pixelvae_results

February 17, 2021

```python
[1]: import torch
     import numpy as np
     import pandas as pd
     import peakutils
     import abel
     import os
     from torch.nn import functional as F
     from matplotlib import pyplot as plt
     from scipy.stats import entropy
     from ruamel.yaml import YAML

     from dii.models.base import valid_models
     from dii.visualization.visualize import radial_profile
     from dii.pipeline.datautils import get_benchmark_imageset

     plt.style.use("publication")
```

/home/kelvin/anaconda3/envs/ion-image/lib/python3.7/site-
packages/pytorch_lightning/utilities/distributed.py:50: UserWarning: Checkpoint
directory /home/kelvin/Dropbox (MIT)/Projects/deep-ion-image/notebooks/reports
exists and is not empty.
  warnings.warn(*args, **kwargs)

```python
[2]: def get_profile_peaks(x: np.ndarray, y: np.ndarray, thres=0.05):
         idx = peakutils.indexes(y, thres=thres)
         centers = peakutils.interpolate(x, y, ind=idx)
         return idx, centers
```

1 Model testing report

This notebook is generated using `papermill`.

1.1 Parameter definitions

```
[3]: # Parameter cell; do not edit!
     model_kwargs = {
         "in_channels": 1,
         "out_channels": 1,
         "latent_dim": 64,
         "activation": "silu"
     }
     image_index = 50
     models_path = "../../models/"
     benchmark_path = "../../data/processed"
     n_images = 128
     model_name = "baseline"
     probabilistic = False
     img_center = (64, 64)
     output_root = "outputs/"
```

```
[4]: # Parameters
     model_kwargs = {
         "in_channels": 1,
         "out_channels": 1,
         "latent_dim": 64,
         "activation": "silu",
         "pixel_hidden": 64,
         "pixel_layers": 5,
     }
     probabilistic = True
     model_name = "pixelvae"
```

```
[5]: # output path is where model specific results go
     # agg path is a YAML with the combined statistics for summarizing across models
     output_path = f"{output_root}{model_name}/"
     agg_path = f"{output_root}combined_statistics.yml"
```

```
[6]: try:
         os.mkdir(output_path)
     except:
         pass
```

1.2 Model determination and loading

```
[7]: # figure out what model we are using with the mapping
     model = valid_models.get(model_name, None)

     if not model:
```

```
        raise KeyError(f"{model_name} is not a valid model in the `dii` codebase!␣
    ↪Try again!")
```

[8]:
```python
model_obj = model(**model_kwargs)
model_obj.load_state_dict(torch.load(f"{models_path}{model_name}.pt"))

# make sure we have the correct behavior for everything
model_obj.eval();
```

1.3 Data set loading

[9]:
```python
input_images, target_images = get_benchmark_imageset(benchmark_path, n_images)
```

1.4 Model predictions

[10]:
```python
with torch.no_grad():
    recon = model_obj(input_images)
```

1.4.1 Calculating the mean reconstruction error

[11]:
```python
recon_error = F.binary_cross_entropy(recon, target_images).item()
```

[12]:
```python
print(f"Mean reconstruction error: {recon_error:.2f}")
```

Mean reconstruction error: 0.14

1.4.2 Finding the best and worst images

[13]:
```python
# this calculates the pixelwise loss
errors = F.binary_cross_entropy(recon, target_images, reduction="none")
```

[14]:
```python
# calculate the highest errors to identify which images are worse
img_errors = errors.mean((1, 2, 3))
worst_idx = torch.argsort(img_errors)[-5:]
best_idx = torch.argsort(img_errors)[:5]

worst_error = img_errors.max().item()
best_error = img_errors.min().item()
```
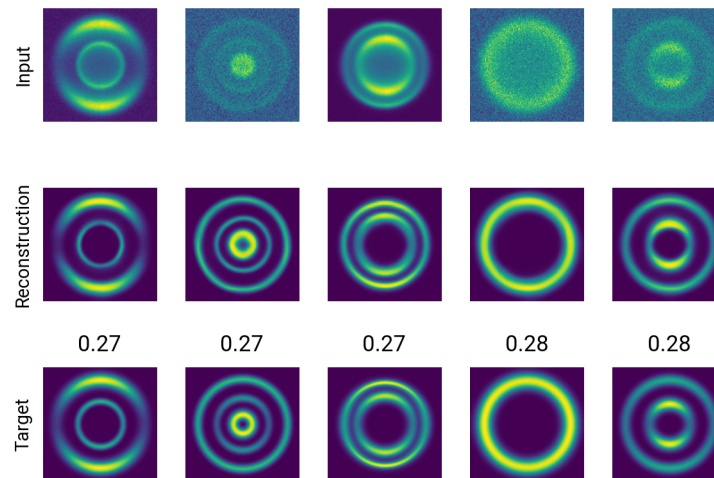
1.4.3 Visualizing the worst images

[15]:
```python
fig, axarray = plt.subplots(3, 5, figsize=(4, 3), sharex=True, sharey=True)

for row, (target, title) in enumerate(zip([input_images, recon, target_images],␣
    ↪["Input", "Reconstruction", "Target"])):
    images = target[worst_idx]
```

```
        for col, image in enumerate(images):
            # get rid of the channel dimension
            axarray[row, col].imshow(image.squeeze())
            axarray[row, col].set(xticks=[], yticks=[])
            for _, spine in axarray[row, col].spines.items():
                spine.set_visible(False)
        axarray[row, 0].set_ylabel(title, rotation=90.)
for col, value in enumerate(img_errors[worst_idx]):
    axarray[-1, col].set(title=f"{value:.2f}")
fig.tight_layout()
fig.savefig(f"{output_path}{model_name}_worstimgs.png", dpi=600)
```


### 1.4.4 Visualizing the best images

```
[16]: fig, axarray = plt.subplots(3, 5, figsize=(4, 3), sharex=True, sharey=True)

for row, (target, title) in enumerate(zip([input_images, recon, target_images],
 ↪["Input", "Reconstruction", "Target"])):
    images = target[best_idx]
    for col, image in enumerate(images):
        # get rid of the channel dimension
        axarray[row, col].imshow(image.squeeze())
        axarray[row, col].set(xticks=[], yticks=[])
        for _, spine in axarray[row, col].spines.items():
            spine.set_visible(False)
    axarray[row, 0].set_ylabel(title, rotation=90.)
for col, value in enumerate(img_errors[best_idx]):
    axarray[-1, col].set(title=f"{value:.2f}")
fig.tight_layout()
```

```
fig.savefig(f"{output_path}{model_name}_bestimgs.png", dpi=600)
```
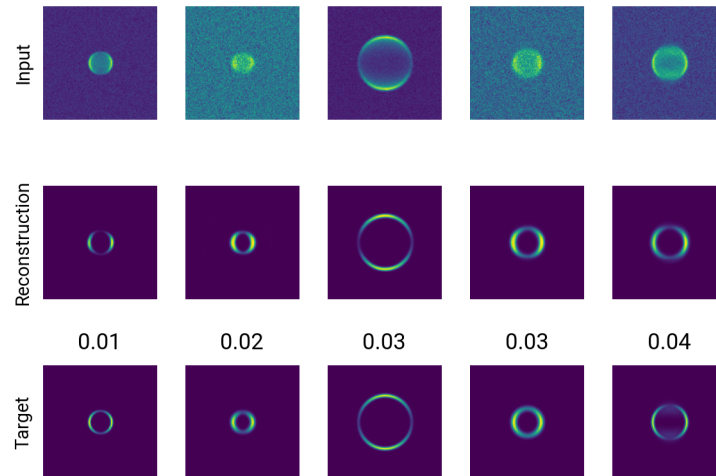

1.5 Common ground: compare one image across models

1.5.1 Show what the reconstruction looks like

```
[17]: fig, axarray = plt.subplots(1, 3, figsize=(2.5, 1), sharex=True, sharey=True)

      for ax, title, target in zip(axarray, ["Input", "Reconstruction", "Target"],
       ↪[input_images, recon, target_images]):
          ax.imshow(target[image_index].squeeze())
          ax.set(title=title, yticks=[], xticks=[])
          for _, spine in ax.spines.items():
              spine.set_visible(False)
      fig.tight_layout()
      fig.savefig(f"{output_path}{model_name}_common_imgs.png", dpi=600)
```
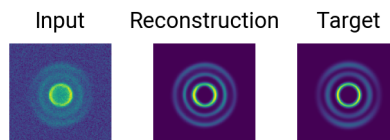
1.5.2 Compare radial profiles

```
[18]:  if probabilistic:
           # get 200 samples from the posterior
           prob_recon = model_obj.predict(input_images[image_index], 200)
           prob_profiles = np.vstack([radial_profile(img.squeeze().numpy(),␣
       ↪img_center) for img in prob_recon])
           # calculate sampling statistics
           profile_mean = prob_profiles.mean(axis=0)
           normalize = profile_mean.sum()
           profile_std = prob_profiles.std(axis=0)
           # get +/- one sigma and the mean
           upper, lower = (profile_mean + profile_std) / normalize, (profile_mean -␣
       ↪profile_std) / normalize
           profile_mean /= normalize
           df = pd.DataFrame(data=list(zip(profile_mean, upper, lower)),␣
       ↪columns=["Model", "Upper", "Lower"])
       else:
           profile = model_obj.model_radial_profile(input_images[image_index])
           profile /= profile.sum()
           df = pd.DataFrame(data=profile, columns=["Model"])

       for target, name in zip([input_images, target_images], ["Input", "Target"]):
           profile = radial_profile(target[image_index].squeeze().numpy(), img_center)
           norm = profile.sum()
           profile /= norm
           df[name] = profile

       op_img = abel.Transform(input_images[image_index].squeeze().numpy(),␣
        ↪method="onion_peeling").transform
       op_profile = radial_profile(op_img, img_center)
       op_profile /= op_profile.sum()
       df["OnionPeeling"] = op_profile
```

```
[19]:  # output the result for overlaying later
       df.to_csv(f"{output_path}{model_name}_common_radial.csv")
```

```
[20]:  fig, ax = plt.subplots(figsize=(2.5, 1.5))

       colors = ["#0051ad", "#d34e60", "#9ac54f"]

       for key, color in zip(["Model", "Target", "OnionPeeling"], colors):
           ax.plot(df[key], lw=1., alpha=0.7, label=key, color=color)

       # if we have a probabilistic model, shade in +/-1 sigma
       if probabilistic:
```
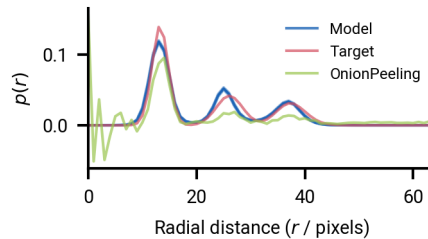
```
      ax.fill_between(np.arange(df["Model"].size), df["Upper"], df["Lower"],␣
   ↪color=colors[0], alpha=0.4)

ax.set(ylabel="$p(r)$", xlabel="Radial distance ($r$ / pixels)", xlim=[0.,␣
   ↪img_center[0]])
ax.legend(fontsize="xx-small")
fig.tight_layout()
fig.savefig(f"{output_path}{model_name}_common_radial.png", dpi=600)
```


1.5.3 Radial error quantification

For the sole exemplar image

```
[21]: # true_quant, true_interp = get_profile_peaks(df.index, df["Target"])
      # recon_quant, recon_interp = get_profile_peaks(df.index, df["Model"])
```

```
[22]: # quant_error = (np.square(true_quant - recon_quant)).mean()
      # interp_error = ((np.square(true_interp - recon_interp)).mean() / df.index.
      ↪size) * 100.
```

```
[23]: # print(f"Quantized pixel error is {quant_error:.2f} pixels")
      # print(f"Interpolated relative error is {interp_error:.2f}%")
```

```
[24]: # # see what the centers actually are
      # print(true_interp, recon_interp)
```

Across the benchmark set

```
[25]: true_num, pred_num = list(), list()
      kl_divs = list()
      for target, predicted in zip(target_images, recon):
          target_profile = radial_profile(target.squeeze().numpy(), img_center)
          recon_profile = radial_profile(predicted.squeeze().numpy(), img_center)
          kl = entropy(pk=target_profile, qk=recon_profile)
          kl_divs.append(kl)
          # get the peaks from the radial profile
          x = np.arange(target_profile.size)
```

```
    true_quant, true_interp = get_profile_peaks(x, target_profile)
    recon_quant, recon_interp = get_profile_peaks(x, recon_profile)
    true_num.append(len(true_quant))
    pred_num.append(len(recon_quant))

true_counts, bins = np.histogram(true_num, bins=np.arange(1, 6))
pred_counts, bins = np.histogram(pred_num, bins=np.arange(1, 6))
```

/home/kelvin/anaconda3/envs/ion-image/lib/python3.7/site-
packages/peakutils/peak.py:246: UserWarning: At least 3 points required for
Gaussian fitting
  warnings.warn(str(e))
/home/kelvin/anaconda3/envs/ion-image/lib/python3.7/site-
packages/peakutils/peak.py:246: UserWarning: Optimal parameters not found:
Number of calls to function has reached maxfev = 800.
  warnings.warn(str(e))

[26]:
```
print(f"Mean KL-divergence, representing the true distribution P with the␣
 ↪predicted Q: {np.mean(kl_divs):.2f}")
```

Mean KL-divergence, representing the true distribution P with the predicted Q:
0.05
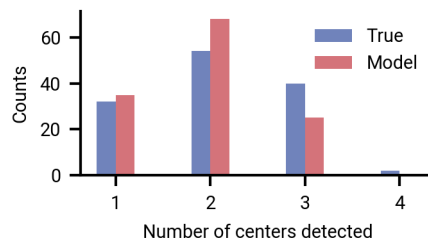
[27]:
```
fig, ax= plt.subplots(figsize=(2.5, 1.5))

ax.bar(bins[:-1] - 0.1, true_counts, label="True", alpha=0.7, width=0.2)
ax.bar(bins[:-1] + 0.1, pred_counts, label="Model", alpha=0.7, width=0.2)
ax.legend(fontsize="x-small")
ax.set(ylabel="Counts", xlabel="Number of centers detected")
```

[27]: [Text(0, 0.5, 'Counts'), Text(0.5, 0, 'Number of centers detected')]

2 Finalizing the results

```python
yaml = YAML()
```

```python
current = None
if os.path.isfile(agg_path):
    with open(agg_path, "r") as results_file:
        current = yaml.load(results_file)
if not current:
    current = dict()
current[f"{model_name}"] = {
    "kl-divergence": str(np.mean(kl_divs)),
    "dev_mean_recon": str(recon_error),
    "best_recon": str(best_error),
    "worst_recon": str(worst_error)
}
with open(agg_path, "w") as results_file:
    yaml.dump(current, results_file)
```