

Supporting Material for 'Diffusion Tempering Improves Parameter Estimation with Probabilistic Integrators for Ordinary Differential Equations'

1 Different schedules

In Fig. 1 we illustrate the comparative performance of different schedules.

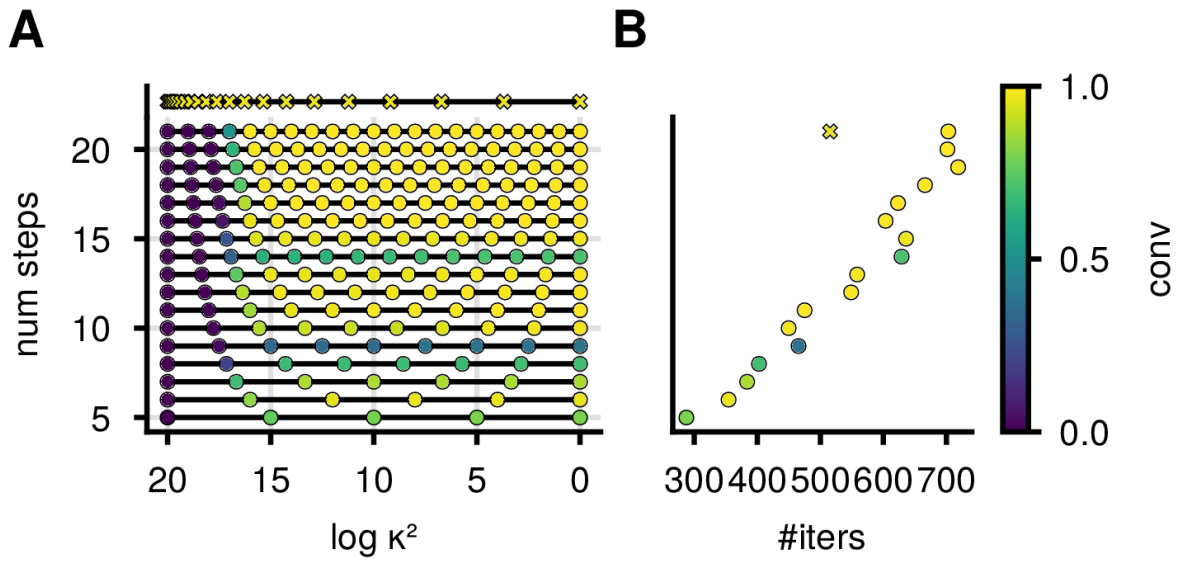


Figure 1: Comparison of different schedules. **A** Percentage of correctly converged runs at every step of the tempering schedule for different schedules. Circles, $\log \kappa^2$ was reduced linearly. Crosses, $\log \kappa^2$ was reduced with an exponential decay. **B** Cost of each schedule and final convergence.

2 Effect of early stopping

Tab.1 shows the effect of early stopping for the pendulum (PD), Lotka Volterra (LV) model and Hodgkin-Huxley (HH) model. The number of parameters is denoted in the model's index.

model	conv	iter	model	conv	iter
PD_1	1.00	303.89 ± 12.43	PD_1	1.00	92.21 ± 0.95
LV_2	0.77	411.18 ± 151.25	LV_2	0.79	132.43 ± 31.01
LV_4	0.43	727.15 ± 482.93	LV_4	0.44	292.05 ± 139.98
HH_2	1.00	696.22 ± 78.10	HH_2	0.96	197.81 ± 40.38

Table 1: Effect of early stopping on the cost of compute. **left** Without early stopping. **right** With early stopping.

3 Updated Table 1

Tab.2 shows the updated Table 1.

ODE	D_θ	ALG	ITER	pRMSE	CONV	tRMSE	N_θ
PD	1	Fenrir	74.12 ± 11.55	0.01 ± 0.08	0.99	0.04 ± 0.26	0.99 ± 0.10
PD	1	RK	34.11 ± 18.45	1.42 ± 1.09	0.32	0.98 ± 0.72	0.32 ± 0.47
PD	1	ours	303.89 ± 12.43	0.00 ± 0.00	1.00	0.02 ± 0.00	1.00 ± 0.00
LV	2	Fenrir	60.68 ± 36.73	1.41 ± 1.01	0.20	2.84 ± 2.71	0.40 ± 0.80
LV	2	RK	97.15 ± 146.95	1.35 ± 1.11	0.24	2.35 ± 1.32	0.48 ± 0.86
LV	2	ours	411.18 ± 151.25	0.41 ± 0.82	0.77	$*0.54 \pm 1.14$	1.54 ± 0.85
LV	4	Fenrir	112.45 ± 47.24	1.31 ± 0.94	0.23	4.18 ± 13.65	1.07 ± 1.70
LV	4	RK	271.49 ± 151.05	1.09 ± 0.76	0.24	6.57 ± 34.45	0.97 ± 1.71
LV	4	ours	727.15 ± 482.93	0.81 ± 0.88	0.43	$*10.41 \pm 69.37$	1.76 ± 1.98
HH ₁	1	Fenrir	46.96 ± 19.08	0.38 ± 0.67	0.68	7.85 ± 10.70	0.68 ± 0.47
HH ₁	1	RK	43.30 ± 43.45	0.42 ± 0.48	0.57	7.54 ± 8.26	0.57 ± 0.50
HH ₁	1	ours	382.08 ± 32.19	0.00 ± 0.00	1.00	0.43 ± 0.02	1.00 ± 0.00
HH ₁	2	Fenrir	110.04 ± 61.70	0.20 ± 0.37	0.75	5.89 ± 10.15	1.53 ± 0.83
HH ₁	2	RK	54.02 ± 62.60	0.28 ± 0.45	0.72	4.88 ± 7.58	1.44 ± 0.90
HH ₁	2	ours	696.22 ± 78.10	0.00 ± 0.00	1.00	0.42 ± 0.04	2.00 ± 0.00
HH ₁	3	Fenrir	122.15 ± 49.74	0.59 ± 0.65	0.51	9.31 ± 9.63	1.53 ± 1.51
HH ₁	3	RK	223.55 ± 117.31	0.90 ± 0.25	0.03	14.33 ± 4.01	0.13 ± 0.56
HH ₁	3	ours	676.33 ± 150.72	0.01 ± 0.10	0.99	0.60 ± 1.51	2.97 ± 0.30
HH ₁	6	Fenrir	108.06 ± 108.49	13.36 ± 6.97	0.00	26.21 ± 7.38	1.05 ± 0.22
HH ₁	6	RK	210.26 ± 120.86	12.27 ± 6.87	0.00	16.80 ± 3.81	1.18 ± 0.39
HH ₁	6	ours	2159.60 ± 532.55	10.36 ± 7.72	0.00	15.20 ± 5.41	1.21 ± 0.46
HH ₂	4	Fenrir	286.54 ± 205.37	0.28 ± 0.44	0.68	12.00 ± 17.37	2.80 ± 1.78
HH ₂	4	RK	136.50 ± 200.20	0.43 ± 0.56	0.50	7.98 ± 9.86	2.08 ± 1.81
HH ₂	4	ours	1492.03 ± 335.17	0.00 ± 0.00	1.00	0.60 ± 0.01	4.00 ± 0.00
HH ₂	6	Fenrir	221.28 ± 144.56	0.62 ± 0.72	0.50	13.01 ± 13.10	3.06 ± 2.96
HH ₂	6	RK	390.34 ± 195.85	0.88 ± 0.22	0.00	19.36 ± 5.54	0.31 ± 0.75
HH ₂	6	ours	1525.57 ± 448.56	0.12 ± 0.32	0.88	$*3.01 \pm 6.70$	5.28 ± 1.96

Table 2: Comparison of different methods, models and model sizes for parameter estimation. LV: Lottka-Volterra, PD: Pendulum, HH_x Hodgkin–Huxley with x compartments, D_θ : Number of parameters, N_θ : The number of correctly identified parameters, CONV: correctly converged. *Runs with a final loss of NaN where excluded from computation if marked with *.*

4 Noisy gradients

In Tab.3 we show the effect of noising the gradients of the RK baseline.

scale	τ_{decay}	conv	pRMSE	iter
0.00	0.00	0.32	1.42 ± 1.09	33.47 ± 18.11
0.01	0.00	0.35	1.40 ± 1.11	33.79 ± 12.84
0.05	0.00	0.34	1.41 ± 1.10	29.89 ± 10.77
0.10	0.00	0.37	1.40 ± 1.13	27.30 ± 11.84
0.50	0.00	0.49	1.14 ± 1.13	15.19 ± 10.72
1.00	0.00	0.63	0.77 ± 1.05	15.52 ± 14.12
5.00	0.00	0.64	0.51 ± 0.88	13.01 ± 8.87
10.00	0.00	0.39	0.64 ± 0.93	10.43 ± 7.19
50.00	0.00	0.45	0.49 ± 0.83	11.66 ± 8.26
100.00	0.00	0.28	0.44 ± 0.74	10.26 ± 7.42
0.00	5.00	0.32	1.42 ± 1.09	33.47 ± 18.11
0.01	5.00	0.31	1.45 ± 1.08	35.94 ± 18.58
0.05	5.00	0.33	1.45 ± 1.10	32.58 ± 13.39
0.10	5.00	0.35	1.40 ± 1.11	33.65 ± 12.85
0.50	5.00	0.43	1.24 ± 1.13	22.23 ± 14.93
1.00	5.00	0.53	0.98 ± 1.08	22.68 ± 18.51
5.00	5.00	0.59	0.67 ± 0.99	15.23 ± 13.33
10.00	5.00	0.45	0.51 ± 0.84	13.11 ± 13.49
50.00	5.00	0.40	0.51 ± 0.79	11.36 ± 11.60
100.00	5.00	0.41	0.58 ± 0.86	12.54 ± 14.20
0.00	10.00	0.32	1.42 ± 1.09	33.47 ± 18.11
0.01	10.00	0.33	1.43 ± 1.10	33.42 ± 12.90
0.05	10.00	0.32	1.44 ± 1.09	34.21 ± 11.00
0.10	10.00	0.34	1.39 ± 1.11	33.40 ± 12.70
0.50	10.00	0.46	1.22 ± 1.14	18.89 ± 13.20
1.00	10.00	0.50	1.08 ± 1.10	18.58 ± 14.95
5.00	10.00	0.61	0.58 ± 0.94	14.28 ± 12.63
10.00	10.00	0.58	0.55 ± 0.90	12.95 ± 10.90
50.00	10.00	0.32	0.41 ± 0.71	9.96 ± 8.40
100.00	10.00	0.37	0.40 ± 0.72	10.92 ± 8.47
Fenrir		0.75	0.20 ± 0.37	110.04 ± 61.70
ours		1.00	0.00 ± 0.00	696.22 ± 78.10

Table 3: Effect of adding noise to the gradients of the RK baseline. The noise was added with different scales / variance and exponential decays.