Optimization Methods for Parameter Identification in Settings with Only Partial Knowledge

Ph.D. Defense

Aleksei Sholokhov

Thursday 8th June, 2023

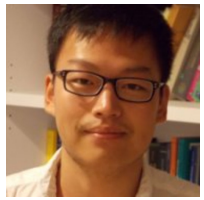
APPLIED MATHEMATICS

UNIVERSITY *of* WASHINGTON

Plan of the Defense

Plan of the Defense





Sparse Relaxed Regularized Regression for Linear Mixed-Effect Models
Together with Aleksandr Aravkin, James Burke, Damian Santomauro, and Peng Zheng

- "A Relaxation Approach to Feature Selection for Linear Mixed Effects Models"
  submitted to Journal of Computational and Graphical Statistics (JCGS)
- "Analysis of Relaxation Methods for Feature Selection in Mixed Effects Models"
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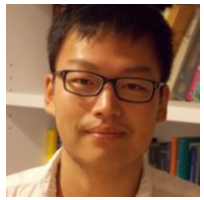


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Together with Hassan Mansour, Saleh Nabi, and Yuying Liu

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  SIAM ADS 2023, arXiv:2211.09419
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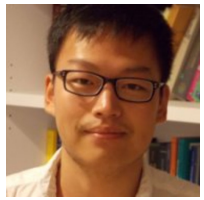





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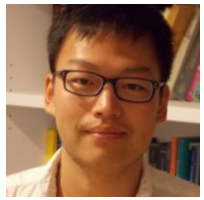





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$\mathcal{MSR}3$ – Sparse Relaxed Regularized Regression for Linear Mixed-Effect Models

Research Objectives and Plan of the Talk

Objectives:

- Extend $\mathcal{SR}3$ relaxation to linear mixed-effects models - $\mathcal{MSR}3$ (see[1]).
- Develop theoretical foundations for it (see[2]).
- Implement it as a `scikit-learn`-compatible Python package – `pysr3` (see[3]).

Plan of the Talk:

1. Proximal Gradient Descent (PGD) for Linear Mixed-Effects Models (LMEs)
2. $\mathcal{MSR}3$ – PGD on $\mathcal{SR}3$-relaxation for LMEs
3. $\mathcal{MSR}3$-fast – practical algorithm for feature selection

[1] Sholokhov, J. V. Burke, et al., A Relaxation Approach to Feature Selection for Linear Mixed Effects Models.

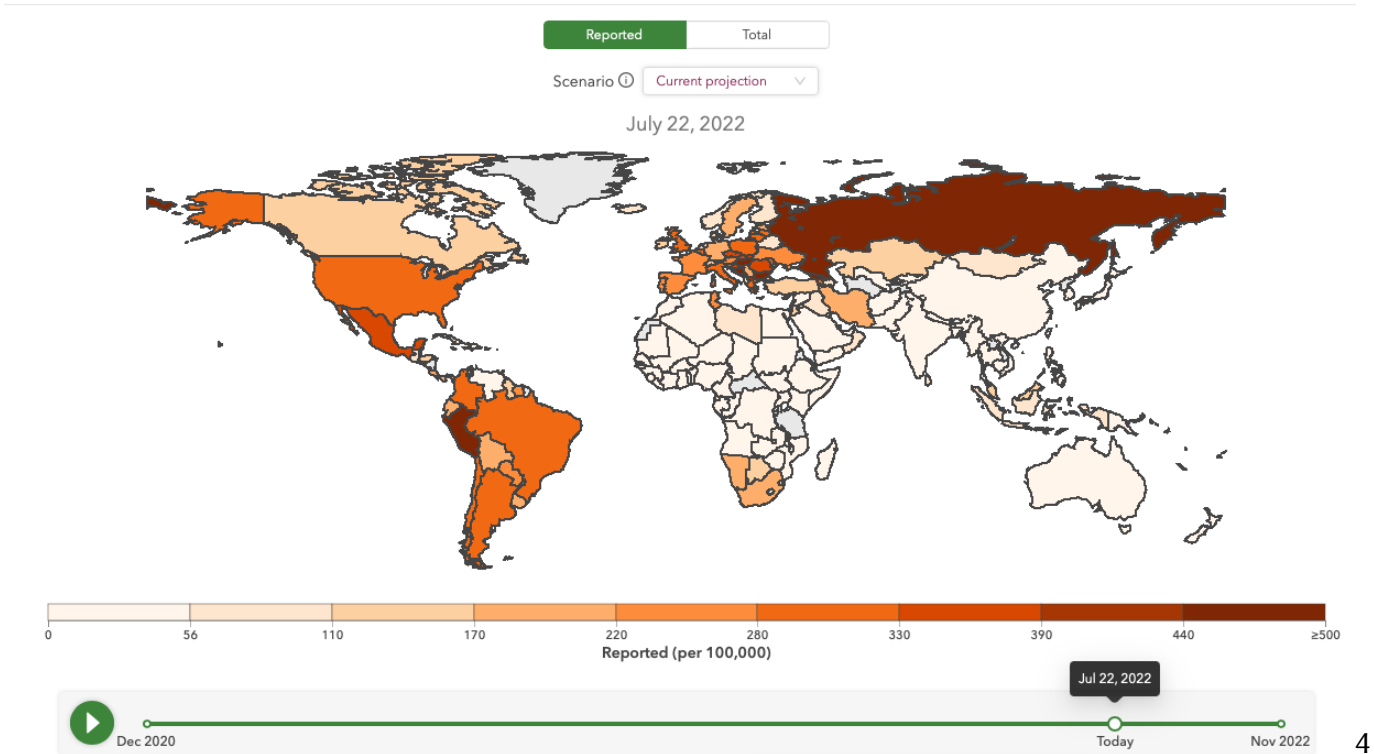
[2] Aravkin et al., Analysis of Relaxation Methods for Feature Selection in Mixed Effects Models.

[3] Sholokhov, Zheng, and Aravkin, "pysr3: A Python Package for Sparse Relaxed Regularized Regression".

Mixed-Effect Models

Mixed-effect models

- Used for analyzing **combined data** across a range of **groups**.
- **Borrow strength** across groups to estimate key statistics.
- Use covariates to separate the **population variability** from the **group variability**.



[4]

[4] Picture is taken from covid19.healthdata.org

Linear Mixed-Effect (LME) Models

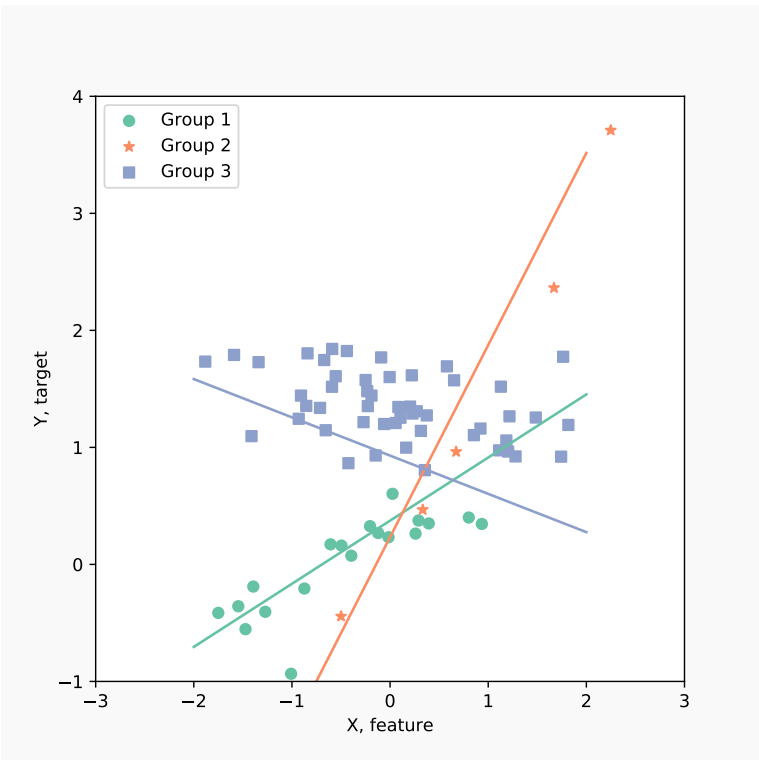
Dataset: m groups (X_i, Z_i, y_i), $\quad i = 1, \ldots m$, each has n_i observations

- $X_i \in \mathbb{R}^{n_i \times p}$ – group i design matrix for fixed features
- $Z_i \in \mathbb{R}^{n_i \times q}$ – group i design matrix for random features
- $y_i \in \mathbb{R}^{n_i}$ – group i observations
- $u_i \in \mathbb{R}^{q}$ – random effects
- $\Gamma \in \mathbb{R}^{q \times q}$ – covariance matrix of random effects, often $\Gamma = \mathrm{diag}(\gamma)$
- $\Lambda_i \in R^{n_i \times n_i}$ – covariance matrix for observation noise

Model:

$$y_i = X_i\beta + Z_i u_i + \varepsilon_i$$
$$\varepsilon_i \sim \mathcal{N}(0, \Lambda_i)$$
$$u_i \sim \mathcal{N}(0, \Gamma)$$

Unknowns: β, u_i, γ, sometimes Λ_i.



Negative Log-Likelihood for Mixed-Effect Models

Optimization problem:

$$\mathcal{FS}-\mathcal{LME} \qquad \min_{\beta\in\mathbb{R}^p,\,\gamma\in\mathbb{R}_+^q} \mathcal{L}(\beta,\gamma)+R(\beta,\gamma) \tag{1}$$

Where $\mathcal{L}$:

$$\begin{aligned}\mathcal{L}(\beta,\gamma) = \sum_{i=1}^{m} \frac{1}{2}(y_i - X_i\beta)^T(Z_i\Gamma Z_i^T + \Lambda_i)^{-1}(y_i - X_i\beta)+ \\ + \frac{1}{2}\log\det(Z_i\Gamma Z_i^T + \Lambda_i), \quad \Gamma = \operatorname{diag}((\gamma))\end{aligned} \tag{2}$$

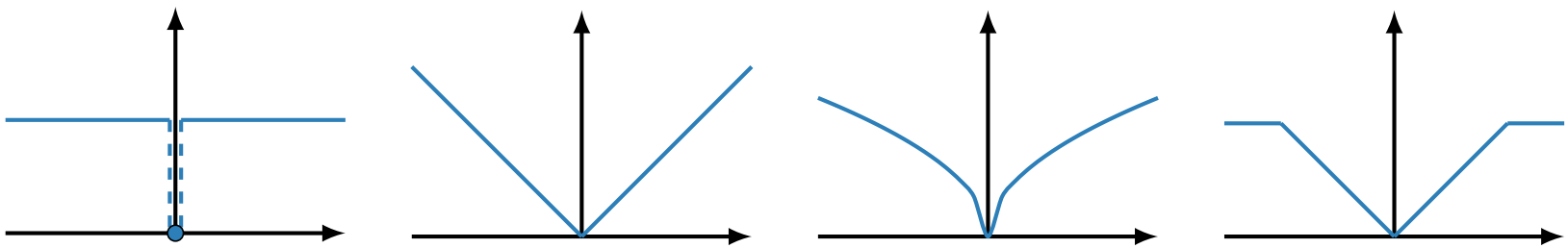
- $\mathcal{L}(\beta,\gamma)$ is smooth on its domain, quadratic w.r.t. β and $\bar{\eta}$-weakly-convex w.r.t. γ.
- $R(\beta,\gamma)$ is closed, proper, with easily computed *prox operator*

Regularization

$R(\beta, \gamma)$ is closed, proper, with easily computed *prox operator*

$$\text{prox}_{\alpha R + \delta_{\mathcal{C}}}(\tilde{\beta}, \tilde{\gamma}) := \underset{(\beta,\gamma)\in\mathcal{C}}{\text{argmin}}\ R(\beta, \gamma) + \frac{1}{2\alpha}\|(\beta, \gamma) - (\tilde{\beta}, \tilde{\gamma})\|_2^2, \tag{3}$$

$$\text{where } \mathcal{C} := \mathbb{R}^p \times \mathbb{R}^q_+$$



(a) ℓ_0 (b) ℓ_1 (c) $\ell_p,\ p = 1/2$ (d) SCAD

Figure: Four commonly-used regularizers which promote sparsity

Proximal Gradient Descent for Feature Selection in MLE

Let

$$x := [\beta, \gamma], \quad \mathcal{C} := \mathbb{R}^p \times \mathbb{R}_+^q \tag{4}$$

Optimization problem $\mathcal{FS} - \mathcal{LME}$:

$$\min_{x \in \mathcal{C}} \mathcal{L}(x) + R(x) \tag{5}$$

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Algorithm: PGD for standard LMEs

$\beta^+ \leftarrow \beta_0, \quad \gamma^+ \leftarrow \gamma_0, \quad \alpha \leftarrow 1/L$ `// Initialization`

$x^+ = [\beta^+, \gamma^+]$;

while making progress **do**

  $x^+ \leftarrow \text{prox}_{\alpha^{-1} R + \delta_{\mathcal{C}}}(x^+ - \alpha \nabla_x \mathcal{L}(x^+))$ `// PGD iterations`

end

return $x^+ = [\beta^+, \gamma^+]$

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Basic Assumptions for the PGD Algorithm[5]:

1. R is a closed proper convex function
2. $\mathcal{L}$ is closed and proper, dom $\mathcal{L}$ convex, dom $R \subset$ *int*(dom $\mathcal{L}$), and $\mathcal{L}$ is L-smooth over *int*(dom $\mathcal{L}$). [×].
3. The problem has an optimal solution[6] with an optimal value $\mathcal{L}^*$

Algorithm converges with backtracking[7].

[5] Beck, First-Order Methods in Optimization, Theorem 10.15.

[6] Aravkin et al., Analysis of Relaxation Methods for Feature Selection in Mixed Effects Models.

[7] J. Burke and Engle, "Line Search and Trust-Region Methods for Convex-Composite Optimization".

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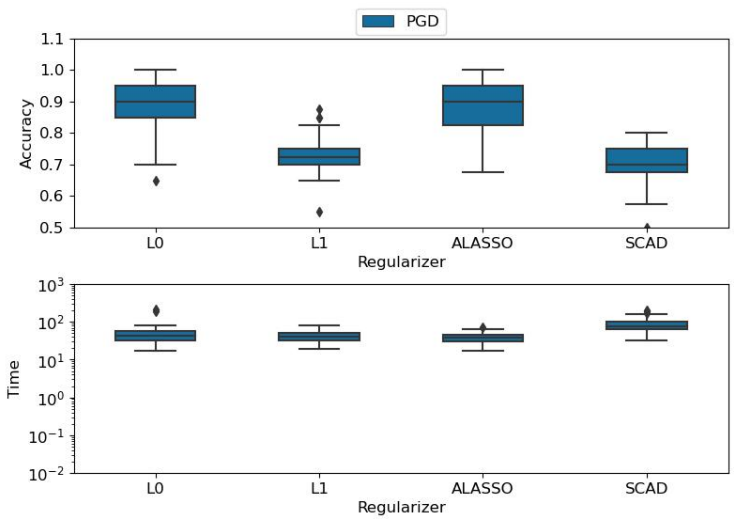
return $x^+ = [\beta^+, \gamma^+]$

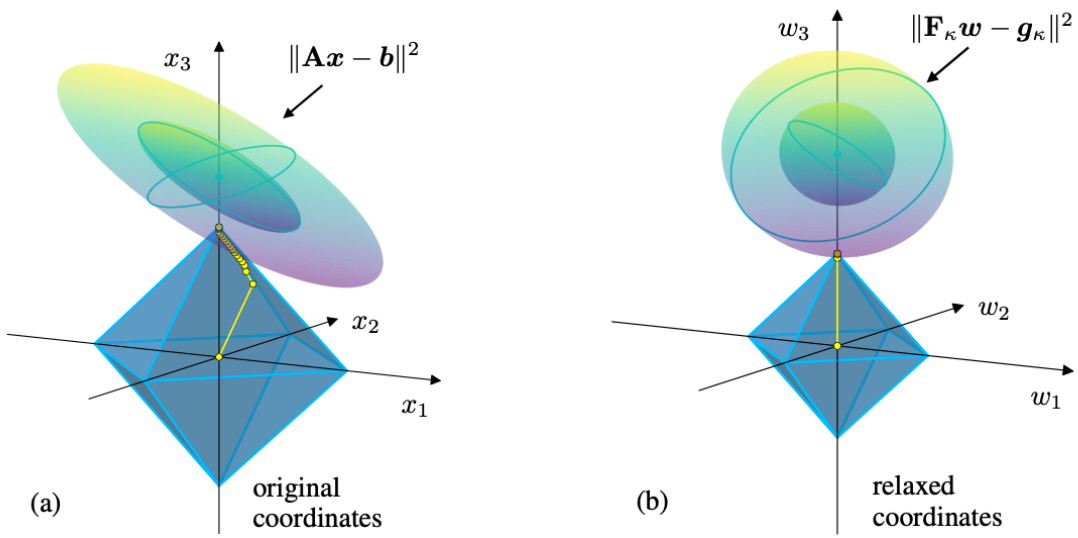
Synthetic Benchmark:

- 100 randomly-generated problems.
- $p = q = 20$.
- $\beta = \gamma = \frac{1}{2}[1, 2, 3, \ldots, 10, 0 \ldots, 0]$
- 9 groups from 3 to 15 observations
- $X_i \sim \mathcal{N}(0, I)^p$, $Z_i = X_i$, $\varepsilon_i \sim \mathcal{N}(0, 0.3^2 I)$
- Golden search for $\lambda \in [0, 10^5]$
- Final model is chosen to maximize BIC



Sparse Relaxed Regularized Regression ($\mathcal{SR}3$)[5]

Original		Decoupled		Value Function
$\min_x f(x) + R(x)$	$\rightarrow$	$\min_{x,w} f(x) + \frac{\eta}{2}\|x - w\|_2^2 + R(w)$	$\rightarrow$	$\min_w v_\eta(w) + R(w)$



[5] Zheng and Aravkin, "Relax-and-split method for nonconvex inverse problems".

SR3-Relaxation for Mixed-Effect Models ($\mathcal{MSR}3$)

Original problem $\mathcal{FS} - \mathcal{LME}$:

$$\min_{x \in \mathcal{C}} \mathcal{L}(x) + R(x) \tag{4}$$

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Decoupled problem:

$$\min_{x, w \in \mathcal{C}} \mathcal{L}(x) + \frac{\eta}{2} ||x - w||_2^2 + R(w) \tag{5}$$

where $w = [\tilde{\beta}, \tilde{\gamma}]$.

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where $w = [\tilde{\beta}, \tilde{\gamma}]$.
By partially minimizing w.r.t. x we get a value function $v_\eta(w)$:

$$v_\eta(w) := \min_{x \in \mathcal{C}} \mathcal{L}(x) + \frac{\eta}{2} ||x - w||_2^2 \tag{6}$$

so $\mathcal{SR}3$-formulation (5) becomes

$$\min_{w \in \mathcal{C}} v_\eta(w) + R(w) \tag{7}$$

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NB: $v_\eta(w)$ is smooth on $\mathcal{C}$ and can be evaluated using Interior Point (IP) method

Value Function of $\mathcal{MSR}3$

$\mathcal{MSR}3$-relaxation replaces the original likelihood $\mathcal{L}$ with a *value function* $v_{\eta,\mu}$:

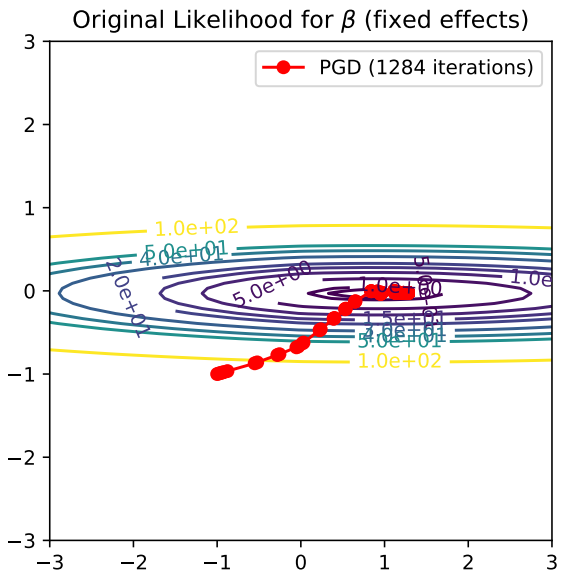
$$v_{\eta,\mu}(w) := \min_{x \in \mathcal{C}} \mathcal{L}(x) + \frac{\eta}{2} \|x - w\|_2^2 + \phi_\mu(x) \tag{8}$$

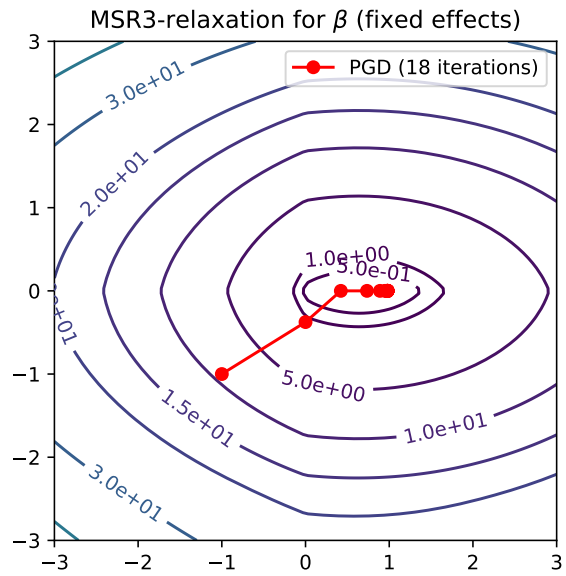
where *perspective mapping* ϕ_μ replaces $\gamma \geq 0$ with a log-barrier

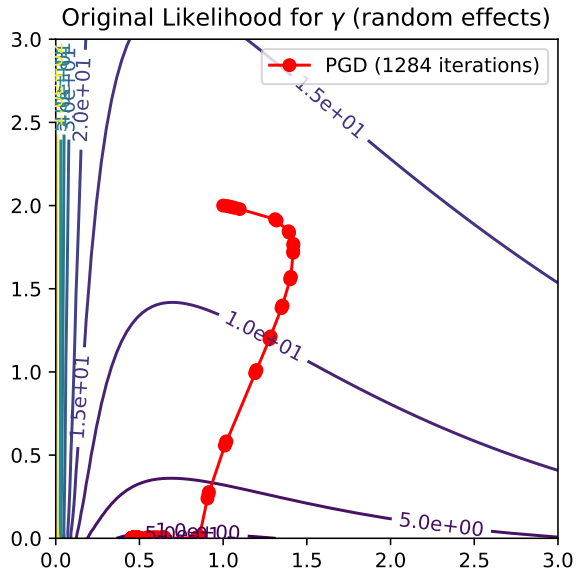
$$\phi_\mu(x) = \phi_\mu(\gamma) := \begin{cases} -\mu \sum_{i=1}^{q} \ln(\gamma_i/\mu), & \mu > 0 \\ \delta_{\mathbb{R}_+^q}(\gamma), & \mu = 0 \\ +\infty, & \mu < 0 \end{cases} \tag{9}$$

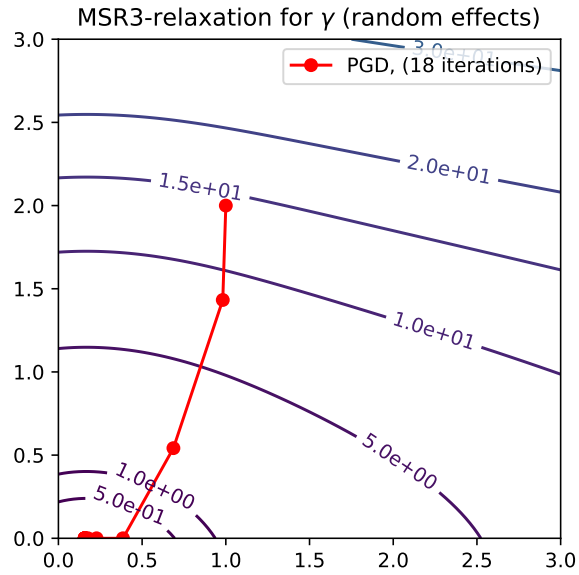
Value Function of $\mathcal{MSR}3$

$$\min_{\beta,\gamma\in\mathcal{C}} \mathcal{L}(\beta,\gamma) + R(\beta,\gamma) \quad \text{vs} \quad \min_{\tilde{\beta},\tilde{\gamma}\in\mathcal{C}} v_{\eta,\mu}(\tilde{\beta},\tilde{\gamma}) + R(\tilde{\beta},\tilde{\gamma})$$









$\mathcal{MSR}3$: Algorithm

Algorithm: PGD for $\mathcal{MSR}3$

$\tilde{\beta}^+ \leftarrow \tilde{\beta}_0, \quad \tilde{\gamma}^+ \leftarrow \tilde{\gamma}_0, \quad \alpha \leftarrow 1/\eta, \quad \eta > \bar{\eta}$ // Initialization

$\tilde{w}^+ := [\tilde{\beta}^+, \tilde{\gamma}^+], \quad x^+ := [\beta, \gamma]$

while making progress in $\tilde{w}$ **do**

  $x^+ \leftarrow$ IP on $\mathcal{L}_{\eta,\mu}(x^+, \tilde{w}^+)$ s.t. $x^+ \in \mathcal{C}$ and $\mu \to 0$ // IP Iterations

  $\nabla_{\tilde{w}} v_{\eta,0}(\tilde{w}^+) \leftarrow \nabla_{\tilde{w}} \mathcal{L}_{\eta,0}(x^+, \tilde{w}^+)$ // Evaluate Gradient of VF

  $\tilde{w}^+ \leftarrow \text{prox}_{\alpha^{-1}R+\delta_{\mathcal{C}}}(\tilde{w}^+ - \alpha \nabla_{\tilde{w}} v_{\eta,0}(\tilde{w}^+))$ // PGD on Value Function

end

return $\tilde{w}^+ = [\tilde{\beta}^+, \tilde{\gamma}^+]$

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end

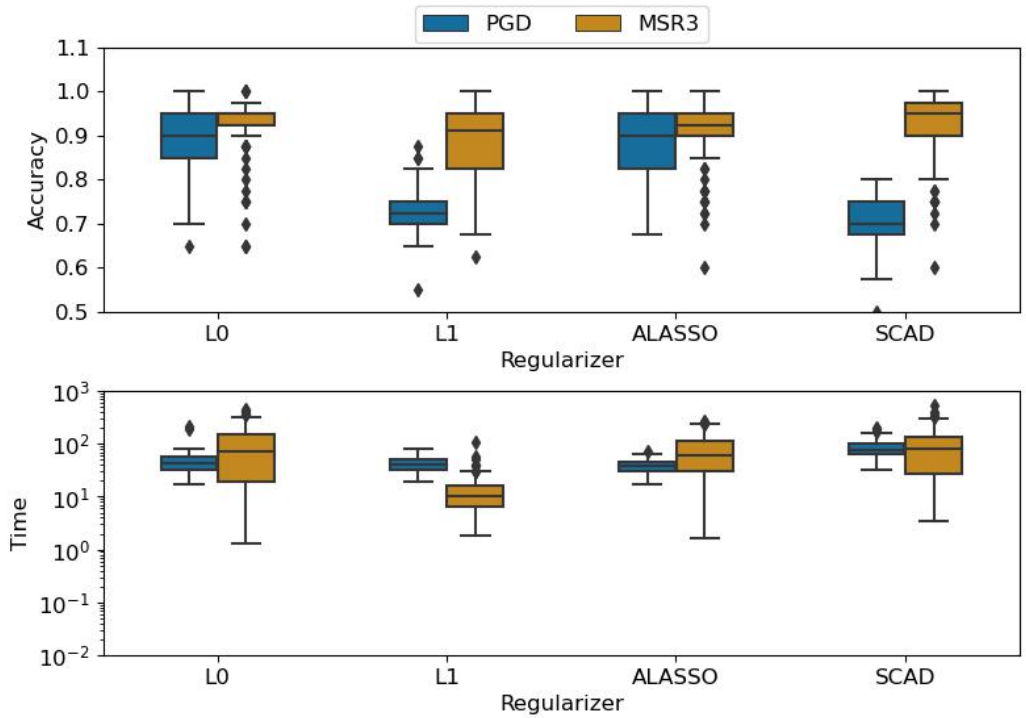
return $\tilde{w}^+ = [\tilde{\beta}^+, \tilde{\gamma}^+]$

Theoretical Results[6]:

1. When $\eta > \bar{\eta}$ the problem has an optimal solution Φ^* (**Theorem 5**)
2. $v_{\eta,\mu}$ is well-defined (**Theorem 5**) and continuously differentiable (**Theorem 10**)
3. When R is 1-coercive $\nabla v_{\eta,\mu}$ is locally $\widetilde{L}$-continuous (**Theorem 14**)
4. Algorithm converges to a stationary point of $v_{\eta,\mu}$ (**Theorem 15**)
5. As $\mu \to 0$ (**Theorem 6**) or $\eta \to \infty$ (**Theorem 7**), cluster points of solutions to $\mathcal{MSR}3$ are FOSPs for $\mathcal{FS} - \mathcal{LME}$

[6] Aleksandr Aravkin et al. Analysis of Relaxation Methods for Feature Selection in Mixed Effects Models. 2022. arXiv: 2209.10575 [stat.ME].

$\mathcal{MSR3}$: Results



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  $\nabla_{\tilde{w}} v_{\eta,0}(\tilde{w}^+) \leftarrow \nabla_{\tilde{w}} \mathcal{L}_{\eta,0}(x^+, \tilde{w}^+)$ // Evaluate Gradient

  $\tilde{w}^+ \leftarrow \mathrm{prox}_{\alpha^{-1} R + \delta_{\mathcal{C}}}(\tilde{w}^+ - \alpha \nabla_{\tilde{w}} v_{\eta,0}(\tilde{w}^+))$ // PGD on Value Function

end

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  $\nabla_{\tilde{w}} v_{\eta,0}(\tilde{w}^+) \leftarrow \nabla_{\tilde{w}} \mathcal{L}_{\eta,0}(x^+, \tilde{w}^+)$ // Evaluate Gradient

  $\tilde{w}^+ \leftarrow \mathrm{prox}_{\alpha^{-1} R + \delta_{\mathcal{C}}}(\tilde{w}^+ - \alpha \nabla_{\tilde{w}} v_{\eta,0}(\tilde{w}^+))$ // PGD on Value Function

end

return $\tilde{w}^+ = [\tilde{\beta}^+, \tilde{\gamma}^+]$

Key Observation: $\nabla_{\tilde{w}} v(\tilde{w})$ does not need to be evaluated exactly. We only need to come close enough to the central path.

$\mathcal{MSR}3$-fast: Algorithm

Algorithm: $\mathcal{MSR}3$-fast

$\tilde{\beta}^+ \leftarrow \tilde{\beta}_0, \quad \tilde{\gamma}^+ \leftarrow \tilde{\gamma}_0, \quad \alpha \leftarrow 1/\eta, \quad \eta > \bar{\eta}$ // Initialization

$\tilde{w}^+ := [\tilde{\beta}^+, \tilde{\gamma}^+], \quad x^+ := [\beta, \gamma]$

while making progress **do**

  while not close enough to the central path **do**

    $x^+ \leftarrow$ IP iteration on $\mathcal{L}_{\eta,\mu}(x^+, \tilde{w}^+)$ s.t. $x^+ \in \mathcal{C}$ // IP Iterations

  end

  Decrease μ

  $\nabla_{\tilde{w}} v_{\eta,\mu}(\tilde{w}^+) \leftarrow \nabla_{\tilde{w}} \mathcal{L}_{\eta,\mu}(x^+, \tilde{w}^+)$ // Evaluate Gradient

  $\tilde{w}^+ \leftarrow \mathrm{prox}_{\alpha^{-1} R + \delta_{\mathcal{C}}}(\tilde{w}^+ - \alpha \nabla_{\tilde{w}} v_{\eta,\mu}(\tilde{w}^+))$ // PGD on Value Function

end

return $\tilde{w}^+ = [\tilde{\beta}^+, \tilde{\gamma}^+]$

Designing an Algorithm

$G_{\nu,\eta}$ encodes both gradient of a Lagrangian (lines 1-2) and the complementarity condition (line 3):

$$G_{\nu,\eta}((\beta,\gamma,v),(\tilde{\beta},\tilde{\gamma})) := \begin{bmatrix} \nabla_\beta \mathcal{L}(\beta,\gamma) + \eta(\beta-\tilde{\beta}) \\ \nabla_\gamma \mathcal{L}(\beta,\gamma) + \eta(\gamma-\tilde{\gamma}) - v \\ v \bigodot \gamma - \mu \mathbf{1} \end{bmatrix} \tag{10}$$

We apply Newton method to G while geometrically decreasing μ.
Lemma: For every $(\mu,\eta) \in \mathbb{R}_+ \times \mathbb{R}_{++}$,

$$\begin{aligned} &(\hat{\beta},\hat{\gamma}) = \underset{(\beta,\gamma)}{\operatorname{argmin}}\, \mathcal{L}_{\eta,\mu}((\beta,\gamma),(\tilde{\beta},\tilde{\gamma})) \\ &\iff \\ &\exists \hat{v} \in \mathbb{R}_+^q \text{ s.t. } G_{\nu,\eta}((\beta,\gamma,\hat{v}),(\tilde{\beta},\tilde{\gamma})) = 0 \end{aligned} \tag{11}$$

If $\mu > 0$, then $\hat{v} = -\nabla\phi_\mu(\hat{\gamma})$, and if $\mu = 0$, then $\hat{v}$ is the unique KKT multiplier associated with the constraint $0 \leq \gamma$.

$\mathcal{MSR}$3-fast Algorithm

progress $\leftarrow$ **True**; iter = 0;

$\beta^+, \tilde{\beta}^+ \leftarrow \beta_0$; $\gamma^+, \tilde{\gamma}^+ \leftarrow \gamma_0$; $v^+ \leftarrow 1 \in \mathbb{R}^q$; $\mu \leftarrow \frac{{v^+}^T \gamma^+}{10q}$

while iter $<$ max_iter and $\|G_\mu(\beta^+, \gamma^+, v^+)\| >$ tol and progress **do**

  $\beta \leftarrow \beta^+$; $\gamma \leftarrow \gamma^+$; $\tilde{\beta} \leftarrow \tilde{\beta}^+$; $\tilde{\gamma} \leftarrow \tilde{\gamma}^+$

  $[dv, d\beta, d\gamma] \leftarrow \nabla G_\mu((\beta, \gamma, v), (\tilde{\beta}, \tilde{\gamma}))^{-1} G_\mu((\beta, \gamma, v), (\tilde{\beta}, \tilde{\gamma}))$

  $\alpha \leftarrow 0.99 \times \min\left(1, -\frac{\gamma_i}{d\gamma_i}, \forall i : \ d\gamma_i < 0\right)$

  $\beta^+ \leftarrow \beta + \alpha d\beta$; $\gamma^+ = \gamma + \alpha d\gamma$; $v^+ \leftarrow v + \alpha dv$

  if $\|\gamma^+ \odot v^+ - q^{-1}{\gamma^+}^T v^+ \mathbf{1}\| > 0.5 q^{-1}{v^+}^T \gamma^+$ **then** continue;

  else

    $\tilde{\beta}^+ = \text{prox}_{\alpha R}(\beta^+)$; $\tilde{\gamma}^+ = \text{prox}_{\alpha R + \delta_{\mathbb{R}_+}}(\gamma^+)$; $\mu = \frac{1}{10}\frac{{v^+}^T \gamma^+}{q}$

  end

  progress = ($\|\beta^+ - \beta\| \geq$ tol or $\|\gamma^+ - \gamma\| \geq$ tol or $\|\tilde{\beta}^+ - \tilde{\beta}\| \geq$ tol or $\|\tilde{\gamma}^+ - \tilde{\gamma}\| \geq$ tol)

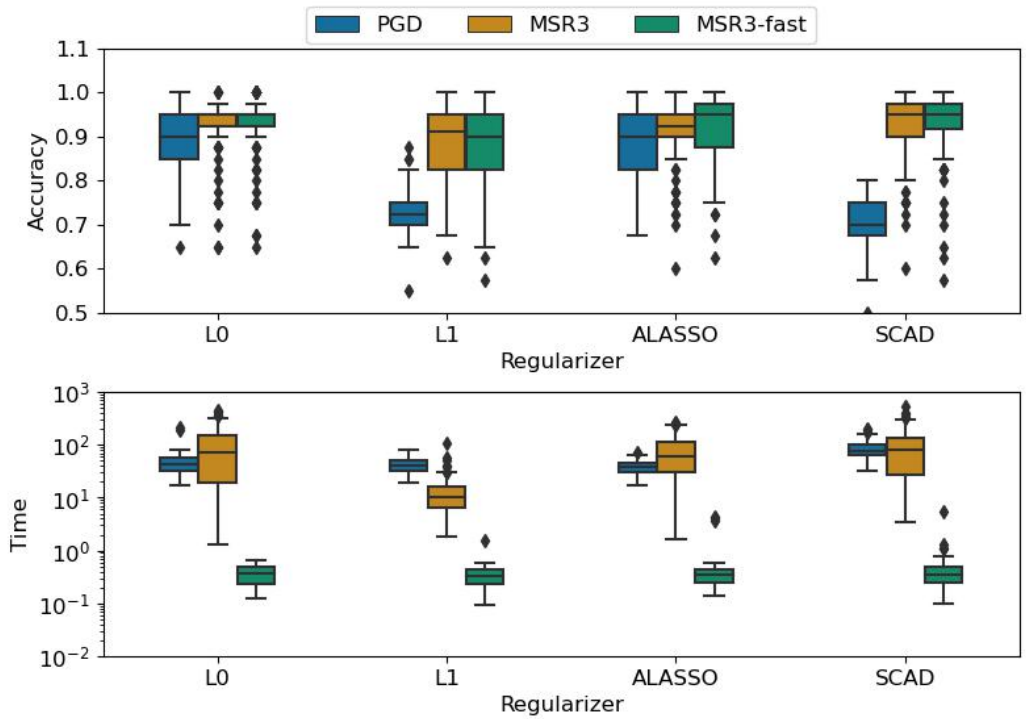
  iter += 1

end

return $\tilde{\beta}^+, \tilde{\gamma}^+$

$\mathcal{MSR}3$-fast: Results

- The number of fixed effects p and random effects q is 20.
- $\beta = \gamma = \frac{1}{2}[1, 2, 3, \ldots, 10, 0 \ldots, 0]$
- 9 groups with sizes $[10, 15, 4, 8, 3, 5, 18, 9, 6]$
- $X_i \sim \mathcal{N}(0, I)^p$, $Z_i = X_i$, $\varepsilon_i \sim \mathcal{N}(0, 0.3^2 I)$
- Each experiment is repeated 100 times.
- Grid-search for $\eta \in [10^{-4}, 10^2]$, golden search for $\lambda \in [0, 10^5]$
- Final model is chosen to maximize BIC



\+ $\mathcal{MSR}3$-relaxation improves feature selection performance of the original likelihood.

\+ $\mathcal{MSR}3$-fast optimization accelerates the compute time by $\sim 10^2$.

– Initialization of η is problem-specific

Comparison to Other Libraries

Algorithm	MSR3-Fast (ℓ_1)	`glmmLasso`[7][8]	`lmmLasso`[9][10]	PGD (ℓ_1)
Accuracy, %	**88**	48	66	73
FE Accuracy, %	**86**	52	47	56
RE Accuracy, %	**91**	45	84	**91**
Time, sec	**0.19**	1.37	11.51	38.39
Iterations, num	34	50	-	7693

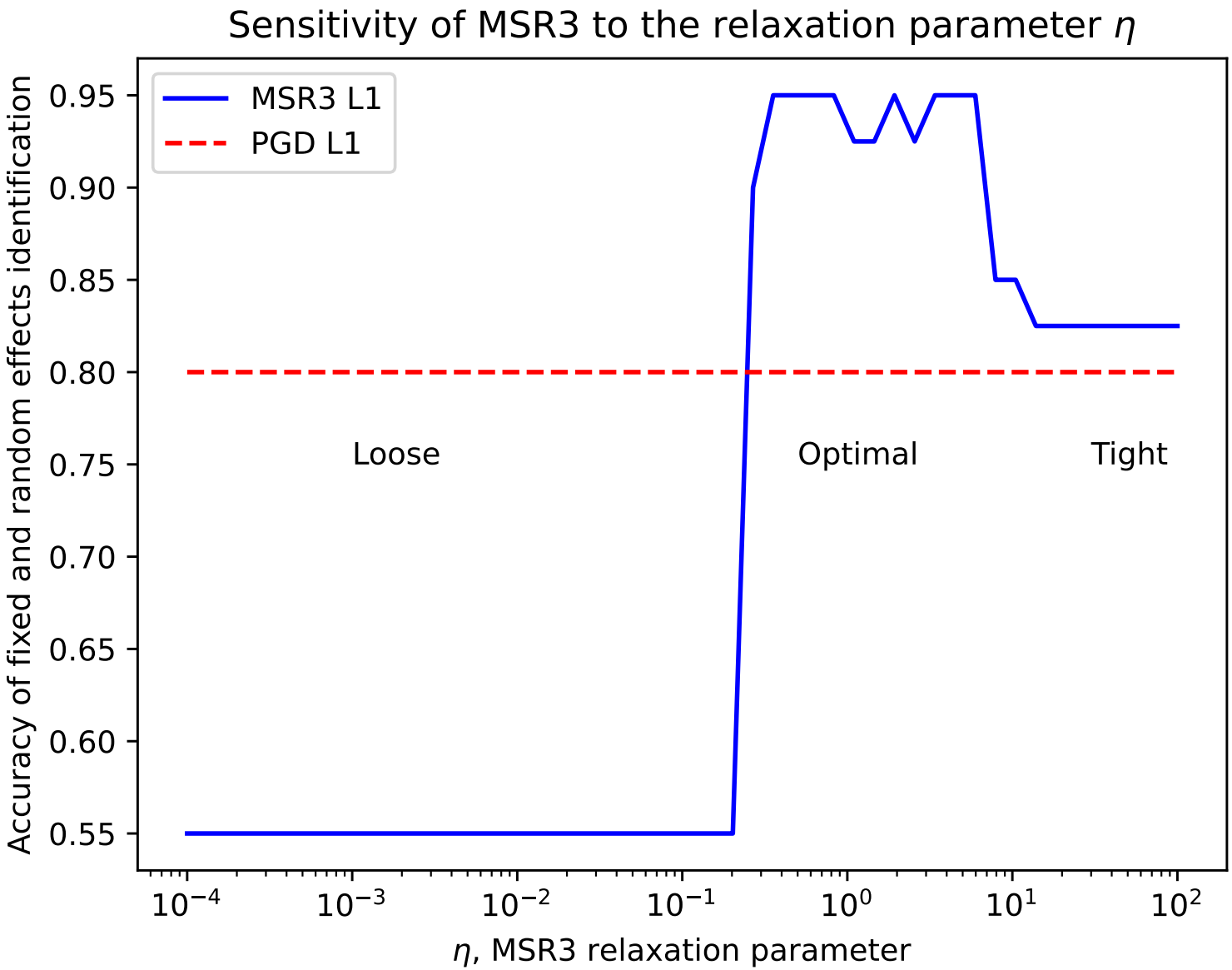
[7] https://rdrr.io/cran/glmmLasso/man/glmmLasso.html

[8] Groll and Tutz, "Variable selection for generalized linear mixed models by L 1-penalized estimation".

[9] https://rdrr.io/cran/lmmlasso/

[10] Schelldorfer, Bühlmann, and DE GEER, "Estimation for high-dimensional linear mixed-effects models using l1-penalization".

Choice of η



ℓ_0-based Covariate Selection for Bullying Study from GBD

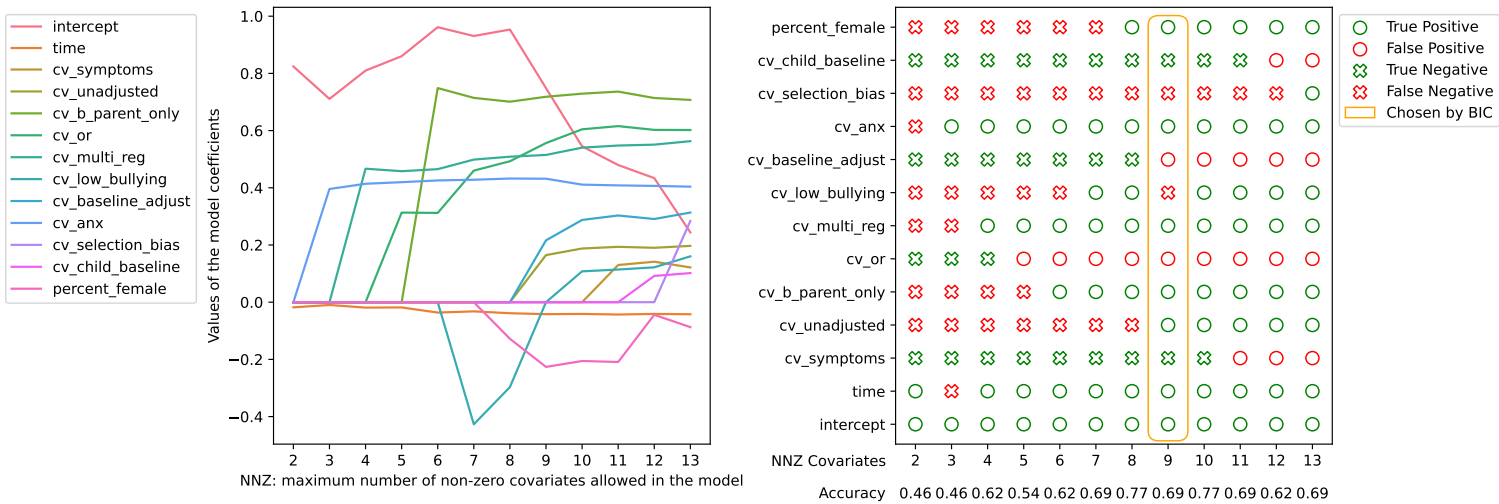
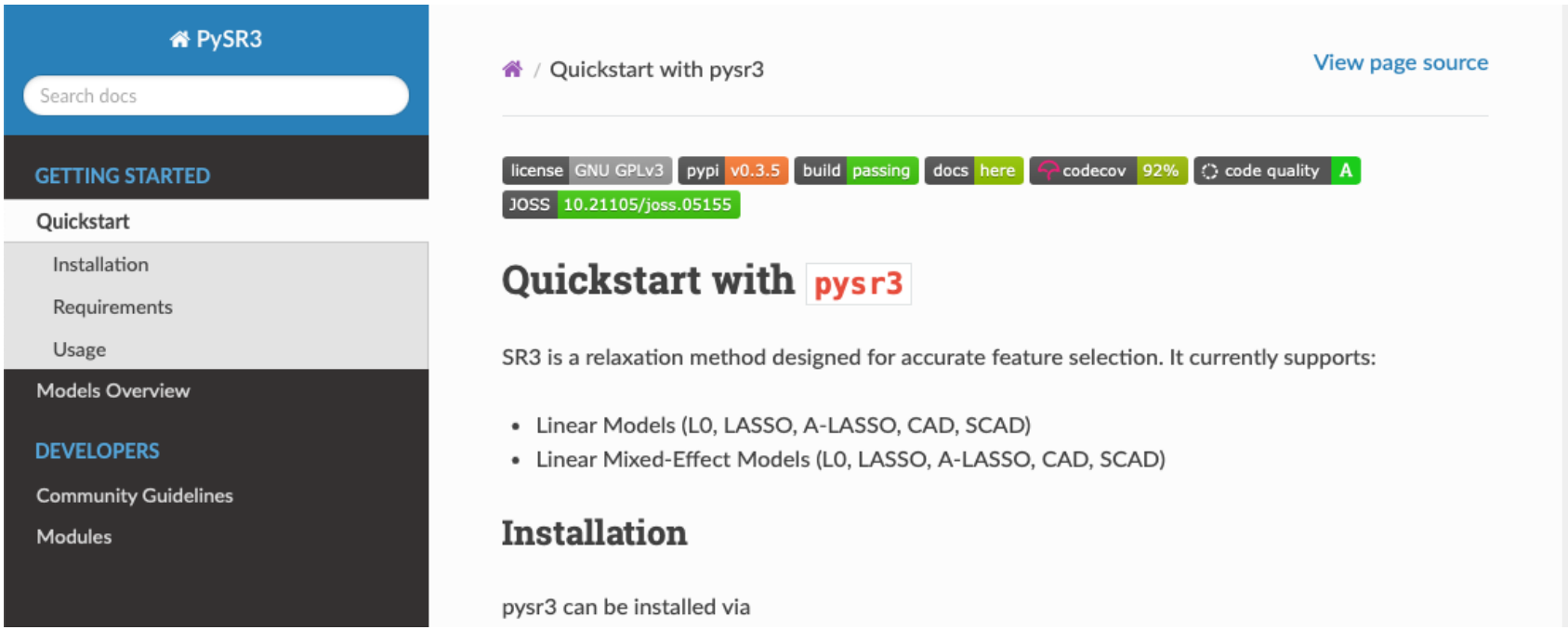


Figure: Fixed and random covariate selection for Bullying dataset[11]. The model selected 9 covariates, 7 of which were historically significant, and did not select 4 covariates, 1 of which was historically significant.

[11] Institute for Health Metrics and Evaluation (IHME). Bullying Victimization Relative Risk Bundle GBD 2020. Seattle, United States of America (USA), 2021.

Software



The code is available on GitHub: https://github.com/aksholokhov/pysr3[12]

- All estimators are fully compatible to `scikit-learn` library.
- Implements SR3 for linear, generalized-linear, and linear mixed-effect models.
- Has tutorials, tests, and documentation.

[12] Aleksei Sholokhov, Peng Zheng, and Aleksandr Aravkin. "pysr3: A Python Package for Sparse Relaxed Regularized Regression". In: Journal of Open Source Software 8.84 (2023), p. 5155.

Physics-Informed Neural ODE (PINODE): Embedding Physics into Models using Collocation Points

Modeling of Physical Systems

[13] Wikipedia: Navier-Stokes

[14] tibco.com

[15] COMSOL Simulations

Modeling of Physical Systems

First-Principle Models

- Require extensive knowledge of the phenomenon
- Require a lot of compute for simulating large-scale phenomena

$$
\begin{cases}
\rho \dfrac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u} \cdot \nabla)\mathbf{u} - \nabla \cdot \boldsymbol{\sigma}(\mathbf{u}, p) = \mathbf{f} & \text{in } \Omega \times (0, T) \\
\nabla \cdot \mathbf{u} = 0 & \text{in } \Omega \times (0, T) \\
\mathbf{u} = \mathbf{g} & \text{on } \Gamma_D \times (0, T) \\
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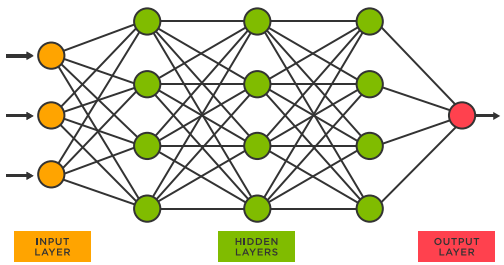
Data-Driven Models

- Require a lot of data
- Often struggle to extrapolate



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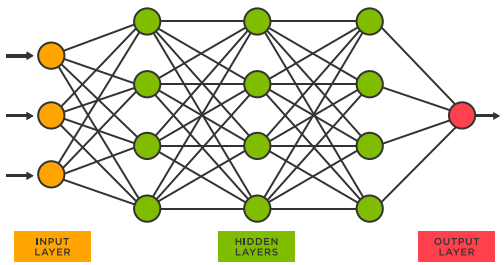
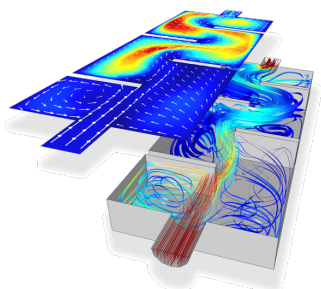


Hybrid Models

- Incorporate elements of both approaches
- Supplement data with knowledge or priors



Pictures sources: [13],[14],[15]

[13] Wikipedia: Navier-Stokes
[14] tibco.com
[15] COMSOL Simulations

Incorporating Knowledge of Physics into Neural Networks

[16] Geiger and Smidt, "e3nn: Euclidean neural networks".

[17] Finzi et al., "Generalizing convolutional neural networks for equivariance to lie groups on arbitrary continuous data".

[18] Chidester, Do, and Ma, Rotation Equivariance and Invariance in Convolutional Neural Networks.

[19] Champion et al., "Data-driven discovery of coordinates and governing equations".

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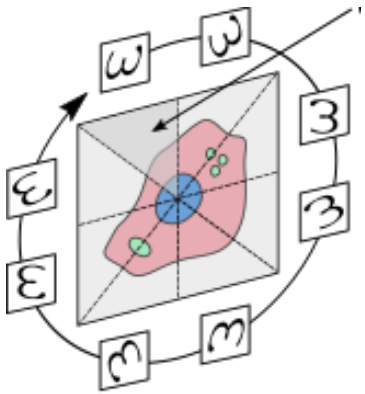

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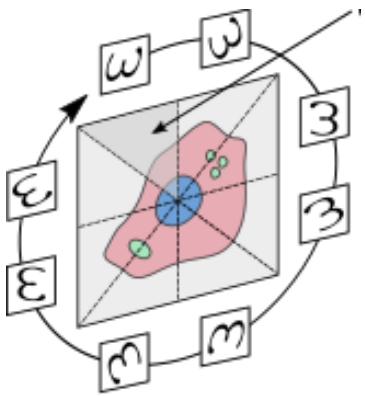

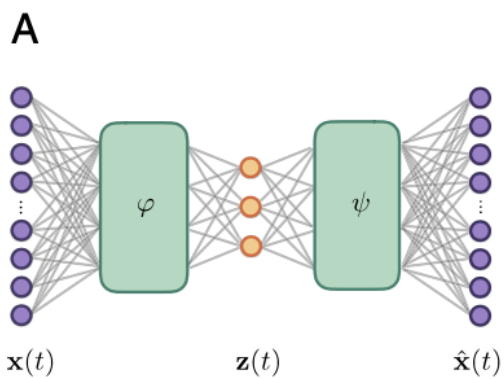

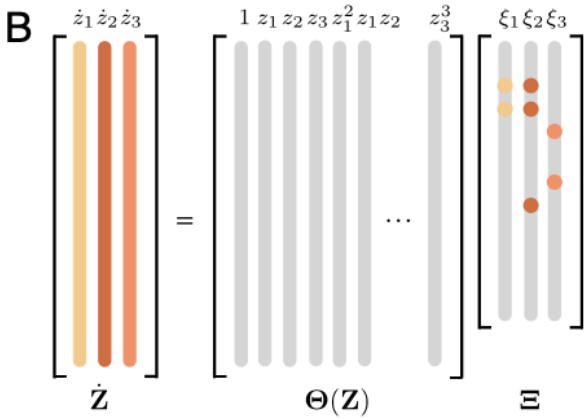

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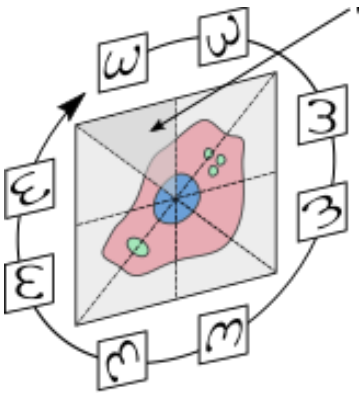
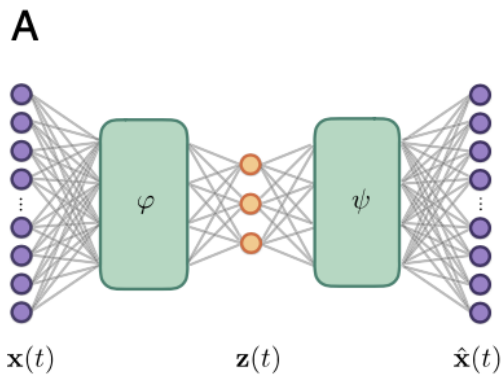
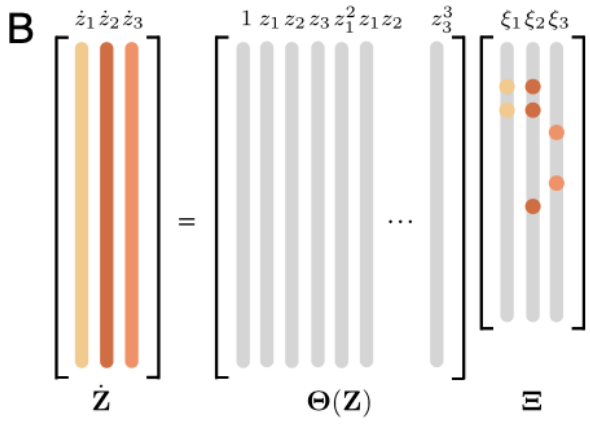
3. **Equation Based:** incorporate first-principle models to aid training of networks: PINNs[21], UDEs[22], *PINODE*







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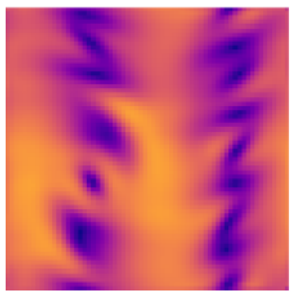
Reduced-Order Models (ROMs)

$$x \in \mathbb{R}^n$$

$$\frac{dx}{dt} = f(x)$$

$$x_0$$



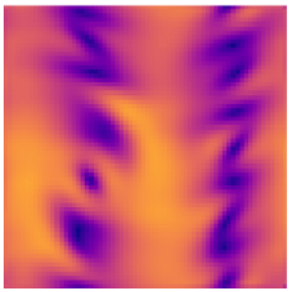
Reduced-Order Models (ROMs)

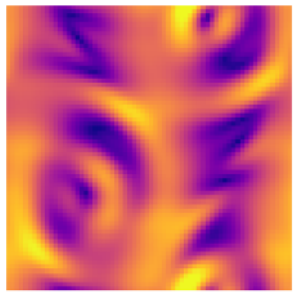
$x \in \mathbb{R}^n$

$$\frac{dx}{dt} = f(x)$$

$$x_T = x_0 + \int_0^T f(x)dt$$

x_0 → x_T





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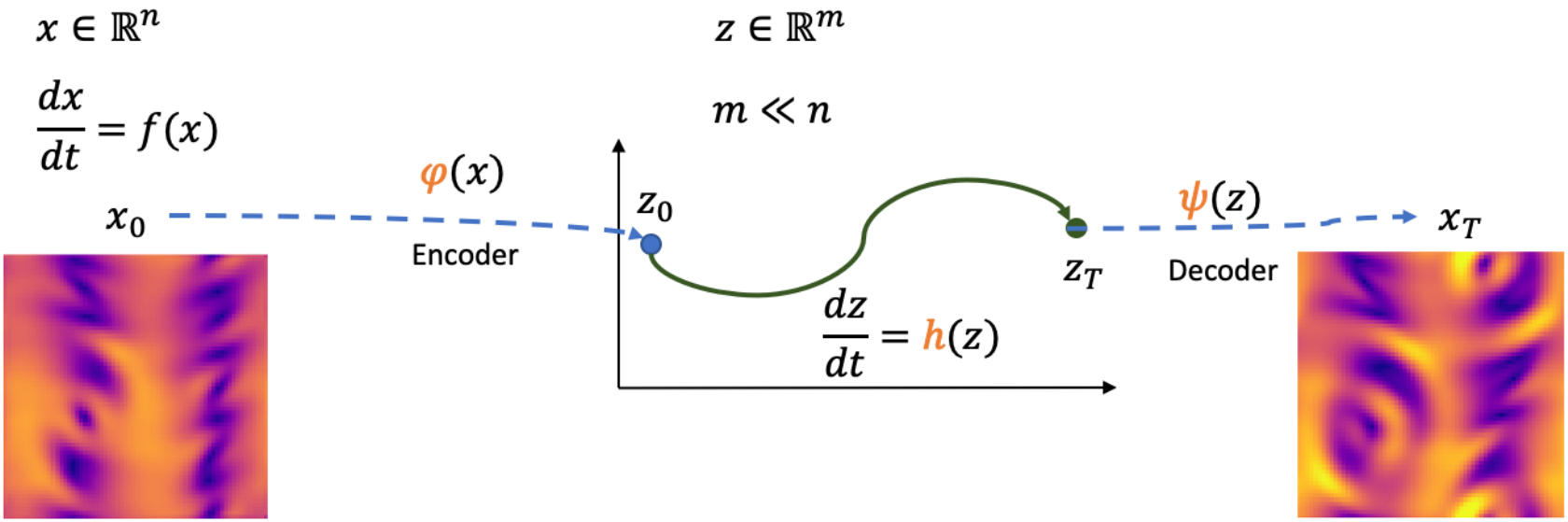

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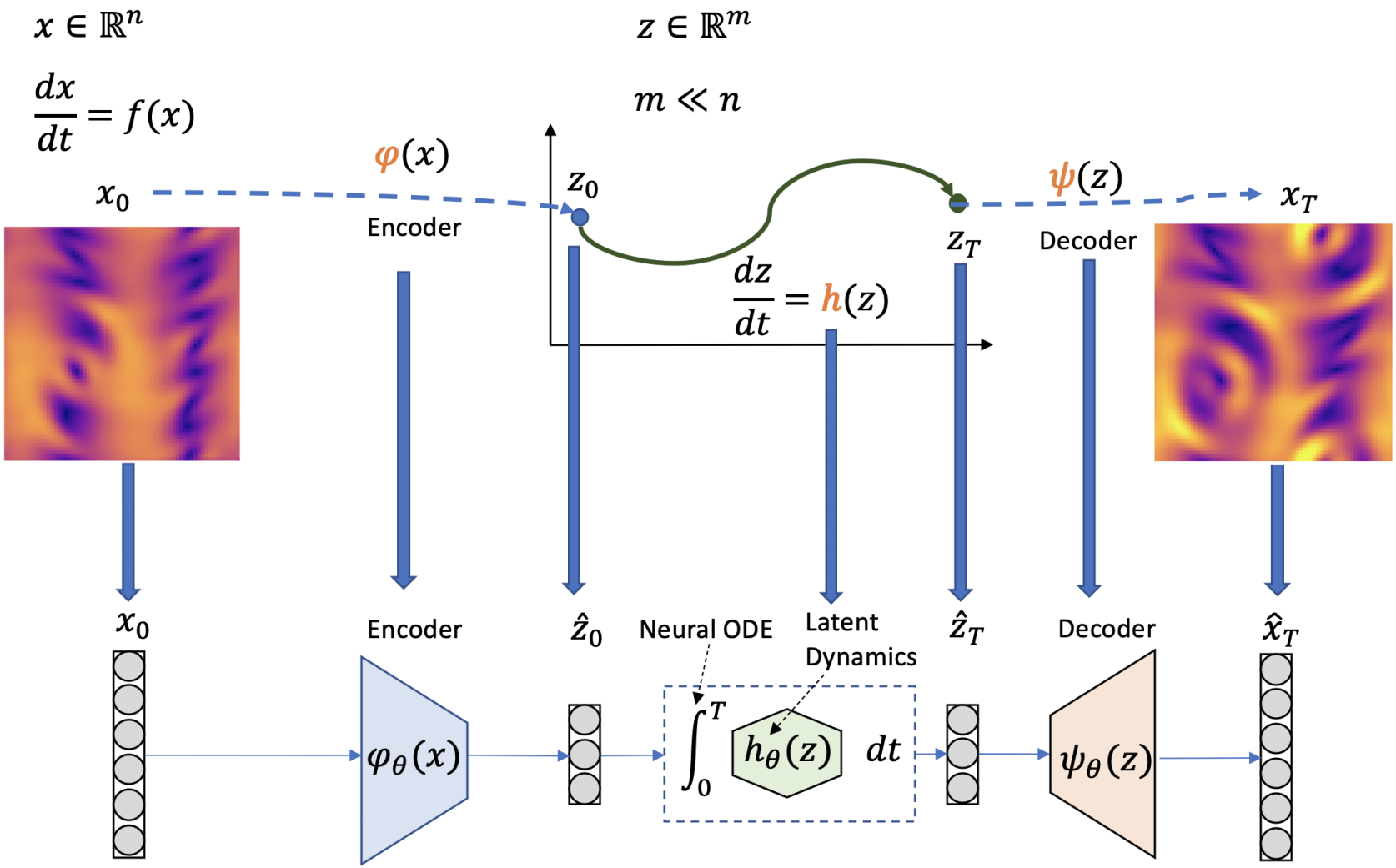
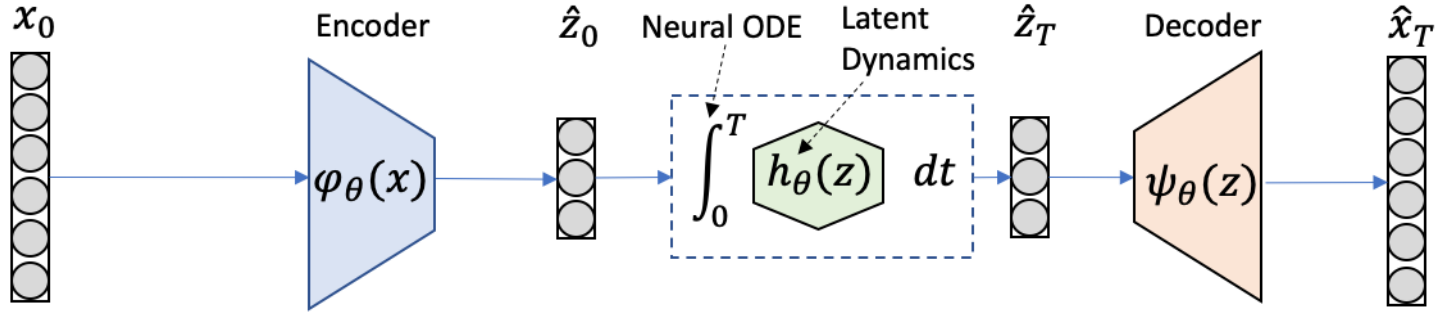


Reduced-Order Models: Data-Driven Loss



Notation:

- k trajectories $x_i(t_j)$, p timesteps each ($i = 1, \ldots, k$, $j = 1, \ldots, p$)
- σ – observation noise variance
- ω_1, ω_2 – weights (hyper-parameters)

$$\mathcal{L}_\theta^{data} = \frac{1}{2\sigma^2} \sum_{i=1}^{k} \left[\frac{\omega_1}{p} \sum_{j=1}^{p} \underbrace{\left\| \boldsymbol{x_i}(t_j) - \psi_\theta(\phi_\theta(\boldsymbol{x_i}(t_j))) \right\|^2}_{\text{reconstruction loss}} + \right. \tag{12}$$

$$\left. + \frac{\omega_2}{p} \sum_{j=1}^{p} \underbrace{\left\| \psi_\theta \left(\phi_\theta(\boldsymbol{x_i}(t_1)) + \int_{t_1}^{t_j} h(z(t))dt \right) - \boldsymbol{x_i}(t_j) \right\|^2}_{\text{prediction loss}} \right] \tag{13}$$

Physics-Informed Loss

Using chain rule:

$$\frac{dz}{dt} = \frac{dz}{dx}\frac{dx}{dt} = \nabla\varphi(x)^T f(x)$$

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1 Let $\dot{x} = f(x)$ be a discretization of $-u_t = u_{yy} + u_{yyyy} + \frac{1}{2}u_y^2$

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Using chain rule:

$$\frac{dz}{dt} = \frac{dz}{dx}\frac{dx}{dt} = \nabla\varphi(x)^T f(x) \qquad \frac{dz}{dt} = h(\varphi(x))$$

$$\mathcal{L}_\theta^{physics} = \sum_{i=1}^{N} \omega_3 \|\nabla\varphi_\theta(\tilde{x}_i)^T f(\tilde{x}_i) - h_\theta(\varphi_\theta(\tilde{x}_i))\|_2^2 + \omega_4 \|\tilde{x}_i - \psi_\theta(\varphi_\theta(\tilde{x}_i))\|_2^2$$

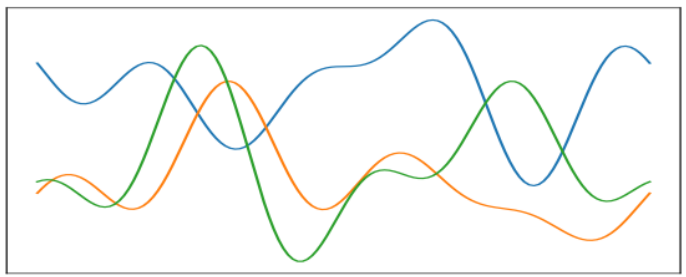
(1) (2) (3)

(1)

Let $\dot{x} = f(x)$ be a discretization of $-u_t = u_{yy} + u_{yyyy} + \frac{1}{2}u_y^2$

Then the **collocations** could be:

$$u(y) = \sum_{w=1}^{30} a(w)\sin(2\pi y) + b(w)\cos(2\pi y)$$



- Diverse
- Cheap
- Representative

Collocations: a set of pairs $(\tilde{x}_i, \dot{\tilde{x}}_i)$, where $\tilde{x}_i$ are s.t. $\dot{\tilde{x}}_i$ are cheap to evaluate.

Physics-Informed Loss

Using chain rule:

$$\frac{dz}{dt} = \frac{dz}{dx}\frac{dx}{dt} = \nabla\varphi(x)^T f(x) \qquad \frac{dz}{dt} = h(\varphi(x))$$

$$\mathcal{L}_\theta^{physics} = \sum_{i=1}^{N} \omega_3 \|\nabla\varphi_\theta(\tilde{x}_i)^T f(\tilde{x}_i) - h_\theta(\varphi_\theta(\tilde{x}_i))\|_2^2 + \omega_4 \|\tilde{x}_i - \psi_\theta(\varphi_\theta(\tilde{x}_i))\|_2^2$$

1

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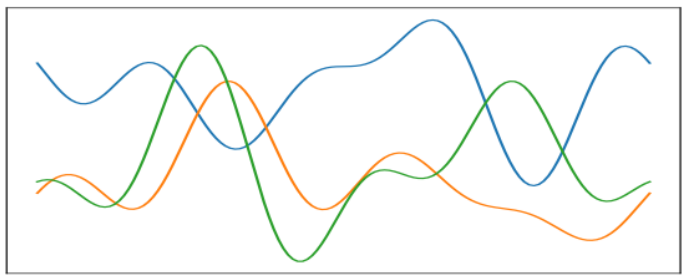

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- Cheap
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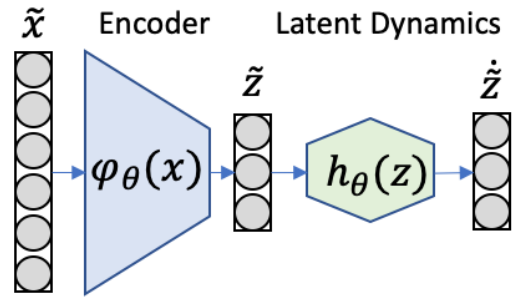
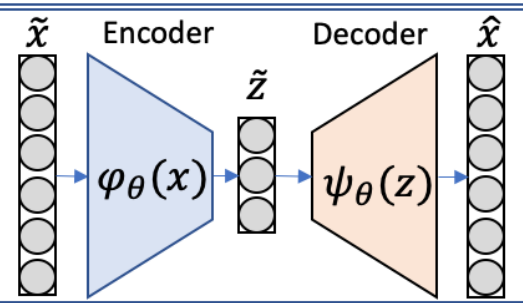
2



3



Collocations: a set of pairs $(\tilde{x}_i, \dot{\tilde{x}}_i)$, where $\tilde{x}_i$ are s.t. $\dot{\tilde{x}}_i$ are cheap to evaluate.

Physics-Informed, Data-Driven, and Hybrid Models

Values of ω_1, ω_2, ω_3, and ω_4 control the type of the ROM:

- If $\omega_1 = \omega_2 = 0$ then $\mathcal{L}_\theta^{\text{data}} = 0$. Thus, the model is purely Physics-Informed
- If $\omega_3 = \omega_4 = 0$ then $\mathcal{L}_\theta^{\text{physics}} = 0$. Thus, the model is purely Data-Driven
- Otherwise the model is Hybrid

Results: Extrapolation to Unknown Regions

Duffing Oscillator on a low-dimensional (2D) manifold:

$$\begin{aligned} \frac{dz_1}{dt} &= z_2 \\ \frac{dz_2}{dt} &= z_1 - z_1^3 \end{aligned} \tag{14}$$

Projection to a high-dimensional (128) space:

$$\boldsymbol{x} := \mathcal{A}(\boldsymbol{z}) = A\boldsymbol{z}^3, \quad A \in \mathbb{R}^{128\times 2}, \quad A_{ij} \sim_{i.i.d.} \mathcal{N}(0,1) \tag{15}$$

Results: Extrapolation to Unknown Regions

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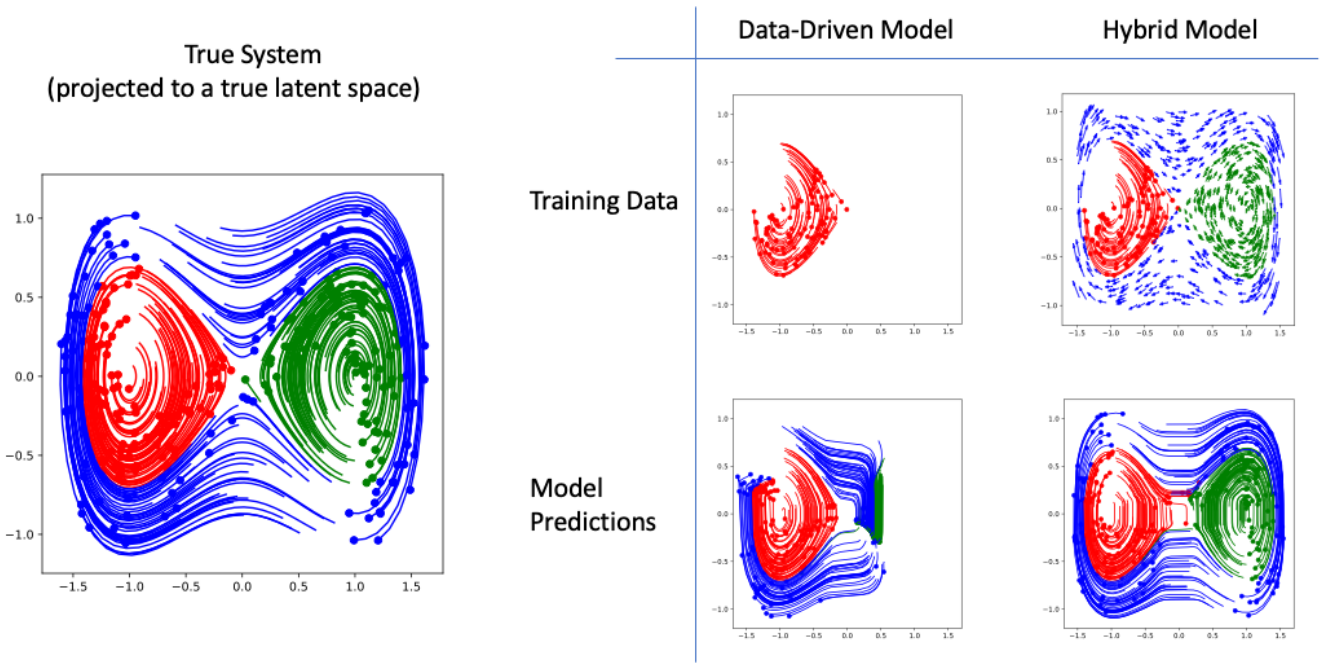
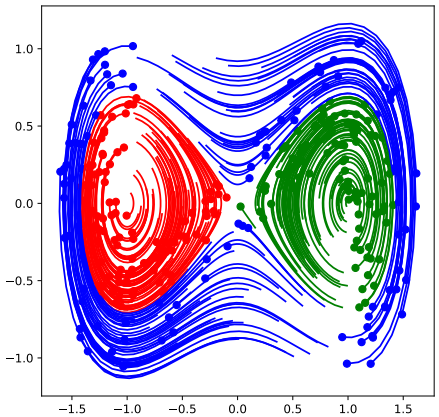
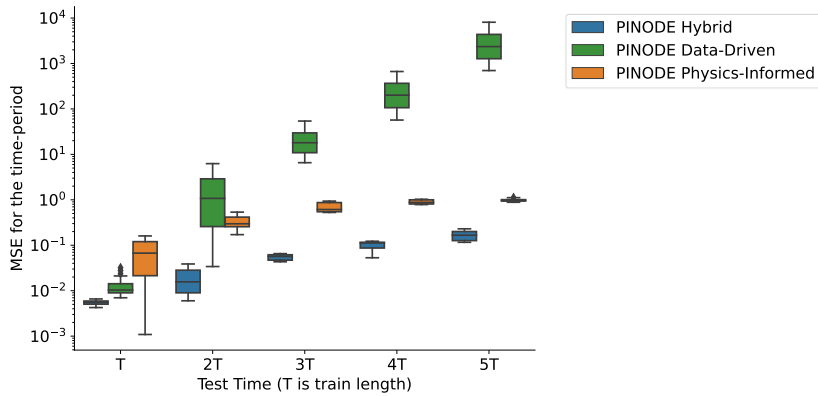
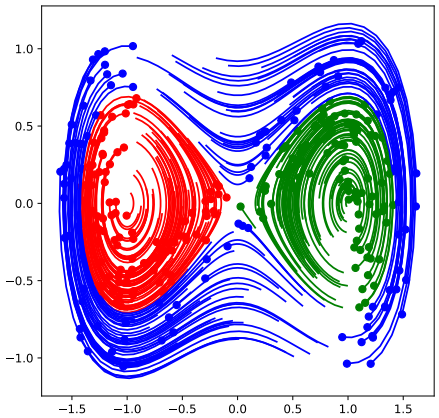


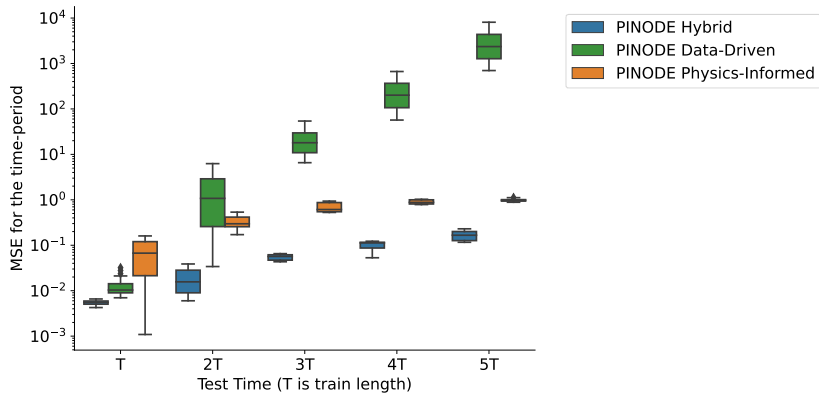
Results: Stable Long-Term Predictions



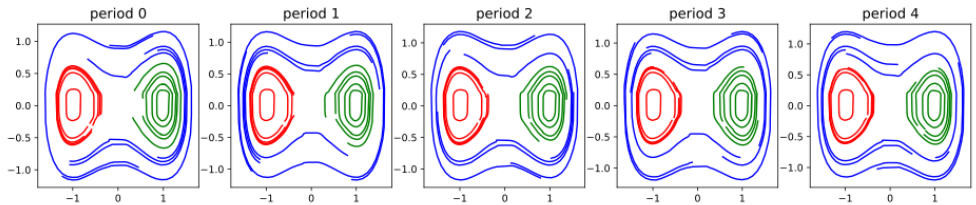


Results: Stable Long-Term Predictions

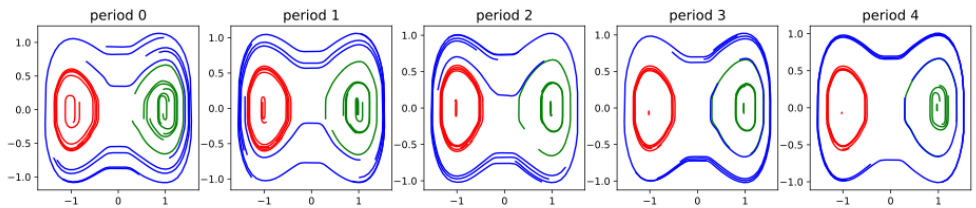




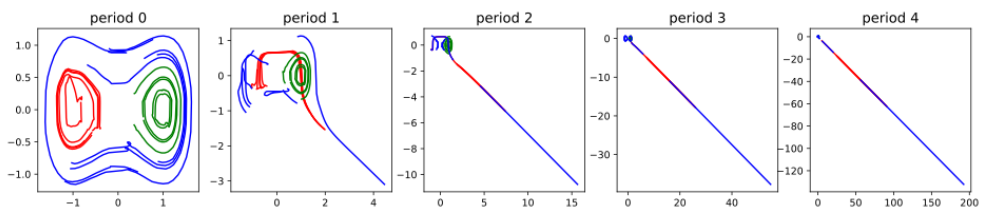
Hybrid Model



Physics-Informed Model



Data-Driven Model



Results: Burgers' Equation

$$
\begin{aligned}
& u_t + u u_x = \nu u_{xx} \\
& u(-\pi, t) = u(\pi, t), \quad \forall t \in [0, T], \quad \nu = 0.01
\end{aligned}
\tag{16}
$$

Results: Burgers' Equation

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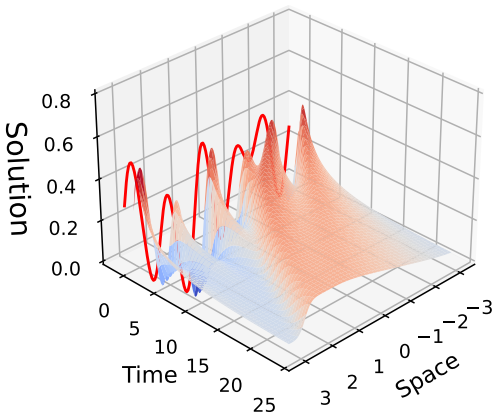
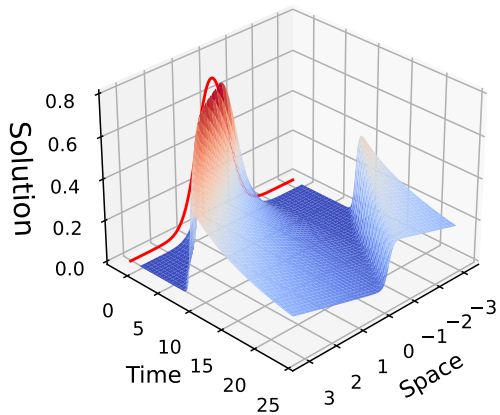
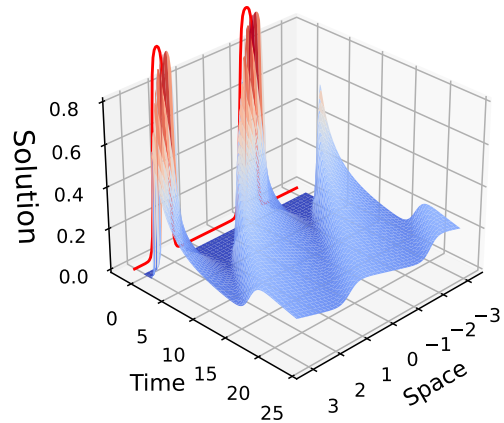
Harmonic: Solution



Bell-Curve: Solution



Bumps: Solution



ICs and Collocations:

Harmonic:

$$u(x) = \sum_{k=1}^{30} a_k \sin(2\pi x/k) + b_k \cos(2\pi x/k)$$
$$a_k = \alpha_k s_k$$
$$\alpha_k \sim \mathcal{U}(0, 1)$$
$$s_k \sim \mathcal{B}e(0.5)$$

Bell-curve:

$$u(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp \frac{-(x-x_0)^2}{2\sigma^2}$$
$$\sigma \sim \mathcal{U}(0, 3)$$
$$x_0 \sim \mathcal{U}(-\pi, \pi)$$

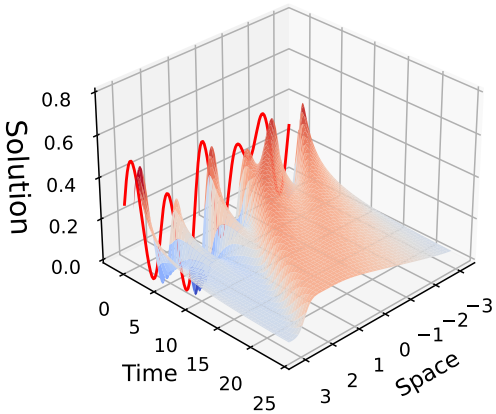
Bumps:

$$u(x) = \frac{a}{1 + \exp^{-k(x-x_0)}} - \frac{a}{1 + \exp^{-k(x-x_1)}}$$
$$k \sim \mathcal{U}(5, 20)$$
$$x_0, x_1 \sim \mathcal{U}(-\pi, \pi)$$

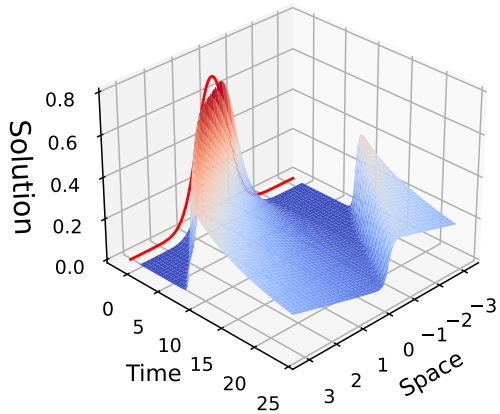
Results: Burgers' Equation

$$u_t + uu_x = \nu u_{xx}$$
$$u(-\pi, t) = u(\pi, t), \quad \forall t \in [0, T], \quad \nu = 0.01 \tag{16}$$

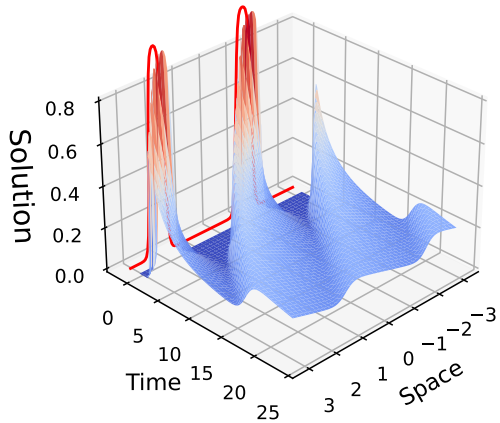
Harmonic: Solution



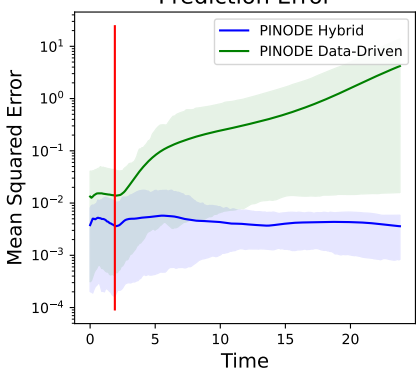
Bell-Curve: Solution



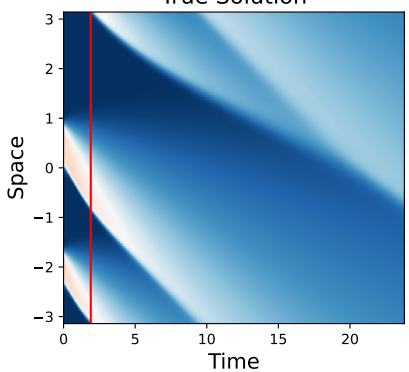
Bumps: Solution



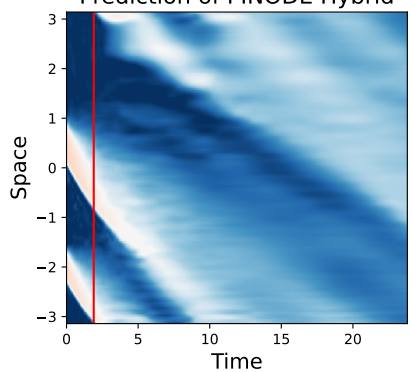
Prediction Error



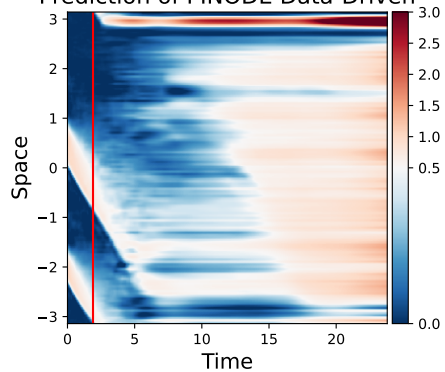
True Solution



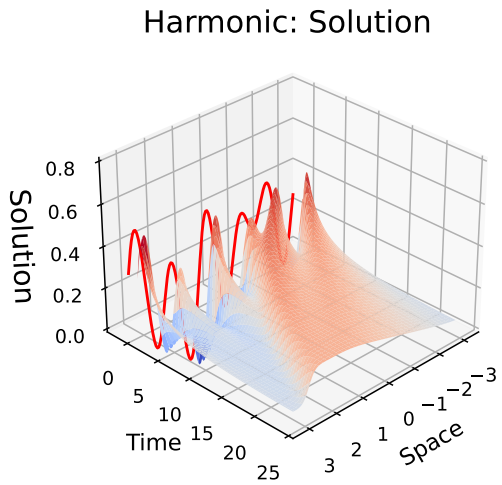
Prediction of PINODE Hybrid

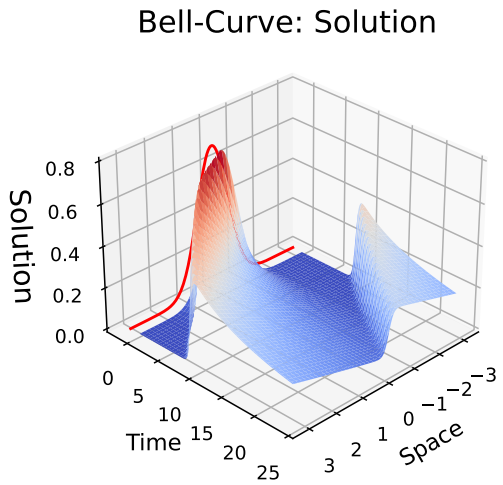


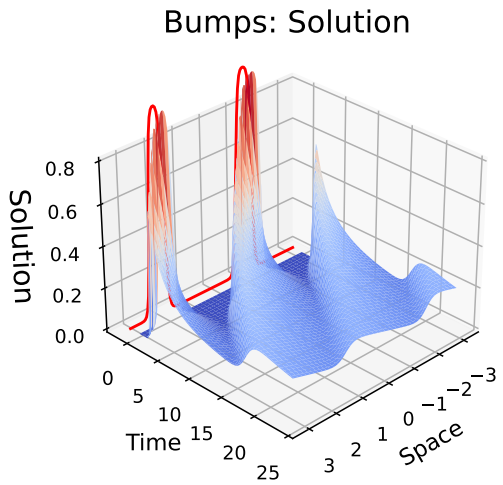
Prediction of PINODE Data-Driven

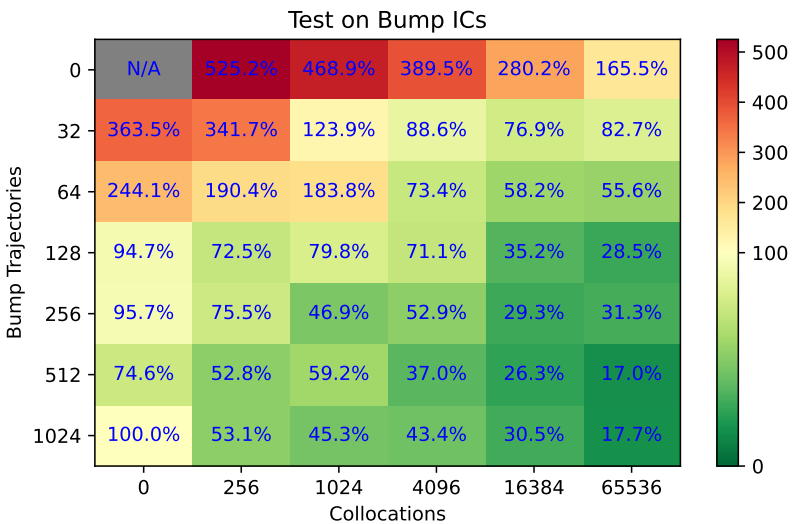


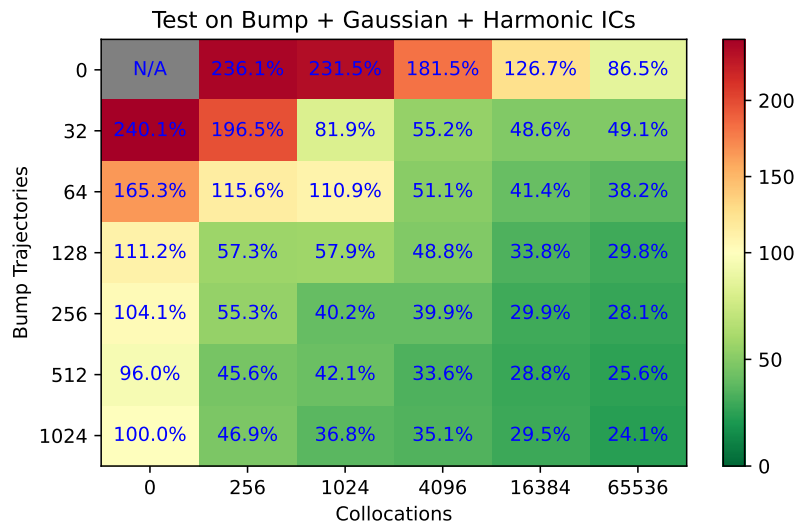
Results: Learning From Collocations











Discussion and Limitations

We showed that:

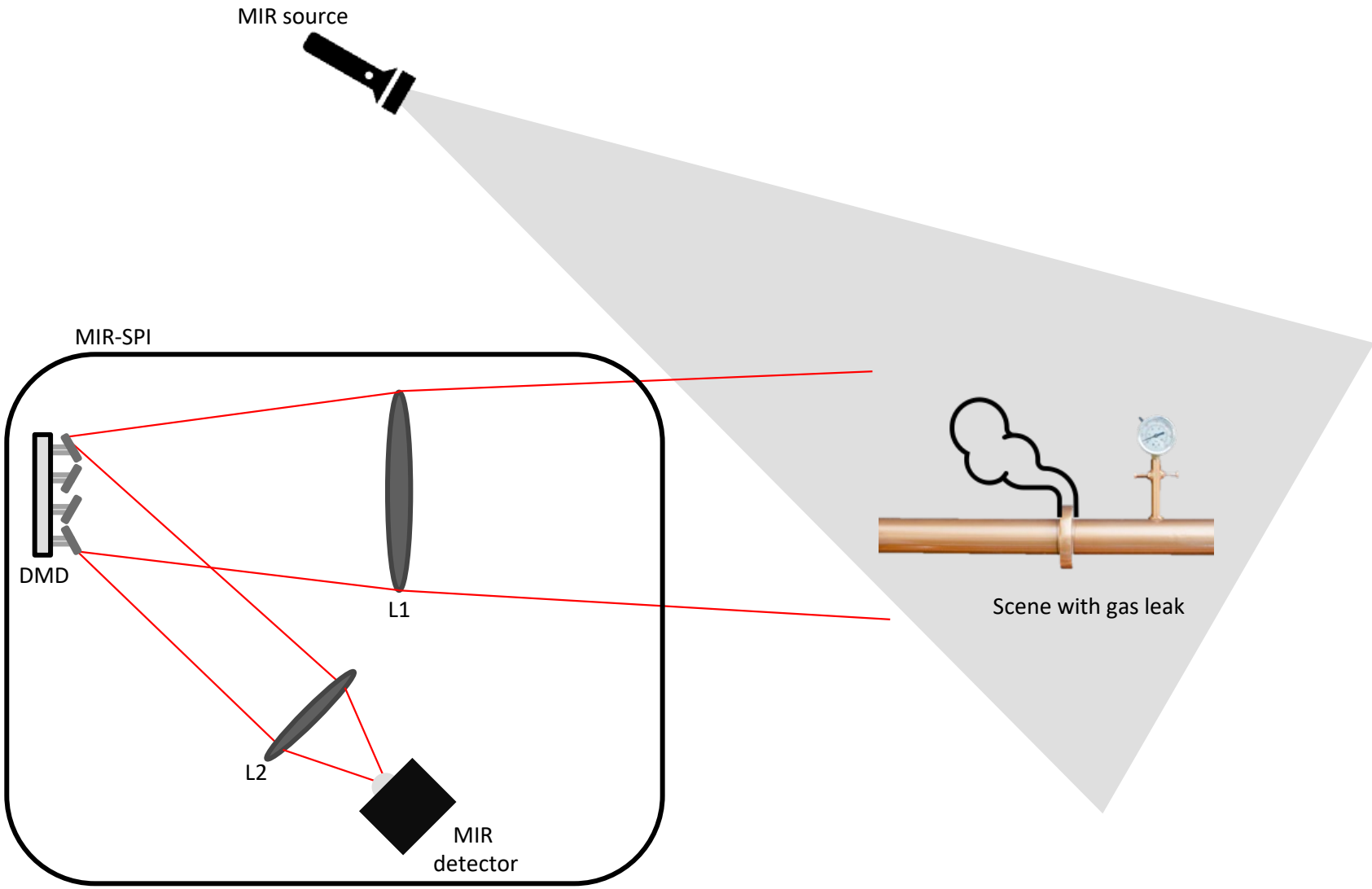
- Physics-informed loss improves accuracy and forecasting stability of ROMs
- Collocations can supplement data to improve model's performance for unseen initial conditions.

Limitations:

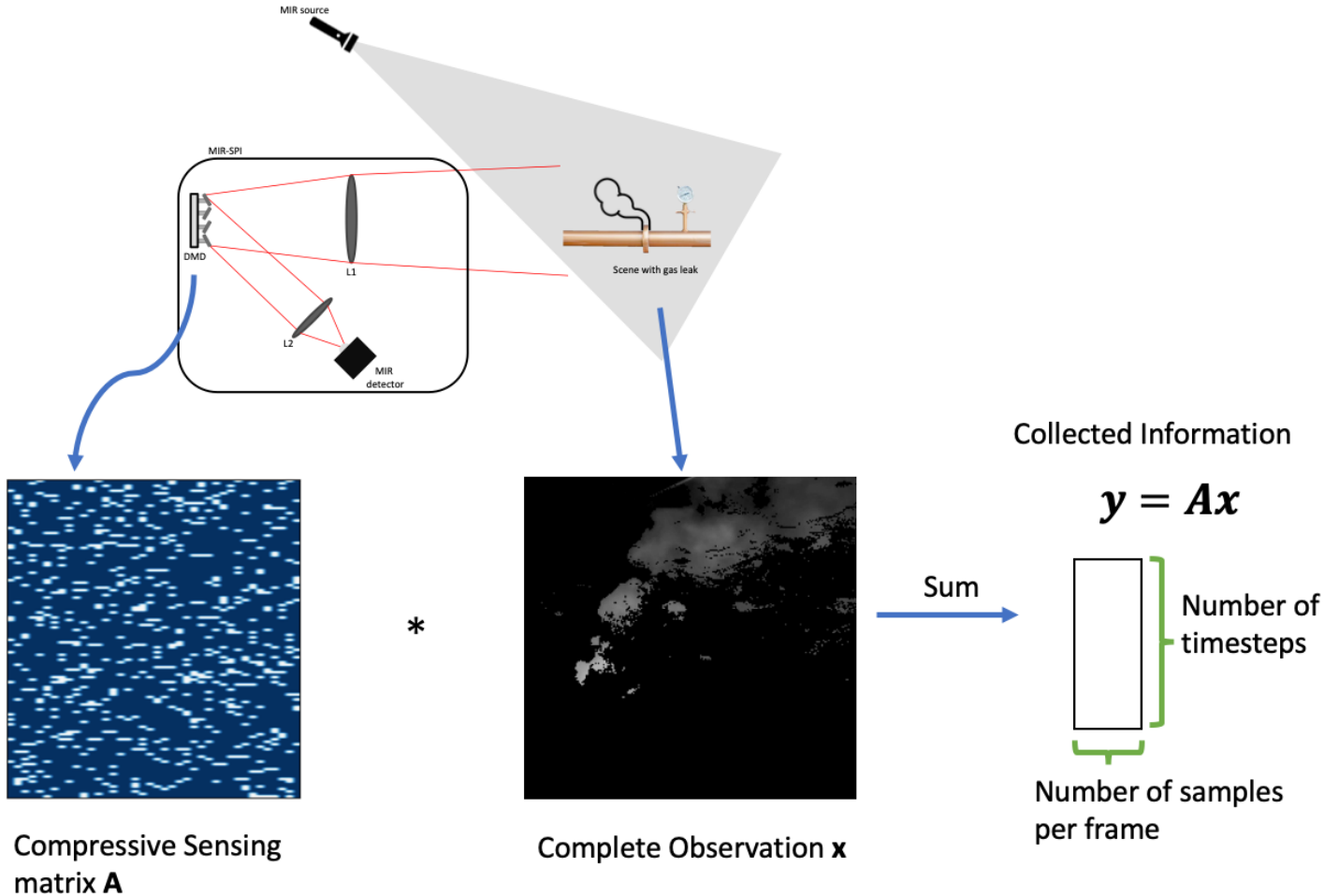
- Optimal choice of collocations is problem-specific
- Need a lot of collocations
  - *Seems* possible to overcome with smarter sampling techniques

Single pixel imaging of spatio-temporal flows using differentiable latent dynamics

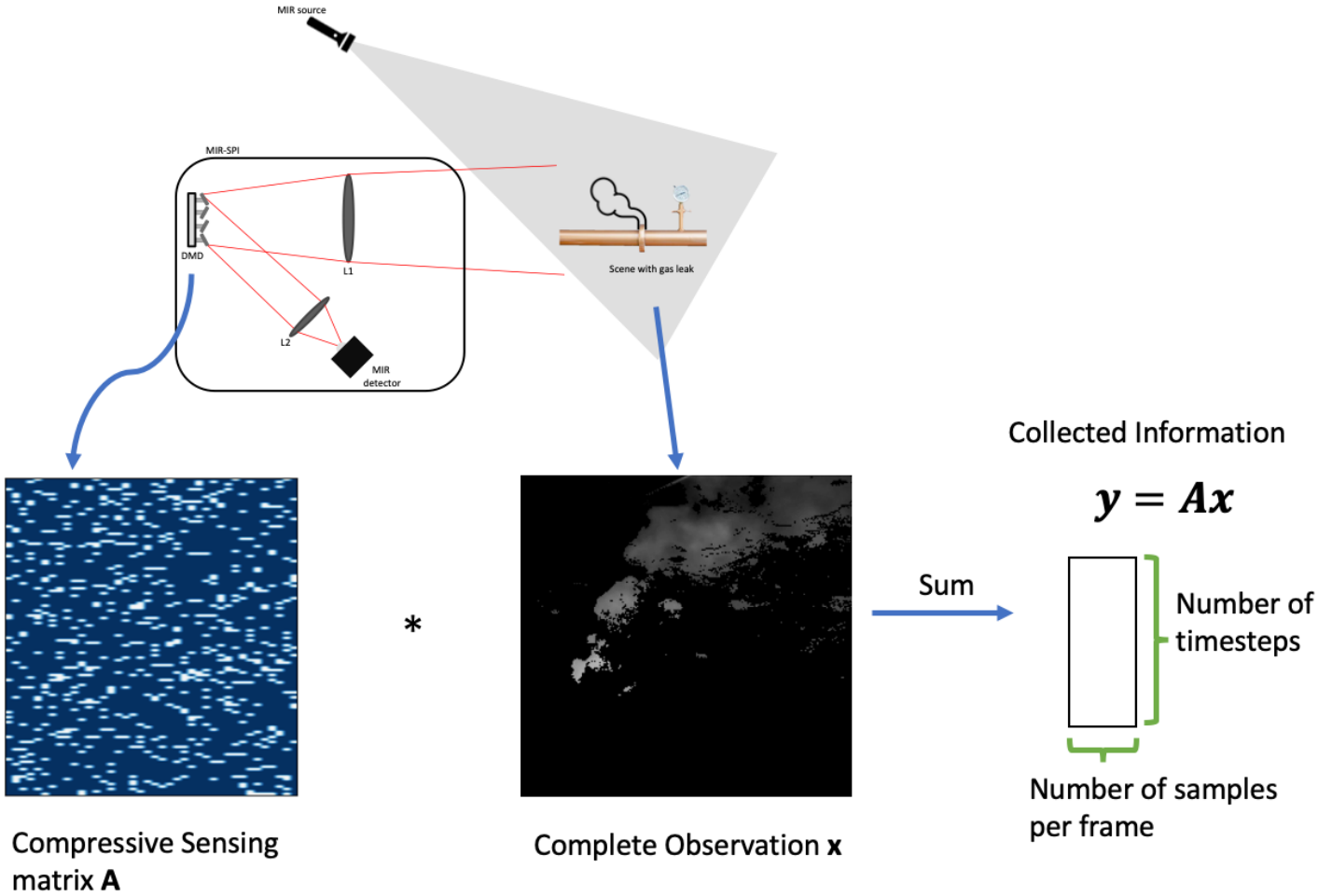
Single-Pixel Imaging



Single-Pixel Imaging



Single-Pixel Imaging

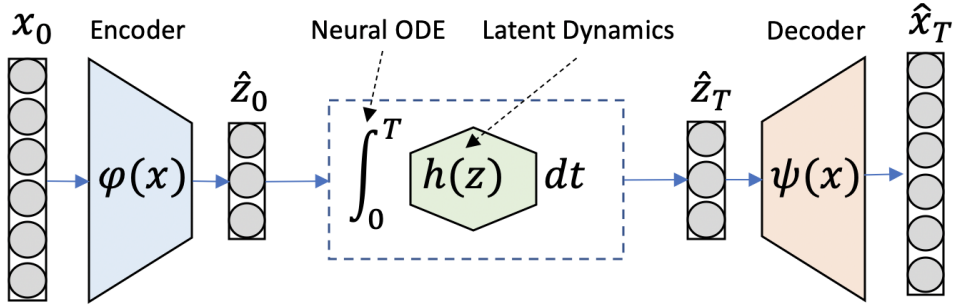


Single-Pixel Image Recovery: find **x** using **y** and **A**.

SPF rate, % = Number of samples per frame / number of pixels per frame * 100

Compressive Sensing with Reduced-Order Models

Offline Step: Train a Data-Driven Reduced-Order Model



Online Step: Reconstruct Complete Observations by Optimizing in Latent Space

Reconstruction Loss

Compressive Sensing Loss

Loss for Prediction in Latent space

$$\mathcal{L}^{recon.}(z) = ||y - A\psi(z)|| + \lambda \left|\left| z - (z_0 + \int_0^T h(z)dz) \right|\right|$$

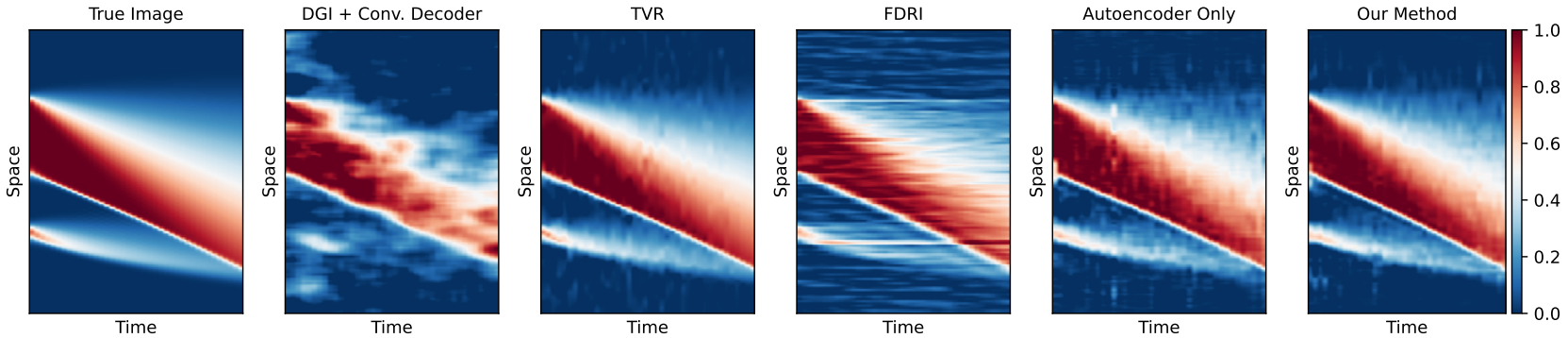
Latent-space representation of the trajectory

"What the data tells us the trajectory should be"

"What the model thinks the trajectory should be"

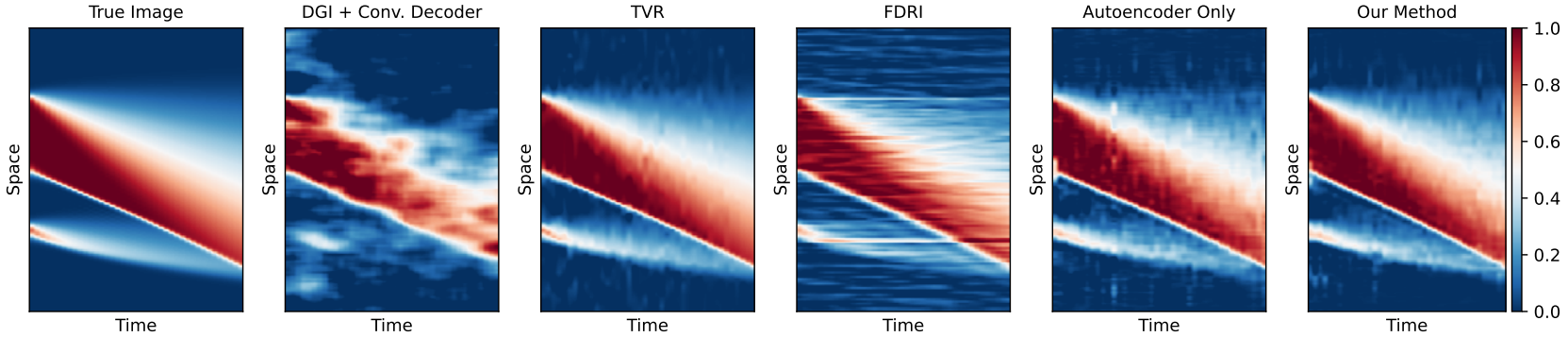
Results: Burger's Equation

Recovery with SPF=25%:

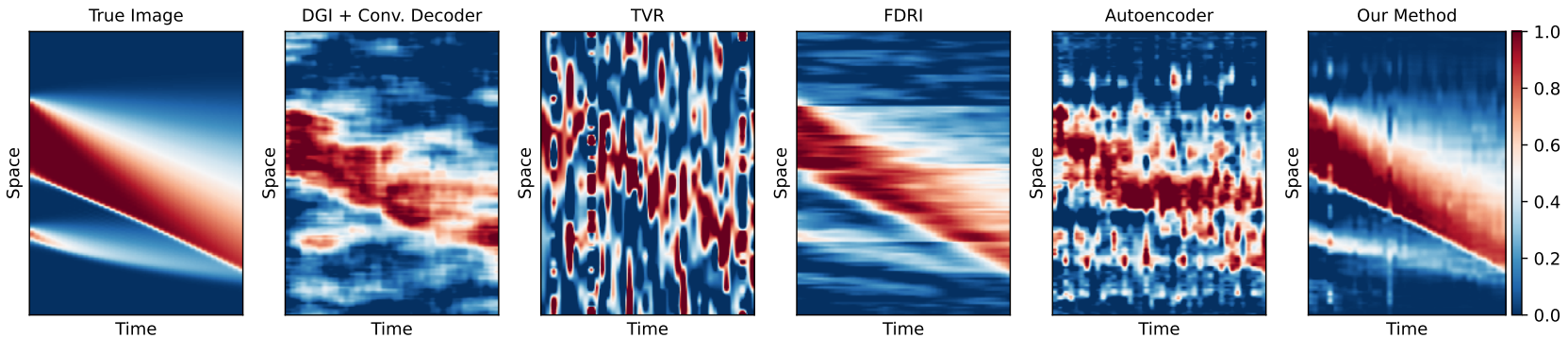


Results: Burger's Equation

Recovery with SPF=25%:

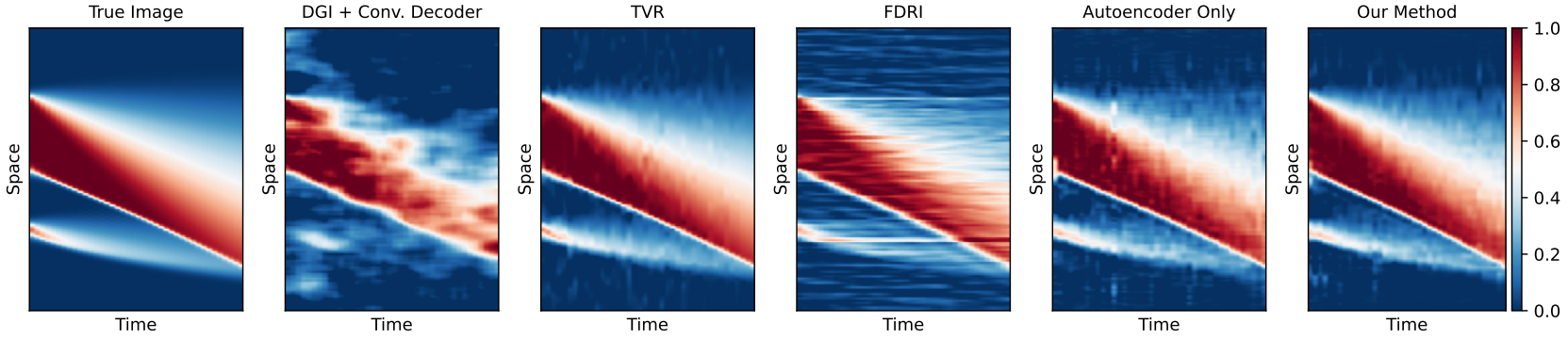


Recovery with SPF=6.25%:

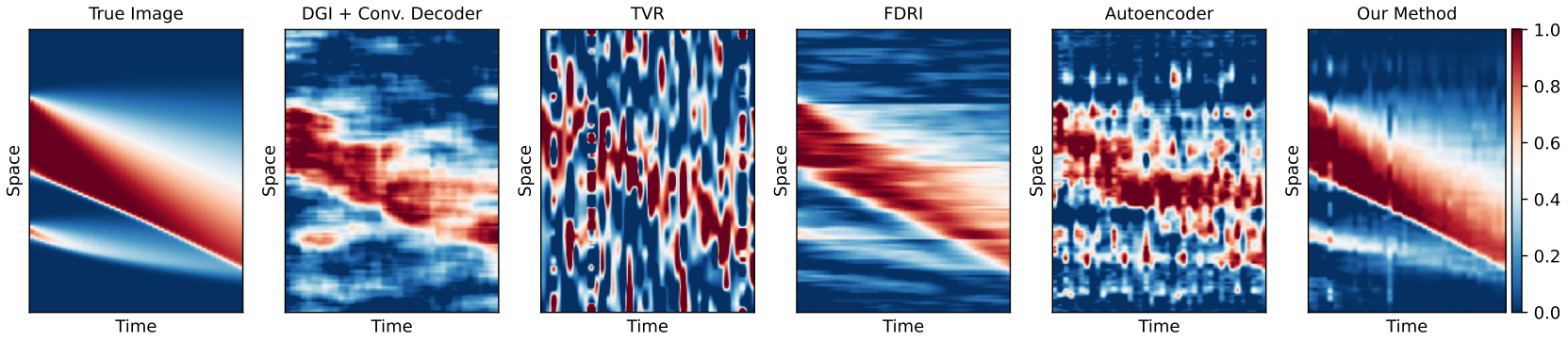


Results: Burger's Equation

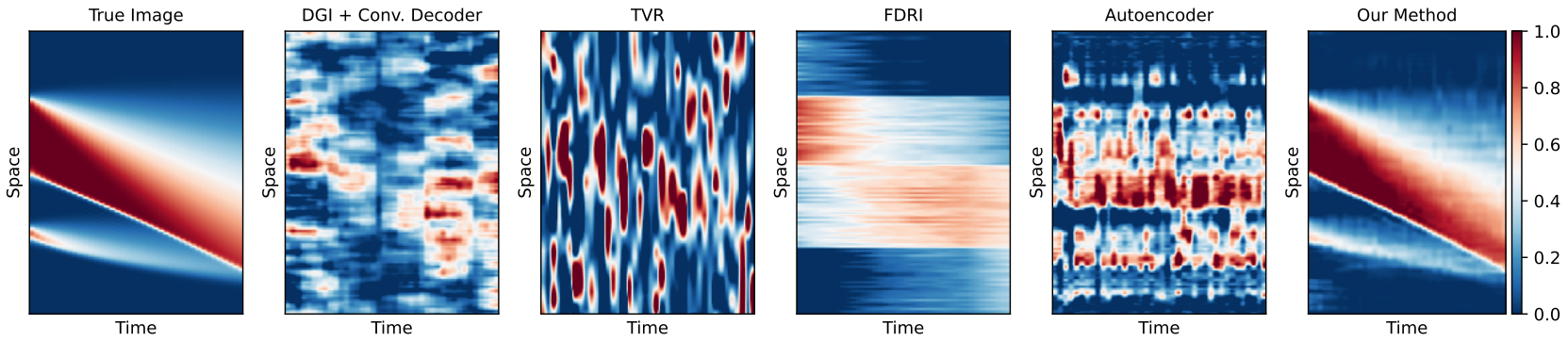
Recovery with SPF=25%:



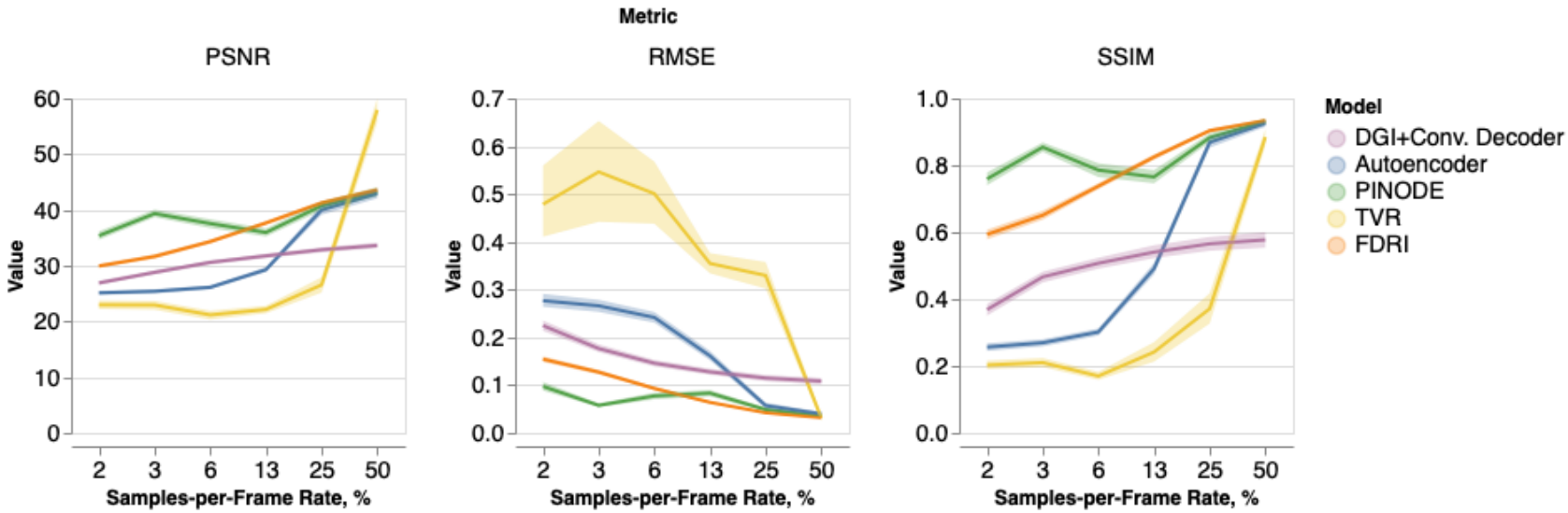
Recovery with SPF=6.25%:



Recovery with SPF=1.5%:



Results: Burger's Equation



Higher is better Lower is better Higher is better

Metrics:

- **PSNR**: Peak Signal-to-Noise Ratio
- **RMSE**: Residual Mean Square Error
- **SSIM**: Structural Similarity Index Measure

Results: Kolmogorov Flow

A 2D velocity field $\boldsymbol{u}(x, y, t)$:

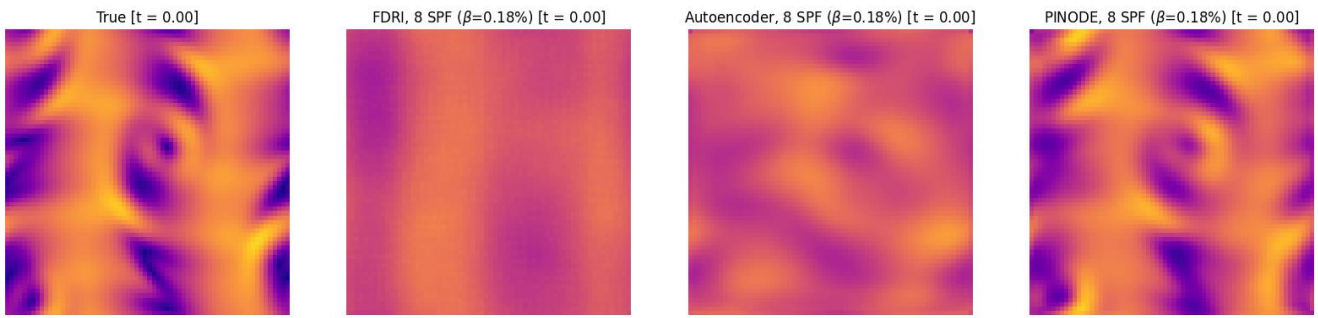
$$\partial_t \boldsymbol{u} + \boldsymbol{u} \cdot \nabla \boldsymbol{u} = -\nabla p + \nu \nabla^2 \boldsymbol{u} + f \tag{17}$$

$$\nabla \cdot \boldsymbol{u} = 0 \tag{18}$$

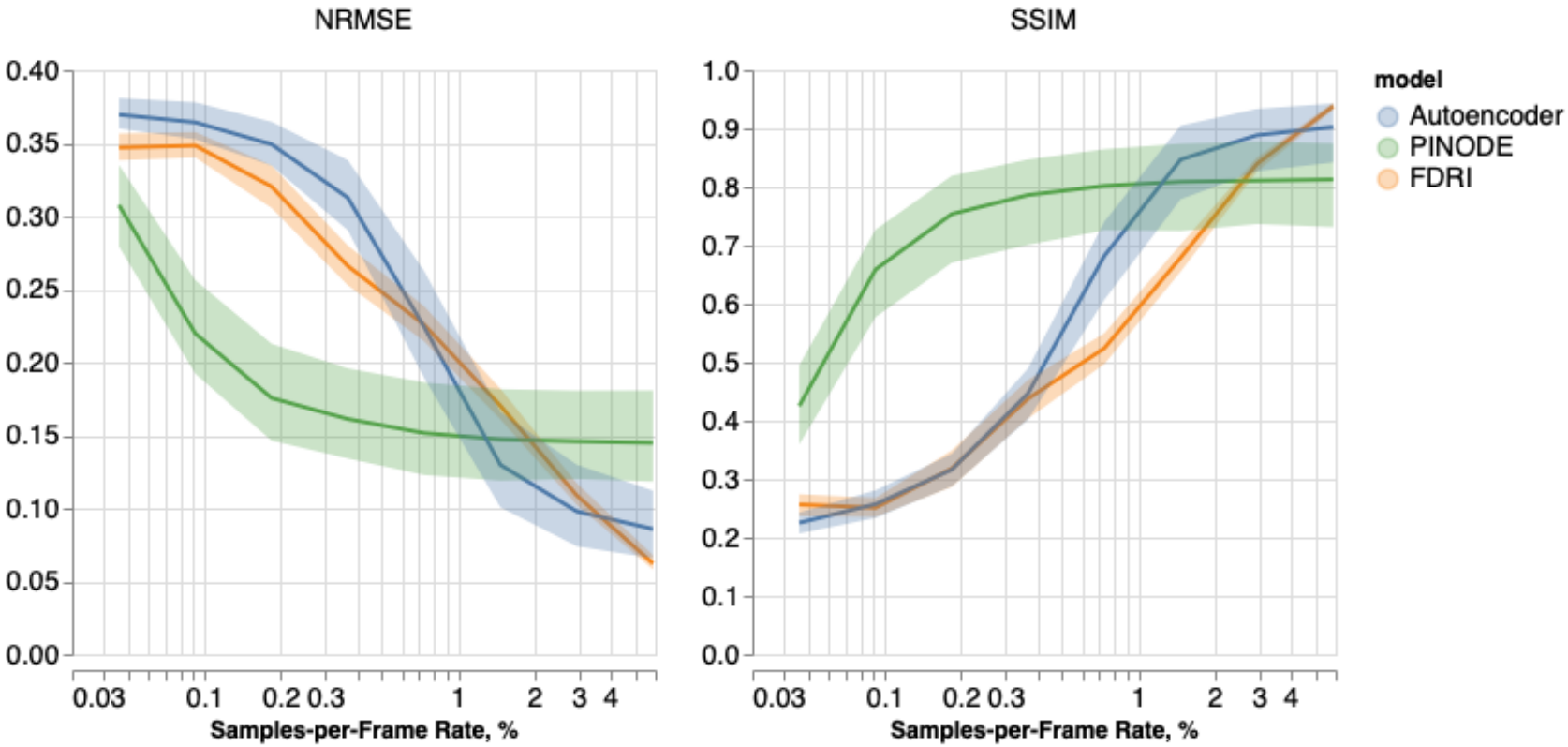
where

- p is a 2D pressure field
- $f = \alpha \sin(ky)x$ - driving force with amplitude A and wavenumber k ($k = 4$)
- $\nu = 1/\mathrm{Re}$ is the non-dimensional viscosity. Re=40

Reconstruction with SPF rate = 0.18% (8 SPI samples per a frame of 66×66 pixels):



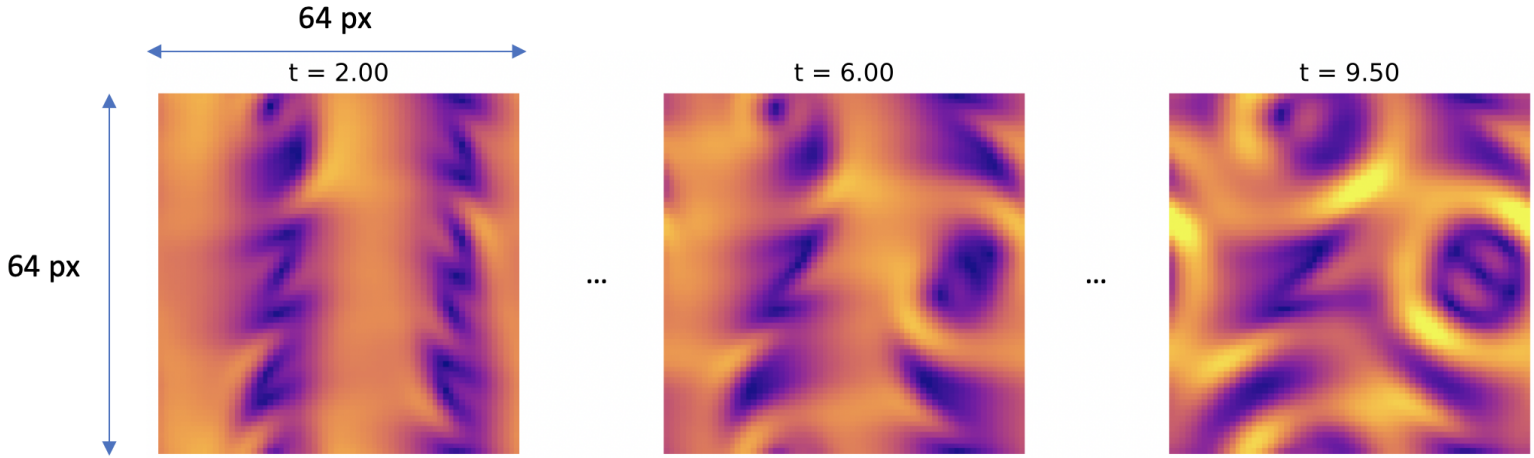
Results: Kolmogorov Flow



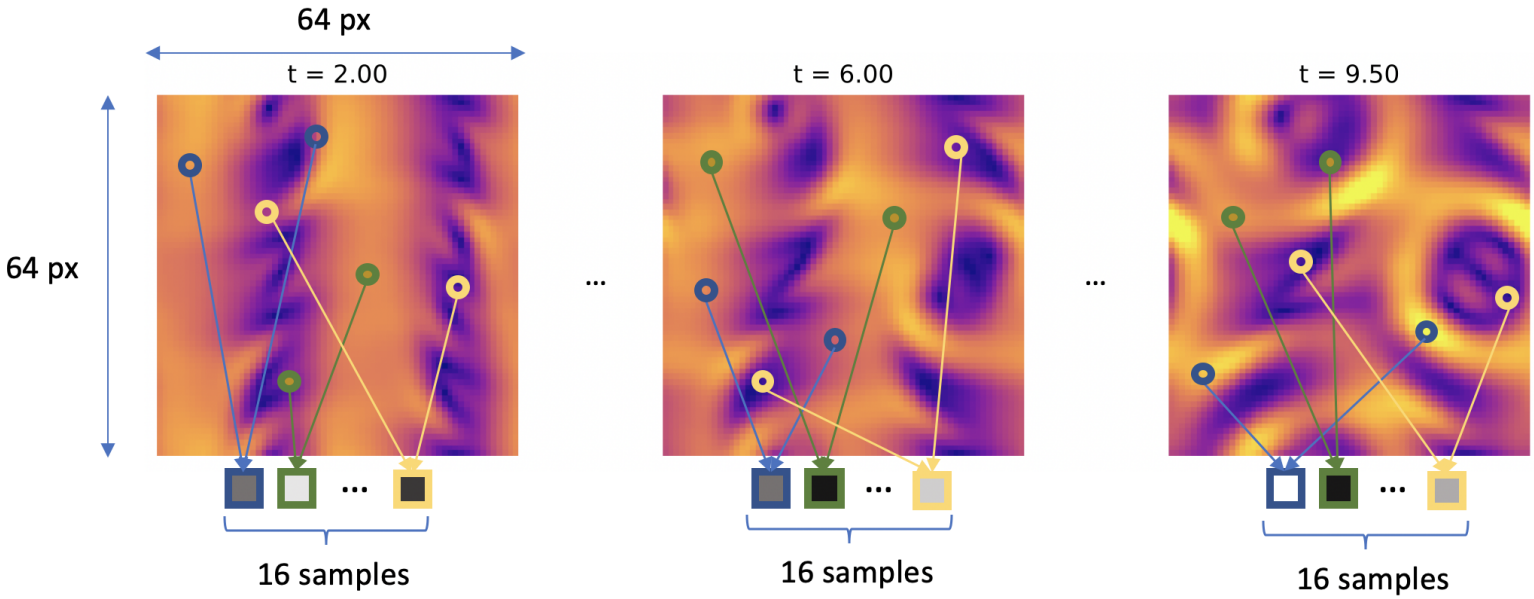
Lower is better

Higher is better

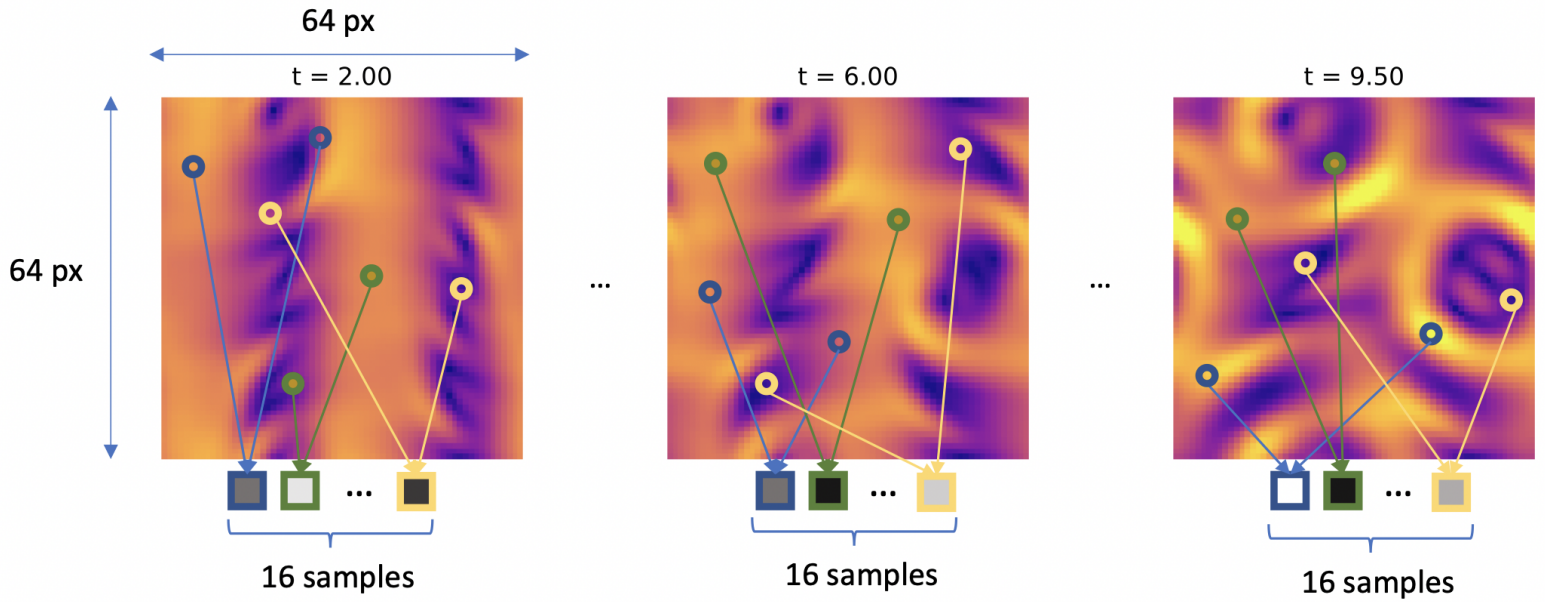
Results: Interpretation

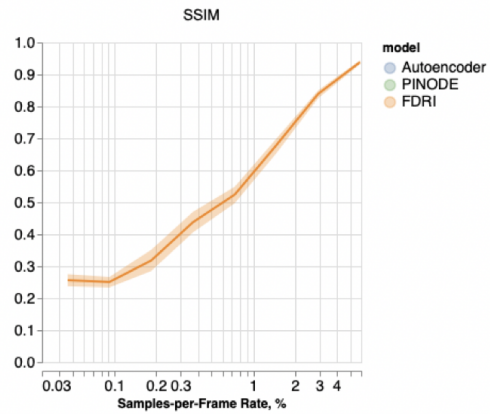


Results: Interpretation

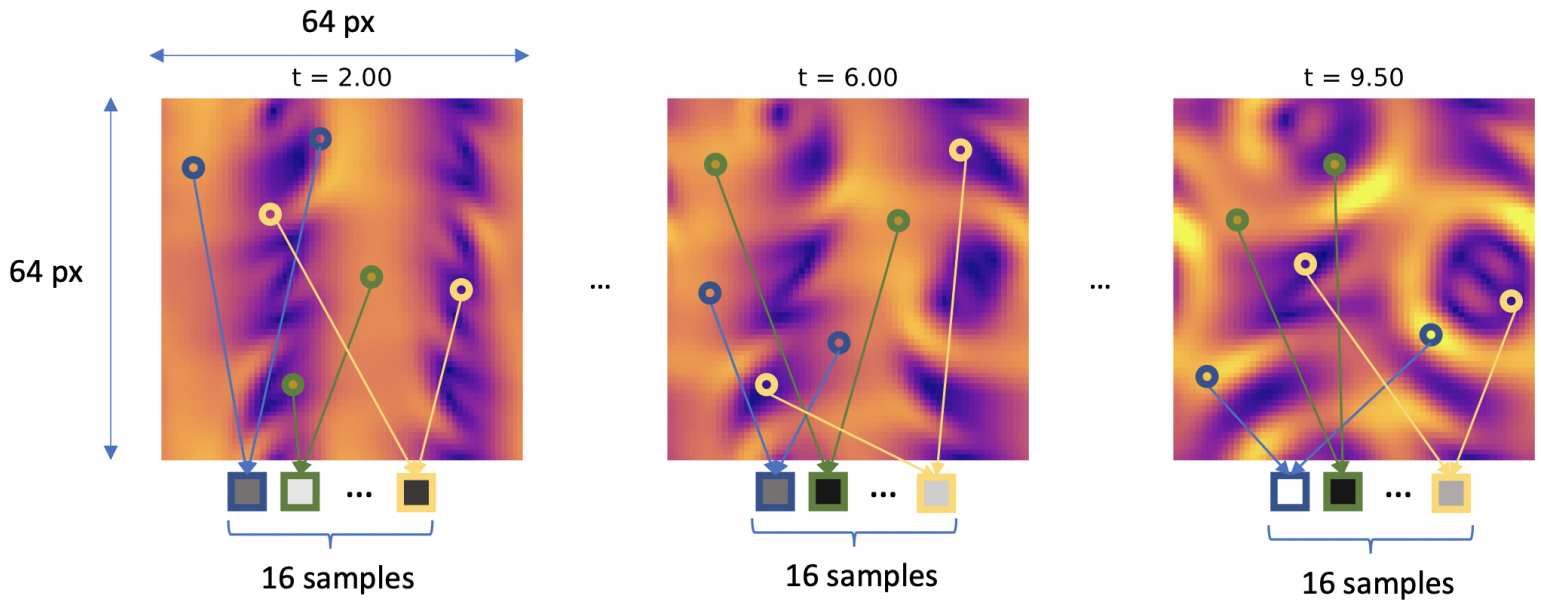


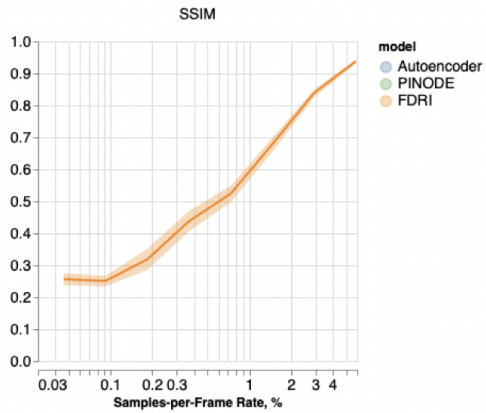
Results: Interpretation



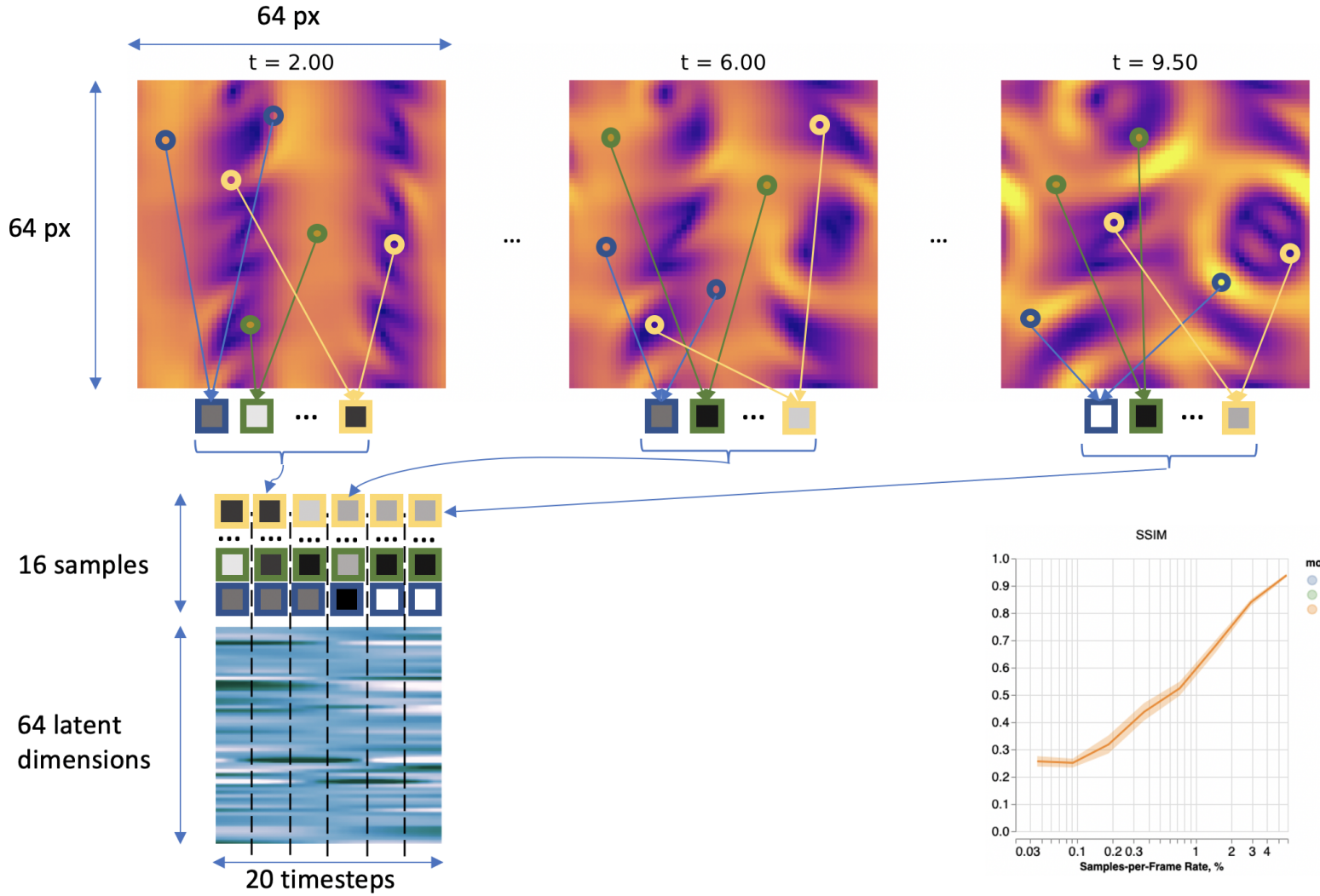


Results: Interpretation

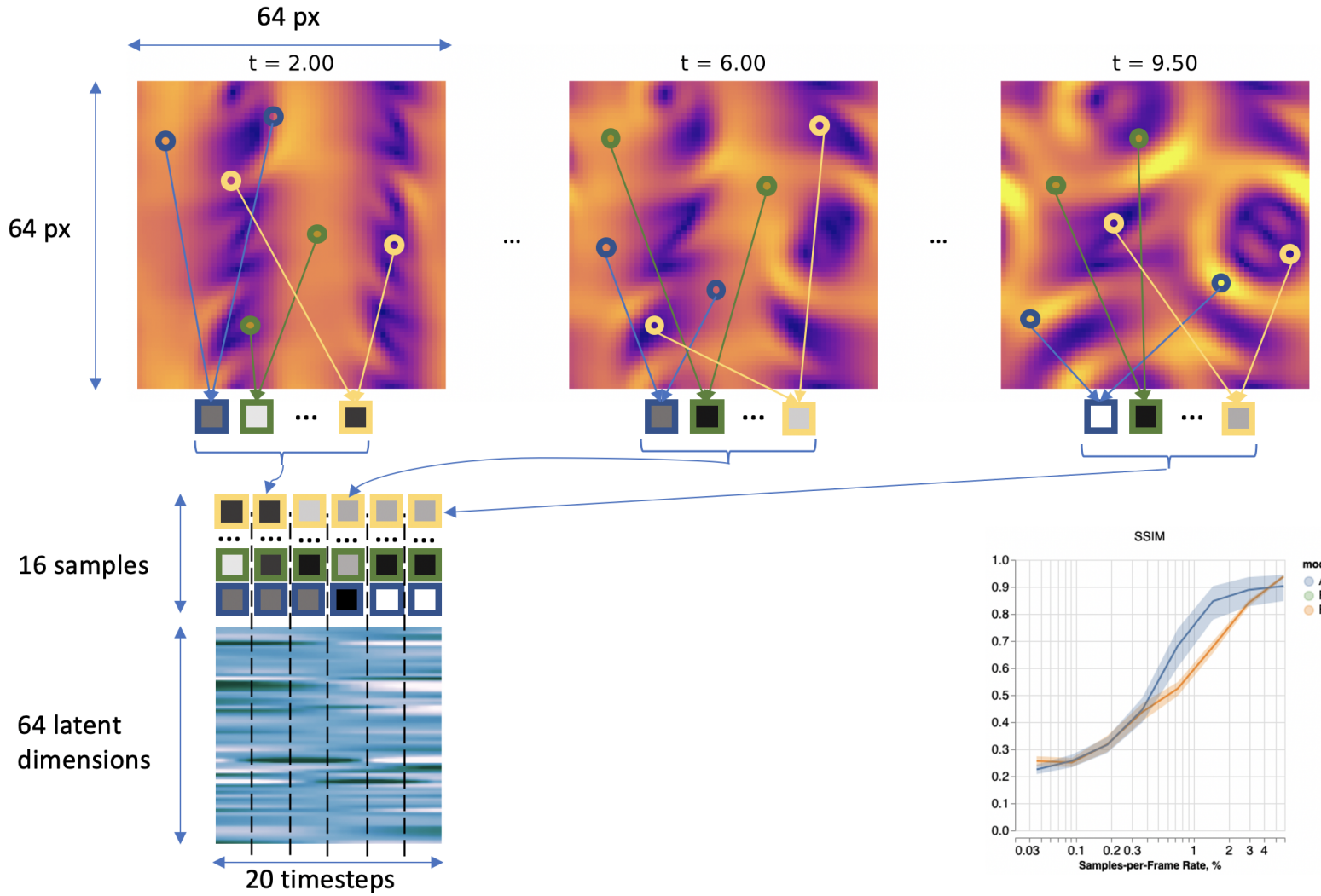




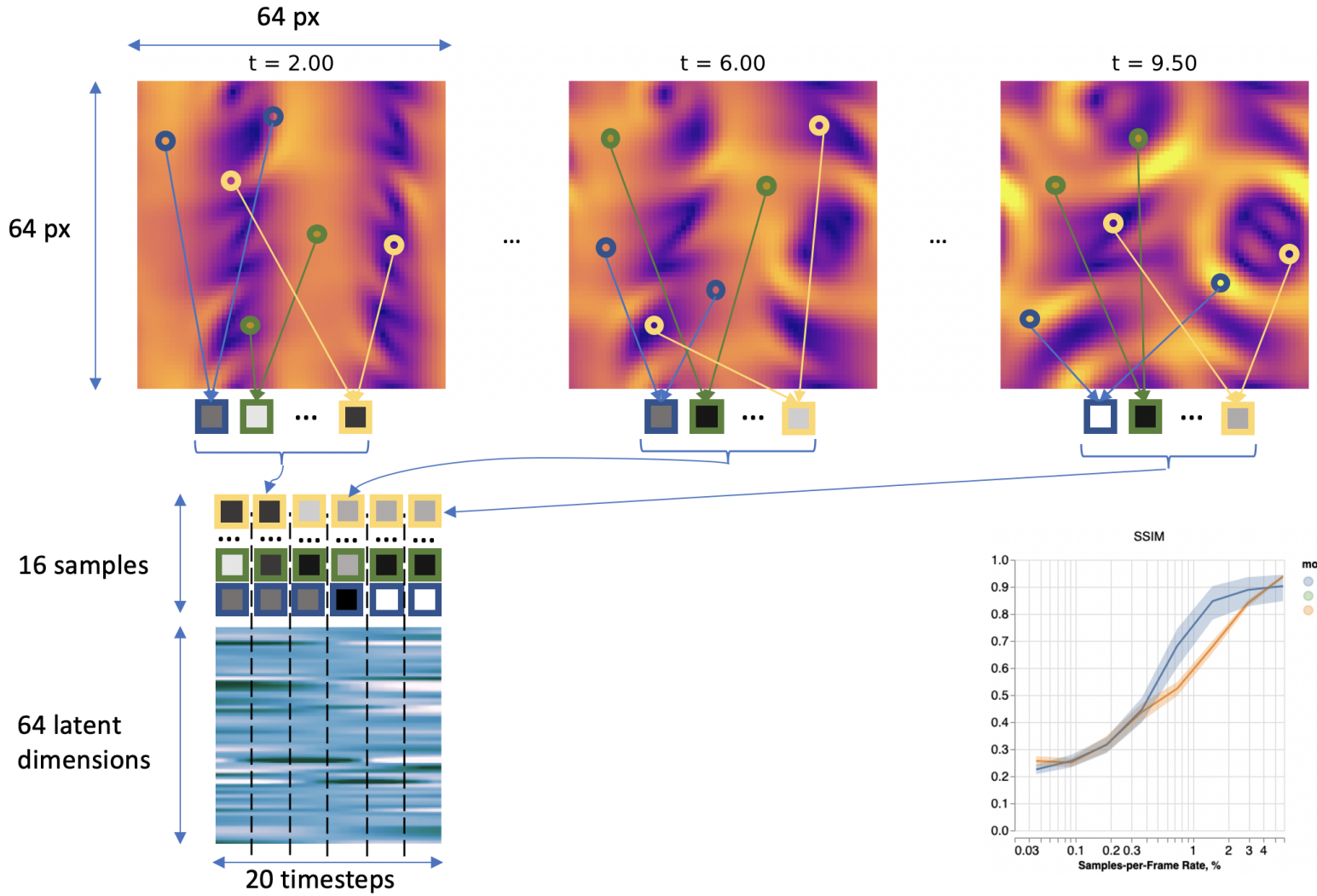
Results: Interpretation



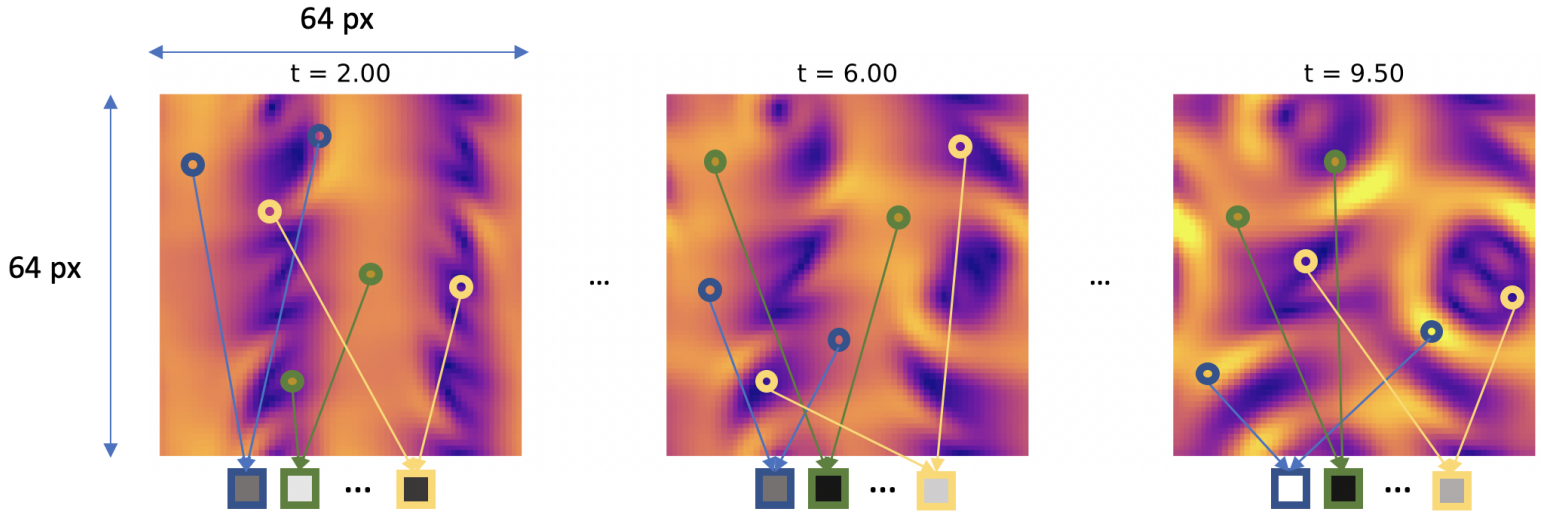
Results: Interpretation

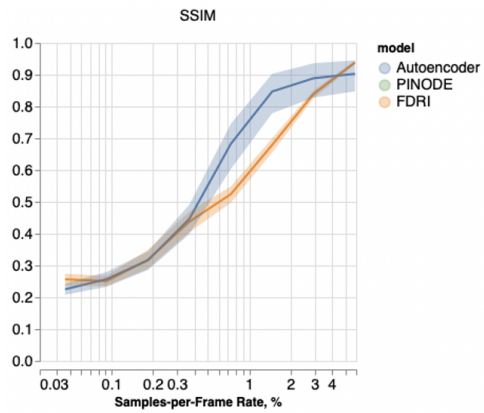


Results: Interpretation

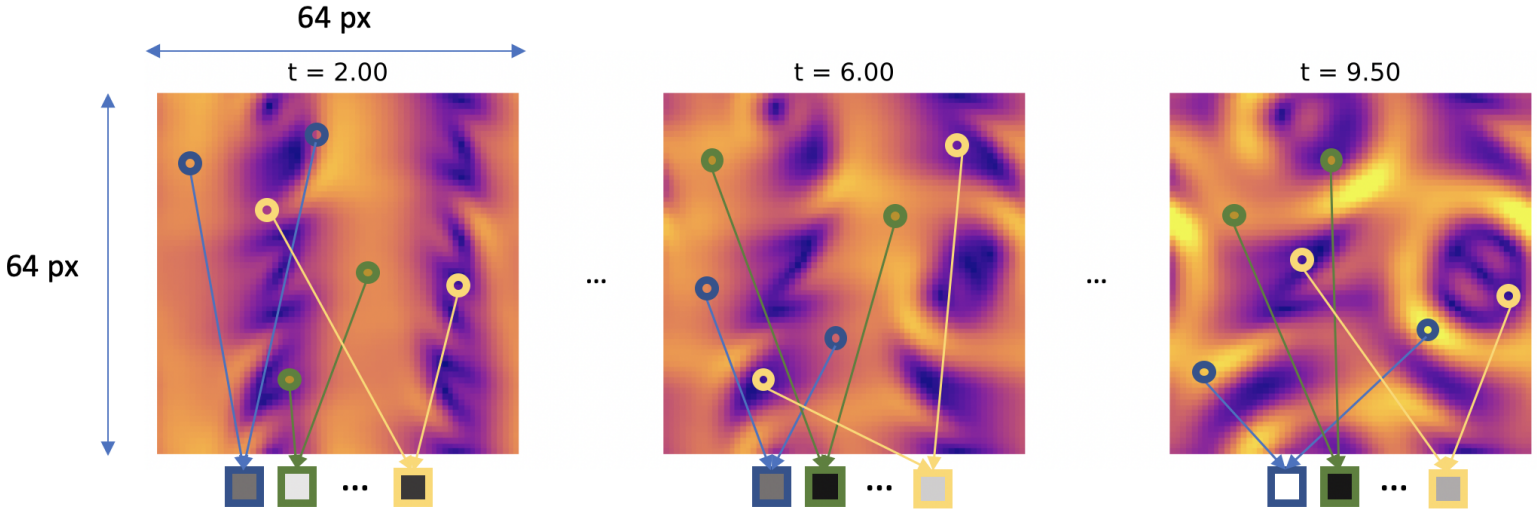


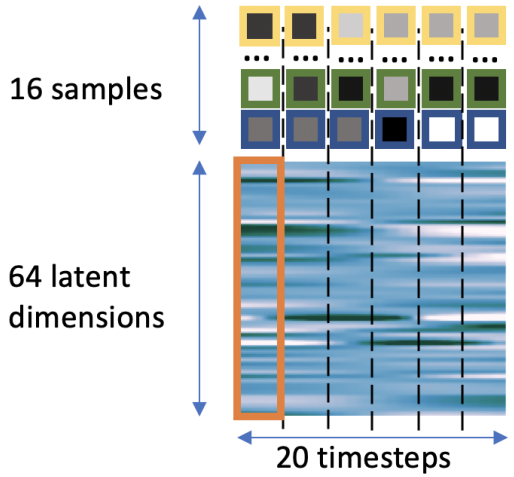
Results: Interpretation





Results: Interpretation





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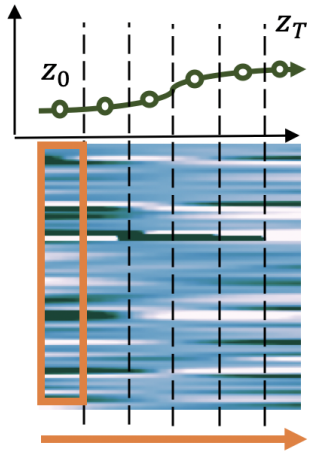
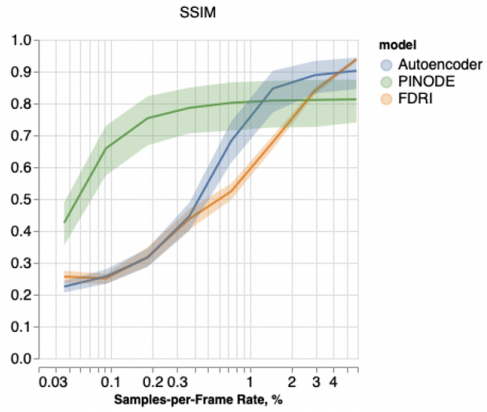


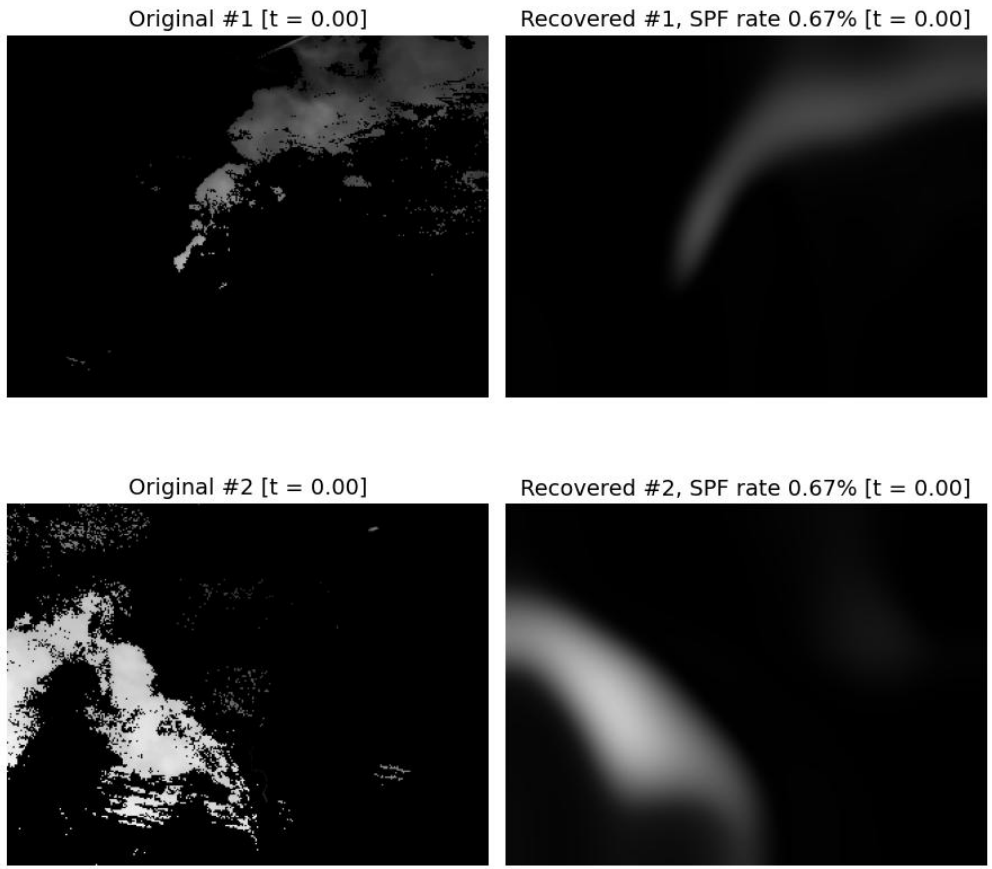
$$\frac{dz}{dt} = h(z)$$



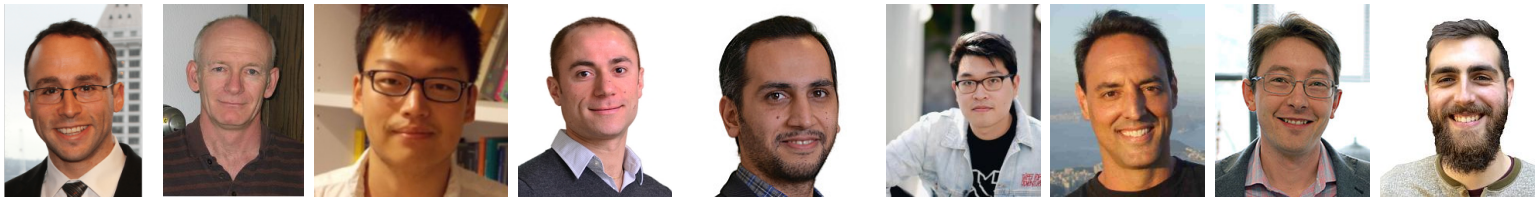
Results: Gas Monitoring

Gas monitoring problem:

- 494 240×320 video recordings, 10 steps each
- 512 samples per frame, SPF rate of 0.67%
- Background noise



Thank You!



Sparse Relaxed Regularized Regression for Linear Mixed-Effect Models
Together with Aleksandr Aravkin, James Burke, Damian Santomauro, and Peng Zheng

- "A Relaxation Approach to Feature Selection for Linear Mixed Effects Models"
  submitted to Journal of Computational and Graphical Statistics (JCGS)
- "Analysis of Relaxation Methods for Feature Selection in Mixed Effects Models"
  submitted to Journal of Computational Optimization and Applications (COAP)
- "`pysr3`: A Python Package for Spare Relaxed Regularized Regression"
  Journal of Open-Source Software (JOSS), 2023, ICCOPT 2022, SIAM OPT 2023

PINODE: Physics-Informed Neural ODEs
Together with Hassan Mansour, Saleh Nabi, and Yuying Liu

- "Physics-Informed Koopman Network"
  SIAM ADS 2023, arXiv:2211.09419
- "Physics-Informed Neural ODE: Embedding Physics into Models using Collocation Points"
  Submitted to Nature Special Issue on Physics-Informed Machine Learning

Single-Pixel Imaging with Reduced-Order Models
Together with J. Nathan Kutz, Steven Brunton, Joshua Rapp, Hassan Mansour, and Saleh Nabi

- "Single pixel imaging of spatio-temporal flows using differentiable latent dynamics" *in preparation*

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Appendix: $\mathcal{MSR}3$