University of Stuttgart
Institute for Parallel and Distributed Systems
Analytic Computing

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ML in the Science
Deep Equilibrium Models

Daniel Frank

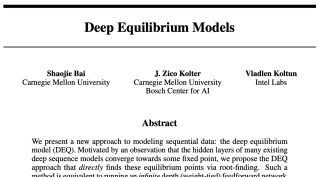
Outline

1. What are deep equilibrium network?
   - Forward Pass
   - Backward Pass
   - Example
2. Monotone equilibrium networks
   - Motivation
   - Formal Definition
   - Existence of a unique solution
3. Connection to System Theory
   - Nonlinear system identification
   - Recurrent Neural Networks as linear, time-invariant (LTI) system
   - Recurrent equilibrium network

What are deep equilibrium network?

Deep equilibrium network in Machine Learning

Where do they come from?



Deep Equilibrium Models

Shaojie Bai
Carnegie Mellon University

J. Zico Kolter
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Bosch Center for AI

Vladlen Koltun
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Abstract

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Deep equilibrium network in Machine Learning

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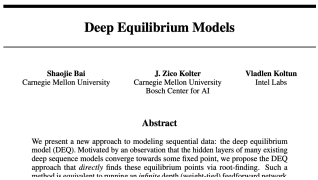

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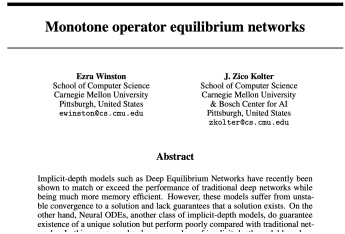

Monotone operator equilibrium networks

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Deep equilibrium network in Machine Learning

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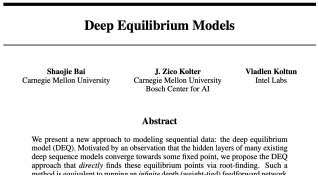

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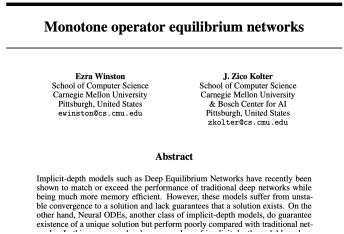

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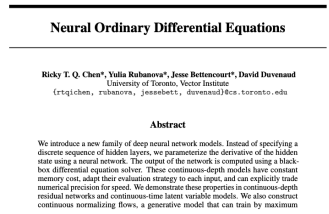

Neural Ordinary Differential Equations

Ricky T. Q. Chen*, Yulia Rubanova*, Jesse Bettencourt*, David Duvenaud
University of Toronto, Vector Institute
{rtqichen, rubanova, jessebett, duvenaud}@cs.toronto.edu

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We introduce a new family of deep neural network models. Instead of specifying a discrete sequence of hidden layers, we parameterize the derivative of the hidden state using a neural network. The output of the network is computed using a black-box differential equation solver. These continuous-depth models have constant memory cost, adapt their evaluation strategy to each input, and can explicitly trade numerical precision for speed. We demonstrate these properties in continuous-depth residual networks and continuous-time latent variable models. We also construct continuous normalizing flows, a generative model that can train by maximum

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Deep equilibrium network in Machine Learning

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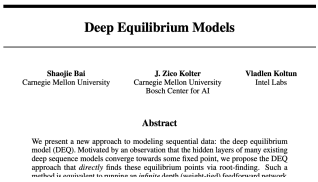

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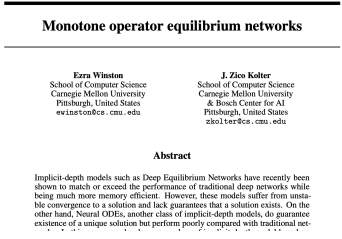

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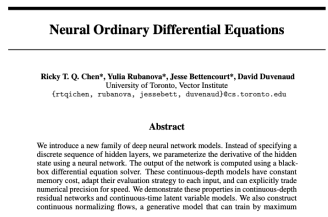

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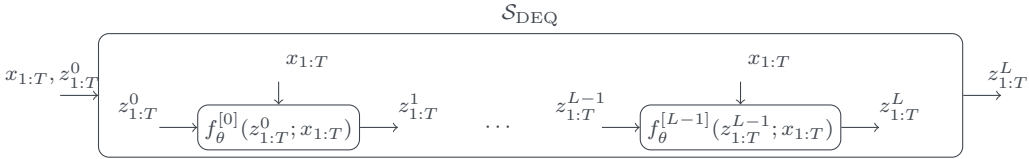
Why are they interesting?

- Training of DEQ only requires constant memory
- Achieve state-of-the-art performance compared to standard deep learning approaches
- DEQ have a strong relation to system theory

Deep equilibrium networks - Forward Pass

[Bai et al., 2019]

- $\mathcal{S}_{\text{DEQ}}$ maps an input sequence $x_{1:T}$ to an output sequence $z^L_{1:T}$. The input is *injected* at each layer, the number of layer is denoted by L.



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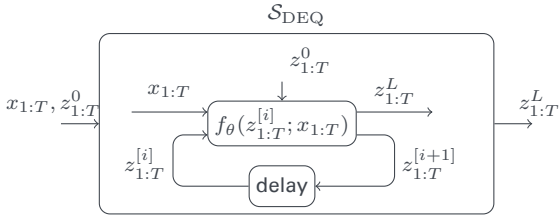

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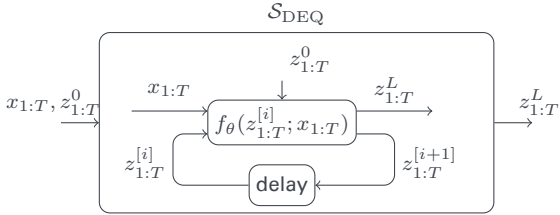

Core idea of DEQs

- What happens for $L \to \infty$?

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$$\mathcal{S}_{\mathrm{DEQ}}: \quad x_{1:T}, z^0_{1:T} \longrightarrow \boxed{\mathrm{RootFind}\left(\underbrace{f_\theta(z_{1:T}; x_{1:T}) - z_{1:T}}_{g_\theta}\right)} \longrightarrow z^*_{1:T}$$

Core idea of DEQs

- What happens for $L \to \infty$?

$$z^*_{1:T} = f_\theta(z^*_{1:T}; x_{1:T})$$

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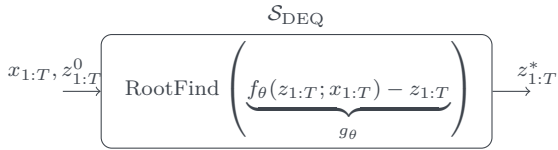

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- How restrictive is weight tying?

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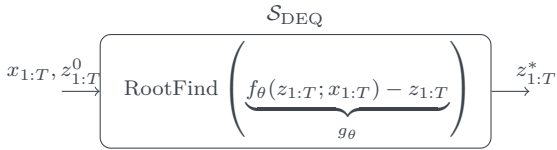

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  - *... Any traditional L-layer deep network (in "standard" format) can be represented by a weight-tied, input-injected network of equivalent depth, with linear increase in width ...*

Deep equilibrium networks - Forward Pass

[Bai et al., 2019]

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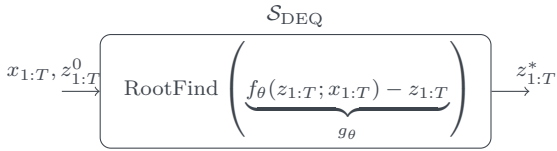

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- How restrictive is weight tying?
  - *... Any traditional L-layer deep network (in "standard" format) can be represented by a weight-tied, input-injected network of equivalent depth, with linear increase in width ...*
- Any *black-box-root-finding* algorithm can be applied to solve the forward pass

Deep equilibrium network - Backward Pass

[Bai et al., 2019]

Traditional backpropagation is not suitable

- Would depend on the root finding method
- Intermediate results are not stored during the forward pass

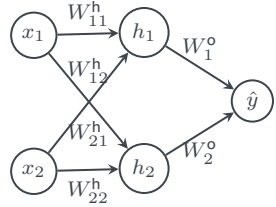

Figure 4: Backpropagation usually takes the same route as the forward pass.

Deep equilibrium network - Backward Pass

[Bai et al., 2019]

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Gradient of the Equilibrium Model

Assume the loss function

$$\ell = \mathcal{L}\left(h\left(\text{RootFind}\left(g_0; x_{1:T}\right)\right), y_{1:T}\right)$$

- $h : \mathbb{R}^{n_z} \mapsto \mathbb{R}^{n_y}$ can be any differentiable function (e.g. linear)
- $y_{1:T}$ is the ground-truth sequence
- $\mathcal{L} : \mathbb{R}^{n_y} \times \mathbb{R}^{n_y} \mapsto \mathbb{R}$ is the loss function

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The loss gradient with respect to $(\cdot)$ is

$$\frac{\partial \ell}{\partial (\cdot)} = -\frac{\partial \ell}{\partial h}\frac{\partial h^\star}{\partial z}_{1:T}\left(J_{g_\theta}^{-1}\Big|_{x^*_{1:T}}\right)\frac{\partial f_\theta\left(z^\star_{1:T}; x_{1:T}\right)}{\partial (\cdot)}$$

- $J_{g_\theta}^{-1}\Big|_{x^*_{1:T}}$ si the inverse Jacobian of g_θ evaluated at x

Simple DEQ - Example

Assume: **Sequence length $T = 3$, size of hidden state $n_z = 10$, input and output size $n_y = n_x = 1$:**

- Weights are randomly initialized
- Initial hidden state $z^0_{1:T} = 0$
- $W_z \in \mathbb{R}^{n_z \times n_z}$, $U_z \in \mathbb{R}^{n_z \times T}$
- Linear output layer $W_y \in \mathbb{R}^{n_y \times n_z}$

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Network with fixed layer size:

$$z^{l+1}_{1:T} = \sigma\left(W_z z^l_{1:T} + U_z x_{1:T} + b_z\right) \qquad l = 1, \ldots, L-1$$
$$\hat{y}_{1:T} = W_y z^*_{1:T} + b_z$$

Listing 1: Traditional forward pass

```
# forward pass for fixed number of layers
z = torch.zeros(size=(1, n_z))
x = torch.tensor(u).reshape(1, n_x)
for l in range(L):
    z = nl(W_z(z) + U_z(x))
y_hat = W_y(z)
```

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DEQ:

$$z_{1:T}^* = \text{RootFind}\left(\sigma\left(W_z z_{1:T} + U_z x_{1:T} + b_z\right) - z_{1:T}\right)$$
$$\hat{y}_{1:T} = W_y z_{1:T}^L + b_z$$

Listing 2: Forward pass of DEQ

```
# DEQ
def g_theta(z):
    z = z.reshape(n_z,1)
    return np.squeeze(np.tanh(W_z_numpy @ z + U_z_numpy @ x + b_z_numpy) - z)

z_star, infodict, ier, mesg = fsolve(g_theta, x0=z_0, full_output=True)
z_star = z_star.reshape(n_z, 1)
y_hat_eq = W_y_numpy @ z_star + b_y_numpy
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DEQ:

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$$\hat{y}_{1:T} = W_y z^L_{1:T} + b_z$$

Comparison:

```
Number of finite layers: 0       || z^L - z^* ||^2: 0.7032
Number of finite layers: 1       || z^L - z^* ||^2: 0.3898
Number of finite layers: 2       || z^L - z^* ||^2: 0.2898
Number of finite layers: 3       || z^L - z^* ||^2: 0.1621
Number of finite layers: 4       || z^L - z^* ||^2: 0.09451
Number of finite layers: 10      || z^L - z^* ||^2: 0.001685
Number of finite layers: 20      || z^L - z^* ||^2: 7.595e-06
Number of finite layers: 30      || z^L - z^* ||^2: 7.069e-08
```

Monotone equilibrium networks

2

Example continued

Do the solutions $z^*_{1:T}$ and $z^L_{1:T}$ always converge for sufficient large L?

- Let the weight of the hidden layer be initialized by a normal distribution

Listing 3: Added line 2

```
1 W_z = torch.nn.Linear(in_features=n_z, out_features=n_z, bias=True)
2 torch.nn.init.normal_(W_z.weight)
3 U_z = torch.nn.Linear(in_features=n_x, out_features=n_z, bias=False)
4 W_y = torch.nn.Linear(in_features=n_z, out_features=n_x, bias=True)
```

Example continued

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```

Comparison:

```
    Number of finite layers: 0       || z^L - z^* ||^2: 0.4664
    Number of finite layers: 1       || z^L - z^* ||^2: 0.332
    Number of finite layers: 2       || z^L - z^* ||^2: 1.035
    Number of finite layers: 3       || z^L - z^* ||^2: 1.834
    Number of finite layers: 4       || z^L - z^* ||^2: 2.348
    Number of finite layers: 10      || z^L - z^* ||^2: 2.75
    Number of finite layers: 20      || z^L - z^* ||^2: 2.724
    Number of finite layers: 30      || z^L - z^* ||^2: 2.927
```

Core idea of monotone equilibrium network (monDEQ)

[Winston and Kolter, 2020]

Finding equilibrium point as operator splitting [Winston and Kolter, 2020, Theorem 1]

Consider (again) a weight-tied input-injected network

$$z^{k+1} = \sigma\left(W_z z^k + U_z x + b_z\right) \tag{1}$$

and an equilibrium point that remains constant after update

$$z^* = \sigma\left(W z_z^* + U_z x + b\right).$$

Finding an equilibrium point of (1) is equivalent of finding a zero of the operator splitting problem $0 \in (F + G)(z^*)$ with the operators

$$F(z) = (I - W_z)(z) - (U_z x + b), \qquad G = \partial f \tag{2}$$

and $\sigma(\cdot) = \text{prox}_f^1(\cdot)$ for some convex closed proper function f, where prox_f^α denotes the proximal operator

$$\text{prox}_f^\alpha(x) \equiv \text{argmin}_z \frac{1}{2}\|x - z\|_2^2 + \alpha f(z)$$

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- An introduction to monotone operator theory would be required to fully appreciate the result, see [Winston and Kolter, 2020, Appendix A]
- Lets view the operator splitting as a *black-box-root-finding* algorithm

Monotone Operator

Monotone operator $F(z) = (I - W_z)(z) - (U_z x + b)$ from (2).

If

$$I - W_z \succeq mI \qquad m > 0$$

is strongly monotone, an unique equilibrium point z^* exists.

- For a scalar, linear function this connection is intuitive

$$F_{\text{scal}}(z) = \underbrace{(1 - w)}_{\text{slope}} z + \underbrace{(ux + b)}_{\text{constant}}$$

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```
min EW of (I-W_z): 0.6272        L: 40   || z^L - z^* ||^2: 3.999e-08
min EW of (I-W_z): 0.3782        L: 40   || z^L - z^* ||^2: 4.184e-08
min EW of (I-W_z): 0.5671        L: 40   || z^L - z^* ||^2: 3.373e-08
min EW of (I-W_z): 0.6786        L: 40   || z^L - z^* ||^2: 6.231e-08
min EW of (I-W_z): 0.8057        L: 40   || z^L - z^* ||^2: 2.551e-08
min EW of (I-W_z): 0.662         L: 40   || z^L - z^* ||^2: 3.364e-08
min EW of (I-W_z): 0.3946        L: 40   || z^L - z^* ||^2: 4.522e-08
min EW of (I-W_z): 0.6532        L: 40   || z^L - z^* ||^2: 2.656e-08
min EW of (I-W_z): 0.4264        L: 40   || z^L - z^* ||^2: 3.059e-08
min EW of (I-W_z): 0.6787        L: 40   || z^L - z^* ||^2: 5.395e-08
```

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```
1  min EW of (I-W_z): -2.172        L: 40   || z^L - z^* ||^2: 3.301
2  min EW of (I-W_z): -2.353        L: 40   || z^L - z^* ||^2: 2.48
3  min EW of (I-W_z): -1.519        L: 40   || z^L - z^* ||^2: 2.585
4  min EW of (I-W_z): -1.657        L: 40   || z^L - z^* ||^2: 2.839
5  min EW of (I-W_z): -0.6791       L: 40   || z^L - z^* ||^2: 2.59
6  min EW of (I-W_z): -2.574        L: 40   || z^L - z^* ||^2: 3.095
7  min EW of (I-W_z): -1.609        L: 40   || z^L - z^* ||^2: 3.514
8  min EW of (I-W_z): -3.02         L: 40   || z^L - z^* ||^2: 2.832
9  min EW of (I-W_z): -1.922        L: 40   || z^L - z^* ||^2: 2.983
10 min EW of (I-W_z): -1.023        L: 40   || z^L - z^* ||^2: 2.722
```

Monotone Operator

Monotone operator $F(z) = (I - W_z)(z) - (U_z x + b)$ from (2).

If

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- For a scalar, linear function this connection is intuitive

$$F_{\text{scal}}(z) = \underbrace{(1 - w)}_{\text{slope}} z + \underbrace{(ux + b)}_{\text{constant}}$$

Introduce constraints on the weight W_z to ensure montonicity

Monotonicity is ensured $I - W_z \succeq mI$ if there exists $A,\ B \in \mathbb{R}^{n_z \times n_z}$ such that

$$W_z = (1 - m)I - A^{\mathrm{T}} A + B - B^{\mathrm{T}}.$$

- The weight W_z is now directly parametrized by A and B

Connection to System Theory

3

Inverted pendulum with torque input

Classical toy example in control

System Identification Problem

If the equations of the pendulum are not available but we are given data $\mathcal{D} = \{(u, y)_i\}_i^N$, which contains input output measurements. Finding the parameter set θ can be seen as a deep learning problem.

- The system states $x_{\text{sys}}^k = [\phi,\ \dot{\phi}]^{\mathrm{T}}$ represents the *angle* and *angular velocity*
- Input u^k represents a torque
- Output y^k is the *angle* ϕ
- One stable and one unstable equilibrium point

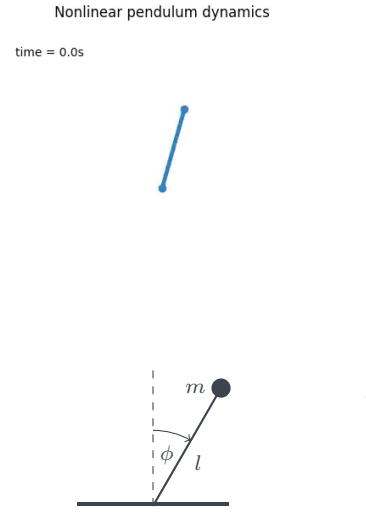


Figure 5: Parameters of single pendulum.

Generalization of Recurrent Neural Networks

LTI system with nonlinear disturbance

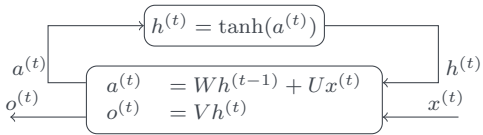
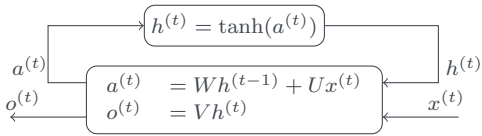


Figure 6: Recurrent neural network from [Goodfellow et al., 2016]

Generalization of Recurrent Neural Networks

LTI system with nonlinear disturbance



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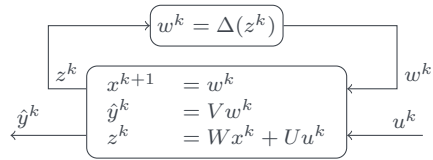
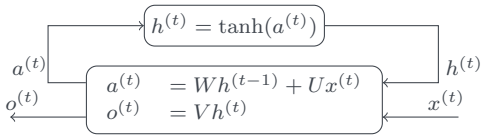


Figure 7: Using common notation from system theory.

Generalization of Recurrent Neural Networks

LTI system with nonlinear disturbance



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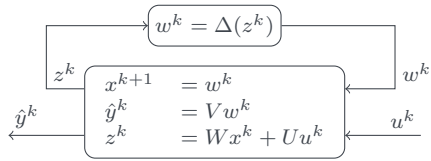


Figure 7: Using common notation from system theory.

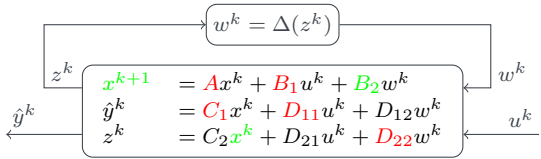


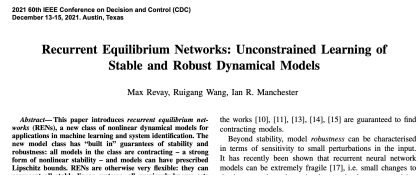
Figure 8: LTI with nonlinear disturbance.

- For $A = B_1 = C_1 = D_{11}, D_{22} = 0$, $B_2 = I$, $\Delta(\cdot) = \tanh(\cdot)$ and $h^{t-1} = x^k$ the networks in Figure 6 and Figure 8 are equivalent

Linear systems with disturbances can be analyzed with tools from robust control

Neural networks with guarantees

- Recurrent neural network (RNN) interpreted as linear systems with nonlinear disturbances can be analyzed with tools from robust control
- The neural network has system theoretic guarantees



2021 60th IEEE Conference on Decision and Control (CDC)
December 13-15, 2021. Austin, Texas

Recurrent Equilibrium Networks: Unconstrained Learning of Stable and Robust Dynamical Models

Max Revay, Ruigang Wang, Ian R. Manchester

***Abstract*— This paper introduces *recurrent equilibrium networks* (RENs), a new class of nonlinear dynamical models for applications in machine learning and system identification. The new model class has "built in" guarantees of stability and robustness: all models in the class are contracting – a strong form of nonlinear stability – and models can have prescribed Lipschitz bounds. RENs are otherwise very flexible: they can**

the works [10], [11], [13], [14], [15] are guaranteed to find contracting models.

Beyond stability, model *robustness* can be characterised in terms of sensitivity to small perturbations in the input. It has recently been shown that recurrent neural network models can be extremely fragile [17], i.e. small changes to

Figure 9: From CDC 2021, *about 8 citations*[Revay et al., 2021]

Linear systems with disturbances can be analyzed with tools from robust control

Figure 10: F16 nonlinear system identification benchmark [Noël and Schoukens, 2017]

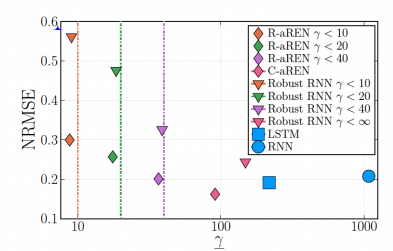


Figure 11: Robustness versus accuracy [Revay et al., 2021, Fig. 2]

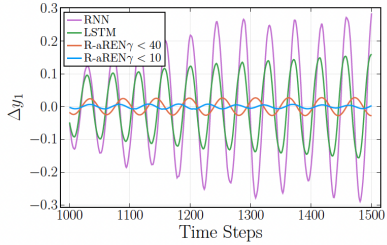


Figure 12: Stability [Revay et al., 2021, Fig. 5]

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2.204

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Monotone operator equilibrium networks.
Advances in neural information processing systems, 33:10718–10728.

Background

Pendulum is also in LTI structure

Same representation as RNNs

Difference equation of pendulum dynamics

$$
\mathcal{G}\begin{cases} x^{k+1} = \underbrace{\begin{pmatrix} 1 & \delta \\ \frac{g\delta}{l} & 1-\frac{\mu\delta}{ml^2} \end{pmatrix}}_{A} x^k + \underbrace{\begin{pmatrix} 0 \\ -\frac{g\delta}{l} \end{pmatrix}}_{B_1} u^k + \underbrace{\begin{pmatrix} 0 \\ \frac{\delta}{ml^2} \end{pmatrix}}_{B_2} w^k \\ y^k = \underbrace{\begin{pmatrix} 1 & 0 \end{pmatrix}}_{C_1} x^k \\ z^k = \underbrace{\begin{pmatrix} 1 & 0 \end{pmatrix}}_{C_2} x^k \end{cases}
$$

$$
w^k = \Delta(z^k) = z^k - \sin(z^k)
$$

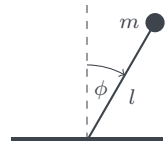

Figure 13: Parameters of single pendulum.

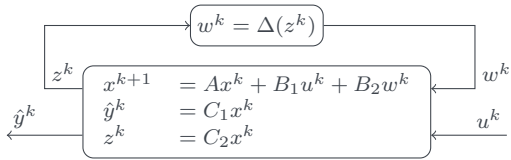

Figure 14: Pendulum dynamics in LTI structure with nonlinearity $\Delta(\cdot)$

Why is this connection interesting?

Linear systems are well understood

- Stability depends on eigenvalues of A matrix
- Well established controller design techniques

Figure 15: [Lunze and Lunze, 1996]

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Linear system with disturbances

- For known disturbances robust control methods can be applied
- Activation function of neural networks can be seen as disturbance

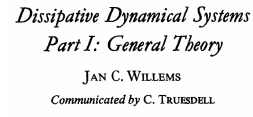

Figure 16: [Willems, 1972]

System Identification Problem

If the equations of the pendulum are not available but we are given data $\mathcal{D} = \{(u, y)_i\}_i^N$, which contains input output measurements. Finding the parameters A, B_1, B_2, C_1, C_2 can be seen as a deep learning problem.

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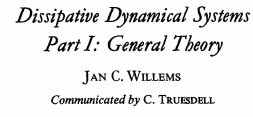

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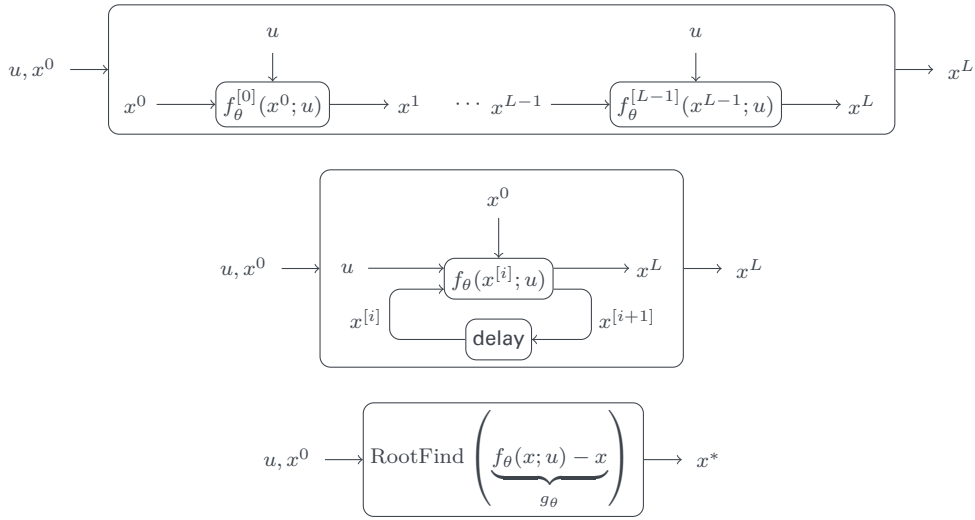
Neural networks that can be represented in LTI structure with nonlinear disturbances can be analyzed with well established tools from robust control.

Figures

5

Figures I


u, x^0
u
x^0
$f_\theta^{[0]}(x^0; u)$
x^1
$\cdots$ x^{L-1}
u
$f_\theta^{[L-1]}(x^{L-1}; u)$
x^L
x^L
u, x^0
x^0
u
$f_\theta(x^{[i]}; u)$
x^L
x^L
$x^{[i]}$
delay
$x^{[i+1]}$
u, x^0
RootFind
$f_\theta(x; u) - x$
g_θ
x^*