sheet05

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1 Sheet 5

[2]: import os import pandas as pd

1.1 1 The logistic sigmoid

1.1.1 (a)

Sigmoid function:

$$\sigma(x) = \frac{1}{1+e^{-x}}$$

Derivative of the sigmoid (quotient rule used):

$$\frac{d}{dx}\sigma(x) = \frac{e^{-x}}{(1+e^{-x})^2}$$

Use:

$$\sigma(x) = \frac{1}{1 + e^{-x}}$$

and

$$1 - \sigma(x) = \frac{e^{-x}}{1 + e^{-x}}$$

Thus:

$$\frac{d}{dx}\sigma(x)=\sigma(x)(1-\sigma(x))$$

1.1.2 (b)

The hyperbolic tangent function is:

$$\tanh(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$$

The logistic sigmoid function is:

$$\sigma(x) = \frac{1}{1 + e^{-x}}$$

Rewrite tanh(x) by factoring e^{-x} from numerator and denominator:

$$\tanh(x) = \frac{1 - e^{-2x}}{1 + e^{-2x}}$$

From $\sigma(x)$, we can write:

$$1 - \sigma(x) = \frac{e^{-x}}{1 + e^{-x}}$$

Thus:

$$\sigma(x) - (1 - \sigma(x)) = 2\sigma(x) - 1 = \frac{2}{1 + e^{-x}} - 1 = \frac{1 - e^{-x}}{1 + e^{-x}}$$

Observe that tanh(x) matches $2\sigma(2x) - 1$.

1.1.3 (c)

The two classes are separated by a line $w^Tx + b$ that goes through the points $x_1 = (1, 1.5)$ and $x_2 = (2, 2.5)$. The points are chosen because they are in the middle between the datapoints of the two classes. The resulting weights are given by w = (1, -1) and the bias b = 0.5. Testing those weights on the data gives values below 0 for class 2 and above 0 for class 1 in the argument of the sigmoid. Therefore the activation separates the classes with the given weights.

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".

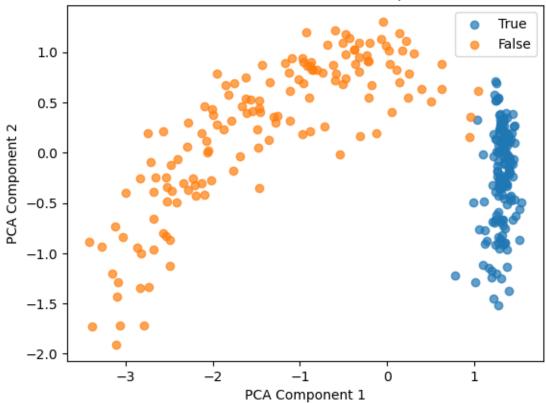
This is how you can load a dataset of LLM activations. Use a new Datamanager if you want to have a new dataset. Use the same data manager if you want to combine datasets.

```
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])
[4]: # 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.
                                                                    Lodz
                                                            1
    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
    8
                       The city of Baoji is in China.
                                                            1
                                                                    Baoji
    9
                   The city of Baoji is in Guatemala.
                                                            0
                                                                    Baoji
                       country correct_country
    0
                       Russia
                                        Russia
    1
                 South Africa
                                        Russia
    2
                       Poland
                                        Poland
    3
       the Dominican Republic
                                        Poland
    4
                    Venezuela
                                     Venezuela
    5
                        China
                                     Venezuela
    6
                   Azerbaijan
                                    Azerbaijan
    7
                      Ukraine
                                    Azerbaijan
    8
                        China
                                         China
    9
                    Guatemala
                                         China
    1.2.1 (a)
[7]: from sklearn.linear_model import LogisticRegression
     from sklearn.metrics import accuracy_score
     from sklearn.decomposition import PCA
     import matplotlib.pyplot as plt
     accuracies = []
```

```
for i, dataset_name in enumerate(dataset names):
   print(f"Processing Dataset {i + 1}")
   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,_
 spath_to_acts=path_to_acts)
   X_train, y_train = dm.get('train')
   X_test, y_test = dm.get('val')
   clf = LogisticRegression(C=1e12, solver='liblinear') # No regularization
   clf.fit(X_train, y_train)
   y_pred = clf.predict(X_test)
   accuracy = accuracy_score(y_test, y_pred)
   accuracies.append({'Dataset': i + 1, 'Accuracy': accuracy})
   print(f"Dataset {i + 1} Performance: Accuracy={accuracy:.2f}")
   activation_vectors = clf.decision_function(X_test).reshape(-1, 1)
   pca = PCA(n_components=2)
   reduced_features = pca.fit_transform(X_test)
   plt.scatter(reduced_features[y_test == 1][:, 0], reduced_features[y_test ==__
 →1][:, 1], label='True', alpha=0.7)
   plt.scatter(reduced_features[y_test == 0][:, 0], reduced_features[y_test ==_
 ⇔0][:, 1], label='False', alpha=0.7)
   plt.title(f'Dataset {i + 1}: Activation Vector Separation')
   plt.xlabel('PCA Component 1')
   plt.ylabel('PCA Component 2')
   plt.legend()
   plt.show()
```

Processing Dataset 1
Dataset 1 Performance: Accuracy=0.99

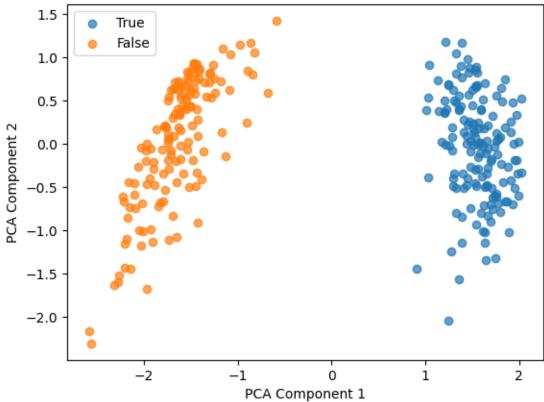
Dataset 1: Activation Vector Separation



Processing Dataset 2

Dataset 2 Performance: Accuracy=1.00

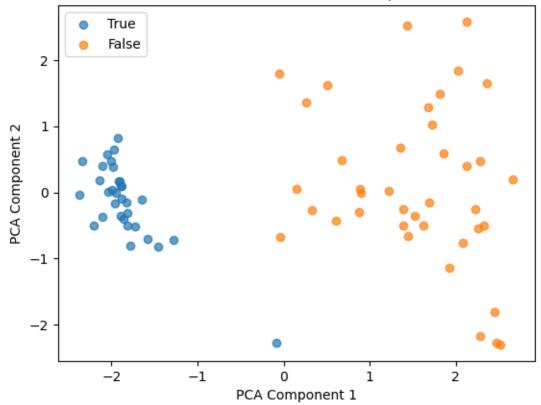




Processing Dataset 3

Dataset 3 Performance: Accuracy=1.00

Dataset 3: Activation Vector Separation



Processing Dataset 4

Dataset 4 Performance: Accuracy=1.00

1.5 1.0 PCA Component 2 0.5 0.0 -0.5 -1.0True -1.5False 1

Dataset 4: Activation Vector Separation

The visualisation of the recuced dimensionality data shows that only dataset 1 in not separable in 2d. The accuracy as it is not 1 shows that the data is also not linearly separable in the original embedding.

0

PCA Component 1

2

-1

1.2.2 (b)

-3

-2

```
[9]: dataset_name = dataset_names[0] # choose dataset cities
     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)
     X_train, y_train = dm.get('train')
     X_test, y_test = dm.get('val')
     clf_no_reg = LogisticRegression(C=1e12, solver='liblinear')
     clf_no_reg.fit(X_train, y_train)
     # With regularization (C=1.0 for L2 regularization)
```

```
clf_with_reg = LogisticRegression(C=1.0, solver='liblinear')
clf_with_reg.fit(X_train, y_train)
accuracies = []
for dataset_name in dataset_names[1:]:
    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)
    X train, y train = dm.get('train')
    X_test, y_test = dm.get('val')
    for model, reg_type in [(clf_no_reg, "No Regularization"), (clf_with_reg,_
 →"With Regularization")]:
        y_pred = model.predict(X_test)
        accuracy = accuracy_score(y_test, y_pred)
        accuracies.append({
            "Train Dataset": "cities",
            "Test Dataset": dataset_name,
            "Regularization": reg type,
            "Accuracy": accuracy
        })
results_df = pd.DataFrame(accuracies)
print(results_df)
```

```
Train Dataset
                   Test Dataset
                                       Regularization Accuracy
0
                                    No Regularization 0.510000
         cities
                      neg_cities
                      neg_cities With Regularization 0.526667
1
         cities
2
        cities
                    sp_en_trans
                                   No Regularization 1.000000
                    sp_en_trans With Regularization 0.971831
3
         cities
                                    No Regularization 0.028169
4
         cities neg_sp_en_trans
                neg_sp_en_trans With Regularization 0.422535
         cities
```

It does not generalize to negated statements, but generalizes well on the translation. Furthermore, the accuracy on neg_ translation is unexpectedly low. It performs much worse than a random classifier. This means that inverting the decision will give a decent classifier again but only in the non regularized case. It is possible that there is a mistake.

1.2.3 (c)

```
[13]: import torch
dataset_name = dataset_names[0] # choose dataset cities
```

```
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)
cities_X_train, cities_y_train = dm.get('train')
cities_X_test, cities_y_test = dm.get('val')
dataset_name = dataset_names[1] # choose dataset neg_cities
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)
neg_cities_X_train, neg_cities_y_train = dm.get('train')
neg_cities_X_test, neg_cities_y_test = dm.get('val')
X_train = torch.cat((cities_X_train, neg_cities_X_train), dim=0)
y_train = torch.cat((cities_y_train, neg_cities_y_train), dim=0)
X_test = torch.cat((cities_X_test, neg_cities_X_test), dim=0)
y_test = torch.cat((cities_y_test, neg_cities_y_test), dim=0)
clf_no_reg = LogisticRegression(C=1e12, solver='liblinear') # No regularization
clf_no_reg.fit(X_train, y_train)
clf_with_reg = LogisticRegression(C=1.0, solver='liblinear') # With_
\hookrightarrow regularization
clf_with_reg.fit(X_train, y_train)
accuracies = []
for dataset name in dataset names[2:]:
    dm = DataManager()
    dm.add_dataset(dataset_name, "Llama3", "8B", "chat", layer=12, split=0.8, u
 ⇔center=False,
                    device='cpu', path_to_datasets=path_to_datasets,_
 →path_to_acts=path_to_acts)
    X_train, y_train = dm.get('train')
    X_test, y_test = dm.get('val')
    for model, reg_type in [(clf_no_reg, "No Regularization"), (clf_with_reg,_
 ⇔"With Regularization")]:
        y_pred = model.predict(X_test)
        accuracy = accuracy_score(y_test, y_pred)
```

```
accuracies.append({
    "Train Dataset": "cities + neg_cities",
    "Test Dataset": dataset_name,
    "Regularization": reg_type,
    "Accuracy": accuracy
})

results_df = pd.DataFrame(accuracies)
print(results_df)
```

```
Train Dataset Test Dataset Regularization Accuracy

O cities + neg_cities sp_en_trans No Regularization 1.000000

1 cities + neg_cities sp_en_trans With Regularization 1.000000

2 cities + neg_cities neg_sp_en_trans No Regularization 0.971831

3 cities + neg_cities neg_sp_en_trans With Regularization 0.971831
```

The trained classifier works for affirmative and negated statements. As before the generalization to translation is successful, even if the accuracy on the negated dataset is 0.03 lower. Regularization makes no difference in this case.

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

1.3.1 (a)

```
import numpy as np
def lse(vec, lam=1):
    return np.log(np.sum(np.exp(lam * vec)))/lam

def softmax(vec, lam=1):
    return np.exp(lam * vec)/np.sum(np.exp(lam * vec))

sig1 = np.array([1,2,3])
sig2 = sig1 + 10
sig3 = sig1 * 10

sigs = [sig1, sig2, sig3]

for sig in sigs:
    print(f"{sig}: softmax={np.round(softmax(sig), decimals=2)}")
```

```
[1 2 3]: softmax=[0.09 0.24 0.67]
[11 12 13]: softmax=[0.09 0.24 0.67]
[10 20 30]: softmax=[0. 0. 1.]
```

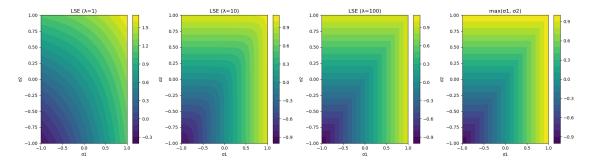
 $\operatorname{Soft}(\operatorname{arg})$ max is invariant under constant offset and not under rescaling.

Proof of invariance under constant offset c:

$$\operatorname{soft}(\operatorname{arg}) \max(c + \sigma) = \frac{\exp(c + \sigma)}{\sum_{j=1}^K \exp(c + \sigma_j)} = \frac{\exp(c)}{\exp(c)} \frac{\exp(\sigma)}{\sum_{j=1}^K \exp(\sigma_j)} = \frac{\exp(\sigma)}{\sum_{j=1}^K \exp(\sigma_j)} = \operatorname{soft}(\operatorname{arg}) \max(\sigma)$$

1.3.2 (b)

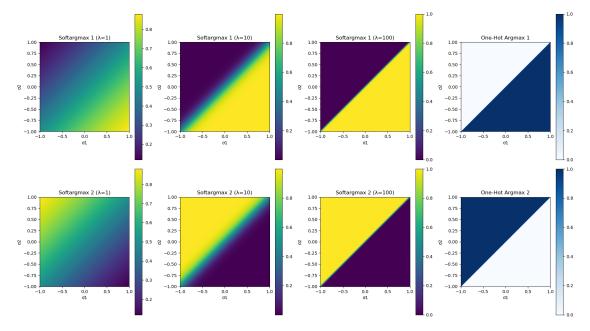
```
[18]: sigma1 = np.linspace(-1, 1, 200)
      sigma2 = np.linspace(-1, 1, 200)
      sigma1, sigma2 = np.meshgrid(sigma1, sigma2)
      lambdas = [1, 10, 100]
      def lse(sigma1, sigma2, lam):
          return (1 / lam) * np.log(np.exp(lam * sigma1) + np.exp(lam * sigma2))
      max_values = np.maximum(sigma1, sigma2)
      fig, axes = plt.subplots(1, len(lambdas) + 1, figsize=(18, 5))
      for i, lam in enumerate(lambdas):
          lse_values = lse(sigma1, sigma2, lam)
          ax = axes[i]
          contour = ax.contourf(sigma1, sigma2, lse_values, levels=20, cmap='viridis')
          ax.set_title(f'LSE (={lam})')
          ax.set_xlabel('1')
          ax.set_ylabel('2')
          fig.colorbar(contour, ax=ax)
      ax = axes[-1]
      contour = ax.contourf(sigma1, sigma2, max_values, levels=20, cmap='viridis')
      ax.set_title('max(1, 2)')
      ax.set_xlabel(' 1')
      ax.set_ylabel('2')
      fig.colorbar(contour, ax=ax)
      plt.tight_layout()
      plt.show()
```



The lse approaches the max function for large λ .

1.3.3 (c)

```
[19]: def softargmax_components(sigma1, sigma2, lam):
          exp_sigma1 = np.exp(lam * sigma1)
          exp_sigma2 = np.exp(lam * sigma2)
          softargmax1 = exp_sigma1 / (exp_sigma1 + exp_sigma2)
          softargmax2 = exp_sigma2 / (exp_sigma1 + exp_sigma2)
          return softargmax1, softargmax2
      def onehot_argmax(sigma1, sigma2):
          onehot1 = (sigma1 > sigma2).astype(float) # 1 if 1 > 2, else 0
          onehot2 = (sigma2 >= sigma1).astype(float) # 1 if 2 1, else 0
          return onehot1, onehot2
      fig, axes = plt.subplots(2, len(lambdas) + 1, figsize=(18, 10))
      for i, lam in enumerate(lambdas):
          softargmax1, softargmax2 = softargmax_components(sigma1, sigma2, lam)
          ax = axes[0, i]
          im = ax.imshow(softargmax1, extent=(-1, 1, -1, 1), origin='lower', __
       ⇔cmap='viridis')
          ax.set_title(f'Softargmax 1 (={lam})')
          ax.set xlabel('1')
          ax.set_ylabel('2')
          fig.colorbar(im, ax=ax)
          ax = axes[1, i]
          im = ax.imshow(softargmax2, extent=(-1, 1, -1, 1), origin='lower', __
       ⇔cmap='viridis')
          ax.set_title(f'Softargmax 2 (={lam})')
          ax.set xlabel('1')
          ax.set_ylabel('2')
          fig.colorbar(im, ax=ax)
      onehot1, onehot2 = onehot_argmax(sigma1, sigma2)
      ax = axes[0, -1]
      im = ax.imshow(onehot1, extent=(-1, 1, -1, 1), origin='lower', cmap='Blues', u
      →vmin=0, vmax=1)
      ax.set_title('One-Hot Argmax 1')
      ax.set xlabel('1')
      ax.set_ylabel('2')
      fig.colorbar(im, ax=ax)
      ax = axes[1, -1]
```



The soft argmax becomes the one-hot argmax for large λ .

1.3.4 (d)

LogSumExp:

$$\operatorname{lse}(\sigma; \lambda) = \frac{1}{\lambda} \log \left(\sum_{i=1}^{k} \exp(\lambda \sigma_i) \right)$$

The derivative of lse with respect to σ_j is:

$$\frac{\partial}{\partial \sigma_j} \mathrm{lse}(\sigma) = \frac{1}{\lambda} \cdot \lambda \cdot \frac{\exp(\lambda \sigma_j)}{\sum_{i=1}^k \exp(\lambda \sigma_i)}$$

This derivative is precisely the softargmax for the \$ j \$-th component:

$$\frac{\exp(\lambda\sigma_j)}{\sum_{i=1}^k \exp(\lambda\sigma_i)}$$

1.3.5 (e)

LogSumExp (LSE):

$$lse(\sigma; \lambda) = \frac{1}{\lambda} log \left(\sum_{i=1}^{n} exp(\lambda \sigma_i) \right)$$

As \$ $\to \infty$ \$, the exponential terms $\exp(\lambda \sigma_i)$ grow rapidly. The largest value of σ_i dominates the sum, so:

$$\sum_{i=1}^{n} \exp(\lambda \sigma_i) \approx \exp(\lambda \sigma_{\max})$$

Thus, the LogSumExp simplifies to:

$$lse(\sigma; \lambda) \approx \frac{1}{\lambda} \log \left(\exp(\lambda \sigma_{\max}) \right) = \sigma_{\max}$$

Therefore:

$$\lim_{\lambda \to \infty} \operatorname{lse}(\sigma; \lambda) = \max(\sigma)$$

1.4 4 Linear regions of MLPs

1.4.1 (a)

Calculate the number of parameters:

 $(\text{num parameters}(w_1) + \text{num parameters}(b_1)) \cdot \text{num neurons} + \text{num parameters}(w_{out}) + \text{num parameters}(b_{out}) = (2+1) \cdot (2+1)$

```
[]: import torch
import torch.nn as nn

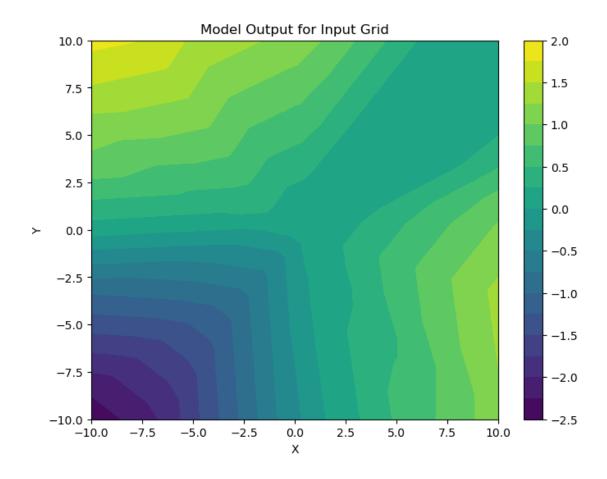
class ShallowNN(nn.Module):
    def __init__(self, input_size, hidden_size, output_size):
        super(ShallowNN, self).__init__()

    self.hidden = nn.Linear(input_size, hidden_size)
        self.output = nn.Linear(hidden_size, output_size)

    def forward(self, x):
        x = torch.relu(self.hidden(x))
        x = self.output(x)
        return x

input_size = 2
hidden_size = 20
```

```
output_size = 1
      model = ShallowNN(input_size, hidden_size, output_size)
      print(model)
      num_params = sum(p.numel() for p in model.parameters())
      print(f"Number of parameters: {num_params}")
     ShallowNN(
       (hidden): Linear(in_features=2, out_features=20, bias=True)
       (output): Linear(in_features=20, out_features=1, bias=True)
     Number of parameters: 81
     1.4.2 (b)
[73]: x_range = np.linspace(-10, 10, 500)
      y_range = np.linspace(-10, 10, 500)
      xx, yy = np.meshgrid(x_range, y_range)
      grid_points = np.vstack([xx.ravel(), yy.ravel()]).T # Stack them into 2D input_
       ⇔for the model
      grid_tensor = torch.tensor(grid_points, dtype=torch.float32)
      with torch.no_grad(): # No need to track gradients for this forward pass
          output = model(grid_tensor)
      output = output.detach().numpy().reshape(xx.shape)
      plt.figure(figsize=(8, 6))
      plt.contourf(xx, yy, output, 20, cmap='viridis')
      plt.colorbar()
      plt.title('Model Output for Input Grid')
      plt.xlabel('X')
      plt.ylabel('Y')
      plt.show()
```



```
[74]: x_range_large = np.linspace(-10000, 10000, 5000)
    y_range_large = np.linspace(-10000, 10000, 5000)

xx_large, yy_large = np.meshgrid(x_range_large, y_range_large)
    grid_points_large = np.vstack([xx_large.ravel(), yy_large.ravel()]).T

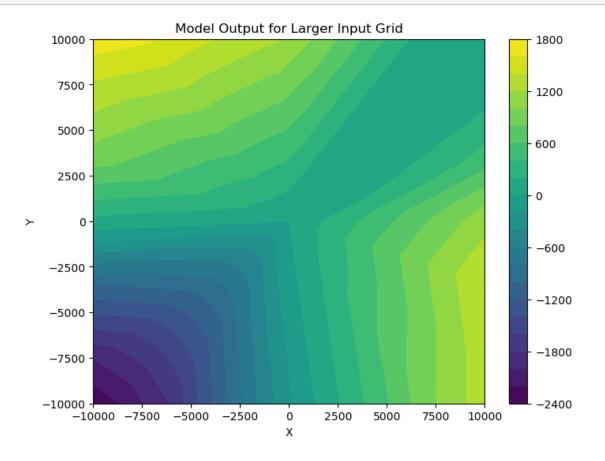
grid_tensor_large = torch.tensor(grid_points_large, dtype=torch.float32)

with torch.no_grad():
    output_large = model(grid_tensor_large)

output_large = output_large.detach().numpy().reshape(xx_large.shape)

plt.figure(figsize=(8, 6))
    plt.contourf(xx_large, yy_large, output_large, 20, cmap='viridis')
    plt.colorbar()
    plt.title('Model Output for Larger Input Grid')
    plt.xlabel('X')
    plt.ylabel('Y')
```





The structure seems to be captured already in the range of -10 to 10.

1.4.3 (c)

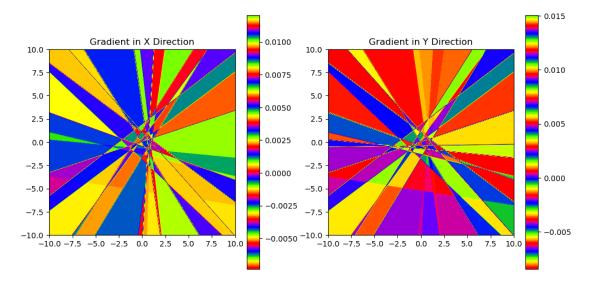
```
[75]: grad_x, grad_y = np.gradient(output, axis=(1, 0))

plt.figure(figsize=(12, 6))

plt.subplot(1, 2, 1)
plt.imshow(grad_x, cmap='prism', extent=[-10, 10, -10, 10])
plt.colorbar()
plt.title('Gradient in X Direction')

plt.subplot(1, 2, 2)
plt.imshow(grad_y, cmap='prism', extent=[-10, 10, -10, 10])
plt.colorbar()
plt.title('Gradient in Y Direction')
```

plt.show()

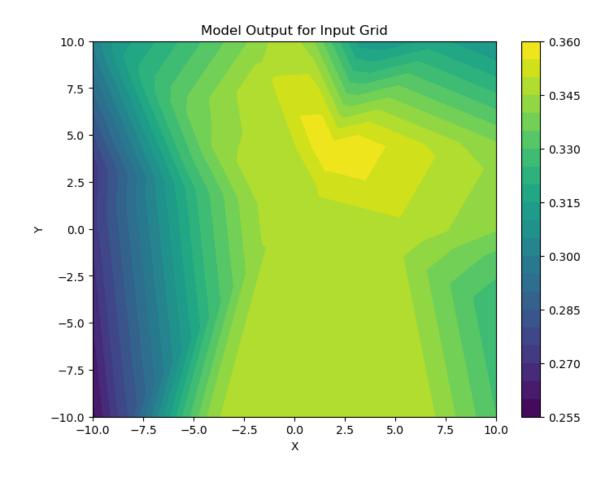


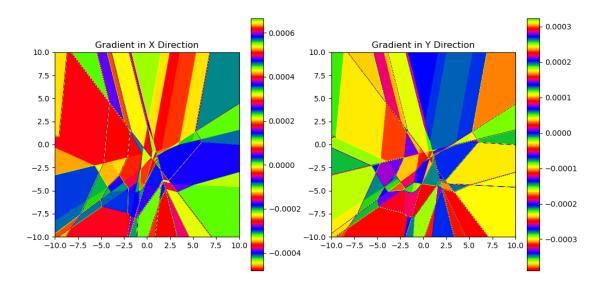
Areas whith constant gradients and the sharp changes of the gradients on the boundaries of those can be seen. This is due to the relu activation function as gradients can become zero or one depending on the sign of the activation.

1.4.4 (d)

```
[79]: class DeeperNN(nn.Module):
          def __init__(self, input_size, hidden_size, output_size):
              super(DeeperNN, self).__init__()
              self.hidden0 = nn.Linear(input_size, hidden_size)
              self.hiddeni = nn.Linear(hidden_size, hidden_size)
              self.output = nn.Linear(hidden_size, output_size)
          def forward(self, x):
              x = torch.relu(self.hidden0(x))
              x = torch.relu(self.hiddeni(x))
              x = torch.relu(self.hiddeni(x))
              x = torch.relu(self.hiddeni(x))
              x = self.output(x)
              return x
      input size = 2
      hidden_size = 5
      output_size = 1
     model = DeeperNN(input_size, hidden_size, output_size)
```

```
x_range = np.linspace(-10, 10, 500)
y_range = np.linspace(-10, 10, 500)
xx, yy = np.meshgrid(x_range, y_range)
grid_points = np.vstack([xx.ravel(), yy.ravel()]).T # Stack them into 2D input_
 ⇔for the model
grid_tensor = torch.tensor(grid_points, dtype=torch.float32)
with torch.no_grad(): # No need to track gradients for this forward pass
    output = model(grid_tensor)
output = output.detach().numpy().reshape(xx.shape)
plt.figure(figsize=(8, 6))
plt.contourf(xx, yy, output, 20, cmap='viridis')
plt.colorbar()
plt.title('Model Output for Input Grid')
plt.xlabel('X')
plt.ylabel('Y')
plt.show()
grad_x, grad_y = np.gradient(output, axis=(1, 0))
plt.figure(figsize=(12, 6))
plt.subplot(1, 2, 1)
plt.imshow(grad_x, cmap='prism', extent=[-10, 10, -10, 10])
plt.colorbar()
plt.title('Gradient in X Direction')
plt.subplot(1, 2, 2)
plt.imshow(grad_y, cmap='prism', extent=[-10, 10, -10, 10])
plt.colorbar()
plt.title('Gradient in Y Direction')
plt.show()
```





The output seems more complex than the one of the shallow network which is recocnizable from the more complex shapes.

1.5 5 Bonus: Number of linear regions

Formula for number of regions:

$$R(n)=1+\frac{n(n+1)}{2}$$

The derivation follows from the reasioning that each neuron with relu activation divides the space into two parts.

[]: