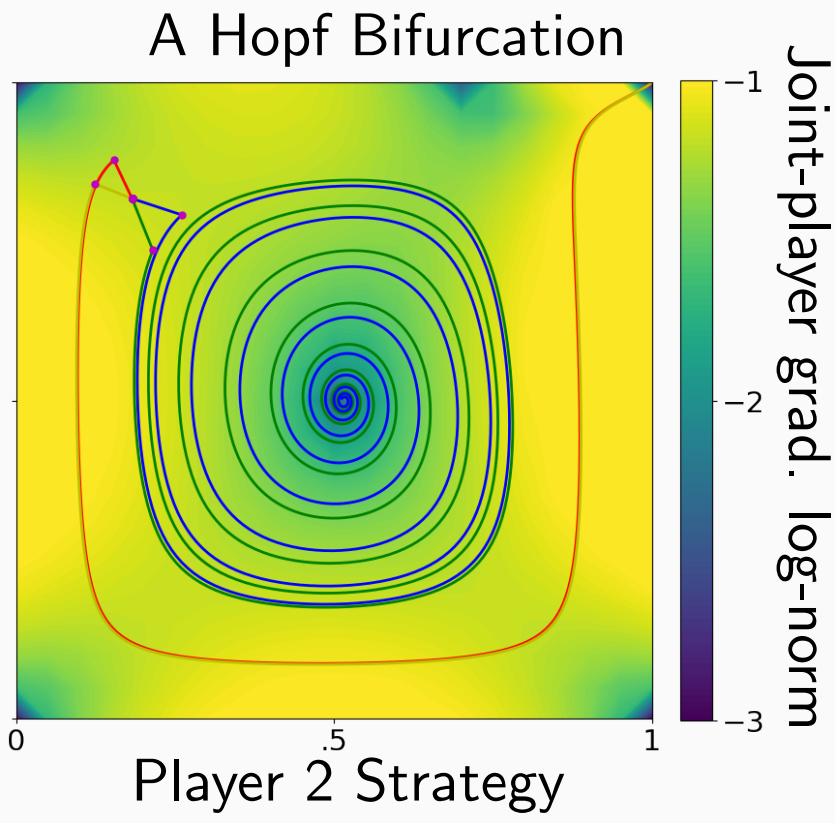

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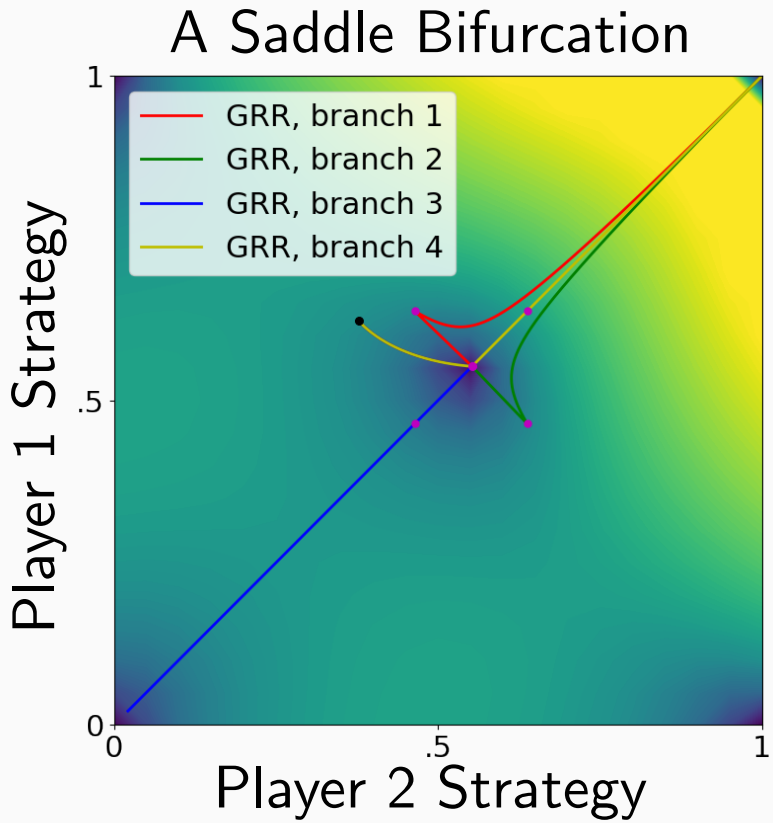
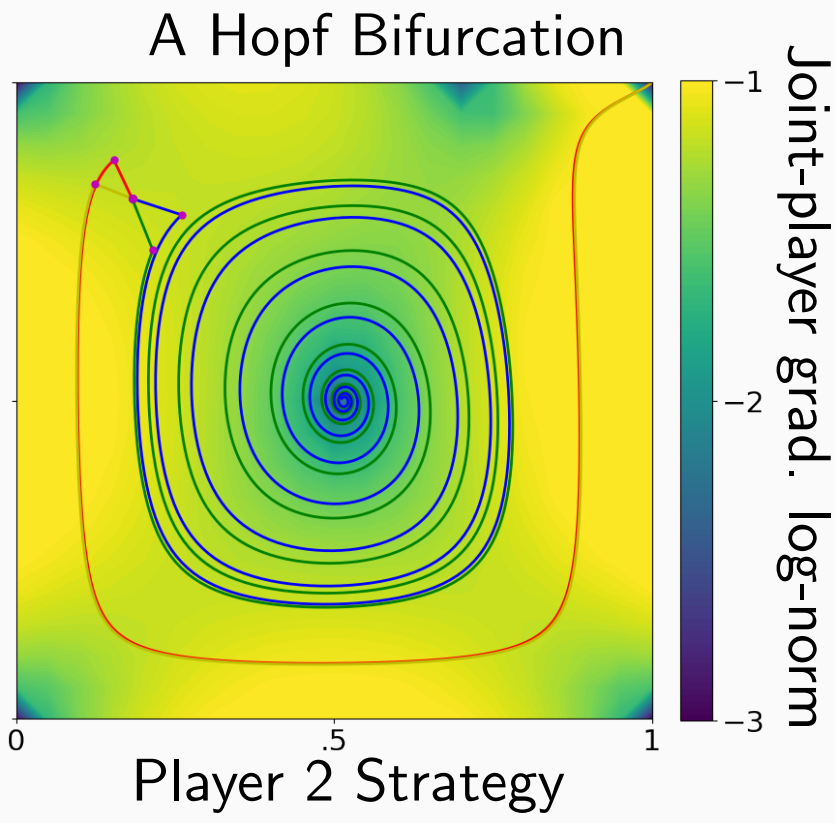
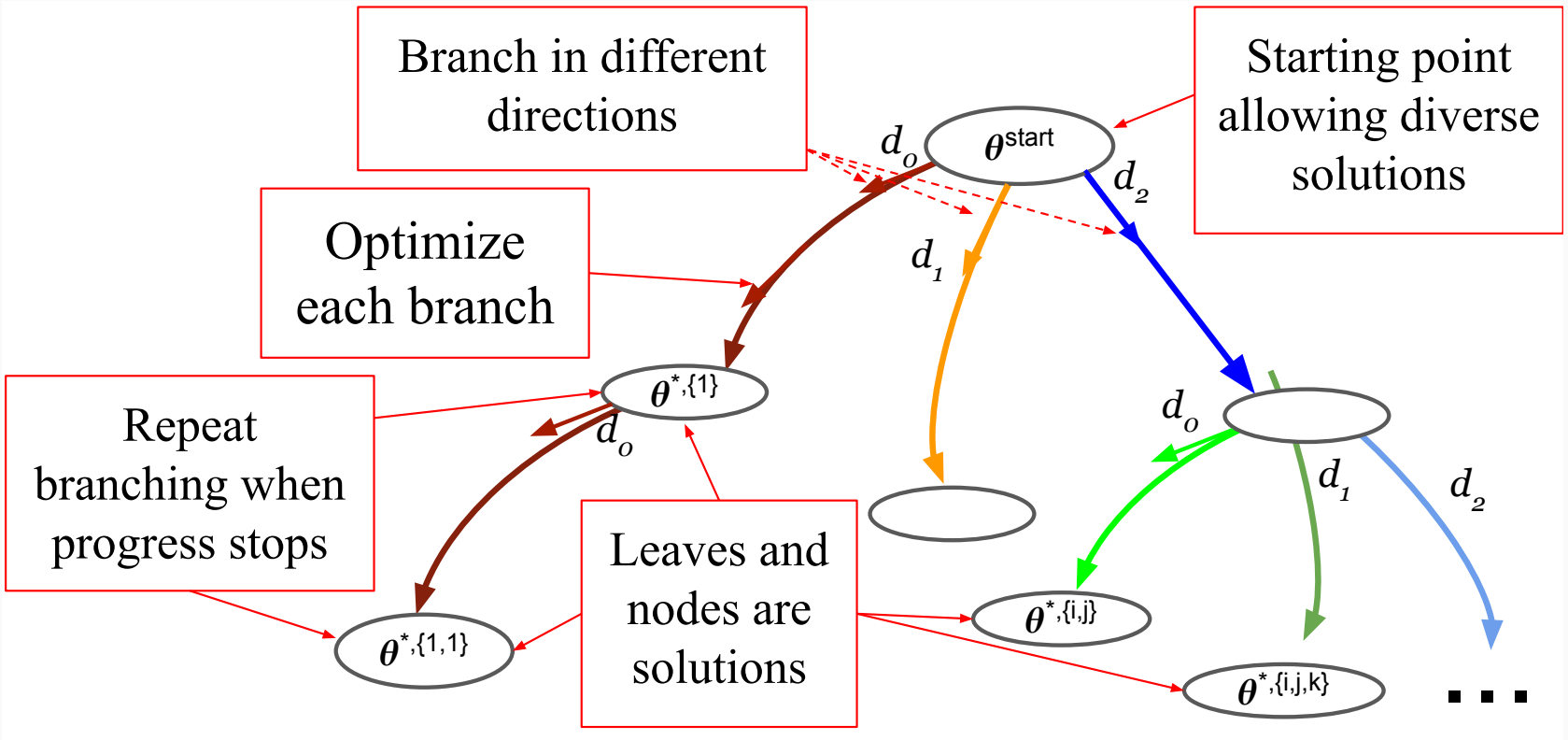




- Now, lets show a framework for finding multiple solutions:

Branching Optimization Tree Search



- Key parts are (1) Selecting the starting point, (2) creating different branches, (3) optimizing each branch, (4) choosing when to re-branch

Notation for Finding Bifurcations

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For example, SGD or LOLA:

$$\boldsymbol{F}_{SGD}(\boldsymbol{\omega}^j) = \boldsymbol{\omega}^j - \alpha \hat{\boldsymbol{g}}^j \tag{4}$$

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- Fixed point operator for SGD:

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What are Lyapunov Exponents?

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- Take limit at opt. horizon $k \to \infty$. We get the (global) Lyapunov exponent in direction $\boldsymbol{d}$ at point $\boldsymbol{\omega}_0$.
- Often interested in the max Lyapunov exponent:

$$\hat{\lambda}_k^{max}(\boldsymbol{\omega}_0) = \max_{\boldsymbol{d}, \|\boldsymbol{d}\|=1} \hat{\lambda}_k(\boldsymbol{\omega}_0, \boldsymbol{d}) \tag{13}$$

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- Can find bifurcations between basins by maxing exponent!

What are Lyapunov Exponents?

- Intuition: just a (log) EVal integrated over a trajectory.

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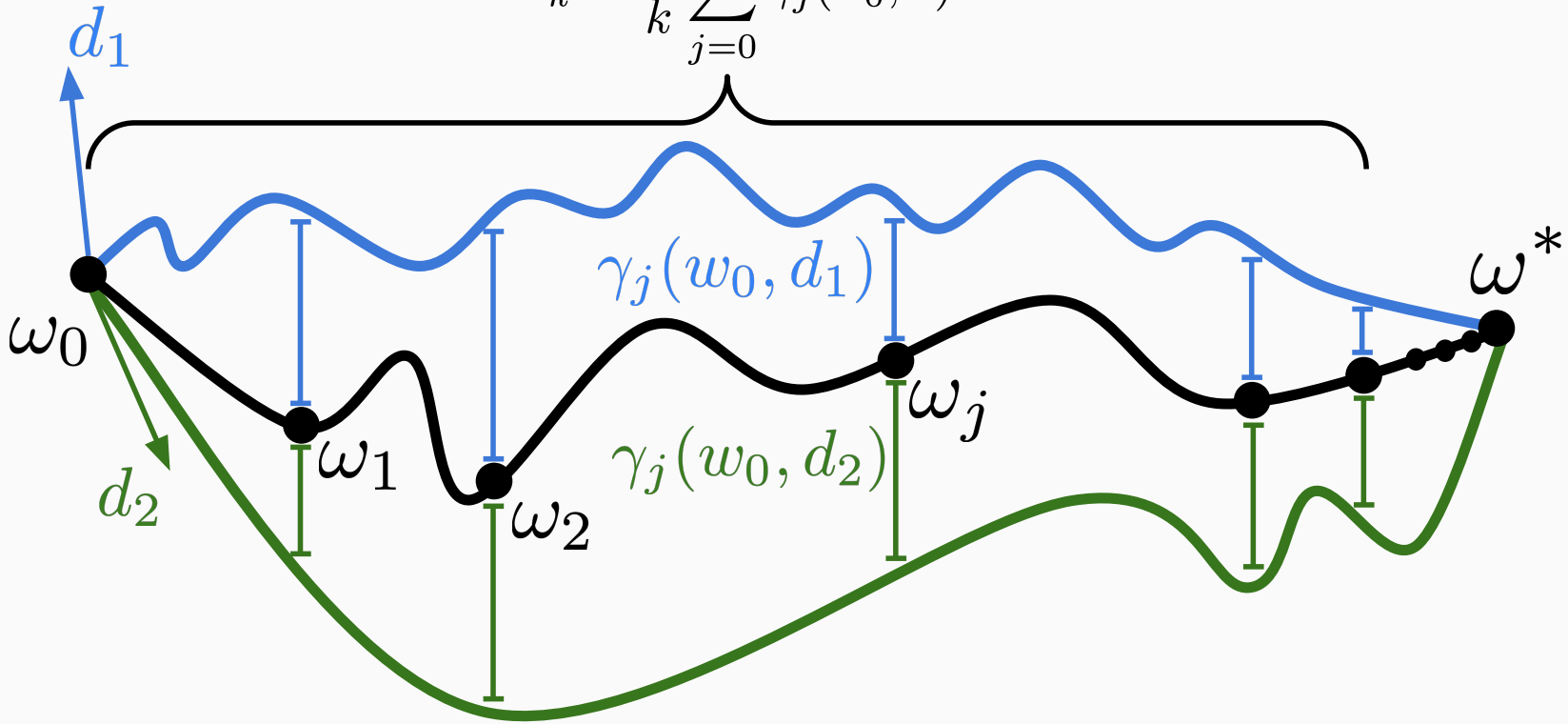
$$\hat{\lambda}_k = \frac{1}{k}\sum_{j=0}^{k} \gamma_j(\omega_0, d)$$



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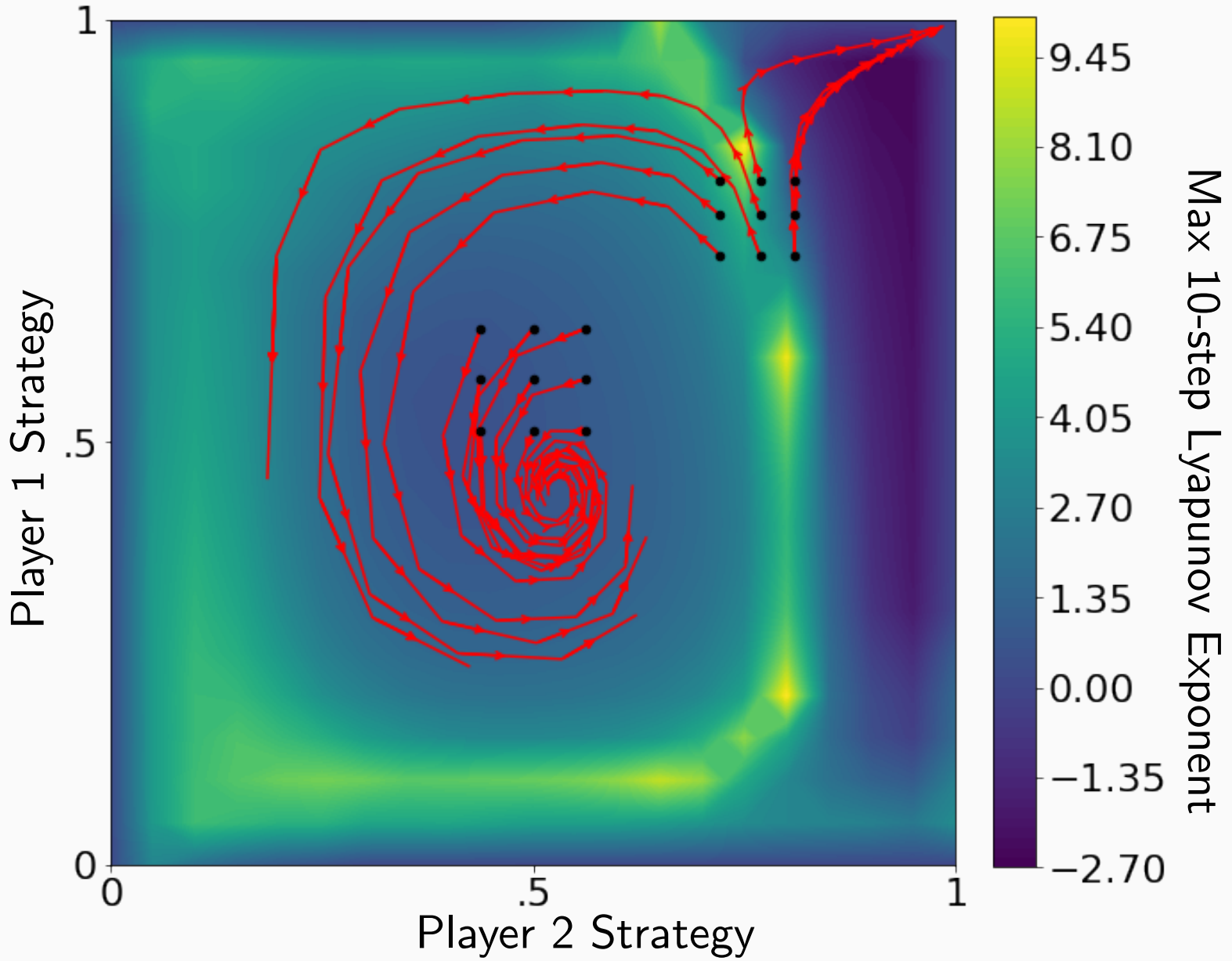
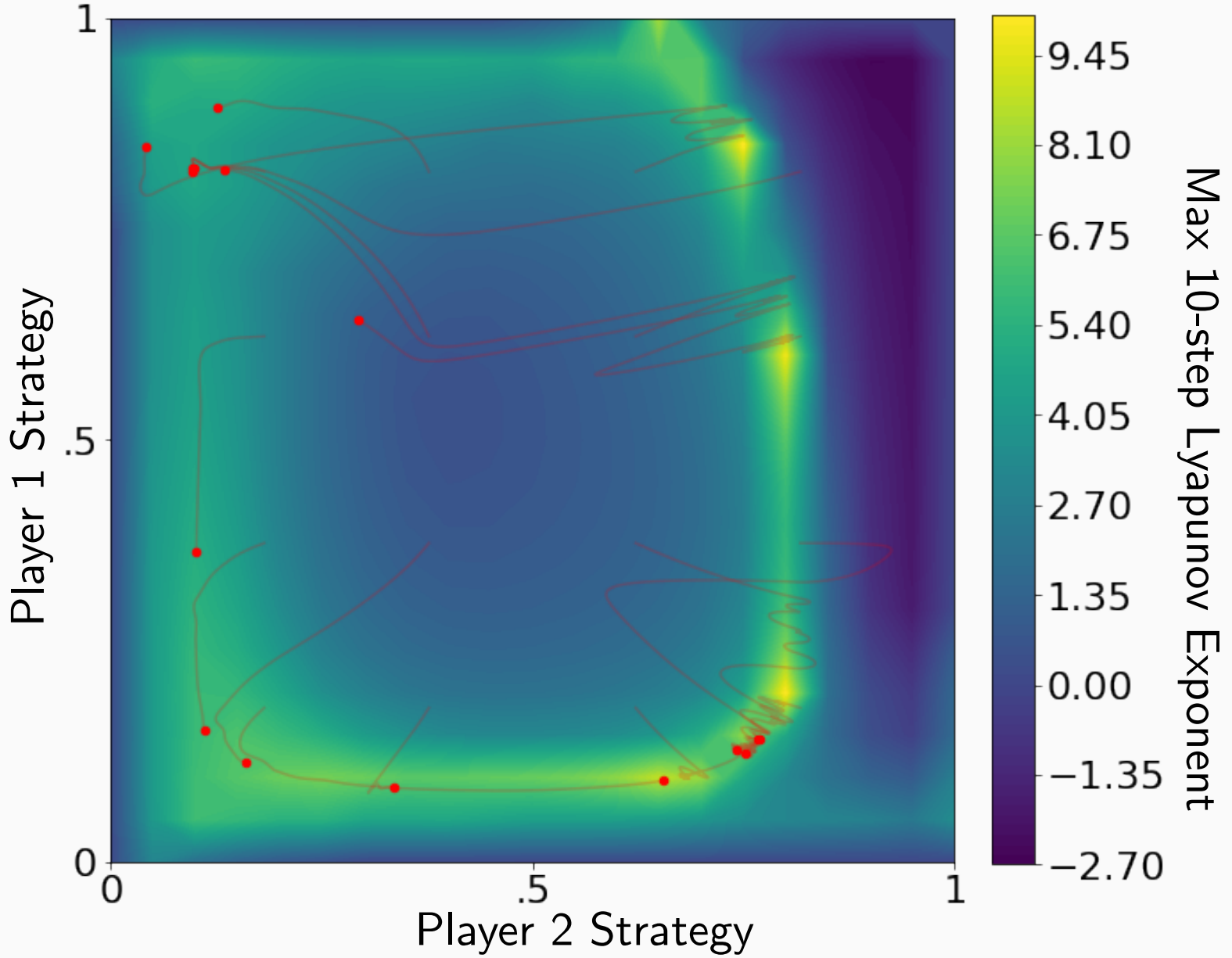
- But, we lose many of the theoretical results.
- The next slides help to build an intuition for the exponent of visualizable toy problems.

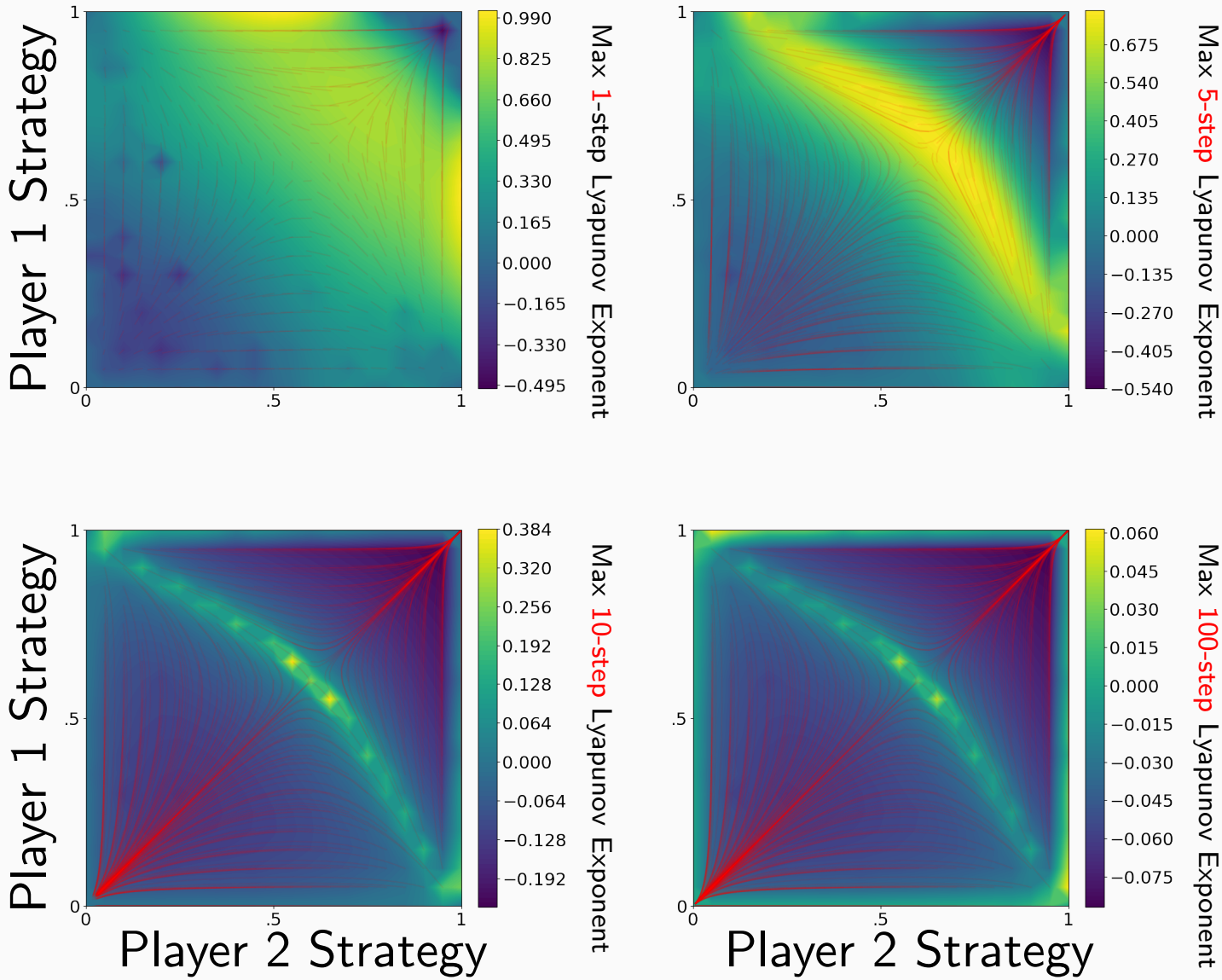
Showing Bifurcations with Lyapunov Exponents - animation



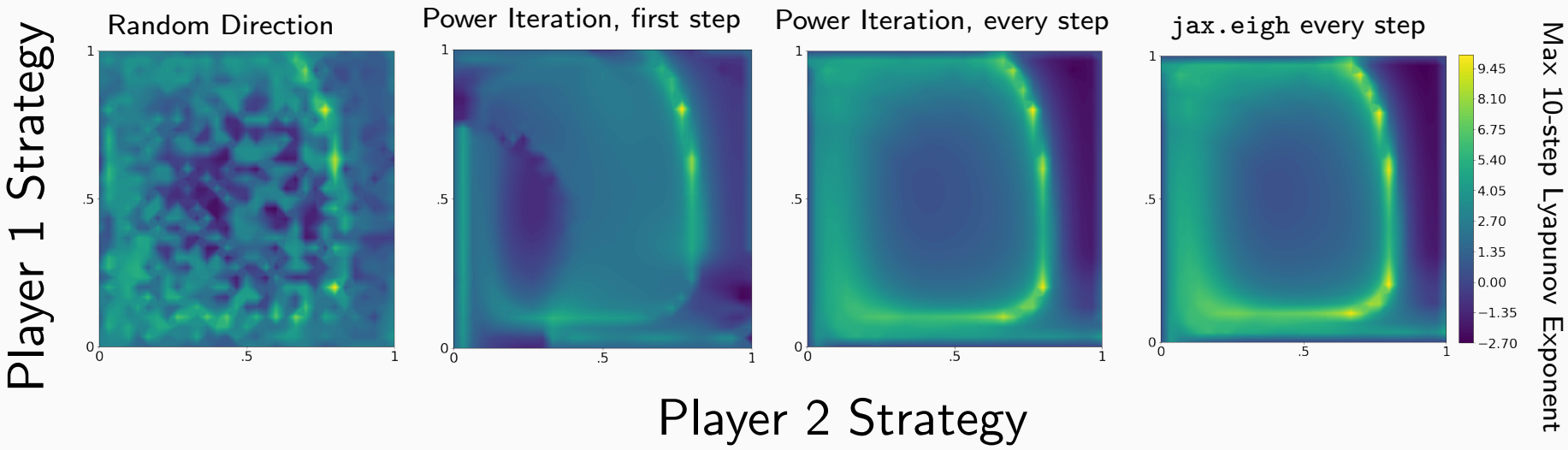
Optimizing Lyapunov Exponents to Find Bifurcations



Impact of Optimization Horizon on Exponent - animation



Impact of Direction Choice on Showing Bifurcations



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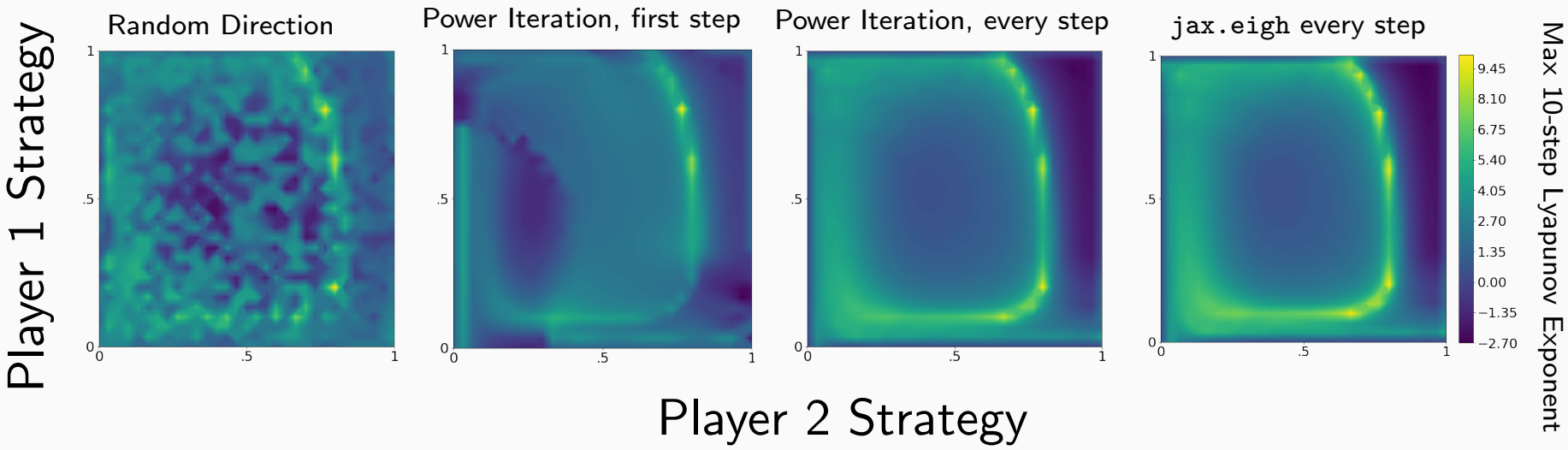
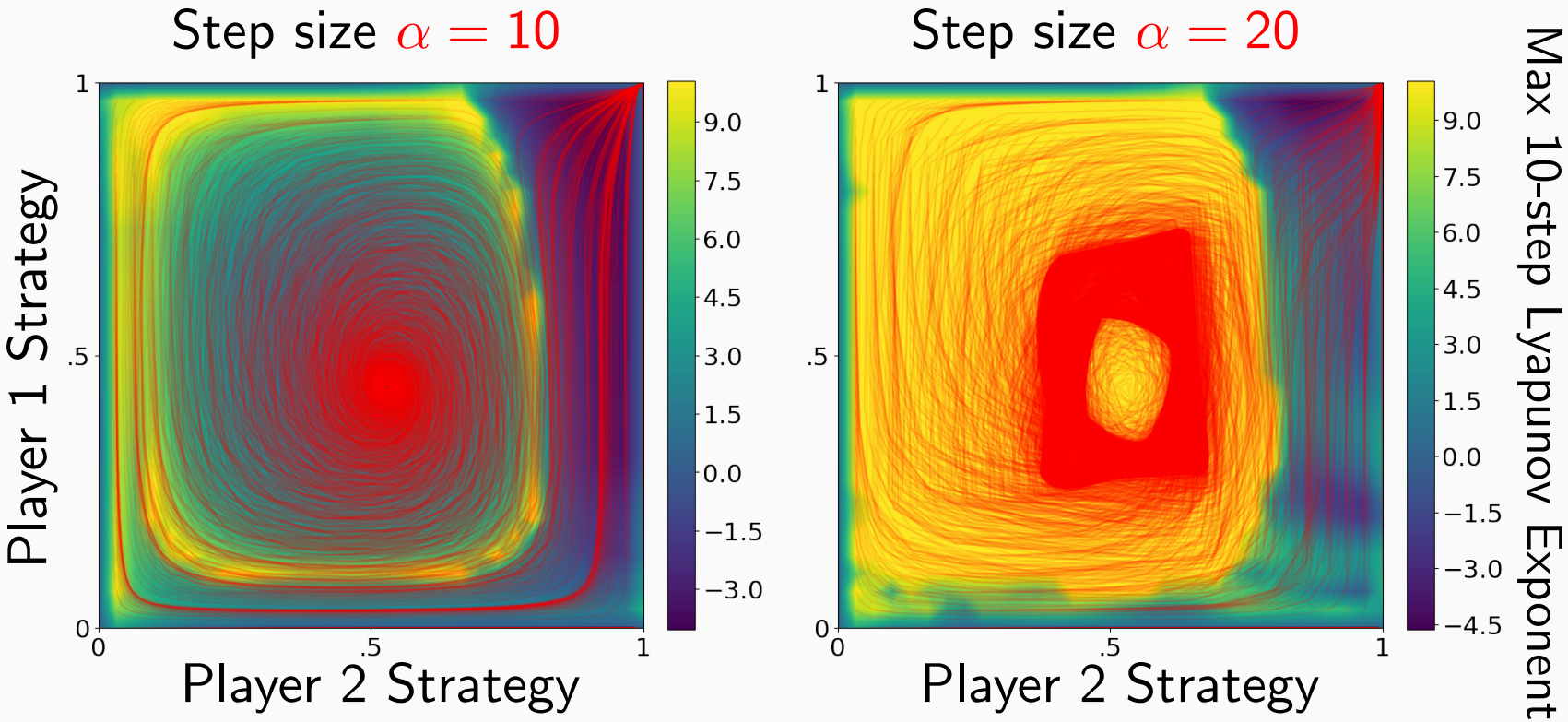


- Re-estimating the top EVecs at each iteration performs best, but is most expensive, and diverges from theory.
- In the optimization limit $k \to \infty$ the choice of direction almost certainly doesn't matter.

What if the Optimizer doesn't Converge?



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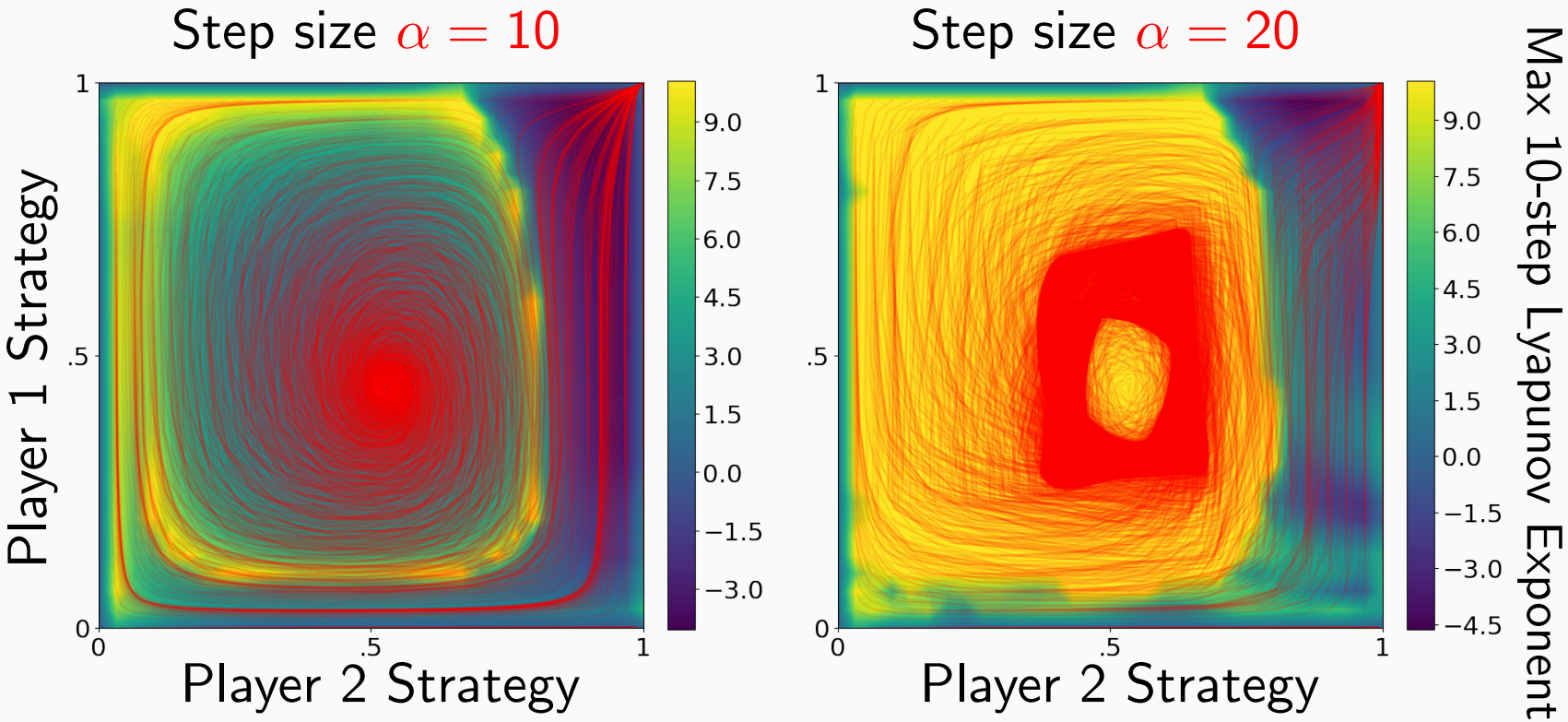

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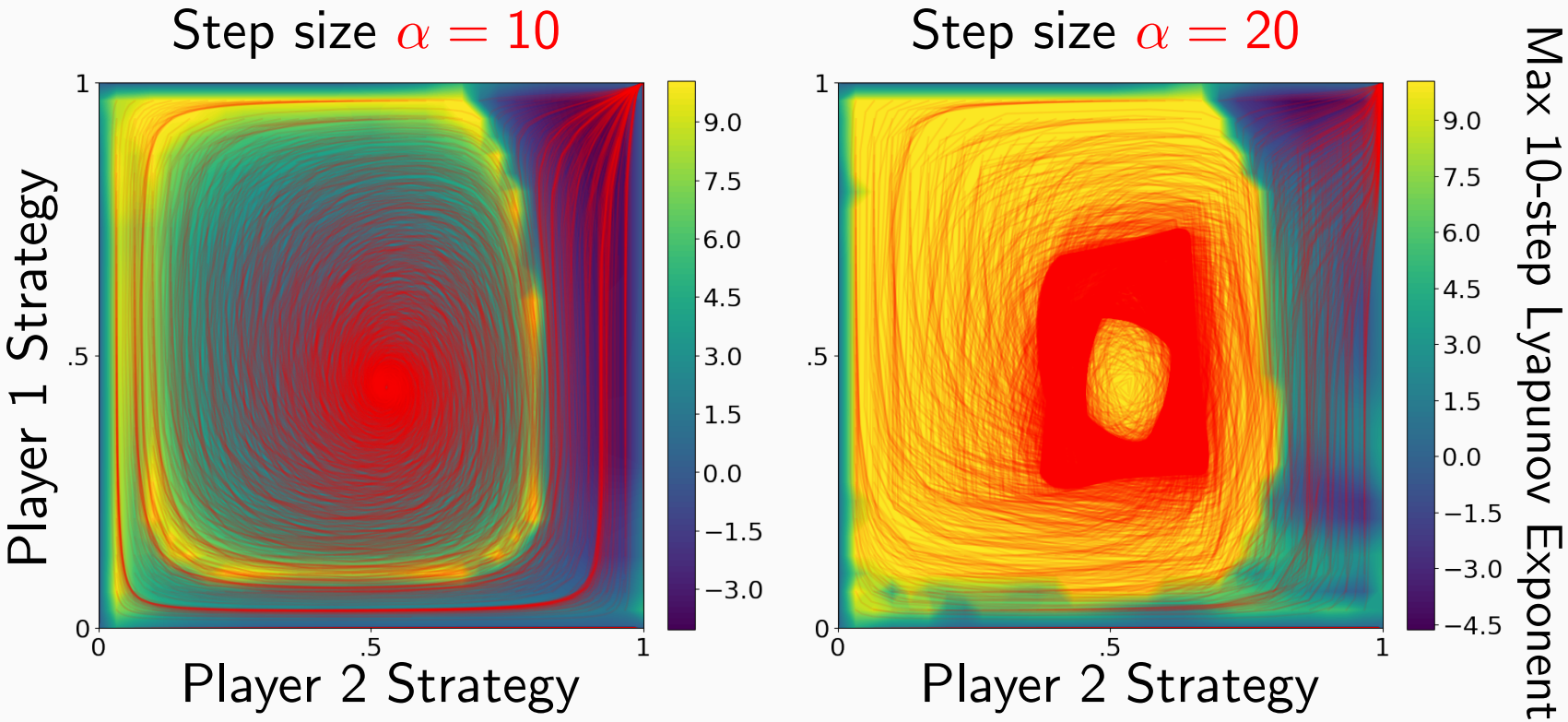

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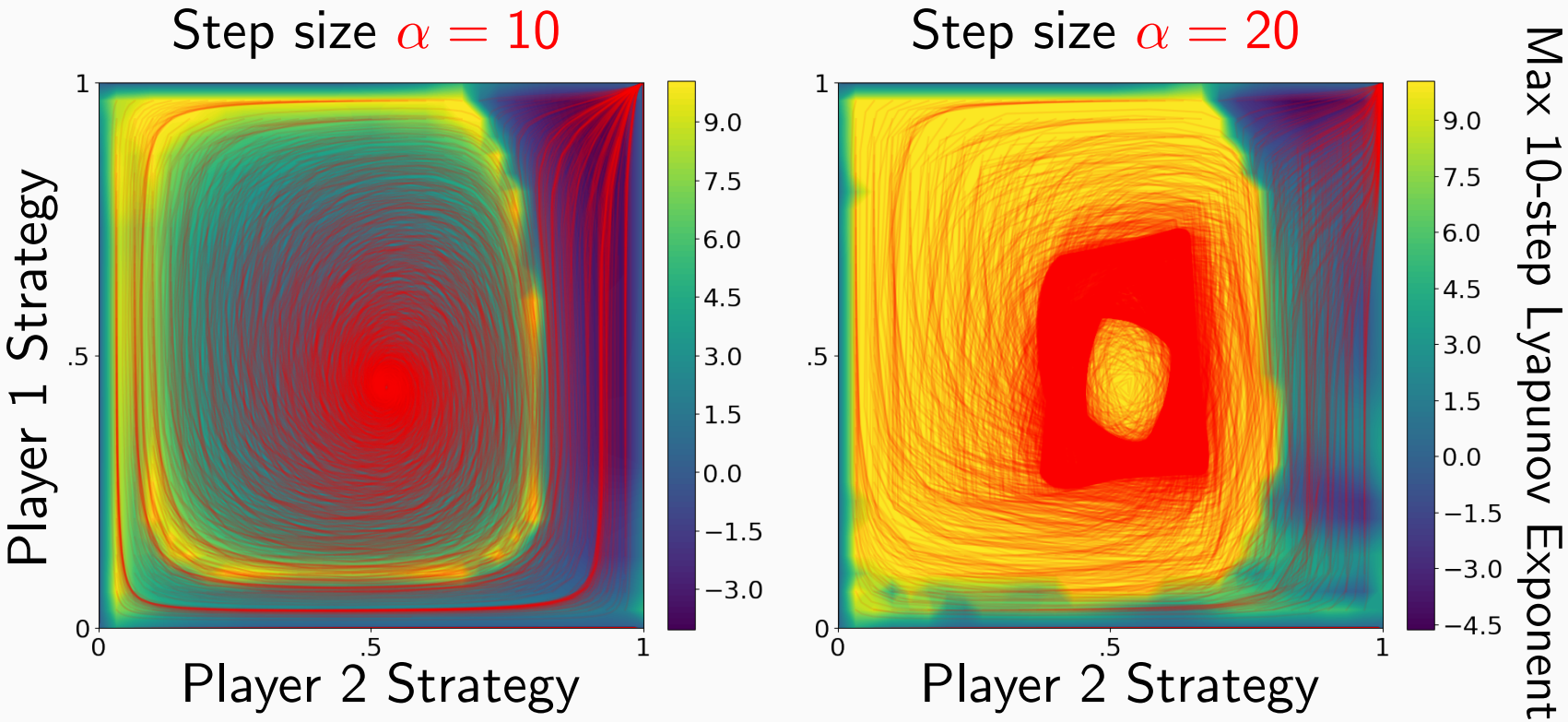

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- If not, exponent maybe max where trajectories don't find soln.
- Can get fractal bifurcation for critical step size: video
- We could use more complicated toy problems...

Random Subspace Problem

- But, we only looked at 2 bifurcations so far. Can we construct toy problems with more types?

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- Idea: take high-dimensional game $\mathcal{L}_A(\theta_A, \theta_B), \mathcal{L}_B(\theta_A, \theta_B)$ and optimize in a subspace. Ex., GAN, IPD, HO, meta-learning,...

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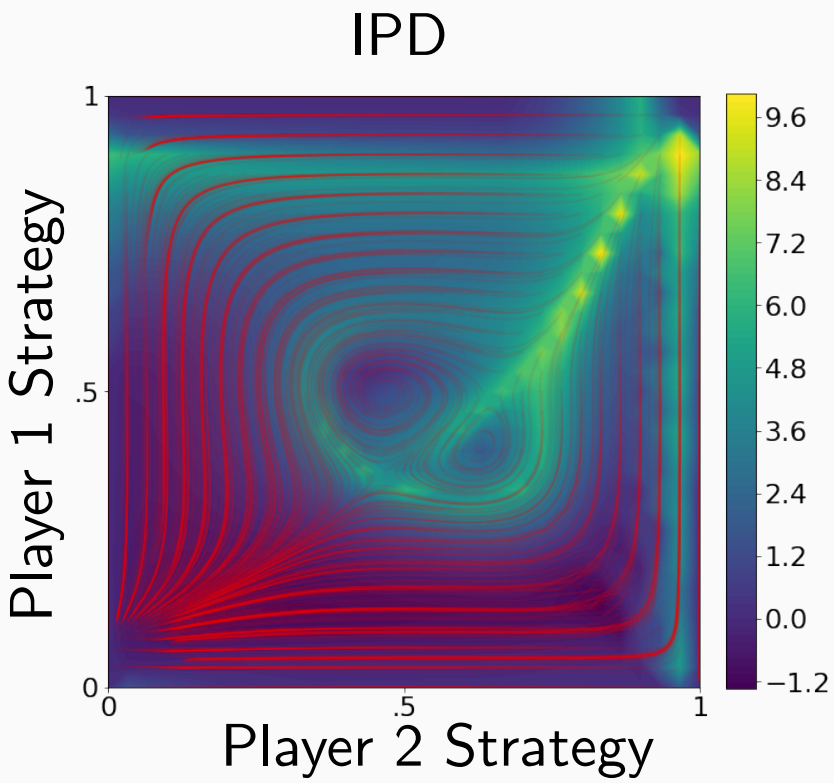
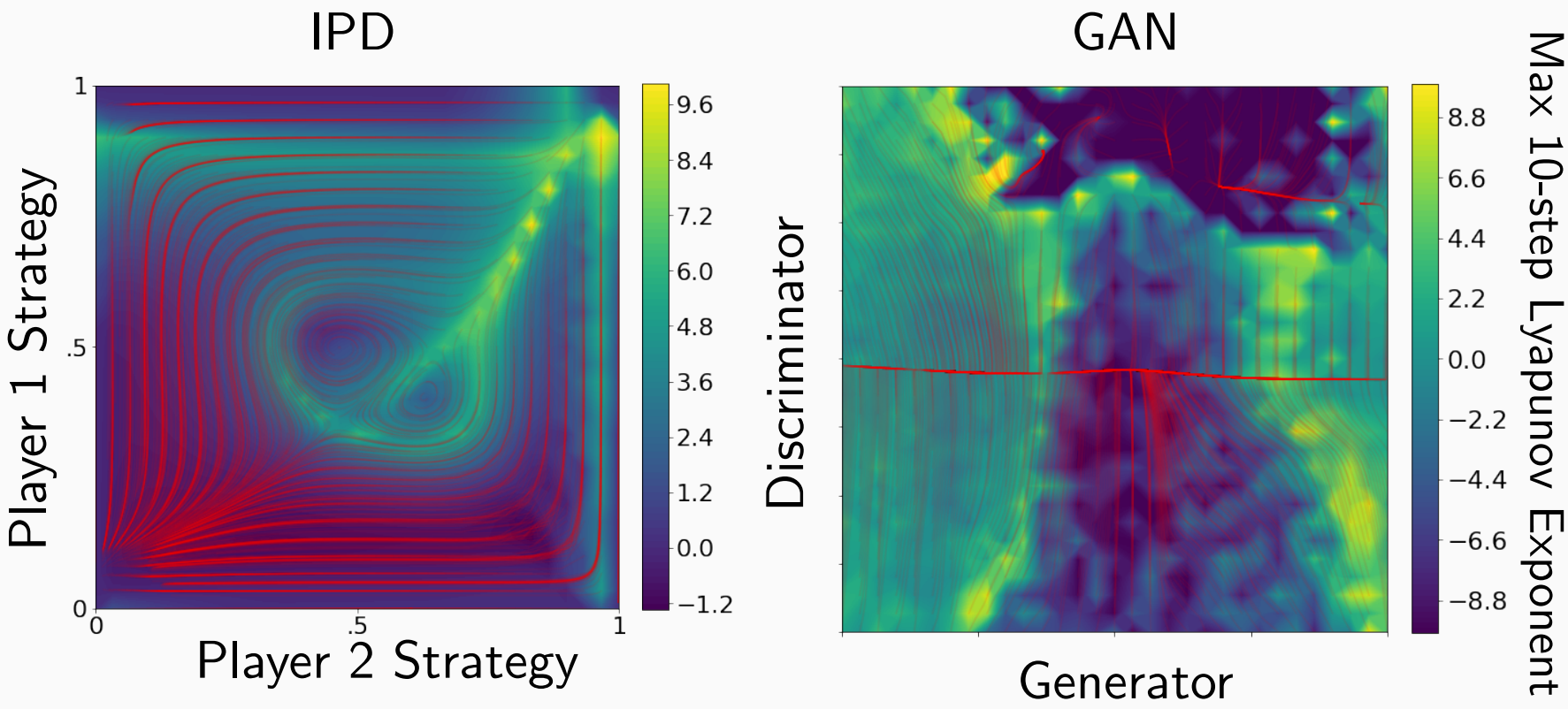
- Specifically, use $\mathcal{L}_A(\mathbf{v}_A x + \mathbf{b}_A, \mathbf{v}_B y + \mathbf{b}_B), \mathcal{L}_B(\mathbf{v}_A x + \mathbf{b}_A, \mathbf{v}_B y + \mathbf{b}_B)$, where $\mathbf{v}$ sampled (ex., uniform) randomly, and offset $\mathbf{b}$ at appropriate value (ex., init., optimal).

Random Subspace Problem



- Exponent peaks near where trajectories separate, showing we find bifurcations.
- Are some bifurcations more prevalent in some games?

Random Subspace Problem



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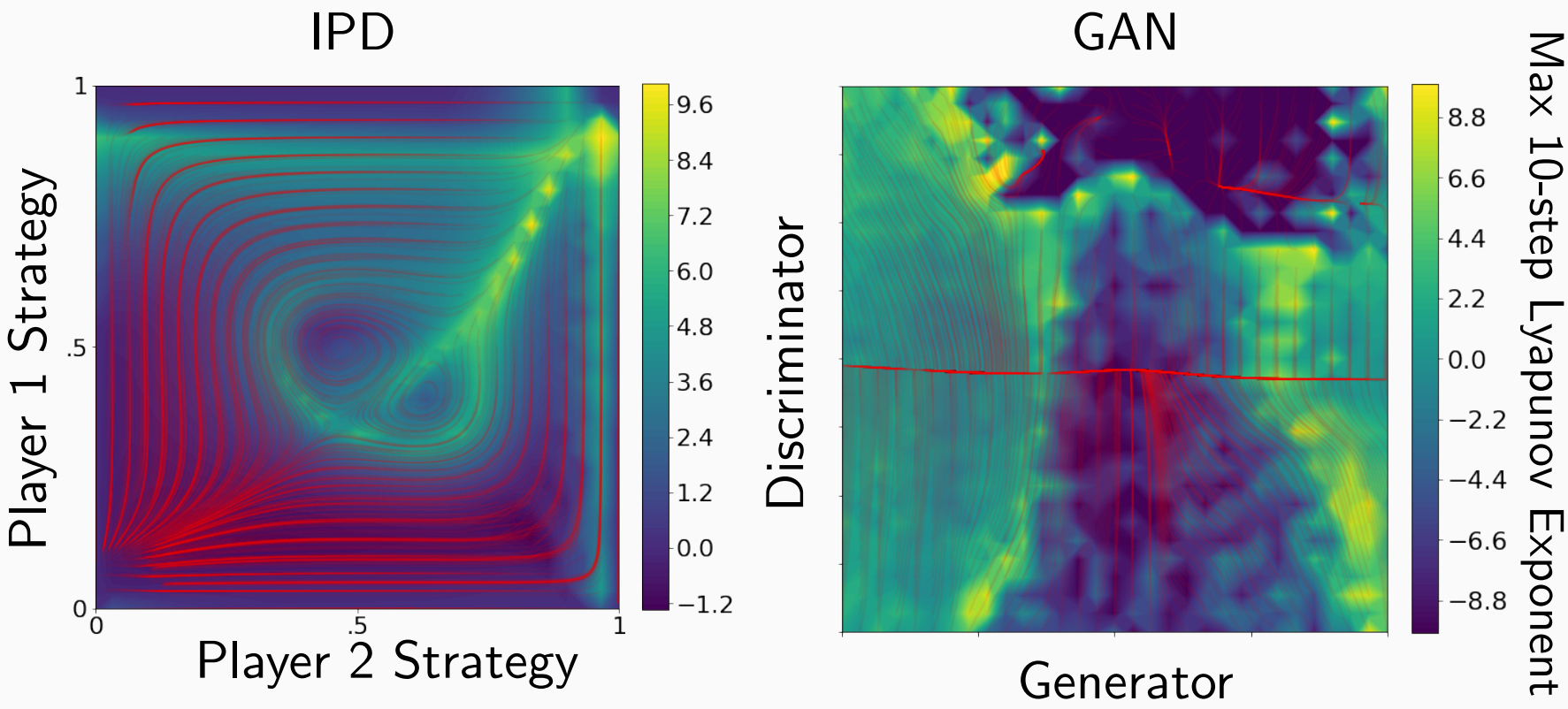

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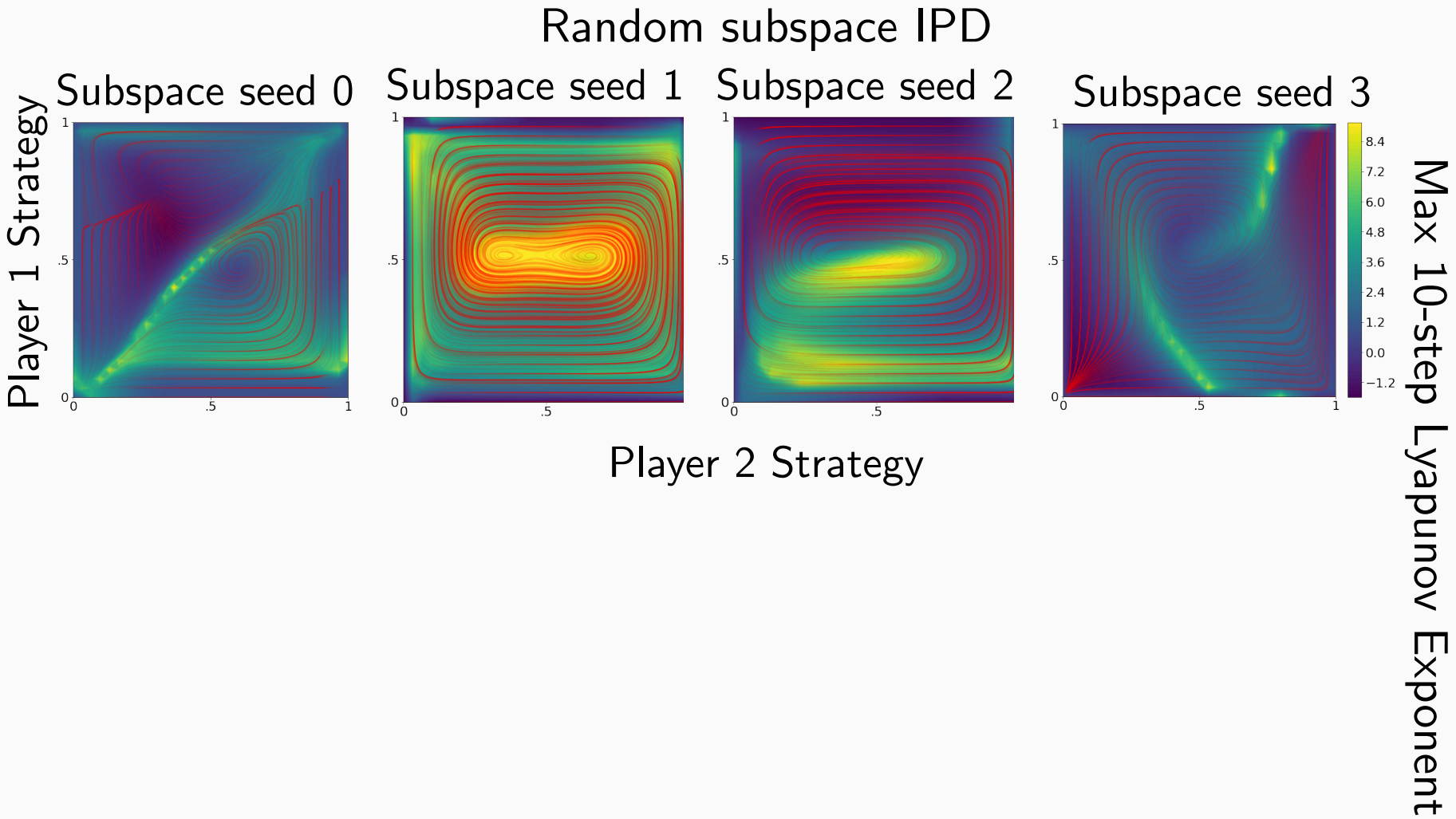

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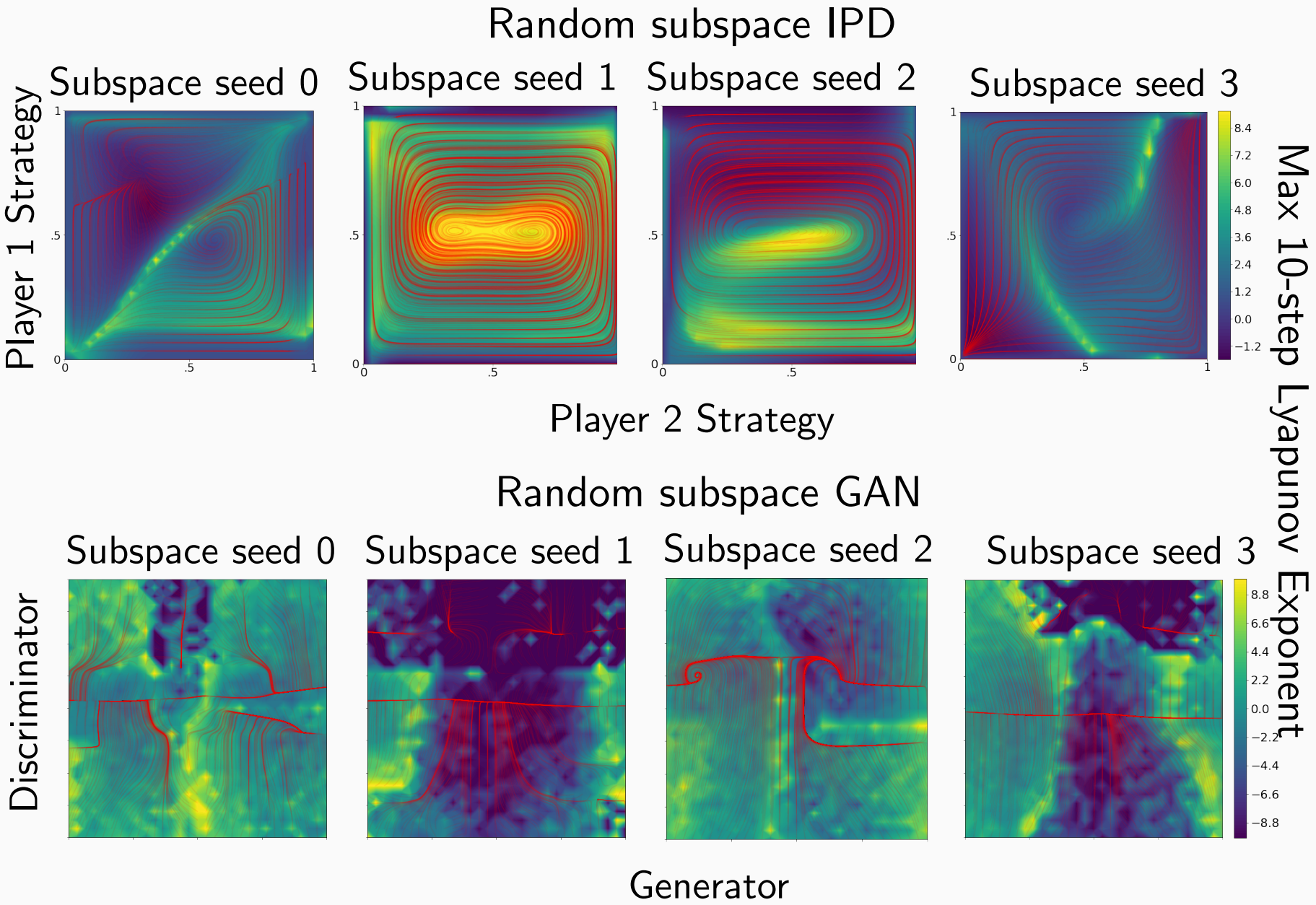

Finding Diverse Solutions in the Iterated Prisoners Dilemma

- Now, try the full branching opt. method – Generalized Ridge Rider (GRR) – on the Iterated Prisoners Dilemma (IPD).

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- We look at these in the following table.

Finding Diverse Solutions in the Iterated Prisoners Dilemma

Search Strategy	Solution Mode: Cooperate	Solution Mode: Defect
$\times 20$ Random init + LOLA [1]	✓	×
$\times 20$ Random init + GD	×	✓

- Randomly init. then applying a training method only finds 1 solution mode. Baselines don't find both.

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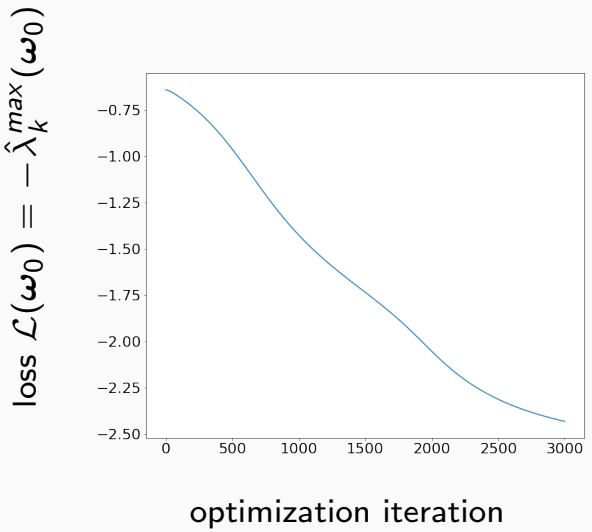
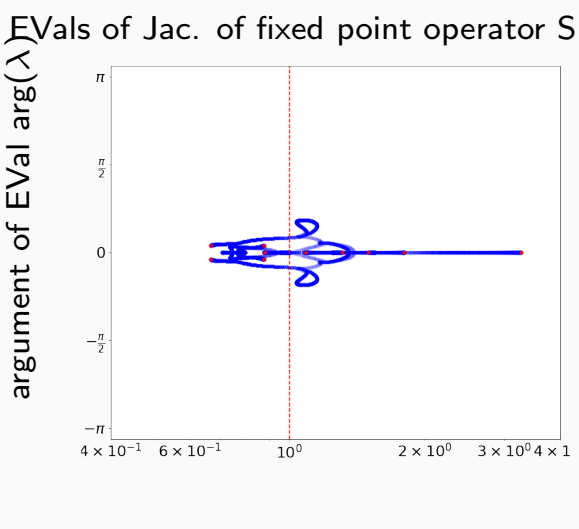
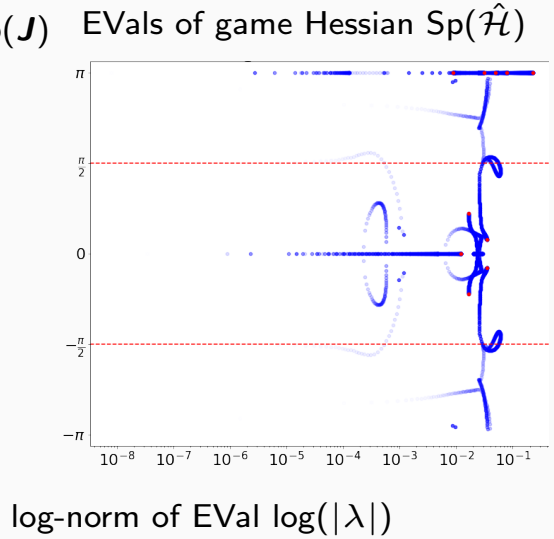
- Our method finds both solution modes (with *any* opt.).
- If we don't tune the Lyapunov exponent, then branching doesn't affect the soln. Evidence we are near a bifurcation.

Analyzing the IPD Optimization







- **Takeaway:** We effectively reduce our loss and correspondingly raise the max EVal of $\boldsymbol{J}$.
- What if we need separation in more than 1 direction?

Connections to Kolmogorov-Sinai Entropy

- Max exponent $\hat{\lambda}_k^{max}(\boldsymbol{\omega}_0) = \max_{\boldsymbol{d}, \|\boldsymbol{d}\|=1} \hat{\lambda}_k(\boldsymbol{\omega}_0, \boldsymbol{d})$ only guarantees separation in 1 direction.

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$$\mathcal{L}_n^{\text{sum}}(\boldsymbol{\omega}_0) = - \max_{\boldsymbol{d}_1, \ldots, \boldsymbol{d}_n} \sum_{l=1}^{n} \hat{\lambda}_k(\boldsymbol{\omega}_0, \boldsymbol{d}_l),$$

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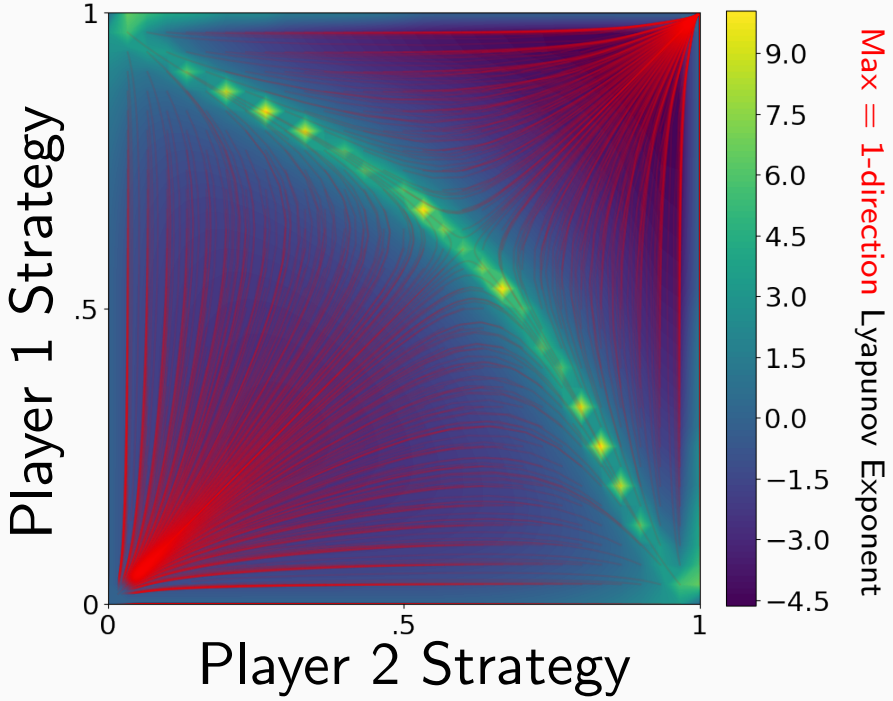
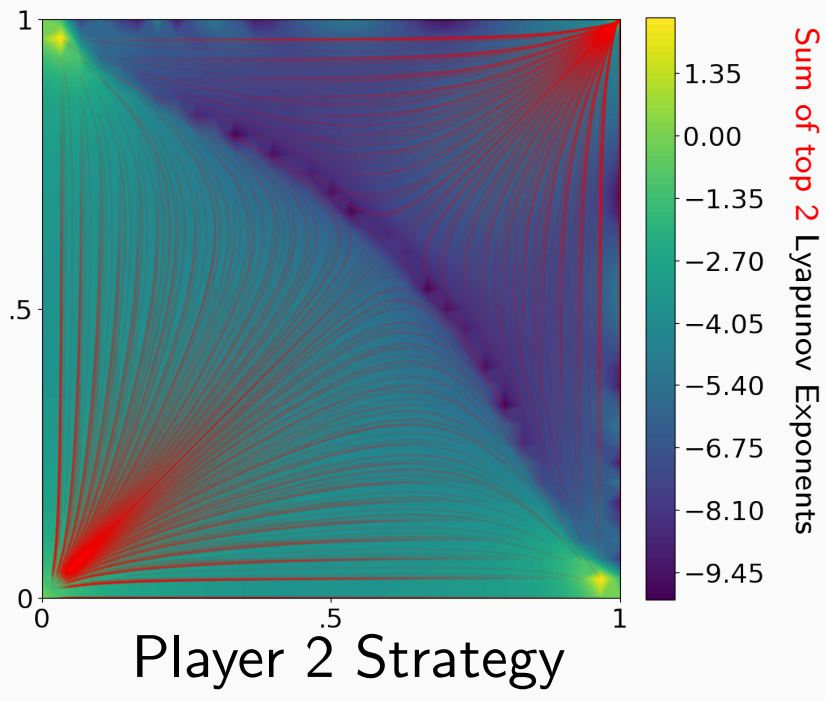
- Cool connection: Kolmogorov-Sinai entropy is $\approx$ # symbols for optimal coding of the particle trajectory. This is $\leq$ sum of positive exponents.

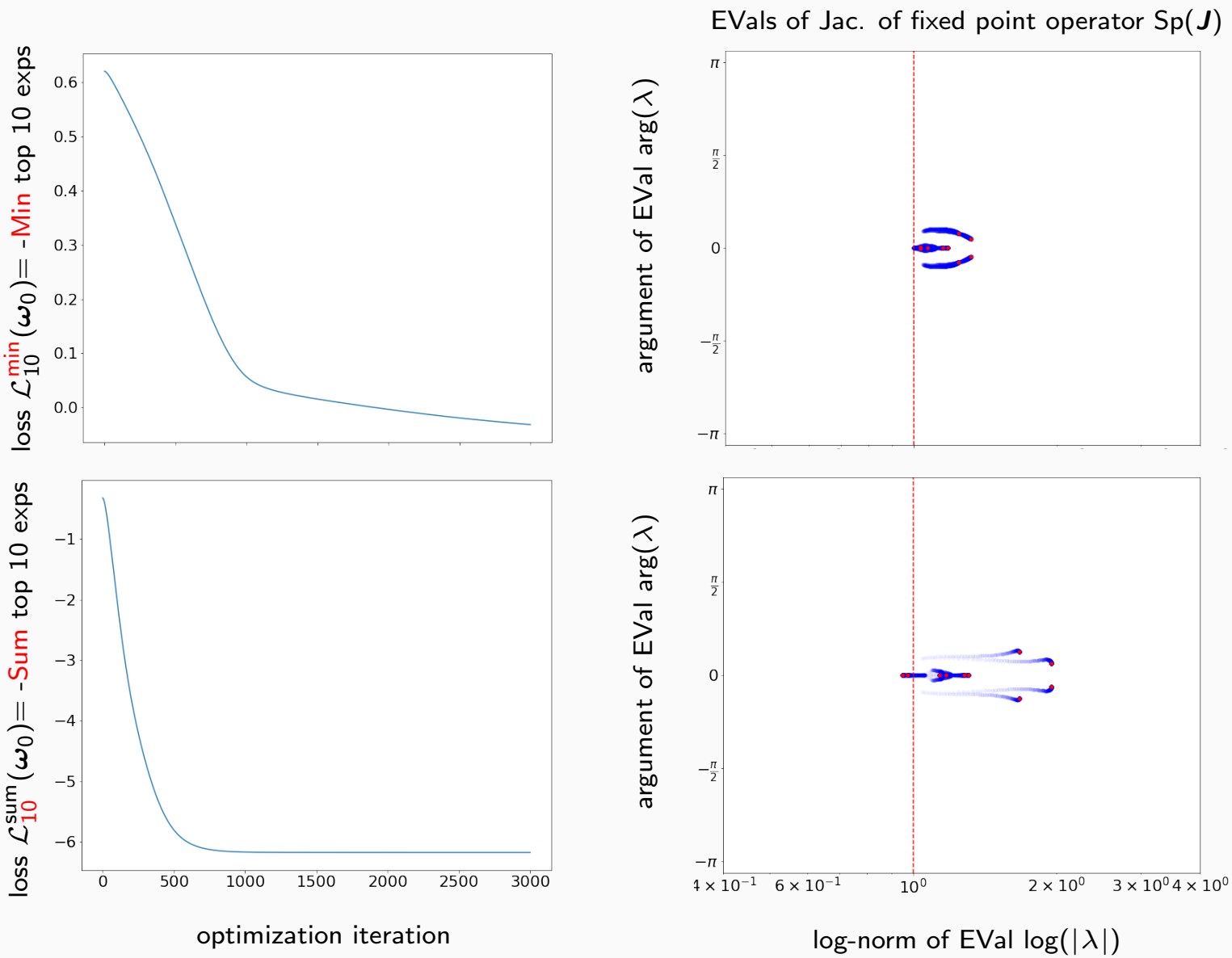
Connections to Kolmogorov-Sinai Entropy





- Local maxima – not saddles – allow trajectory separation in all directions here.

Trajectory Separation in Multiple Directions



Scaling up to GANs

Init scale, step size	Max Lyap Coeff	Ensemble log-prob
0.001, 1.0	0.952 ± 0.834	$-16\,342 \pm 817$
0.1, 1.0	6.485 ± 1.155	$-13\,691 \pm 1317$
10.0, 1.0	0.053 ± 0.128	$-46\,659 \pm 26\,793$
0.001, 0.1	0.849 ± 0.765	$-12\,321 \pm 126$
0.1, 0.1	6.571 ± 0.953	$-10\,846 \pm 256$
10.0, 0.1	-0.012 ± 0.014	$-23\,459 \pm 12\,693$

- Goal: Exponent calculation is scalable to larger problems.
- Mean and std. dev. (over 10 runs) of the max 10-step exponent and the log-prob. of an ensemble of 5 GANs branching in the top 5 directions at the init.
- Higher exponent then better ensemble performance?
- Each branch's GAN may be learning a different part of the data distribution.

Estimating EVecs in Single Objective

	MNIST Accuracy	
# HVP Evaluations	Our method	Method from RR
10 000	19%(+8%)	11%
100 000	89%(+6%)	83%
1 000 000	93%(+2%)	91%

- How many HVP evaluations to reach different MNIST classifier accuracies by following EVecs, repeating the exp. in RR's Fig. 4.
- Not designed to train a single strong classifier! But, to test our ability to efficiently follow negative EVecs.
- Takeaway: Estimate largest EVecs of Jacobian of fixed-point op. is an efficient way to estimate most negative EVecs of Hessian, and generalizes idra to other setups.

Thanks!

Jonathan Lorraine

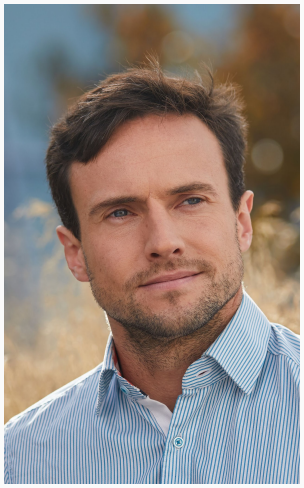
Paul Vicol

Jack Parker-Holder

Tal Kachman

Luke Metz

Jakob Foerster



Connecting to my other work

Hyperparameter Optimization is Nested Optimization

- $\mathcal{L}_T$ is training loss.
- $\mathcal{L}_V$ is validation loss.
- $\mathbf{w}$ are (elementary or NN) parameters.
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- Want to optimize validation loss using optimal parameters:

$$\mathcal{L}_V^*(\boldsymbol{\lambda}) := \mathcal{L}_V(\mathbf{w}^*(\boldsymbol{\lambda}))$$

Hypergradient Decomposition

- The gradient is difficult to compute because we may need the **Jacobian of the best-response**, which could require differentiating through optimization:

$$\underbrace{\frac{\partial \mathcal{L}_V^*(\boldsymbol{\lambda})}{\partial \boldsymbol{\lambda}}}_{\text{hypergradient}} = \frac{\partial \mathcal{L}_V(\mathbf{w}^*(\boldsymbol{\lambda}))}{\partial \mathbf{w}^*(\boldsymbol{\lambda})} \frac{\partial \mathbf{w}^*(\boldsymbol{\lambda})}{\partial \boldsymbol{\lambda}}$$

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$$\frac{\partial \mathcal{L}_V^*}{\partial \boldsymbol{\lambda}} = \frac{\partial \mathcal{L}_V}{\partial \mathbf{w}} \frac{\partial \mathbf{w}^*}{\partial \boldsymbol{\lambda}}$$

IFT Hypergradient [8]

Theorem (Implicit Function Theorem)

If $\frac{\partial \mathcal{L}_T}{\partial \mathbf{w}}|_{\boldsymbol{\lambda}', \mathbf{w}'} = 0$ *for some* $(\boldsymbol{\lambda}', \mathbf{w}')$ *and regularity conditions are satisfied, then surrounding* $(\boldsymbol{\lambda}', \mathbf{w}')$ *there exists a function* $\mathbf{w}^*(\boldsymbol{\lambda})$ *s.t.* $\frac{\partial \mathcal{L}_T}{\partial \mathbf{w}}|_{\boldsymbol{\lambda}, \mathbf{w}^*(\boldsymbol{\lambda})} = 0$ *and*

$$\left.\frac{\partial \mathbf{w}^*}{\partial \boldsymbol{\lambda}}\right|_{\boldsymbol{\lambda}'} = -\left[\frac{\partial^2 \mathcal{L}_T}{\partial \mathbf{w} \partial \mathbf{w}}\right]^{-1} \left.\frac{\partial^2 \mathcal{L}_T}{\partial \mathbf{w} \partial \boldsymbol{\lambda}}\right|_{\boldsymbol{\lambda}', \mathbf{w}^*(\boldsymbol{\lambda}')}$$

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So,

$$\begin{aligned}\left.\frac{\partial \mathcal{L}_V^*}{\partial \boldsymbol{\lambda}}\right|_{\boldsymbol{\lambda}'} &= \frac{\partial \mathcal{L}_V}{\partial \mathbf{w}} \frac{\partial \mathbf{w}^*}{\partial \boldsymbol{\lambda}} \\ &= -\frac{\partial \mathcal{L}_V}{\partial \mathbf{w}} \left[\frac{\partial^2 \mathcal{L}_T}{\partial \mathbf{w} \partial \mathbf{w}}\right]^{-1} \left.\frac{\partial^2 \mathcal{L}_T}{\partial \mathbf{w} \partial \boldsymbol{\lambda}}\right|_{\boldsymbol{\lambda}', \mathbf{w}^*(\boldsymbol{\lambda}')}\end{aligned}$$

Learned Data Augmentation

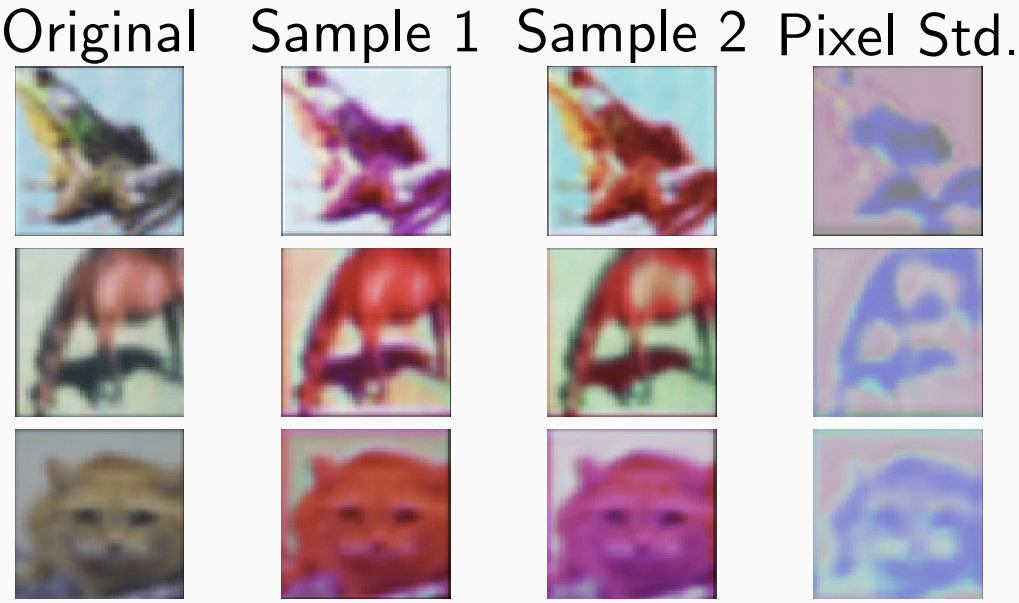

Figure 2: The original image is on the left, followed by two augmented samples and the standard deviation of the pixel intensities from the augmentation distribution.

The hyperparameters are weights in a U-Net [9], which learns a stochastic data augmentation: $\mathbf{x}' = U_{\boldsymbol{\lambda}}(\mathbf{x}, \epsilon), \epsilon \sim \mathcal{N}(0, I), \mathbf{x} \sim \mathcal{D}$.

IFT for meta-learning/pre-training [10]

- What if we want to tune pre-training parameters? Or have a meta-learning setup with more than 2 levels?
- Well, we can use the IFT for each level.

Hyperparameter Optimization through Hypernetworks [6, 7]

- Remember that:

$$\mathbf{w}^*(\boldsymbol{\lambda}) = \arg\min_{\mathbf{w}} \mathcal{L}_T(\boldsymbol{\lambda}, \mathbf{w})$$

- Idea: approximate the response with a neural network. In this case, a hypernetwork with parameters ϕ:

$$\mathbf{w}^*(\boldsymbol{\lambda}) \approx \hat{\boldsymbol{w}}_\phi(\boldsymbol{\lambda})$$

1st Order Optimization in Differentiable Games

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$$\frac{\partial \mathcal{L}_V^*}{\partial \boldsymbol{\lambda}} = \left(\frac{\partial \mathcal{L}_V}{\partial \boldsymbol{\lambda}} + \frac{\partial \mathcal{L}_V}{\partial \mathbf{w}} \frac{\partial \mathbf{w}^*}{\partial \boldsymbol{\lambda}} \right) \Bigg|_{\boldsymbol{\lambda}, \mathbf{w}^*(\boldsymbol{\lambda})}$$

1st Order Optimization in Differentiable Games

- The **direct gradient** is often identically 0 for hyperparameter optimization.
- If the **direct gradient** available, we can simple use first-order methods.
- These can be much simpler to implement, compute, and analyze.
- Minimax games, $\mathcal{L}_A = -\mathcal{L}_B$, always have a **direct gradient** – ex., GANs.

Complex Momentum [11] - animation

Actual JAX implementation: changes in green

```
mass = .7 + .2j

def momentum(step_size, mass):
  ...
  def update(i, g, state):
    x, velocity = state
    velocity = mass * velocity + g
    x = x - jnp.real(step_size(i)*velocity)
    return x, velocity
  ...
```

- Gradient descent in differentiable games (like GANs) rotates around solutions.
- We solve this with a simple trick: complex momentum damps the oscillations.

References

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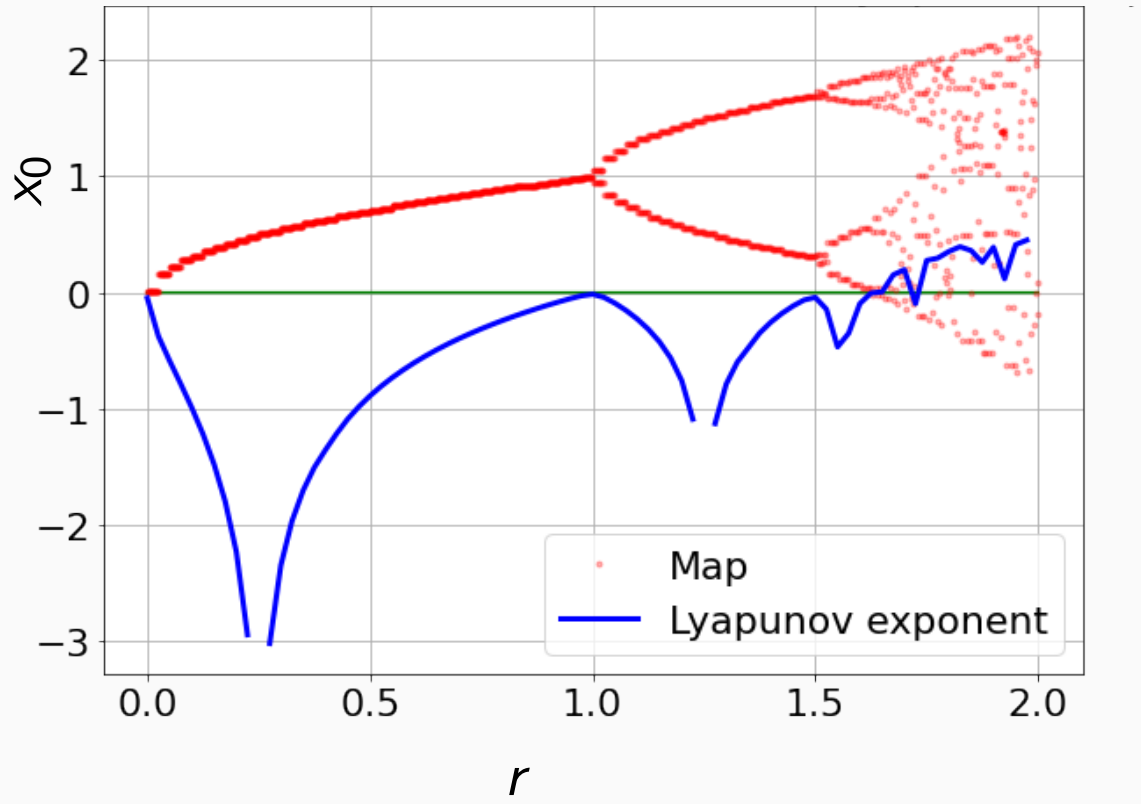
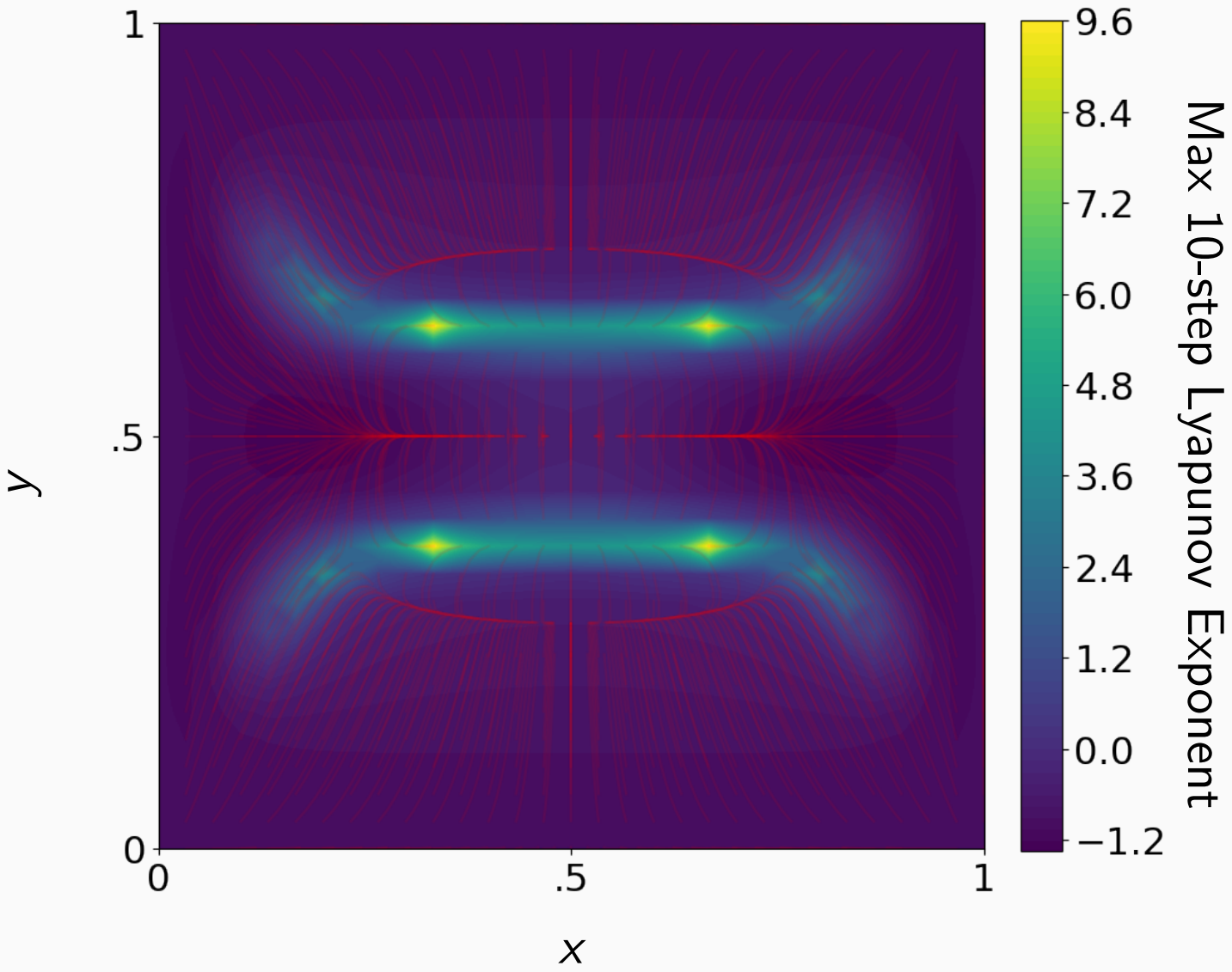
Extra Slides

The Logistic Map Example



- A canonical 1-dimensional example for bifurcations:
  $x(t+1) = x(t) + r + x(t)^2$

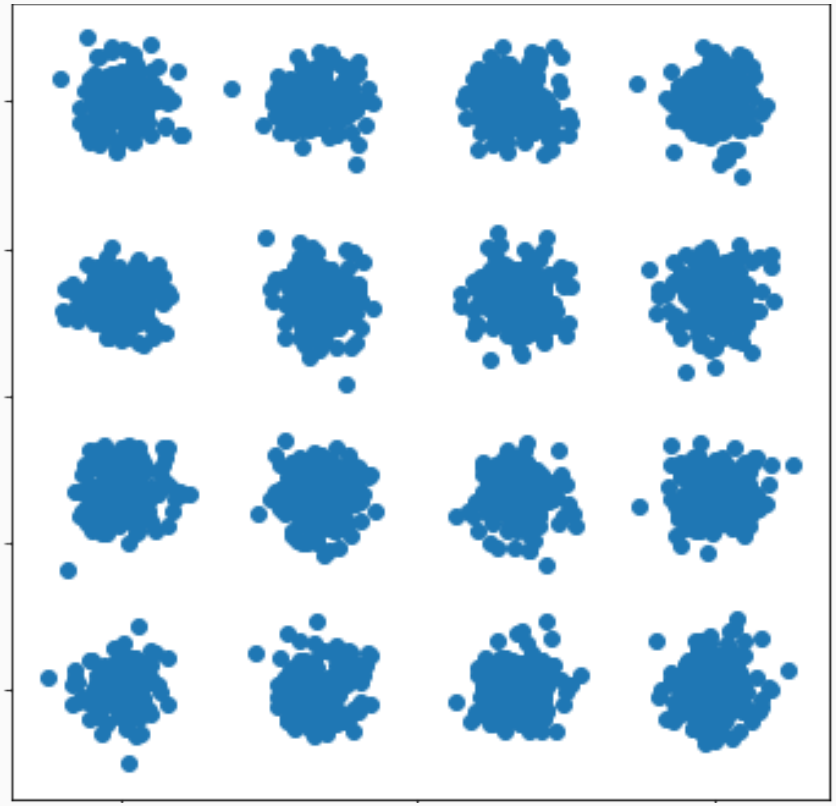
Single-objective Optimization Example



Branching Optimization Tree Search– RR/GRR changes in red

1: Select optimization parameters α
2: Find starting parameters $\boldsymbol{\omega}^{start} = \text{FindStartingPoint}(\alpha)$
3: Initialize a branch $\psi^{init} = \text{InitBranch}(\boldsymbol{\omega}^{start}, \alpha)$
4: Initialize the set of branches $\mathcal{B} = \text{SplitBranch}(\psi^{init})$
5: Initialize the set of solutions $\mathcal{S} = \emptyset$
6: **while** Branches $\mathcal{B}$ non-empty **do**
7: $\quad \psi, \mathcal{B} = \text{ChooseBranch}(\mathcal{B})$
8: $\quad \boldsymbol{\omega}^* = \text{Optimize}(\psi.\boldsymbol{\omega}, \psi.\alpha)$ # Optimize our parameters
9: $\quad$ **if** $\text{VerifySolution}(\boldsymbol{\omega}^*)$ **then**
10: $\quad\quad \mathcal{S} = \mathcal{S} \cup \{\boldsymbol{\omega}^*\}$
11: $\quad$ Make new branch to split $\psi' = \text{copy}(\psi)$
12: $\quad$ Store the optimized parameters $\psi'.\textit{parameters} = \boldsymbol{\omega}^*$
13: $\quad$ **if** $\text{ContinueBranching}(\psi')$ **then**
14: $\quad\quad \mathcal{B} = \mathcal{B} \cup \text{SplitBranch}(\psi')$
15: **return** $\mathcal{S}$

GAN Samples



- Ground truth samples for our GAN Mixture of Gaussian experiment.
- Designed to test mode dropping.