

Intern Project

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Abstract

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1 Second-order Algorithm

Assume we define a field with $x_t = \alpha_t x_0 + \beta_t x_1$, we can manually calculate \dot{x}_t and \ddot{x} , representing the first-order and second-order gradient, respectively.

Definition 1.1. *The loss function for second order method contain two parts. We define the first part which is trying to using \dot{x}_t , x_t and t to learn function $u_{1,t}$, thus the loss is*

$$L_{2,1,\theta_1} := \|\dot{x}_t - u_{1,\theta_1}(x_t, t)\|_2^2 \quad (1)$$

Next, we define the second part which is trying to use \ddot{x}_t , $u_{1,\theta_1}(x_t, t)$, x_t and t to learn u_{2,θ_2} function, thus the loss is

$$L_{2,2,\theta_2,\theta_1} := \|\ddot{x}_t - u_{2,\theta_2}(u_{1,\theta_1}(x_t, t), \textcolor{red}{x}_t, t)\|_2^2 \quad (2)$$

Overall the total loss is

$$L_{2,\theta} := L_{2,1,\theta_1,\theta_2} + L_{2,2,\theta_2} \quad (3)$$

Algorithm 1

```

1: procedure OURSECONDORDERALG()
2:   for each iteration do
3:     Random sample  $x_0$  and time  $t$ , with target  $x_1$ 
4:      $x_t \leftarrow \alpha_t \cdot x_0 + \sqrt{1 - \alpha_t^2} \cdot x_1$ 
5:     Compute gradient with respect to  $L_{2,\theta}$  ▷ see Def. 1.1
6:   end for
7:   return  $u_1, u_2$  ▷ Two network functions
8: end procedure
9: /* Below is an inference algorithm that only use first-order learner  $u_1$  */
10: procedure INF1( $u_1$ )
11:    $x_0 \sim \mathcal{N}(0, 1)$ 
12:   Initial  $x \leftarrow x_0$ 
13:   for  $t$  from 0 to 1 with step  $\Delta t = 0.01$  do
14:      $x \leftarrow x + \Delta t \cdot u_1(x, t)$ 
15:   end for
16:   return  $x$ 
17: end procedure

```

Algorithm 2 Second Order Inference Algorithm 3

```
1: /* Option 3 */
2: procedure INF2NDOORDERALG3( $u_1, u_2$ )
3:    $x_0 \sim \mathcal{N}(0, 1)$ 
4:   Initial  $x \leftarrow x_0$ 
5:   for  $t$  from 0 to 1 with step  $\Delta t = 0.01$  do
6:      $x \leftarrow x + \Delta t \cdot u_1(x, t) + \frac{(\Delta t)^2}{2} \cdot u_2(u_1(x, t), x, t)$ 
7:   end for
8:   return  $x$ 
9: end procedure
```

2 Experimental Details

IMPORTANT! Please modify [this colab](#) for the code task.

2.1 Stage 1 instructions

We would like to implement the second order version VP ODE framework from [LGL22], the algorithm is written in Algorithm 2.

Recall that we have defined the original trajectory as

$$z_t = \alpha_t z_0 + \beta_t z_1$$

in VP ODE, we choose $\alpha_t = \exp(-\frac{1}{4}a(1-t)^2 - \frac{1}{2}b(1-t))$ and $\beta_t = \sqrt{1 - \alpha_t^2}$, with hyperparameters $a = 19.9$ and $b = 0.1$.

We calculate the first order ground truth by

$$\frac{dz_t}{dt} = \frac{d\alpha_t}{dt} z_0 + \frac{d\beta_t}{dt} z_1$$

We calculate the second order ground truth by

$$\frac{d^2 z_t}{dt^2} = \frac{d^2 \alpha_t}{dt^2} z_0 + \frac{d^2 \beta_t}{dt^2} z_1$$

The first-order derivatives are given by

$$\frac{d\alpha_t}{dt} = \alpha_t \cdot \frac{1}{2}(a(1-t) + b)$$

and

$$\frac{d\beta_t}{dt} = -\frac{\alpha_t}{\sqrt{1 - \alpha_t^2}} \cdot \frac{d\alpha_t}{dt}$$

The second-order derivatives are

$$\frac{d^2 \alpha_t}{dt^2} = \frac{1}{2}(\alpha_t \cdot (a(1-t) + b)^2 - a \cdot \alpha_t)$$

and

$$\frac{d^2 \beta_t}{dt^2} = -\frac{1}{(1 - \alpha_t^2)\sqrt{1 - \alpha_t^2}} \cdot \frac{d\alpha_t}{dt} + \frac{d\beta_t}{dt} \cdot \frac{d^2 \alpha_t}{dt^2}$$

The **loss** should be calculate as (3)

2.2 Stage 1 expected results

You should get a result similar to Figure 1.

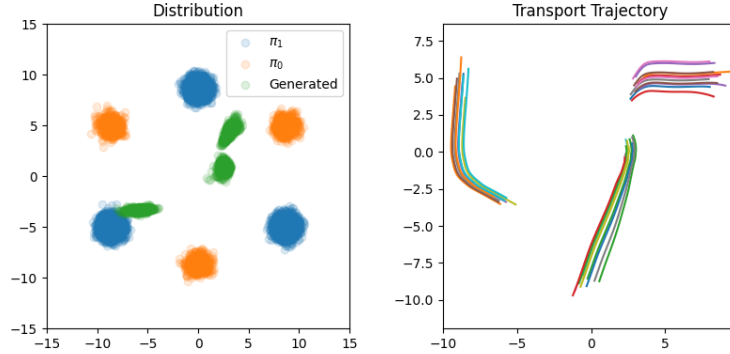


Figure 1: Stage 1 expected results.

2.3 Stage 2 instructions

Please observe the loss curve of first order loss (Eq.(1)) and second order loss (Eq. (2)).

It can be easily find that second order loss has a greater magnitude than first order loss. However, we expect first and second order loss should have the same magnitude. So we change the total loss as

$$L_{2,\theta} := \lambda_1 \cdot L_{2,1,\theta_1,\theta_2} + \lambda_2 \cdot L_{2,2,\theta_2}$$

For simplicity, we would like to fix λ_1 here to 1. Please find the correct λ_2 to make sure that $\lambda_1 \cdot L_{2,1,\theta_1,\theta_2}$ and $\lambda_2 \cdot L_{2,2,\theta_2}$ are in the same magnitude.

2.4 Stage 2 expected results

If you choose the correct λ_2 , you will probably get result like Figure 2.

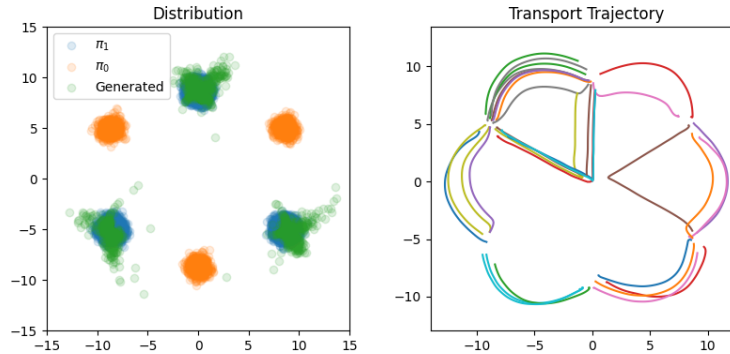


Figure 2: Stage 2 expected results

References

- [LGL22] Xingchao Liu, Chengyue Gong, and Qiang Liu. Flow straight and fast: Learning to generate and transfer data with rectified flow. *arXiv preprint arXiv:2209.03003*, 2022.