assignment2

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1 MATH5472 Assignment 2

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1.1 Problem 1

1.1.1 (a)

Since $X \in \mathbb{R}^{n\times p}$ has full rank , we have that for $n \geq p$, (X^TX) is revertible, and for $n < p$, (XX^T) is revertible.

(i) For $n \geq p$, $\|y - Xb\|_2^2 = (y - Xb)^T(y - Xb) = y^Ty - b^TX^Ty - y^TXb + b^TX^TXb = y^Ty - 2b^TX^Ty + b^TX^TXb$,

let $S(b) = \frac{1}{2}\|y - Xb\|_2^2$,

then $\frac{dS}{db} = -X^Ty + (X^TX)b$.

Since (X^TX) is revertible, let $S(b) = 0$, we have $b = (X^TX)^{-1}X^Ty$.

Therefore, for $n \geq p$, $\hat{\beta} = (X^TX)^{-1}X^Ty$ minimizes $S(b)$, and thus minimizes $\frac{S(b)}{n}$.

(ii) For $n < p$, let $\beta = X^T(XX^T)^{-1}y$, we have that $X\beta = XX^T(XX^T)^{-1}y = y$.

So $\frac{1}{2n}\|y - X\beta\|_2^2 = 0$, meanwhile $\frac{1}{2n}\|y - Xb\|_2^2 \geq 0$.

Thus $\hat{\beta} = X^T(XX^T)^{-1}y$ minimizes $\frac{1}{2n}\|y - X\beta\|_2^2$.

(iii) Based on the Stein's lemma, $df = E[\sum_i \frac{\partial \hat{y}_i}{\partial y_i}]$.

For $n \geq p$, $\hat{y} = X\hat{\beta} = X\left(X^TX\right)^{-1}X^Ty = Hy$,

where $H = X\left(X^TX\right)^{-1}X^T$ satisfies $H^T = H, H^2 = H$, thus H is symmetric and idempotent. Thus $\text{trace}(H) = \text{rank}(H) = p$.

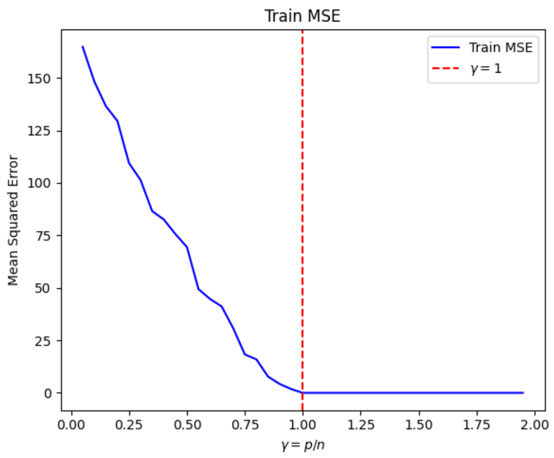
And $\frac{\partial \hat{y}}{\partial y} = H$, $\sum_{i=1}^n \frac{\partial \hat{y}_i}{\partial y_i} = \text{trace}(H) = p$. Thus $df = p$ for $n \geq p$.

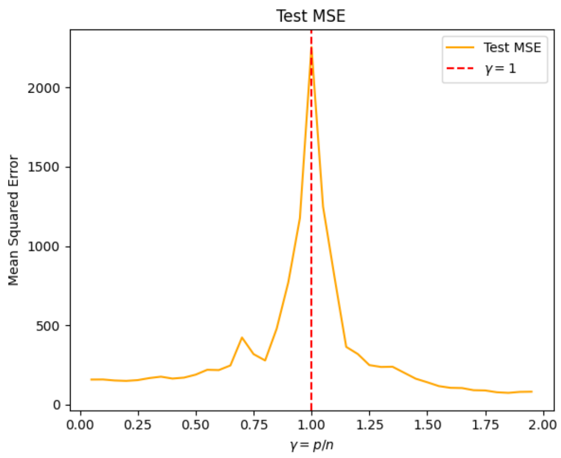
For $n < p$, $\hat{y} = X\hat{\beta} = XX^T\left(XX^T\right)^{-1}y = y$, so $\frac{\partial \hat{y}_i}{\partial y_i} = 1$, thus $df = n$ for $n < p$.

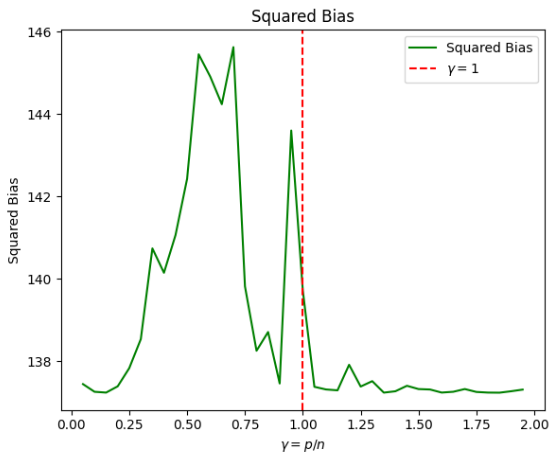
1.1.2 (b)

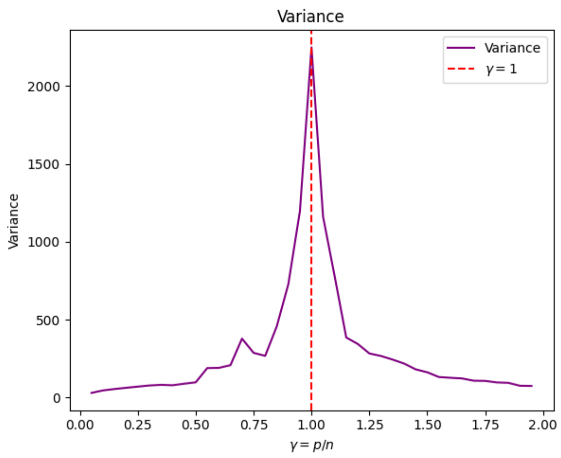
[1]:
```
import numpy as np
import matplotlib.pyplot as plt

np.random.seed(42)

n = 100  # number of samples
p_max = 200  # maximum number of features
p_list = np.arange(5, p_max, 5)  # number of features
gamma_list = p_list / n

# True coefficients
beta_true = np.random.randn(p_max)

X_full = np.random.randn(n, p_max)
y = X_full @ beta_true + np.random.randn(n) * 0.5

X_test = np.random.randn(n, p_max)
y_test = X_test @ beta_true + np.random.randn(n) * 0.5
y_test_true = X_test @ beta_true

train_errors = []
test_errors = []
bias2_list = []
var_list = []

for p in p_list:
    X = X_full[:, :p]
    X_test_p = X_test[:, :p]

    # Fit linear model
    if n >= p:
        beta_hat = np.linalg.inv(X.T @ X) @ X.T @ y
    else:
        beta_hat = X.T @ np.linalg.inv(X @ X.T) @ y

    y_train_pred = X @ beta_hat
    y_test_pred = X_test_p @ beta_hat

    train_error = np.mean((y - y_train_pred) ** 2)
    test_error = np.mean((y_test - y_test_pred) ** 2)
    bias2 = np.mean((np.mean(y_test_pred) - y_test_true) ** 2)
    variance = np.var(y_test_pred)

    train_errors.append(train_error)
    test_errors.append(test_error)
```

```python
    bias2_list.append(bias2)
    var_list.append(variance)

# 1. Plot train/test MSE side by side
plt.figure(figsize=(12, 5))
plt.subplot(1, 2, 1)
plt.plot(gamma_list, train_errors, label='Train MSE', color='blue')
plt.axvline(1, color='r', linestyle='--', label=r'$\gamma = 1$')
plt.xlabel(r'$\gamma = p/n$')
plt.ylabel('Mean Squared Error')
plt.title('Train MSE')
plt.legend()

plt.subplot(1, 2, 2)
plt.plot(gamma_list, test_errors, label='Test MSE', color='orange')
plt.axvline(1, color='r', linestyle='--', label=r'$\gamma = 1$')
plt.xlabel(r'$\gamma = p/n$')
plt.ylabel('Mean Squared Error')
plt.title('Test MSE')
plt.legend()

plt.tight_layout()
plt.show()

# 2. Plot bias and variance side by side
plt.figure(figsize=(12, 5))
plt.subplot(1, 2, 1)
plt.plot(gamma_list, bias2_list, label='Squared Bias', color='green')
plt.axvline(1, color='r', linestyle='--', label=r'$\gamma = 1$')
plt.xlabel(r'$\gamma = p/n$')
plt.ylabel('Squared Bias')
plt.title('Squared Bias')
plt.legend()

plt.subplot(1, 2, 2)
plt.plot(gamma_list, var_list, label='Variance', color='purple')
plt.axvline(1, color='r', linestyle='--', label=r'$\gamma = 1$')
plt.xlabel(r'$\gamma = p/n$')
plt.ylabel('Variance')
plt.title('Variance')
plt.legend()

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









1.1.3 (c)

Our goal is to show that $\lim_{k\to\infty} \beta^{(k)} = (X^TX)^{-1}X^Ty$.

Expanding $\beta^{(k)}$:

$$\beta^{(k)} = \beta^{(k-1)} + \epsilon\frac{X^T}{n}(y - X\beta^{(k-1)}) = \beta^{(k-1)} + \epsilon(\frac{X^Ty}{n} - \frac{X^TX}{n}\beta^{(k-1)})$$

Let $A = \frac{X^TX}{n}$ and $b = \frac{X^Ty}{n}$, we have:

$$\beta^{(k)} = \beta^{(k-1)} + \epsilon b - \epsilon A\beta^{(k-1)} = (I - \epsilon A)\beta^{(k-1)} + \epsilon b$$

And let $M = I - \epsilon A$, we have:

$$\beta^{(k)} = M\beta^{(k-1)} + \epsilon b = M^k\beta^{(0)} + (I + M + ... + M^{k-1})\epsilon b = (I + M + ... + M^{k-1})\epsilon b$$

If $\lim_{k\to\infty} M = 0$, then $I + M + M^2 + ... = (I - M)^{-1}$, and so we have:

$$\lim_{k\to\infty} \beta^{(k)} = (I - M)^{-1}\epsilon b = (\epsilon A)^{-1}\epsilon b = A^{-1}b$$

Substituting $A = \frac{X^TX}{n}$ and $b = \frac{X^Ty}{n}$ back to the equation:

$$\lim_{k\to\infty} \beta^{(k)} = (\frac{X^TX}{n})^{-1}\frac{X^Ty}{n} = (X^TX)^{-1}X^Ty$$

The condition for $\lim_{k\to\infty} M = 0$ is that the absolute value of every eigenvalue of M is strictly smaller than 1, that is, if we let λ_i be the eigenvalues of A, we need $|1 - \epsilon\lambda_i| < 1 \ \forall i$, and this condition is true when $0 < \epsilon \leq 1/\lambda_{max}(A)$.

1.1.4 (d)

Given $\frac{d\beta}{dt} + \frac{X^TX}{n}\beta = \frac{X^Ty}{n}$ and $\beta(0) = 0$, we will solve this differential equation using the method of integration factors.

We define the function $\mu(t)$:

$$\mu(t) = e^{\int_0^t \frac{X^TX}{n}dt} = e^{t\frac{X^TX}{n}}$$

Then $\beta(t)$ is

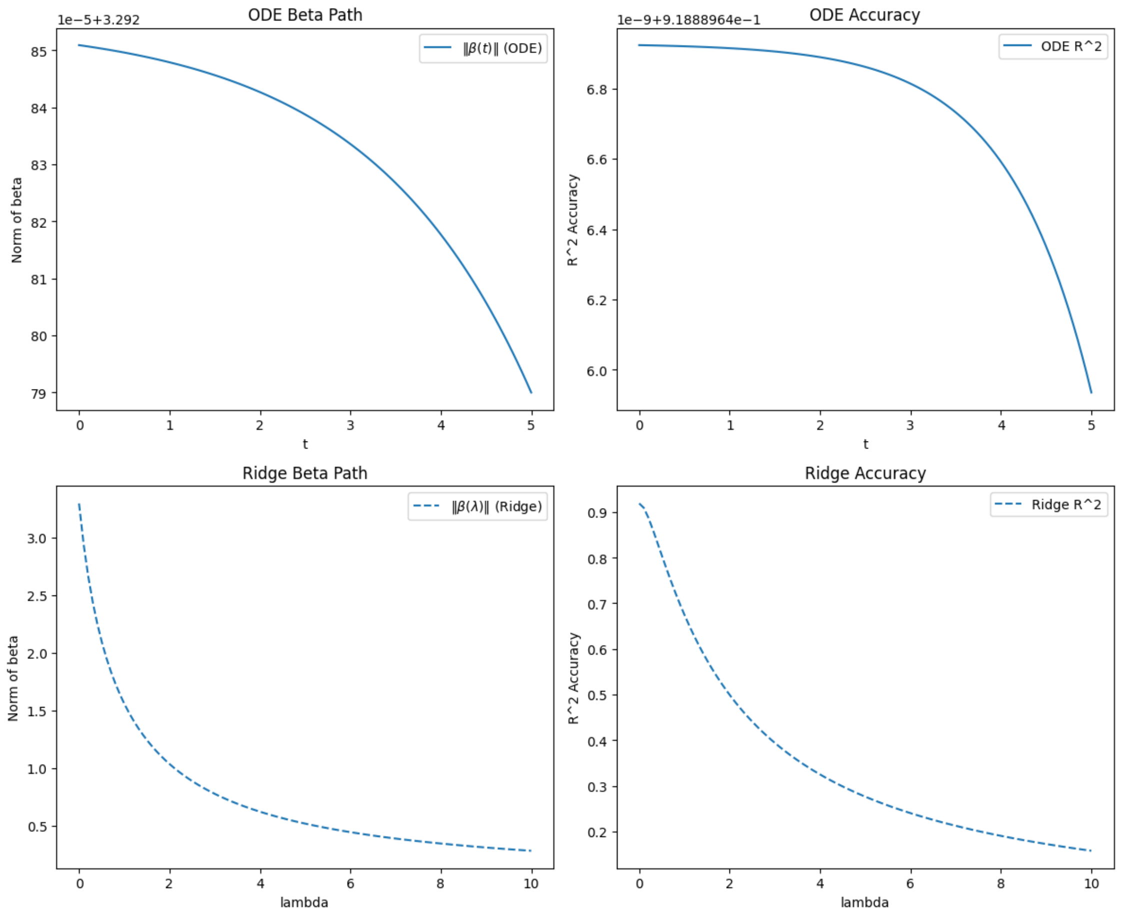
$$\begin{aligned}
\beta(t) &= \frac{1}{\mu(t)}(\beta(0) + \int_0^t e^{s\frac{X^TX}{n}}\frac{X^Ty}{n}ds) \\
&= \frac{1}{\mu(t)}\int_0^t e^{s\frac{X^TX}{n}}\frac{X^Ty}{n}ds \\
&= \frac{1}{\mu(t)}[(\frac{X^TX}{n})^{-1}e^{s\frac{X^TX}{n}}\frac{X^Ty}{n}]_0^t \\
&= \frac{1}{\mu(t)}(e^{t\frac{X^TX}{n}} - I)(X^TX)^{-1}X^Ty \\
&= (I - e^{-t\frac{X^TX}{n}})(X^TX)^{-1}X^Ty
\end{aligned}$$

1.1.5 (e)

In Ridge regression, $\hat{\beta}(\lambda) = (X^TX + n\lambda I)^{-1}X^Ty$

[2]:
```
import numpy as np
import matplotlib.pyplot as plt
from scipy.linalg import expm
```

```python
np.random.seed(42)

n = 50
p = 5
X = np.random.randn(n, p)
beta_true = np.random.randn(p)
y = X @ beta_true + np.random.randn(n)

XtX = X.T @ X
XtX_inv = np.linalg.inv(XtX)
Xt_y = X.T @ y

# ODE solution for OLS: beta(t) = (I - exp(-t * XtX / n)) @ XtX_inv @ Xt_y
t_grid = np.linspace(17, 22, 100)
beta_ols_path = np.array([ (np.eye(p) - expm(-t * XtX / n)) @ XtX_inv @ Xt_y␣
 ↪for t in t_grid ])

# Ridge regression path: beta(lambda) = (X^T X + n*lambda*I)^{-1} X^T y
lambda_grid = np.linspace(0.0001, 10, 100)
beta_ridge_path = np.array([np.linalg.inv(XtX + n * l * np.eye(p)) @ Xt_y for l␣
 ↪in lambda_grid])

def r2_score(beta):
    y_pred = X @ beta
    ss_res = np.sum((y - y_pred) ** 2)
    ss_tot = np.sum((y - np.mean(y)) ** 2)
    return 1 - ss_res / ss_tot

r2_ols = [r2_score(beta) for beta in beta_ols_path]
r2_ridge = [r2_score(beta) for beta in beta_ridge_path]

plt.figure(figsize=(12, 10))

# Plot ODE beta(t) and accuracy
plt.subplot(2, 2, 1)
plt.plot(22-t_grid, np.linalg.norm(beta_ols_path, axis=1),␣
 ↪label=r'$\|\beta(t)\|$ (ODE)')
plt.xlabel('t')
plt.ylabel('Norm of beta')
plt.title('ODE Beta Path')
plt.legend()

plt.subplot(2, 2, 2)
plt.plot(22-t_grid, r2_ols, label='ODE R^2')
plt.xlabel('t')
plt.ylabel('R^2 Accuracy')
plt.title('ODE Accuracy')
plt.legend()

# Plot Ridge beta(lambda) and accuracy
plt.subplot(2, 2, 3)
plt.plot(lambda_grid, np.linalg.norm(beta_ridge_path, axis=1),␣
 ↪label=r'$\|\beta(\lambda)\|$ (Ridge)', linestyle='--')
plt.xlabel('lambda')
plt.ylabel('Norm of beta')
plt.title('Ridge Beta Path')
plt.legend()

plt.subplot(2, 2, 4)
plt.plot(lambda_grid, r2_ridge, label='Ridge R^2', linestyle='--')
plt.xlabel('lambda')
plt.ylabel('R^2 Accuracy')
plt.title('Ridge Accuracy')
plt.legend()

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



The $\hat{\beta}(t)$ and $\hat{\beta}(\lambda)$ show similar behavior (The norm of beta and R^2 decay) in certain region of t and λ. This show that ridge regression and early stopping are related.

1.2 Problem 2

1.2.1 (a)

Given 1. $z_{A,i}|\mu_{A,i} \sim N(\mu_{A,i}, 1)$ and $z_{B,i}|\mu_{B,i} \sim \mathcal{N}(\mu_{B,i}, 1)$, 2. $i = 1, ..., N$, 3. $z_{A,i}$ and $z_{B,i}$ are observed.

Assume:

$$\begin{pmatrix} \mu_{A,i} \\ \mu_{B,i} \end{pmatrix} \sim \mathcal{N}(\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \Sigma)$$

where

$$\Sigma = \begin{pmatrix} \sigma_A^2 & \rho\sigma_A\sigma_B \\ \rho\sigma_A\sigma_B & \sigma_B^2 \end{pmatrix}$$

Our goal is to derive an algorithm to estimate Σ, then estimate $\mu_{A,i}^{(\rho)}$ and $\mu_{B,i}^{(\rho)}$.

Step 1: Estimate Σ (Covariance Matrix)

$(z_{A,i}, z_{B,i})$ are observed and each is distributed as $\mathcal{N}(0, \Sigma + I)$.

1. Collect all observed pairs $(z_{A,i}, z_{B,i})$ for $i = 1, \dots, N$.
2. Compute the sample mean for each variable:
   - $\bar{z}_A = \frac{1}{N}\sum_{i=1}^N z_{A,i}$
   - $\bar{z}_B = \frac{1}{N}\sum_{i=1}^N z_{B,i}$
3. Compute the sample covariance matrix S:

$$S = \frac{1}{N}\sum_{i=1}^N \begin{pmatrix} z_{A,i} - \bar{z}_A \\ z_{B,i} - \bar{z}_B \end{pmatrix} \begin{pmatrix} z_{A,i} - \bar{z}_A & z_{B,i} - \bar{z}_B \end{pmatrix}$$

4. Since $S \approx \Sigma + I$, we estimate Σ as:

$$\hat{\Sigma} = S - I$$

Step 2: Estimate Posterior Means $\mu_{A,i}^{(\rho)}, \mu_{B,i}^{(\rho)}$ For each $i = 1, \dots, N$: 1. Form the observed vector $z_i = \begin{pmatrix} z_{A,i} \\ z_{B,i} \end{pmatrix}$. 2. Compute the posterior mean:

$$\hat{\mu}_i = \hat{\Sigma}(\hat{\Sigma} + I)^{-1} z_i$$

3. The first entry of $\hat{\mu}_i$ is $\mu_{A,i}^{(\rho)}$, the second is $\mu_{B,i}^{(\rho)}$.

1.2.2 (b)

Correct specification

[3]:
```python
import numpy as np

np.random.seed(42)

# Simulation parameters
N = 100  # number of samples
rho = 0.8  # correlation coefficient
sigma_A = 1.2
sigma_B = 1.6

# True covariance matrix
Sigma_true = np.array([[sigma_A**2, rho*sigma_A*sigma_B],
                       [rho*sigma_A*sigma_B, sigma_B**2]])

# Generate true means (mu_A, mu_B) for each i
mu = np.random.multivariate_normal([0, 0], Sigma_true, size=N)

# Generate observed data with noise
z = mu + np.random.randn(N, 2)

# --- New algorithm: Estimate Sigma and posterior means ---
# Estimate sample means
z_mean = np.mean(z, axis=0)
# Estimate sample covariance (biased, but fine for large N)
S = np.cov(z, rowvar=False, bias=True)
# Subtract noise variance
Sigma_hat = S - np.eye(2)

# Posterior mean for each i
Sigma_hat_plus_I = Sigma_hat + np.eye(2)
Sigma_hat_inv = np.linalg.inv(Sigma_hat_plus_I)
mu_hat = (Sigma_hat @ Sigma_hat_inv @ z.T).T  # shape (N,2)

# --- James-Stein Estimator (JSE, rho=0) ---
# JSE shrinks each coordinate separately
sigma_A2_hat = S[0,0] - 1
sigma_B2_hat = S[1,1] - 1
# Shrinkage factor for each coordinate
def james_stein(z_col, sigma2):
    return (sigma2 / (sigma2 + 1)) * z_col

mu_hat_jse = np.zeros_like(z)
mu_hat_jse[:,0] = james_stein(z[:,0], sigma_A2_hat)
mu_hat_jse[:,1] = james_stein(z[:,1], sigma_B2_hat)

# --- Compute expected squared losses ---
loss_new = np.mean(np.sum((mu_hat - mu)**2, axis=1))
```

```
loss_jse = np.mean(np.sum((mu_hat_jse - mu)**2, axis=1))

print(f"Expected squared loss (New): {loss_new:.4f}")
print(f"Expected squared loss (JSE):  {loss_jse:.4f}")
```

```
Expected squared loss (New): 1.0759
Expected squared loss (JSE):  1.3271
```

Misspecification

[4]:
```
import numpy as np

np.random.seed(42)

# Simulation parameters
N = 100  # number of samples
rho = 0.8  # correlation coefficient
sigma_A = 1.2
sigma_B = 1.6

# True covariance matrix
Sigma_true = np.array([[sigma_A**2, rho*sigma_A*sigma_B],
                      [rho*sigma_A*sigma_B, sigma_B**2]])

# Generate true means (mu_A, mu_B) for each i
mu = np.random.multivariate_normal([2, -2], Sigma_true, size=N)

# Generate observed data with noise
z = mu + np.random.randn(N, 2)

# --- New algorithm: Estimate Sigma and posterior means ---
# Estimate sample means
z_mean = np.mean(z, axis=0)
# Estimate sample covariance (biased, but fine for large N)
S = np.cov(z, rowvar=False, bias=True)
# Subtract noise variance
Sigma_hat = S - np.eye(2)

# Posterior mean for each i
Sigma_hat_plus_I = Sigma_hat + np.eye(2)
Sigma_hat_inv = np.linalg.inv(Sigma_hat_plus_I)
mu_hat = (Sigma_hat @ Sigma_hat_inv @ z.T).T  # shape (N,2)

# --- James-Stein Estimator (JSE, rho=0) ---
# JSE shrinks each coordinate separately
sigma_A2_hat = S[0,0] - 1
sigma_B2_hat = S[1,1] - 1
# Shrinkage factor for each coordinate
```

```
def james_stein(z_col, sigma2):
    return (sigma2 / (sigma2 + 1)) * z_col

mu_hat_jse = np.zeros_like(z)
mu_hat_jse[:,0] = james_stein(z[:,0], sigma_A2_hat)
mu_hat_jse[:,1] = james_stein(z[:,1], sigma_B2_hat)

# --- Compute expected squared losses ---
loss_new = np.mean(np.sum((mu_hat - mu)**2, axis=1))
loss_jse = np.mean(np.sum((mu_hat_jse - mu)**2, axis=1))

print(f"Expected squared loss (New): {loss_new:.4f}")
print(f"Expected squared loss (JSE):  {loss_jse:.4f}")
```

```
Expected squared loss (New): 5.8422
Expected squared loss (JSE):  3.3914
```

1.2.3 (c)

The simulation shows that the algorithm generally achieves lower expected squared loss than the James-Stein estimator, especially when the correlation ρ is large/nonzero. But when the model is misspecified, the preformance drops drastically.

1.3 Problem 3

1.3.1 (a)

[5]:
```
import numpy as np
from numpy.linalg import inv

np.random.seed(42)

n = 70
p = 30

X = np.random.randn(n, p)
beta = np.random.randn(p)
y = X @ beta + np.random.randn(n)

# Compute OLS estimate: beta_hat
XtX = X.T @ X
XtX_inv = inv(XtX)
Xt_y = X.T @ y
beta_hat = XtX_inv @ Xt_y

# Compute y_hat
y_hat = X @ beta_hat
```

```
# Compute the hat matrix H
H = X @ XtX_inv @ X.T

# df = trace(H)
df = np.trace(H)

print(f"Degrees of freedom (df) of OLS estimate: {df:.2f}, expected p = {p}")
```

```
Degrees of freedom (df) of OLS estimate: 30.00, expected p = 30
```

1.3.2 (b)

Given m linear constraints of the form $A\beta = 0$, where $A \in \mathbb{R}^{m\times p}$. The constrained minimization can be solved using Lagrange multipliers.

Forming the Lagrangian:

$$\mathcal{L}(\beta, \lambda) = \|y - X\beta\|_2^2 + 2\lambda^\top A\beta$$

and the derivative with respect to β is:

$$\frac{\partial \mathcal{L}}{\partial \beta} = -2X^\top y + 2X^\top X\beta + 2A^\top\lambda = 0$$

By reordering the equation, we have:

$$X^\top X\beta + A^\top\lambda = X^\top y$$
$$\beta = (X^\top X)^{-1}(X^\top y - A^\top\lambda)$$

Since $A\beta = 0$, we have:

$$A(X^\top X)^{-1}(X^\top y - A^\top\lambda) = 0$$
$$\lambda = (A(X^\top X)^{-1}A^\top)^{-1}A(X^\top X)^{-1}X^\top y$$

Substitute λ back into the expression for β:

$$\beta = (X^\top X)^{-1}(X^\top y - A^\top(A(X^\top X)^{-1}A^\top)^{-1}A(X^\top X)^{-1}X^\top y) = [I - (X^\top X)^{-1}A^\top\left(A(X^\top X)^{-1}A^\top\right)^{-1}A](X^\top X)^{-1}X^\top y$$

Let $P = I - Q$ and $Q = (X^\top X)^{-1}A^\top\left(A(X^\top X)^{-1}A^\top\right)^{-1}A$, we have:

$$\beta = P(X^\top X)^{-1}X^\top y$$

Since Q has a rank of m, P has rank $p - m$.

The fitted values are $\hat{y}_c = X\beta = H_c y$, where $H_c = XP(X^\top X)^{-1}X^\top$ is the constrained hat matrix, which projects onto a subspace of dimension $p-m$. The effective degrees of freedom is trace$(H_c) = p - m$.

[6]:
```
import numpy as np
from numpy.linalg import inv

np.random.seed(42)

n = 70
p = 30
m = 10  # number of constraints

X = np.random.randn(n, p)
beta = np.random.randn(p)
y = X @ beta + np.random.randn(n)

# Generate a random constraint matrix A (m x p), full rank
A = np.random.randn(m, p)
while np.linalg.matrix_rank(A) < m:
    A = np.random.randn(m, p)

# Compute unconstrained OLS estimate: beta_hat
XtX = X.T @ X
XtX_inv = inv(XtX)
Xt_y = X.T @ y
beta_hat = XtX_inv @ Xt_y

# Compute Q and P matrices
Q = XtX_inv @ A.T @ inv(A @ XtX_inv @ A.T) @ A
P = np.eye(p) - Q
beta_hat_c = P @ beta_hat

print(f"Validate that A @ beta_hat_c is close to zero: {np.linalg.norm(A @␣
 ↪beta_hat_c):.2e}")

# Compute y_hat for constrained estimator
y_hat_c = X @ beta_hat_c

# Compute the constrained hat matrix H_c
H_c = X @ P @ XtX_inv @ X.T

# Degrees of freedom for constrained OLS
df_c = np.trace(H_c)

print(f"Degrees of freedom (df) of constrained OLS estimate: {df_c:.2f},␣
 ↪expected p - m = {p - m}")
```

```
Validate that A @ beta_hat_c is close to zero: 5.28e-15
Degrees of freedom (df) of constrained OLS estimate: 20.00, expected p - m = 20
```