Sheet#04 Proposed Solution MLPH_W24

J. Schubert, M. Schümann

November 24, 2024

1 Sheet 5

1.1 1

 $\begin{array}{l} \text{(a)} \\ \frac{\partial \sigma(x))}{\partial x} = \frac{\partial}{\partial x} \frac{1}{1 + \exp(-x)} = \frac{-(-\exp(-x))}{(1 + \exp(-x))^2} = \exp(-x)\sigma(x)^2 \\ \text{(b)} \\ \text{Consider } 2\sigma(2x) - 1 = 2\frac{1}{1 + \exp(-2x)} - 1 = 2\frac{\exp(x)}{\exp(x) + \exp(-x)} - 1 = \frac{2\exp(x) - \exp(x) - \exp(x) - \exp(-x)}{\exp(x) + \exp(-x)} = \tanh(x). \\ \text{(c)} \\ a = (1, 1)^{\mathrm{T}}, \ c = (2, 2)^{\mathrm{T}}, \ d = (1, 2)^{\mathrm{T}}, \ f = (2, 3)^{\mathrm{T}}, \\ \text{Consider } w = (4, -3), \ b = 0: \\ \sigma(a; w, b) = \sigma(1) > 0.5 \\ \sigma(c; w, b) = \sigma(2) > 0.5 \\ \sigma(d; w, b) = \sigma(-2) < 0.5 \end{array}$

 $\sigma(f; w, b) = \sigma(-1) < 0.5$

1.2 2 Logistic regression: an LLM lie detector

Download the data from https://heibox.uni-heidelberg.de/f/38bd3f2a9b7944248cc2/ Unzip it and place the lie_detection folder in the folder named data to get the following structure: "data/lie_detection/datasets" and "data/lie_detection/acts".

This is how you can load a dataset of LLM activations. Use a new Datamanager if you want to have a new dataset. Use the same data manager if you want to combine datasets.

```
[2]: from lie_detection_utils import DataManager

path_to_datasets = "data/datasets"

path_to_acts = "data/acts"
```

```
# check if the datasets and activations are available
     assert os.path.exists(path_to_datasets), "The path to the datasets does not_
     assert os.path.exists(path_to_acts), "The path to the activations does not__
      ⇔exist."
     \# these are the different datasets containing true and false factual statements \sqcup
      ⇔about different topics
     dataset_names = ["cities", "neg_cities", "sp_en_trans", "neg_sp_en_trans"]
     dataset_name = dataset_names[0] # choose some dataset from the above datasets,
      →index "0" loads the "cities" dataset for example
     # the dataloader automatically loads the training data for us
     dm = DataManager()
     dm.add_dataset(dataset_name, "Llama3", "8B", "chat", layer=12, split=0.8, __
      ⇔center=False,
                     device='cpu', path_to_datasets=path_to_datasets,_
      →path_to_acts=path_to_acts)
     acts_train, labels_train = dm.get('train') # train set
     acts_test, labels_test = dm.get('val')
     print(acts_train.shape, labels_train.shape)
    torch.Size([1196, 4096]) torch.Size([1196])
[3]: # have a look at the statements that were fed to the LLM to produce the
     →activations:
     df = pd.read_csv(f"{path_to_datasets}/{dataset_name}.csv")
     print(df.head(10))
                                             statement label
                                                                    city \
    0
                  The city of Krasnodar is in Russia.
                                                            1 Krasnodar
    1
            The city of Krasnodar is in South Africa.
                                                            0 Krasnodar
    2
                       The city of Lodz is in Poland.
                                                            1
                                                                    Lodz
    3
       The city of Lodz is in the Dominican Republic.
                                                            0
                                                                    Lodz
    4
                 The city of Maracay is in Venezuela.
                                                            1
                                                                 Maracay
    5
                     The city of Maracay is in China.
                                                            0
                                                                 Maracay
    6
                   The city of Baku is in Azerbaijan.
                                                            1
                                                                    Baku
    7
                      The city of Baku is in Ukraine.
                                                                    Baku
                                                            0
    8
                       The city of Baoji is in China.
                                                            1
                                                                   Baoji
    9
                   The city of Baoji is in Guatemala.
                                                                   Baoji
                      country correct_country
    0
                       Russia
                                       Russia
                 South Africa
    1
                                       Russia
                       Poland
                                       Poland
    3 the Dominican Republic
                                       Poland
```

```
4
                 Venezuela
                                  Venezuela
                                  Venezuela
5
                     China
6
                Azerbaijan
                                 Azerbaijan
7
                   Ukraine
                                 Azerbaijan
8
                     China
                                       China
9
                 Guatemala
                                       China
 (a)
```

```
tensor(0.0002) tensor(0.0985)
torch.Size([1196, 4096]) torch.Size([1196])
score cities 0.99666666666666667 0.9378154589707266
tensor(-0.0002) tensor(0.1108)
torch.Size([1196, 4096]) torch.Size([1196])
score neg_cities 1.0 0.48106144589465705
tensor(-0.0027) tensor(0.1095)
torch.Size([283, 4096]) torch.Size([283])
score sp_en_trans 1.0 0.6866930208929193
tensor(-0.0009) tensor(0.1103)
torch.Size([283, 4096]) torch.Size([283])
score neg_sp_en_trans 1.0 0.3806657749382361
```

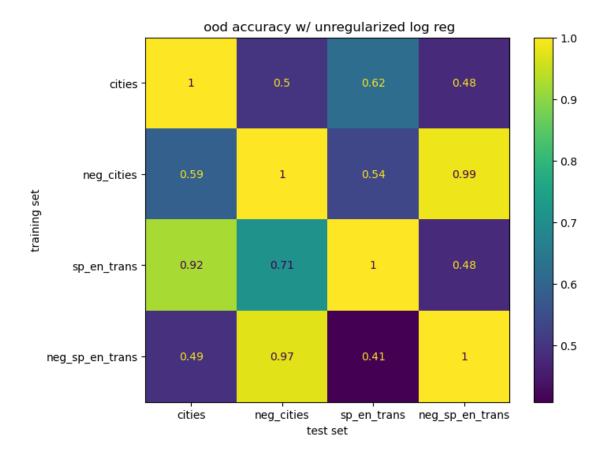
If our inputs were linearly separable, we would expect at least one very large value in the weights vectors $w, y = \sigma(w \cdot x + b)$, because then the sigmoid turns into a step function along that dimension of data. However, the maximum is on the order of unity for all datasets, suggesting that in our chosen representation the classes are not linearly separable and have some overlap.

(b)

```
[5]: from sklearn.metrics import ConfusionMatrixDisplay
     # Plot of accuracy when train and test data come from different datasets, ___
     ⇔without regularization
    scores = []
    for train_set_name in dataset_names:
        for test_set_name in dataset_names:
            dm1 = DataManager()
            dm1.add_dataset(train_set_name, "Llama3", "8B", "chat", layer=12, u
      ⇒split=0.8, center=False,
                            device='cpu', path_to_datasets=path_to_datasets,_
      →path_to_acts=path_to_acts)
            acts_train, labels_train = dm1.get('train') # train set
            dm2 = DataManager()
            dm2.add_dataset(test_set_name, "Llama3", "8B", "chat", layer=12,__
      ⇒split=0.8, center=False,
                            device='cpu', path_to_datasets=path_to_datasets,_
      spath_to_acts=path_to_acts)
            acts_test, labels_test = dm2.get('val')
            logreg = LogisticRegression(n_jobs=10, C=1e6, random_state=0)
            logreg.fit(acts_train, labels_train)
            score = logreg.score(acts_test, labels_test)
            print("score", train_set_name, test_set_name, score)
            scores.append(logreg.score(acts_test, labels_test))
    score cities cities 1.0
    score cities neg cities 0.49666666666666665
    score cities sp_en_trans 0.6197183098591549
    score cities neg_sp_en_trans 0.4788732394366197
    score neg_cities cities 0.59
    score neg_cities neg_cities 1.0
    score neg_cities sp_en_trans 0.5352112676056338
    score neg_cities neg_sp_en_trans 0.9859154929577465
    score sp_en_trans neg_cities 0.71
    score sp_en_trans sp_en_trans 1.0
    score sp_en_trans neg_sp_en_trans 0.4788732394366197
    score neg_sp_en_trans cities 0.49333333333333333
    score neg_sp_en_trans neg_cities 0.9733333333333333334
    score neg_sp_en_trans sp_en_trans 0.4084507042253521
```

score neg_sp_en_trans neg_sp_en_trans 1.0

[6]: Text(0.5, 1.0, ' ood accuracy w/ unregularized log reg')



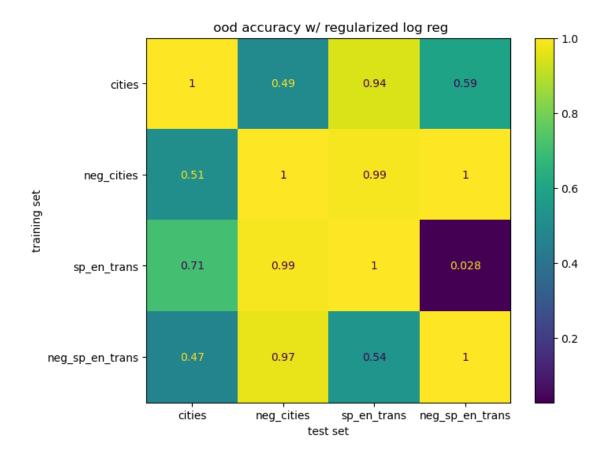
```
[7]: from sklearn.metrics import ConfusionMatrixDisplay

# Plot of accuracy when train and test data come from different datasets,
without regularization

scores = []
for train_set_name in dataset_names:
    for test_set_name in dataset_names:
```

```
dm1 = DataManager()
      dm1.add_dataset(train_set_name, "Llama3", "8B", "chat", layer=12, ___
⇔split=0.8, center=False,
                       device='cpu', path_to_datasets=path_to_datasets,__
→path_to_acts=path_to_acts)
      acts_train, labels_train = dm1.get('train') # train set
      dm2 = DataManager()
      dm2.add_dataset(test_set_name, "Llama3", "8B", "chat", layer=12,__
⇔split=0.8, center=False,
                       device='cpu', path_to_datasets=path_to_datasets,_
path_to_acts=path_to_acts)
      acts_test, labels_test = dm2.get('val')
      logreg = LogisticRegression(n_jobs=10, C=1, random_state=0)
      logreg.fit(acts_train, labels_train)
      score = logreg.score(acts_test, labels_test)
       print("score", train_set_name, test_set_name, score)
      scores.append(logreg.score(acts_test, labels_test))
```

[8]: Text(0.5, 1.0, ' ood accuracy w/ regularized log reg')



We see that regularizing training on the cities dataset improves the out-of-distribution test accuracy, especially in the case of the sp_en_trans test set. Overall however the regularized model performs poorer than the unregularized model, for instance training on sp_en_trans and testing on cities or neg_sp_en_trans leads to lower accuracy (.91-> .77 and .52 -> 0.07) in the regularized case.

(c)

```
cities_train, labels_train = dm.get('train')
cities_test, labels_test = dm.get('val')
logreg = LogisticRegression(n_jobs=1, C=1e-1, random_state=0)
logreg.fit(cities_train, labels_train)
# verifying city training
print("city score", logreg.score(cities_test, labels_test))
dm = DataManager()
# adding both cities set to data
dm.add_dataset(test_sets[0], "Llama3", "8B", "chat", layer=12, split=0.8, __
 ⇔center=False,
                device='cpu', path_to_datasets=path_to_datasets,_
→path_to_acts=path_to_acts)
dm.add_dataset(test_sets[1], "Llama3", "8B", "chat", layer=12, split=0.8, __
 ⇔center=False,
                device='cpu', path_to_datasets=path_to_datasets,_
 →path_to_acts=path_to_acts)
trans_test, trans_labels_test = dm.get('val')
print("trans score", logreg.score(trans_test, trans_labels_test))
```

city score 0.9983333333333333 trans score 0.9788732394366197

Training on both of the cities datasets shows a very high (<0.98) test score for both the cities and the trans test sets.

1.3 3 Log-sum-exp and soft(arg)max

1.3.1 (a)

(i) :

$$\operatorname{softmax}(a\sigma, b\lambda)_{k} = \frac{\exp(ab\lambda\sigma_{k})}{\sum_{i=1}^{n} \exp(ab\sigma_{i}\lambda)}$$

$$= \frac{(\exp(\lambda\sigma_{k}))^{ab}}{\sum_{i=1}^{n} (\exp(\sigma_{i}\lambda))^{ab}}$$

$$\neq \frac{\exp(\lambda\sigma_{k})}{\sum_{i=1}^{n} \exp(\sigma_{i}\lambda)}$$

$$(3)$$

$$= \frac{\left(\exp(\lambda \sigma_k)\right)^{ab}}{\sum_{i=1}^{n} \left(\exp(\sigma_i \lambda)\right)^{ab}} \tag{2}$$

$$\neq \frac{\exp(\lambda \sigma_k)}{\sum_{i=1}^n \exp(\sigma_i \lambda)} \tag{3}$$

The function is not invariant under rescaling.

(ii) :

$$\operatorname{softmax}(a\sigma, b\lambda)_k = \frac{\exp(\lambda\sigma_k + c)}{\sum_{i=1}^n \exp(ab\sigma_i\lambda + c)} \tag{4}$$

$$= \frac{\exp(c)\exp(\lambda\sigma_k)}{\sum_{i=1}^n \exp(c)\exp(\sigma_i\lambda)}$$
 (5)

$$= \frac{\exp(c)\exp(\lambda\sigma_k)}{\exp(c)\sum_{i=1}^n \exp(\sigma_i\lambda)}$$
(6)

$$= \frac{\exp(\lambda \sigma_k)}{\sum_{i=1}^n \exp(\sigma_i \lambda)} \tag{7}$$

So the function is invariant under a constant offset. Therefore σ^1 and σ^2 produce the same result while σ^3 is diffrent.

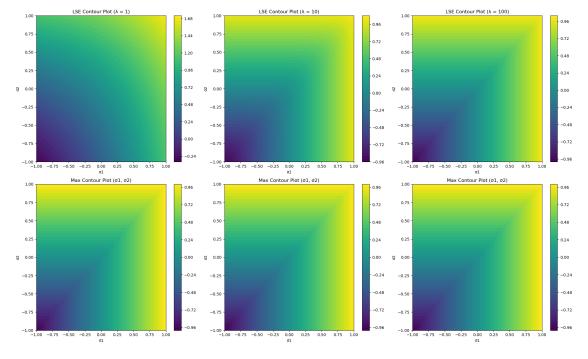
1.3.2 (b)

```
[10]: def lse(sigma, lamda):
          return (1 / lamda) * np.log(np.sum(np.exp(np.array(sigma) * lamda)))
      lambda_values = np.array([1, 10, 100])
      sigma values = np.linspace(-1, 1, 100)
      sigma_1, sigma_2 = np.meshgrid(sigma_values, sigma_values)
      def evaluate_lse(lamda):
          Z = np.zeros_like(sigma_1)
          for i in range(sigma_1.shape[0]):
              for j in range(sigma_1.shape[1]):
                  Z[i, j] = lse([sigma_1[i, j], sigma_2[i, j]], lamda)
          return Z
      def max_sigma(sigma_1, sigma_2):
          return np.maximum(sigma_1, sigma_2)
      fig, axes = plt.subplots(2, len(lambda_values), figsize=(20, 12))
      for idx, lam in enumerate(lambda_values):
          Z_lse = evaluate_lse(lam)
          ax = axes[0, idx]
          cp = ax.contourf(sigma_1, sigma_2, Z_lse, levels=50, cmap='viridis')
          fig.colorbar(cp, ax=ax)
          ax.set_title(f"LSE Contour Plot ( = {lam})")
          ax.set_xlabel(" 1")
```

```
ax.set_ylabel("2")

Z_max = max_sigma(sigma_1, sigma_2)
for idx in range(len(lambda_values)):
    ax = axes[1, idx]
    cp = ax.contourf(sigma_1, sigma_2, Z_max, levels=50, cmap='viridis')
    fig.colorbar(cp, ax=ax)
    ax.set_title(f"Max Contour Plot (1, 2)")
    ax.set_xlabel("1")
    ax.set_ylabel("2")

plt.tight_layout()
plt.show()
```

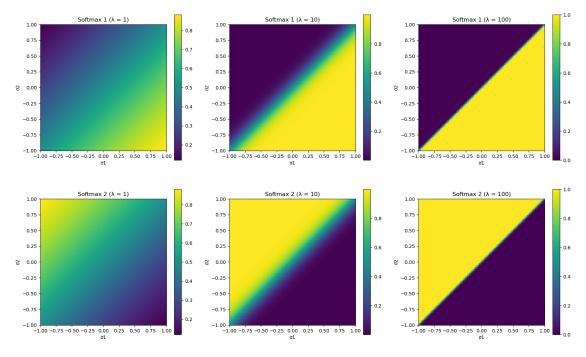


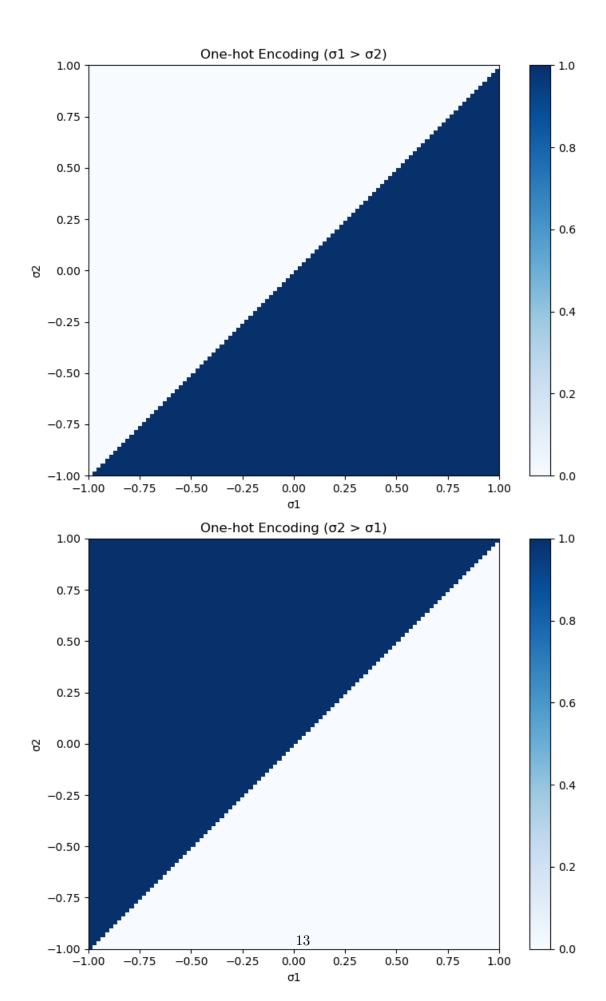
1.3.3 (c)

```
def onehot_argmax(sigma):
   return np.array([1, 0] if sigma[0] > sigma[1] else [0, 1])
def evaluate_softmax_components(lamda):
    softmax_1_vals = np.zeros_like(sigma_1)
    softmax_2_vals = np.zeros_like(sigma_1)
   for i in range(sigma_1.shape[0]):
       for j in range(sigma_1.shape[1]):
            softmax_1_vals[i, j] = softmax_1([sigma_1[i, j], sigma_2[i, j]],
 →lamda)
           softmax_2_vals[i, j] = softmax_2([sigma_1[i, j], sigma_2[i, j]],__
 →lamda)
   return softmax_1_vals, softmax_2_vals
def evaluate_onehot():
   onehot_vals_1 = np.zeros((sigma_1.shape[0], sigma_1.shape[1]))
    onehot_vals_2 = np.zeros_like(onehot_vals_1)
   for i in range(sigma_1.shape[0]):
       for j in range(sigma_1.shape[1]):
           onehot_vec = onehot_argmax([sigma_1[i, j], sigma_2[i, j]])
           onehot_vals_1[i, j] = onehot_vec[0]
           onehot_vals_2[i, j] = onehot_vec[1]
   return onehot_vals_1, onehot_vals_2
fig, axes = plt.subplots(2, len(lambda_values), figsize=(20, 12))
for idx, lam in enumerate(lambda_values):
    softmax_1_vals, softmax_2_vals = evaluate_softmax_components(lam)
   ax1 = axes[0, idx]
   im1 = ax1.imshow(softmax_1_vals, extent=[-1, 1, -1, 1], origin='lower',__
 fig.colorbar(im1, ax=ax1)
   ax1.set_title(f"Softmax 1 ( = {lam})")
   ax1.set xlabel("1")
   ax1.set_ylabel(" 2")
   ax2 = axes[1, idx]
   im2 = ax2.imshow(softmax_2_vals, extent=[-1, 1, -1, 1], origin='lower',_
 fig.colorbar(im2, ax=ax2)
   ax2.set_title(f"Softmax 2 ( = {lam})")
```

```
ax2.set_xlabel("1")
    ax2.set_ylabel(" 2")
onehot_vals_1, onehot_vals_2 = evaluate_onehot()
fig2, axes2 = plt.subplots(2, 1, figsize=(8, 12))
ax1 = axes2[0]
im1 = ax1.imshow(onehot_vals_1, extent=[-1, 1, -1, 1], origin='lower', ___
⇔cmap='Blues', vmin=0, vmax=1)
fig2.colorbar(im1, ax=ax1)
ax1.set_title("One-hot Encoding (1 > 2)")
ax1.set_xlabel(" 1")
ax1.set_ylabel(" 2")
ax2 = axes2[1]
im2 = ax2.imshow(onehot_vals_2, extent=[-1, 1, -1, 1], origin='lower',_

¬cmap='Blues', vmin=0, vmax=1)
fig2.colorbar(im2, ax=ax2)
ax2.set_title("One-hot Encoding (2 > 1)")
ax2.set_xlabel(" 1")
ax2.set_ylabel(" 2")
plt.tight_layout()
plt.show()
```





1.3.4 (d)

$$\frac{d\text{LSE}(\sigma_k, \lambda)}{d\sigma_k} = \frac{d}{d\sigma_k} \left(\frac{1}{\lambda} \log \left(\sum_{i=1}^n \exp(\sigma_i \lambda) \right) \right)$$
 (8)

$$= \frac{1}{\lambda} \frac{1}{\sum_{i=1}^{n} \exp(\sigma_i \lambda)} \exp(\lambda \sigma_j \delta_{jk}) \lambda \tag{9}$$

$$= \frac{\exp(\lambda \sigma_k)}{\sum_{i=1}^n \exp(\sigma_i \lambda)} \tag{10}$$

$$= \operatorname{softmax}_{2}(\sigma, \lambda) \tag{11}$$

1.4 4 Linear regions of MLPs

(a)

```
[12]: import torch
from torch.nn import ReLU, Linear
```

```
[16]: def shallow_model(x):
          x = x.astype("float32")
          x = x.T
          \#assert\ np.shape(x)[0] == 2
          # initializing the input linear layer that broadcasts all the input to all,
       → the hidden units
          torch.manual seed(0)
          input_layer = Linear(in_features=2, out_features=20)
          # initialize activation function
          sigma = ReLU()
          # initializing the linear layer taht sums the activations into a scalar
          output_layer = Linear(in_features=20, out_features=1)
          # input vector
          \#x = np.random.normal(size=(10,2)).astype("float32")
          # input vector as tensor
          input_as_tensor = torch.from_numpy(x)
          # apply the ReLU after applying linear transformation to the input
          activation = sigma(input_layer(input_as_tensor))
          # summing the activations to a scalar
```

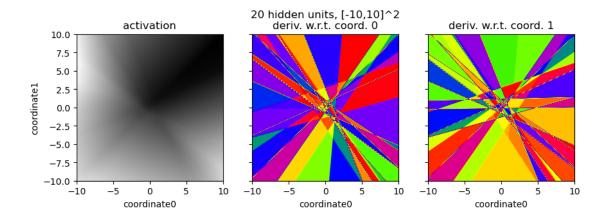
```
y = output_layer(activation)
return y
```

The model has 2 * 20 (w) + 20 (b) parameters on the input side and 1*20 + 1 parameters on the output. That makes a total of 81 parameters. It should be noted that only the linear layers have parameters and the ReLU has no parameter. Any scaling of the activation fct. would be absorbed into the data itself or explicit scaling layers.

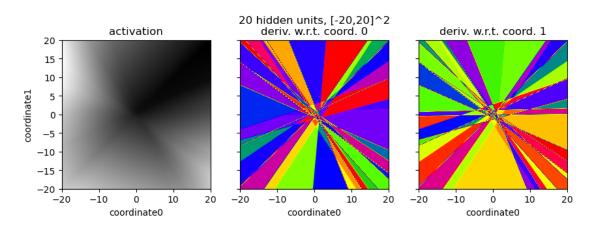
(b), (c)

```
[17]: | def plot_model_output(scale=10, model = shallow_model, title = ""):
          n points = 2000
          scale = scale
          arr = np.mgrid[-n_points//2:n_points//2, -n_points//2:n_points//2] *__
       ⇒(scale*2/n_points)
          # print("arr.shape = ", arr.shape)
          y = model(arr).detach().numpy()
          # remove scalar dimension
          y = np.squeeze(y)
          # print("output shape= ", y.shape)
          extent = (-scale, scale, -scale, scale)
          fig, (ax0, ax1, ax2) = plt.subplots(1,3, figsize=(10,6), sharey = True)
          ax0.imshow(y, cmap="gray", extent = extent, origin="lower")
          ax1.imshow(np.gradient(y, axis=1), cmap="prism", extent = extent,
       ⇔origin="lower")
          ax2.imshow(np.gradient(y, axis=0), cmap="prism", extent = extent,
       ⇔origin="lower")
          ax0.set_ylabel("coordinate1")
          ax0.set_xlabel("coordinate0")
          ax1.set_xlabel("coordinate0")
          ax2.set_xlabel("coordinate0")
          ax0.set_title("activation")
          ax1.set_title("deriv. w.r.t. coord. 0")
          ax2.set_title("deriv. w.r.t. coord. 1")
          if title:
              ax1.set_title(title+"\n"+str(ax1.title.get_text()))
```

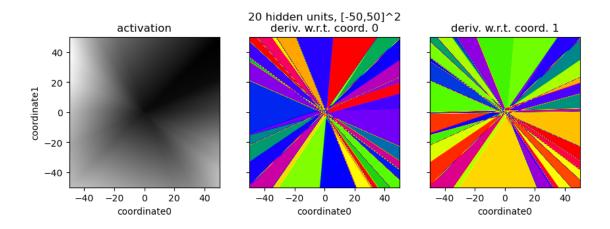
```
[18]: plot_model_output(title="20 hidden units, [-10,10]^2")
```



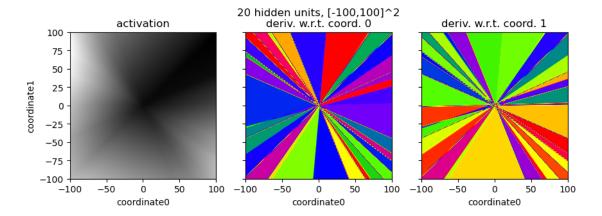
[19]: plot_model_output(scale=20, title="20 hidden units, [-20,20]^2")



[20]: plot_model_output(scale=50, title="20 hidden units, [-50,50]^2")



[21]: plot_model_output(scale=100, title="20 hidden units, [-100,100]^2")

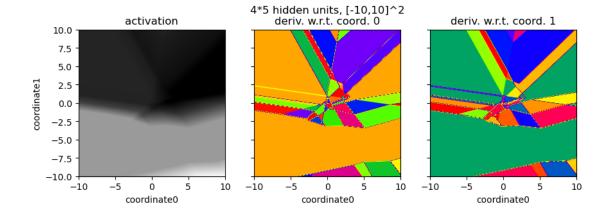


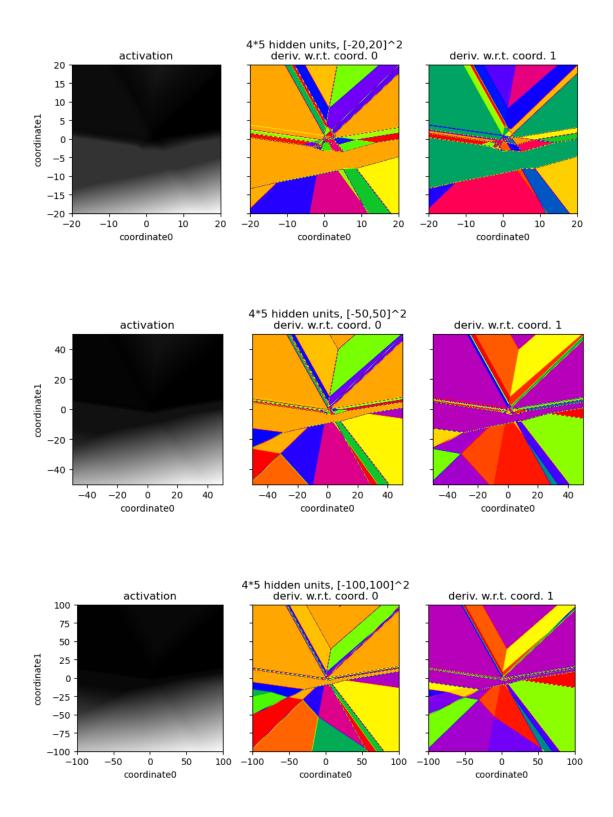
We conclude that the structure disappears at $[-100, 100]^2$ and is mostly centered around the origin within $[-5, 5]^2$, judging from the derivatives.

(d)

```
[22]: def deep_model(x):
          x = x.astype("float32")
          x = x.T
          # input vector as tensor
          input_as_tensor = torch.from_numpy(x)
          # initialize activation function
          relu = ReLU()
          torch.manual_seed(2)
          # initializing the input linear layer that broadcasts all the input to all \sqcup
       ⇔the hidden units
          input_layer = Linear(in_features=2, out_features=5)
          # deep layers
          second_layer = Linear(in_features=5, out_features=5)
          third_layer = Linear(in_features=5, out_features=5)
          fourth_layer = Linear(in_features=5, out_features=5)
          # initializing the linear layer taht sums the activations into a scalar
          output_layer = Linear(in_features=5, out_features=1)
          # chaining
          y = output_layer(
```

```
relu(
            fourth_layer(
                 relu(
                     third_layer(
                         relu(
                              second_layer(
                                  relu(
                                       input_layer(input_as_tensor)
                              )
                         )
                     )
                 )
            )
        )
    )
return y
```





For the deeper model with 4 hidden layers (the non-linear activation fct. is applied four times, hence four hidden layers, even though there is a fifth linear layer to the output), the shapes in the output appear more sophisticated judging from the derivatives. It seems like the model activation

resembles curved shapes in some instances which is unseen in the linear model, though it is hard to tell with N=1 since the weights are initialized randomly. The structure also does not disappears at larger ranges and as opposed to the shallow model.

1.5 5 Number of linear regions

We consider the construction from the lecture where the non-linearity of the ReLU is represented by a line in two dimensional feature space. In that case, a MLP with no ReLUs has no lines dissecting it, thus it is characterized by a single partition, or linear region. By adding one line, two linear regions appear, such that the total number of regions has risen by one as compared to the case of none. If another line is added such that it intersects the first, the total number of regions grows by two. A third line can be added such that it intersects the first two, the number of intersections will grow by three since the two existing lines will intersect the new line in two points, creating three new regions. This rule generalizes: Any n-1 existing lines intersect the nth line n-1 times such that n new regions are created (think of the fencepost problem), assuming that none of the lines are parallel. Thus, the total number N of regions created by a single hidden layer with n units is given by

$$N = 1 + \sum_{i=1}^{n} i = \frac{n(n+1)}{2}$$

where the 1 one the left is due to the fact that without lines there is exactly one partition.