



Forecasting Multiscale Image-Level Trajectories of Disease Progression with Irregularly-Sampled Longitudinal Medical Images

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ImageFlowNet: Forecasting Multiscale Image-Level Trajectories of Disease Progression with Irregularly-Sampled Longitudinal Medical Images

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What are we doing?

Predicting the progression of diseases in the image space



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Malignant mass lesion. Malignant cancer in dog, malignant cancer in cat. Skin cancer dog, skin cancer cat. Benign tumour on dog; benign growth on dog; non cancerous tumors in dogs Source: https://cdn.britannica.com/64/91764-004-0294A28A.jpg

Longitudinal Medical Images

Repeated scanning of the same patient over time



Temporal Sparsity

Unlike videos (many frames per second), these longitudinal images are separated by weeks, months or years.

Sampling Irregularity

Irregularly sampled over time for the same patient, and different sampling schedules among patients.

Spatial Misalignment

Almost never spatially aligned.

Why Interpolate on Image-Level?



Preliminaries

Neural ODE

$$egin{aligned} rac{\mathrm{d}y(au)}{\mathrm{d} au} &= f_ heta(y(au), au) \ y(t_1) &= y(t_0) + \int_{t_0}^{t_1} f_ heta(y(au), au) \mathrm{d} au \end{aligned}$$

Parameterize the continuous dynamics of hidden units using an ordinary differential equation (ODE) specified by a neural network.

$$y(t_1) = \text{ODESolve}(f(y(t), t, \theta), y(t_0), t_0, t_1)$$



Figure 1: *Left:* A Residual network defines a discrete sequence of finite transformations. *Right:* A ODE network defines a vector field, which continuously transforms the state. *Both:* Circles represent evaluation locations.

Chen, R. T., Rubanova, Y., Bettencourt, J., & Duvenaud, D. K. (2018). Neural Ordinary Differential Equations. *Advances in neural information processing systems*, *31*.

Preliminaries

Neural SDE

$$dX_{t} = f(t, X_{t}) dt + g(t, X_{t}) \circ dW_{t}$$

$$f(t, X_{t}) dt$$
Deterministic term
$$g(t, X_{t}) \circ dW_{t}$$
Stochastic term
$$\int g(t, X_{t}) \circ dW_{t}$$
Stochastic term

1.5 -

Kidger, P., Foster, J., Li, X., & Lyons, T. J. (2021). Neural SDEs as Infinite-Dimensional GANs. *International conference on machine learning* (pp. 5453-5463). PMLR.

Preprocessing



Figure S2: Our image registration pipeline. (A) Moving and fixed images come from the same eye at different time points. (B) SuperRetina is used to detect consistent and descriptive keypoints. (C) Keypoints are matched by descriptor similarity and filtered by distance heuristics. (D) The moving image is aligned under the constraint of a perspective transformation.

Methods (1/3)

ImageFlowNet predicts future image from earlier image and time gap.



Methods (2/3)

Latent features extracted by UNet are flowed with ODE or SDE.



Methods (3/3)

The flowed latent features are collected to construct the future image.



Optimization objective

Loss components affect different modules.



visual features $loss = l_r + \lambda_v l_v + \lambda_c l_v$ reconstruction contra	smoothness $l_c + \lambda_s l_s$ stive
Loss Component	Modules Affected
$l_r = MSE(\widehat{x_j}, x_j)$	
$l_{v} = D_{cos}\left(e(\widehat{x}_{j}), e(x_{j})\right)$	
$l_c = D_{cos}\left(z_{t_i}, z_{t_j}\right)$	Road
$l_s = f_{\theta} _2^2$	
$\lambda_v, \lambda_c, \lambda_s$: weighting coefficient	ents
MSE: pixel-level mean-	squared error
D_{cos} : cosine distance of	of vectors

(C)

- $e(\cdot)$: a pre-trained vision encoder
- ODE: ordinary differential equation
- SDE: stochastic differential equation

Optimization objective



1 Image reconstruction objective is achieved by a MSE loss, attending to low-level features on the pixel level.

2 Visual feature regularization guides the network to produce images that resemble the ground truth on high-level features judged by an encoder pretrained on ImageNet [15].

3 Contrastive learning regularization organizes a wellstructured ImageFlowNet latent space, by encouraging proximity of representations from images within the same longitudinal series, following the SimSiam formulation [16].

4 Trajectory smoothness regularization leverages a theorem in convex optimization (Lemma 2.2 in [17]) to enforce smoothness of trajectories by regularizing the norm of the field. Notably, this achieves Lipschitz continuity, satisfying a crucial assumption for our theoretical results.

Flowed latent features are collected hierarchically to form an image.



$$\frac{\mathrm{d}z_{\tau}^{(b)}}{\mathrm{d}\tau} = f_{\theta}^{(b)}(z_{\tau}^{(b)}) \quad \text{for } b \in [1, B] \quad (3a) \quad z_{t_j}^{(b)} = z_{t_i}^{(b)} + \int_{t_i}^{t_j} f_{\theta}^{(b)}(z_{\tau}^{(b)}) \mathrm{d}\tau \quad \text{for } b \in [1, B] \quad (3b)$$

 $\widehat{x_{j}} = \operatorname{ResBlock}(\operatorname{Concat}(\widetilde{z}_{t_{j}}^{(2)}, z_{t_{j}}^{(1)})), \text{ where}$ $\widetilde{z}_{t_{j}}^{(b)} = \operatorname{Upsample}(\operatorname{ResBlock}(\operatorname{Concat}(\widetilde{z}_{t_{j}}^{(b+1)}, z_{t_{j}}^{(b)}))) \text{ for } b \in [2, B-1], \text{ with } \widetilde{z}_{t_{j}}^{(B)} = z_{t_{j}}^{(B)}$ (4)

NOTE: We used a novel ODE formulation, which we call a *position-parameterized* ODE.

$$\frac{\mathrm{d}y(\tau)}{\mathrm{d}\tau} = f_{\theta}(y(\tau), \tau)$$

Standard ODE

$$\frac{\mathrm{d} z_\tau^{(b)}}{\mathrm{d} \tau} = f_\theta^{(b)}(z_\tau^{(b)})$$

Our ODE

Change of variable to make the comparison more obvious.

$$rac{\mathrm{d} z_{ au}^{(b)}}{\mathrm{d} au} = f_{ heta}^{(b)}(z_{ au}^{(b)}, au)$$
Standard ODE

$$\frac{\mathrm{d}z_{\tau}^{(b)}}{\mathrm{d}\tau} = f_{\theta}^{(b)}(z_{\tau}^{(b)})$$



Why the position-parameterized ODE?





Why the position-parameterized ODE?



Theoretical Results (1/2)

Equivalent Expressiveness of our ODE and standard ODE.

Proposition IV.1. Let f_{θ} be a continuous function that satisfies the Lipschitz continuity and linear growth conditions. Also, let the initial state $y(t_0) = y_0$ satisfy the finite second moment requirement. Suppose $z(t_0)$ is the latent representation learned by ImageFlowNet in the initial state corresponding to t_0 . Then, our neural ODEs are at least as expressive as the original neural ODEs, and their solutions capture the same dynamics.

Theoretical Results (2/2)

Connection between ImageFlowNet and dynamic optimal transport.

Proposition IV.2. If we consider an image as a distribution over a 2D grid, ImageFlowNet is equivalently solving a dynamic optimal transport problem, as it meets 3 essential criteria: (1) matching the density, (2) smoothing the dynamics, and (3) minimizing the transport cost, where the ground distance is the Euclidean distance in the latent joint embedding space.

Empirical Results (1/3)

Future Image Forecasting

Datasets:

- 1. Retinal geographic atrophy
 - a. 2-5 years
 - b. <24 month gap
- 2. Brain multiple sclerosis
 - a. ~5 years
 - b. ~4.4 time points per person
- 3. Brain glioblastoma
 - a. <5 years
 - b. 2-18 time points per person

	Ground Truth	Input	Linear	Cubic Spline	T-UNet	T-Diffusion		ImageFlowNet _{ODE} ++		mageFlowNetsoc++
	x_j	x _i	x_j	x_j	x_j	xj	xj	xj	xj	xj
Image	PSNR/SSIM	20.09/0.572	18.72 / 0.540	18.72 / 0.540	19.15/0.550	19.76 / 0.543	20.27 / 0.539	21.5670.587	21.27/0.558	21.98/0.597
Residual Map	MAE / MSE	.156/0.039	0.17770.054	0.17770.054	0.16870.049	0.13070.026	0.137/0.029	0.13170.028	0.13970.030	.125/0.025
Disease Region	DSC/HD	0.810 / 7.28	0.848 / 7.00	0.848 / 7.00	0.850 / 6.94	0.841/6.35	0.902 / 5.39	0.876 / 6.71	0.884/5.83	0.925/6.32
	PSNR / SSIM	30.98 / 0.914	30.38 / 0.911	25.19 / 0.878	31.34 / 0.913	30.94 / 0.914	31.61 / 0.913	33.81/0.913	31.29 / 0.909	33.93 / 0.915
Image										
	MAE / MSE	0.024/0.003	0.028 / 0.003	0.057/0.012	0.025/0.003	0.025 / 0.003	0.023 / 0.003	0.019/0.002	0.025 / 0.003	0.019/0.002
Residual Map		-+©	* O	+0	+0	*	*	+0		
	DSC / HD	0.803 / 8.00	0.494 / 28.86	0.311/35.36	0.823 / 8.00	0.803 / 8.00	0.846 / 7.00	0.844 / 3.16	0.813/6.00	0.854/3.16
Disease Region										
	PSNR / SSIM	30.98 / 0.914	29.20 / 0.865	32.60 / 0.899	31.34 / 0.909	29.72 / 0.889	31.88 / 0.914	33.80 / 0.909	32.81/0.911	31.37 / 0.903
Image			-			· · ·		L. C.	1	-
Residual Map	MAE / MSE	0.026 / 0.004	0.031 / 0.005	0.023/0.003	0.022/0.003	0.026 / 0.004	0.021/0.003	0.019/0.002	0.021/0.002	0.022/0.003
	DSC / HD	0.136 / 45.54	0.006 / 47.54	0.000 / 63.19	0.127 / 45.88	0.138 / 45.54	0.078 / 44.60	0.150 / 16.12	0.093 / 42.95	0.103 / 51.97
Disease Region							- C	2-1-1	Ů	

Empirical Results (1/3)



Empirical Results (1/3)

Dataset	Metric	Linear [†] [24]	Cubic Spline [†] [25]	T-UNet [33]	T-Diffusion [28]	ImageFlowNet _{ODE} (ours)	ImageFlowNet _{ODE} ++ (ours)	ImageFlowNet _{SDE} (ours)	ImageFlowNet _{SDE} ++ (ours)
Retinal	PSNR \uparrow	$20.22 {\pm} 0.00$	19.79 ± 0.00	$\textbf{22.06} {\pm 0.33}$	$\textbf{22.29} {\pm}~\textbf{0.33}$	$22.63 {\pm}~0.26$	22.74± 0.25	$22.32{\pm}~0.29$	22.89 ± 0.28
Images	SSIM ↑	0.535 ± 0.000	0.505 ± 0.000	0.635 ± 0.015	0.624 ± 0.016	0.646 ± 0.012	0.647 ± 0.013	0.651 ± 0.015	0.651 ± 0.012
all	$MAE \downarrow$	0.163 ± 0.000	0.177 ± 0.000	0.126 ± 0.005	0.122 ± 0.004	0.119 ± 0.004	0.118 ± 0.004	0.124 ± 0.005	0.115 ± 0.004
cases	$MSE \downarrow$	0.050 ± 0.000	0.060 ± 0.000	0.029 ± 0.002	0.027 ± 0.002	0.024 ± 0.001	0.024 ± 0.001	0.027 ± 0.002	0.023 ± 0.001
1	DSC ↑	0.833 ± 0.000	0.756 ± 0.000	0.872 ± 0.012	0.867 ± 0.014	0.874 ± 0.012	0.873 ± 0.011	0.885 ± 0.011	0.883 ± 0.012
	HD↓	51.64 ± 0.00	54.30 ± 0.00	44.59 ± 4.66	44.41 ± 4.74	42.68 ± 4.82	47.10 ± 4.89	48.14 ± 4.87	45.14 ± 4.89
minor	PSNR ↑	$21.36 {\pm 0.00}$	21.08 ± 0.00	$22.56 {\pm 0.55}$	$22.99 {\pm}~0.55$	$23.23 {\pm}~0.34$	23.44 ± 0.33	$23.28 {\pm}~ 0.36$	$\textbf{23.63}{\scriptstyle\pm}~0.43$
atrophy	SSIM ↑	$0.599 {\pm}~0.000$	0.586 ± 0.000	0.662 ± 0.023	0.657 ± 0.024	$0.682 {\pm} 0.018$	0.685 ± 0.018	$\textbf{0.693} {\pm 0.018}$	0.687± 0.019
growth	$MAE \downarrow$	$0.141 {\pm}~0.000$	0.147 ± 0.000	$0.121 {\pm}~0.007$	$0.114 {\pm} 0.007$	$0.110 {\pm 0.005}$	$\underline{0.108} \pm 0.004$	$0.109 {\pm 0.005}$	0.106 ± 0.005
2	$MSE\downarrow$	$0.038 {\pm}~0.000$	0.042 ± 0.000	$0.027 {\pm}~0.003$	$0.024 {\pm} 0.002$	$0.021 {\pm}~0.002$	$\textbf{0.020} \pm 0.002$	$0.021 {\pm}~0.002$	$\textbf{0.020} \pm 0.002$
	$DSC\uparrow$	0.900 ± 0.000	$0.874 {\pm 0.000}$	$\textbf{0.949} {\pm}~\textbf{0.004}$	$\textbf{0.949} {\pm}~0.004$	$0.936 {\pm 0.009}$	$0.939 {\pm}~0.007$	$0.948 {\pm 0.005}$	0.948 ± 0.006
	$\text{HD}\downarrow$	$38.15 {\pm}~0.00$	41.67 ± 0.00	35.74 ± 5.67	$29.40 {\pm}~ 4.77$	$34.59 {\scriptstyle \pm 6.20}$	$39.86 {\pm}~6.40$	$\underline{31.66} \pm 5.21$	$36.98 \pm \textbf{6.04}$
maior	PSNR ↑	19.02 ± 0.00	18.41 ± 0.00	21.40 ± 0.33	21.68 ± 0.32	21.94 ± 0.34	22.01 ± 0.33	22.01 ± 0.30	22.10 ± 0.31
atrophy	SSIM †	0.468 ± 0.000	0.420 ± 0.000	0.607 ± 0.017	0.588 ± 0.017	0.607 ± 0.014	0.606 ± 0.014	0.607 ± 0.014	0.613 ± 0.013
growth	MAE 🗼	$0.186 {\pm 0.000}$	0.210 ± 0.000	$\overline{0.135} \pm 0.006$	$0.131 {\pm 0.006}$	$\overline{0.129} \pm 0.006$	$0.129 {\pm 0.006}$	0.128 ± 0.005	0.126 ± 0.005
3	MSE ↓	0.063 ± 0.000	0.080 ± 0.000	$0.032 {\pm} 0.003$	$0.030 {\pm}~0.002$	$0.028 {\pm 0.002}$	0.028 ± 0.002	0.027± 0.002	$\textbf{0.027} {\pm}~0.002$
	DSC ↑	$0.762 {\pm} 0.000$	$0.631 {\pm} 0.000$	$0.784 {\pm} \hspace{0.05cm} 0.016$	$0.779 {\pm}~ 0.019$	$0.807 {\pm 0.014}$	0.803 ± 0.012	$\textbf{0.817} {\pm 0.016}$	$\underline{0.814} \pm 0.017$
	$\mathrm{HD}\downarrow$	$65.97 {\pm}~0.00$	67.73 ± 0.00	$61.43 \pm \textbf{7.26}$	$60.36 {\pm}~7.37$	$\textbf{51.28} \pm 7.13$	$54.79 \pm \textbf{7.19}$	$65.65 \pm \textbf{7.17}$	<u>53.81</u> ± 7.49
Brain	PSNR ↑	30.07 ± 0.00	29.56 ± 0.00	31.55 ± 0.20	31.57±0.23	32.01±0.19	32.34± 0.20	32.40 ± 0.20	32.41 ± 0.20
MS	SSIM †	0.895 ± 0.000	0.888 ± 0.000	0.909 ± 0.003	0.907 ± 0.003	0.914 ± 0.002	0.915 ± 0.002	0.913 ± 0.002	0.915 ± 0.002
Images	MAE 🗼	$0.028 {\pm 0.000}$	0.030 ± 0.000	0.024 ± 0.000	0.024 ± 0.001	0.023 ± 0.000	$\textbf{0.021} {\pm 0.000}$	$\textbf{0.021} {\pm}~0.000$	0.021 ± 0.000
4	MSE ↓	$0.004 {\pm} 0.000$	0.005 ± 0.000	0.004 ± 0.000	0.004 ± 0.000	0.003 ± 0.000	$\textbf{0.003} {\pm 0.000}$	0.003 ± 0.000	$\textbf{0.003} {\pm 0.000}$
	DSC ↑	$0.739 {\pm} 0.000$	$0.682 {\pm 0.000}$	$0.774 {\pm}~0.007$	0.771 ± 0.007	$0.775 {\scriptstyle \pm 0.007}$	0.777 ± 0.007	0.777 ± 0.007	0.774 ± 0.007
	$HD\downarrow$	22.73 ± 0.00	26.23 ± 0.00	22.00 ± 1.30	$\textbf{20.91} \pm 1.23$	$\textbf{22.38} {\pm}~ \textbf{1.28}$	$21.72 {\pm}~1.16$	$22.21 {\pm}~1.27$	$\underline{21.28} \pm 1.27$
Brain	PSNR ↑	35.32 ± 0.00	33.60 ± 0.00	35.73 ± 0.13	35.49 ± 0.17	35.86± 0.12	35.90 ± 0.14	35.77 ± 0.12	35.79± 0.15
GBM	SSIM †	$0.929 {\pm 0.000}$	0.895 ± 0.000	$0.935 {\pm 0.001}$	0.940 ± 0.001	$\overline{0.940} \pm 0.001$	0.943 ± 0.001	$0.937 {\pm 0.001}$	$0.939 {\pm 0.001}$
Images	$MAE\downarrow$	$0.017 {\pm}~0.000$	0.024 ± 0.000	0.015 ± 0.000	$\overline{0.014} \pm 0.000$	0.014 ± 0.000	$\textbf{0.014} {\pm 0.000}$	$0.015 {\pm 0.000}$	0.015 ± 0.000
5	MSE ↓	0.002 ± 0.000	0.005 ± 0.000	$\textbf{0.001} \pm 0.000$	0.002 ± 0.000	$\textbf{0.001} \pm 0.000$	0.001 ± 0.000	0.001 ± 0.000	$\textbf{0.001} \pm 0.000$
	DSC †	$\underline{0.300} \pm 0.000$	$0.287 {\pm 0.000}$	$0.258 {\pm}~0.018$	$0.253 {\pm} 0.017$	$0.302 {\pm 0.019}$	$0.266 {\pm} 0.018$	$0.286 {\pm 0.019}$	$0.287 {\pm 0.017}$
	$HD\downarrow$	$\underline{170.44} \pm 0.00$	165.62 ± 0.00	$195.52 \pm \textbf{7.69}$	$189.61{\pm}7.64$	$198.19 {\pm}~7.78$	$185.14{\scriptstyle\pm}7.69$	$196.37{\scriptstyle\pm}~7.74$	$181.66 \pm \textbf{7.66}$
1.4.5	Rank	6.3 ± 1.6	7.3±2.0	4.9 ±1.4	4.6 ±1.9	2.9 ±1.9	2.3 ± 1.6	3.4 ±2.0	2.1 ±1.3
-, -, -		65	76.10	10.15	15.00	21	27.17	30.10	20110

Table 1: Image forecasting performance: metric $(x_j, \hat{x_j})$. $\hat{x_j} = \mathcal{F}(x_i, t_i, t_j), \forall i < j$. [†]Extrapolation methods use the entire history. "++" means using the 3 regularizations in Eqn (6)

Empirical Results (2/3)

Latent Space Regularization



Figure 4: Joint representation space and the effect of contrastive learning regularization. Red dots are the observed disease states and arrows connect adjacent transitions. Normalized time is color coded. (A) Without regularization ($\lambda_c = 0$). (B) With contrastive learning regularization ($\lambda_c = 0.01$).

Empirical Results (3/3)

Test-Time Optimization

(Using the entire history to locally fine-tune the vector field)

Iterations	Learning Rate	PSNR ↑	SSIM ↑	MAE↓	MSE↓	DSC↑	HD↓
N/A	N/A	22.31	0.643	0.123	0.027	0.827	51.07
1	10^{-4}	22.52	0.646	0.120	0.025	0.829	48.97
1	10^{-5}	22.36	0.643	0.122	0.027	0.827	51.02
1	10^{-6}	22.31	0.643	0.123	0.027	0.827	51.07
10	10^{-4}	20.63	0.605	0.157	0.042	0.749	64.79
10	10^{-5}	<u>22.59</u>	0.646	0.119	0.025	0.829	49.92
10	10^{-6}	22.36	0.644	0.122	0.027	0.827	51.01
100	10^{-4}	19.63	0.571	0.177	0.056	0.726	70.12
100	10^{-5}	20.92	0.614	0.152	0.040	0.759	58.76
100	10^{-6}	22.61	0.646	0.119	0.025	0.829	<u>49.74</u>

Table 2: Effect of test-time optimization.

Ablation

TABLE II

FLOW FIELD FORMULATION.

	PSNR ↑	SSIM ↑	MAE↓	MSE↓	DSC ↑	HD↓
$f_{ heta}(z_t,t)$	22.42	0.643	0.123	0.027	0.872	48.38
$f_{ heta}(z_t)$	22.63	0.646	0.119	0.024	0.874	42.68

TABLE III

LATENT REPRESENTATION.

	PSNR ↑	SSIM↑	MAE↓	MSE↓	DSC↑	HD↓
bottleneck only	22.33	0.639	0.122	0.026	0.850	48.13
all unique resolutions	22.49	0.643	0.122	0.025	0.859	43.39
all unique layers	22.63	0.646	0.119	0.024	0.874	42.68

TABLE IV VISUAL FEATURE REGULARIZATION.

λ_v	PSNR ↑	SSIM ↑	MAE↓	MSE↓	DSC↑	HD↓
0	22.63	0.646	0.119	0.024	0.874	42.68
0.001	22.65	0.658	0.118	0.024	0.872	44.27
0.01	22.64	0.650	0.120	0.025	0.872	45.89
0.1	22.57	0.647	0.120	0.025	0.869	50.69
1	22.54	0.634	0.124	0.027	0.867	48.13

TABLE V

CONTRASTIVE REGULARIZATION.

λ_c	PSNR ↑	SSIM ↑	MAE↓	MSE↓	DSC↑	HD↓
0	22.63	0.646	0.119	0.024	0.874	42.68
0.001	22.63	0.646	0.119	0.025	0.872	46.23
0.01	22.65	0.652	0.118	0.024	0.875	42.18
0.1	22.38	0.651	0.121	0.025	0.871	45.30
1	22.25	0.644	0.121	0.025	0.868	46.85

TABLE VI

SMOOTHNESS REGULARIZATION.

λ_s	PSNR ↑	SSIM ↑	MAE↓	MSE↓	DSC↑	HD↓
0	22.63	0.646	0.119	0.024	0.874	42.68
0.001	22.38	0.649	0.123	0.027	0.870	46.91
0.01	22.65	0.648	0.119	0.024	0.870	45.71
0.1	22.70	0.657	0.118	0.024	0.878	47.44
1	22.69	0.655	0.118	0.024	0.875	45.16

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