Machine learning under physical constraints
Technical details of DAN

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Outline

Model design of DAN

Pytorch implementation of DAN

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DAN: model design in detail

- How to parameterize $\mathbf{a}, \mathbf{b}, \mathbf{c}$ so that $p_t^{\mathbf{a}} \approx q_t^{\mathbf{a}}$ and $p_t^{\mathbf{b}} \approx q_t^{\mathbf{b}}$?
- What is the training and test procedure?

$$
\begin{array}{ccccc}
 & & & y_t & \\
 & & & | & \\
h_{t-1}^{\mathrm{a}} & \xrightarrow{\boxed{b}} & h_t^{\mathrm{b}} & \xrightarrow{\boxed{a}} & h_t^{\mathrm{a}} \\
\downarrow \boxed{c} & & \downarrow \boxed{c} & & \downarrow \boxed{c} \\
q_{t-1}^{\mathrm{a}} & & q_t^{\mathrm{b}} & & q_t^{\mathrm{a}}
\end{array}
$$

Design of procoder c: Gaussian model

- Let $\{c(h)\}_{h\in\mathbb{H}}$ represent a family of Gaussian distributions.
- How to parameterize a Gaussian distribution

$$\mathcal{N}(\mu,\Sigma)?$$

- $x \in \mathbb{R}^n \Rightarrow \mu \in \mathbb{R}^n$.
- Σ is a positive-definite matrix on $\mathbb{R}^{n\times n}$.
- **Challenge**: How to parameterize Σ?

Design of procoder c: parameterize Σ

- Cholesky representation of covariance matrices by lower-triangular matrix Λ

$$\mathcal{N}(\mu, \Lambda\Lambda^\intercal).$$

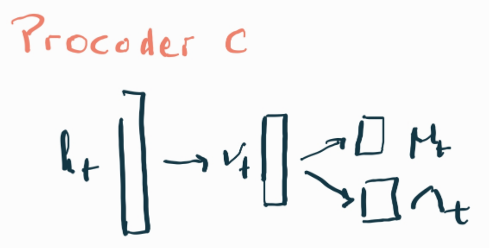
- If $\det(\Lambda) > 0$, then $\Lambda\Lambda^\intercal$ is positive definite.
- If Λ has strictly positive diagonal elements, then Λ is invertible. Denote $\mu = (v_0, \cdots, v_{n-1})^\intercal$, and

$$\Lambda = \begin{pmatrix} e^{v_n} & 0 & \cdots & 0 \\ v_{2n} & e^{v_{n+1}} & \cdots & 0 \\ \cdots & \cdots & \cdots & 0 \\ v_{n+\frac{n(n+1)}{2}-1} & \cdots & v_{3n-2} & e^{v_{2n-1}} \end{pmatrix}$$

Design of procoder $\mathbf{c}$: One-layer model

- How to build $(\mu_t, \Lambda_t) = \mathbf{c}(h_t)$ for $h_t \in \mathbb{H}$?
- Assume $\mathbb{H} \in \mathbb{R}^{mn}$ (m as ensemble size, n dim. of x).
- Associate (μ, Λ) with a vector $\mathbf{v} = (v_0, \cdots, v_{n+\frac{n(n+1)}{2}-1}) \in \mathbb{R}^{n+n(n+1)/2}$.
- $\Rightarrow$ use one linear layer with **parameter** $\theta^{\mathbf{c}} = (W, b)$

$$(\mu_t, \Lambda_t) := \mathbf{v}_t = \mathbf{c}(h_t) = Wh_t + b.$$



Design of propagator $\mathbf{b}$: need non-linearity

- How to build $h^{\mathbf{b}}_{t+1} = \mathbf{b}(h^{\mathbf{a}}_t)$?
- Why using non-linear multiple-layers of NN?

$$h^{\mathbf{b}}_{t+1} = F_L \circ F_{L-1} \circ \cdots \circ F_1(h^{\mathbf{a}}_t).$$

- Problem of gradient vanishing/explosion when L is big

Design of propagator $\mathbf{b}$: Residual networks

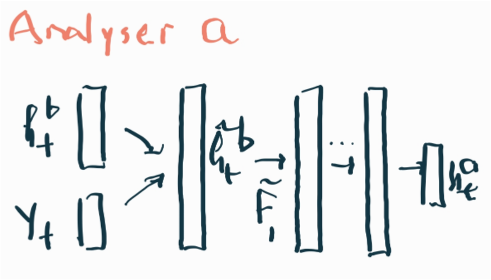
- For large L, we use residual networks with depth L to represent $\mathbf{b}$.
- The layer ℓ is a mapping of $\mathbb{H} \to \mathbb{H}$, with parameter $(W_\ell, b_\ell, \alpha_\ell)$:

$$h \mapsto F_\ell(h) = h + \alpha_\ell \rho(W_\ell h + b_\ell).$$

- The non-linearity ρ is element-wise and it can be chosen to be tanh or (leaky-)relu.
- To be close to the identify mapping, initialize $\alpha_\ell = 0$.
- The **parameter** of $\mathbf{b}$ is $\theta^{\mathbf{b}} = (W_\ell, b_\ell, \alpha_\ell)_{\ell \leq L}$.

Design of analyser $\mathbf{a}$: Augmented residual networks

- How to build $h_t^a = a(h_t^b, y_t)$?
- Consider an augmented input: $\tilde{h}_t^b = (h_t^b, y_t) \in \mathbb{H} \times \mathbb{R}^d$.
- Use a similar residual networks with depth L to transform $\tilde{h}_t^b$.
- Need an extra layer to map from $\mathbb{H} \times \mathbb{R}^d$ to $\mathbb{H}$.



Design of analyser **a**: Augmented residual networks

- For layer $\ell \leq \tilde{L}$, with parameter $(\tilde{W}_\ell, \tilde{b}_\ell, \tilde{\alpha}_\ell)$, is a mapping of $\mathbb{H} \times \mathbb{R}^d \to \mathbb{H} \times \mathbb{R}^d$:

$$\tilde{h} \mapsto \tilde{F}_\ell(\tilde{h}) = \tilde{h} + \tilde{\alpha}_\ell \rho(\tilde{W}_\ell \tilde{h} + \tilde{b}_\ell).$$

- As in **c**, define the extra layer to be a linear mapping from $\mathbb{H} \times \mathbb{R}^d \to \mathbb{H}$ with parameters $(\tilde{W}, \tilde{b})$.
- The **parameter** of **a** is $\theta^{\mathbf{a}} = (\tilde{W}_\ell, \tilde{b}_\ell, \tilde{\alpha}_\ell, \tilde{W}, \tilde{b})_{\ell \leq L}$.

The objective $L_0(q_0^{\mathbf{a}})$

- Since $q_0^{\mathbf{a}}$ is Gaussian, we evaluate the negative log-likelihood of Gaussian distributions.
- Let $(\mu_0^{\mathbf{a}}, \Lambda_0^{\mathbf{a}}) := c(h_0^{\mathbf{a}}) = Wh_0^{\mathbf{a}} + b$, then

$$L_0(q_0^{\mathbf{a}}) = \int \frac{(x_0 - \mu_0^{\mathbf{a}})^\intercal (\Lambda_0^{\mathbf{a}} (\Lambda_0^{\mathbf{a}})^\intercal)^{-1} (x_0 - \mu_0^{\mathbf{a}})}{2} p(x_0) dx_0 \\ + \log |2\pi \Lambda_0^{\mathbf{a}} (\Lambda_0^{\mathbf{a}})^\intercal|^{1/2}.$$

- As $\Lambda_0^{\mathbf{a}}$ is a triangular matrix, it is easy to compute $|\Lambda_0^{\mathbf{a}}|$.
- How about $(\Lambda_0^{\mathbf{a}})^{-1}$? e.g. given $(a, b, c) \in \mathbb{R}^3$,

$$\Lambda = \begin{pmatrix} 1 & 0 & 0 \\ a & 1 & 0 \\ b & c & 1 \end{pmatrix}, \quad \Lambda^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ -a & 1 & 0 \\ ac - b & -c & 1 \end{pmatrix}$$

Training procedure: supervised learning

- Optimize the training objective from I training sequences $\{(x_t(i), y_t(i))\}_{i\leq I, t\leq T}$,

$$\mathcal{L}_{train} = \frac{1}{T}\sum_{t\leq T}(\mathcal{L}_t(q_t^{\mathbf{b}}) + \mathcal{L}_t(q_t^{\mathbf{a}})) + \mathcal{L}_0(q_0^{\mathbf{a}})$$

- Each term in $\mathcal{L}_{train}$ is a Monte-Carlo estimation of $L_t(q_t^{\mathbf{b}})$, $L_t(q_t^{\mathbf{a}})$ or $L_0(q_0^{\mathbf{a}})$.
- For example, $L_0(q_0^{\mathbf{a}})$ is estimated by

$$\mathcal{L}_0(q_0^{\mathbf{a}}) = \frac{1}{I}\sum_{i\leq I}\frac{(x_0(i) - \mu_0^{\mathbf{a}})^\intercal(\Lambda_0^{\mathbf{a}}(\Lambda_0^{\mathbf{a}})^\intercal)^{-1}(x_0(i) - \mu_0^{\mathbf{a}})}{2} + \log|2\pi\Lambda_0^{\mathbf{a}}(\Lambda_0^{\mathbf{a}})^\intercal|^{1/2}.$$

Training procedure: full mode

- Step 1 Pre-training: Optimize $\mathbf{c}$ from I training sequences at $t = 0$,

$$\min_{\theta^{\mathbf{c}}} \mathcal{L}_0(q_0^{\mathbf{a}})$$

- Step 2 Full-training: Optimize $\mathbf{a}, \mathbf{b}, \mathbf{c}$ from I training sequences $t = 1, \cdots, T$,

$$\min_{\theta^{\mathbf{a}}, \theta^{\mathbf{b}}, \theta^{\mathbf{c}}} \frac{1}{T} \sum_{t \leq T} (\mathcal{L}_t(q_t^{\mathbf{b}}) + \mathcal{L}_t(q_t^{\mathbf{a}})) + \mathcal{L}_0(q_0^{\mathbf{a}})$$

- Deterministic optimization: solved by GD, L-BFGS, etc.

Test procedure

- Goal: evaluate the trained model
- Generalization (loss): use I test sequences to estimate how small the **objective function** is

$$\frac{1}{T}\sum_{t\leq T}(L_t(q_t^{\mathbf{a}}) + L_t(q_t^{\mathbf{b}})) + L_0(q_0^{\mathbf{a}})$$

- Generalization (error): for a test trajectory (x_t, y_t) of ODS, compute (μ_t^a, μ_t^b) for $t \leq T$, and then evaluate **RMSE**

$$\frac{1}{T}\sum_{t\leq T}\|x_t - \mu_t^a\|, \quad \frac{1}{T}\sum_{t\leq T}\|x_t - \mu_t^b\|$$

- Prediction: what happens for $t > T$?

Training procedure: online mode

- Minimization of $\mathcal{L}_t(q_t^{\mathbf{b}}) + \mathcal{L}_t(q_t^{\mathbf{a}})$ at each t, by truncated BPTT.
- Example, $\mathcal{L}_t(q_t^{\mathbf{a}}) = \frac{1}{I}\sum_i \mathcal{L}_t(q_t^{\mathbf{a}}(i))$, the truncated gradients $\tilde{\nabla}\mathcal{L}_t(q_t^{\mathbf{a}}(i))$ with respect to $(\theta^{\mathbf{a}}, \theta^{\mathbf{b}}, \theta^{\mathbf{c}})$ at time-step t are

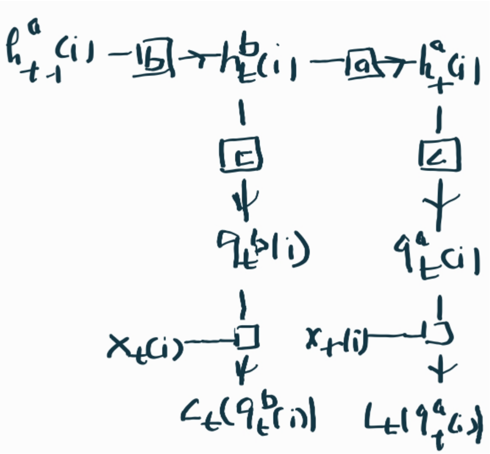
$$\tilde{\nabla}_{\theta^{\mathbf{c}}}\mathcal{L}_t(q_t^{\mathbf{a}}(i)) = \left(\frac{\partial q_t^{\mathbf{a}}(i)}{\partial \theta_t^{\mathbf{c}}}\right)^{\mathsf{T}} \nabla_{q_t^{\mathbf{a}}(i)}\mathcal{L}_t(q_t^{\mathbf{a}}(i))$$

$$\tilde{\nabla}_{\theta^{\mathbf{b}}}\mathcal{L}_t(q_t^{\mathbf{a}}(i)) = \left(\frac{\partial h_t^{\mathbf{b}}(i)}{\partial \theta_t^{\mathbf{b}}}\right)^{\mathsf{T}} \nabla_{h_t^{\mathbf{b}}(i)}\mathcal{L}_t(q_t^{\mathbf{a}}(i))$$

$$\tilde{\nabla}_{\theta^{\mathbf{a}}}\mathcal{L}_t(q_t^{\mathbf{a}}(i)) = \left(\frac{\partial h_t^{\mathbf{a}}(i)}{\partial \theta_t^{\mathbf{a}}}\right)^{\mathsf{T}} \nabla_{h_t^{\mathbf{a}}(i)}\mathcal{L}_t(q_t^{\mathbf{a}}(i))$$

Training procedure: online mode

- Computational graph (truncated) from i-th sample sequence $(x_s(i), y_s(i))_{s \leq t}$



Training procedure: online mode

- Let $\mathcal{L}_t(\theta) = \mathcal{L}_t(q_t^{\mathbf{b}}) + \mathcal{L}_t(q_t^{\mathbf{a}})$ with parameters $\theta = (\theta^{\mathbf{a}}, \theta^{\mathbf{b}}, \theta^{\mathbf{c}})$
- Online: update model parameters using truncated gradients.
- Truncated GD optimiser with learning rate $\eta_k > 0$:

$$\theta^{(k+1)} = \theta^{(k)} - \eta_k \tilde{\nabla}_\theta \mathcal{L}_{k+1}(\theta^{(k)})$$

- Truncated Adam optimiser: adaptive control of η_k:

$$\theta^{(k+1)} = \theta^{(k)} - \mathrm{Adam}_k(\tilde{\nabla}_\theta \mathcal{L}_{k+1}(\theta^{(k)}))$$

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Data generation

- Propagation step: $x_t = Mx_{t-1} + \eta_t$
  - Linear 2d: Periodic (Hamiltonian) dynamics
  - Lorentz (non-linear) 40d: Chaotic dynamics
  - η_t white noise
- Observation step: $y_t = Hx_t + \epsilon_t$
  - Identity case: $H = I$
  - ϵ_t white noise

Forward steps of $(\mathbf{a}, \mathbf{b}, \mathbf{c})$ in DAN

- Compute the loss (and the gradient) over t.
- Initial $h_0^{\mathbf{a}}$
- Input: $h_{t-1}^{\mathbf{a}}, x_t, y_t$
- Output: $\mathcal{L}_t(q_t^{\mathbf{b}}) + \mathcal{L}_t(q_t^{\mathbf{a}})$, $h_t^{\mathbf{a}}$
- Key internal steps:
  - Compute $h_t^{\mathbf{b}} = \mathbf{b}(h_{t-1}^{\mathbf{a}})$
  - Compute $q_t^{\mathbf{b}} = \mathbf{c}(h_t^{\mathbf{b}})$
  - Compute $h_t^{\mathbf{a}} = \mathbf{a}(h_t^{\mathbf{b}}, y_t)$
  - Compute $q_t^{\mathbf{a}} = \mathbf{c}(h_t^{\mathbf{a}})$

Summary: Training

- **Input**: net, data, optimizer, dimensions, training time
- **Output**: a trained net
- Optimize and compute how fast the training loss decreases.
  - 2 modes: full vs. online
- Full mode
  - Generate training data: I sequences of $\{(x_t(i), y_t(i))\}_{i \le I, t \le T}$.
  - Optimize the total loss $\frac{1}{T} \sum_{t \le T} (\mathcal{L}_t(q_t^{\mathbf{b}}) + \mathcal{L}_t(q_t^{\mathbf{a}})) + \mathcal{L}_0(q_0^{\mathbf{a}})$.
- Online mode
  - At each $t \in \mathbb{Z}_+$, generate $\{(x_t(i), y_t(i))\}_{i \le I}$ on the fly, and optimize the loss $\mathcal{L}_t(q_t^{\mathbf{b}}) + \mathcal{L}_t(q_t^{\mathbf{a}})$ with truncated gradients.

Summary: Test

- **Input**: net, data, dimensions, test time
- **Output**: RMSE over $t \leq T$ (or $t > T$)
- Generate test data, e.g. I sequences of $\{(\tilde{x}_t(i), \tilde{y}_t(i))\}_{i \leq I, t \leq T}$ (independent of the training sequences).
- Use net to compute $\tilde{\mu}_t^a(i)$ from $\tilde{Y}_t(i)$, resp. $\tilde{\mu}_t^b(i)$ from $\tilde{Y}_{t-1}(i)$.
- Compute the RMSE based on $\tilde{x}_t(i)$,

$$\frac{1}{I} \sum_i \|\tilde{x}_t(i) - \tilde{\mu}_t^a(i)\|, \quad \frac{1}{I} \sum_i \|\tilde{x}_t(i) - \tilde{\mu}_t^b(i)\|$$