sheet03

November 10, 2024

1 Sheet 3

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[1]:
```
import numpy as np
from matplotlib import pyplot as plt
from sklearn.linear_model import LinearRegression
```

1.2 1 Regularization and Intercept

1.2.1 (a)

$$\text{Loss}_{\text{Ridge}} = \sum_{i=1}^{N}(y_i - \beta_0 - \beta_1 x_{1i} - \beta_2 x_{2i})^2 + \lambda(\beta_0^2 + \beta_1^2 + \beta_2^2),$$

where $x_i = (1, x_{1i}, x_{2i})$, λ is regularization strength. Higher λ makes β_0 smaller in regression.

1.2.2 (b)

$$\text{Loss}_{\text{Ridge Modified}} = \sum_{i=1}^{N}(y_i - \beta_0 - \beta_1 x_{1i} - \beta_2 x_{2i})^2 + \lambda(\beta_1^2 + \beta_2^2),$$

1.2.3 (c)

For (a), regularization penalty is $\lambda(\beta_0^2 + \beta_1^2 + \beta_2^2)$. The regularization contours are **spheres**.

For (b), regularization penalty is $\lambda(\beta_1^2 + \beta_2^2)$. The regularization contours are **cylinder surfaces**, the height is along β_0 axis.

1.3 2 σ^2 Estimation

1.3.1 (a)

$$\mathcal{N}(y_n|\beta^T x_n, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp[-\frac{(y_n - \beta^T x_n)^2}{2\sigma^2}],$$

$$\log \mathcal{N}(y_n|\beta^T x_n, \sigma^2) = -\frac{1}{2}\log(2\pi\sigma^2) - \frac{(y_n - \beta^T x_n)^2}{2\sigma^2},$$

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

$$= \text{arg max}_\beta[-\frac{N}{2}\log(2\pi\sigma^2) - \frac{1}{2\sigma^2}\sum_{n=1}^{N}(y_n - \beta^T x_n)^2],$$

$$= \text{arg min}_\beta \frac{1}{2\sigma^2}\sum_{n=1}^{N}(y_n - \beta^T x_n)^2,$$

which is SSQ formulation with a factor of $\frac{1}{2\sigma^2}$.

1.3.2 (b)

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

$$= \text{arg max}_{\sigma^2}[-\frac{N}{2}\log(2\pi\sigma^2) - \frac{1}{2\sigma^2}\sum_{n=1}^{N}(y_n - \beta^T x_n)^2],$$

$$= \text{arg min}_{\sigma^2} \frac{N}{2}\log(2\pi) + \frac{N}{2}\log(\sigma^2) + \frac{1}{2\sigma^2}\sum_{n=1}^{N}(y_n - \beta^T x_n)^2,$$

$$= \text{arg min}_{\sigma^2} \frac{A}{\sigma^2} + B\log(\sigma^2)$$

where $A = \frac{1}{2}\sum_{n=1}^{N}(y_n - \beta^T x_n)^2$, $B = N/2$. This can be solved simply by let the derivative respect to σ^2 equals 0, which gives

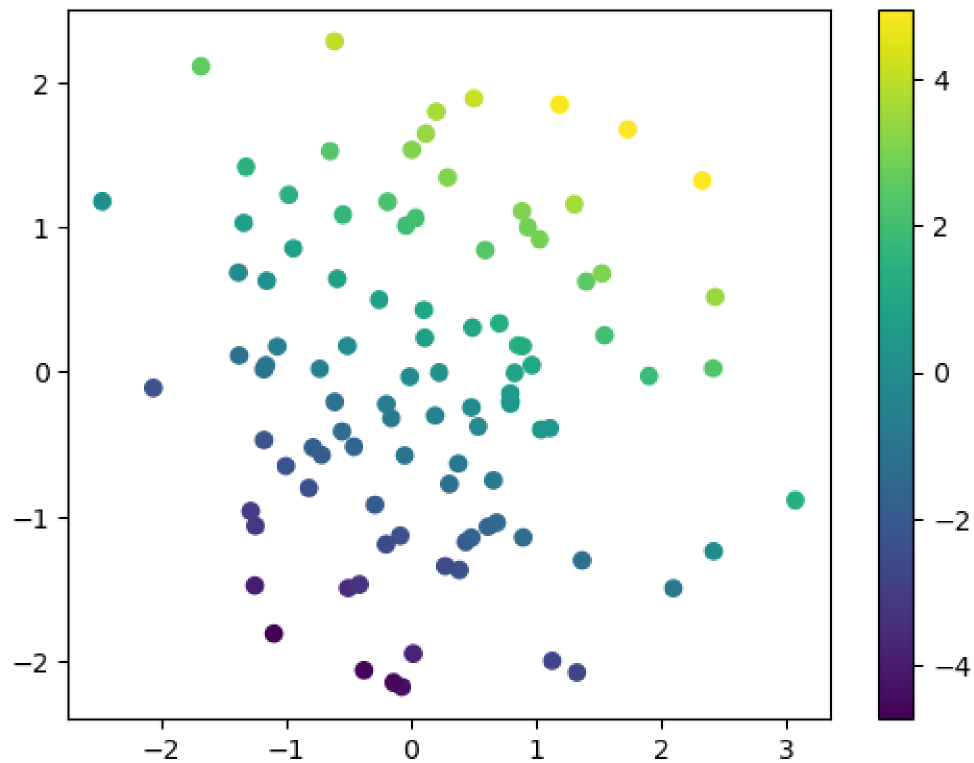
$$\hat{\sigma}^2 = \frac{A}{B} = \frac{1}{N}\sum_{n=1}^{N}(y_n - \beta^T x_n)^2,$$

which is simply the average sum of squared residuals.

1.4 3 Visualize Regularization Contours

[2]:
```
# 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)
```



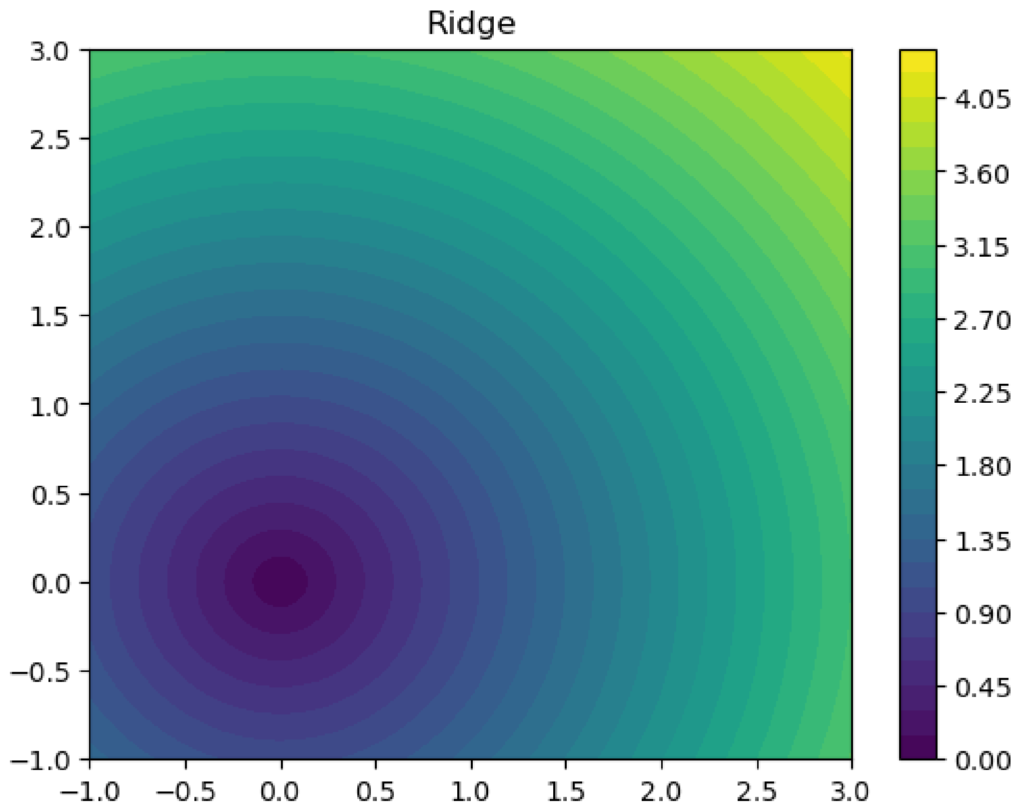
[3]:
```
# create a grid of points in the parameter space
b1, b2 = np.linspace(-1, 3, 100), np.linspace(-1, 3, 100)
bs = np.stack(np.meshgrid(b1, b2, indexing='ij'), axis=-1)
bs.shape
```

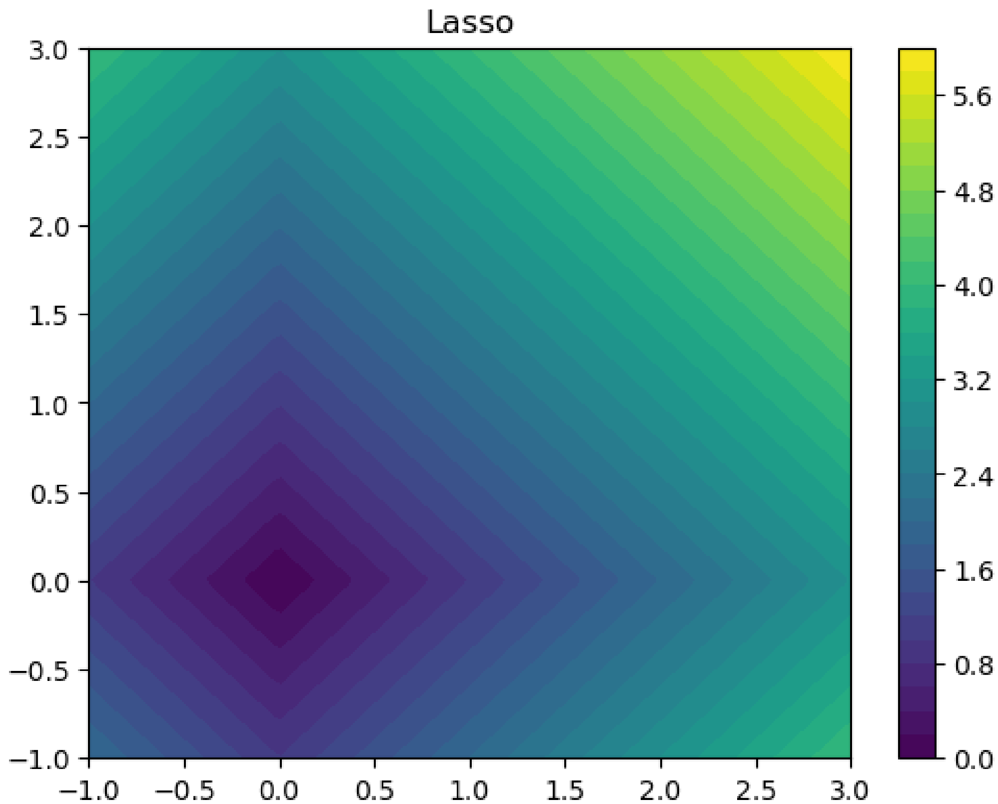
[3]: (100, 100, 2)

1.4.1 (a)

[4]:
```
# Plt the Ridge regression regularisation term as well as Lasso regularisation␣
  ↪term
# Ridge
ridge = np.linalg.norm(bs, axis=-1)
plt.contourf(b1, b2,ridge, levels=30)
plt.colorbar()
plt.title('Ridge')
plt.show()

# Lasso
lasso = np.sum(np.abs(bs), axis=-1)
plt.contourf(b1, b2, lasso, levels=30)
plt.colorbar()
```

```
plt.title('Lasso')
plt.show()
```





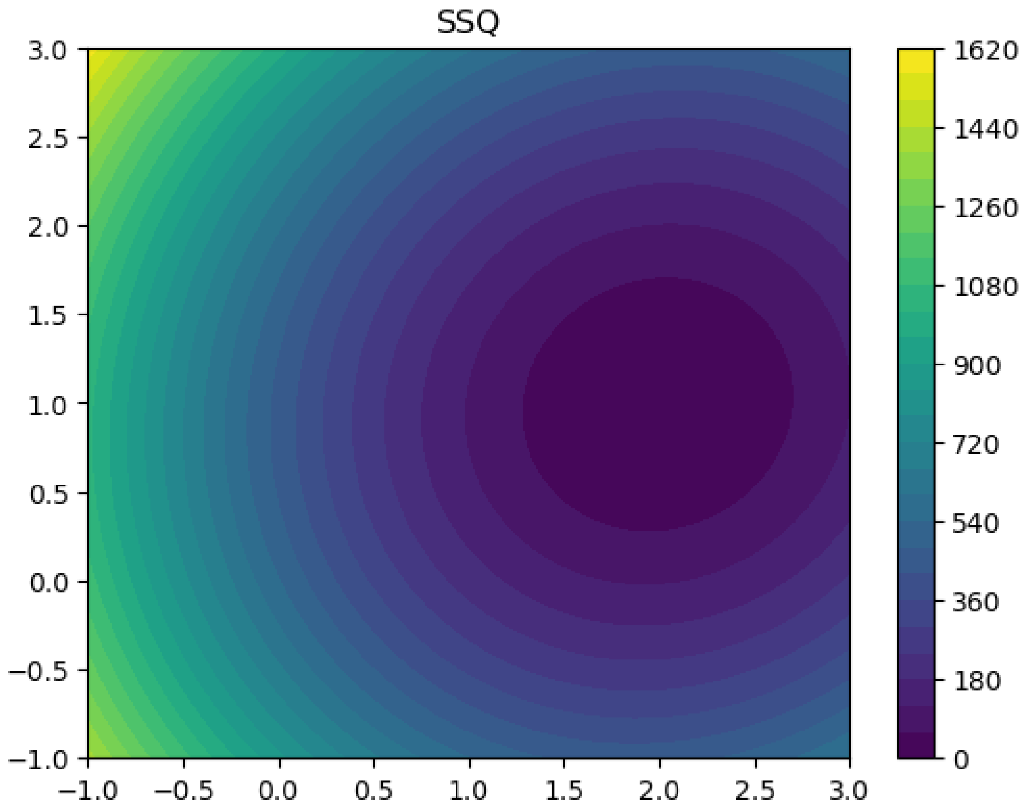
1.4.2 (b)

[5]:
```
y.shape
```

[5]: (1, 100)

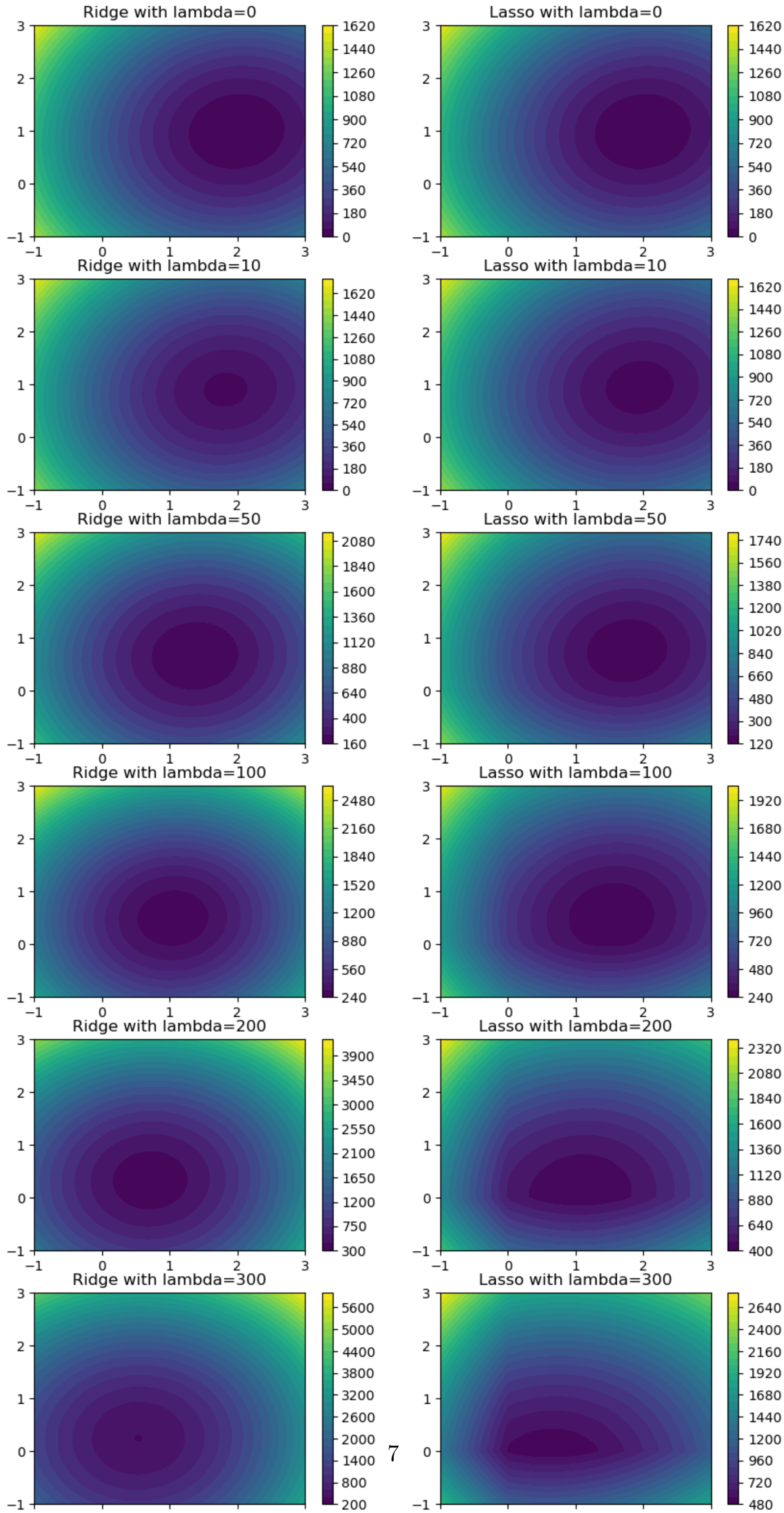
[6]:
```
#For the data set linreg.npz plot the sum of squares (SSQ) of a linear␣
 ↪regression as a function of
#over the same range as in i), i.e. over the grid [−1, 3] × [−1, 3].

# use bs grid from above
ssq = np.sum((y[:, None] - bs @ x)**2, axis=2)
print(ssq.shape)
plt.contourf(b1, b2, ssq, levels=30)
plt.colorbar()
plt.title('SSQ')
plt.show()
```

```
(100, 100)
```



1.4.3 (c)

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

fig, ax = plt.subplots(6, 2, figsize=(10, 20))
for i in range(len(lambdas)):
    l = lambdas[i]
    ridge = np.linalg.norm(bs, axis=-1)**2
    lasso = np.sum(np.abs(bs), axis=-1)
    ssq = np.sum((y[:, None] - bs @ x)**2, axis=2)
    im = ax[i,0].contourf(b1, b2, ssq + l*ridge, levels=30)
    plt.colorbar(im, ax=ax[i, 0])
    ax[i,0].set_title(f'Ridge with lambda={l}')

    im = ax[i,1].contourf(b1, b2, ssq + l*lasso, levels=30)
    plt.colorbar(im, ax=ax[i, 1])
    ax[i,1].set_title(f'Lasso with lambda={l}')

plt.show()
```


Ridge with lambda=0
Lasso with lambda=0
Ridge with lambda=10
Lasso with lambda=10
Ridge with lambda=50
Lasso with lambda=50
Ridge with lambda=100
Lasso with lambda=100
Ridge with lambda=200
Lasso with lambda=200
Ridge with lambda=300
Lasso with lambda=300

As λ increases the centre of the contours shifts towards the origin For the ridge regression, the contour shape stays the same. Whereas for the Lasso, the countours deform about the axes.

1.5 4 CT Reconstruction

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

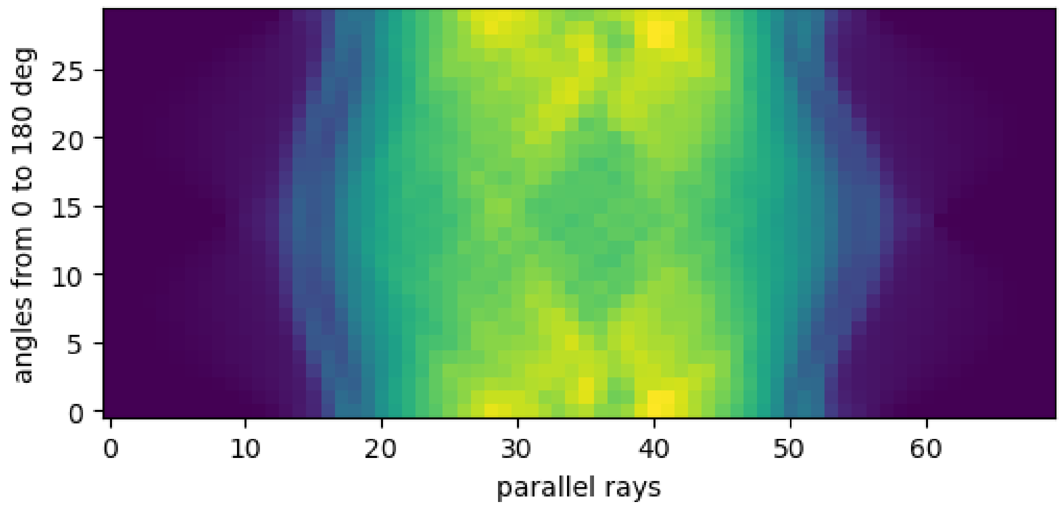
[8]:
```
# create design matrix
# don't change any of this, just run it once to create and save the design␣
↪matrix
import os

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
```

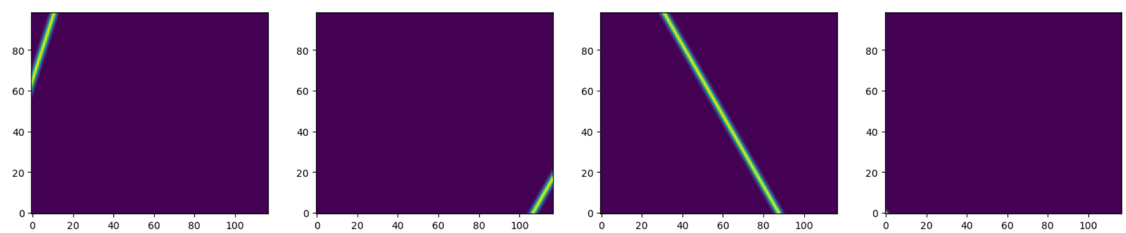
[9]:
```
sino = np.load('data/sino.npy')

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)
```



1.5.1 (a)

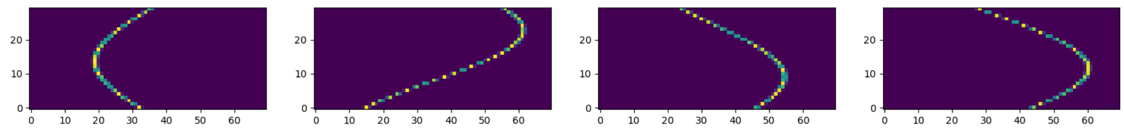
```
[10]: design_matrix = np.load('data/design_matrix.npy')

# TODO: visualize four random columns as images, using an image shape of (99,␣
 ↪117)
fig, ax = plt.subplots(1, 4, figsize=(20, 5))
for i in range(4):
    ax[i].imshow(design_matrix[:, np.random.randint(design_matrix.shape[1])].
 ↪reshape(99, 117), origin='lower')
plt.show()
```



The columns show for a given detector and angle, the response it can receive from different pixels. (If it can receive signal from that pixel, and the strength of the signal.)

1.5.2 (b)

[11]:
```
# TODO: visualize four random rows as images, using an images
fig, ax = plt.subplots(1, 4, figsize=(20, 10))
for i in range(4):
    ax[i].imshow(design_matrix[np.random.randint(design_matrix.shape[0])].
 ↪reshape(30, 70), origin='lower')
plt.show()
```



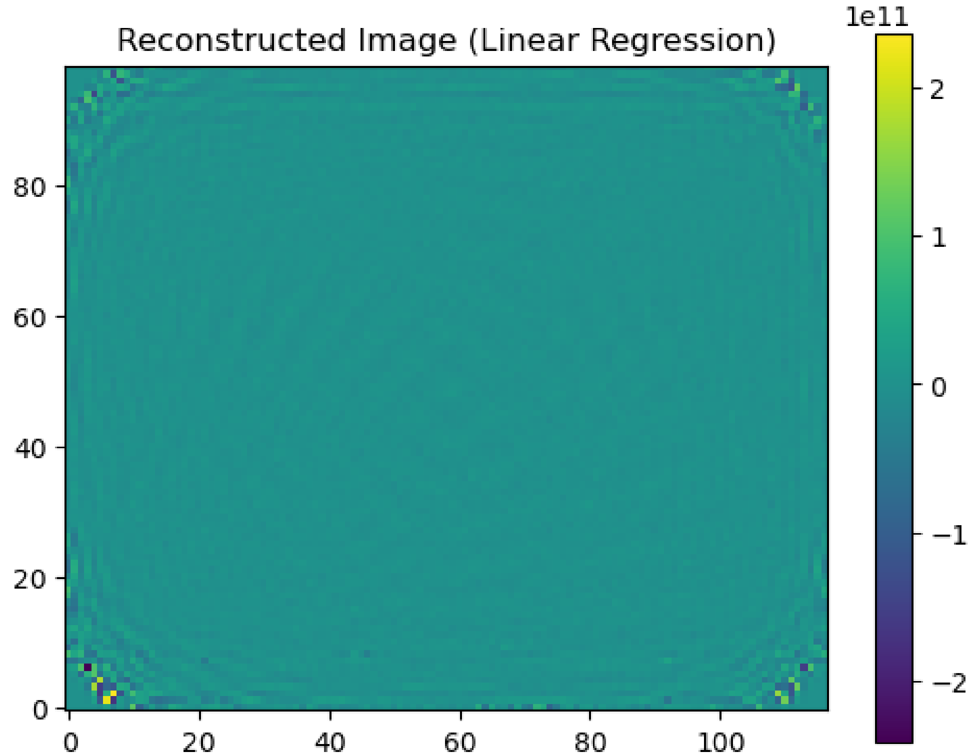
The rows show which detectors and angles can receive signals and the strength of that signal from a given pixel.

1.5.3 (c)

[12]:
```
sino.shape, design_matrix.shape
```

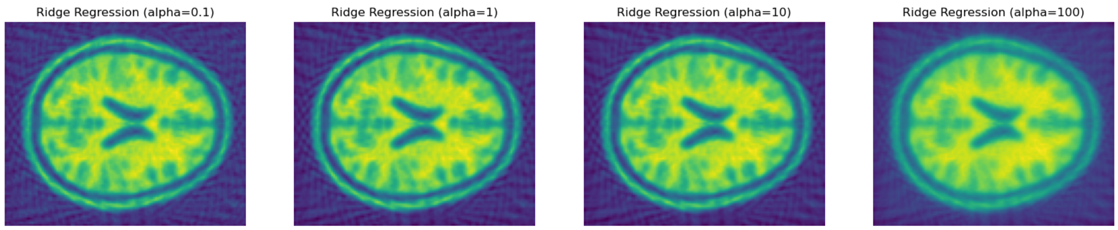
[12]: ((1, 2100), (11583, 2100))

[13]:
```
# TODO: solve the reconstruction with linear regression (no regularisation) and␣
 ↪visualize the result
# Load the design matrix and sinogram
#design_matrix = np.load('data/design_matrix.npy')
#sino = sino.reshape(n_angles * n_parallel_rays)

# Perform linear regression
model = LinearRegression()
model.fit(design_matrix.T, sino.flatten())
reconstructed_image = model.coef_.reshape(res)

# Visualize the reconstructed image
plt.imshow(reconstructed_image, origin='lower')
plt.title('Reconstructed Image (Linear Regression)')
plt.colorbar()
plt.show()
```



[14]:

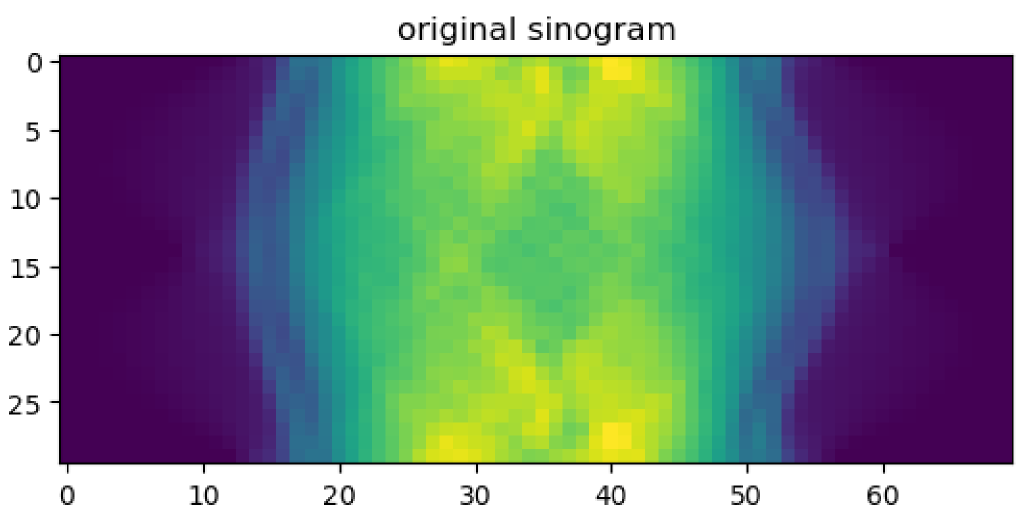
```python
# TODO: solve the reconstruction with ridge regression and visualize the result
# Optional: try out different regularization strengths and oberve the influence
from sklearn.linear_model import Ridge

# Perform ridge regression with different regularization strengths
alphas = [0.1, 1, 10, 100]
fig, ax = plt.subplots(1, len(alphas), figsize=(20, 5))

for i, alpha in enumerate(alphas):
    ridge_model = Ridge(alpha=alpha)
    ridge_model.fit(design_matrix.T, sino.flatten())
    reconstructed_image_ridge = ridge_model.coef_.reshape(res)

    ax[i].imshow(reconstructed_image_ridge, origin='lower')
    ax[i].set_title(f'Ridge Regression (alpha={alpha})')
    ax[i].axis('off')

plt.show()
```

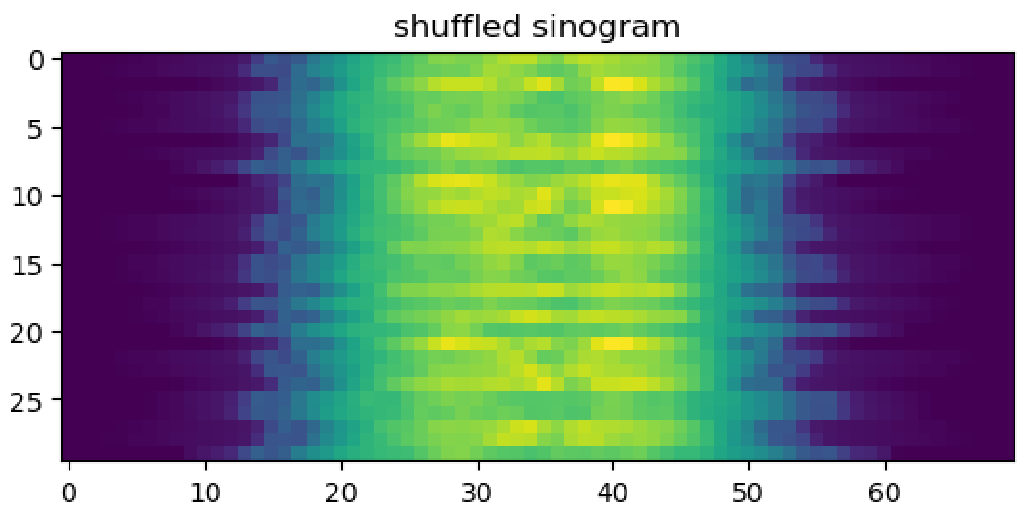


The Ridge regression considerably outperforms the Linear Regression, which is unable to reconstruct the image in any useful way.

1.6 5 Bonus: X-Ray Free-Electron Lasers

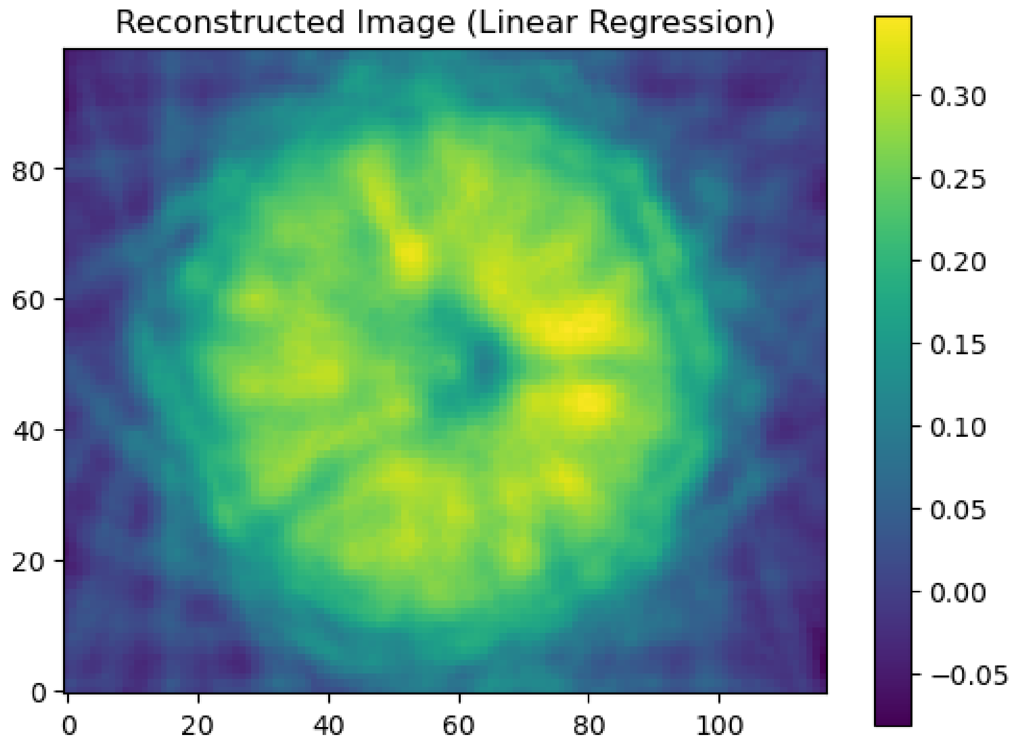
[15]:
```
sino = np.load('data/sino.npy').reshape(n_angles, n_parallel_rays)
plt.imshow(sino)
plt.title('original sinogram')
plt.show()

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





[16]:
```
#Try to reconstruct the image from the data of task 4, after shuffling the␣
↪sinogram along the angle axis
#Perturbatively perform Ridge regression

import time

t1=time.time()

alphas = [100, 50, 20, 10, 1, 0.1]
sino_pert = sino_shuffled
#print(sino_pert.shape)
for i, alpha in enumerate(alphas):
    model = Ridge(alpha=alpha)
    model.fit(design_matrix.T, sino_pert.flatten())
    reconstructed_image = model.coef_.reshape(res)
    sino_pert = (model.coef_[:,np.newaxis].T @ design_matrix).reshape(30,70)
    #print(sino_pert.shape)

t2=time.time()
print(f"Runtime: {t2-t1}")

# Visualize the reconstructed image
plt.imshow(reconstructed_image, origin='lower')
plt.title('Reconstructed Image (Linear Regression)')
plt.colorbar()
plt.show()
```

```
Runtime: 3.3538594245910645
```



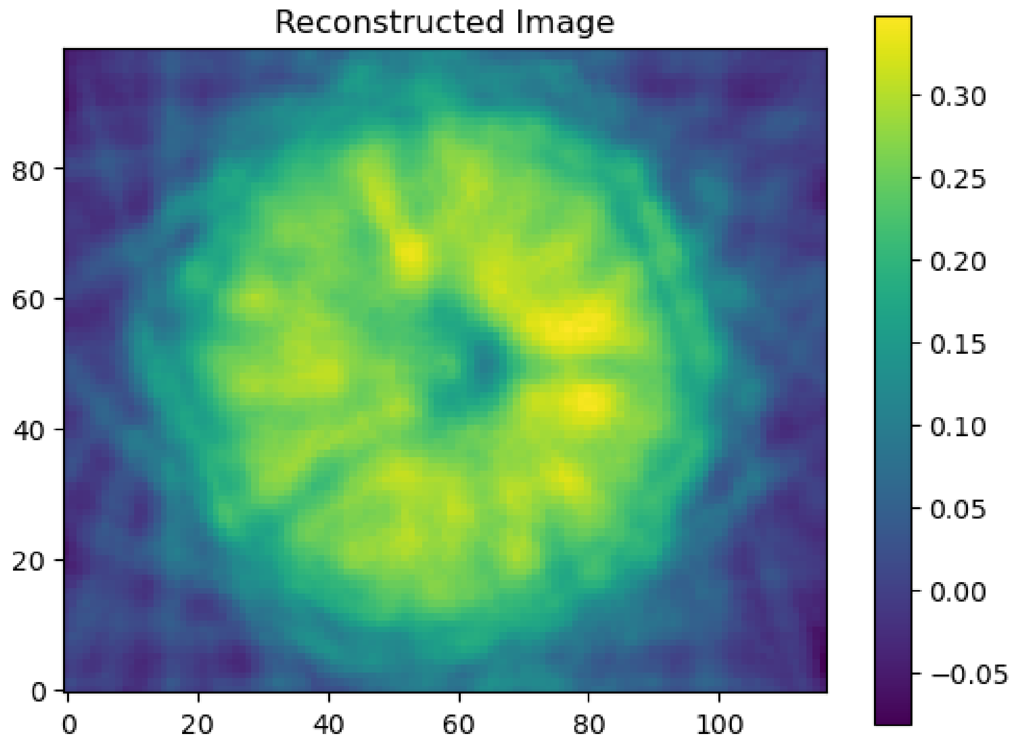
We can try all the full permutation and choose the one with lowest loss function value, but it will be very expensive. Notice that the shuffle performed above still makes every data that have same angle in the same row, we can just try every permutations with of angles, this will give a O(a!) time. This is still very expensive for large a. To make this cheaper, we can divided both X and Y into a = n_angles submatrixs, each with shape (p, r) and (1, r), and try to run regression on these smaller datasets for every pair of X_i and Y_j, and for every X_i, use the results that returns minimum loss. This gives O(a^2) time, which is faster, but the performance could be lower than trying out every permutations.

[17]:
```
x_sub = []
y_sub = []
for i in range(n_angles):
    x_sub.append(design_matrix[:, i*n_parallel_rays: (i+1)*n_parallel_rays])
    y_sub.append(sino_shuffled[i])
```

[18]:
```
# submatrix pair
def loss_ridge(x, y, beta, alpha):
    m = y - beta.T @ x

    return np.dot(m.flatten(), m.flatten()) + alpha * np.dot(beta.flatten(),␣
 ↪beta.flatten())

t1=time.time()
```

```
permuts = []
for i in range(n_angles):
    score = np.inf
    ind = -1
    for j in range(n_angles):
        if j in set(permuts):
            continue

        model = Ridge(alpha=1)
        model.fit(x_sub[i].T, y_sub[j].flatten())
        score_tmp = loss_ridge(x_sub[i], y_sub[j].reshape(1, n_parallel_rays),␣
 ↪model.coef_.reshape(res[0]*res[1], 1), 1)
        if score > score_tmp:
            ind = j
            score = score_tmp
    permuts.append(ind)

y_guess = np.array([x for _, x in sorted(zip(permuts, y_sub))]).flatten()

ridge_model = Ridge(alpha=1)
ridge_model.fit(design_matrix.T, y_guess)
reconstructed_image_ridge = ridge_model.coef_.reshape(res)

t2=time.time()
print(f"Runtime: {t2-t1}")

plt.imshow(reconstructed_image, origin='lower')
plt.title('Reconstructed Image')
plt.colorbar()
plt.show()
```

```
Runtime: 2.5525357723236084
```


Reconstructed Image
0
20
40
60
80
0
20
40
60
80
100
0.30
0.25
0.20
0.15
0.10
0.05
0.00
−0.05