Learning trajectories

joint work with Paul Zhang

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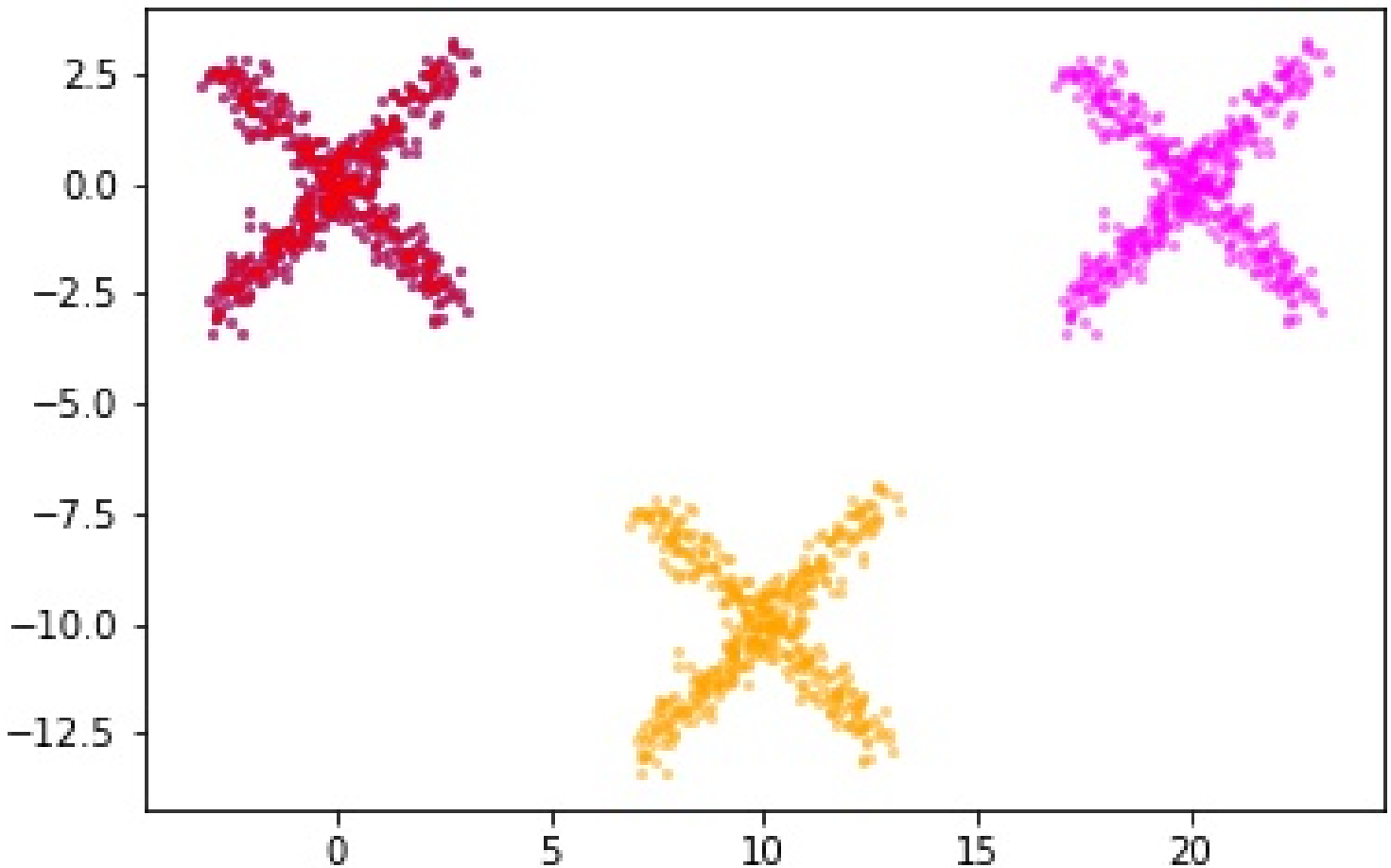
Trajectory Learning



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- **Goal** : Learn the vector field f

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- $\mathrm{x}(t_i, \theta)$ point cloud of solutions to the ODE with initial condition $\mathrm{x}(t_0) = \mathrm{x}_{t_0}$.
- Loss ensures that point cloud of observations $x(t_i)$ matches the point cloud of solutions $\mathrm{x}(t_i, \theta)$ at all times t_i.

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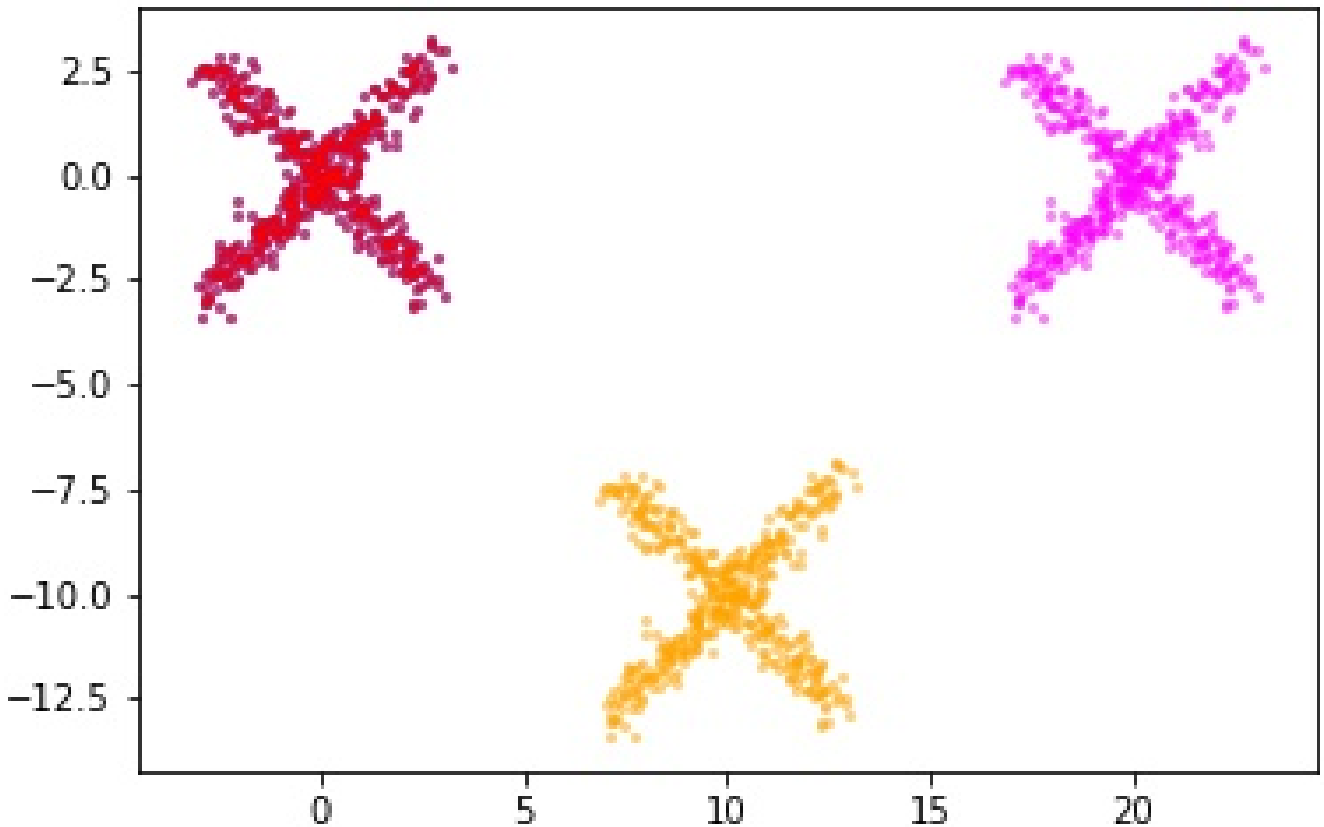
- Adjoint method is implemented in Torchdiffeq library

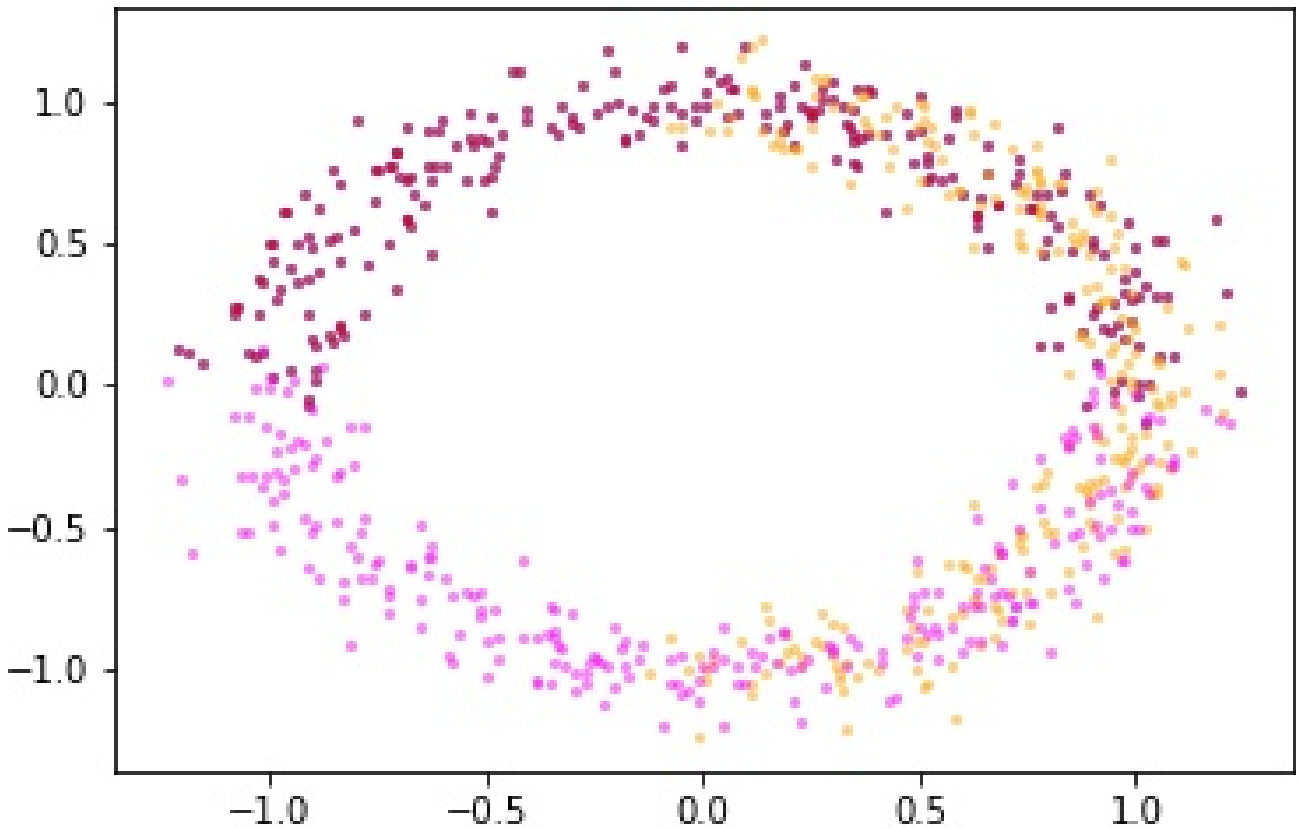
First experiments



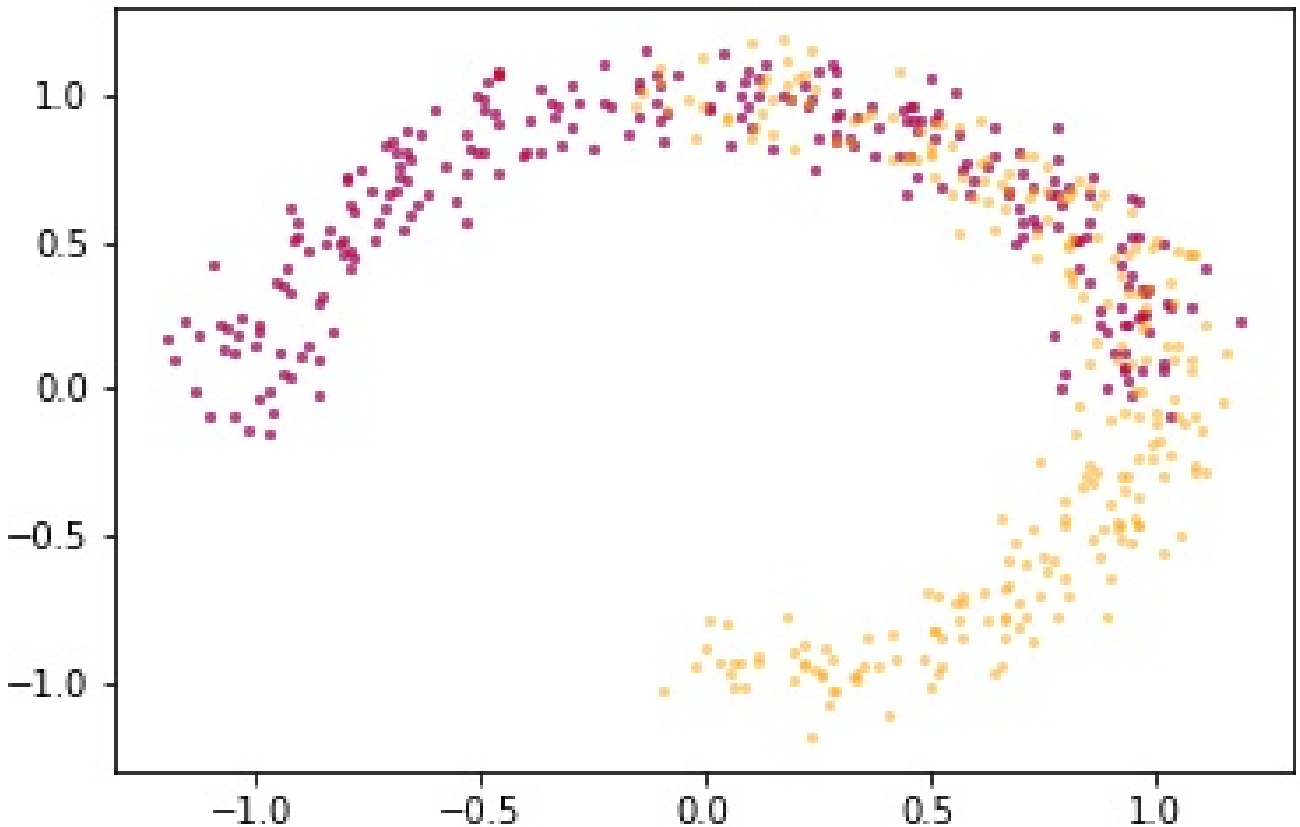
Some remarks about the trajectory :

- Good
  - Smooth trajectory
  - Good data fidelity
- Bad
  - Not symmetric : rotates $0/rightarrow1$ but translates $1/rightarrow2$

Half-moon with 3 steps



Half-moon with 2 steps



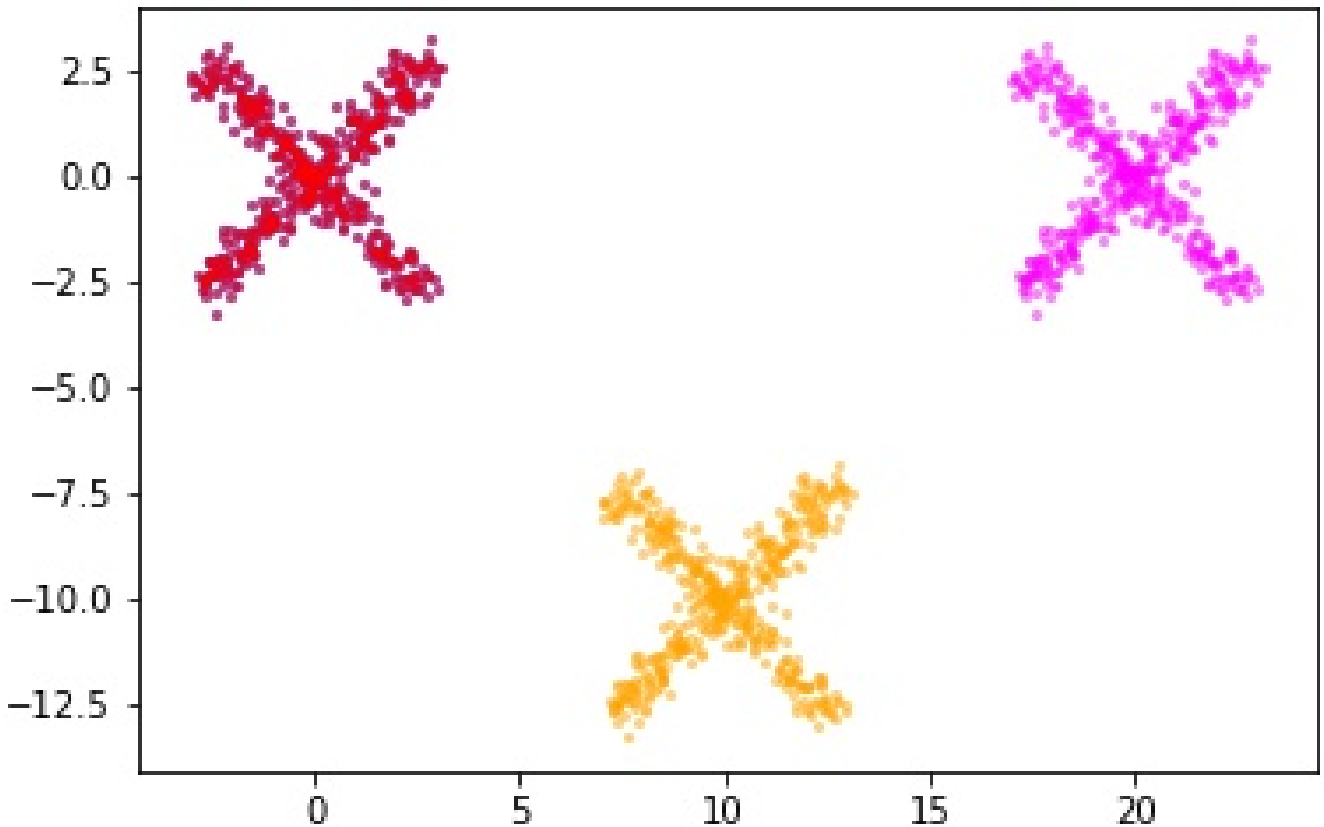
Adding prior knowledge

We can favor certain behaviors by penalizing the loss with the following energy :

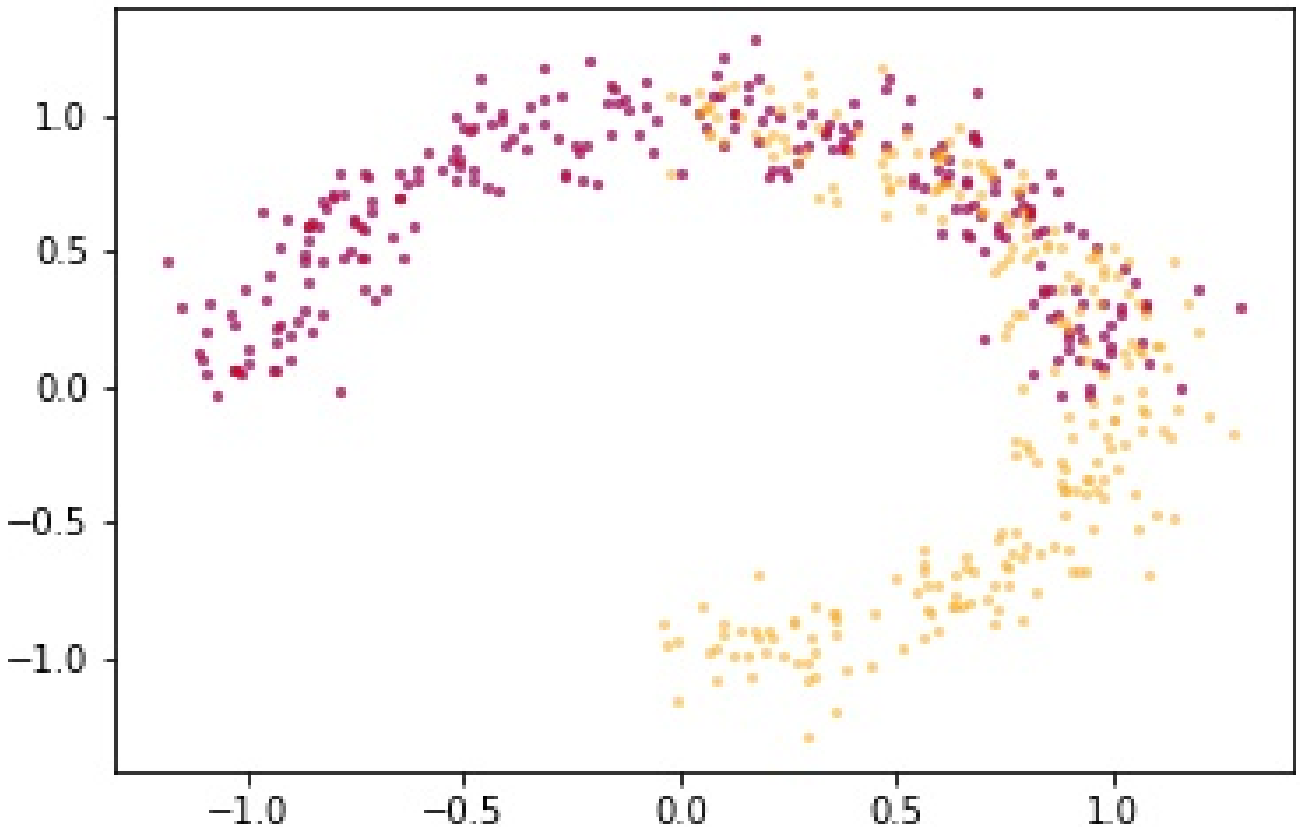
$$E(\theta) = \int_{\Omega \times [0,T]} \left\| L \left[\frac{\partial f(\mathbf{x}, t, \theta)}{\partial x} \right] \right\|_F^2 d\mathbf{x} dt \tag{2}$$

- $L_d[A] = \mathrm{Tr}[A]$ computes a divergence based energy,
- $L_r[A] = A + A^T$ computes a rigidity based energy,
- $L_\times[A] = A - A^T$ computes a curl based energy.

Crosses with 3 steps, no curl



Adding negative curl loss



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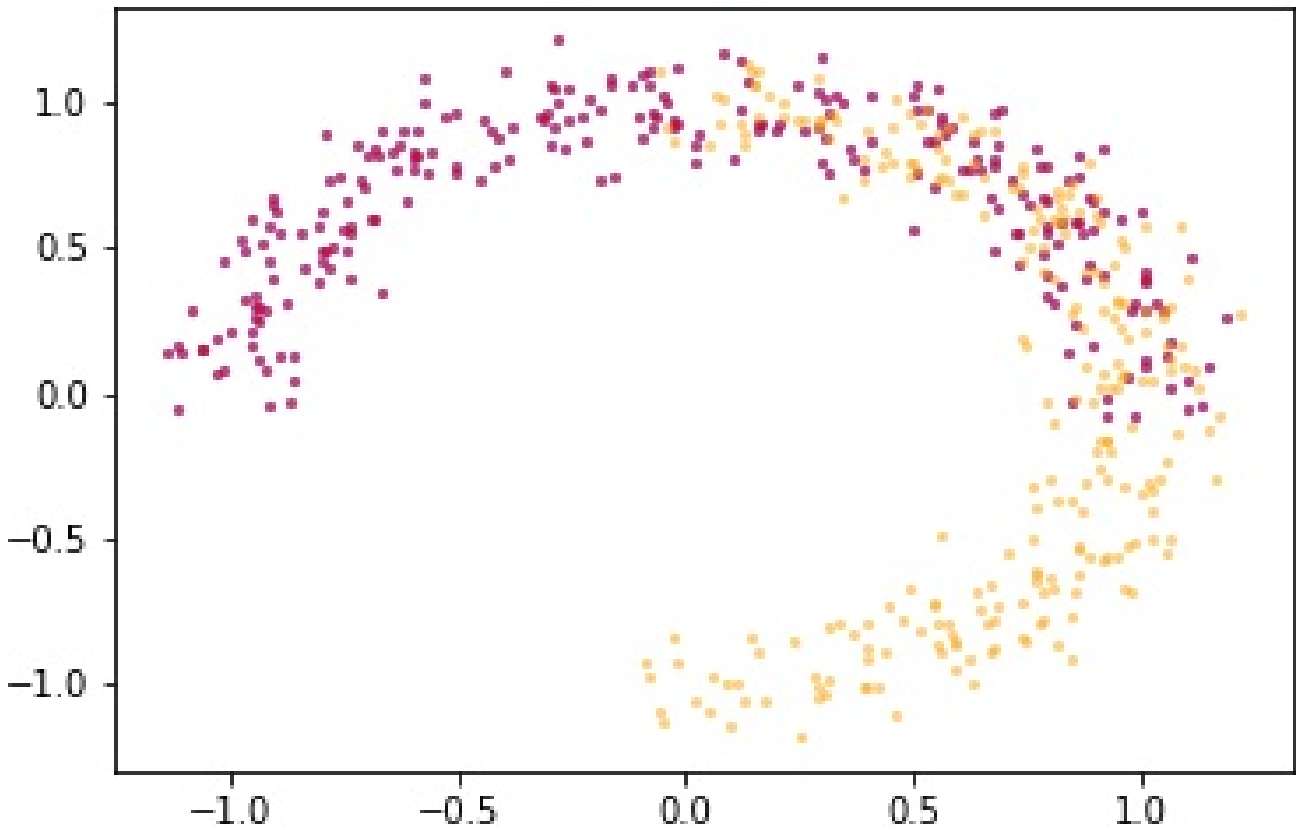
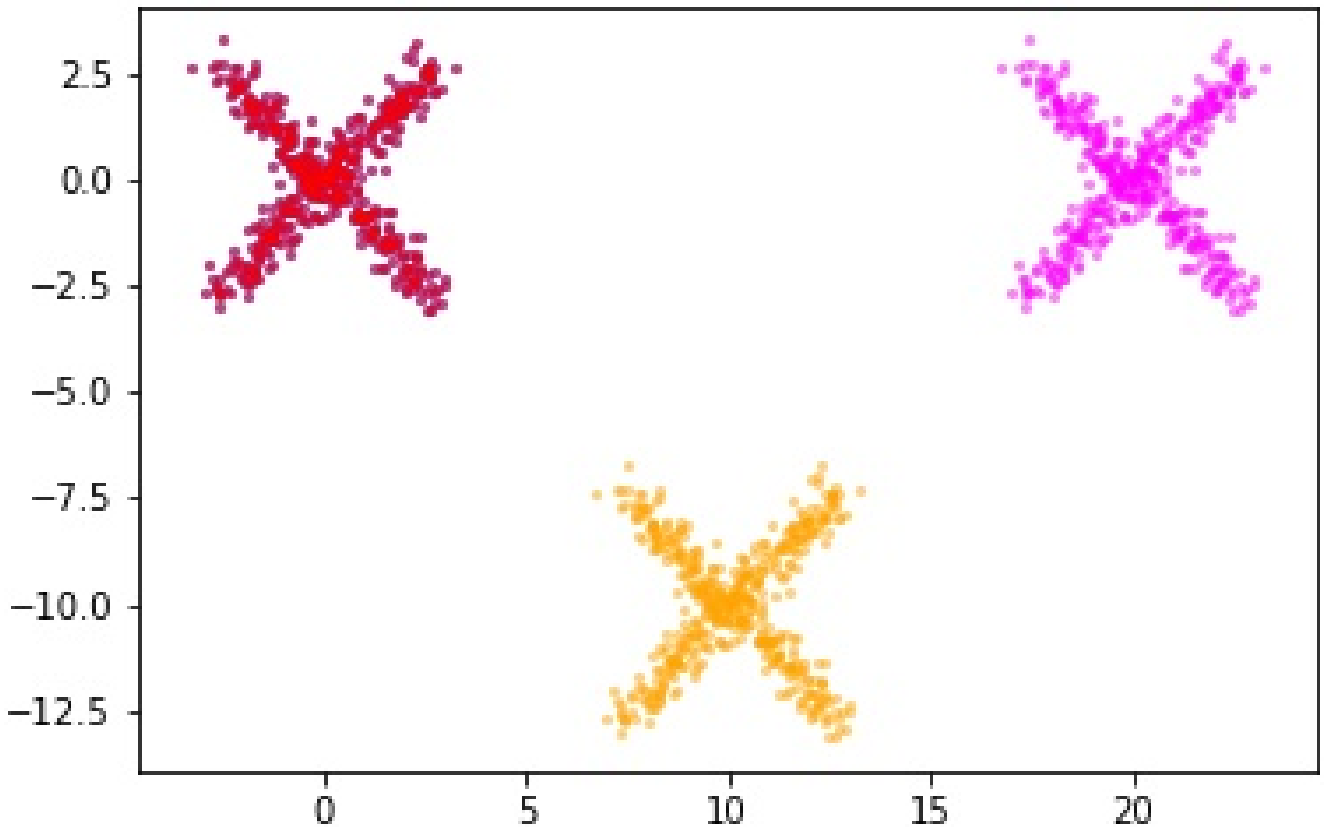
- Solution : Clamp the curl loss (using torch.clamp) to ignore large values

Adding clamped negative curl loss



Crosses with 3 steps, clamped curl



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  - how many observation time steps can we handle ?
  - what are meaningful regularizers in high dimensional gene expression space ?