Neural ODE & ODE^2VAE

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Benefits

- Memory Efficiency
- Continuous time-series model
- Adaptive computation

How to optimize?

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- **ASM**: Computes gradients by solving a second, augmented ODE backwards in time

ASM

Consider

$$L(z(t_1)) = L(ODESolve(z(t_0, f, t_0, t_1, \theta))) \tag{3}$$

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$$a(t) = \frac{\partial L}{\partial z(t)} \text{ [} Adjoint \text{]} \tag{4a}$$

$$\frac{da(t)}{dt} = -a(t)\frac{\partial f}{\partial z(t)} \tag{4b}$$

$$\frac{dL}{d\theta} = -\int_{t_1}^{t_0} a(t)\frac{\partial f}{\partial \theta}\, dt \tag{4c}$$

ODE for supervised learning

- Comparison with:
  - ResNet which down samples the input twice then applies 6 standard residual blocks
  - RK-Net where gradients are back-propagated directly through a Runge-Kutta integrator

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	Test Error	Param	Memory	Time
1-Layer MLP	1.60%	0.24 M	-	-
ResNet	0.41%	0.60 M	O(L)	O(L)
RK-Net	0.47%	0.22 M	$O(L*)$	$O(L*)$
ODE-Net	0.42%	0.22 M	O(1)	$O(L*)$

Continuous Normalizing flow

Normalizing flow:

$$log(p(z_1)) = log(p(z_0)) - log|det\frac{\partial f}{\partial z_0}| \tag{5}$$

Bottleneck: Computing the determinant

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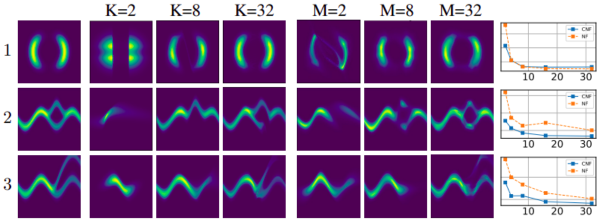
Bottleneck: Computing the determinant
Moving to a continuous transformation, where an ODE describe the transformation in z(t):

$$\frac{\partial log(p(z(t)))}{\partial t} = -tr(\frac{\partial f}{\partial z(t)}) \tag{6}$$

Experiments

- Compare the continuous and discrete planar flows at learning to sample from a known distribution and shows that a planar CNF with M hidden units can be at least as expressive as a NF with K = M layers.
- Train CNF for 10,000 iterations using Adam and NF for 500,000 iterations using RMSprop. We minimize $KL(q(x)||p(x))$ as the loss function where q is the flow model and the target density $p()$



(a) Target (b) NF (c) CNF (d) Loss vs. K/M

Time series modeling

- Represent each time series by a latent trajectory
- Given a local initial state z_{t_0}, ODE solver produces $z_{t_1}, ...z_{t_n}$ at each observation time

$$z_{t_0} \sim p(z_{t_0}) \tag{7a}$$

$$z_{t_1}, ...z_{t_n} = ODESolve(z_{t_0}, f, \theta_f, t_0, ..., t_n) \tag{7b}$$

$$each\ x_{t_i} \sim p(x|z_{t_i}, \theta_x) \tag{7c}$$

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z_{t_1}, ...z_{t_n} &= ODESolve(z_{t_0}, f, \theta_f, t_0, ..., t_n) && \text{(7b)} \\
each\ x_{t_i} &\sim p(x|z_{t_i}, \theta_x) && \text{(7c)}
\end{aligned}
$$

Training:

- Encode the data points sequentially using RNN to output $q_\phi(z_0|x_1, x_2, ..., x_n)$ from which local initial state can be sampled
- Using ODEs as a generative model allows us to make predictions for arbitrary time points with maximizing ELBO

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ODE + VAE ?

- Can we model the latent dynamic state with an ODE as previously shown?
- Learning low-rank latent representations of possibly high-dimensional sequential data trajectories
- Extend VAEs for sequential data with a latent space governed by a continuous-time probabilistic ODE

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$$\ddot{z}_t = \frac{d^2 f(z_t)}{d^2 t} = f_W(z_t, \dot{z}_t) \tag{8}$$

The above equation can be decomposed as:

$$\dot{s}_t = v_t \tag{9a}$$
$$\dot{v}_t = f_W(s_t, v_t) \tag{9b}$$

$$\begin{bmatrix} s_t \\ v_t \end{bmatrix} = \begin{bmatrix} s_0 \\ v_0 \end{bmatrix} + \int_0^T \begin{bmatrix} v_t \\ f_W(s_t, v_t) \end{bmatrix} \tag{10}$$

where $z_t = (s_t, v_t)$, s_t is state position and v_t is state velocity. The $f_W(s_t, v_t)$ is governed by a BNN.

ODE^2VAE Model

- VAE formalism $+ \ 2^{nd}$ order Bayesian neural ODE model in the latent space to model the data dynamics
- Infer continuous-time latent position and velocity trajectories while matching data as well

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Consider a generative model defined as:

$$
\begin{aligned}
s_0 &\sim p(s_0) && \text{(11a)}\\
v_0 &\sim p(v_0) && \text{(11b)}\\
s_t &= s_0 + \int_0^t v_t \, dt && \text{(11c)}\\
v_t &= v_0 + \int_0^t f(s_t, v_t) \, dt && \text{(11d)}\\
x_i &\sim p(x_i | s_i) && \text{(11e)}
\end{aligned}
$$

ODE^2VAE Model

- Position encoder maps the first item (x_0) of a high-dimensional data sequence into a distribution of the initial position s_0 characterized by μ_s, σ_s
- Velocity encoder maps the first m items of a high-dimensional data sequence ($x_{0:m}$) into a distribution of the initial position v_0 characterized by μ_v, σ_v
- Probabilistic latent dynamics are implemented by a second order ODE model f parameterised by a Bayesian deep neural network

Variational Inference

Variational approximation for unobserved quantities:

$$q(\mathcal{W}, z_{0:N}|x_{0:N}) = q(\mathcal{W})q_{enc}(z_0|x_{0:N})q_{ode}(z_{1:N}|x_{0:N}, z_0, W) \tag{12}$$

where

$$q(\mathcal{W}) = \mathcal{N}(\mathcal{W}|m, s\mathcal{I}) \tag{13}$$

$$q_{enc}(z_0|x_{0:N}) = \mathcal{N}(\begin{bmatrix} \mu_s(x_0) \\ \mu_v(x_{0:m}) \end{bmatrix}, \begin{bmatrix} diag(\sigma_s(x_0)) & 0 \\ 0 & diag(\sigma_v(x_{0:m})) \end{bmatrix}) \tag{14}$$

$$\frac{\partial log(q_{ode}(z(t)|\mathcal{W}))}{\partial t} = -tr(\frac{\partial f_{\mathcal{W}}}{\partial v_t}) \tag{15}$$

Variational Inference

ELBO

$$log(p(X)) \geq ODE\ \ regularization\ +\ VAE\ \ loss\ +\ dynamic\ \ loss \tag{16}$$

$$ODE\ \ regularization = -KL[q(\mathcal{W})||p(\mathcal{W})] \tag{17}$$

$$VAE\ \ loss = \mathbb{E}_{q_{enc}(z_0|X)}[-log\frac{q_{enc}(z_0|X)}{p(z_0)} + log(p(x_0|z_0))] \tag{18}$$

$$dynamic\ \ loss = \sum_{i=1}^{N} \mathbb{E}_{q_{ode}(\mathcal{W},z_i|X,z_0)}[-log\frac{q_{ode}(z_i|\mathcal{W},X)}{p(z_i)} + log(p(x_i|z_i))] \tag{19}$$

Penalized Variational loss

- Optimizing the ELBO objective does not necessarily result in accurate inference
- To counteract the imbalance between the KL term and reconstruction likelihood : Weight the regularization term by β where,

$$\beta = \frac{|q|}{|\mathcal{W}|} \tag{20}$$

Penalized Variational loss

- Optimizing the ELBO objective does not necessarily result in accurate inference
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- In long input sequences, dynamic loss term can easily dominate VAE loss, which may cause the encoders to underfit
- Propose to minimize the distance between the encoder distribution and the distribution induced by the ODE flow

$ODE^2VAE - KL$

Alternative penalized target function:

$$\mathcal{L}_{ODE^2VAE} = -\beta KL[q(\mathcal{W})||p(\mathcal{W})] - \gamma KL[q_{ode}(Z|X)||q_{enc}(Z|\mathcal{W}, X)]$$

$$+ \mathrm{E}_{q(\mathcal{W},Z|X)}[-log\frac{q(Z|\mathcal{W},X)}{p(Z)} + log(p(X|\mathcal{W}, Z)](21)$$

- Choose the constant γ by cross-validation

- CMU walking data: First two-third of each sequence is reserved for training and validation, and the rest is used for testing

Model	Test error: Mocap-1	Test error: Mocap-2	Reference
GPDM	126.46 ± 34	N/A	Wang et al. (2008)
VGPLVM	142.18 ± 1.92	N/A	Damianou et al. (2011)
DTSBN-S	80.21 ± 0.04	34.86 ± 0.02	Gan et al. (2015)
NPODE	45.74	22.96	Heinonen et al. (2018)
NEURALODE	87.23 ± 0.02	22.49 ± 0.88	Chen et al. (2018b)
ODE^{2}VAE	93.07 ± 0.72	10.06 ± 1.4	current work
ODE^{2}VAE-KL	$\mathbf{15.99 \pm 4.16}$	$\mathbf{8.09 \pm 1.95}$	current work

Experiments and Results

- CMU walking data: First two-third of each sequence is reserved for training and validation, and the rest is used for testing
- Rotating MNIST: Constructing a dataset by rotating the images of handwritten "3" digits with 16 rotation angles. Moreover, four rotation angles are randomly removed from each rotation sequence to introduce non-uniform sequences and missing data.

Model	Test Error
GPPVAE-DIS$^{\diamond}$	0.0309 ± 0.00002
GPPVAE-JOINT$^{\diamond}$	0.0288 ± 0.00005
ODE^{2}VAE	0.0194 ± 0.00006
ODE^{2}VAE-KL	$\mathbf{0.0188 \pm 0.0003}$

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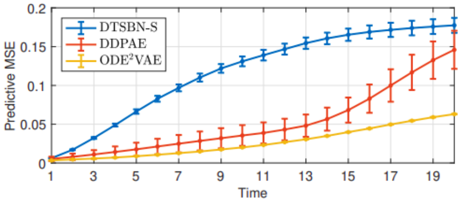
- Rotating MNIST: Constructing a dataset by rotating the images of handwritten "3" digits with 16 rotation angles. Moreover, four rotation angles are randomly removed from each rotation sequence to introduce non-uniform sequences and missing data.
- Bouncing Balls: Generated a training set of 10000 sequences of length 20 frames and a test set of 500 sequences where each frame is 32x32x1



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- A spectral density field can be formed over graph nodes, where nodes can act as a measurement point of spectral density creating kernel at each node with entanglement with other nearby nodes. The evolution of latent space of spectral density can be done via neural ODEs.

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- A spectral density field can be formed over graph nodes, where nodes can act as a measurement point of spectral density creating kernel at each node with entanglement with other nearby nodes. The evolution of latent space of spectral density can be done via neural ODEs.
- One go place for all stuff: `https://yogeshverma1998.github.io/`

Repository

./ yogeshverma1998.github.io

View on GitHub

An evolving trajectory in drug design

The purpose of this note is to act as a one place repository for all the literature read, presentations and ideas which have been formulated reside here and act as a one go place. The literature read has been segregated in different domains ranging from dynamics to representing molecule as a 3d object. Paper which are being currently read and analyzed are marked with . The slides presented by me in subsequent meetings are dated and can be found at the end of this page.

Research Ideas (:lock:)

>> Dynamics

- >> ODE^{2}VAE
- >> Neural ODEs
- >> Neural Flows
- >> FFJORD
- >> Review of Normalizing flows

>> Conformer generation and molecule as 3d object

- >> ODE^{2}VAE

>> Slides Presented:

- >> 26/01/2022 [Regular meeting]

THANK YOU