Non-reversible Gaussian processes for identifying latent dynamical structure in neural data

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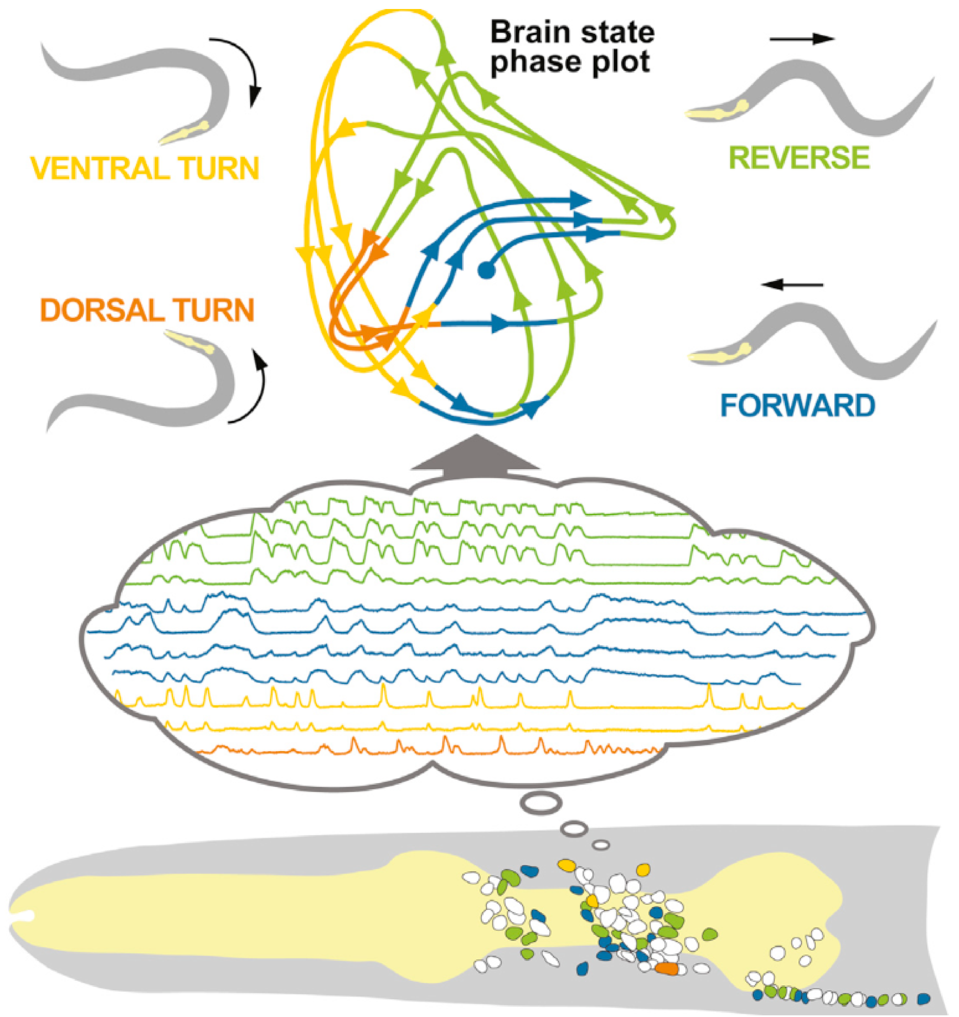
EXECUTIVE SUMMARY

- In neuroscience, we aim to uncover how the dynamics of brain circuits give rise to a variety of behaviours. As a key step, we often smooth and denoise high-dimensional timeseries of neural activity by reducing their dimensionality.



[Reproduced from Kato et al., 2015]

- Bayesian methods exist for doing this (e.g. GPFA [1]), offering data efficiency, uncertainty quantification and principled model selection.
- Ideally, low-D trajectories would retain the phase portrait of the underlying dynamics. However, most methods developed thus far aim at capturing variance; one can only hope that high-variance components also reflect dynamics.
- Here, we extend Gaussian process-based methods to capture dynamical structure. We do this by constructing multi-output GP kernels that express a key property of dynamical systems: **temporal non-reversibility**.
- **Non-reversible kernels** are interesting in their own right for regression, yielding better fit to data coming from dynamical systems.
- We propose Gaussian Process Factor Analysis with Dynamical Structure (**GPFADS**), which uses non-reversible kernels to enable simultaneous dimensionality reduction, smoothing and demixing of dynamical state trajectories in toy and real data.

NON-REVERSIBLE GP KERNELS

Second-order reversibility:

let $K(\tau) \in \mathbb{R}^{M\times M}$ be a M-output stationary covariance function. Define non-reversibility index:

$$\zeta^2 = \frac{\int d\tau \|K(\tau) - K(-\tau)\|_F^2}{\int d\tau \|K(\tau) + K(-\tau)\|_F^2}$$

One can show $0 \le \zeta \le 1$.

Any $K(\tau) = \mathbb{E}[x(t)x(t+\tau)^\top]$ can be "Kronecker"-decomposed:

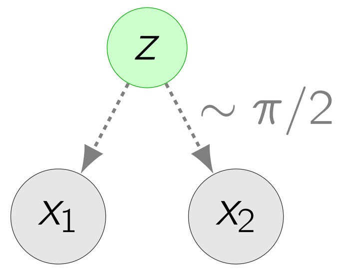
$$K(\tau) = \underbrace{\sum_{\ell=1}^{n^+} \lambda_\ell^+ A_\ell^+ f_\ell^+(\tau)}_{\text{reversible}} + \underbrace{\sum_{\ell=1}^{n^-} \lambda_\ell^- A_\ell^- f_\ell^-(\tau)}_{\text{breaks reversibility}} \qquad \zeta^2 = \frac{\sum (\lambda_\ell^-)^2}{\sum (\lambda_\ell^+)^2}$$

General planar construction:

$$K(\tau) \propto \begin{pmatrix} \nu & \rho \\ \rho & 1/\nu \end{pmatrix} \underbrace{f(\tau)}_{\text{any scalar covariance...}} + \alpha\sqrt{1-\rho^2}\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \underbrace{\mathcal{H}[f](\tau)}_{\text{...its Hilbert transform}}, \quad |\alpha| \le 1$$

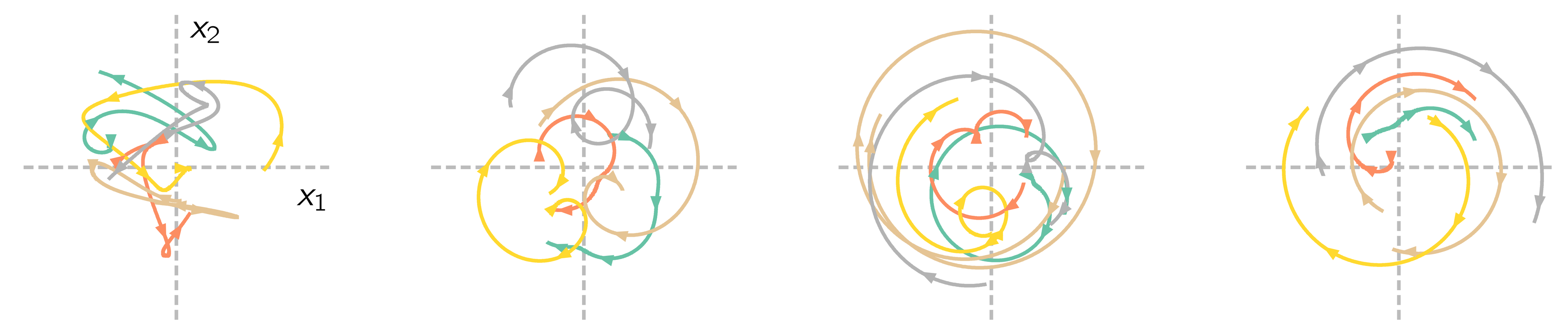
max. $\zeta = |\alpha|$ when $\nu = 1$ and $\rho = 0$ (spherical process)

In the Fourier domain, this corresponds to the two outputs being entrained to a shared latent process $z \sim \mathcal{GP}(0, f)$ with some spectral coherence $|\alpha|$ and frequency-independent phase shifts separated by $\pi/2$ (the Fourier transform of $\mathcal{H}[f]$ is $-j\,\mathrm{sgn}(\omega)\hat{f}(\omega)$).

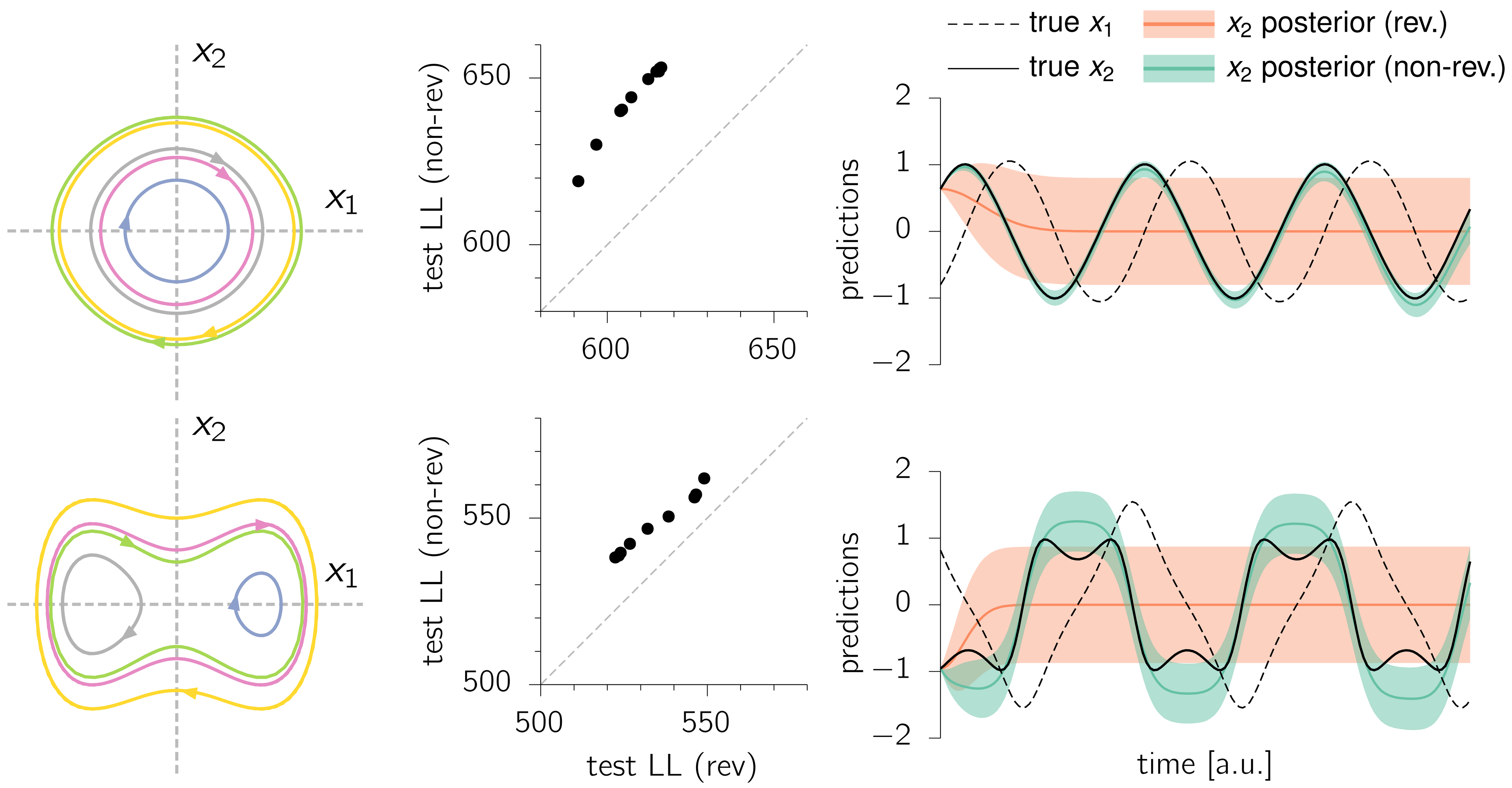


In the maximally non-reversible samples shown below (for three different marginal kernels, and $\zeta = 1$), any subset of any sample trajectory has zero probability density under time-reversal:

squared exponential	squared exponential	sinc	spectral mixture
reversible ($\zeta = 0$)	non-reversible ($\zeta = 1$)	non-reversible ($\zeta = 1$)	non-reversible ($\zeta = 1$)



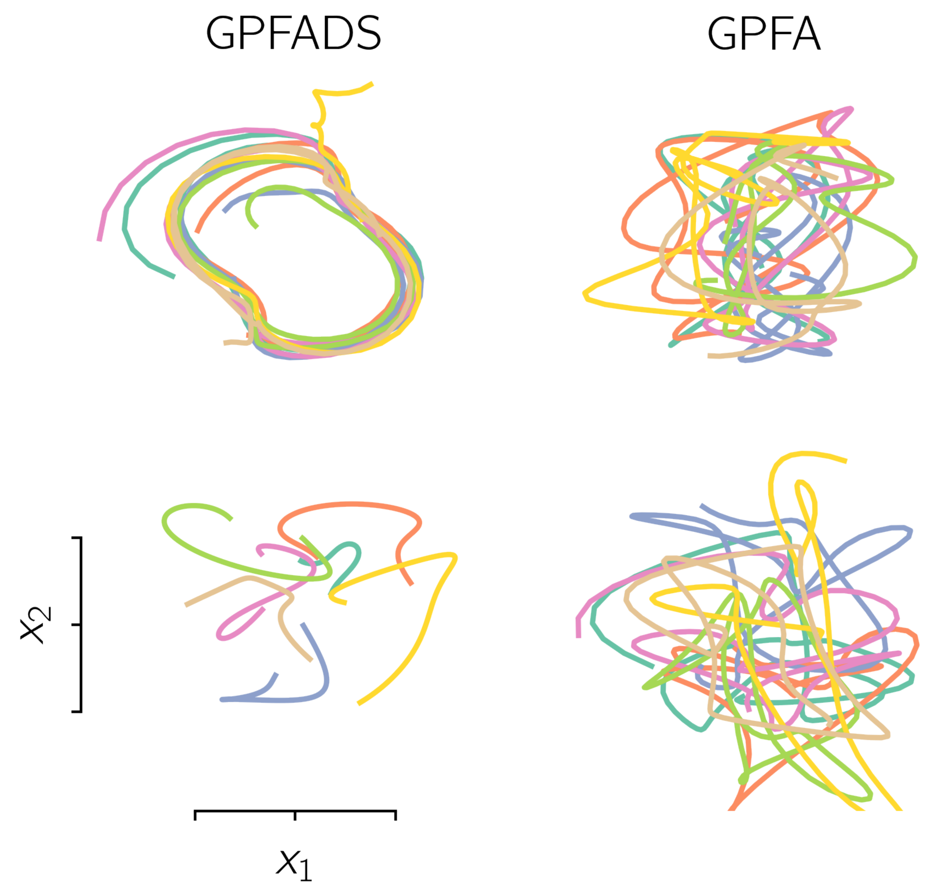
REGRESSION



GPFADS

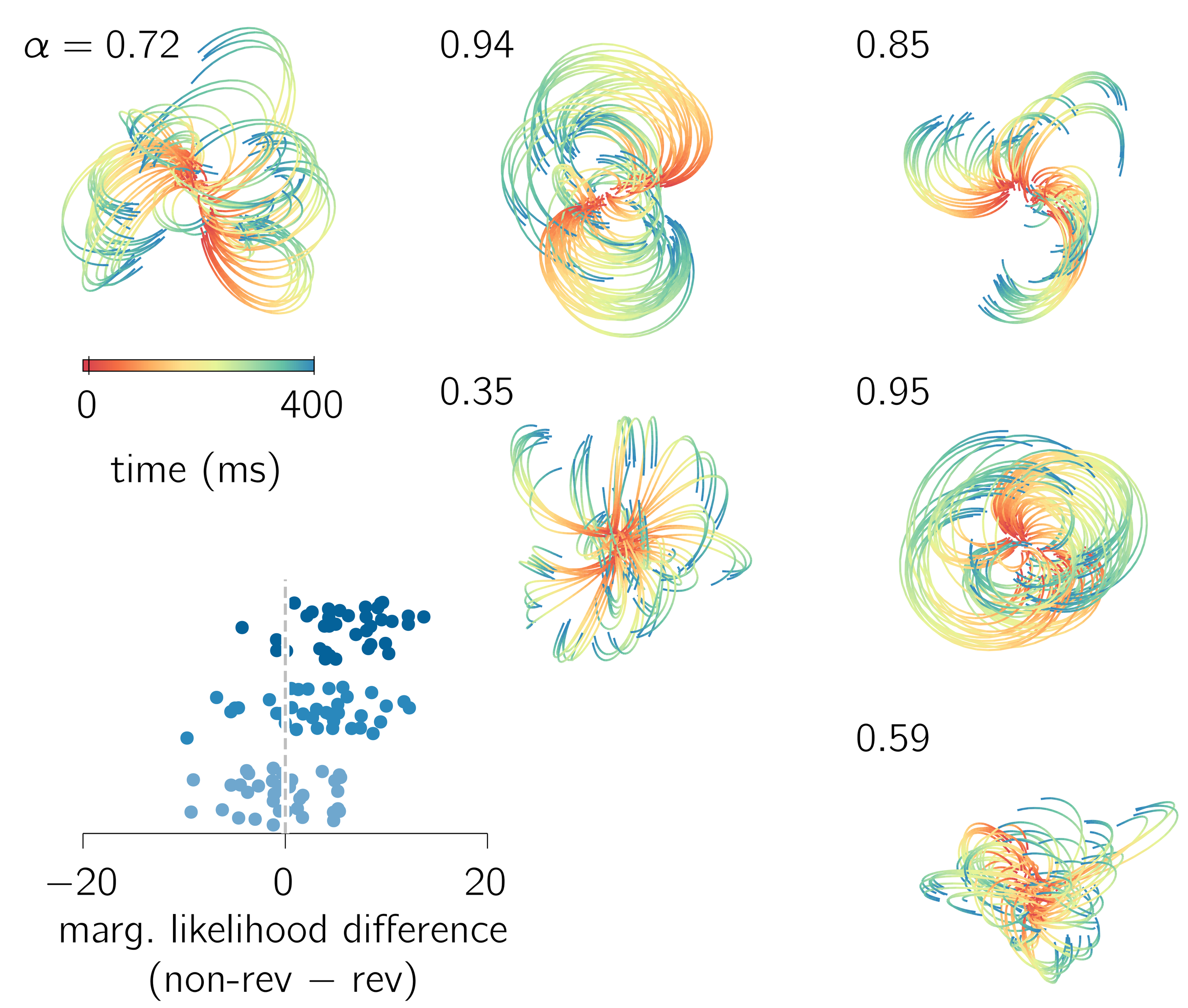
$x(t) \sim \mathcal{GP}(0, K(\cdot))$ with a non-reversible stationary M-output covariance $K(\cdot)$

$y(t)|x(t) \sim \mathcal{N}(Cx(t), \sigma^2 I)$ with some mixing matrix $C \in \mathbb{R}^{N\times M}$



- Van der Pol oscillations embedded in high dimensions, together with a distractor noisy planar process of matching time scales
- GPFADS (fit with two independent latent planes), unlike GPFA, demixes the two processes
- learns a non-reversible prior, effectively a *simpler* model which does not place probability mass on time-reversed trajectories, which never occur

We applied GPFADS to M1 reaching data: 218 neurons and 108 movement conditions. With a single latent plane, GPFADS finds the same latents as GPFA – maximum variance. With more room, GPFADS cleaning isolates very non-reversible components, which need not be pure rotations (thus generalizes jPCA [2]):



REFERENCES

[1] Yu et al., *NIPS* (2009)

[2] Churchland et al., *Nature* (2012)