HW3

November 21, 2022

1 Homework 3

1.0.1 1.

We consider the LASSO problem :

$$\begin{aligned}
&\min_{w}\frac{1}{2}||Xw-y||_2^2+\lambda||w||_1\\
\iff &\min_{w,z}\frac{1}{2}||z||_2^2+\lambda||w||_1\\
&\text{s.t.} z = Xw-y
\end{aligned}$$

where we introduce the dummy variable z to compute the dual of the problem in a useful form.

Indeed, using this form of the problem, the Lagrangian is, with ν denoting the Lagrange multiplier :

$$\begin{aligned}
\mathscr{L}(w,z,\nu) &= \frac{1}{2}||z||_2^2+\lambda||w||_1+\nu^T\left(z-Xw+y\right)\\
&= \frac{1}{2}||z||_2^2+\nu^T z+\lambda\left(||w||_1-\frac{1}{\lambda}\left(X^T\nu\right)^T w\right)+\nu^T y
\end{aligned}$$

Minimizing $\mathscr{L}(z,w,\nu)$ over w is equivalent to :

$$\max_{w}\lambda\left(\frac{1}{\lambda}\left(X^T\nu\right)^T w-||w||_1\right)$$

where we recognize the conjugate norm $\lambda||\frac{1}{\lambda}X^T\nu||_1^*$, therefore :

$$\begin{aligned}
\min_{w}\mathscr{L}(w,z,\nu) &= -\infty \text{ if } ||\frac{1}{\lambda}X^T\nu||_\infty > 1\\
&= \frac{1}{2}||z||_2^2+\nu^T z+\nu^T y \text{ otherwise}\\
&= z^T\left(\frac{1}{2}z+\nu\right)+\nu^T y
\end{aligned}$$

We compute the gradient of $\mathscr{L}$ with respect to z to minimize it (i.e. compute the Lagrange dual function $g(\nu)$) :

$$\begin{aligned} \nabla\mathscr{L}(z) &= \frac{1}{2}z + \nu + \frac{1}{2}z \\ &= z + \nu \\ \implies \nabla\mathscr{L}(z) = 0 &\iff z = -\nu \end{aligned}$$

Therefore, we obtain :

$$g(\nu) = -\frac{1}{2}\nu^T\nu + \nu^T y$$

and the dual problem expressed as a quadratic program is :

$$\begin{aligned} \min_v \ & -g(v) = v^TQv + p^Tv \\ \text{s.t.} \ & Av \leq b \end{aligned}$$

where $v = \nu, Q = \frac{1}{2}I, p = -y$,

$$A = \begin{bmatrix} X^T \\ -X^T \end{bmatrix} \tag{1}$$

and $b = \lambda\mathbb{1}_{2d}$ (which is $||\frac{1}{\lambda}X^T\nu||_\infty \leq 1$ written in matrix form)

1.0.2 2.

Let us now implement the barrier method to solve this dual problem.

[1]:
```
import numpy as np
import matplotlib.pyplot as plt
from typing import Callable, Union, Tuple
import sys
```

[2]:
```
# Backtracking Line Search params
BLS_ALPHA = 0.1
BLS_BETA = 0.7

# Newton precision
NEWTON_EPSILON = 1e-8

LOGBARR_MU = 10.  # path update : t <- μ * t
LOGBARR_T0 = 1.  # first t value (start of path)
```

[3]:
```
def log_barrier(vals: np.ndarray) -> float:
    """
    Log barrier function. Expects NEGATIVE values as inputs.
    (This is the function "phi" from slide 7 of Lecture 5)

    :param vals: value of constraint functions
    :return: log barrier evaluation
    """
    if np.any(vals >= 0):
        raise ValueError('[log_barrier] Positive value encountered')

    return -np.sum(np.log(-vals))
```

[4]:
```
def check_objective_def(A: np.ndarray,
                        b: np.ndarray,
):
    """
    Create a function that checks if the objective is defined

    :param A: the inequality constraint matrix
    :param b: the inequality constraint vector
    :return: A function of x that returns True if Ax - b < 0
    """
    def _check(x):
        u = A @ x
        u = u - b
        return np.all(u < 0)

    return _check
```

[5]:
```
def bls(f: Callable,
        gradf_x: Union[np.ndarray, float],
        x: Union[np.ndarray, float],
        delta_x: Union[np.ndarray, float],
        alpha: float,
        beta: float,
        check_def: Callable,
        ) -> float:
    """
    Backtracking Line Search algorithm.
    The algorithm may not converge if we are very close to the optimum,
    therefore we break out of the loop if the step length becomes zero
    (the loop becomes infinite in this case)

    :param f: the objective function (real-valued)
    :param gradf_x: the gradient of f at x
    :param x: the current point from which to descent
    :param delta_x: the descent direction
    :param alpha: parameter in [0, 1/2]
    :param beta: shrinkage parameter in [0, 1)
    :param check_def: function that returns True on an input v if f(v) is␣
↪defined
    :return: the optimal (if reached) step length t
    """
    t = 1.

    while (
            not check_def(x + t * delta_x)
            or f(x + t * delta_x) >= f(x) + alpha * t * np.dot(gradf_x, delta_x)
    ):
        t = beta * t
        if t < sys.float_info.epsilon:
            break

    return t
```

Computation of the gradient and the Hessian The gradient and Hessian of $g_t(v) = t\left(v^TQv + p^Tv\right) - \sum_{k=1}^{2d} \log\left(b - Av\right)_k$ are :

$$\nabla g_t(v) = t(2Qv + p) - \sum_{k=1}^{2d} \frac{1}{(Av-b)_k} A_k^T$$

where A_k^T is the k-th column of A^T i.e. the k-th line of A, and

$$\nabla^2 g_t(v) = t2Q + \sum_{k=1}^{2d} \frac{1}{(Av-b)_k^2} M(k)$$

where

$$M(k)_{ij} = A_{ki}A_{kj}$$

i.e. $M(k)$ is the "tensor product" of the k-th line of A with itself :

$$M(k) = \begin{bmatrix} A_{k1} \\ \vdots \\ A_{kn} \end{bmatrix} \begin{bmatrix} A_{k1} \dots A_{kn} \end{bmatrix} \tag{2}$$

Using the element-wise multiplication rule of NumPy arrays, these weighted sums are written in short expressions in the code below.

[6]:
```python
def centering_step(
        Q: np.ndarray,
        p: np.ndarray,
        A: np.ndarray,
        b: np.ndarray,
        t: float,
        v0: np.ndarray,
        eps: float
) -> np.ndarray:
    """
    Perform the centering step of the log-barrier algorithm.
    Compute the steepest descent in local Hessian norm (Newton algorithm)
    and choose a step length using backtracking line search

    :param Q: Hessian of the original objective
    :param p: linear coefficients of the original objective
    :param A:
    :param b:
    :param t:
    :param v0:
    :param eps:
    :return:
    """

    objective_f = lambda v: t * (v.T @ Q @ v + p @ v) + log_barrier(A @ v - b)
    def_checker = check_objective_def(A, b)
    v = v0
    v_history = [v]
    previous_decrement = None # debug purposes (check decreasing decrement)

    while True:
        # Compute gradient and Hessian of the objective
        u = A @ v - b
        grad = t * (2 * Q @ v + p) - np.sum(1 / u * A.T, axis=1)  # sum( 1/
 ↪(Av-b)[k]*(k-th line of A) )

        barrier_hess = (1 / u**2 * A.T) @ A
        hess = t * 2 * Q + barrier_hess

        delta_v = np.linalg.solve(hess, -grad)  # Newton descent direction
        newton_decrement_sq = np.dot(grad, -delta_v)

        # Sanity check
        if previous_decrement is None:
            previous_decrement = newton_decrement_sq
        if newton_decrement_sq - previous_decrement > 0.:
            print('[WARNING][centering_step] Newton decrement increasing')
        # Stop
        if 0.5 * newton_decrement_sq <= eps:
            return np.array(v_history, dtype=float)

        # Descend
        step_l = bls(
            f=objective_f,
            gradf_x=grad,
            x=v,
            delta_x=delta_v,
            alpha=BLS_ALPHA,
            beta=BLS_BETA,
            check_def=def_checker,
        )
        reached_zero = step_l < sys.float_info.epsilon
        if reached_zero:
            return np.array(v_history, dtype=float)

        v = v + step_l * delta_v
        v_history.append(v)
```

[7]:
```
def barr_method(
        Q: np.ndarray,
        p: np.ndarray,
        A: np.ndarray,
        b: np.ndarray,
        v0: np.ndarray,
        eps: float,
        mu=LOGBARR_MU,
        t0=LOGBARR_T0
) -> np.ndarray:
    def_checker = check_objective_def(A, b)
    if not def_checker(v0):
        raise ValueError('The log barrier is not defined for the input v0')

    m = len(b)
    t = t0
    v_history = [v0]
    v = v0

    while True:
        v = centering_step(Q=Q,
                           p=p,
                           A=A,
                           b=b,
                           t=t,
                            v0=v,
                            eps=NEWTON_EPSILON)[-1]

        v_history.append(v)

        if m / t < eps:
            break

        t = mu * t

    return np.array(v_history, dtype=float)
```

1.0.3 3.

We now test the implemented LASSO solver using random data

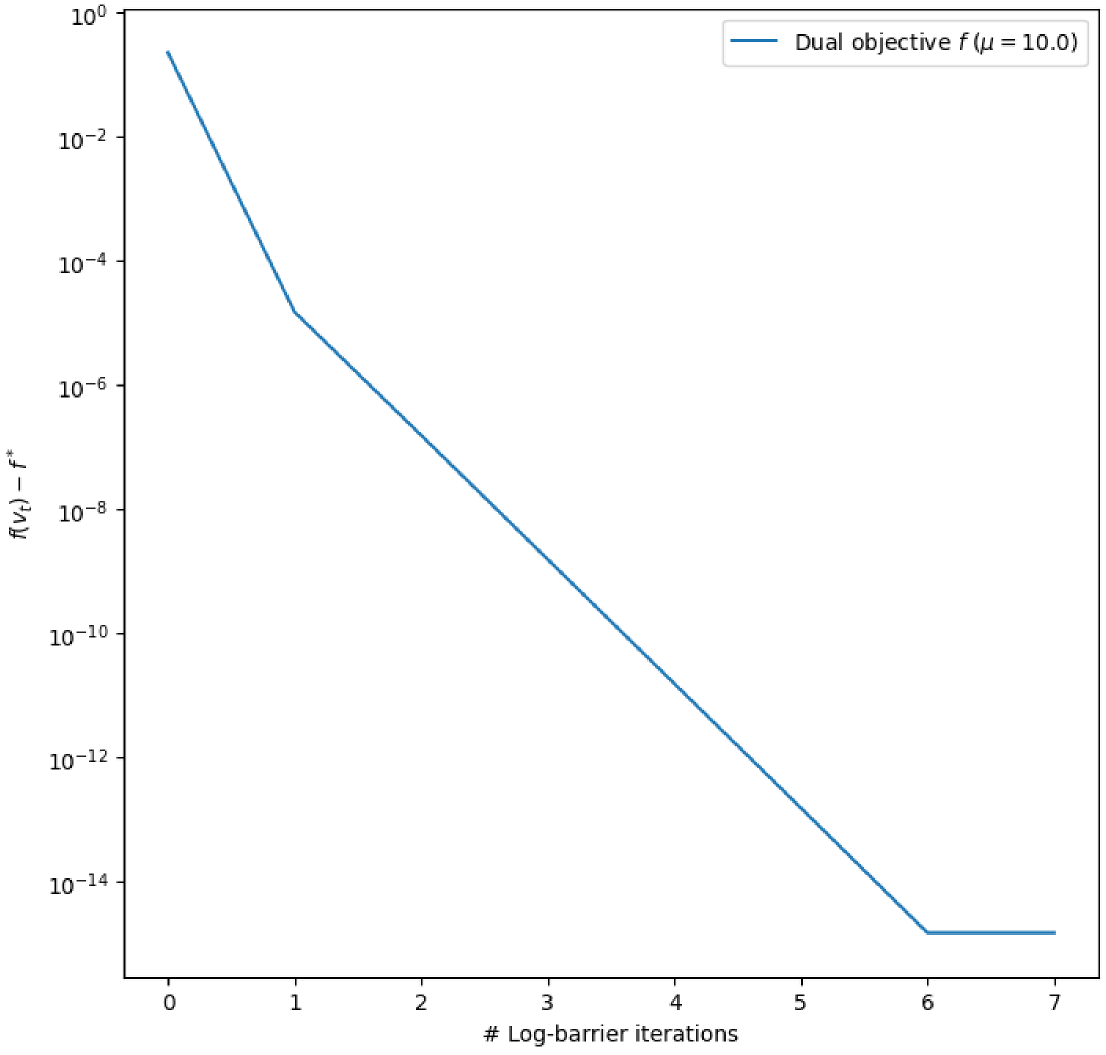
[8]:
```
# A very small example
n = 3
d = 2
scale = 1.
X = scale * 2 * (np.random.rand(n, d) - 0.5)  # n x's in R^d, in rows
y = 2 * (np.random.rand(n) - 0.5)  # n observations
_lambda = 10.

Q = 0.5 * np.eye(n)
p = -y
A = np.vstack([X.T, -X.T])
b = np.full(shape=2 * d, fill_value=_lambda)
```

[9]:
```
v0 = np.zeros(shape=n) # v0 stricly feasible (for all lambda > 0)
v_hist = barr_method(Q=Q,
                     p=p,
                     A=A,
                     b=b,
                     v0=v0,
                     eps=1e-6)
```

[10]:
```
def dual_objective(v):
    res = np.zeros(len(v), dtype=float)
    for i, _v in enumerate(v):
        res[i] = np.dot(_v, np.dot(Q, _v)) + np.dot(p, _v)
    return res
```

[11]:
```
plt.figure(figsize=(8, 8))
plt.semilogy(dual_objective(v_hist[:-1]) - dual_objective([v_hist[-1]]),␣
 ↪label=f'Dual objective $f$ ($\mu = {LOGBARR_MU})$')
plt.legend()
plt.ylabel('$f(v_t) - f^*$')
_ = plt.xlabel('# Log-barrier iterations')
```



As expected, a linear convergence in semilog scale

[12]:
```
# A more complex example
n = 25
d = 200

scale = 1.
X = scale * 2 * (np.random.rand(n, d) - 0.5)  # n x's in R^d, in rows
y = 2 * (np.random.rand(n) - 0.5)  # n observations
_lambda = 10.
```

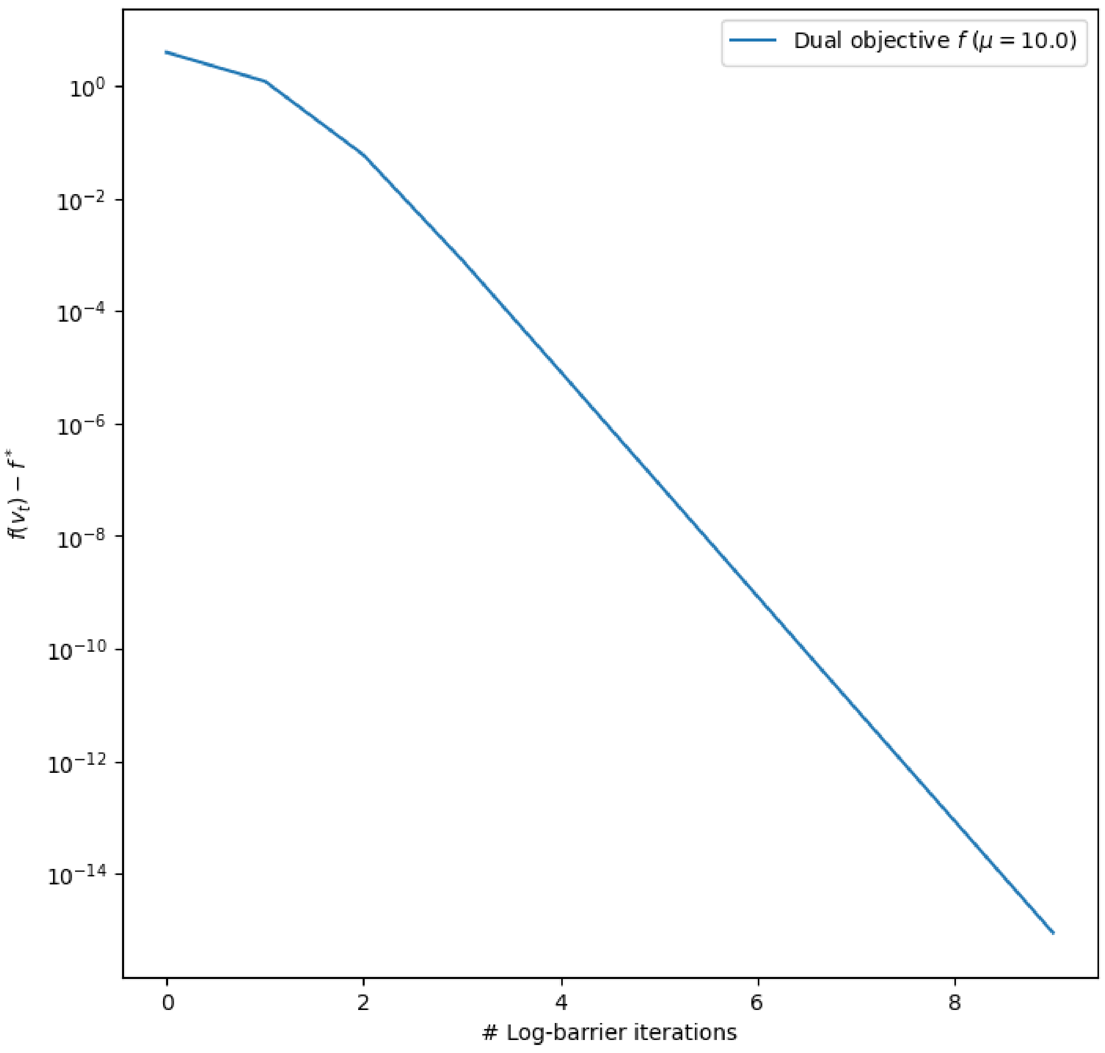
```
Q = 0.5 * np.eye(n)
p = -y
A = np.vstack([X.T, -X.T])
b = np.full(shape=2 * d, fill_value=_lambda)
```

```
[13]: print(f'X^T X is singular : {np.linalg.cond(X.T @ X) >= 1 / sys.float_info.
        ↪epsilon}')
```

```
X^T X is singular : True
```

```
[14]: v0 = np.zeros(shape=n) # v0 stricly feasible (for all lambda > 0)
      v_hist = barr_method(Q=Q,
                           p=p,
                           A=A,
                           b=b,
                           v0=v0,
                           eps=1e-6)
```

```
[15]: plt.figure(figsize=(8, 8))
      plt.semilogy(dual_objective(v_hist[:-1]) - dual_objective([v_hist[-1]]),␣
        ↪label=f'Dual objective $f$ ($\mu = {LOGBARR_MU})$')
      plt.legend()
      plt.ylabel('$f(v_t) - f^*$')
      _ = plt.xlabel('# Log-barrier iterations')
```



Still a very quick convergence, both in number of iterations and in time !

We must now relate the optimum of the dual with the optimum of the primal. The primal

$$\begin{aligned} & \min_{w} \frac{1}{2}||Xw - y||_2^2 + \lambda||w||_1 \\ \iff & \min_{w,z} \frac{1}{2}||z||_2^2 + \lambda||w||_1 \\ & \text{s.t. } \ z = Xw - y \end{aligned}$$

is convex (by convexity of norms in the objective function, and convexity of the linear inequality constraints), and it is strictly feasible as any $w \in \mathbb{R}^d$ is feasible. Therefore, strong duality holds, and we have for the optimal parameters (w^*, z^*, ν^*) :

$$\begin{aligned} z^* &= -\nu^* \text{ by definition of the Lagrange dual function (from } \nabla\mathscr{L}(z,\nu)=0 \iff z=-\nu \text{)} \\ Xw^* &= z^* + y \text{ by constraints} \\ \iff w^* &= \left(X^TX\right)^{-1} X^T(z^*+y) \text{ if } \operatorname{rank}(X)=d \end{aligned}$$

In practice, if $n < d$, we always have $\operatorname{rank}(X) < d$. However, solving the system to get a value of w^* still results in a solution of the primal, with the same l_1 norm and the same fitted values (and therefore, the same residues) as shown by Tibshirani (2012), The Lasso Problem and Uniqueness. It may be difficult to choose the "right" w^* value as it is difficult to define such a notion, particularly when different candidates have different non-zero coefficients (supports). In the same paper, Tibshirani derives a sufficient condition for uniqueness : considering the set

$$\varepsilon = \{i \in \{1, ..., d\}, |X_i^T(Xw^* - y)| = \lambda\}$$

where $X_i \in \mathbb{R}^n$ denotes a column of X, and the matrix X_ε defined by the concatenation of the columns $X_j, j \in \varepsilon$, then the solution is unique if $\operatorname{rank}(X_\varepsilon) = \operatorname{Card}(\varepsilon)$, and, denoting s the vector containing the signs of the elements of $X_\varepsilon^T(y - Xw^*)$:

$$\begin{aligned} w_\varepsilon^* &= \left(X_\varepsilon^T X_\varepsilon\right)^{-1}\left(X_\varepsilon^T y - \lambda s\right) \\ w_{\bar{\varepsilon}}^* &= 0 \end{aligned}$$

where w_ε^* denotes the vector of components of w^* whose indices are in ε

We can try to apply this criterion to get the solution.

[16]:
```python
def compute_epsilon_set(X,
                        resid,
                        _lambda,
                        tol=1e-6
                        ):
    X_cols = X.T
    epsilon_set = []
    for i, col in enumerate(X_cols):
        if abs(abs((np.dot(col, resid)) - _lambda) < tol:
            epsilon_set.append(i)

    return epsilon_set
```

[17]:
```python
compute_epsilon_set(X, -v_hist[-1], _lambda=_lambda)
```

[17]:
```
[]
```

Since the definition of the ε set is quite restrictive, we can't seem to compute it explicitly (or maybe it is always null in this example ?). We will thus simply resort to solving w.r.t. w

$$X^T X w = X^T (z^* + y)$$

[18]:
```
z_star = -v_hist[-1]
w_star = np.linalg.solve(X.T @ X, np.dot(X.T, z_star + y))
```

[19]:
```
print(f'Minimal component of w_star : {np.min(np.abs(w_star))}\n'
      f'l1-norm : {np.linalg.norm(w_star, ord=1)}')  # not very sparse in some␣
 ↪cases (likely not best solution found by NumPy ?)
```

```
Minimal component of w_star : 1.981015739935525e-12
l1-norm : 6.260402014420241e-07
```

Let us now study the impact of μ on w^*.

[20]:
```
mus = np.array([2., 10., 30., 70., 100., 130.,])
histories = []
z_stars = []
w_stars = []

for mu in mus:
    histories.append(barr_method(
        Q,
        p,
        A,
        b,
        v0,
        eps=1e-6,
        mu=mu,
        t0=LOGBARR_T0,
    ))

    z_stars.append(-histories[-1][-1])

    w_stars.append(
        np.linalg.solve(X.T @ X, np.dot(X.T, z_star + y))
    )

z_stars = np.array(z_stars)
w_stars = np.array(w_stars)
```

[21]:
```
# Check residue coherence
print(f'Residues are all close : '
      f'{np.allclose(z_stars, [z_stars[0] for _ in range(len(z_stars))],␣
 ↪atol=1e-16)}')

# Check if w_stars are all close
print(f'w_stars are all close : '
    f'{np.allclose(w_stars, [w_stars[0] for _ in range(len(w_stars))],␣
↪atol=1e-16)}')
```

```
Residues are all close : True
w_stars are all close : True
```

w^* is not impacted at all by the choice of μ, therefore, we can simply choose any value of μ for which the convergence is empirically fast. Moreover, the above check seems to show that the solution to the problem is in fact unique, as predicted by Lemma 4 in Tibshirani 2012, which states that if the points are drawn from a continuous distribution on $\mathbb{R}^{np}$, the solution is almost surely unique. Since we draw points uniformly, we indeed get a unique optimum.

In fact, we are minimizing a convex function over a polytope, and unless the optimal values lie on a face of the polytope (which is of probability 0), the optimal value is indeed unique and located at a vertex of the polytope. Starting from an interior point, we thus converge to this vertex.

[21]:
```

```