Exercise Sheet 3

Due: 10.11.25 14h00

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General Regulations.

- Please hand in your solutions in groups of two (preferably from the same tutorial group).
- Your solutions to theoretical exercises can be either handwritten notes (scanned), or typeset using LaTeX. For scanned handwritten notes, please ensure they are legible and not blurry.
- For the practical exercises, always provide the (commented) code as well as the output, and don't forget to explain/interpret the latter.
- Please hand in a **single PDF** that includes both the exported notebook and your solutions to the theoretical exercises. Submit the PDF to the Übungsgruppenverwaltung once per group, making sure to include the names of both group members in the submission.
- You can find all the data in the GitHub Repository.

1 Regularization and Intercept

Consider a regression problem with two explanatory variables x_1, x_2. As introduced in the lecture, the intercept β_0 can be incorporate by considering $y = \boldsymbol{\beta}^T \mathbf{x}$ with $\boldsymbol{\beta} = (\beta_0, \beta_1, \beta_2)^T$ and $\mathbf{x} = (1, x_1, x_2)^T$.

(a) In this setting, write down the loss function for ridge regression, penalizing the L^2-norm of $\boldsymbol{\beta}$, in components. What is the influence of the regularization strength on the intercept β_0? (1 pt)

(b) Oftentimes, a regularization of the intercept term is unwanted. How would you modify the loss function to account for this? (1 pt)

(c) Which shapes in $\mathbb{R}^3$ do the regularization contours (i.e. sets of parameters with equal regularization penalty) of versions (a) and (b) have? (1 pt)

2 Visualize Regularization Contours

For two-dimensional parameter vectors β, we can visualize the error/loss surface of linear regression using contour plots. In this exercise, you will create a set of such plots in order to familiarize yourself further with the influence of regularization. For example, you can visualize the contours via `plt.contour` or `plt.contourf`.[1]

(a) Plot the Ridge regression regularization term as well as the Lasso[2] regularization term for $\beta_1, \beta_2 \in [-1, 3]$. (2 pts)

(b) For the data set `linreg.npz`, plot the sum of squares (SSQ) of a linear regression as a function of $\boldsymbol{\beta}$ over the same range as in **(a)**, i.e., over the grid $[-1, 3] \times [-1, 3]$. (2 pts)

(c) Plot the ridge and Lasso loss functions, i.e., $\text{SSQ}(\boldsymbol{\beta}) + \lambda ||\boldsymbol{\beta}||_2^2$ and $\text{SSQ}(\boldsymbol{\beta}) + \lambda ||\boldsymbol{\beta}||_1$, for $\lambda \in \{0, 10, 50, 100, 200, 300\}$ in the same $\boldsymbol{\beta}$ grid as before and *discuss your observations!* (2 pts)

[1] See https://matplotlib.org/stable/gallery/images_contours_and_fields/contour_demo.html for an example.
[2] The abbreviation comes from *least absolute shrinkage and selection operator*.

3 CT Reconstruction

Linear regression plays an important role in reconstructing computer tomography (CT) scans. In this task, you will do this on simulated data in the 2D case. You are given a sinogram $Y \in \mathbb{R}^{ar}$, i.e., a matrix where each row corresponds to a (1D) projection of the image consisting of r detector readouts along one of a distinct, evenly spaced angles. Additionally, you are given the design matrix $\mathbf{X} \in \mathbb{R}^{p \times ar}$. Excluding noise, one has $Y = I\mathbf{X}$, with the image $I \in \mathbb{R}^p$ which should be reconstructed.

(a) What is the interpretation of a column of $\mathbf{X}$? Visualize a choice of four columns as images. (2 pts)

(b) What is the interpretation of a row of $\mathbf{X}$? Visualize a choice of four rows as images. (2 pts)

(c) Solve the reconstruction problem with linear regression without any regularization and with ridge regression. What do you observe? (3 pts)

4 Bayes Classifiers

In the lecture, we derived the Bayes classifier for the 0-1 loss. In this exercise, you will find the optimal classifier for another loss function.

Consider classification with k classes in the ground-truth $y \in \{1, \dots, k\}$, but adding 0 as an additional "reject class" to the prediction $\hat{y} \in 0, 1, \dots, k$. For a fixed $\alpha \in (0, 1)$, consider a loss function L with

$$\begin{aligned} L(y, \hat{y}) &= 1 - \delta_{y\hat{y}} = \begin{cases} 0, \text{ for } y = \hat{y} \\ 1, \text{ else} \end{cases} && \text{for} \quad y, \hat{y} = 1, \dots, k \\ L(y, 0) &= \alpha && \text{for} \quad y = 1, \dots, k\,. \end{aligned}$$

Derive the optimal Bayes Classifier in this setting. What is the influence of α? When would you prefer this classifier over the one discussed in the lecture? (4 pts)

(5)

a) $L_\lambda^{ridge}(\vec{\beta}) = (\vec{y} - \underline{X}\vec{\beta})^T(\vec{y} - \underline{X}\vec{\beta}) + \lambda \|\vec{\beta}\|_2^2$

$= \sum_{i=1}^{N} (y_i - \vec{x}_i^T \vec{\beta})^2 + \lambda \sum_{j=0}^{2} \beta_j^2$

It can be seen here that the intercept β_0 grows linearly with the regularisation strength λ.

b) We would like the regularisation term to have no β_0 anymore. Change:

$\lambda \|\vec{\beta}\|_2^2 \rightarrow \lambda \|\underline{D}\vec{\beta}\|_2^2$

where

$$\underline{D} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

c) Ridge regularisation has a spherical contour, as $\beta_0 + \beta_1 + \beta_2 = \text{const.}$ for specific λ.
When β_0 is excluded, the contour becomes circular, inside the β_1, β_2 plane.

(4)

A BAYES classifier has chooses with

$$f^*(\vec{x}) = \underset{C_j}{\operatorname{argmin}}\, R(C_j|\vec{x}) = \underset{C_j}{\operatorname{argmin}} \sum_k L(C_k, C_j)\, p(C_k, \vec{x})$$

We have

$$L(C_k, C_j) = \begin{cases} 0, \text{ for } k = j \\ \alpha, \text{ for } j = 0 \\ 1, \text{ else} \end{cases}$$

So

$$R(C_j|\vec{x}) = \sum_{k \neq j} L(C_k, C_j)\, p(C_k, \vec{x})$$

$$\Rightarrow R(0|\vec{x}) = \sum_k \alpha\, p(C_k, \vec{x}) = \alpha$$

$$\Rightarrow R(C_j|\vec{x})^{j \neq 0} = \sum_{k \neq j} \alpha\, p(C_k, \vec{x}) = 1 - p(C_k, \vec{x})$$

Then

$$f^*(\vec{x}) = \begin{cases} \underset{C_k}{\operatorname{argmax}}\, p(C_k, \vec{x}), \text{ if } 1 - \max_{C_k} p(C_k, \vec{x}) < \alpha \\ 0, \text{ else} \end{cases}$$

α makes it possible to add general "reject class"

when one prefers not to assign a class at all, rather than misclassifying. We can also write:

$$f^*(\vec{x}) = \begin{cases} \underset{C_k}{\operatorname{argmax}}\, p(C_k, \vec{x}), & \text{if } \max_{C_k} p(C_k, \vec{x}) > 1-\alpha \\ 0 & \text{if } \max_{C_k} p(C_k, \vec{x}) \leq 1-\alpha \end{cases}$$

sheet03_notebook

November 10, 2025

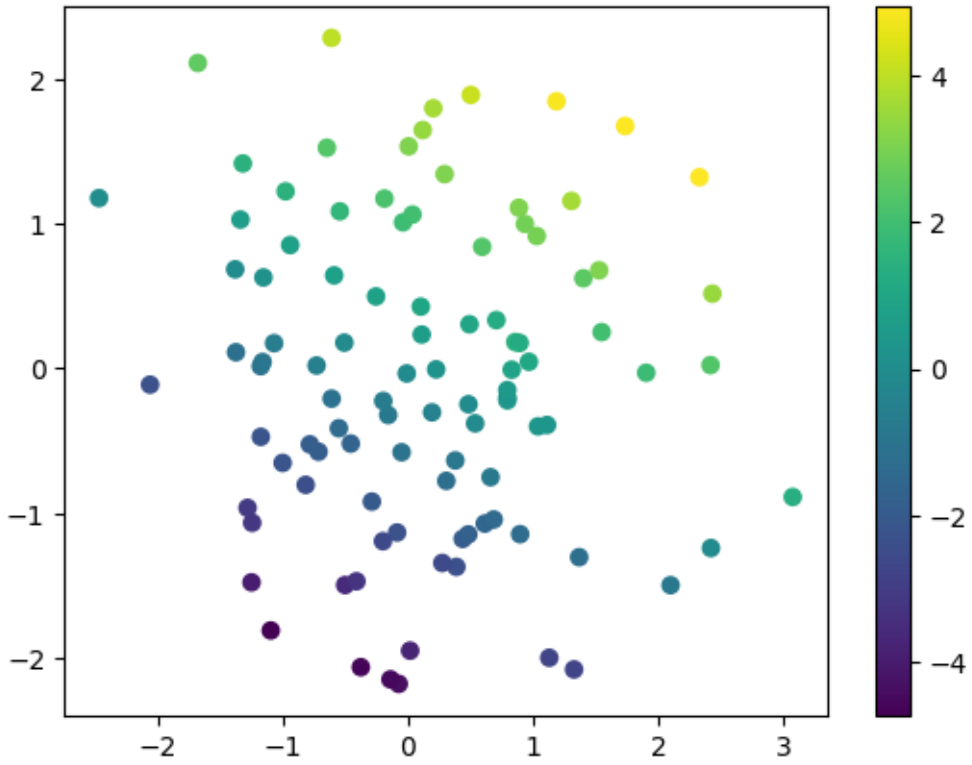
1 Sheet 03

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

1.1 (2) 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)
```



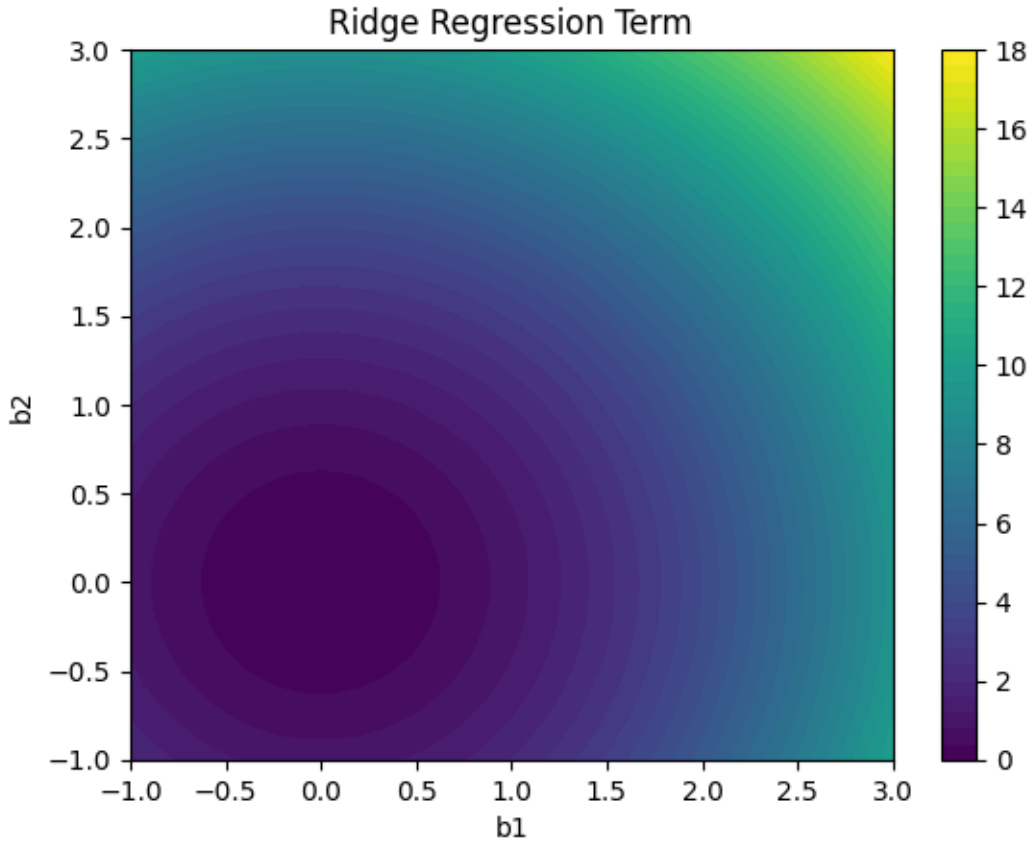
[3]:
```
# create a grid of points in the parameter space
b1, b2 = np.linspace(-1, 3, 101), np.linspace(-1, 3, 101)
bs = np.stack(np.meshgrid(b1, b2, indexing='ij'), axis=-1)
bs.shape
```

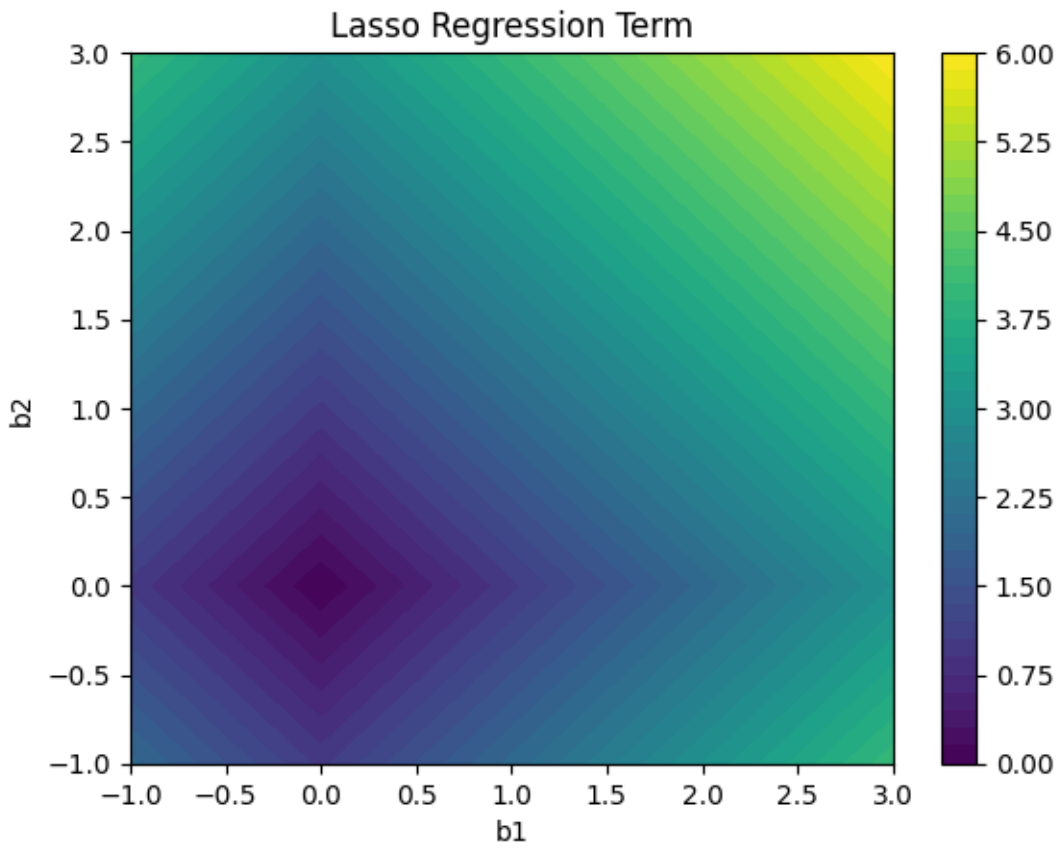
[3]:
```
(101, 101, 2)
```

1.1.1 (a)

[5]:
```
# Define ridge regression term
def ridge_term(b, alpha=1.0):
    return alpha * np.sum(b**2, axis=-1)

# Plot ridge regression contour
plt.contourf(b1, b2, ridge_term(bs), levels=50)
plt.colorbar()
plt.xlabel('b1')
plt.ylabel('b2')
plt.title('Ridge Regression Term')
plt.show()

# define lasso regression term
```

```python
def lasso_term(b, alpha=1.0):
    return alpha * np.sum(np.abs(b), axis=-1)

# Plot lasso regression contour
plt.contourf(b1, b2, lasso_term(bs), levels=50)
plt.colorbar()
plt.xlabel('b1')
plt.ylabel('b2')
plt.title('Lasso Regression Term')
plt.show()
```





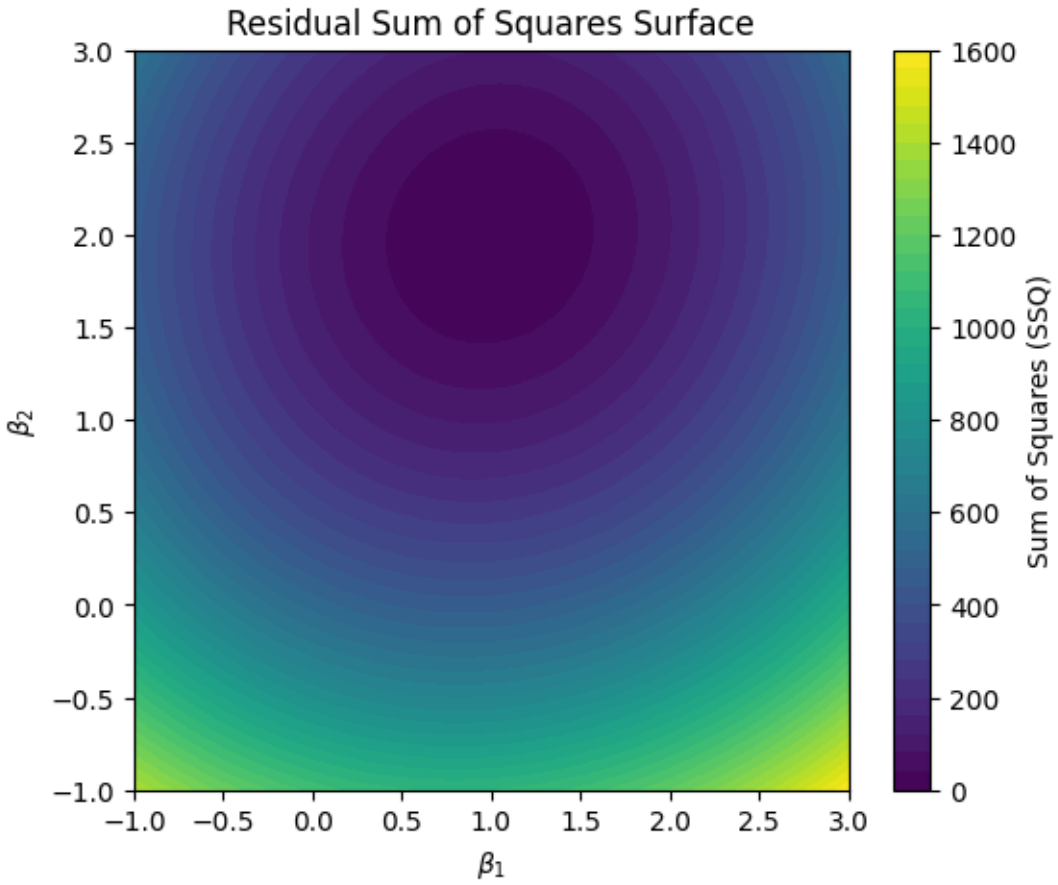
[13]:
```
x.shape
```

[13]:
```
(2, 100)
```

1.1.2 (b)

[14]:
```
# Initialise SSQ array
SSQ = np.zeros((len(b1), len(b2)))

# Compute SSQ for each ( ,  ) pair
for i in range(len(b1)):
    for j in range(len(b2)):
        beta = bs[i, j, :]  # ( ,  )
        X_T = x.T  # before (2,100), now (100, 2)
        y_pred = X_T @ beta  # works! (100,2) @ (2,) -> (100,)
        SSQ[i, j] = np.sum((y - y_pred)**2)

# Plot contour
plt.figure(figsize=(6, 5))
plt.contourf(b1, b2, SSQ.T, levels=50, cmap="viridis")
```

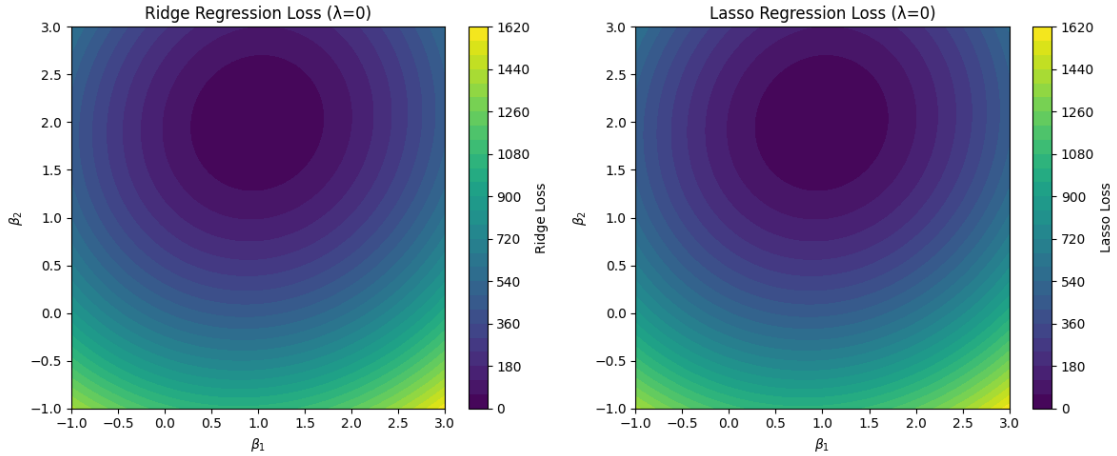
```
plt.colorbar(label="Sum of Squares (SSQ)")
plt.xlabel(r"$\beta_1$")
plt.ylabel(r"$\beta_2$")
plt.title("Residual Sum of Squares Surface")
plt.show()
```

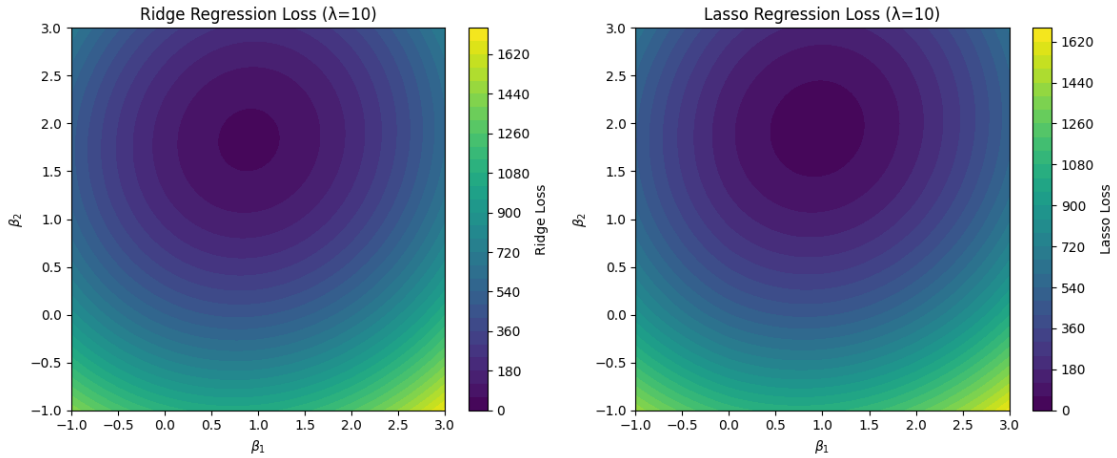


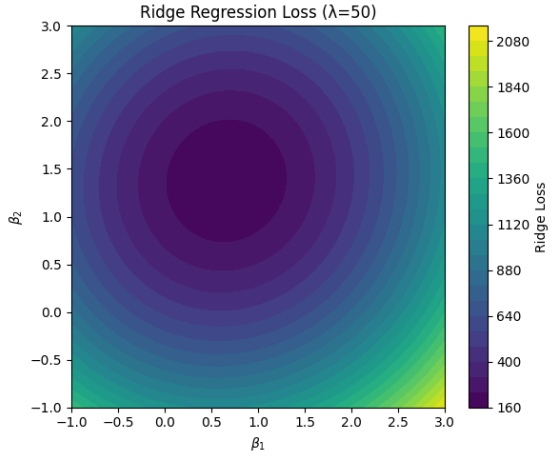
1.1.3 (c)

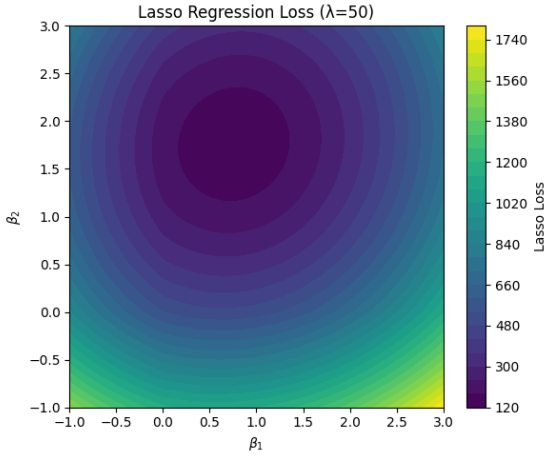
[24]:
```
# TODO: for each lambda, plot both ridge regression and lasso loss functions
lambdas = [0, 10, 50, 100, 200, 300]

for lam in lambdas:
    ridge_loss = SSQ + ridge_term(bs, alpha=lam)
    lasso_loss = SSQ + lasso_term(bs, alpha=lam)

    # Plot ridge regression loss
    plt.figure(figsize=(12, 5))
```

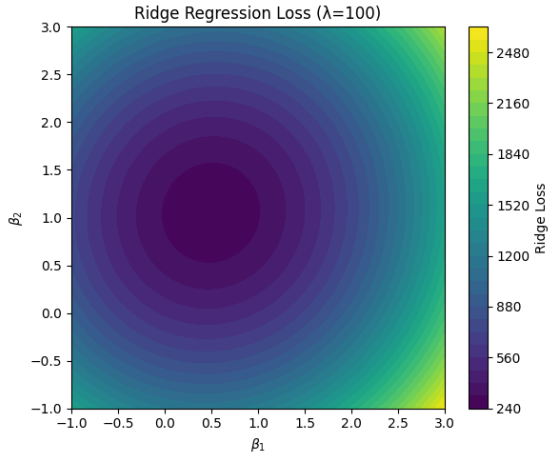
```
    plt.subplot(1, 2, 1)
    plt.contourf(b1, b2, ridge_loss.T, levels=30, cmap="viridis")
    plt.colorbar(label="Ridge Loss")
    plt.xlabel(r"$\beta_1$")
    plt.ylabel(r"$\beta_2$")
    plt.title(f"Ridge Regression Loss ( ={lam})")

    # Plot lasso regression loss
    plt.subplot(1, 2, 2)
    plt.contourf(b1, b2, lasso_loss.T, levels=30, cmap="viridis")
    plt.colorbar(label="Lasso Loss")
    plt.xlabel(r"$\beta_1$")
    plt.ylabel(r"$\beta_2$")
    plt.title(f"Lasso Regression Loss ( ={lam})")

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

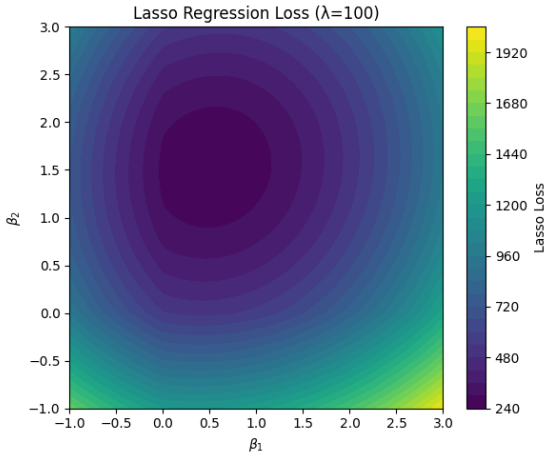


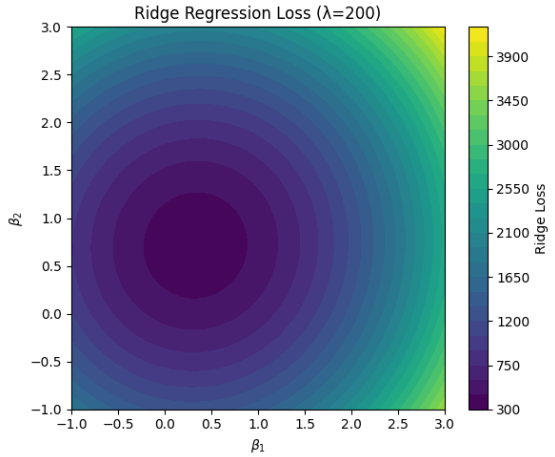


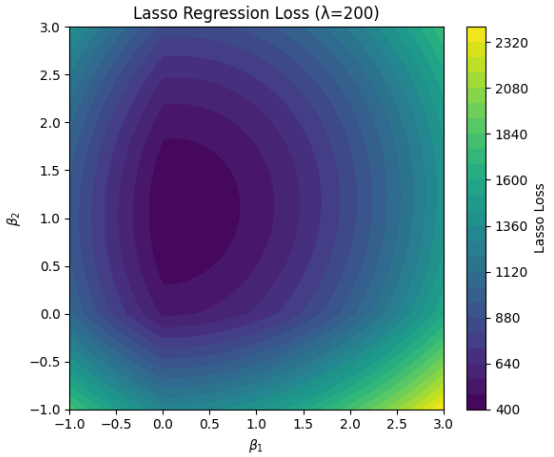

Ridge Regression Loss (λ=50)
β_1
β_2
Ridge Loss

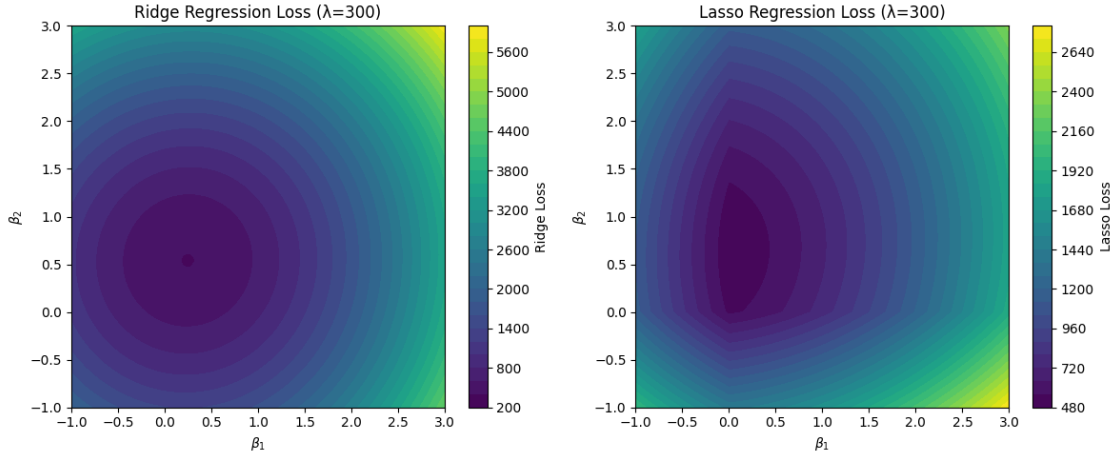

Lasso Regression Loss (λ=50)
β_1
β_2
Lasso Loss


Ridge Regression Loss (λ=100)
β_1
β_2
Ridge Loss


Lasso Regression Loss (λ=100)
β_1
β_2
Lasso Loss


Ridge Regression Loss (λ=200)
β_1
β_2
Ridge Loss


Lasso Regression Loss (λ=200)
β_1
β_2
Lasso Loss



1.2 (3) CT Reconstruction

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

[25]:
```
# 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
```

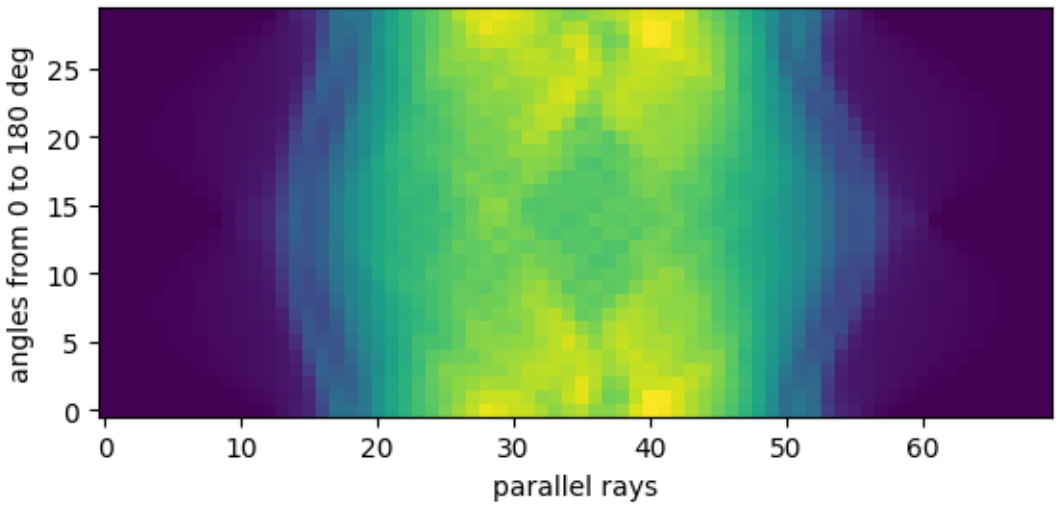
```
    ray_angles = np.linspace(0, np.pi, n_ray_angles, endpoint=False) + np.pi/
↪n_ray_angles

    # 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
created and saved design matrix of shape (11583, 2100) at data/design_matrix.npy
```

[26]:
```
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)
```



1.2.1 (a)

[50]:
```
design_matrix = np.load('data/design_matrix.npy')

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

fig, axs = plt.subplots(1, 4, figsize=(12, 4))
for i in range(4):
    # select random column index
    col_idx = np.random.randint(design_matrix.shape[1])
    print(design_matrix[:, col_idx].shape)

    # reshape column to image shape
    img = design_matrix[:, col_idx].reshape(99, 117)

    # plot the image
    axs[i].imshow(img, origin='lower')
    axs[i].set_title(f'Column {col_idx}')
    axs[i].axis('off')
plt.tight_layout()
```

```
plt.show()
```

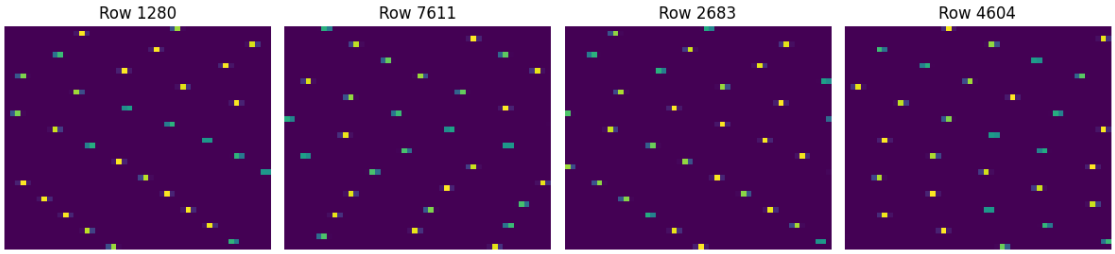
```
(11583,)
(11583,)
(11583,)
(11583,)
```

The columns give the different detector readings, meaning one specific column corresponds to a single pixel of the image and how it contributes to all detector readings.

1.2.2 (b)

[40]:
```
# TODO: visualize four random rows as images
fig , axs = plt.subplots(1, 4, figsize=(12, 4))
for i in range(4):
    # Select random row index
    row_idx = np.random.randint(design_matrix.shape[0])
    print(design_matrix[row_idx, :].shape)

    # Reshape row to image shape (2100 = 42*50)
    img = design_matrix[row_idx, :].reshape(42, 50)

    # Plot the image
    axs[i].imshow(img, origin='lower')
    axs[i].set_title(f'Row {row_idx}')
    axs[i].axis('off')
plt.tight_layout()
plt.show()
```

```
(2100,)
(2100,)
(2100,)
(2100,)
```



The rows give the different 2D slices. One individual row corresponds to a single detector reading.

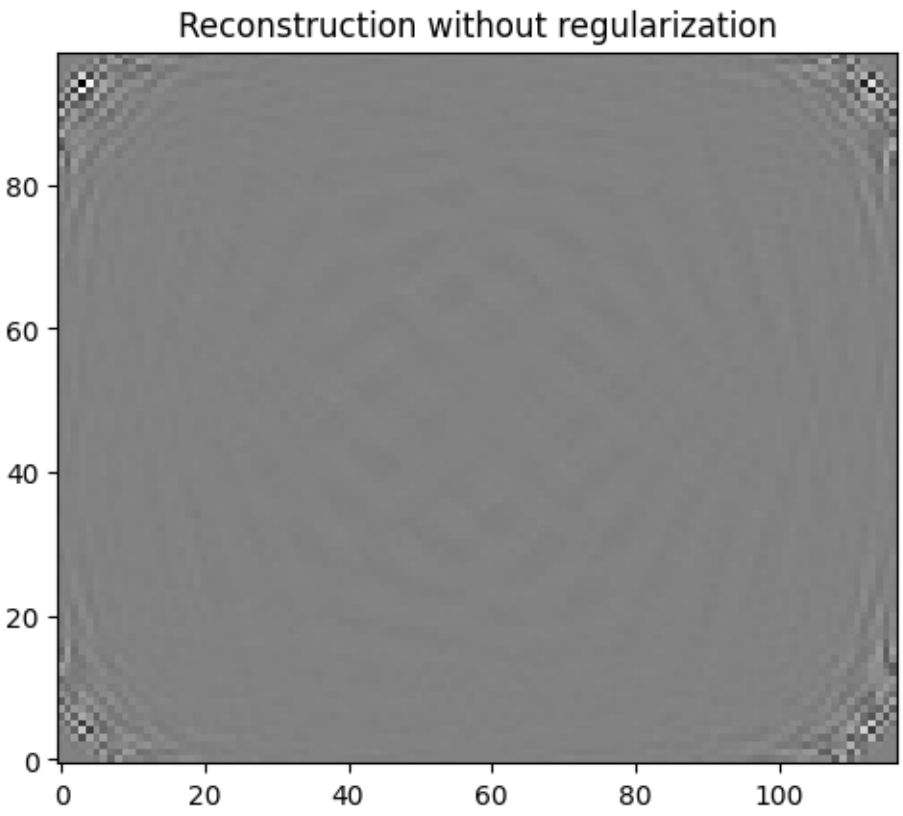
1.2.3 (c)

[62]:
```
# check shapes and solve (adapt names A and sino to your variables)
A = design_matrix.T             # expected shape (m, n)
b = sino.T                      # expected shape (m,)  or (m, 1) or (m, k)

print("A.shape (m,n) =", A.shape)
print("b.shape (m,) or (m,k) =", b.shape)

# ensure b is a 1D or 2D array with matching first dimension
b = b.ravel() if b.ndim == 2 and b.shape[1] == 1 else b
assert A.shape[0] == b.shape[0], "number of rows in A must equal length of b␣
 ↪(m)"
```

```
A.shape (m,n) = (2100, 11583)
b.shape (m,) or (m,k) = (2100, 1)
```

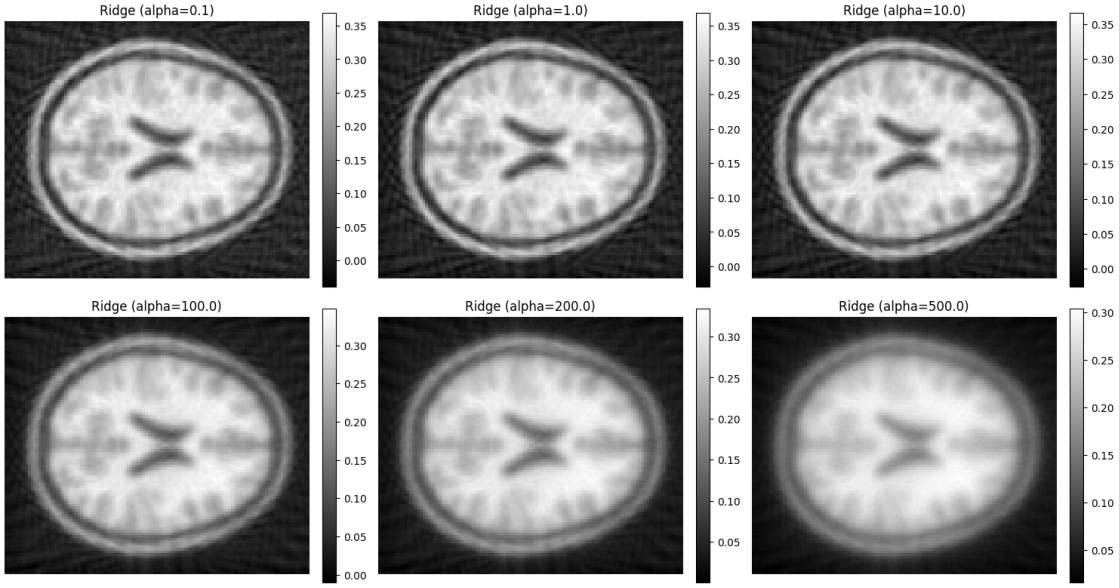
[63]:
```
# TODO: solve the reconstruction with linear regression and visualize the result
I_hat = np.linalg.lstsq(A, b, rcond=None)[0]
image_recon = I_hat.reshape(99, 117)
plt.imshow(image_recon, cmap='gray', origin='lower')
plt.title('Reconstruction without regularization')
plt.show()
```

```
(2, 100) (1, 100) (11583,)
```



[69]:
```python
# TODO: Same with ridge regression for different alphas
from sklearn.linear_model import Ridge

# define range of alphas to test
alphas = [0.1, 1.0, 10.0, 100.0, 200.0, 500.0]
fig, axs = plt.subplots(2, 3, figsize=(15, 8))

# loop over alphas and plot reconstructions
for ax, alpha in zip(axs.flat, alphas):
    # fit ridge regression model
    ridge = Ridge(alpha=alpha, fit_intercept=False)
    ridge.fit(A, b)
    I_ridge = ridge.coef_.ravel()

    # reshape and plot the reconstructed image
    im = ax.imshow(I_ridge.reshape(99, 117), cmap='gray', origin='lower')
    ax.set_title(f'Ridge (alpha={alpha})')
    ax.axis('off')
    fig.colorbar(im, ax=ax, fraction=0.046, pad=0.04)

plt.tight_layout()
```

```
plt.show()
```



With ridge regularisation a brain cut is visible. For larger regularisation strengths it becomes more blurry.