Watching SGD in action with constant step sizes

In [1]:
```
import numpy as np
import matplotlib.pyplot as plt
from numpy import linalg as LA
```

In [2]:
```
def compute_loss_avg(X, y, w):
    return (1/X.shape[0])*LA.norm(X@w - y, ord=2)**2
```

In [6]:
```
def SGD_update(X, y, w, eta):
    return w - (2.0 * eta/X.shape[0])*(X.transpose()@(X@w - y))
```

Part (1). Under-parameterized ($n > d$) Noiseless ($\sigma = 0$) Regime

Generate data

In [3]:
```
# Generate data
np.random.seed(0)

# Set number of samples
N = 2000
# Set the dimension
d = 200

# Generate data matrix X_train
X_train = np.random.randn(N, d)
# Generate ground truth w_star
w_star = np.random.randn(d, 1)

# Generate outputs y_train
y_train = X_train @ w_star
# Set mini batch size
batch_size = 64
# Set step size
eta = 0.01
# Set number of iterations
N_iteration = 10000

# Evaluate the largest and smallest eigenvalue
_, s, _ = np.linalg.svd(X_train/np.sqrt(N))
print('largest eigenvalue: ', s[0]**2)
print('smallest eigenvalue: ', s[-1]**2)
```

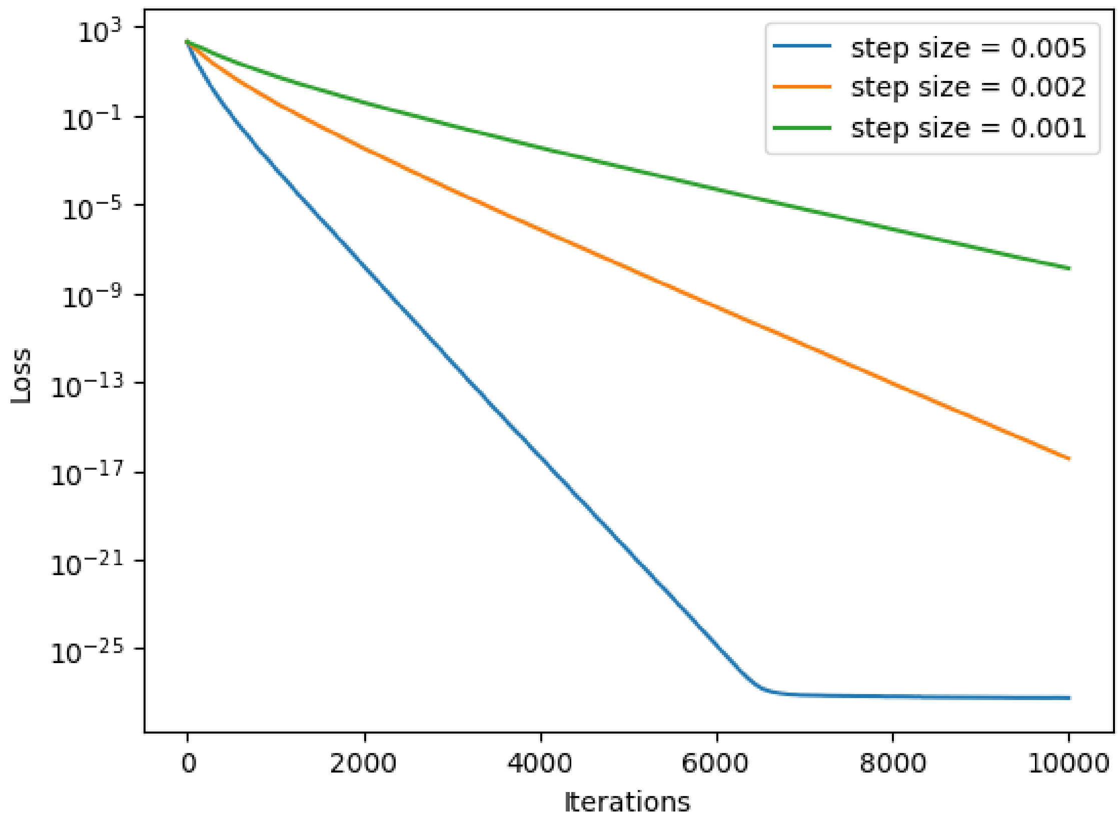
```
largest eigenvalue:  1.7095023515203154
smallest eigenvalue:  0.47581318789985916
```

```
In [4]: BatchSizeList = [1, 64, 128]
        EtaList = [0.005, 0.002, 0.001]
```

Study the effect of step size η

```
In [7]: w_init = (np.random.randn(d, 1)) * 0.0

        Losses = []
        batch_size = 64
        for eta in EtaList:
            loss = []
            w = w_init.copy()
            for i in range(N_iteration):
                random_index = np.random.choice(N, batch_size)
                X_i = X_train[random_index, :]
                y_i = y_train[random_index]
                w = SGD_update(X_i, y_i, w, eta)
                loss.append(compute_loss_avg(X_train, y_train, w))
            Losses.append(loss)
```

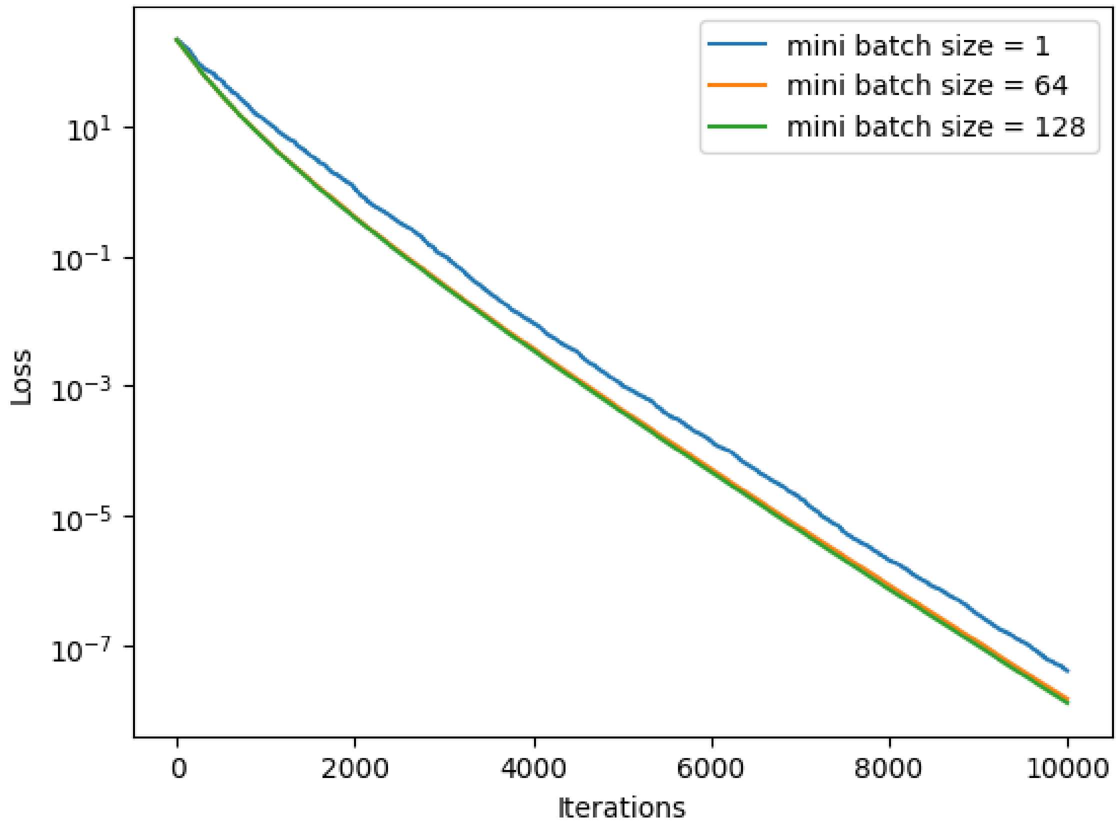
```
In [8]: plt.figure()
        idx = 0
        for eta in EtaList:
            plt.semilogy(range(N_iteration), Losses[idx], label = 'step size = {}'.format(et
            idx += 1
        plt.axis('tight')
        plt.xlabel("Iterations")
        plt.ylabel("Loss")
        plt.legend()
        plt.show()
```



Study the effect of mini batch size $|\mathcal{S}_t|$

In [9]:
```
w_init = (np.random.randn(d, 1)) * 0.0
Losses = []
eta = 0.001
for batch_size in BatchSizeList:
    loss = []
    w = w_init.copy()
    for i in range(N_iteration):
        random_index = np.random.choice(N, batch_size)
        X_i = X_train[random_index, :]
        y_i = y_train[random_index]
        w = SGD_update(X_i, y_i, w, eta)
        loss.append(compute_loss_avg(X_train, y_train, w))
    Losses.append(loss)
```

In [10]:
```
plt.figure()
idx = 0
for batch_size in BatchSizeList:
    plt.semilogy(range(N_iteration), Losses[idx], label = 'mini batch size = {}'.for
    idx += 1
plt.axis('tight')
plt.xlabel("Iterations")
plt.ylabel("Loss")
plt.legend()
plt.show()
```



Part (2). Over-parameterized ($n < d$) Noiseless ($\sigma = 0$) Regime

Generate data

In [11]:
```
# Generate data
np.random.seed(0)

# Set number of samples
N = 500
# Set the dimension
d = 1000

# Generate data matrix X_train
X_train = np.random.randn(N, d)
# Generate ground truth w_star
w_star = np.random.randn(d, 1)

# Generate outputs y_train
y_train = X_train @ w_star
# Set mini batch size
batch_size = 64
# Set step size
eta = 0.001
# Set number of iterations
N_iteration = 50000


# Evaluate the largest and smallest eigenvalue
_, s, _ = np.linalg.svd(X_train/np.sqrt(N))
print('largest eigenvalue: ', s[0]**2)
print('smallest singular value (square): ', s[-1]**2)
```

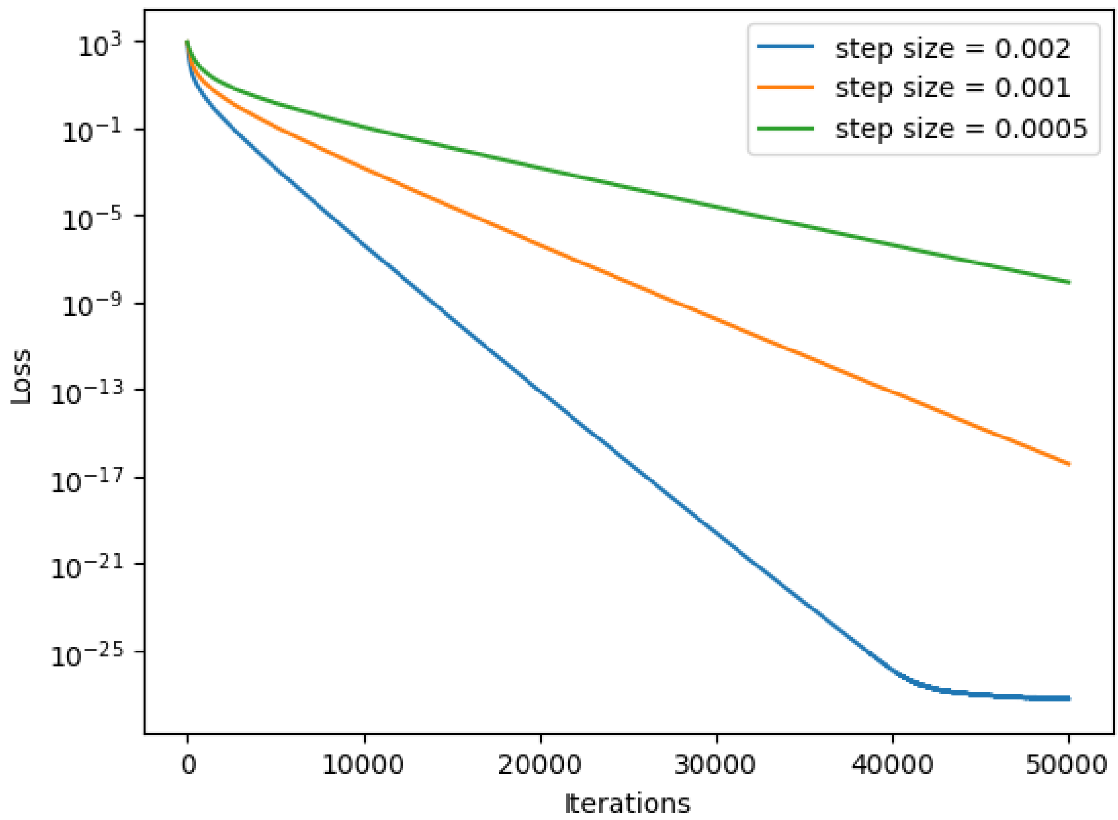
```
largest eigenvalue:  5.771623003224577
smallest singular value (square):  0.17331335068830736
```

In [12]:
```
BatchSizeList = [1, 64, 128]
EtaList = [0.002, 0.001, 0.0005]
```

Study the effect of step size η

In [14]:
```
w_init = (np.random.randn(d, 1)) * 0.0

Losses = []
batch_size = 64
for eta in EtaList:
    loss = []
    w = w_init.copy()
    for i in range(N_iteration):
        random_index = np.random.choice(N, batch_size)
        X_i = X_train[random_index, :]
        y_i = y_train[random_index]
        w = SGD_update(X_i, y_i, w, eta)
        loss.append(compute_loss_avg(X_train, y_train, w))
    Losses.append(loss)
```

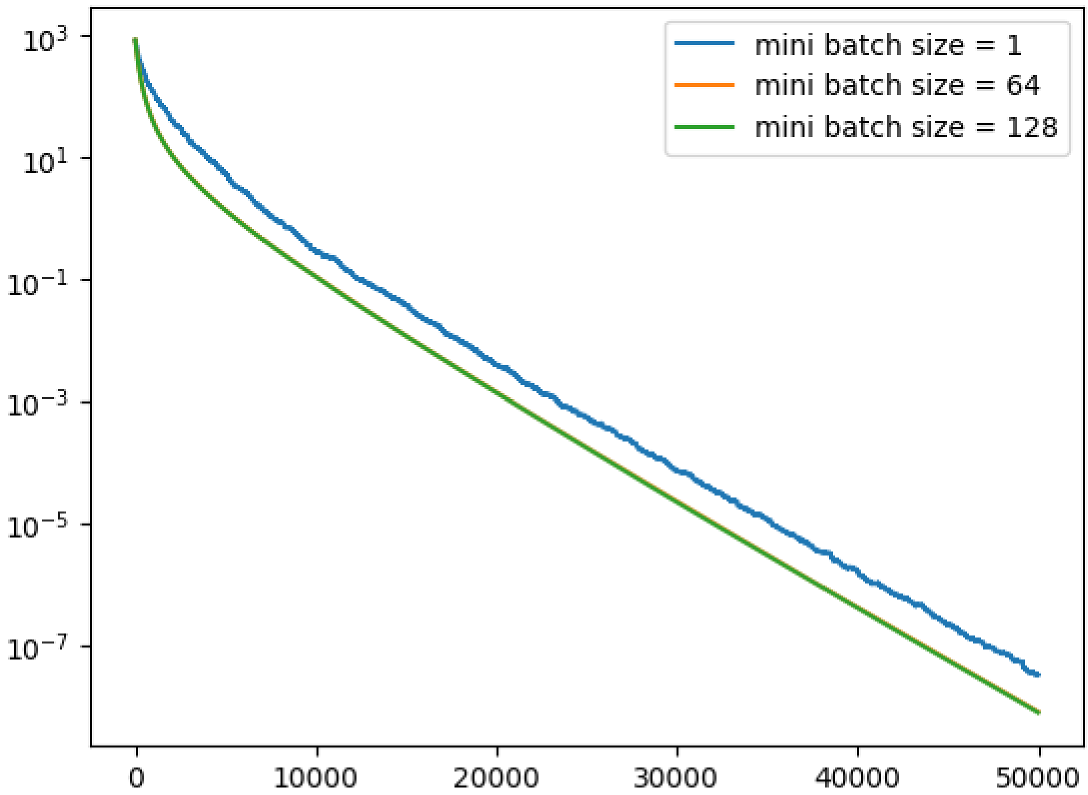
In [15]:
```
plt.figure()
idx = 0
for eta in EtaList:
    plt.semilogy(range(N_iteration), Losses[idx], label = 'step size = {}'.format(et
    idx += 1
plt.axis('tight')
plt.xlabel("Iterations")
plt.ylabel("Loss")
plt.legend()
plt.show()
```



Study the effect of mini batch size $|S_t|$

In [16]:
```
w_init = (np.random.randn(d, 1)) * 0.0
Losses = []
eta = 0.0005
for batch_size in BatchSizeList:
    loss = []
    w = w_init.copy()
    for i in range(N_iteration):
        random_index = np.random.choice(N, batch_size)
        X_i = X_train[random_index, :]
        y_i = y_train[random_index]
        w = SGD_update(X_i, y_i, w, eta)
        loss.append(compute_loss_avg(X_train, y_train, w))
    Losses.append(loss)
```

In [17]:
```
plt.figure()
idx = 0
for batch_size in BatchSizeList:
    plt.semilogy(range(N_iteration), Losses[idx], label = 'mini batch size = {}'.for
    idx += 1
plt.axis('tight')
plt.legend()
plt.show()
```



Part (3). Over-parameterized ($n < d$) Noise ($\sigma > 0$) Regime

Generate data

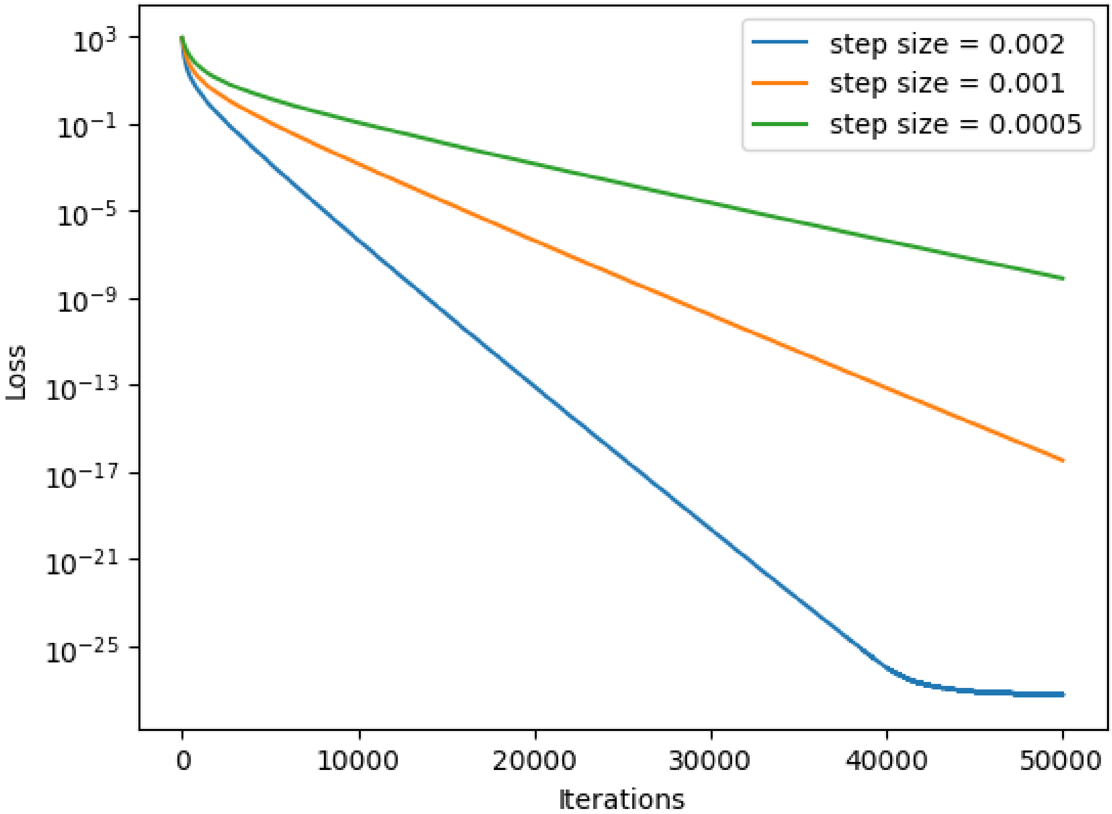
In [18]:
```
# Generate data
np.random.seed(0)

# Set number of samples
N = 500
# Set the dimension
d = 1000

# Generate data matrix X_train
X_train = np.random.randn(N, d)
# Generate ground truth w_star
w_star = np.random.randn(d, 1)

# Generate outputs y_train
y_train = X_train @ w_star + 0.1 * np.random.randn(N, 1)
# Set mini batch size
batch_size = 64
# Set step size
eta = 0.001
# Set number of iterations
N_iteration = 50000


# Evaluate the largest and smallest eigenvalue
X_train = np.concatenate((X_train, 0.1 * np.eye(N)), axis=1)
_, s, _ = np.linalg.svd(X_train/np.sqrt(N))
print('largest eigenvalue: ', s[0]**2)
print('smallest singular value (square): ', s[-1]**2)
```

```
largest eigenvalue:  5.77164300322458
smallest singular value (square):  0.17333335068830757
```

Study the effect of step size η

In [19]:
```
w_init = (np.random.randn(d + N, 1)) * 0.0

Losses = []
batch_size = 64
for eta in EtaList:
    loss = []
    w = w_init.copy()
    for i in range(N_iteration):
        random_index = np.random.choice(N, batch_size)
        X_i = X_train[random_index, :]
        y_i = y_train[random_index]
        w = SGD_update(X_i, y_i, w, eta)
        loss.append(compute_loss_avg(X_train, y_train, w))
    Losses.append(loss)
```

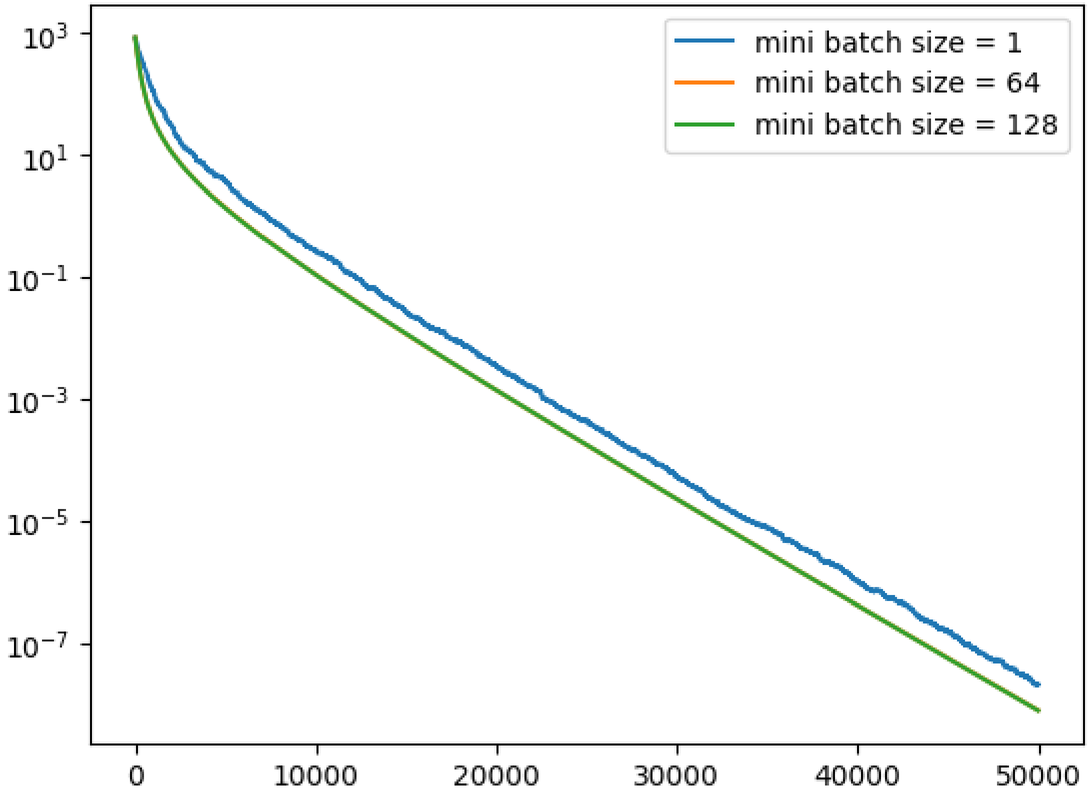
In [20]:
```
plt.figure()
idx = 0
for eta in EtaList:
    plt.semilogy(range(N_iteration), Losses[idx], label = 'step size = {}'.format(et
    idx += 1
plt.axis('tight')
plt.xlabel("Iterations")
plt.ylabel("Loss")
plt.legend()
plt.show()
```



Study the effect of mini batch size $|S_t|$

In [21]:
```
w_init = (np.random.randn(d + N, 1)) * 0.0
Losses = []
eta = 0.0005
for batch_size in BatchSizeList:
    loss = []
    w = w_init.copy()
    for i in range(N_iteration):
        random_index = np.random.choice(N, batch_size)
        X_i = X_train[random_index, :]
        y_i = y_train[random_index]
        w = SGD_update(X_i, y_i, w, eta)
        loss.append(compute_loss_avg(X_train, y_train, w))
    Losses.append(loss)
```

In [22]:
```
plt.figure()
idx = 0
for batch_size in BatchSizeList:
    plt.semilogy(range(N_iteration), Losses[idx], label = 'mini batch size = {}'.for
    idx += 1
plt.axis('tight')
plt.legend()
plt.show()
```



Part (4). Under-parameterized ($n > d$) Noise ($\sigma > 0$) Regime

Compare SGD on original ridge regression and feature-augmented regression

In [23]:
```
# Generate data
np.random.seed(0)

# Set number of samples
N = 500
# Set the dimension
d = 50

# Generate data matrix X_train
X_train = np.random.randn(N, d)
# Generate ground truth w_star
w_star = np.random.randn(d, 1)

# Generate outputs y_train
y_train = X_train @ w_star + 0.1 * np.random.randn(N, 1)
y_train_clean = X_train @ w_star
# Set mini batch size
batch_size = 64
# Set step size
eta = 0.001
# Set number of iterations
N_iteration = 500000


alpha = 0.01

w_star = np.linalg.inv(X_train.transpose()@X_train + N * alpha * np.eye(d))@X_train
w_star_clean = np.linalg.inv(X_train.transpose()@X_train)@X_train.transpose()@y_tra


# Evaluate the largest and smallest eigenvalue
X_train_aug = np.concatenate((X_train, np.sqrt(N * alpha) * np.eye(N)), axis=1)
_, s, _ = np.linalg.svd(X_train_aug/np.sqrt(N))
print('largest eigenvalue: ', s[0]**2)
print('smallest singular value (square): ', s[-1]**2)
```

```
largest eigenvalue:  1.6696575471365793
smallest singular value (square):  0.009999999999999981
```

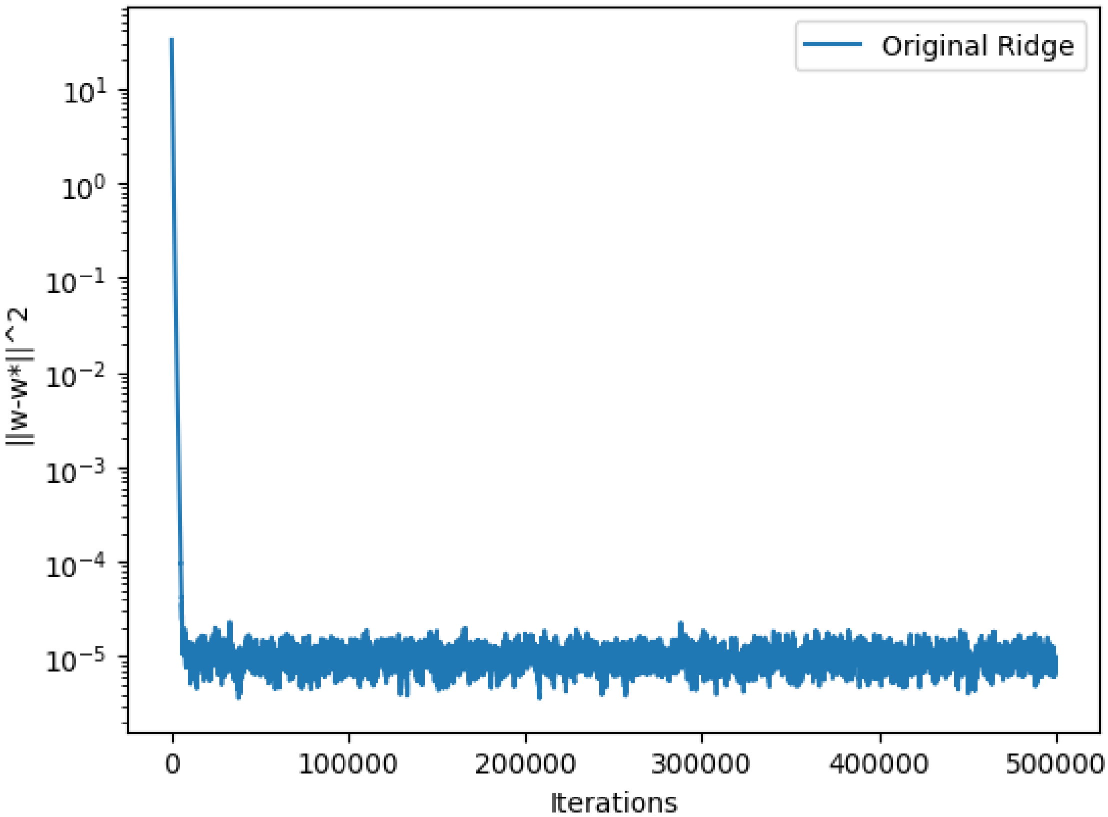
In [24]:
```
def compute_diff_norm(w, w_star):
    return LA.norm(w - w_star, ord=2)**2
```

In [25]:
```
def SGD_update_ridge(X, y, w, eta, alpha = 0.01):
    return w - (2.0 * eta/X.shape[0])*(X.transpose()@(X@w - y)) - 2.0 * eta * alph
```

Run SGD on original ridge regression

In [26]:
```
w_init = (np.random.randn(d, 1)) * 0.0
loss_ridge = []
w = w_init.copy()
for i in range(N_iteration):
    random_index = np.random.choice(N, batch_size)
    X_i = X_train[random_index, :]
    y_i = y_train[random_index]
    w = SGD_update_ridge(X_i, y_i, w, eta, alpha)
    loss_ridge.append(compute_diff_norm(w, w_star))
```

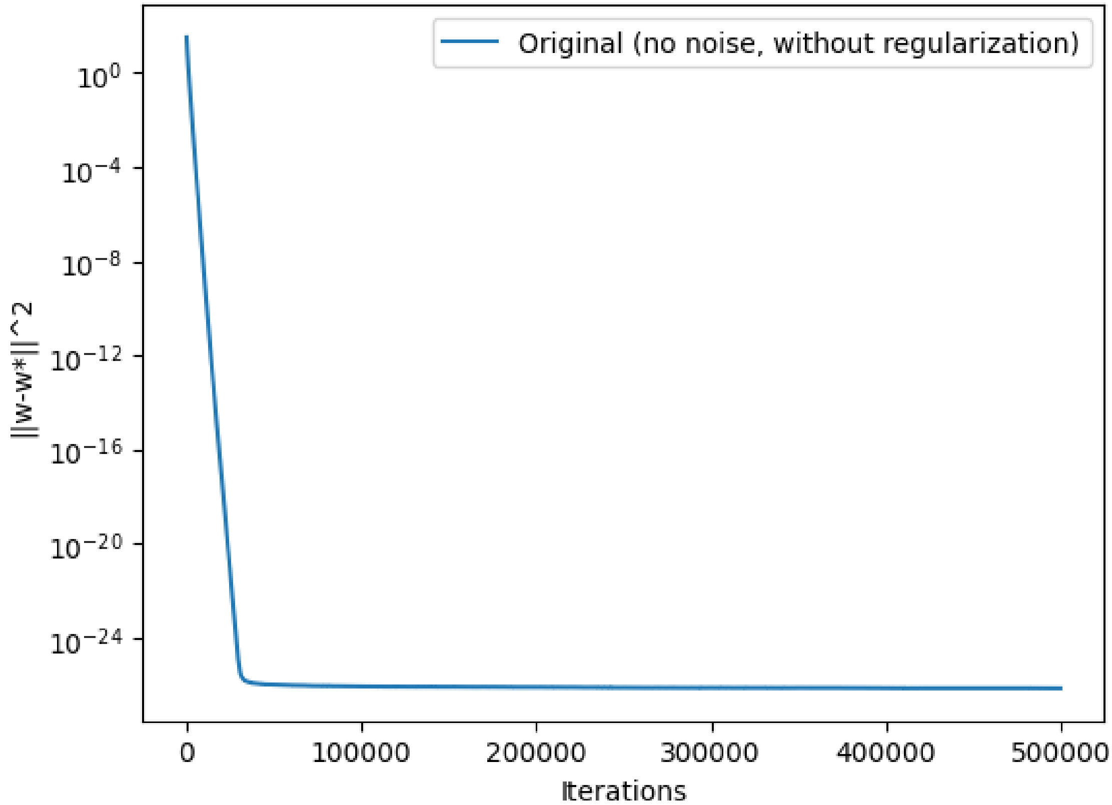
In [27]:
```
plt.figure()
plt.semilogy(range(N_iteration), loss_ridge, label = 'Original Ridge')
plt.axis('tight')
plt.xlabel("Iterations")
plt.ylabel("||w-w*||^2")
plt.legend()
plt.show()
```



Run SGD on original regression (but with no noise in y, i.e., $\sigma = 0.0$)

In [28]:
```
w_init = (np.random.randn(d, 1)) * 0.0
loss_ridge_clean = []
w = w_init.copy()
for i in range(N_iteration):
    random_index = np.random.choice(N, batch_size)
    X_i = X_train[random_index, :]
    y_i = y_train_clean[random_index]
    w = SGD_update(X_i, y_i, w, eta)
    loss_ridge_clean.append(compute_diff_norm(w, w_star_clean))
```

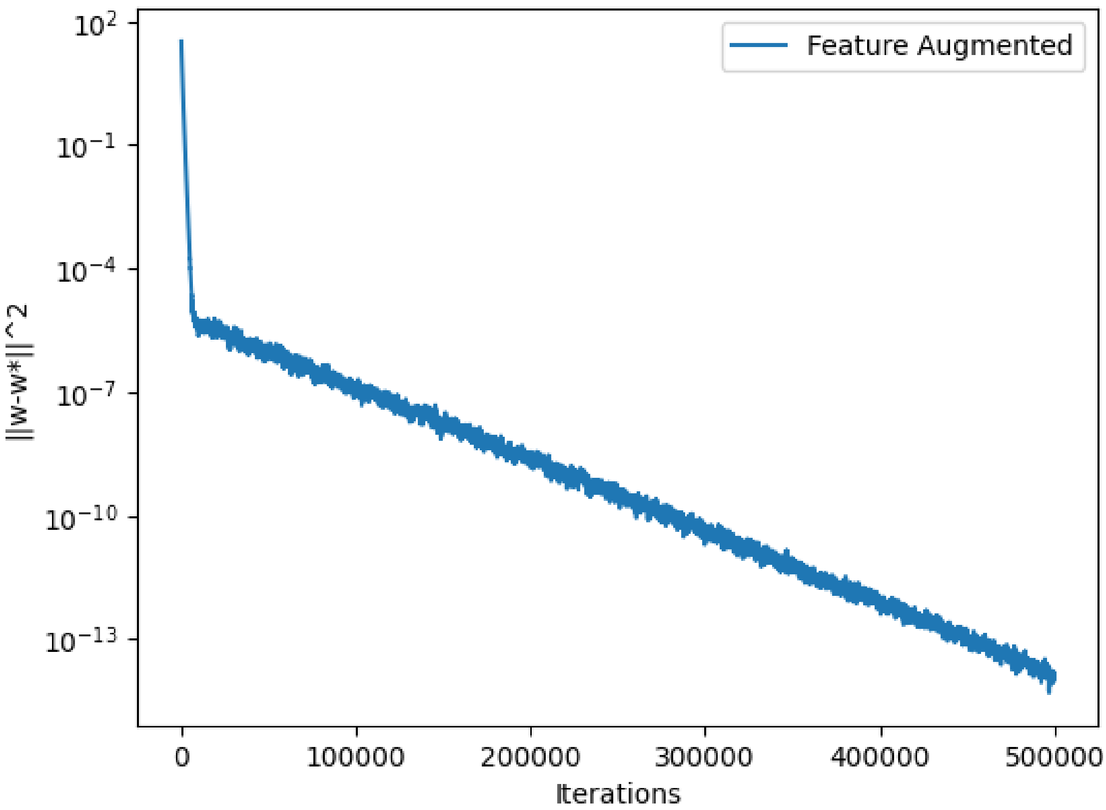
In [29]:
```
plt.figure()
plt.semilogy(range(N_iteration), loss_ridge_clean, label = 'Original (no noise, with
plt.axis('tight')
plt.xlabel("Iterations")
plt.ylabel("||w-w*||^2")
plt.legend()
plt.show()
```



Run SGD on augmented regression

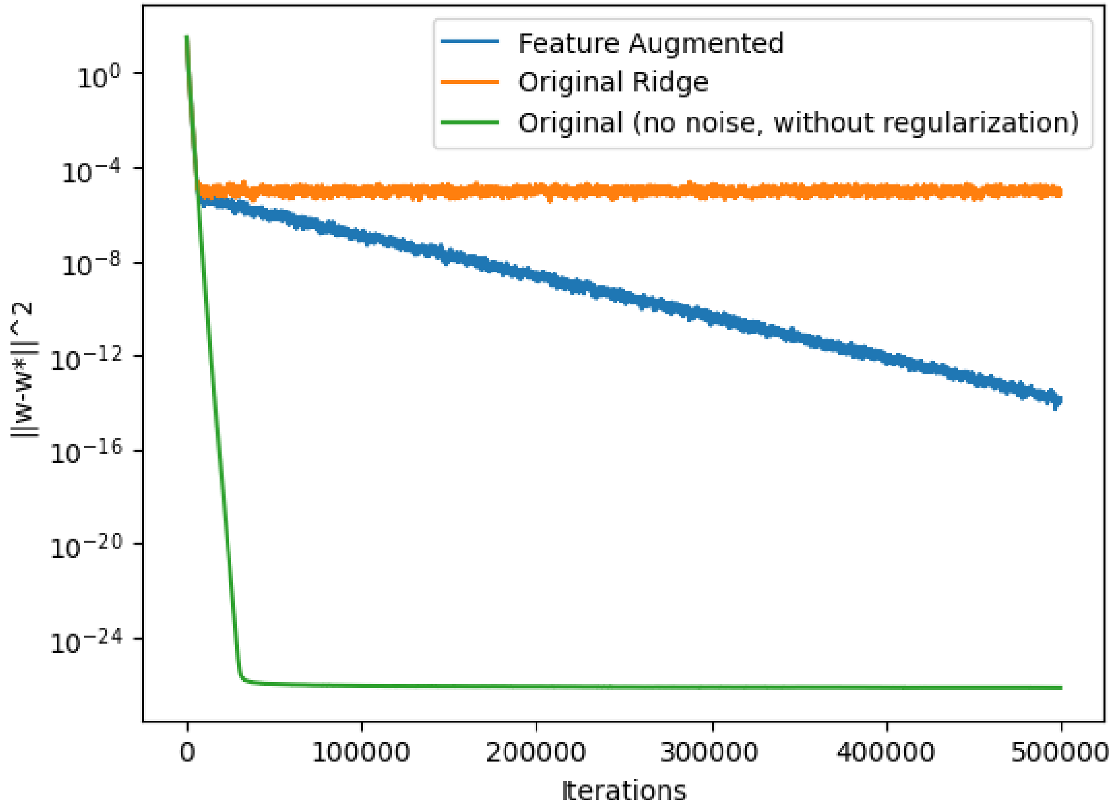
In [30]:
```
w_aug_init = (np.random.randn(d + N, 1)) * 0.0

loss_aug = []
w_aug = w_aug_init.copy()
for i in range(N_iteration):
    random_index = np.random.choice(N, batch_size)
    X_i = X_train_aug[random_index, :]
    y_i = y_train[random_index]
    w_aug = SGD_update(X_i, y_i, w_aug, eta)
    loss_aug.append(compute_diff_norm(w_aug[:d], w_star))
```

In [31]:
```
plt.figure()
plt.semilogy(range(N_iteration), loss_aug, label = 'Feature Augmented')
plt.axis('tight')
plt.xlabel("Iterations")
plt.ylabel("||w-w*||^2")
plt.legend()
plt.show()
```



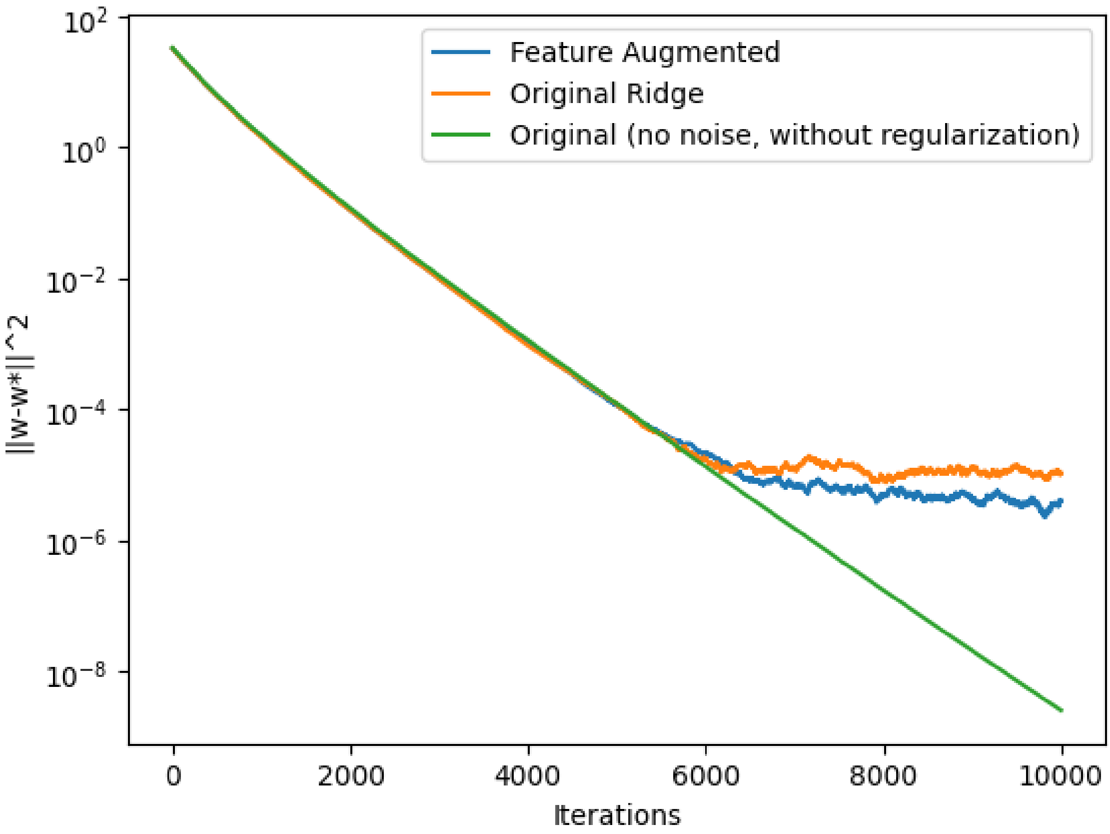
Compare the above three figures

In [32]:
```
plt.figure()
plt.semilogy(range(N_iteration), loss_aug, label = 'Feature Augmented')
plt.semilogy(range(N_iteration), loss_ridge, label = 'Original Ridge')
plt.semilogy(range(N_iteration), loss_ridge_clean, label = 'Original (no noise, with
plt.axis('tight')
plt.xlabel("Iterations")
plt.ylabel("||w-w*||^2")
plt.legend()
plt.show()
```



Zoom in Visualization

In [33]:
```
plt.figure()
plt.semilogy(range(N_iteration)[:10000], loss_aug[:10000], label = 'Feature Augmente
plt.semilogy(range(N_iteration)[:10000], loss_ridge[:10000], label = 'Original Ridge
plt.semilogy(range(N_iteration)[:10000], loss_ridge_clean[:10000], label = 'Original
plt.axis('tight')
plt.xlabel("Iterations")
plt.ylabel("||w-w*||^2")
plt.legend()
plt.show()
```



In [ ]: