

Deep Learning with JAX

Fitting neural state-space models

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State-space models

We consider state-space models in the form:

$$\begin{aligned}x(k+1) &= f(x(k), u(k); p) \\y(k) &= g(x(k); p)\end{aligned}$$

- $x(k) \in \mathbb{R}^{n_x}$ is the state vector. Latent, hidden, unobserved variable
- $u(k) \in \mathbb{R}^{n_u}$ is the input vector. External, exogenous variable
- $y(k) \in \mathbb{R}^{n_y}$ is the output vector
- $p \in \mathbb{R}^{n_p}$ is the parameter vector

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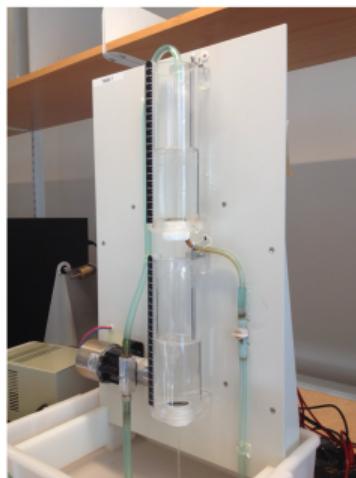
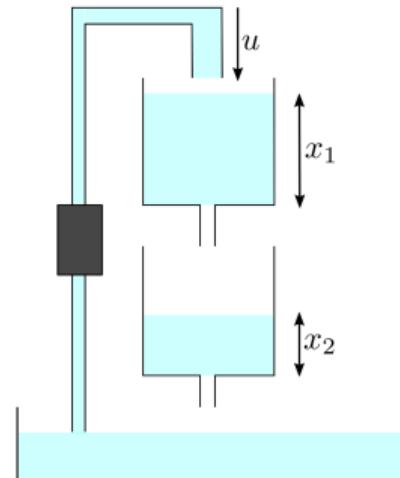
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- We will see how to fit state-space models to data using JAX
- f, g represented as neural networks.

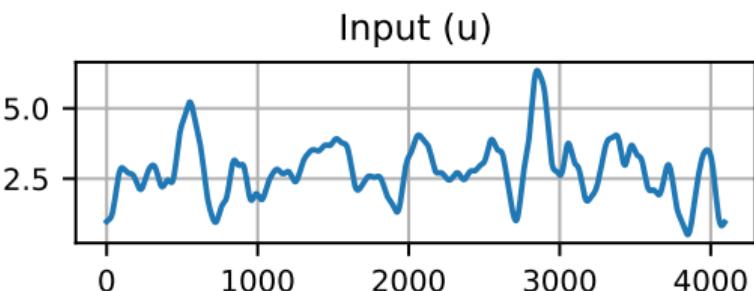
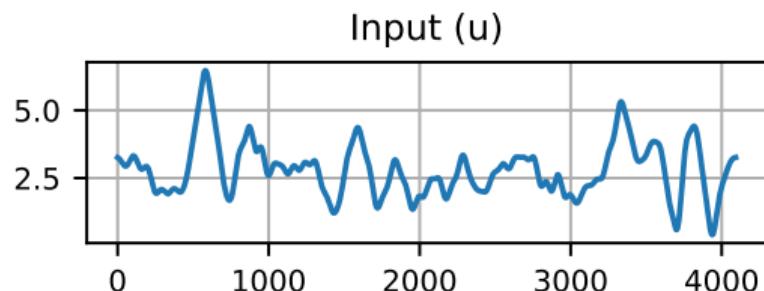
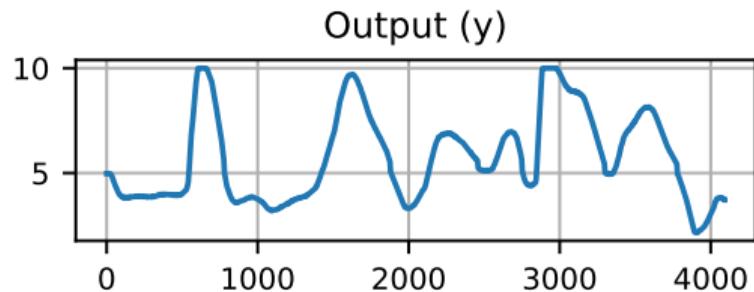
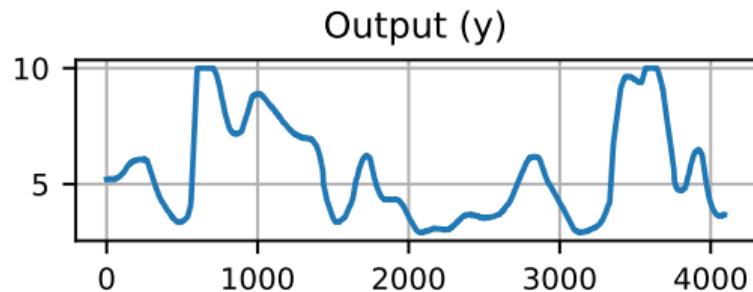
Benchmark Dataset: Cascaded Tanks

Non-linear SISO system. Input: upper tank inlet flow u . Output: lower tank level x_2 .

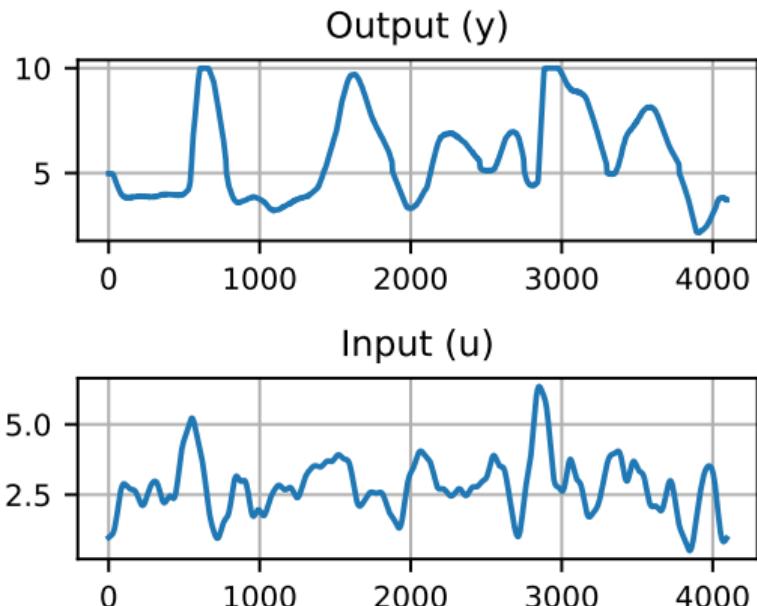
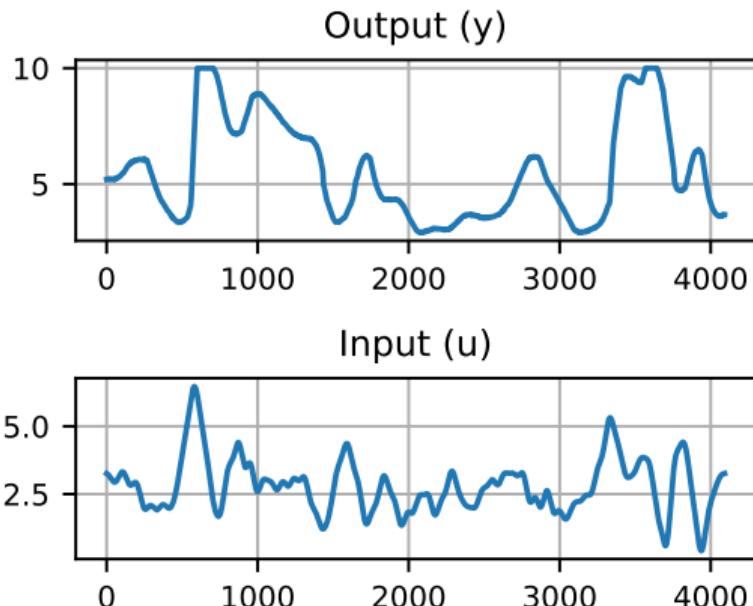


A pretty common **benchmark** for system identification algorithms.

Training (left) and test (right) data



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```
u_tr.shape, y_tr.shape, u_te.shape, y_te.shape
```

```
((1024, 1), (1024, 1), (1024, 1), (1024, 1))
```

Pre-processing

Learning algorithms perform better with favorable **scaling** (e.g., standardization)

```
u_mean = jnp.mean(u_tr); u_std = jnp.std(u_tr)
u_tr_sc = (u_tr - u_mean) / u_std
u_te_sc = (u_te - u_mean) / u_std # use training mean and std!
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```
# Same shapes as before...
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```
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```
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```

```
((1024, 1), (1024, 1))
```

```
# ... but normalized to zero mean and unit variance
```

```
u_tr_sc.mean(), u_tr_sc.std()
```

```
(Array(-4.246831e-07, dtype=float32), Array(1., dtype=float32))
```

Same procedure applied to the output...

Model fitting

- Among several valid options, we choose the model structure:

$$\begin{aligned}x(k+1) &= x(k) + W_2 \tanh(W_1[x(k)^\top u(k)^\top]^\top + b_1) + b_2 \\y(k) &= Cx(k)\end{aligned}$$

State update: previous state + FF(x, u). Output: linear.

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- We will implement simulation error minimization:

$$\hat{p}, \hat{x}(1) = \arg \min_{p, x(1)} \frac{1}{T} \sum_{k=1}^T \|y^{\text{sim}}(k) - y(k)\|^2$$

- $y^{\text{sim}}(k)$: output *simulated* by iterating the model, starting from $x(1)$
- Loss minimized w.r.t. the parameters p and the initial state $x(1)$
- It enhances learning of long-term dependencies

Define optimization variables

We will need to optimize both wrt parameters and initial condition. Let's define:

```
nu = 1; nx = 2; ny = 1; nh = 16
params = {
    "W1": jr.normal(keys[0], shape=(nh, nu+nx)), # nu + nx inputs
    "b1": jr.normal(keys[1], shape=(nh,)),
    "W2": jr.normal(keys[2], shape=(nx, nh)) * 1e-3, # nx outputs
    "b2": jr.normal(keys[3], shape=(nx,)) * 1e-3,
    "C": jr.normal(keys[4], shape=(ny, nx)), # nx inputs, ny outputs
}

x0 = jnp.zeros((nx,)) # initial state, also to be optimized
```

Single step (left) and whole simulation (right)

We need `y_sim = sim(params, x0, u_tr_sc).`

```
def f(p, x, u):
    xu = jnp.concatenate([x, u])
    z = jnp.tanh(p["W1"]@xu + p["b1"])
    x_new = x + p["W2"]@z + p["b2"]
    return x_new

def g(p, x):
    y = p["C"] @ x
    return y
```

```
def sim(p, x, us):
    # x: (nx), us:(T, nu)
    T = us.shape[0]; y_sim = []
    for t in range(T):
        y_sim.append(g(p, x))
        x = f(p, x, us[t])

    y_sim = jnp.stack(y_sim)
    return y_sim # (T, ny)
```

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- For nerds: see `sim` implementation with `jax.lax.scan` (equivalent, faster)

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- Then, write `loss_fn` with first argument `ov` with same structure as `opt_vars`

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def loss_fn(ov, ys, us):  
    y_sim = sim(ov["params"], ov["x0"], us)  
    return jnp.mean((ys - y_sim)**2)
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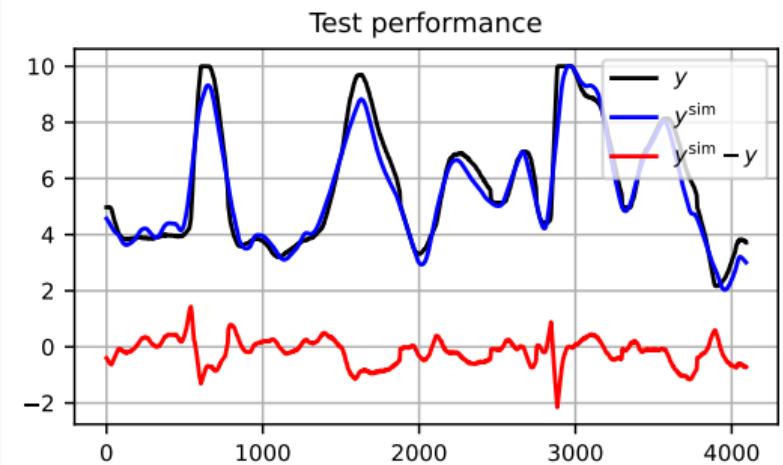
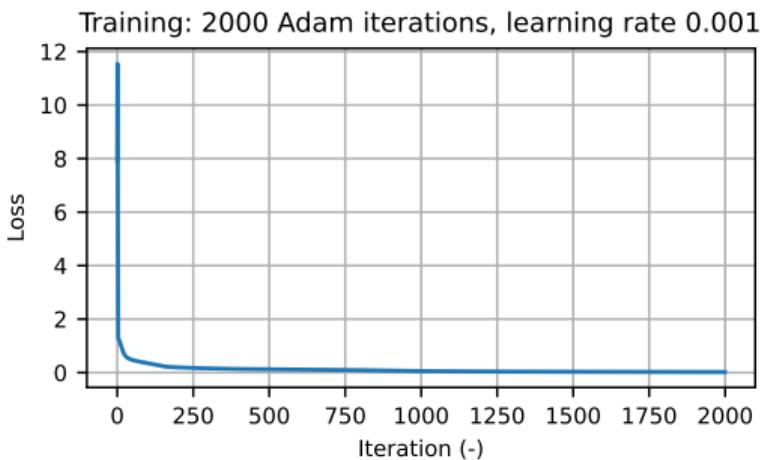
Loss function available, together with its derivatives. In a sense, the problem is *solved*.

```
loss_fn(opt_vars, y_tr_sc, u_tr_sc)
```

```
Array(7.950006, dtype=float32)
```

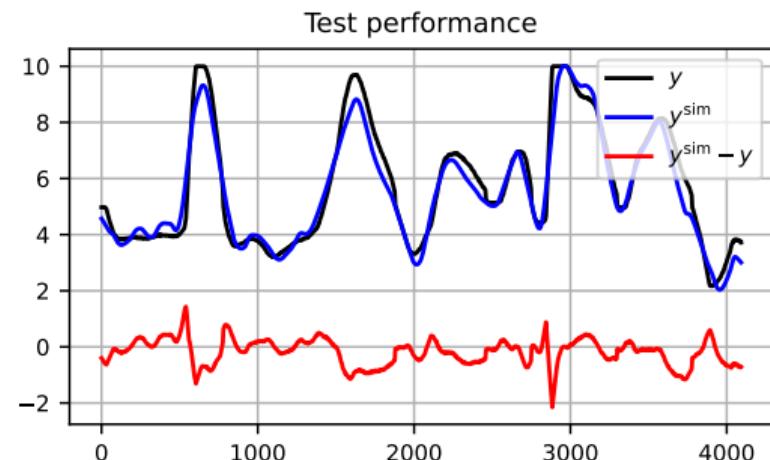
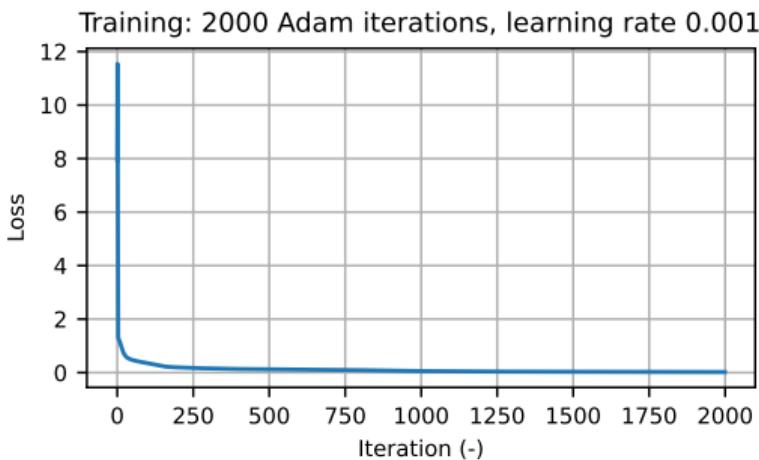
Training loss and test performance

After training (left), we assess test-set performance (right).



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```
rmse = jnp.sqrt(jnp.mean((y_te_sim - y_te)**2)); rmse
```

Array(0.5024492, dtype=float32)

Not too bad! Check out the official **Benchmark Results**

Exercise

- Reproduce the training at the previous slide
 - Hint: adapt the optimization code from the feed-forward example.
- Try out different models. You may modify:
 - Hyper-parameters and optimization settings
 - Parameter initialization
 - Number of states
 - Output equation as one of the two states
 - Output equation as another feedforward neural net
 - ...
- Try out a different dataset

Some links

- A more extensive JAX tutorial: <https://github.com/forgi86/jax-tutorial>
- Re-implementation of existing SYSID methods from the literature:
<https://github.com/forgi86/jax-ident>
- Same in PyTorch: <https://github.com/forgi86/pytorch-ident>
- PyTorch SYSID package from TU/e:
<https://github.com/MaartenSchoukens/deepSI>
- JAX SYSID package from IMT: <https://github.com/bemporad/jax-sysid>

Actually many more... the ones above I have either authored or tested!

Remarks

- Training a feedforward neural network in JAX is quite easy
- Most of the effort to specify the model and initialize its parameters
 - higher-level JAX libraries like `flax` help you out with that
- Once you have the model and the loss as functions, the rest is boilerplate

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 - higher-level JAX libraries like `flax` help you out with that
- Once you have the model and the loss as functions, the rest is boilerplate
- JAX adopts a native functional interface. Other libraries (eg, PyTorch) are primarily object-oriented.