PGD_BlockPGD_AccPGD_for_epsilon=0.0_and_eta=1.

March 4, 2019

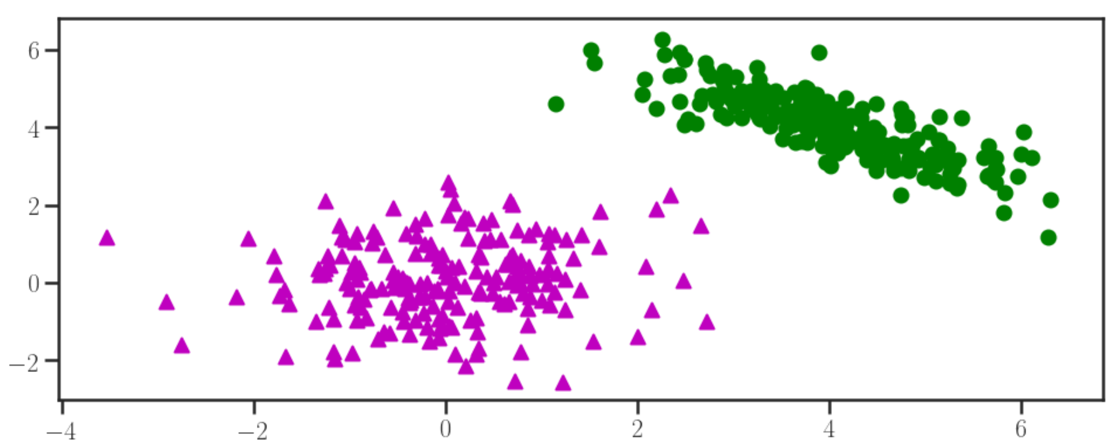
In [2]:
```
# NUMPY
import numpy as np

# MATPLOTLIB
import matplotlib.pyplot as plt
plt.style.context('dark_background')
%matplotlib inline
from matplotlib import rc
rc('font', **{'family': 'sans-serif', 'sans-serif': ['Computer Modern Roman']})
params = {'axes.labelsize': 8, # 12
          'font.size': 8, # 12
          'legend.fontsize': 8, # 12
          'xtick.labelsize': 8, # 10
          'ytick.labelsize': 8, # 10
          'text.usetex': True,
          'figure.figsize': (16, 6)}
plt.rcParams.update(params)

# SEABORN
import seaborn as sns
sns.set_context("poster")
sns.set_style("ticks")

# SKLEARN
from sklearn.metrics import pairwise_distances

# POT
import ot
from ot import sinkhorn, emd
# from ot.bregman import sinkhorn, greenkhorn

# PATH
import sys
path_files = '/Users/mzalaya/PycharmProjects/OATMIL/oatmilrouen/'
sys.path.insert(0, path_files)

# GREENKHORN
```

```
# from greenkhorn.sinkhorn import sinkhorn as sinkhgreen
# SCREENKHORN
from screenkhorn.screenkhorn import Screenkhorn
# np.random.seed(3946)

import warnings
warnings.filterwarnings("ignore", category=FutureWarning)
```

0.1 Data generation

In [3]:
```
n_1 = 200# nb samples
n_2 = 200
mu_s = np.array([0, 0])
cov_s = np.array([[1, 0], [0, 1]])

mu_t = np.array([4, 4])
cov_t = np.array([[1, -.8], [-.8, 1]])

xs = ot.datasets.make_2D_samples_gauss(n_1, mu_s, cov_s)
xt = ot.datasets.make_2D_samples_gauss(n_2, mu_t, cov_t)

a = np.ones((n_1,)) / n_1
b = np.ones((n_2,)) / n_2  # uniform distribution on samples

# loss matrix
M = ot.dist(xs, xt)
M /= M.max()
reg = 1.

K = np.exp(-M/reg)
```

In [4]:
```
plt.scatter(xs[:,0], xs[:,1], marker='^', c='m')
plt.scatter(xt[:,0], xt[:,1], marker='o', c='g');
```

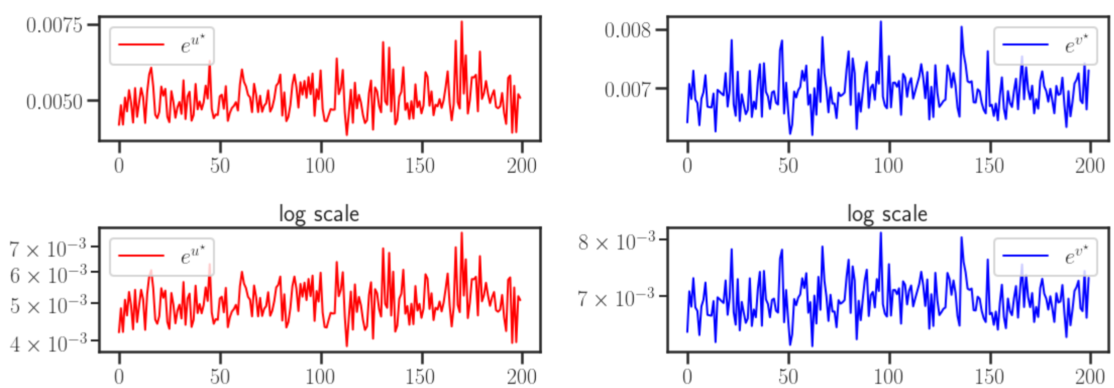


0.2 Sinkhorn's algorithm from POT

```
In [5]: P_sink = sinkhorn(a, b, M, reg, log=True)

        # Print P^star, u_sink = e^{u^star}, v_sink = e^{v^star}
        P_star = P_sink[0]
        outputs_dict = P_sink[1]
        exp_u_star = outputs_dict['u']
        exp_v_star = outputs_dict['v']
```

0.3 Plots of $e^{u^\star}$ and $e^{v^\star}$

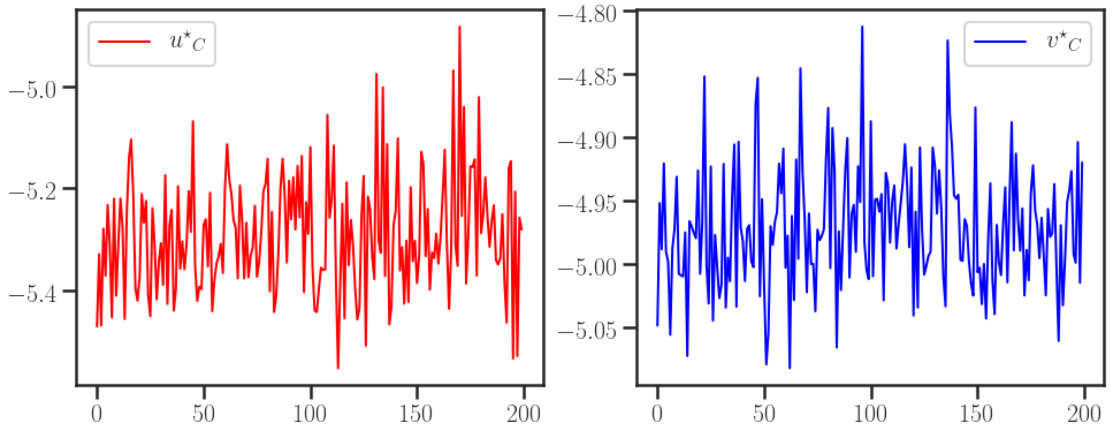
```
In [6]: figure, axes= plt.subplots(nrows=2, ncols=2)

        axes[0,0].plot(exp_u_star, linewidth=2, color='r', label=r'$e^{u^\star}$')
        axes[0,1].plot(exp_v_star, linewidth=2, color='b', label=r'$e^{v^\star}$')
        axes[0,0].legend()
        axes[0,1].legend();

        axes[1,0].semilogy(exp_u_star, linewidth=2, color='r', label=r'$e^{u^\star}$')
        axes[1,1].semilogy(exp_v_star, linewidth=2, color='b', label=r'$e^{v^\star}$')
        axes[1,0].legend()
        axes[1,0].set_title("log scale")
        axes[1,1].set_title("log scale")
        axes[1,1].legend();
        plt.subplots_adjust(hspace=.5)
        plt.tight_layout()
```



0.3.1 Plots of $u^\star$ and $v^\star$

```
In [7]: u_star = np.log(exp_u_star)
        v_star = np.log(exp_v_star)

        figure, axes= plt.subplots(ncols=2)
```

```
axes[0].plot(u_star, linewidth=2, color='r', label=r'${u^\star}_C$')
axes[1].plot(v_star, linewidth=2, color='b', label=r'${v^\star}_C$')
axes[0].legend()
axes[1].legend();
```



0.4 Choosing of the intervals I_u and J_v

```
In [8]: epsilon = 0.0
        I = np.where(exp_u_star >= epsilon)[0].tolist()
        Ic = np.where(exp_u_star < epsilon)[0].tolist()
        len(I), len(Ic)

Out[8]: (200, 0)

In [9]: J = np.where(exp_v_star >= epsilon)[0].tolist()
        Jc = np.where(exp_v_star < epsilon)[0].tolist()
        len(J), len(Jc)

Out[9]: (200, 0)
```

1 screenkhorn

```
In [10]: screenkhorn = Screenkhorn(a, b, M, reg, epsilon)
```

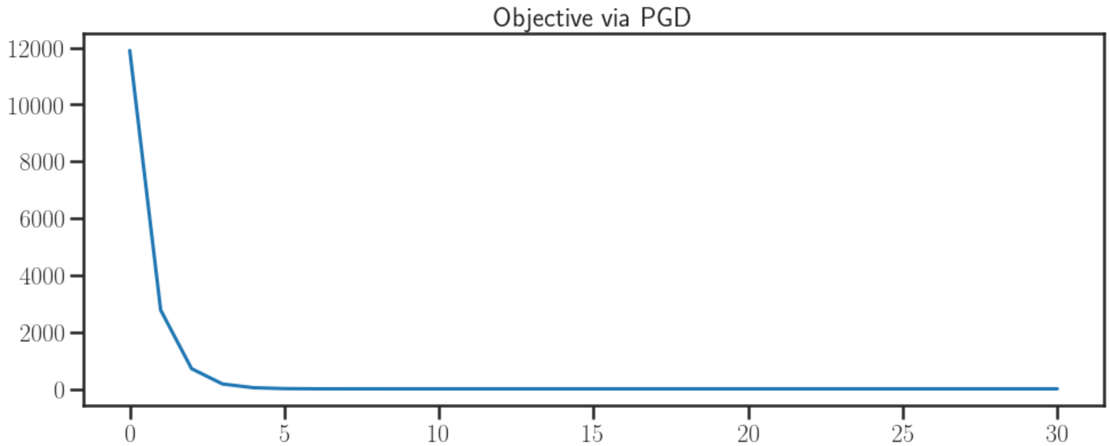
1.1 Projected Gradient Descent

```
In [36]: proj_grad_ord = \
         screenkhorn.projected_grad(np.zeros(n_1), np.zeros(n_2), I, J, max_iter_backtracking=
                                    step_size=100., max_iter=1000, tol=1e-10, verbose=False)

  2%|          | 18/1000 [00:00<00:21, 45.34it/s]
```

```
Achieved relative tolerance at iteration 30
```

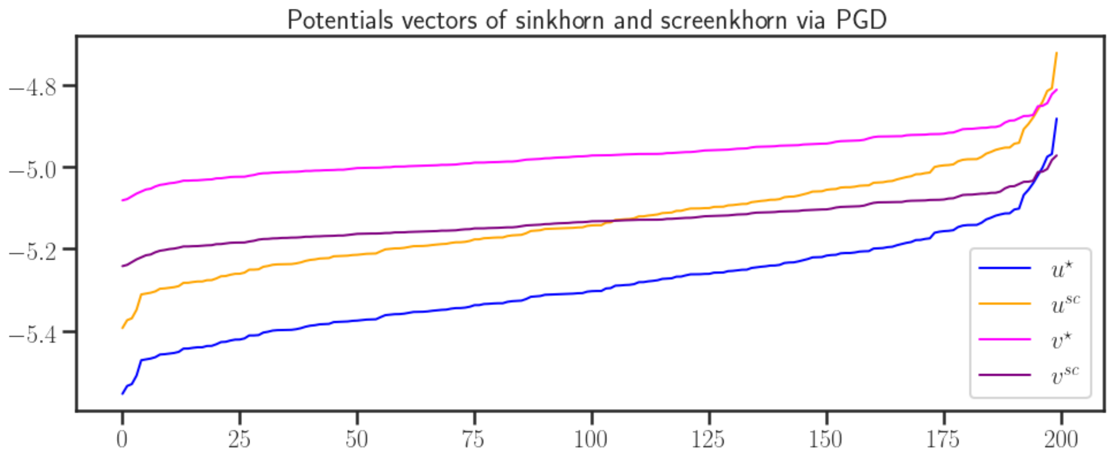
1.1.1 Curve of the objective function

```
In [37]: obj_ord = proj_grad_ord["trace_obj"]
         plt.plot(obj_ord);
         plt.title("Objective via PGD");
```



1.1.2 Sort of the solution by `screenkhorn`

```
In [38]: plt.plot(np.sort(u_star), 'blue', linewidth=2, label =r'${u^\star}$')
         plt.plot(np.sort(proj_grad_ord["usc"]), 'orange', linewidth=2, label =r'${u^{{sc}}}$'
         plt.plot(np.sort(v_star), 'magenta', linewidth=2, label =r'${v^\star}$')
         plt.plot(np.sort(proj_grad_ord["vsc"]), 'purple', linewidth=2, label =r'${v^{{sc}}}$'
         plt.legend(loc='best');
         plt.title(r'Potentials vectors of sinkhorn and screenkhorn via PGD');
```



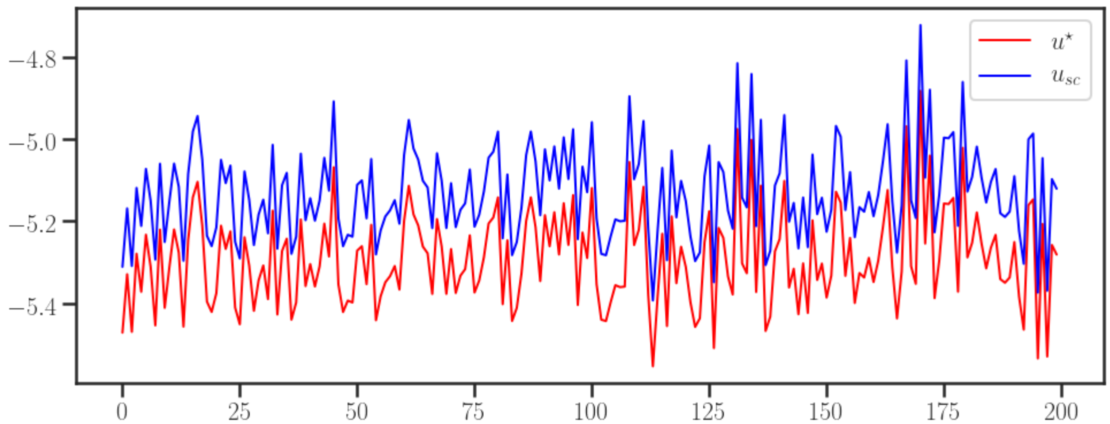
1.1.3 Checking the solutions of Block PDG

In [39]:
```
# sinkhorn
P_star = np.diag(np.exp(u_star)) @ K @ np.diag(np.exp(v_star))
a_star = P_star @ np.ones(n_2)
b_star = P_star.T @ np.ones(n_1)

# screenkhorn via pgd
usc_ord = proj_grad_ord["usc"]
vsc_ord = proj_grad_ord["vsc"]
P_sc_ord = np.diag(np.exp(usc_ord)) @ K @ np.diag(np.exp(vsc_ord))
a_sc_ord = P_sc_ord @ np.ones(n_2)
b_sc_ord = P_sc_ord.T @ np.ones(n_1)

print("sum of the marginals in sinkhorn are: %s, \t %s" %(sum(a_star), sum(b_star)))
print("\t")
print("sum of the marginals in screenkhorn are: %s, \t %s" %(sum(a_sc_ord), sum(b_sc_
print("\t")
print("Difference in sinkhorn: %s \t %s:" %(abs(1 - sum(a_star)), abs(1 - sum(b_star)
print("\t")
print("Difference in screenkhorn: %s \t  %s:" %(abs(1 - sum(a_sc_ord)), abs(1 - sum(b
print("\t")
print("Frobenius norm of difference solution matrices %s " %np.linalg.norm(P_star - P
print('\t')
print("Max norm of difference solution matrices %s "  %abs(P_star - P_sc_ord).max())
```

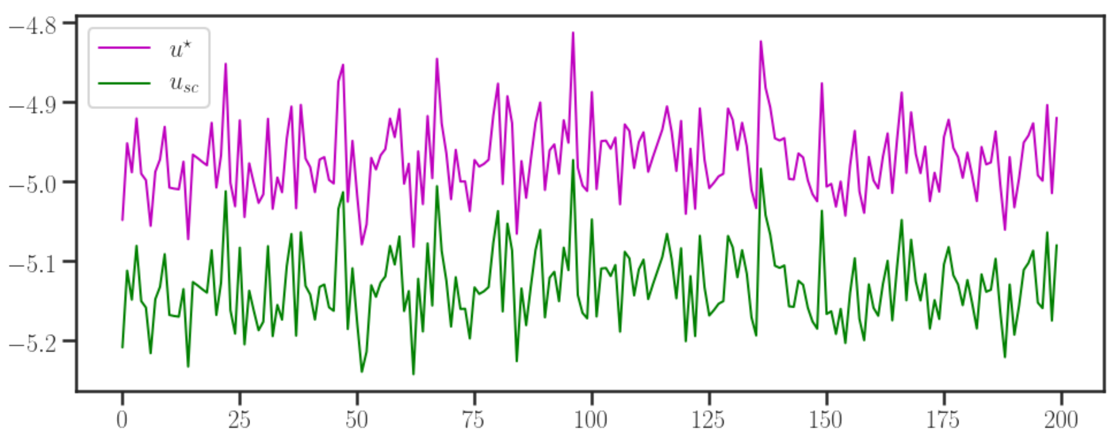
```
sum of the marginals in sinkhorn are: 1.0000000000000007,          1.0000000000000007

sum of the marginals in screenkhorn are: 1.0,          1.0

Difference in sinkhorn: 6.661338147750939e-16          6.661338147750939e-16:
```

```
Difference in screenkhorn: 0.0           0.0:

Frobenius norm of difference solution matrices 2.9337889936761695e-12

Max norm of difference solution matrices 8.53493233661691e-14
```

```
In [40]: plt.plot(u_star, linewidth=2, color='r', label=r'${u^\star}$')
         plt.plot(usc_ord, linewidth=2, color='b', label=r'$u_{sc}$')
         plt.legend()
         plt.legend();
```




```
In [41]: plt.plot(v_star, linewidth=2, color='m', label=r'${u^\star}$')
         plt.plot(vsc_ord, linewidth=2, color='g', label=r'$u_{sc}$')
         plt.legend()
         plt.legend();
```

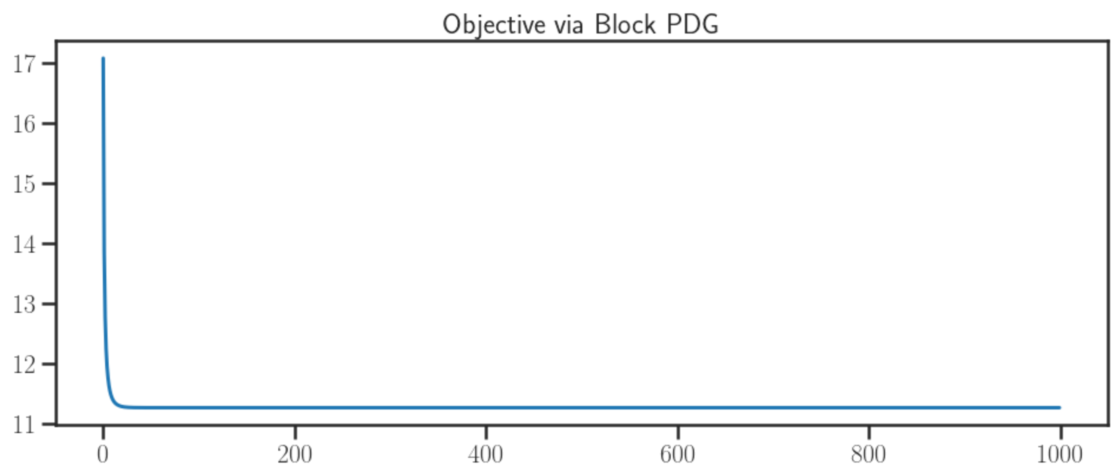


1.2 Block Projected Gradient Decsent

```
In [182]: proj_grad_alt = \
          screenkhorn.block_projected_grad(-3*np.ones(n_1), -3*np.ones(n_2), I, J, max_iter_bac
                                            step_size=8., max_iter=1000, tol=1e-10, verbose=Fals
```

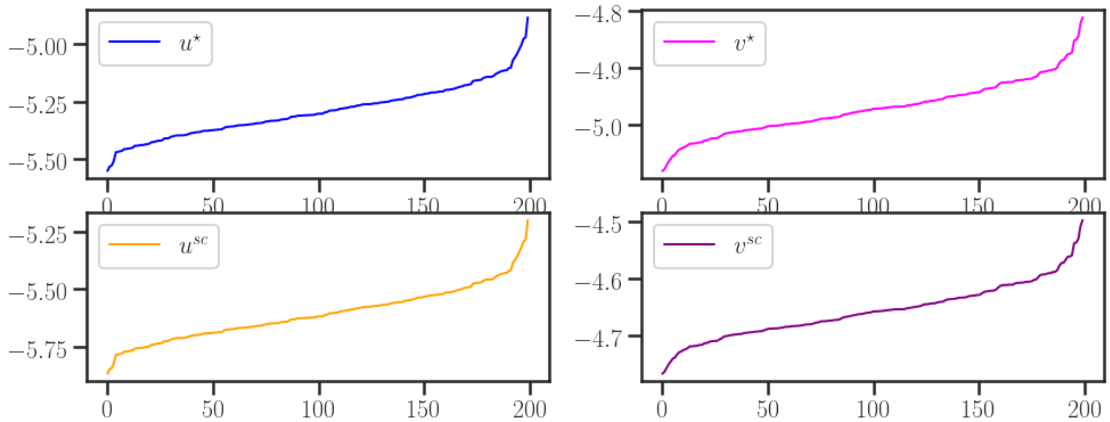
```
/Users/mzalaya/PycharmProjects/OATMIL/oatmilrouen/screenkhorn/screenkhorn.py:335: RuntimeWarnin
  usc[Ic] = np.log(self.epsilon) * np.ones(len(Ic))
/Users/mzalaya/PycharmProjects/OATMIL/oatmilrouen/screenkhorn/screenkhorn.py:336: RuntimeWarnin
  vsc[Jc] = np.log(self.epsilon) * np.ones(len(Jc))
  0%|          | 0/1000 [00:00<?, ?it/s]/Users/mzalaya/PycharmProjects/OATMIL/oatmilrouen/scree
  u_proj[np.where(u < np.log(self.epsilon))] = np.log(self.epsilon)
/Users/mzalaya/PycharmProjects/OATMIL/oatmilrouen/screenkhorn/screenkhorn.py:87: RuntimeWarning
  u_param_Ic = np.log(self.epsilon) * np.ones(len(Ic))
/Users/mzalaya/PycharmProjects/OATMIL/oatmilrouen/screenkhorn/screenkhorn.py:88: RuntimeWarning
  v_param_Jc = np.log(self.epsilon) * np.ones(len(Jc))
100%|| 1000/1000 [00:07<00:00, 132.44it/s]
```

```
In [183]: obj_alt= proj_grad_alt["trace_obj"]
          plt.plot(obj_alt)
          plt.title("Objective via Block PDG");
```




```
In [184]: figure, axes = plt.subplots(nrows=2, ncols=2)
          axes[0,0].plot(np.sort(u_star), 'blue', linewidth=2, label =r'${u^\star}$')
          axes[1,0].plot(np.sort(proj_grad_alt["usc"]), 'orange', linewidth=2, label =r'${u^{{s
          axes[0,1].plot(np.sort(v_star), 'magenta', linewidth=2, label =r'${v^\star}$')
          axes[1,1].plot(np.sort(proj_grad_alt["vsc"]), 'purple', linewidth=2, label =r'${v^{{s

          axes[0,0].legend()
          axes[0,1].legend()
          axes[1,0].legend()
```

```
axes[1,1].legend();

# plt.plot(np.sort(u_star), 'blue', linewidth=2, label =r'${u^\star}$')
# plt.plot(np.sort(proj_grad_alt["usc"]), 'orange', linewidth=2, label =r'${u^{{sc}}
# plt.plot(np.sort(v_star), 'magenta', linewidth=2, label =r'${v^\star}$')
# plt.plot(np.sort(proj_grad_alt["vsc"]), 'purple', linewidth=2, label =r'${v^{{sc}}
# plt.axhline(y =np.log(epsilon), linewidth=, color='r', label=r'$\log(\varepsilon)$
# plt.legend(loc='best');
# plt.title(r'log-potentials vectors of sinkhorn and screenkhorn with ${maxIter}=100
# plt.title(r'Potentials vectors of sinkhorn and screenkhorn via Block PGD');
```



1.2.1 Checking the solutions of Block PDG

In [185]:
```
# screenkhorn via block pgd
usc_alt = proj_grad_alt["usc"]
vsc_alt = proj_grad_alt["vsc"]
P_sc_alt = np.diag(np.exp(usc_alt)) @ K @ np.diag(np.exp(vsc_alt))
a_sc_alt = P_sc_alt @ np.ones(n_2)
b_sc_alt  = P_sc_alt.T @ np.ones(n_1)

print("sum of the marginals in sinkhorn are: %s, \t %s" %(sum(a_star), sum(b_star)))
print("\t")
print("sum of the marginals in screenkhorn are: %s, \t %s" %(sum(a_sc_alt), sum(b_sc_
print("\t")
print("Difference in sinkhorn: %s \t %s:" %(abs(1 - sum(a_star)), abs(1 - sum(b_star
print("\t")
print("Difference in screenkhorn: %s \t  %s:" %(abs(1 - sum(a_sc_alt)), abs(1 - sum(

print("\t")
print("Frobenius norm of %s ",  np.linalg.norm(P_star - P_sc_alt,'fro'))
print('\t')
print("Max norm of %s ",  abs(P_star - P_sc_alt).max())
```

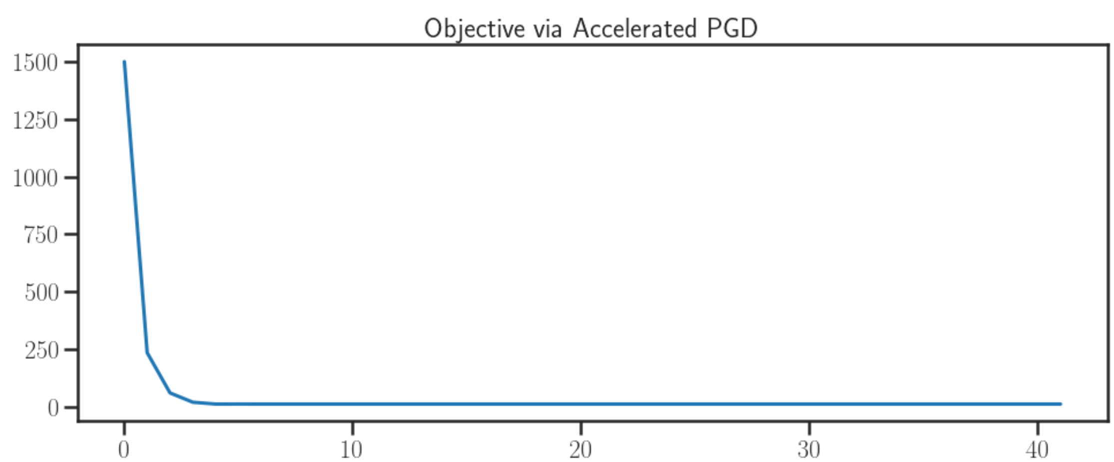
```
sum of the marginals in sinkhorn are: 1.0000000000000007,          1.0000000000000007

sum of the marginals in screenkhorn are: 0.9999999999999994,          1.0000000000000002

Difference in sinkhorn: 6.661338147750939e-16          6.661338147750939e-16:

Difference in screenkhorn: 5.551115123125783e-16           2.220446049250313e-16:

Frobenius norm of %s  6.900367487577692e-17

Max norm of %s  6.301925127571995e-19
```

1.3 Accelerated Projected Gradient Descent

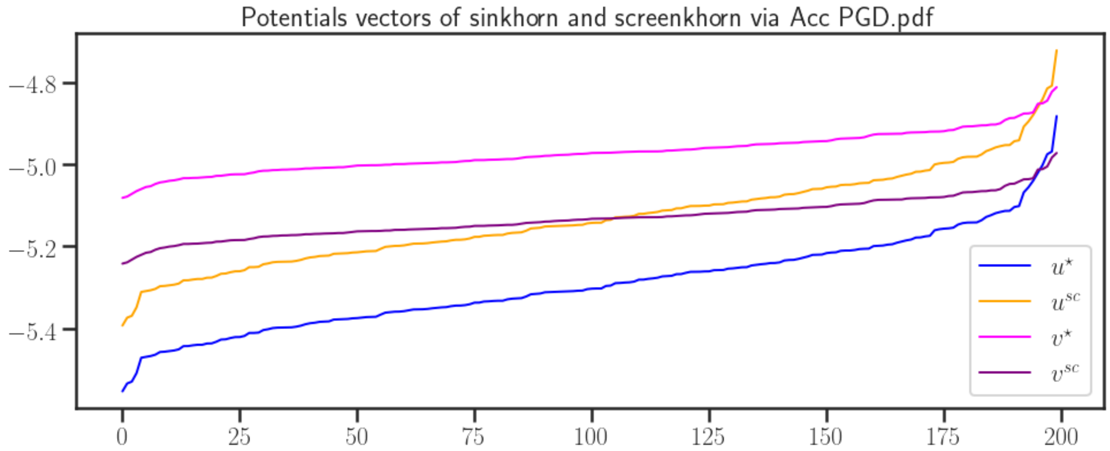
```
In [174]: proj_grad_acc = \
          screenkhorn.accelerated_projected_grad(-np.ones(n_1), -np.ones(n_2), I, J,
                                                  max_iter_backtracking=70,
                                                  step_size=100., max_iter=1000, tol=1e-10, ve
```

```
  4%|         | 37/1000 [00:00<00:28, 33.57it/s]

Achieved relative tolerance at iteration 41
```

```
In [175]: #plt.yscale("log")
          obj_acc= proj_grad_acc["trace_obj"]
          plt.plot(obj_acc)
          plt.title("Objective via Accelerated PGD");
```



In [176]:
```
plt.plot(np.sort(u_star), 'blue', linewidth=2, label =r'${u^\star}$')
plt.plot(np.sort(proj_grad_acc["usc"]), 'orange', linewidth=2, label =r'${u^{{sc}}}$
plt.plot(np.sort(v_star), 'magenta', linewidth=2, label =r'${v^\star}$')
plt.plot(np.sort(proj_grad_acc["vsc"]), 'purple', linewidth=2, label =r'${v^{{sc}}}$
# plt.axhline(y =np.log(epsilon), linewidth=, color='r', label=r'$\log(\varepsilon)$
plt.legend(loc='best');
# plt.title(r'log-potentials vectors of sinkhorn and screenkhorn with ${maxIter}=100
plt.title(r'Potentials vectors of sinkhorn and screenkhorn via Acc PGD.pdf');
```

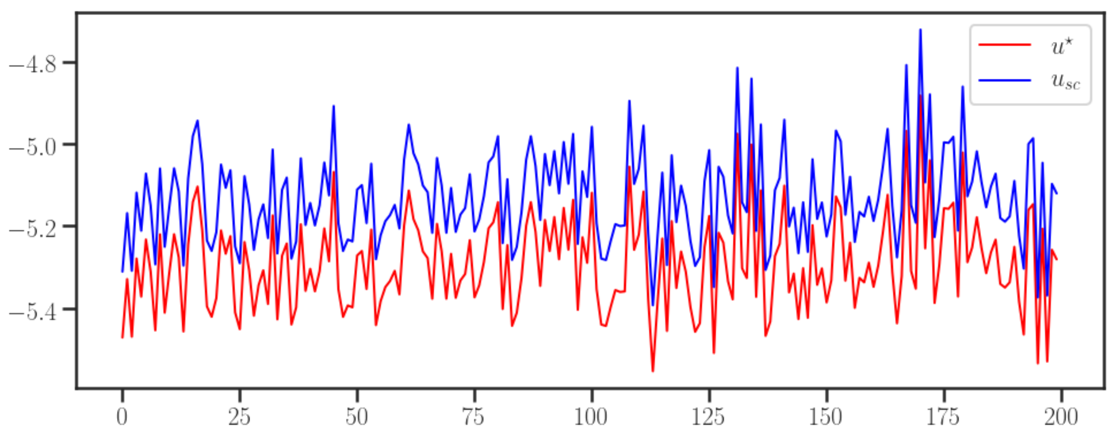


1.3.1 Checking the solutions of Block PDG

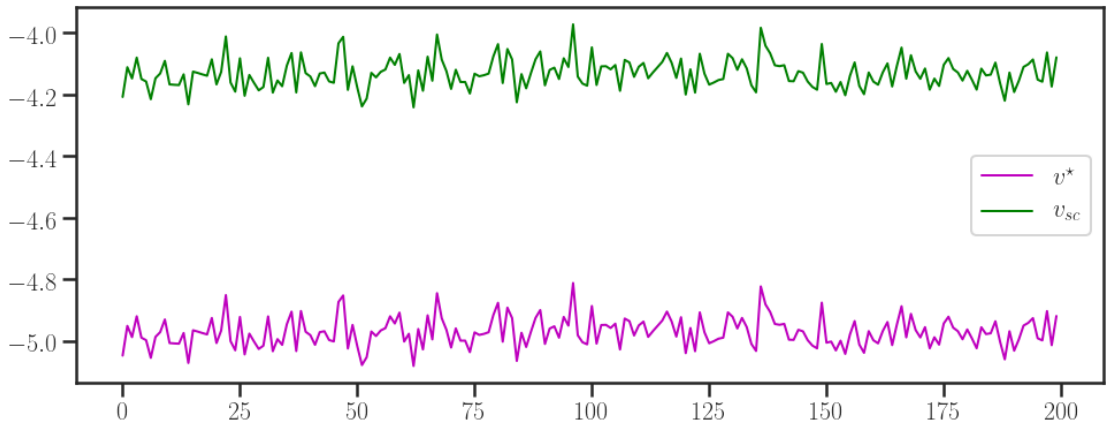
In [177]:
```
# screenkhorn via pgd
usc_acc = proj_grad_acc["usc"]
vsc_acc = proj_grad_acc["vsc"]
P_sc_acc = np.diag(np.exp(usc_acc)) @ K @ np.diag(np.exp(vsc_acc))
a_sc_acc = P_sc_acc @ np.ones(n_2)
b_sc_acc  = P_sc_acc.T @ np.ones(n_1)

print("sum of the marginals in sinkhorn are: %s, \t %s" %(sum(a_star), sum(b_star)))
print("\t")
print("sum of the marginals in screenkhorn are: %s, \t %s" %(sum(a_sc_acc), sum(b_sc_
print("\t")
print("Difference in sinkhorn: %s \t %s:" %(abs(1 - sum(a_star)), abs(1 - sum(b_star)
print("\t")
print("Difference in screenkhorn: %s \t  %s:" %(abs(1 - sum(a_sc_acc)), abs(1 - sum(b

print("\t")
print("Frobenius norm of %s " %np.linalg.norm(P_star - P_sc_acc,'fro'))
print('\t')
print("Max norm of %s "  %abs(P_star - P_sc_acc).max())
```

```
sum of the marginals in sinkhorn are: 1.0000000000000007,         1.0000000000000007

sum of the marginals in screenkhorn are: 0.9999999999999999,         0.9999999999999999

Difference in sinkhorn: 6.661338147750939e-16         6.661338147750939e-16:

Difference in screenkhorn: 1.1102230246251565e-16          1.1102230246251565e-16:

Frobenius norm of 4.601991702378369e-12

Max norm of 7.934753250499954e-14
```

In [165]:
```python
usc_alt = proj_grad_acc["usc"]
vsc_alt = proj_grad_acc["vsc"]

plt.plot(u_star, linewidth=2, color='r', label=r'${u^\star}$')
plt.plot(usc_acc, linewidth=2, color='b', label=r'$u_{sc}$')
plt.legend()
plt.legend();
```



In [160]:
```python
plt.plot(v_star, linewidth=2, color='m', label=r'${v^\star}$')
plt.plot(vsc_acc, linewidth=2, color='g', label=r'$v_{sc}$')
plt.legend()
plt.legend();
```



In [ ]: