TP - Least Squares

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1 TP Least squares

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1.1 Import libraries

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

1.2 Import data and helper functions

[ ]:
```
from data_center_helper import *
```

1.3 Preliminary data analysis

[ ]:
```
data = data.iloc[:, 1:]
data["TIME"] = pd.to_datetime(data["TIME"], format="mixed")
```

[ ]:
```
data.head()
```

[ ]:
```
                               TIME     VALUE BUILDING  \
0 2022-05-01 19:24:38.178000+00:00  348307.0    bat01
1 2022-05-02 16:04:38.148000+00:00  348497.0    bat01
2 2022-05-30 05:24:37.188000+00:00  353967.0    bat01
3 2022-05-03 06:32:38.127000+00:00      15.5    bat01
4 2022-05-04 11:28:38.085000+00:00       2.6    bat01

                   DETAILS                                       NAME  \
0  auxiliary_inverter_1_ge  bat01.r01.b.cfo.tgtbqb.dis124.cpt.ea.mes
1  auxiliary_inverter_1_ge  bat01.r01.b.cfo.tgtbqb.dis124.cpt.ea.mes
2  auxiliary_inverter_1_ge  bat01.r01.b.cfo.tgtbqb.dis124.cpt.ea.mes
3  auxiliary_inverter_1_ge  bat01.r01.b.cfo.tgtbqb.dis124.cpt.pa.mes
4  auxiliary_inverter_1_ge  bat01.r01.b.cfo.tgtbqb.dis124.cpt.pa.mes

                SUBCATEGORY          LIBELLE UNITE
0  active_energy_auxiliary_ge   Energie active   kWh
1  active_energy_auxiliary_ge   Energie active   kWh
```

```
2  active_energy_auxiliary_ge    Energie active   kWh
3   active_power_auxiliary_ge  Puissance active    kW
4   active_power_auxiliary_ge  Puissance active    kW
```

[ ]:
```
data.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 456700 entries, 0 to 456699
Data columns (total 8 columns):
 #   Column       Non-Null Count   Dtype
---  ------       --------------   -----
 0   TIME         456700 non-null  datetime64[ns, UTC]
 1   VALUE        456700 non-null  float64
 2   BUILDING     456700 non-null  object
 3   DETAILS      456700 non-null  object
 4   NAME         456700 non-null  object
 5   SUBCATEGORY  456700 non-null  object
 6   LIBELLE      456700 non-null  object
 7   UNITE        430055 non-null  object
dtypes: datetime64[ns, UTC](1), float64(1), object(6)
memory usage: 27.9+ MB
```

[ ]:
```
data.describe(include='all')
```

[ ]:
```
                                       TIME         VALUE BUILDING  \
count                                456700  4.567000e+05   456700
unique                                  NaN           NaN        1
top                                     NaN           NaN    bat01
freq                                    NaN           NaN   456700
mean    2022-05-16 19:26:29.192930048+00:00  1.066365e+04      NaN
min        2022-04-30 22:44:38.208000+00:00 -3.270629e+03      NaN
25%     2022-05-07 05:36:37.988999936+00:00  2.195044e+01      NaN
50%     2022-05-17 15:40:37.625999872+00:00  5.029004e+01      NaN
75%     2022-05-25 15:52:37.347000064+00:00  1.505638e+03      NaN
max               2022-05-31 21:59:59+00:00  1.133439e+06      NaN
std                                     NaN  6.062515e+04      NaN

           DETAILS                               NAME  \
count       456700                             456700
unique         125                               1794
top     rt_16_b1_3  bat01.r01.b.cvc.rt_10b15.gf.fct.mes
freq         32240                               1087
mean           NaN                                NaN
min            NaN                                NaN
25%            NaN                                NaN
50%            NaN                                NaN
75%            NaN                                NaN
max            NaN                                NaN
```

```
std            NaN                                 NaN

                    SUBCATEGORY      LIBELLE   UNITE
count                    456700       456700  430055
unique                      455          126      13
top     temperature_it_room_b1  température       %
freq                       8312        19106  116749
mean                        NaN          NaN     NaN
min                         NaN          NaN     NaN
25%                         NaN          NaN     NaN
50%                         NaN          NaN     NaN
75%                         NaN          NaN     NaN
max                         NaN          NaN     NaN
std                         NaN          NaN     NaN
```

[ ]:
```
print(
    f"""
    Number of features:\t{len(names)},
    Train data shape:\t{data_matrix_train.shape},
    Test data shape:\t{data_matrix_test.shape},
    Train KPI shape:\t{COP_train.shape},
    Test KPI shape:\t{COP_test.shape}
    """
)
```

```
    Number of features: 892,
    Train data shape:   (722, 892),
    Test data shape:    (361, 892),
    Train KPI shape:    (722, 4),
    Test KPI shape:     (361, 4)
```

[ ]:
```
print(f"""
A's (x, 1, -y*x) train shape: {A.shape},
b's (KPI number 3) traint shape: {b.shape}
A's (x, 1, -y*x) test shape: {A_test.shape},
b's (KPI number 3) test shape: {b_test.shape}
""")
```

```
A's (x, 1, -y*x) train shape: (722, 1785),
b's (KPI number 3) traint shape: (722,)
A's (x, 1, -y*x) test shape: (361, 1785),
b's (KPI number 3) test shape: (361,)
```

1.4 3. Least squares

1.4.1 Question 3.1.

By focusing on the key performance indicator (KPI) number 3, and simplifying $(w_{i=3,0}, w_{i=3,1}, w_{i=3,2})$ as (w_0, w_1, w_2), we consider the model:

$$y(t) = \frac{w_1^T \tilde{x}(t) + w_0 + \epsilon(t)}{w_2^T \tilde{x}(t) + 1}$$

Where we aim to solve the least square problem:

$$\min_w \frac{1}{2} \|Aw - b\|^2$$

,

where:

$$\begin{aligned}(Aw)_t &= \tilde{x}(t)^T w_1 + w_0 - y(t) \times \tilde{x}(t)^T w_2 \\ b_t &= y(t)\end{aligned}$$

In this context, $\hat{w} = (A^T A)^{-1} A^T b$.

If $Aw = b$:

$$\begin{aligned}\tilde{x}(t)^T w_1 + w_0 - y(t) \times \tilde{x}(t)^T w_2 &= y(t) \\ \tilde{x}(t)^T w_1 + w_0 &= y(t) \times \tilde{x}(t)^T w_2 + y(t) \\ \frac{\tilde{x}(t)^T w_1 + w_0}{\tilde{x}(t)^T w_2 + 1} &= y(t) \\ \Rightarrow y(t) &= \frac{w_1^T \tilde{x}(t) + w_0}{w_2^T \tilde{x}(t) + 1}\end{aligned}$$

Thus, $Aw = b \iff y(t) = \frac{w_1^T \tilde{x}(t) + w_0}{w_2^T \tilde{x}(t) + 1}$

1.4.2 Question 3.2.

[ ]:
```
w_lstsq = np.linalg.lstsq(A, b, rcond=None)[0]
```

1.4.3 Question 3.3.

To evaluate the found solution on the test sample, we can proceed by calculating $\frac{1}{2}||Aw - b||^2$, on the training sample and on the test sample:

[ ]:
```
print(f"""
Training sample: {(1/2)*np.linalg.norm(b - A @ w_lstsq)**2},
Test sample: {(1/2)*np.linalg.norm(b_test - A_test @ w_lstsq)**2}
```

```
""")
```

```
Training sample: 4.237266019148281e-25,
Test sample: 140952.175523103
```

Despite the promising outcome observed on the training sample, with the minimized function yielding a value close to 0, the determined weights exhibit subpar performance on the test sample. This discrepancy is apparent in the considerably large value produced by the minimized function, serving as a clear indicator of an overfitted model.

1.4.4 Question 3.4.

```
[ ]: lambd = 100
```

```
[ ]: w_l2_regularization = np.linalg.lstsq(
         A.T @ A + lambd * np.identity(A.shape[1]), A.T @ b, rcond=None
     )[0]
```

To evaluate the found solution on the test sample, we can proceed by calculating $\frac{1}{2}\|Aw-b\|^2+\frac{\lambda}{2}\|w\|^2$, on the training sample and on the test sample:

```
[ ]: print(f"""
     Training sample: {(1/2)*np.linalg.norm(b - A @ w_l2_regularization)**2 + (lambd/
      ↪2)*np.linalg.norm(w_l2_regularization)**2},
     Test sample: {(1/2)*np.linalg.norm(b_test - A_test @ w_l2_regularization)**2 +␣
      ↪(lambd/2)*np.linalg.norm(w_l2_regularization)**2}
     """)
```

```
Training sample: 301.51532425463233,
Test sample: 54565.04853323527
```

Once again, despite the promising outcome observed on the training sample, the determined weights demonstrate subpar performance on the test sample. This discrepancy is evident in the considerably large value produced by the minimized function, serving as a clear indicator of an overfitted model. It is important to note, however, that this ℓ_2 regularized model is significantly less overfitted than the previous Least Squares model, as its performance on the test sample is not as abysmal. As evidence of this, in the next cell, we compute $\|Aw-b\|$ for both models:

```
[ ]: print(f"""
     Train sample:
     LSTSQ: {np.linalg.norm(b - A @ w_lstsq)},
     L2 regularization: {np.linalg.norm(b - A @ w_l2_regularization)}

     Test sample
     LSTSQ: {np.linalg.norm(b_test - A_test @ w_lstsq)},
```

```
L2 regularization: {np.linalg.norm(b_test - A_test @ w_l2_regularization)}
""")
```

```
Train sample:
LSTSQ: 9.205722154343223e-13,
L2 regularization: 12.398650226890355

Test sample
LSTSQ: 530.9466555560982,
L2 regularization: 329.66770079188836
```

1.4.5 Question 3.5.

The gradient of the function $f_1 : w \mapsto \frac{1}{2}\|Aw - b\|^2 + \frac{\lambda}{2}\|w\|^2$ is obtained by computing the partial derivatives with respect to $ w $:

$$\begin{aligned}
\nabla f_1(w) &= \frac{\partial}{\partial w}(\frac{1}{2}\|Aw - b\|^2) + \frac{\partial}{\partial w}(\frac{\lambda}{2}\|w\|^2) \\
&= \frac{1}{2}\frac{\partial}{\partial w}\|Aw - b\|^2 + \frac{\lambda}{2}\frac{\partial}{\partial w}\|w\|^2 \\
&= \frac{1}{2}\frac{\partial}{\partial w}((Aw - b)^T \cdot (Aw - b)) + \frac{\lambda}{2}\frac{\partial}{\partial w}(w^T w)
\end{aligned}$$

Focusing on the term $\frac{\partial}{\partial w}((Aw - b)^T \cdot (Aw - b))$:

$$\begin{aligned}
\frac{\partial}{\partial w}((Aw - b)^T \cdot (Aw - b)) &= \frac{\partial}{\partial w}(w^T A^T Aw - w^T A^T b - b^T Aw + b^T b) \\
&= A^T Aw + w^T A^T A - A^T b - A^T b + 0 \\
&= 2A^T(Aw - b)
\end{aligned}$$

Substituting this result back in the original expression, we get:

$$\begin{aligned}
\nabla f_1(w) &= \frac{1}{2} \cdot 2A^T(Aw - b) + \frac{\lambda}{2} \cdot 2Iw \\
&= A^T(Aw - b) + \lambda Iw \\
\Rightarrow \nabla f_1(w) &= (A^T A + \lambda I)w - A^T b
\end{aligned}$$

The Hessian matrix of $ f_1(w) $ is given by $ H = A^T A + I $, where $ I $ is the identity matrix. To verify the convexity of $ f_1(w) $, we examine the terms involved:

1. $ A^T A $ is positive semi-definite since $ A^T A = |A|^2 0 $ for any matrix $ A $. The L_2 norm of a matrix A, denoted as $\|A\|_2$, is equal to zero if and only if every element a_{ij} of the matrix A is zero, expressed as $\|A\|^2 = 0 \iff a_{ij} = 0$ for all i and j. As A is specified not to be the zero matrix, it implies that there exist non-zero entries in A. Consequently, the product $A^T A$ is positive definite.
2. $ I $, where $ > 0 $, is positive definite as it scales the identity matrix.

The sum of positive definite matrices is positive definite. Therefore, $ H = A^T A + I $ is positive definite, and by the second-order condition for convexity, $ f_1(w) $ is convex.

1.4.6 Question 3.6.

[ ]:
```
def gradient_descent(
    max_iterations,
    step_size,
    w_init,
    obj_func,
    grad_func,
    threshold=1,
    verbose=False,
):
    w = w_init
    w_history = w
    f_history = obj_func(w)

    for iteration in range(max_iterations):
        w -= step_size * grad_func(w)

        if iteration % 10000 == 0 and verbose:
            w_history = np.vstack((w_history, w))
            f_history = np.vstack((f_history, obj_func(w)))
            print(f"Step: {iteration}, Norm of grad: {np.linalg.
↪norm(grad_func(w))}")

        if np.linalg.norm(grad_func(w)) <= threshold and verbose:
            print(f"Number of iterations: {iteration}")
            print(f"Norm of grad: {np.linalg.norm(grad_func(w))}")
            break

    if verbose:
        return w, w_history, f_history

    return w
```

By utilizing Proposition 1.4.1 from the course's handout, we can apply its insights to calculate the value of L, consequently establishing an upper limit for the step size, denoted as $\frac{2}{L}$.

Referring to information from Question 3.5, where $H = A^T A + \lambda I \Rightarrow \|H\| = \|A^T A\| + \lambda = L$, we recognize that if we choose $\gamma < \frac{2}{L}$, the gradient descent algorithm will converge to x^* such that

$\|\nabla f_1(x^*)\| = 0$.

[ ]:
```
L = np.linalg.norm(A.T @ A) + lambd

2/L
```

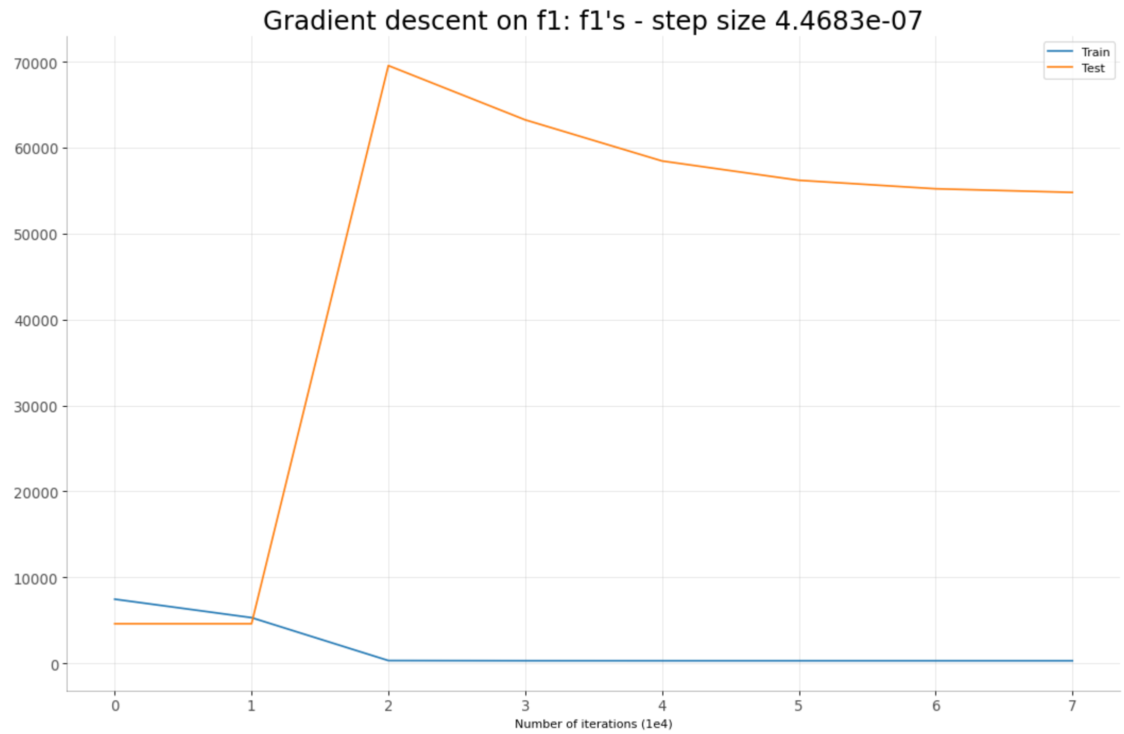
[ ]: 4.7034672060866193e-07

[ ]:
```
f1 = (
    lambda w, A, b, lambd: (1 / 2) * np.linalg.norm(A @ w - b) ** 2
    + (lambd / 2) * np.linalg.norm(w) ** 2
)

t1 = A.T @ A + lambd * np.identity(A.shape[1])
t2 = A.T @ b
f1_gradient_train = lambda w: t1 @ w - t2

step_size = 1.9/L

w_gradient_descent, w_gradient_descent_history, f_history_train = 
 ↪gradient_descent(
    max_iterations=100000,
    step_size=step_size,
    w_init=np.zeros(A.shape[1]),
    obj_func=lambda w: f1(w, A, b, lambd),
    grad_func=f1_gradient_train,
    verbose=True,
)
```

```
Step: 0, Norm of grad: 62015.478885047545
Step: 10000, Norm of grad: 111.41470490888052
Step: 20000, Norm of grad: 31.804547649277545
Step: 30000, Norm of grad: 11.861728117279583
Step: 40000, Norm of grad: 5.0911285958091455
Step: 50000, Norm of grad: 2.384909948503544
Step: 60000, Norm of grad: 1.1835979888228894
Number of iterations: 62503
Norm of grad: 0.9999737158935562
```

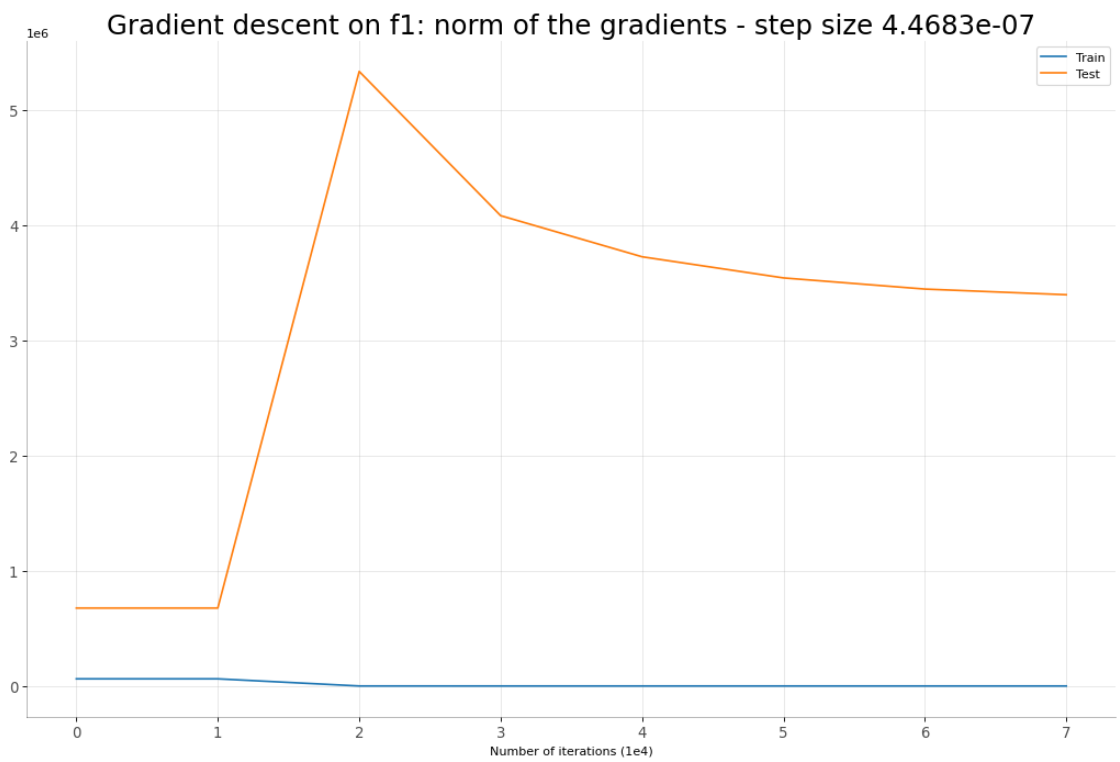
[ ]:
```
f_history_test = [f1(w, A_test, b_test, lambd) for w in 
 ↪w_gradient_descent_history]

plt.figure(figsize=(16, 10), dpi=80)

plt.plot(range(len(f_history_train)), f_history_train, label="Train")
plt.plot(range(len(f_history_test)), f_history_test, label="Test")

plt.xticks(rotation=0, fontsize=12, horizontalalignment="center", alpha=0.7)
```

```
plt.yticks(fontsize=12, alpha=0.7)
plt.title(f"Gradient descent on f1: f1's - step size {step_size:.5g}",␣
↪fontsize=22)
plt.xlabel("Number of iterations (1e4)")
plt.grid(axis="both", alpha=0.3)
plt.legend()

plt.gca().spines["top"].set_alpha(0.0)
plt.gca().spines["bottom"].set_alpha(0.3)
plt.gca().spines["right"].set_alpha(0.0)
plt.gca().spines["left"].set_alpha(0.3)
plt.show()
```



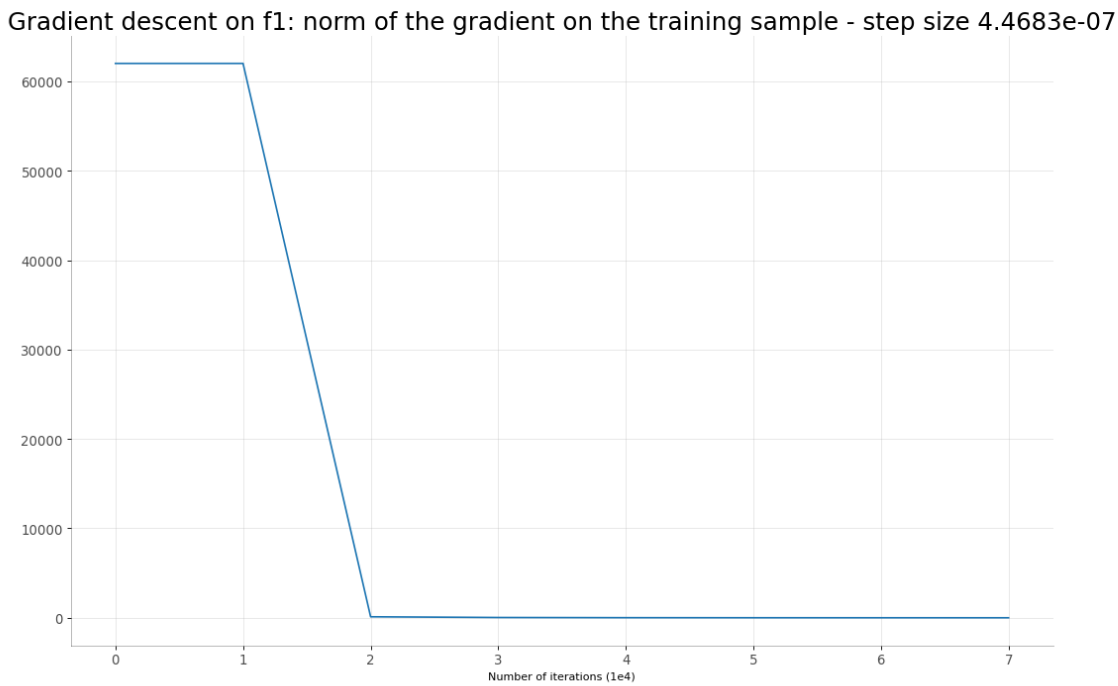
[ ]:
```
t1_test = A_test.T @ A_test + lambd * np.identity(A_test.shape[1])
t2_test = A_test.T @ b_test
f1_gradient_test = lambda w: t1_test @ w - t2_test

gradient_history_train = np.vstack(
    [np.linalg.norm(f1_gradient_train(w)) for w in w_gradient_descent_history]
)
gradient_history_test = np.vstack(
    [np.linalg.norm(f1_gradient_test(w)) for w in w_gradient_descent_history]
)
```

[ ]:
```
plt.figure(figsize=(16, 10), dpi=80)

plt.plot(range(len(gradient_history_train)), gradient_history_train,␣
 ↪label="Train")
plt.plot(range(len(gradient_history_test)), gradient_history_test, label="Test")

plt.xticks(rotation=0, fontsize=12, horizontalalignment="center", alpha=0.7)
plt.yticks(fontsize=12, alpha=0.7)
plt.title(f"Gradient descent on f1: norm of the gradients - step size␣
 ↪{step_size:.5g}", fontsize=22)
plt.xlabel("Number of iterations (1e4)")
plt.grid(axis="both", alpha=0.3)
plt.legend()

plt.gca().spines["top"].set_alpha(0.0)
plt.gca().spines["bottom"].set_alpha(0.3)
plt.gca().spines["right"].set_alpha(0.0)
plt.gca().spines["left"].set_alpha(0.3)
plt.show()
```



[ ]:
```
plt.figure(figsize=(16, 10), dpi=80)
```

```python
plt.plot(range(len(gradient_history_train)), gradient_history_train,␣
 ↪label="Train")

plt.xticks(rotation=0, fontsize=12, horizontalalignment="center", alpha=0.7)
plt.yticks(fontsize=12, alpha=0.7)
plt.title(f"Gradient descent on f1: norm of the gradient on the training sample␣
 ↪- step size {step_size:.5g}", fontsize=22)
plt.xlabel("Number of iterations (1e4)")
plt.grid(axis="both", alpha=0.3)

plt.gca().spines["top"].set_alpha(0.0)
plt.gca().spines["bottom"].set_alpha(0.3)
plt.gca().spines["right"].set_alpha(0.0)
plt.gca().spines["left"].set_alpha(0.3)
plt.show()
```



From the graphs above, we can observe that the gradient descent algorithm is a method of slow convergence.

[ ]:
```python
print(f"""
Training sample: {f1(w_gradient_descent, A, b, lambd)},
Test sample: {f1(w_gradient_descent, A_test, b_test, lambd)}
""")
```

```
Training sample: 301.5187865344042,
```

```
Test sample: 54737.17259875137
```

[ ]:
```python
print(f"""
Train sample:
LSTSQ: {np.linalg.norm(b - A @ w_lstsq)},
L2 regularization: {np.linalg.norm(b - A @ w_l2_regularization)}
Gradient Descent: {np.linalg.norm(b - A @ w_gradient_descent)}

Test sample
LSTSQ: {np.linalg.norm(b_test - A_test @ w_lstsq)},
L2 regularization: {np.linalg.norm(b_test - A_test @ w_l2_regularization)}
Gradient Descent: {np.linalg.norm(b_test - A_test @ w_gradient_descent)}
""")
```

```
Train sample:
LSTSQ: 9.205722154343223e-13,
L2 regularization: 12.398650226890355
Gradient Descent: 12.427240132697595

Test sample
LSTSQ: 530.9466555560982,
L2 regularization: 329.66770079188836
Gradient Descent: 330.1904661278845
```

Nevertheless, in terms of results, we can see that the gradient descent algorithm has a similar performance as the ℓ_2 regularized model. In terms of computational complexity and time ressources, the gradient descent algorithm is subpar if compared to the other models.

1.5 4. Regularization for a sparse model

1.5.1 Question 4.1.

The proximal operator of a convex lower-semicontinuous function g_2 is defined as: $\text{prox}_{g_2}(v) = \arg\min_w \left(g(w) + \frac{1}{2}\|w - v\|^2\right)$. Additionally, the proximal operator of the 1-norm is the element-wise soft-thresholding operator: $S_\lambda(x) = \text{sign}(x) \cdot \max(|x| - \lambda, 0)$.

The objective function is given by: $F_2(w) = \frac{1}{2}\|Aw - b\|_2^2 + \lambda\|w\|_1$. From there, we can identify f_2 and g_2: - $f_2(w) = \frac{1}{2}\|Aw - b\|^2$; - $g_2(w) = \lambda\|w\|_1$. Thus: $\text{prox}_{g_2}(v)_i = \text{sign}(v_i) \cdot \max(|v_i| - \lambda, 0)$.

Now, let's calculate the gradient of f_2:

$$
\begin{aligned}
\nabla f_2(w) &= \frac{\partial}{\partial w}(\frac{1}{2}\|Aw-b\|^2) \\
&= \frac{1}{2}\frac{\partial}{\partial w}\|Aw-b\|^2 \\
&= \frac{1}{2}\frac{\partial}{\partial w}((Aw-b)^T\cdot(Aw-b)) \\
&= \frac{1}{2}\cdot 2A^T(Aw-b) \\
\Rightarrow \nabla f_2(w) &= A^T(Aw-b)
\end{aligned}
$$

1.5.2 Question 4.2.

[ ]:
```
def soft_thresholding(x, threshold):
    return np.sign(x) * np.maximum(np.abs(x) - threshold, 0)

def proximal_gradient_descent(
    max_iterations,
    step_size,
    w_init,
    lambd,
    obj_func,
    grad_func,
    threshold=1,
    verbose=False,
):
    w = w_init
    w_history = w
    f_history = obj_func(w)

    for iteration in range(max_iterations):
        w = soft_thresholding(w - step_size * grad_func(w), lambd*step_size)

        if iteration % 10000 == 0 and verbose:
            w_history = np.vstack((w_history, w))
            f_history = np.vstack((f_history, obj_func(w)))
            print(f"Step: {iteration}, Norm of grad: {np.linalg.
 ↪norm(grad_func(w))}")

        if np.linalg.norm(grad_func(w)) <= threshold and verbose:
            print(f"Number of iterations: {iteration}")
            print(f"Norm of grad: {np.linalg.norm(grad_func(w))}")
            break

    if verbose:
        return w, w_history, f_history
```

```
    return w
```

[ ]:
```
L = np.linalg.norm(A.T @ A)

2/L
```

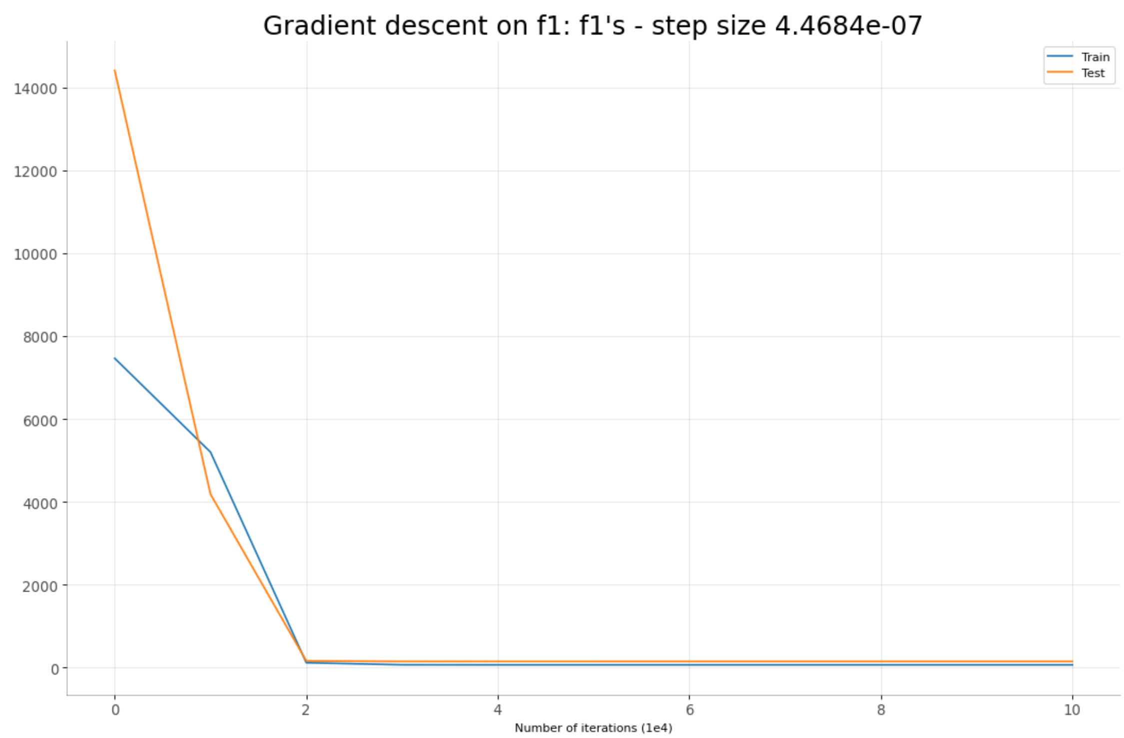
[ ]: 4.7035778217067977e-07

[ ]:
```
f2 = lambda w, A, b: (1 / 2) * np.linalg.norm(A @ w - b) ** 2

t1 = A.T @ A
t2 = A.T @ b
f2_gradient_train = lambda w: t1 @ w - t2

step_size = 1.9/L

w_proximal_gradient_descent, w_proximal_gradient_descent_history,␣
 ↪f_history_train = proximal_gradient_descent(
    max_iterations=100000,
    step_size=step_size,
    lambd=200,
    w_init=np.zeros(A.shape[1]),
    obj_func=lambda w: f2(w, A, b),
    grad_func=f2_gradient_train,
    verbose=True
)
```

```
Step: 0, Norm of grad: 55331.84301502639
Step: 10000, Norm of grad: 2701.562236512747
Step: 20000, Norm of grad: 2529.0167347005845
Step: 30000, Norm of grad: 2521.379567226735
Step: 40000, Norm of grad: 2521.0137470842424
Step: 50000, Norm of grad: 2520.9946775190647
Step: 60000, Norm of grad: 2520.9936819598274
Step: 70000, Norm of grad: 2520.993629982604
Step: 80000, Norm of grad: 2520.993627268924
Step: 90000, Norm of grad: 2520.993627127221
```

[ ]:
```
f_history_test = np.vstack(
    [f2(w, A_test, b_test) for w in w_proximal_gradient_descent_history]
)

plt.figure(figsize=(16, 10), dpi=80)

plt.plot(range(len(f_history_train)), f_history_train, label="Train")
plt.plot(range(len(f_history_test)), f_history_test, label="Test")

plt.xticks(rotation=0, fontsize=12, horizontalalignment="center", alpha=0.7)
```

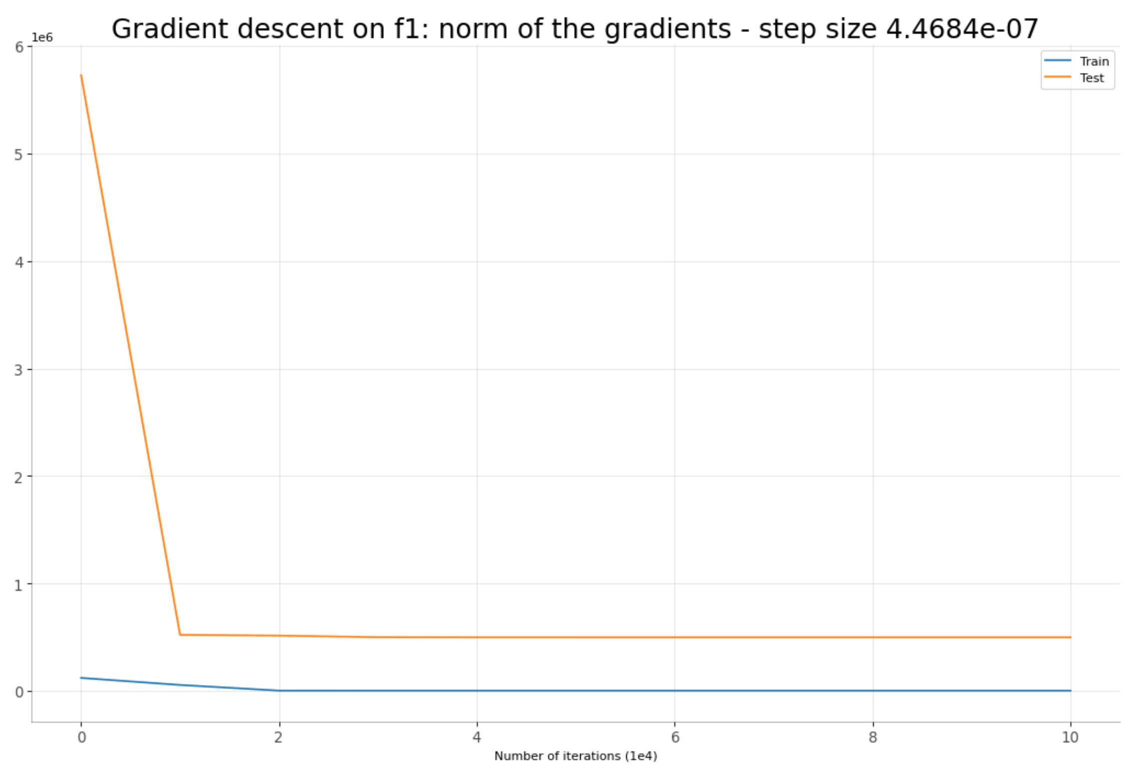
```
plt.yticks(fontsize=12, alpha=0.7)
plt.title(f"Gradient descent on f1: f1's - step size {step_size:.5g}",␣
↪fontsize=22)
plt.xlabel("Number of iterations (1e4)")
plt.grid(axis="both", alpha=0.3)
plt.legend()

plt.gca().spines["top"].set_alpha(0.0)
plt.gca().spines["bottom"].set_alpha(0.3)
plt.gca().spines["right"].set_alpha(0.0)
plt.gca().spines["left"].set_alpha(0.3)
plt.show()
```



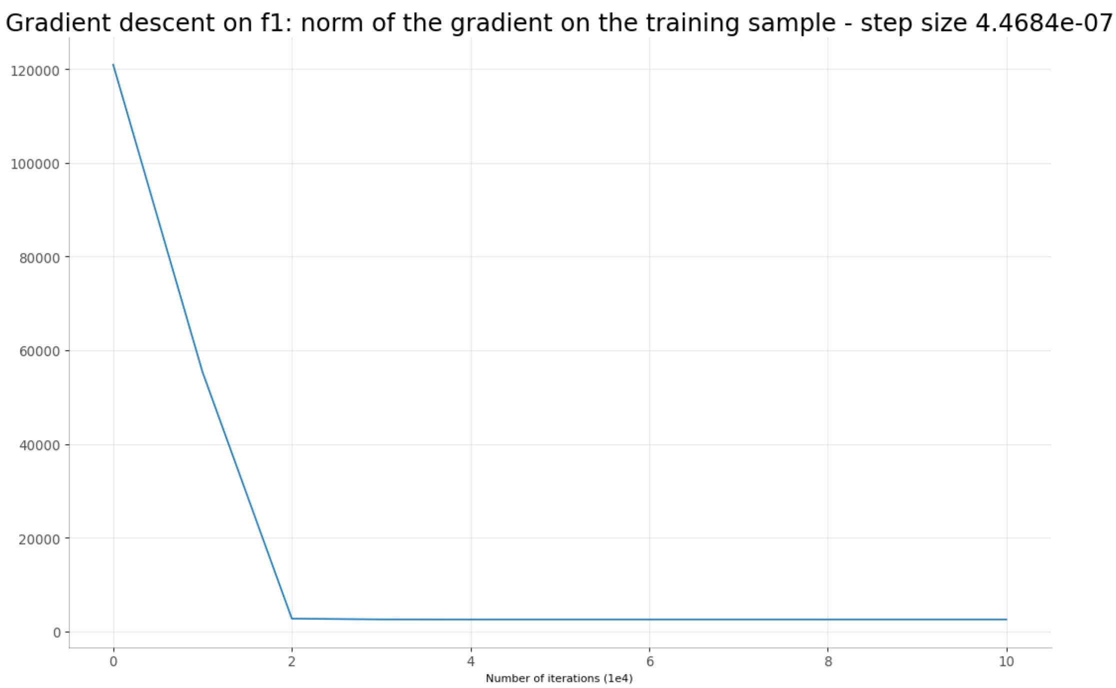
[ ]:
```
t1_test = A_test.T @ A_test
t2_test = A_test.T @ b_test
f2_gradient_test = lambda w: t1_test @ w - t2_test

gradient_history_train = np.vstack(
    [np.linalg.norm(f2_gradient_train(w)) for w in␣
↪w_proximal_gradient_descent_history]
)
gradient_history_test = np.vstack(
```

```
    [np.linalg.norm(f2_gradient_test(w)) for w in␣
 ↪w_proximal_gradient_descent_history]
)
```

[ ]:
```
plt.figure(figsize=(16, 10), dpi=80)

plt.plot(range(len(gradient_history_train)), gradient_history_train,␣
 ↪label="Train")
plt.plot(range(len(gradient_history_test)), gradient_history_test, label="Test")

plt.xticks(rotation=0, fontsize=12, horizontalalignment="center", alpha=0.7)
plt.yticks(fontsize=12, alpha=0.7)
plt.title(f"Gradient descent on f1: norm of the gradients - step size␣
 ↪{step_size:.5g}", fontsize=22)
plt.xlabel("Number of iterations (1e4)")
plt.grid(axis="both", alpha=0.3)
plt.legend()

plt.gca().spines["top"].set_alpha(0.0)
plt.gca().spines["bottom"].set_alpha(0.3)
plt.gca().spines["right"].set_alpha(0.0)
plt.gca().spines["left"].set_alpha(0.3)
plt.show()
```



[ ]:
```
plt.figure(figsize=(16, 10), dpi=80)

plt.plot(range(len(gradient_history_train)), gradient_history_train,␣
 ↪label="Train")

plt.xticks(rotation=0, fontsize=12, horizontalalignment="center", alpha=0.7)
plt.yticks(fontsize=12, alpha=0.7)
plt.title(f"Gradient descent on f1: norm of the gradient on the training sample␣
 ↪- step size {step_size:.5g}", fontsize=22)
plt.xlabel("Number of iterations (1e4)")
plt.grid(axis="both", alpha=0.3)

plt.gca().spines["top"].set_alpha(0.0)
plt.gca().spines["bottom"].set_alpha(0.3)
plt.gca().spines["right"].set_alpha(0.0)
plt.gca().spines["left"].set_alpha(0.3)
plt.show()
```



[ ]:
```
print(f"""
Training sample: {np.linalg.
 ↪norm(f2_gradient_train(w_proximal_gradient_descent))},
Test sample: {np.linalg.norm(f2_gradient_test(w_proximal_gradient_descent))}
""")
```

```
Training sample: 2520.99362711994,
Test sample: 498277.4725469157
```

```
[ ]: print(f"""
     Training sample: {f2(w_proximal_gradient_descent, A, b)},
     Test sample: {f2(w_proximal_gradient_descent, A_test, b_test)}
     """)
```

```
Training sample: 68.77295241761897,
Test sample: 151.68325403149103
```

```
[ ]: print(f"""
     Train sample:
     LSTSQ: {np.linalg.norm(b - A @ w_lstsq)},
     L2 regularization: {np.linalg.norm(b - A @ w_l2_regularization)}
     Gradient Descent: {np.linalg.norm(b - A @ w_gradient_descent)}
     Proximal gradient Descent: {np.linalg.norm(b - A @ w_proximal_gradient_descent)}

     Test sample
     LSTSQ: {np.linalg.norm(b_test - A_test @ w_lstsq)},
     L2 regularization: {np.linalg.norm(b_test - A_test @ w_l2_regularization)}
     Gradient Descent: {np.linalg.norm(b_test - A_test @ w_gradient_descent)}
     Proximal gradient Descent: {np.linalg.norm(b_test - A_test @
       ↪w_proximal_gradient_descent)}
     """)
```

```
Train sample:
LSTSQ: 9.205722154343223e-13,
L2 regularization: 12.398650226890355
Gradient Descent: 12.427240132697595
Proximal gradient Descent: 11.727996624967025

Test sample
LSTSQ: 530.9466555560982,
L2 regularization: 329.66770079188836
Gradient Descent: 330.1904661278845
Proximal gradient Descent: 17.417419672930375
```

The proximal gradient descent algorithm, differently than the gradient descent algorithm, is able to minimize the functions both on the training and test samples, it converges much more quickly, despite being similar in computational complexity and time ressources employed. Nevertheless, it is important to take notice that the proximal gradient descent was not able to minimize the norm of the gradient to a magnitude less than 1, even in $1 \cdot 10^5$ iterations. Furthermore, it is remarkable how the proximal gradient descent seems to be more robust to overfitting.

1.5.3 Question 4.3.

```
[ ]: def line_search(a, b, w, obj_func, grad_func):
    step_size = b
    wp = w - step_size * grad_func(w)
    delta_w = wp - w

    while (
        obj_func(wp)
        > obj_func(w)
        + grad_func(w) @ delta_w
        + 1 / (2 * step_size) * np.linalg.norm(wp - w) ** 2
    ):
        step_size *= a
        wp = w - step_size * grad_func(w)
        delta_w = wp - w

    return step_size


def proximal_gradient_descent_line_search(
    max_iterations,
    a,
    b,
    w_init,
    lambd,
    obj_func,
    grad_func,
    threshold=1,
    verbose=False,
):
    w = w_init
    w_history = w
    f_history = obj_func(w)

    for iteration in range(max_iterations):
        step_size = line_search(a, b, w, obj_func, grad_func)
        w = soft_thresholding(w - step_size * grad_func(w), lambd * step_size)

        if iteration % 10000 == 0 and verbose:
            w_history = np.vstack((w_history, w))
            f_history = np.vstack((f_history, obj_func(w)))
            print(f"Step: {iteration}, Norm of grad: {np.linalg.
↪norm(grad_func(w))}")

        if np.linalg.norm(grad_func(w)) <= threshold and verbose:
            print(f"Number of iterations: {iteration}")
```

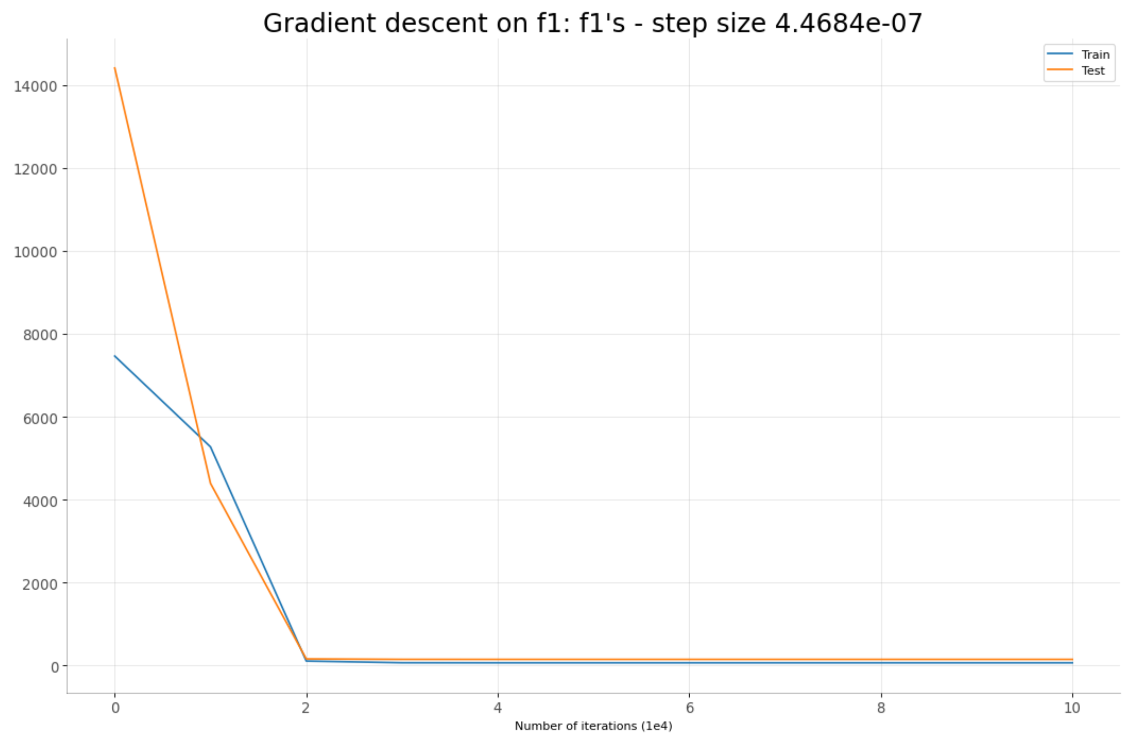
```
            print(f"Norm of grad: {np.linalg.norm(grad_func(w))}")
            break

    if verbose:
        return w, w_history, f_history

    return w
```

[ ]:
```
(
    w_proximal_gradient_descent_line_search,
    w_proximal_gradient_descent_line_search_history,
    f_history_train,
) = proximal_gradient_descent_line_search(
    max_iterations=100000,
    a=0.5,
    b=2/L,
    lambd=200,
    w_init=np.zeros(A.shape[1]),
    obj_func=lambda w: f2(w, A, b),
    grad_func=f2_gradient_train,
    verbose=True,
)
```

```
Step: 0, Norm of grad: 45469.48298434487
Step: 10000, Norm of grad: 2673.438426248707
Step: 20000, Norm of grad: 2526.7012032004936
Step: 30000, Norm of grad: 2521.2356282697565
Step: 40000, Norm of grad: 2521.004434231764
Step: 50000, Norm of grad: 2520.994110120992
Step: 60000, Norm of grad: 2520.9936487061404
Step: 70000, Norm of grad: 2520.9936280836805
Step: 80000, Norm of grad: 2520.9936271618726
Step: 90000, Norm of grad: 2520.99362712089
```

[ ]:
```
f_history_test = np.vstack(
    [f2(w, A_test, b_test) for w in␣
 ↪w_proximal_gradient_descent_line_search_history]
)

plt.figure(figsize=(16, 10), dpi=80)

plt.plot(range(len(f_history_train)), f_history_train, label="Train")
plt.plot(range(len(f_history_test)), f_history_test, label="Test")

plt.xticks(rotation=0, fontsize=12, horizontalalignment="center", alpha=0.7)
plt.yticks(fontsize=12, alpha=0.7)
```

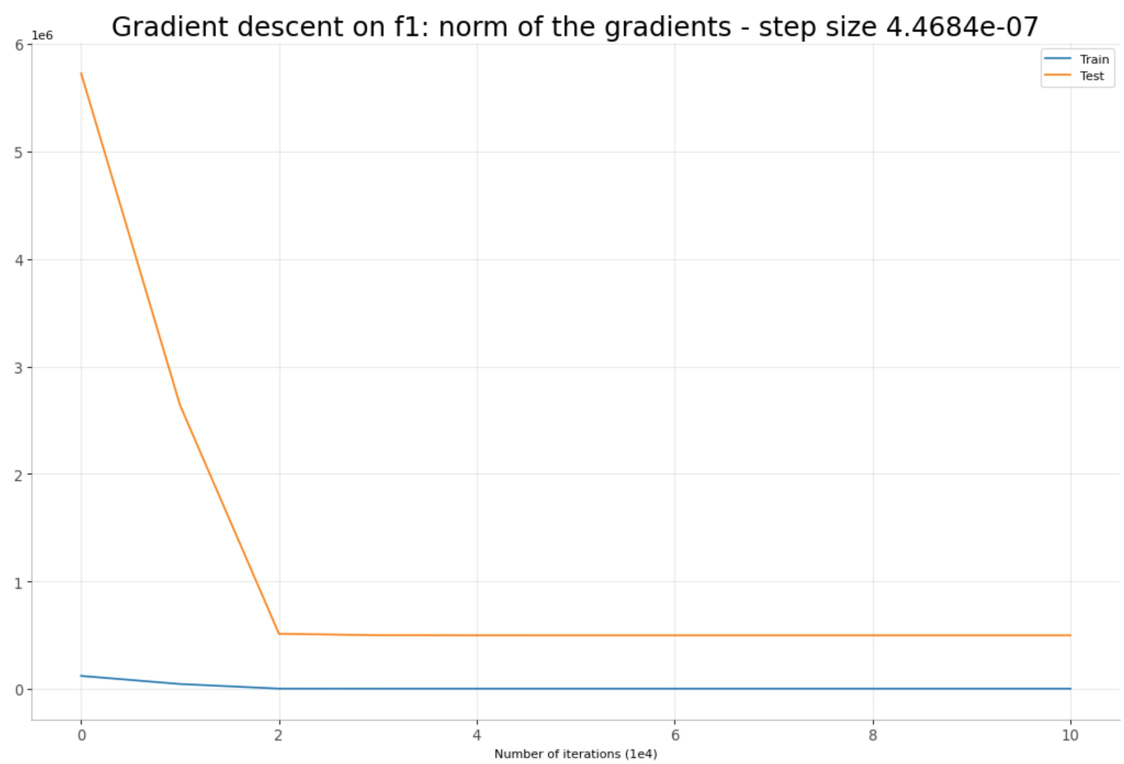
```
plt.title(f"Gradient descent on f1: f1's - step size {step_size:.5g}",␣
↪fontsize=22)
plt.xlabel("Number of iterations (1e4)")
plt.grid(axis="both", alpha=0.3)
plt.legend()

plt.gca().spines["top"].set_alpha(0.0)
plt.gca().spines["bottom"].set_alpha(0.3)
plt.gca().spines["right"].set_alpha(0.0)
plt.gca().spines["left"].set_alpha(0.3)
plt.show()
```



[ ]:
```
gradient_history_train = np.vstack(
    [np.linalg.norm(f2_gradient_train(w)) for w in␣
↪w_proximal_gradient_descent_line_search_history]
)
gradient_history_test = np.vstack(
    [np.linalg.norm(f2_gradient_test(w)) for w in␣
↪w_proximal_gradient_descent_line_search_history]
)
```

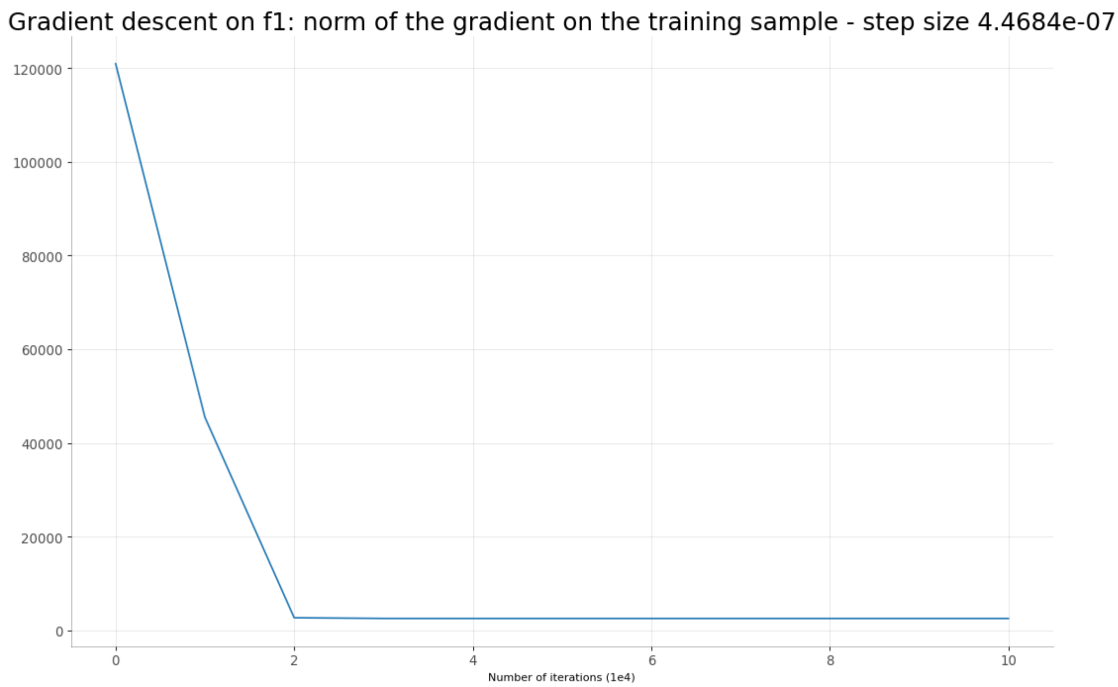
[ ]:
```
plt.figure(figsize=(16, 10), dpi=80)
```

```
plt.plot(range(len(gradient_history_train)), gradient_history_train,␣
 ↪label="Train")
plt.plot(range(len(gradient_history_test)), gradient_history_test, label="Test")

plt.xticks(rotation=0, fontsize=12, horizontalalignment="center", alpha=0.7)
plt.yticks(fontsize=12, alpha=0.7)
plt.title(f"Gradient descent on f1: norm of the gradients - step size␣
 ↪{step_size:.5g}", fontsize=22)
plt.xlabel("Number of iterations (1e4)")
plt.grid(axis="both", alpha=0.3)
plt.legend()

plt.gca().spines["top"].set_alpha(0.0)
plt.gca().spines["bottom"].set_alpha(0.3)
plt.gca().spines["right"].set_alpha(0.0)
plt.gca().spines["left"].set_alpha(0.3)
plt.show()
```



[ ]:
```
plt.figure(figsize=(16, 10), dpi=80)

plt.plot(range(len(gradient_history_train)), gradient_history_train,␣
 ↪label="Train")
```

```
plt.xticks(rotation=0, fontsize=12, horizontalalignment="center", alpha=0.7)
plt.yticks(fontsize=12, alpha=0.7)
plt.title(f"Gradient descent on f1: norm of the gradient on the training sample␣
 ↪- step size {step_size:.5g}", fontsize=22)
plt.xlabel("Number of iterations (1e4)")
plt.grid(axis="both", alpha=0.3)

plt.gca().spines["top"].set_alpha(0.0)
plt.gca().spines["bottom"].set_alpha(0.3)
plt.gca().spines["right"].set_alpha(0.0)
plt.gca().spines["left"].set_alpha(0.3)
plt.show()
```



[ ]:
```
print(f"""
Training sample: {np.linalg.
 ↪norm(f2_gradient_train(w_proximal_gradient_descent_line_search))},
Test sample: {np.linalg.
 ↪norm(f2_gradient_test(w_proximal_gradient_descent_line_search))}
""")
```

```
Training sample: 2520.9936271193674,
Test sample: 498277.47254682577
```

```
[ ]: print(f"""
Training sample: {f2(w_proximal_gradient_descent_line_search, A, b)},
Test sample: {f2(w_proximal_gradient_descent_line_search, A_test, b_test)}
""")
```

```
Training sample: 68.77295241745867,
Test sample: 151.68325403143805
```

```
[ ]: print(f"""
Train sample:
LSTSQ: {np.linalg.norm(b - A @ w_lstsq)},
L2 regularization: {np.linalg.norm(b - A @ w_l2_regularization)}
Gradient descent: {np.linalg.norm(b - A @ w_gradient_descent)}
Proximal gradient descent: {np.linalg.norm(b - A @ w_proximal_gradient_descent)}
Proximal gradient descent with line search: {np.linalg.norm(b - A @␣
↪w_proximal_gradient_descent_line_search)}

Test sample
LSTSQ: {np.linalg.norm(b_test - A_test @ w_lstsq)},
L2 regularization: {np.linalg.norm(b_test - A_test @ w_l2_regularization)}
Gradient descent: {np.linalg.norm(b_test - A_test @ w_gradient_descent)}
Proximal gradient descent: {np.linalg.norm(b_test - A_test @␣
↪w_proximal_gradient_descent)}
Proximal gradient descent with line search: {np.linalg.norm(b_test - A_test @␣
↪w_proximal_gradient_descent_line_search)}
""")
```

```
Train sample:
LSTSQ: 9.205722154343223e-13,
L2 regularization: 12.398650226890355
Gradient descent: 12.427240132697595
Proximal gradient descent: 11.727996624967025
Proximal gradient descent with line search: 11.727996624953358

Test sample
LSTSQ: 530.9466555560982,
L2 regularization: 329.66770079188836
Gradient descent: 330.1904661278845
Proximal gradient descent: 17.417419672930375
Proximal gradient descent with line search: 17.417419672927334
```

The proximal gradient descent algorithm with line search achieves similar results as the proximal gradient descent algorithm, it is able to minimize the functions both on the training and test samples, it converges even more quickly, despite being similar in computational complexity and time ressources employed. Nevertheless, it is important to take notice that the proximal gradient descent was not able to minimize the norm of the gradient to a magnitude less than 1, even in $1 \cdot 10^5$ iterations.

1.6 6. Comparison

1.6.1 Question 6.1.

The comparison between the two types of regularization was done throughout this academic report in previous sections.