sheet03_Rename

November 11, 2024

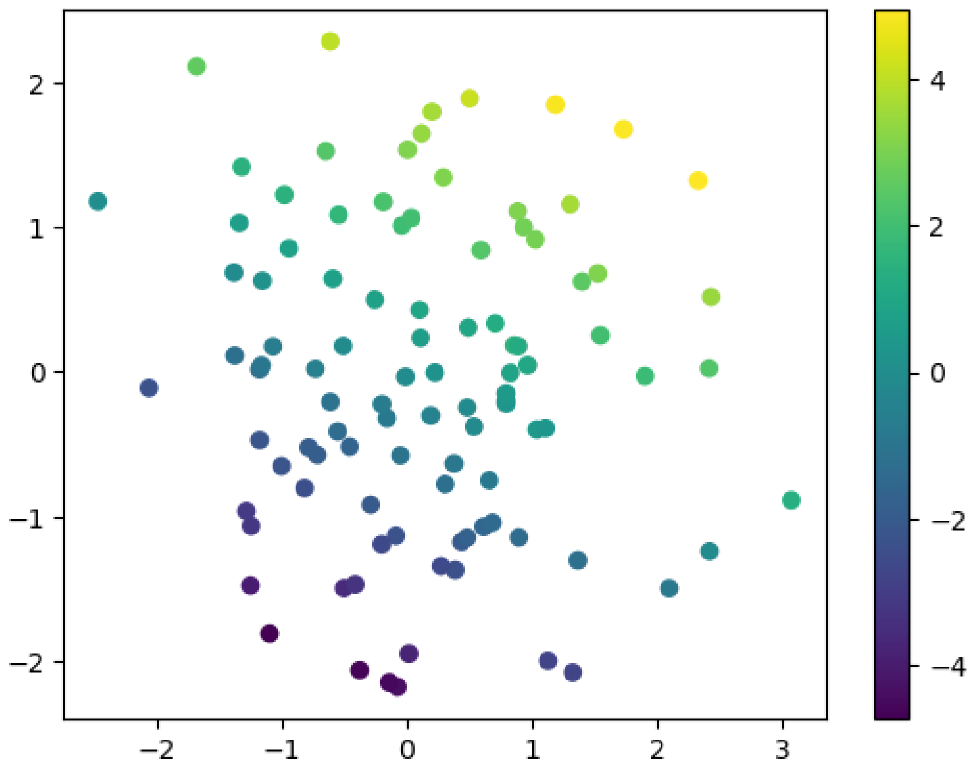
From Oliver Sange, Elias Huber and Sam Rouppe van der Voort

[ ]:
```
import numpy as np
from matplotlib import pyplot as plt
from sklearn.linear_model import LinearRegression
```

0.1 3 Visualize Regularization Contours

[25]:
```
# load the data
data = np.load('data/linreg.npz')
x = data['X']
y = data['Y']
print(f'x.shape: {x.shape}, "y.shape:" {y.shape}')
plt.scatter(*x, c=y);
plt.colorbar()
plt.show()
```

```
x.shape: (2, 100), "y.shape:" (1, 100)
```



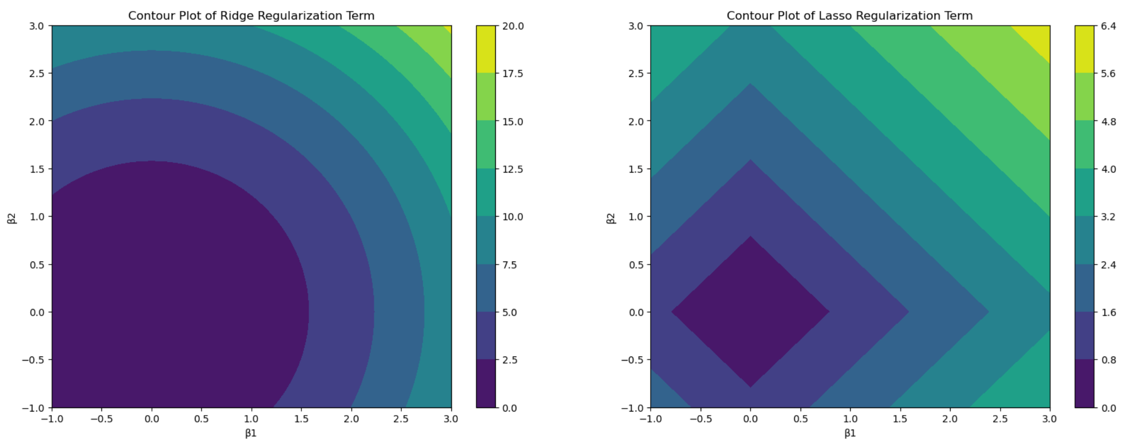
```
[26]: # create a grid of points in the parameter space
b1, b2 = np.linspace(-1, 3, 101), np.linspace(-1, 3, 101)
bs = np.stack(np.meshgrid(b1, b2, indexing='ij'), axis=-1)
bs.shape
```

```
[26]: (101, 101, 2)
```

0.1.1 (a)

```
[27]: ridge_term = bs[..., 0]**2 + bs[..., 1]**2
lasso_term = np.abs(bs[..., 0]) + np.abs(bs[..., 1])

# Plotting
fig, ax = plt.subplots(1, 2, figsize=(20, 7))

# Ridge regression
contour1 = ax[0].contourf(bs[..., 0], bs[..., 1], ridge_term, cmap='viridis')
fig.colorbar(contour1, ax=ax[0])
ax[0].set_title('Contour Plot of Ridge Regularization Term')
ax[0].set_xlabel(' 1')
ax[0].set_ylabel(' 2')
```

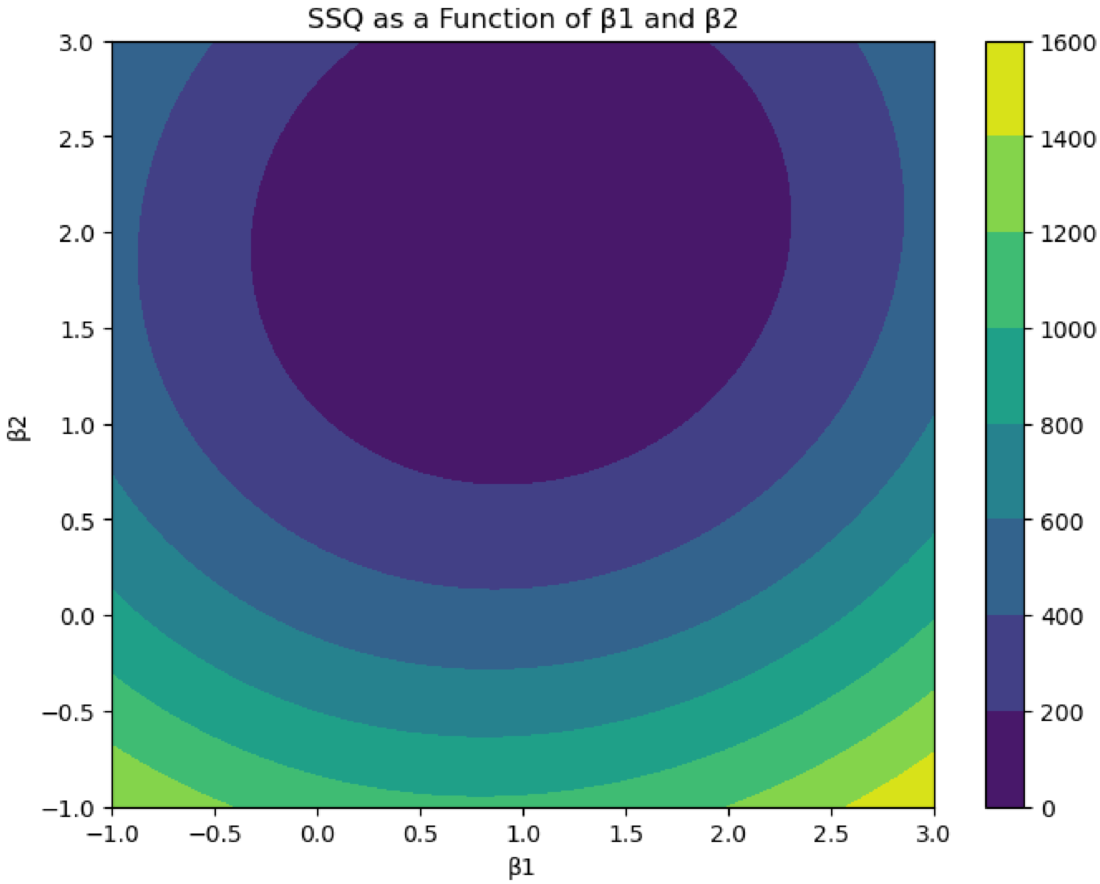
```python
# Lasso regression
contour2 = ax[1].contourf(bs[..., 0], bs[..., 1], lasso_term, cmap='viridis')
fig.colorbar(contour2, ax=ax[1])
ax[1].set_title('Contour Plot of Lasso Regularization Term')
ax[1].set_xlabel(' 1')
ax[1].set_ylabel(' 2')

plt.show()
```



0.1.2 (b)

[28]:
```python
# Reshape bs
b1_vals = bs[..., 0]
b2_vals = bs[..., 1]

# Compute predictions
y_pred_grid = b1_vals[:, :, np.newaxis] * x[0] + b2_vals[:, :, np.newaxis] *
 ↪x[1]

# Compute residuals
residuals = y - y_pred_grid

# Compute SSQ
SSQ = np.sum(residuals**2, axis=-1)

# Plot
fig, ax = plt.subplots(figsize=(8, 6))
contour = ax.contourf(b1_vals, b2_vals, SSQ, cmap='viridis')
fig.colorbar(contour, ax=ax)
ax.set_title('SSQ as a Function of  1 and  2')
ax.set_xlabel(' 1')
```

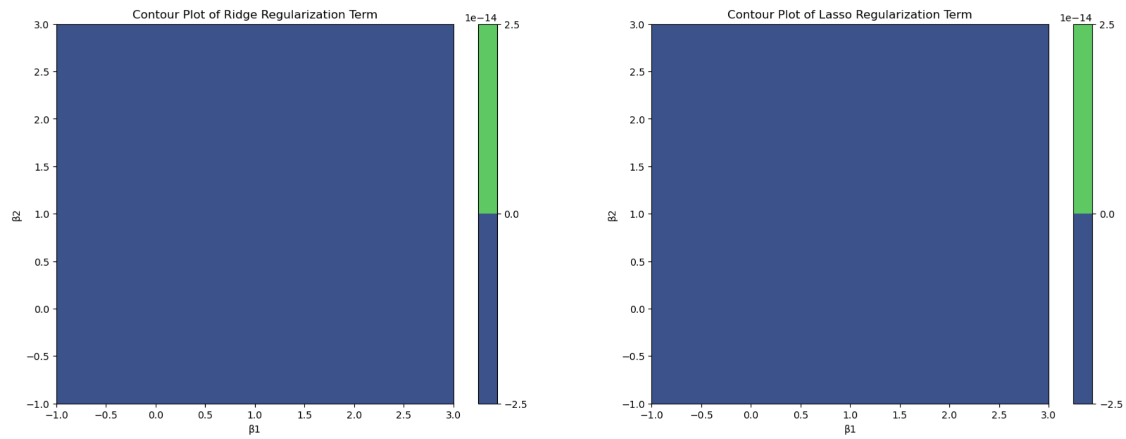
```
ax.set_ylabel(' 2')
plt.show()
```

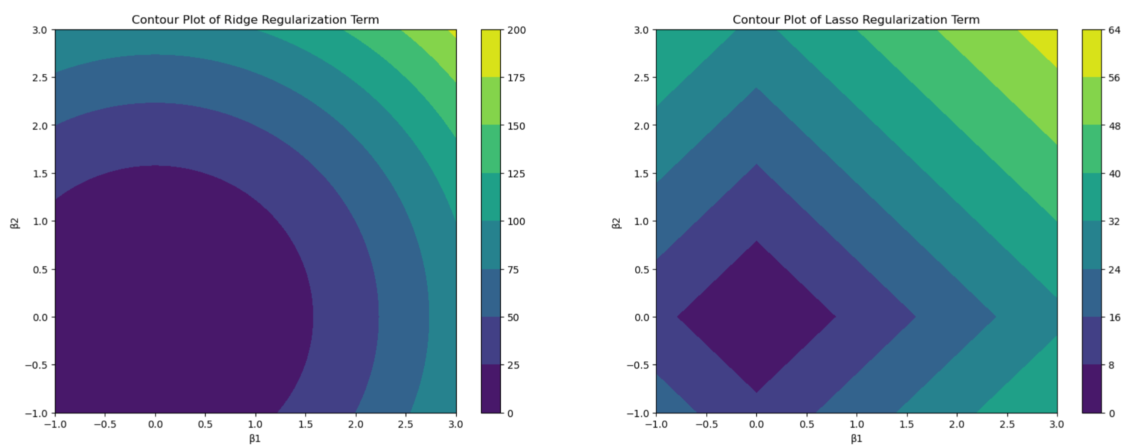


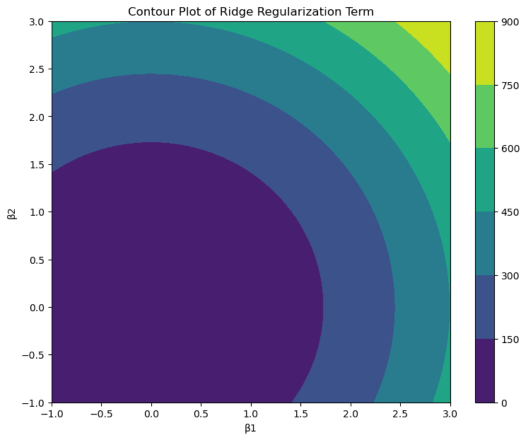
0.1.3 (c)

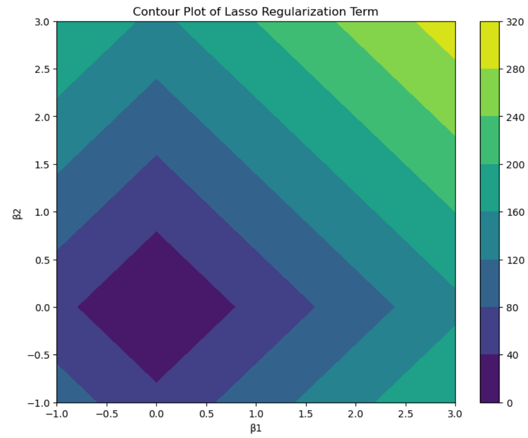
[29]:
```
# TODO: for each lambda, plot both ridge regression and lasso loss functions
lambdas = [0, 10, 50, 100, 200, 300]

for lam in lambdas:
    ridge_term = lam * (bs[..., 0]**2 + bs[..., 1]**2)
    lasso_term = lam * (np.abs(bs[..., 0]) + np.abs(bs[..., 1]))

    # Plotting
    fig, ax = plt.subplots(1, 2, figsize=(20, 7))

    # Ridge regression
    contour1 = ax[0].contourf(bs[..., 0], bs[..., 1], ridge_term,␣
 ↪cmap='viridis')
```

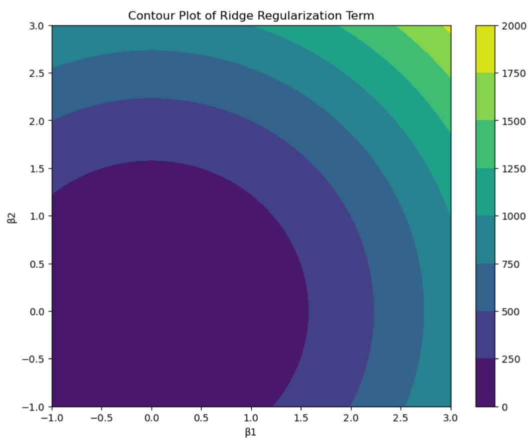
```
    fig.colorbar(contour1, ax=ax[0])
    ax[0].set_title('Contour Plot of Ridge Regularization Term')
    ax[0].set_xlabel(' 1')
    ax[0].set_ylabel(' 2')

    # Lasso regression
    contour2 = ax[1].contourf(bs[..., 0], bs[..., 1], lasso_term, cmap='viridis')
    fig.colorbar(contour2, ax=ax[1])
    ax[1].set_title('Contour Plot of Lasso Regularization Term')
    ax[1].set_xlabel(' 1')
    ax[1].set_ylabel(' 2')

    plt.show()
```

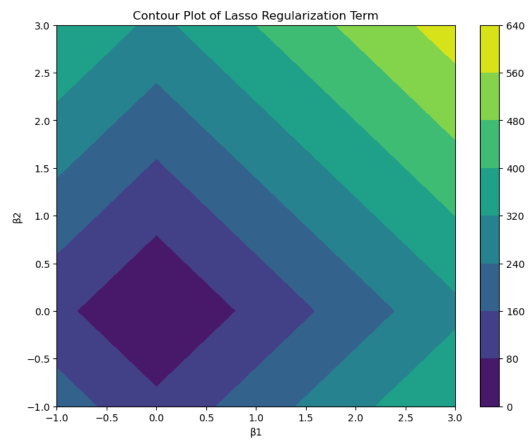


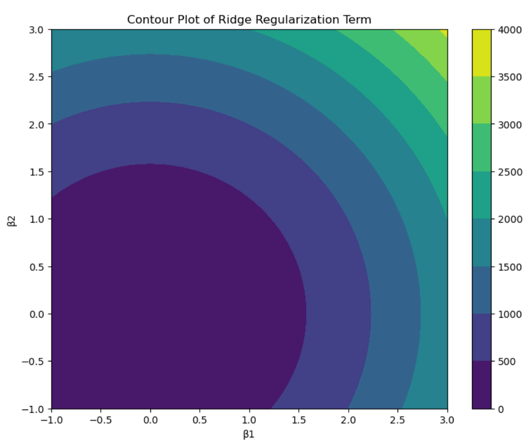


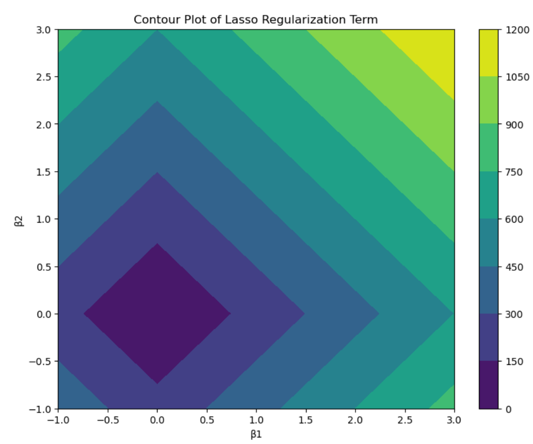

Contour Plot of Ridge Regularization Term
β1
β2
0 150 300 450 600 750 900

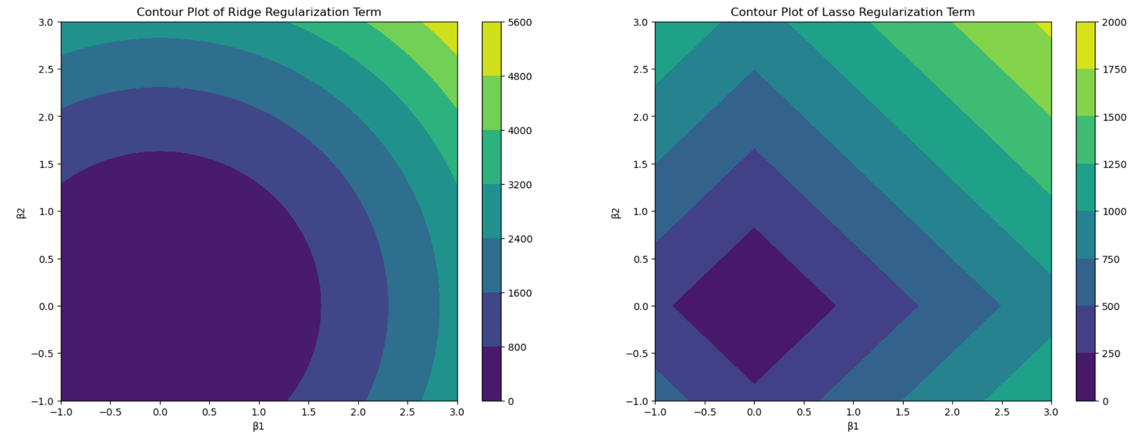

Contour Plot of Lasso Regularization Term
β1
β2
0 40 80 120 160 200 240 280 320


Contour Plot of Ridge Regularization Term
β1
β2
0 250 500 750 1000 1250 1500 1750 2000


Contour Plot of Lasso Regularization Term
β1
β2
0 80 160 240 320 400 480 560 640


Contour Plot of Ridge Regularization Term
β1
β2
0 500 1000 1500 2000 2500 3000 3500 4000


Contour Plot of Lasso Regularization Term
β1
β2
0 150 300 450 600 750 900 1050 1200



For a larger , the colorbar will extend to higher values. This means that the colors in the plot will represent a stronger penalty, and the "cost" of larger coefficients beta1 and beta2 becomes more pronounced in the optimization.

0.2 4 CT Reconstruction

First, set up the design matrix. (Run this once to save it to the disk)

[15]:
```
# create design matrix
# don't change any of this, just run it once to create and save the design matrix
import os

n_parallel_rays = 70
n_ray_angles = 30
res = (99, 117)
print("Number of pixels in the 2d image:", np.prod(res))
print("Total number of rays:", n_parallel_rays * n_ray_angles)

def rot_mat(angle):
    c, s = np.cos(angle), np.sin(angle)
    return np.stack([np.stack([c, s], axis=-1), np.stack([-s, c], axis=-1)], axis=-1)

kernel = lambda x: np.exp(-x**2/sigma**2/2)

if not os.path.exists('data/design_matrix.npy'):
    xs = np.arange(0, res[1]+1) - res[1]/2 # np.linspace(-1, 1, res[1] + 1)
    ys = np.arange(0, res[0]+1) - res[0]/2 # np.linspace(-1, 1, res[0] + 1)

    # rays are defined by origin and direction
    ray_offset_range = [-res[1]/1.5, res[1]/1.5]
```

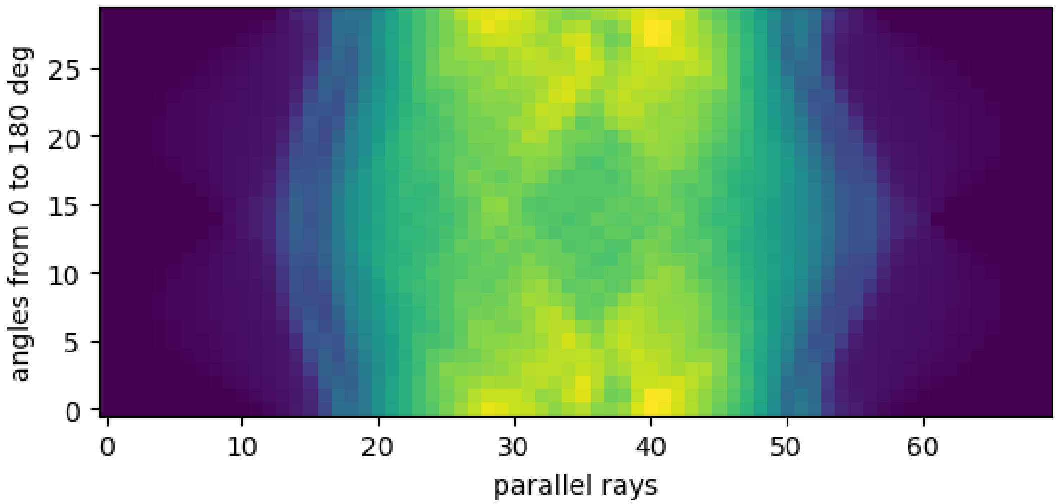
```
    n_rays = n_parallel_rays * n_ray_angles

    ray_angles = np.linspace(0, np.pi, n_ray_angles, endpoint=False) + np.pi/
↪n_ray_angles

    # offsets for ray_angle = 0, i.e. parallel to x-axis
    ray_0_offsets = np.stack([np.zeros(n_parallel_rays), np.
↪linspace(*ray_offset_range, n_parallel_rays)], axis=-1)
    ray_0_directions = np.stack([np.ones(n_parallel_rays), np.
↪zeros(n_parallel_rays)], axis=-1)



    ray_rot_mats = rot_mat(ray_angles)

    ray_offsets = np.einsum('oi,aij->aoj', ray_0_offsets, ray_rot_mats).
↪reshape(-1, 2)
    ray_directions = np.einsum('oi,aij->aoj', ray_0_directions, ray_rot_mats).
↪reshape(-1, 2)

    sigma = 1
    xsc = (xs[1:] + xs[:-1]) / 2
    ysc = (ys[1:] + ys[:-1]) / 2
    b = np.stack(np.meshgrid(xsc, ysc), axis=-1).reshape(-1, 2)
    a = ray_offsets
    v = ray_directions
    v = v / np.linalg.norm(v, axis=-1, keepdims=True)
    p = ((b[None] - a[:, None]) * v[:, None]).sum(-1, keepdims=True) * v[:,␣
↪None] + a[:, None]
    d = np.linalg.norm(b - p, axis=-1)
    d = kernel(d)
    design_matrix = d.T

    np.save('data/design_matrix.npy', design_matrix)
    print(f'created and saved design matrix of shape {design_matrix.shape} at␣
↪data/design_matrix.npy')
```

```
Number of pixels in the 2d image: 11583
Total number of rays: 2100
```

[16]:
```
sino = np.load('data/sino.npy')

print(f'sino shape: {sino.shape}')

# visualize sinogram as image
n_parallel_rays = 70
n_angles = 30
```

```
plt.imshow(sino.reshape(n_angles, n_parallel_rays), origin='lower')
# plt.colorbar()
plt.xlabel('parallel rays')
plt.ylabel('angles from 0 to 180 deg')
plt.show();
```

```
sino shape: (1, 2100)
```

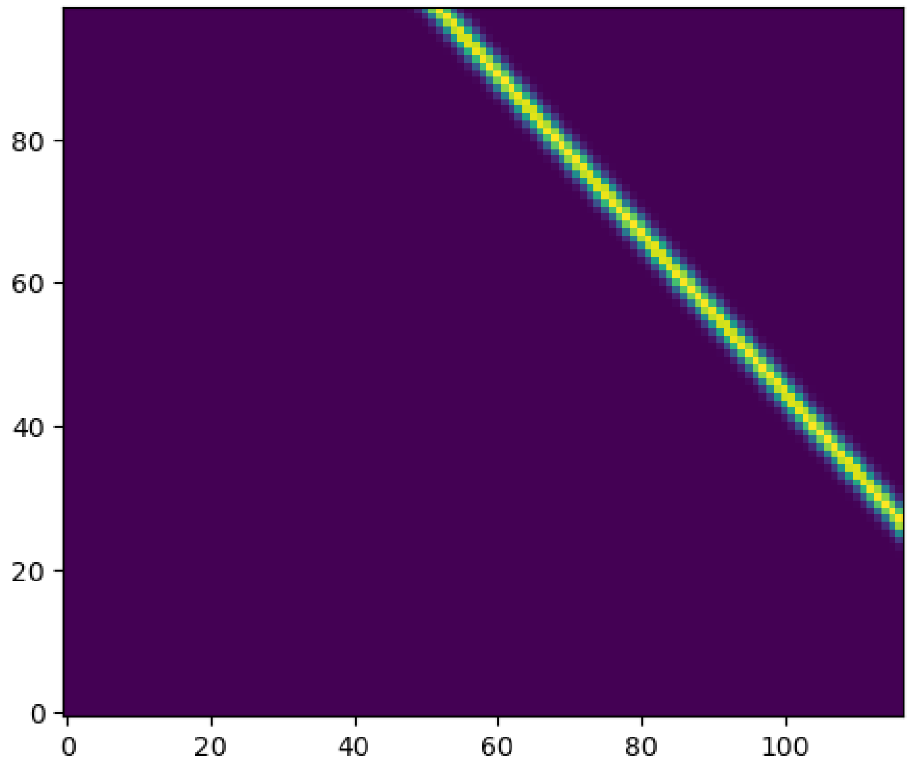


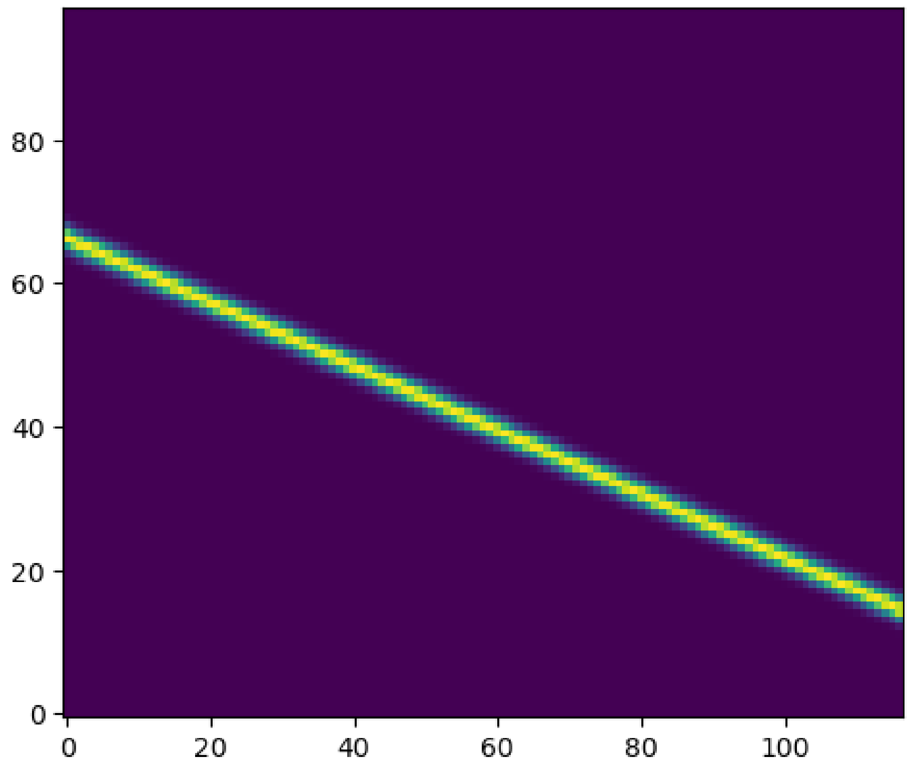
0.2.1 (a)

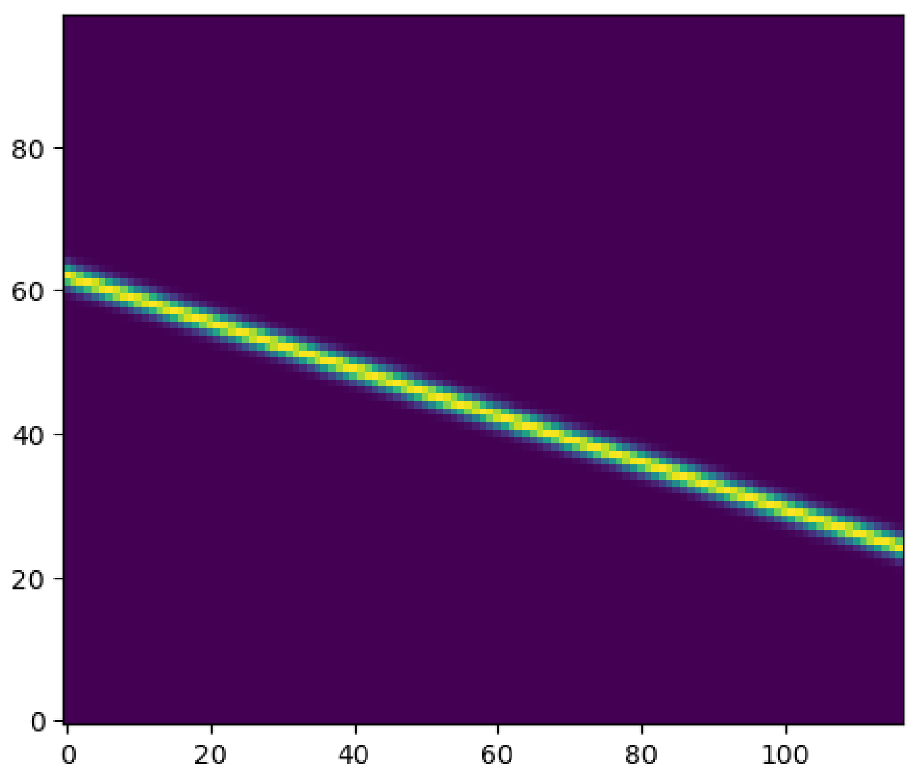
[17]:
```
design_matrix = np.load('data/design_matrix.npy')
numbers = np.random.randint(0,design_matrix.shape[1],size = 4)
print(f"shape design matrix: {design_matrix.shape}")


image1 = design_matrix[:,numbers[0]].reshape(res)
image2 = design_matrix[:,numbers[1]].reshape(res)
image3 = design_matrix[:,numbers[2]].reshape(res)
image4 = design_matrix[:,numbers[3]].reshape(res)


plt.imshow(image1, origin='lower')
plt.show()
plt.imshow(image2, origin='lower')
plt.show()
plt.imshow(image3, origin='lower')
plt.show()
plt.imshow(image4, origin='lower')
plt.show()
```

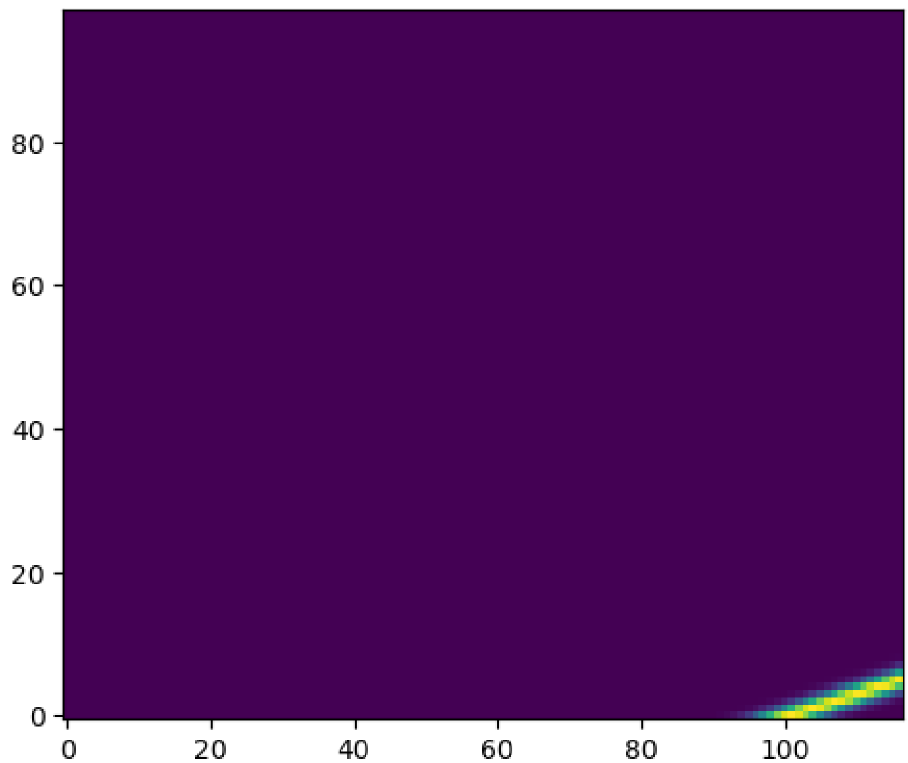
```
# Each image shows the trajectory and its corresponding intensity through the
 ↪final image


# TODO: visualize four random columns as images, using an image shape of (99,
 ↪117)
```

```
shape design matrix: (11583, 2100)
```




80
60
40
20
0
0
20
40
60
80
100

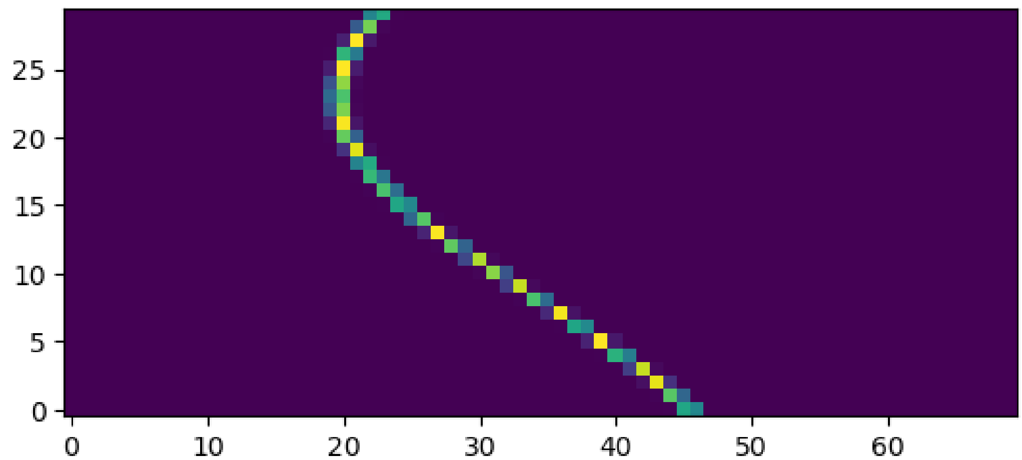

80
60
40
20
0
0
20
40
60
80
100

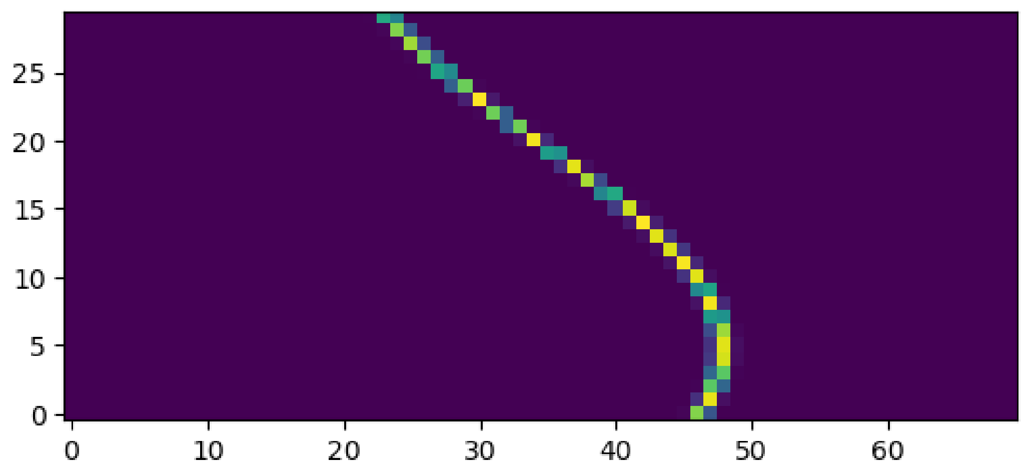


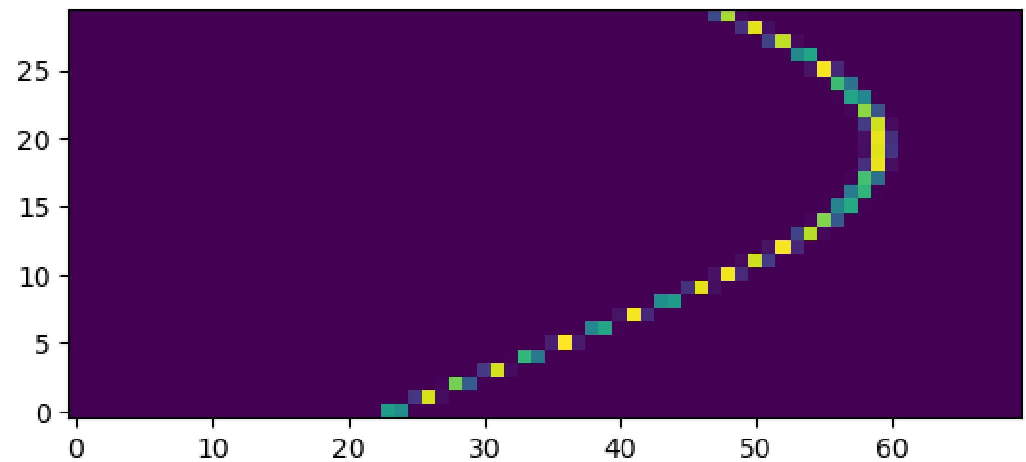
0.2.2 (b)

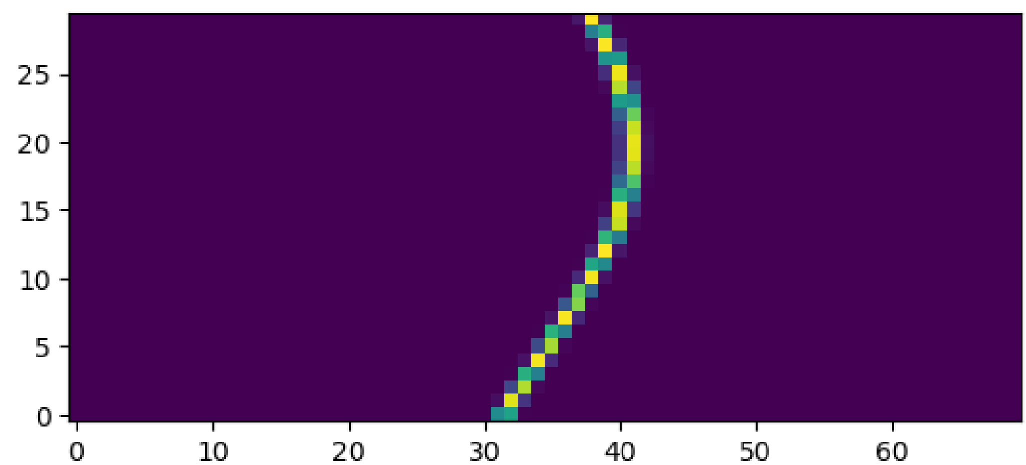
[18]:
```
# TODO: visualize four random rows as images, using an images
numbers = np.random.randint(0,design_matrix.shape[0],size = 4)
res2 = (30,70)

image1 = design_matrix[numbers[0]].reshape(res2)
image2 = design_matrix[numbers[1]].reshape(res2)
image3 = design_matrix[numbers[2]].reshape(res2)
image4 = design_matrix[numbers[3]].reshape(res2)


plt.imshow(image1, origin='lower')
plt.show()
plt.imshow(image2, origin='lower')
plt.show()
plt.imshow(image3, origin='lower')
plt.show()
plt.imshow(image4, origin='lower')
```

```
plt.show()
# The images map the readout intensity of a detector to the corresponding ray␣
↪and angle
```







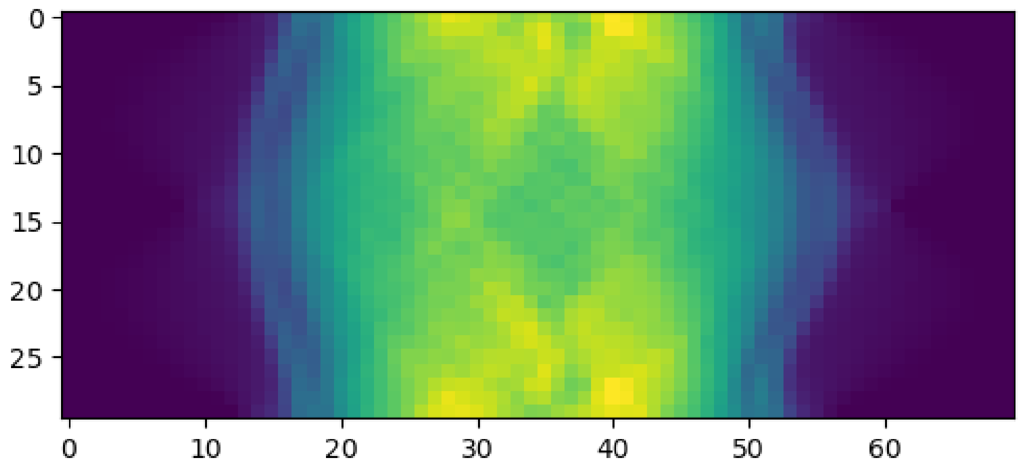


0.2.3 (c)

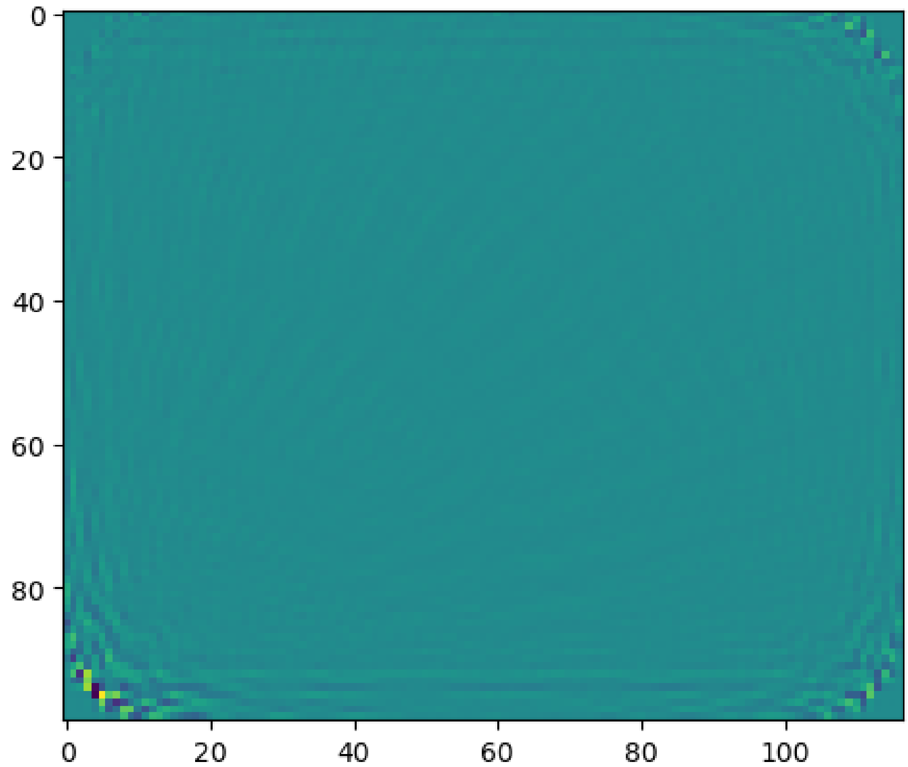
[19]:
```
# TODO: solve the reconstruction with linear regression and visualize the result
print(f"shapes: sino {sino.shape} design_matrix: {design_matrix.shape}")
# project components onto sino
Y = sino.squeeze()
reg = LinearRegression().fit(design_matrix.T, Y)
print(reg.score(design_matrix.T,Y))
prediction = reg.predict(design_matrix.T)
new_sino = prediction.reshape((30,70))
plt.imshow(new_sino)
plt.show()
# double check if sinogram fits
```

```
image = reg.coef_.reshape(res)
plt.imshow(image)

# we observe that the reconstructed image is not interpretable
```

```
shapes: sino (1, 2100) design_matrix: (11583, 2100)
0.9999999900717896
```



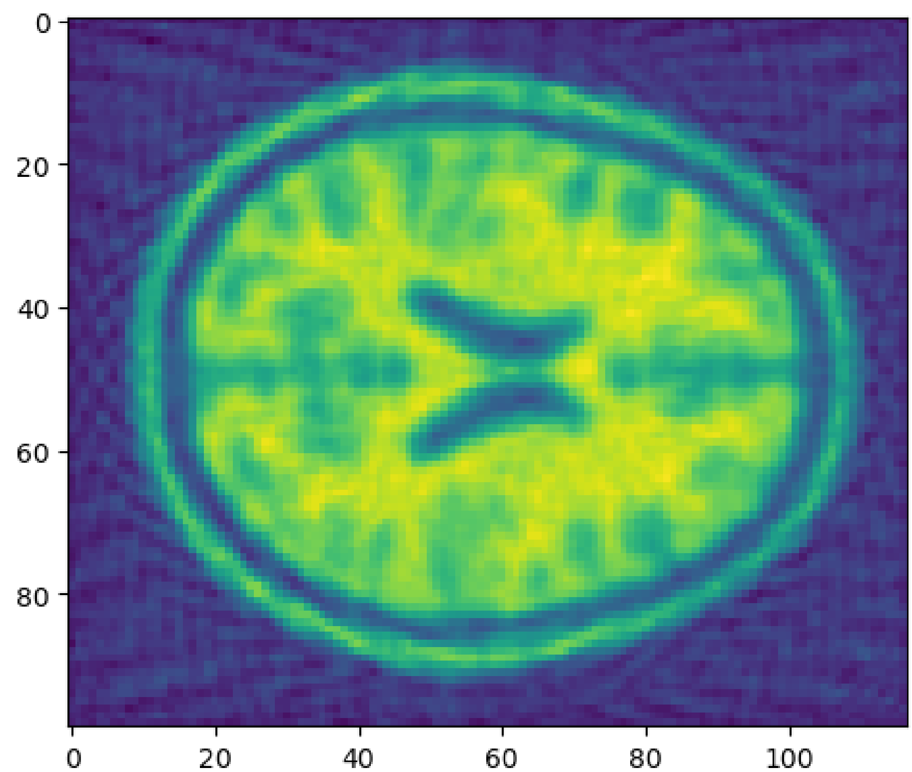
[19]: `<matplotlib.image.AxesImage at 0x7f5ce8aa6e80>`



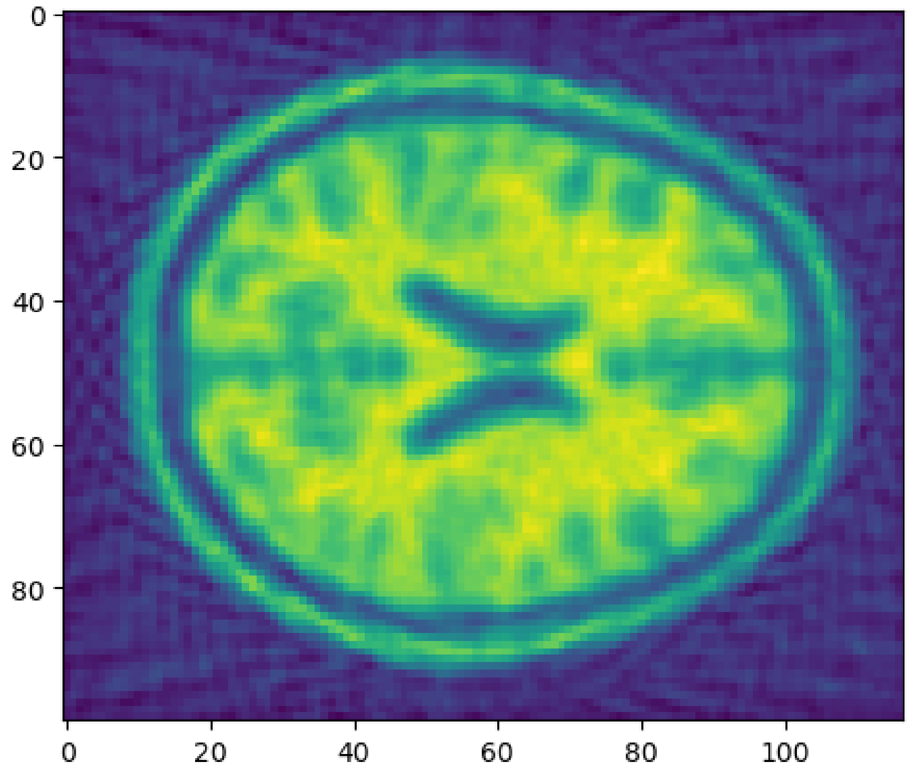
[11]:
```
# TODO: solve the reconstruction with ridge regression and visualize the result
# Optional: try out different regularization strengths and observe the influence
from sklearn.linear_model import Ridge

reg = Ridge(alpha=0.1).fit(design_matrix.T, Y)
print(reg.score(design_matrix.T,Y))
prediction = reg.predict(design_matrix.T)
image = reg.coef_.reshape(res)
plt.imshow(image)
plt.show()

reg = Ridge(alpha=1).fit(design_matrix.T, Y)
print(reg.score(design_matrix.T,Y))
prediction = reg.predict(design_matrix.T)
image = reg.coef_.reshape(res)
plt.imshow(image)
plt.show()

reg = Ridge(alpha=10).fit(design_matrix.T, Y)
print(reg.score(design_matrix.T,Y))
prediction = reg.predict(design_matrix.T)
image = reg.coef_.reshape(res)
```

```
plt.imshow(image)
plt.show()

# We observe that alpha= 0.1 delivers the best image quality as well as the␣
↪highest prediction score
```

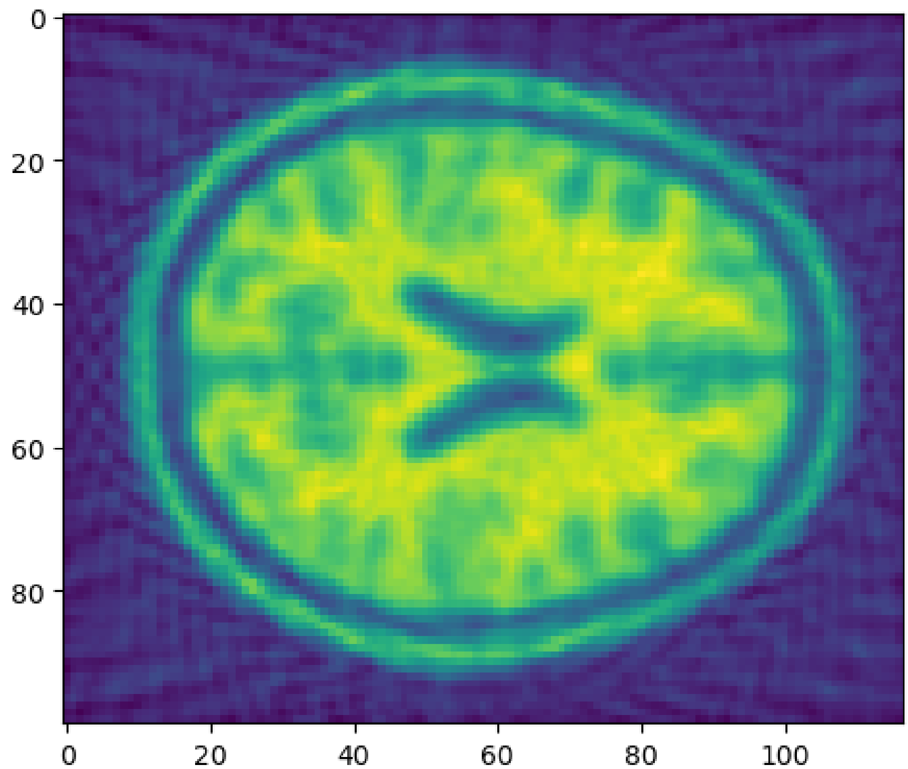
0.9999999710587341



0.9999997054099179

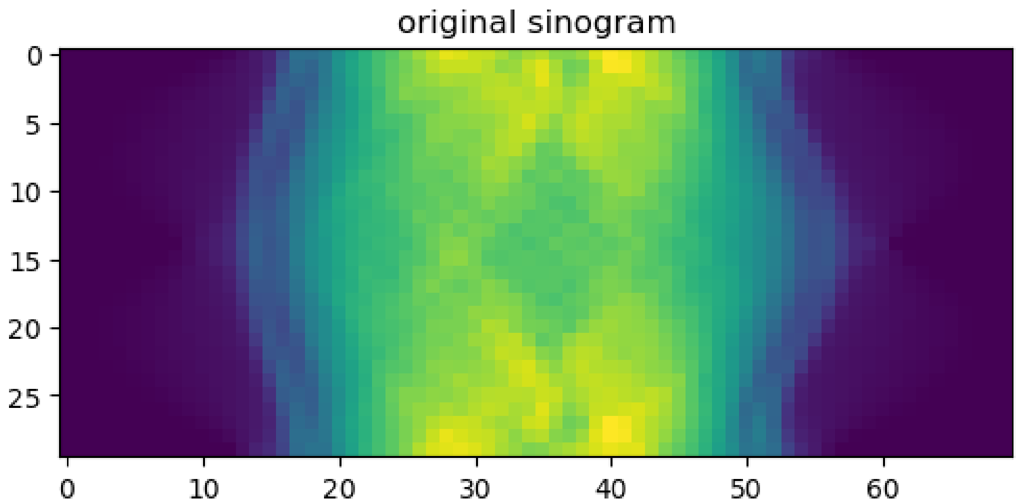


0.9999783629561321

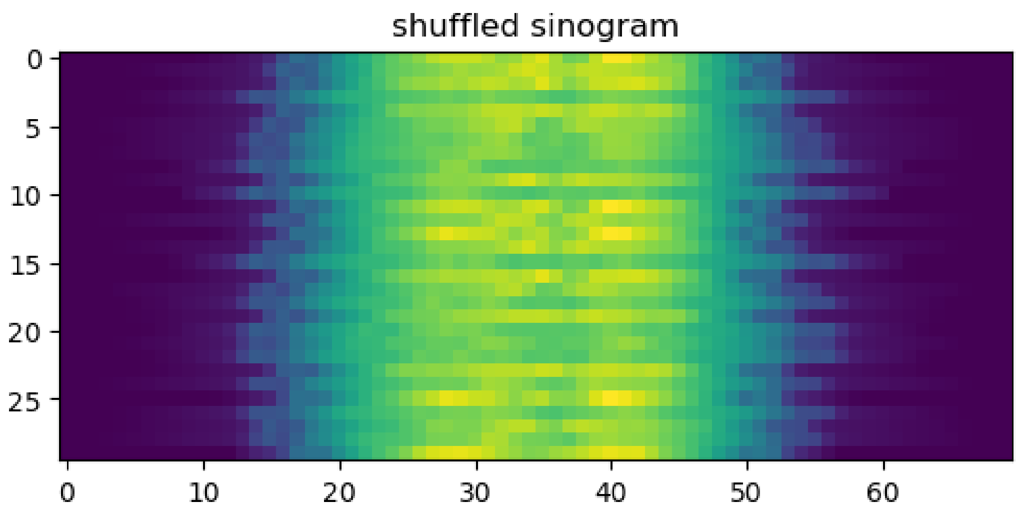


0.3 5 Bonus: X-Ray Free-Electron Lasers

[9]:
```
sino = np.load('data/sino.npy').reshape(n_angles, n_parallel_rays)
plt.imshow(sino)
plt.title('original sinogram')
plt.show()

order = np.arange(n_angles)
np.random.shuffle(order)
sino_shuffled = sino[order]
plt.imshow(sino_shuffled)
plt.title('shuffled sinogram')
plt.show()
```



original sinogram
0
5
10
15
20
25
0
10
20
30
40
50
60



shuffled sinogram
0
5
10
15
20
25
0
10
20
30
40
50
60


```
[ ]:
```

Machine Learning and Physics Sheet 08

① a) $\hat{\beta}_{ridge} = \arg\min_{\beta} \|y - X^T\beta\|_2^2 + \lambda\|\beta\|_2^2$

$$= \arg\min_{\beta} \hat{\sum_{i=1}} \left(y_i - (\beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i})\right)^2 + \lambda(\beta_0^2 + \beta_1^2 + \beta_2^2)$$

We then get $\hat{\beta}_{ridge} = (XX^T + \lambda I)^{-1} X y$

→ Since the regularization ~~punishes~~ ~~big~~ values of β_i, This results in a bias for the intercept β_0 towards values close to 0.

b) We modify: $\hat{\beta}_{ridge,mod} = \arg\min_{\beta} \|y - X^T\beta\|_2^2 + \lambda\|\beta\|_2^2 - \lambda\beta_0^2$

to remove the punishment of the β_0 component.

c) Since we remove the dependency on β_0 of the penalty term, The total penalty losses read:

$\lambda(\beta_1^2 + \beta_2^2)$ for b) and $\lambda(\beta_0^2 + \beta_1^2 + \beta_2^2)$ for a).

If we now assume we find a minimal value L, the regularization contour (~~sets~~ of parameters with same value) then a solves the equation

$\lambda(\beta_1^2 + \beta_2^2) = L$ for b) and $\lambda(\beta_0^2 + \beta_1^2 + \beta_2^2)$ for a).

We thus have the surface of a sphere for a) and the surface of a cylinder for b).

(Since for all values of β_0 we have the same penalty).

(2) a) $y_n = \beta^T x_n + \varepsilon_n$ with $\varepsilon_n \sim \mathcal{N}(0, \sigma^2)$

$$\hat{\beta} = \underset{\beta}{\arg\max} \sum_{n=1}^{N} \log \mathcal{N}(y_n | \beta^T x, \sigma^2)$$

$$= \underset{\beta}{\arg\max} \sum_{n=1}^{N} \log e^{-(y_n - x^T\beta)^T(y_n - x^T\beta)/\sigma^2}$$

$$= \underset{\beta}{\arg\max} \log \prod_{n=1}^{N} e^{-(y_n - x^T\beta)^T(y_n - x^T\beta)/\sigma^2}$$

$$= \underset{\beta}{\arg\max} -\sum_{n=1}^{N} (y_n - x^T\beta)^T(y_n - x^T\beta)/\sigma^2$$

$$= \underset{\beta}{\arg\min} \sum_{n=1}^{N} (y_n - x^T\beta)^T(y_n - x^T\beta)$$

b) $$\hat{\sigma}^2 = \underset{\sigma^2}{\arg\max} \sum_{n=1}^{N} \log \mathcal{N}(y_n | \hat{\beta}^T x, \sigma^2)$$

$$\overset{a)}{=} \underset{\sigma^2}{\arg\min} \sum_{n=1}^{N} (y_n - x^T\hat{\beta})^T(y_n - x^T\hat{\beta})/\sigma^2 \quad \Big| \; \hat{\beta} = (XX^T)^{-1} X y$$

$$= \underset{\sigma^2}{\arg\min} \left(Y - (X^T(XX^T)^{-1}XY)\right)^T\left(Y - X^T(XX^T)^{-1}XY\right)/\sigma^2 \quad \Big| \; Y = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}$$