Exercise 4

May 26, 2025

1 Advanced Deep Learning for Physics (IN2298):

1.1 Exercise 4: Supervised Network Training

1.1.1 Analytic trajectories

def. analytic state function

```
[66]: def exact_state( dt: float, p0: tensor, v0: tensor):
    g = math.vec(x=0.,y=-9.8)
    return p0 + v0*dt + 0.5*g*dt**2, v0 + g*dt
```

plot analytic trajectories

```
[67]: # initial conditions
p0 = math.vec(x=10., y=10.)
v0 = math.vec(x=1.,y=13.)
dt = 1
t = 100
n_step = int(t/dt)

# first trajectory
p_traj,v_traj = iterate(lambda p, v: exact_state(dt ,p, v),batch(time=n_step),u
p0, v0)

# plot trajectory
plot(p_traj,color='#28d642', animate='time')
```

[67]: <matplotlib.animation.FuncAnimation at 0x7f807c8c7250>

1.1.2 Simulation

```
def. simulation state function
```

```
[68]: def sim_state(dt: float, p0: tensor, v0: tensor):
    g = math.vec(x=0.,y=-9.8)
    return p0 + v0 * dt, v0 + g * dt
```

plot simulated trajectories

```
[69]: # initial conditions
p0 = math.vec(x=10., y=10.)
v0 = math.vec(x=1.,y=13.)
dt = 1
t = 100
n_step = int(t/dt)

# first trajectory
p_sim_traj,v_sim_traj = iterate(lambda p, v: sim_state(dt ,p,u ov),batch(time=n_step), p0, v0)

# plot trajectory
plot(p_sim_traj,color = '#d62828', animate='time')
```

[69]: <matplotlib.animation.FuncAnimation at 0x7f807c906290>

<Figure size 640x480 with 0 Axes>

plot trajectories together

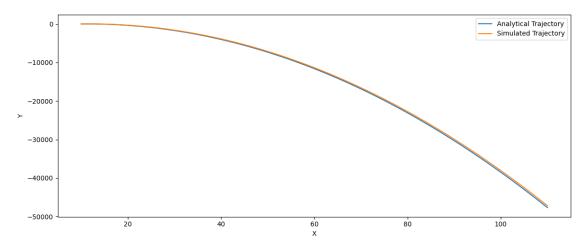
```
[70]: traj = math.stack([p_traj,p_sim_traj],instance('trajectory'))
color = color = wrap(['#28d642','#d62828'],instance(traj))
plot(traj,color = color, animate='time')
```

```
/usr/local/lib/python3.11/dist-packages/phiml/math/_tensors.py:1379:
RuntimeWarning: invalid value encountered in power
  result = op(n1, n2)
```

[70]: <matplotlib.animation.FuncAnimation at 0x7f808079fd10>

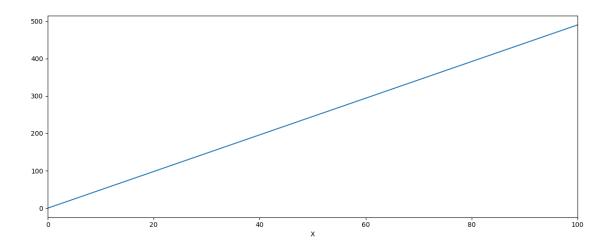
<Figure size 640x480 with 0 Axes>

/usr/local/lib/python3.11/dist-packages/phiml/math/_tensors.py:1379:
RuntimeWarning: invalid value encountered in power
 result = op(n1, n2)



plot error for positions

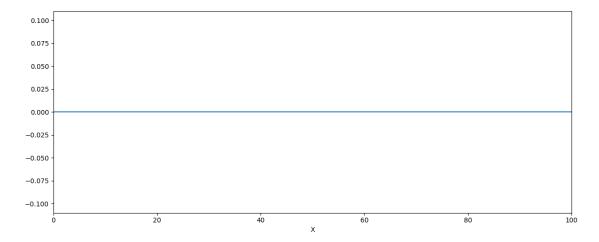
```
[72]: x = p_traj.vector['x']
    error = p_sim_traj - p_traj
    error = math.pack_dims(error, dims='time', packed_dim='x')
    x = math.pack_dims(x, dims='time', packed_dim='x')
    show(error.vector['y'])
```



plot error for velocities

```
[73]: x = v_traj.vector['x']
    error = v_sim_traj - v_traj
    print(error)
    error = math.pack_dims(error, dims='time', packed_dim='x')
    x = math.pack_dims(x, dims='time', packed_dim='x')
    show(error.vector['y'])
```

(time =101, vector =x,y) const 0.0



1.1.3 Data Set

```
[74]: # Set the seed to have always the same Dataset
      torch.manual_seed(42)
      sample_list = []
      an_sample_list = []
      n_samples = 500
      n_step = 100
      dt = 1
      scaling = math.linspace(0.0, n_step, batch(time=n_step+1))
      scaling = math.expand(scaling, channel(vector='x,y'))
      for sample in range(n_samples):
        # Defining p0,v0
        p0 = math.random_uniform(channel(vector='x,y'))*10
        v0 = math.random uniform(channel(vector='x,y'))*10
        # Defining analytical and simulated trajectories
        an_pos_traj, an_vel_traj = iterate(lambda p, v: exact_state(dt ,p,u
       →v),batch(time=n_step), p0, v0)
        sim_pos_traj,sim_vel_traj = iterate(lambda p, v: sim_state(dt ,p,_
       →v),batch(time=n step), p0, v0)
        #print(an_pos_traj)
        sample_state = math.concat([sim_pos_traj,sim_vel_traj],'vector')
        sample_an_state = math.concat([an_pos_traj,an_vel_traj],'vector')
        sample_list.append(sample_state)
        an_sample_list.append(sample_an_state)
      state = math.concat(sample_list, 'time')
      an_state = math.concat(an_sample_list, 'time')
      print(state)
      print(an_state)
     (time =50500, vector =x,y,x,y) -4.03e+03 \pm 1.0e+04
     (-5e+04...1e+03)
     (time = 50500, vector = x, y, x, y) -4.09e + 03 \pm 1.0e + 04
```

1.1.4 Neural Corrector

(-5e+04...1e+03)

```
[75]: net = dense_net(4, 4, layers=[32, 32], activation='ReLU') optimizer = adam(net, 1e-3)
```

```
[76]: @math.jit_compile
      def loss_function(state: tensor,an_state: tensor):
        predicted_delta_state = math.native_call(net,state)
        predicted_delta_state = math.
       Grename_dims(predicted_delta_state,channel('vector'),channel(vector='x,y,x,y'))
        delta_state = state - an_state
        diff = delta_state-predicted_delta_state
        return math.12_loss(diff)
[77]: for i in range(5000):
        loss = update_weights(net,optimizer,loss_function,state,an_state)
        if i % 1000 == 0: print(loss)
     (time = 50500) 9.73e + 05 \pm 1.2e + 06 (2e - 02...5e + 06)
     (time = 50500) 1.066 \pm 1.083 (2e-05...1e+01)
     (time = 50500) 1.026 \pm 1.017 (4e-05...9e+00)
     (time = 50500) 1.205 \pm 1.221 (2e-04...9e+00)
     (time = 50500) 1.011 \pm 1.019 (8e-05...1e+01)
     Visualize results
[78]: # Defining p0, v0
      p0 = math.random_uniform(channel(vector='x,y'))*10
      v0 = math.random_uniform(channel(vector='x,y'))*10
      # Defining analytical and simulated trajectories
      an_pos_traj, an_vel_traj = iterate(lambda p, v: exact_state(dt ,p,__
       ⇒v),batch(time=n_step), p0, v0)
      sim_pos_traj,sim_vel_traj = iterate(lambda p, v: sim_state(dt ,p,_
       ⇒v),batch(time=n step), p0, v0)
      print(an_pos_traj)
      state = math.concat([sim_pos_traj,sim_vel_traj],'vector')
      an_state = math.concat([an_pos_traj,an_vel_traj],'vector')
      predictions = math.native_call(net,state)
      print(predictions)
     (time = 101, vector = x, y) -7.81e + 03 \pm 1.3e + 04
      (-5e+04...1e+03)
     (time = 101, vector = 4) 61.193 \pm 128.390
     (-2e+00...5e+02)
     Visualize trajectories
[79]: # True Trajectory
      traj = math.stack([an_pos_traj,sim_pos_traj],instance('trajectory'))
      color = color = wrap(['#28d642', '#d62828'], instance(traj))
```

```
plot(traj,color = color, animate='time')
```

[79]: <matplotlib.animation.FuncAnimation at 0x7f807cf70f10>

<Figure size 640x480 with 0 Axes>

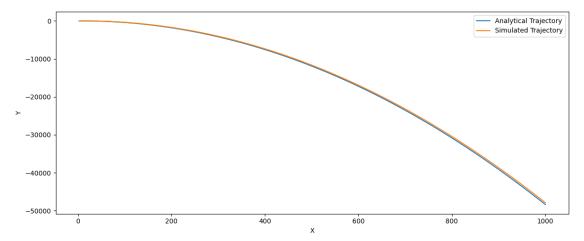
```
#Frame visualization

# Extract x and y vectors and combine into a spatial field
an_xy = math.stack([an_pos_traj.vector['x'], an_pos_traj.vector['y']],___
channel(vector='x,y'))

corr_xy = math.stack([sim_pos_traj.vector['x'], sim_pos_traj.vector['y']],__
channel(vector='x,y'))

# Pack time dimension into sample points
an_xy = math.pack_dims(an_xy, 'time', 't')
corr_xy = math.pack_dims(corr_xy, 'time', 't')

# Plot both trajectories on the same plot
show(math.stack({'Analytical Trajectory': an_xy, 'Simulated Trajectory':___
corr_xy}, channel('trajectory')))
```



```
[82]: # Corrected Trajectory
traj = math.stack([an_pos_traj,corrected_traj],instance('trajectory'))
color = color = wrap(['#28d642','#d62828'],instance(traj))
plot(traj,color = color, animate='time')
```

[82]: <matplotlib.animation.FuncAnimation at 0x7f807cef8250>

<Figure size 640x480 with 0 Axes>

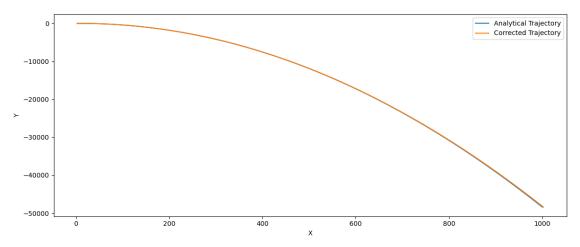
```
#Frame visualization

# Extract x and y vectors and combine into a spatial field
an_xy = math.stack([an_pos_traj.vector['x'], an_pos_traj.vector['y']],___
channel(vector='x,y'))

corr_xy = math.stack([corrected_traj.vector['x'], corrected_traj.vector['y']],__
channel(vector='x,y'))

# Pack time dimension into sample points
an_xy = math.pack_dims(an_xy, 'time', 't')
corr_xy = math.pack_dims(corr_xy, 'time', 't')

# Plot both trajectories on the same plot
show(math.stack({'Analytical Trajectory': an_xy, 'Corrected Trajectory':___
corr_xy}, channel('trajectory')))
```

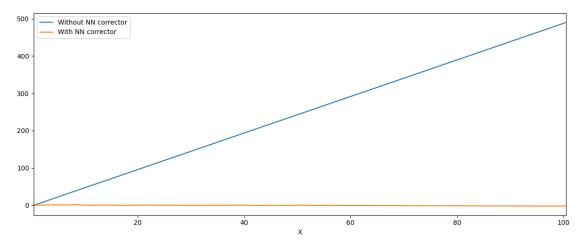


Errors

```
[84]: # Error without Neural corrector
x = sim_pos_traj.vector['x']
errore = sim_pos_traj - an_pos_traj
errore = math.pack_dims(errore, dims='time', packed_dim='x')
x = math.pack_dims(x, dims='time', packed_dim='x')

# Error with neural corrector
x = corrected_traj.vector['x']
error = corrected_traj - an_pos_traj
error = math.pack_dims(error, dims='time', packed_dim='x')
```

```
x = math.pack_dims(x, dims='time', packed_dim='x')
show(CenteredGrid(math.stack({
    "Without NN corrector": errore.vector['y'],
    "With NN corrector": error.vector['y']
},channel('trajectory'))))
```



[87]: \[\%\capture \] !jupyter nbconvert --to pdf --output /content/drive/MyDrive/Fisica/ADL4P/ \[\times \text{Exercise_4.pdf /content/drive/MyDrive/Fisica/ADL4P/Exercise_4.ipynb} \]