## **Problem Set 1. Solution**

2020-11

### 1 Problem 1

(1) Show that  $X \sim \mathcal{N}(0,1)$  is the maximum entropy distribution such that  $\mathbb{E}X = 0$  and  $\mathbb{E}X^2 = 1$ .

Solution.

$$\begin{aligned} & \min_{p} & & \int_{\mathcal{X}} p(x) \log p(x) \, \mathrm{d}x \\ & \text{s.t.} & & \int_{\mathcal{X}} p(x) \, \mathrm{d}x = 1 \\ & & & \int_{\mathcal{X}} x \, p(x) \, \mathrm{d}x = 0 \\ & & & \int_{\mathcal{X}} x^2 p(x) \, \mathrm{d}x = 1 \end{aligned}$$

The Lagrangian is

$$\mathcal{L}(p; \boldsymbol{\lambda}, \mu) = \int p(x) \log p(x) \, \mathrm{d}x + \lambda_0 \left( \int p(x) \, \mathrm{d}x - 1 \right) + \lambda_1 \int x \, p(x) \, \mathrm{d}x + \lambda_2 \left( \int x^2 p(x) \, \mathrm{d}x - 1 \right)$$

which is convex in p. Then taking

$$\frac{\partial \mathcal{L}}{\partial p} = \log p(x) + 1 + \lambda_0 + \lambda_1 x + \lambda_2 x^2 = 0$$

we have

$$p(x) = \exp\left(-\left(\lambda_0 + \lambda_1 x + \lambda_2 x^2\right) - 1\right) \geqslant 0.$$

 $p(x) = \exp\left(-\left(\lambda_0 + \lambda_1 x + \lambda_2 x^2\right) - 1\right)$  with  $\int x p(x) dx = 0$ , we have  $\lambda_1 = 0$ .

$$p(x) = \exp\left(-\left(\lambda_0 + \lambda_2 x^2\right) - 1\right) \text{ with } \int x^2 p(x) \, \mathrm{d}x = 1 \text{ and } \int p(x) \, \mathrm{d}x = 1, \text{ we have } \lambda_0 = \log \sqrt{2\pi} - 1, \lambda_2 = \frac{1}{2}.$$

Therefore, 
$$p(x) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{1}{2}x^2\right)$$
, i.e.,  $X \sim \mathcal{N}(0,1)$ .

(2) Generalize the result in (1) for the maximum entropy distribution given the first k moments, i.e.,  $\mathbb{E}X^i = m_i, i = 1, \ldots, k$ .

**Solution.** Write the problem as

$$\label{eq:problem} \begin{split} \min_p & \quad \int_{\mathcal{X}} p(x) \log p(x) \, \mathrm{d}x \\ \mathrm{s.t.} & \quad \int_{\mathcal{X}} x^n p(x) \, \mathrm{d}x = m_n, \quad n=0,\dots,k, \quad m_0 := 1 \end{split}$$

The Lagrangian is

$$\mathcal{L}(p; \lambda) = \int p(x) \log p(x) dx + \sum_{0 \leqslant n \leqslant k} \lambda_n \left( \int x^n p(x) dx - m_n \right)$$

which is convex in p. Then taking

$$\frac{\partial \mathcal{L}}{\partial p} = \log p(x) + 1 + \sum_{0 \leqslant n \leqslant k} \lambda_n x^n = 0$$

we have

$$p(x) = \exp\left(-\sum_{0 \leqslant n \leqslant k} \lambda_n x^n - 1\right),$$

an exponential family, then  $\lambda$  is determined by the constraints  $\int x^n p(x) dx = m_n, \ n = 0, \dots, k$ .

## 2 Problem 2

Let  $Y_1, \ldots, Y_n$  be a set of independent random variables with the following pdfs

$$p(y_i \mid \theta_i) = \exp(y_i b(\theta_i) + c(\theta_i) + d(y_i)), \quad i = 1, \dots, n$$

Let  $\mathbb{E}(Y_i) = \mu_i(\theta_i)$ ,  $g(\mu_i) = x_i^\mathsf{T} \beta$ , where g is the link function and  $\beta \in \mathbb{R}^d$  is the vector of model parameters.

(1) Denote  $g(\mu_i)$  as  $\eta_i$ , and let s be the score function of  $\beta$ . Show that

$$s_{j} = \sum_{i=1}^{n} \frac{(y_{i} - \mu_{i}) x_{ij}}{\mathbb{V}ar(Y_{i})} \frac{\partial \mu_{i}}{\partial \eta_{i}}, \quad j = 1, \dots, d$$

**Solution.** Let  $L_i := \log p(y_i \mid \theta_i) = y_i b(\theta_i) + c(\theta_i) + d(y_i)$ , then

$$s_{j} = \sum_{i=1}^{n} \frac{\partial L_{i}}{\partial \beta_{j}} = \sum_{i=1}^{n} \frac{\partial L_{i}}{\partial \theta_{i}} \frac{\partial \theta_{i}}{\partial \mu_{i}} \frac{\partial \mu_{i}}{\partial \eta_{i}} \frac{\partial \eta_{i}}{\partial \beta_{j}} = \sum_{i=1}^{n} \left( y_{i} \frac{\partial b(\theta_{i})}{\partial \theta_{i}} + \frac{\partial c(\theta_{i})}{\partial \theta_{i}} \right) \frac{\partial \theta_{i}}{\partial \mu_{i}} \frac{\partial \mu_{i}}{\partial \eta_{i}} x_{ij}, \quad j = 1, \dots, d.$$

By interchanging the differentiation  $\frac{\partial}{\partial \theta_i}$  and integration  $\mathbb{E}1, \mathbb{E}Y_i$ , we have

$$0 = \frac{\partial}{\partial \theta_i} \mathbb{E} 1 = \mu_i \frac{\partial b(\theta_i)}{\partial \theta_i} + \frac{\partial c(\theta_i)}{\partial \theta_i}$$
$$\frac{\partial \mu_i}{\partial \theta_i} = \frac{\partial}{\partial \theta_i} \mathbb{E} Y_i = (\mathbb{E} Y_i^2) \frac{\partial b(\theta_i)}{\partial \theta_i} + \mu_i \frac{\partial c(\theta_i)}{\partial \theta_i}.$$

then

$$\begin{split} y_i \frac{\partial b(\theta_i)}{\partial \theta_i} + \frac{\partial c(\theta_i)}{\partial \theta_i} &= \left( y_i \frac{\partial b(\theta_i)}{\partial \theta_i} + \frac{\partial c(\theta_i)}{\partial \theta_i} \right) - \left( \mu_i \frac{\partial b(\theta_i)}{\partial \theta_i} + \frac{\partial c(\theta_i)}{\partial \theta_i} \right) = \left( y_i - \mu_i \right) \frac{\partial b(\theta_i)}{\partial \theta_i} \\ &\frac{\partial \mu_i}{\partial \theta_i} &= \frac{\partial \mu_i}{\partial \theta_i} - \mu_i \left( \mu_i \frac{\partial b(\theta_i)}{\partial \theta_i} + \frac{\partial c(\theta_i)}{\partial \theta_i} \right) = \mathbb{V} \text{ar} \left( Y_i \right) \frac{\partial b(\theta_i)}{\partial \theta_i}. \end{split}$$

therefore

$$s_{j} = \sum_{i=1}^{n} \frac{(y_{i} - \mu_{i}) \frac{\partial b(\theta_{i})}{\partial \theta_{i}}}{\mathbb{V}\operatorname{ar}(Y_{i}) \frac{\partial b(\theta_{i})}{\partial \theta_{i}}} \frac{\partial \mu_{i}}{\partial \eta_{i}} x_{ij} = \sum_{i=1}^{n} \frac{(y_{i} - \mu_{i}) x_{ij}}{\mathbb{V}\operatorname{ar}(Y_{i})} \frac{\partial \mu_{i}}{\partial \eta_{i}}, \quad j = 1, \dots, d.$$

(2) Let  $\mathcal{I}$  be the Fisher information matrix. Show that

$$\mathcal{I}_{jk} = \mathbb{E}\left(s_j s_k\right) = \sum_{i=1}^n \frac{x_{ij} x_{ik}}{\mathbb{V} \text{ar}\left(Y_i\right)} \left(\frac{\partial \mu_i}{\partial \eta_i}\right)^2, \quad \forall \, 1 \leq j, k \leq d$$

$$\begin{split} \mathcal{I}_{jk} &= \mathbb{E} \left( s_j s_k \right) \\ &= \mathbb{E} \bigg( \sum_{i=1}^n \frac{\left( y_i - \mu_i \right) x_{ij}}{\mathbb{V} \mathrm{ar} \left( Y_i \right)} \frac{\partial \mu_i}{\partial \eta_i} \sum_{l=1}^n \frac{\left( y_l - \mu_l \right) x_{lk}}{\mathbb{V} \mathrm{ar} \left( Y_l \right)} \frac{\partial \mu_l}{\partial \eta_l} \bigg) \\ &= \sum_{1 \leqslant i,l \leqslant n} \frac{x_{ij} x_{lk} \mathbb{E} \left( y_i - \mu_i \right) \left( y_l - \mu_l \right)}{\mathbb{V} \mathrm{ar} \left( Y_l \right)} \frac{\partial \mu_i}{\partial \eta_i} \frac{\partial \mu_l}{\partial \eta_l} \\ &= \sum_{i=1}^n \frac{x_{ij} x_{ik}}{\mathbb{V} \mathrm{ar} \left( Y_i \right)} \left( \frac{\partial \mu_i}{\partial \eta_i} \right)^2, \quad \text{by independence.} \end{split}$$

#### 3 Problem 3

Use the following code to generate co-variate matrices X.

```
import numpy as np

np.random.seed(1234)

n = 100

X = np.random.normal(size=(n,2))
```

(1). Generate n = 100 observations Y following the logistic regression model with true parameter  $\beta_0 = (-2, 1)$ .

#### Solution.

```
import numpy as np
   from scipy.special import expit as sigmoid
   def generate_data(beta0, n=100):
       X = np.random.normal(size=(n, beta0.shape[0]))
       logits = X @ beta0
       probs = sigmoid(logits)
       return {"X":X, "logits":logits, "probs":probs}
   def generate_y(probs):
10
       y = np.random.binomial(1, probs)
11
       return y
   seed = 1234
14
   np.random.seed(seed)
15
beta0 = np.array([-2., 1.])
   data = generate_data(beta0, n=100)
   X, probs = data["X"], data["probs"]
   y = generate_y(probs=probs)
   print(y)
   [0\ 0\ 1\ 0\ 0\ 1\ 0\ 0\ 0\ 1\ 0\ 0\ 0\ 1\ 1\ 0\ 0\ 1\ 1\ 0\ 1\ 1\ 0\ 1\ 1\ 0\ 0\ 1\ 1\ 0
    1 0 0 0 0 1 1 0 0 1 0 0 0 1 0 0 0 0 1 0 0 1 0 1 1 1 1 1 0 0 0 1 1 0 0 0 1
    1 1 0 0 1 1 1 0 1 0 0 0 1 0 0 0 1 0 1 1 1 0 0 0 0 0]
```

(2). Find the MLE using the iteratively reweighted least square algorithm.

```
import numpy as np
from scipy import sparse
from scipy.special import expit as sigmoid
from numpy.linalg import inv as inverse
from numpy.linalg import norm
```

```
''' Readme:
            this function is defined to estimate
            the parameters of logistic regression model
            by IRLS, Iteratively Reweighted Least Square Algorithm.
        # initialization
        n, d = X.shape
        beta = inverse(X.TaX) a (X.Tay)
        W = sparse.dia_matrix((n, n))
16
        err_path = []
18
        # main
19
        for i in range(1, max_itr+1):
            logits = X @ beta
            probs = sigmoid(logits)
            W = sparse.diags(probs*(1-probs))
23
            beta_ = beta + inverse(X.TaWaX) a (X.Ta(y-probs))
            err = norm(beta_-beta)/norm(beta)
            err_path.append(err)
            beta = beta
28
            if i % 5 == 0:
                if not quiet:
30
                    print(f"err: {err:.3e}, itr: {i}")
            if err < epsilon:</pre>
32
                if not quiet:
                    print(f"err: {err:.3e}, itr: {i}")
34
                    print(f"MLE: {list(beta)}")
                break
        # returns
37
        out = {"beta":beta, "itr":i, "errs":err_path}
38
        return out
   out = irls_lr(X, y, quiet=0)
  err: 2.217e-06, itr: 5
  err: 1.627e-16, itr: 7
   MLE: [-1.3708659534317205, 0.6698777671314895]
```

def irls\_lr(X, y, max\_itr=200, epsilon=1e-12, quiet=True):

(3). Repeat (1) and (2) for 100 instances. Compare the MLEs with the asymptotical distribution  $\hat{\beta} \sim \mathcal{N}\left(\beta_0, \mathcal{I}^{-1}\left(\beta_0\right)\right)$ . Present your result with a scatter plot for MLEs with contours for the PDF of the asymptotical distribution.

```
W = sparse.diags(probs*(1-probs))
Fisher = X.T @ W @ X
cov = inverse(Fisher)
print(cov)

[[ 0.19350715 -0.0440933 ]
[-0.0440933    0.10205911]]
```

```
from scipy import stats
   import matplotlib.pyplot as plt
4 radius = 0.8
x0 = np.linspace(beta0[0]-radius, beta0[0]+radius, 50)
6 x1 = np.linspace(beta0[1]-radius, beta0[1]+radius, 50)
   X0, X1 = np.meshgrid(x0, x1) # create x0-x1 meshgrid
   pos = np.dstack((X0, X1))
                               # shape-(num1,num2,d)
  binorm_rv1 = stats.multivariate_normal(beta0, cov)
   Z1 = binorm_rv1.pdf(pos)
12
plt.figure(figsize=(6, 6))
plt.plot(betas[:, 0], betas[:, 1], 'o', mfc='none')
                                                        # scatter
cS = plt.contour(X0, X1, Z1, cmap='cool')
                                                        # contour
plt.clabel(CS, inline=1)
plt.title(r'Comparison ($n=100$)')
plt.savefig('./comparison_100.pdf', bbox_inches='tight')
plt.show()
```

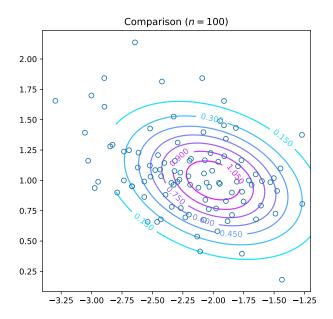


Figure 3.1: Comparison

(4). Try the same for n = 10000. Does the asymptotical distribution provide a better fit to the MLEs? You can use the empirical covariance matrix of the MLEs for comparison.

```
seed = 1234
   np.random.seed(seed)
   beta0 = np.array([-2., 1.])
   data = generate_data(beta0, n=100)
   X, probs = data["X"], data["probs"]
   betas_ = experiment(X, probs, num_tri=100)
   betas_cov_ = np.cov(betas_.T)
   W = sparse.diags(probs*(1-probs))
10
   Fisher = X.T a W a X
   cov_ = inverse(Fisher)
   print(cov_)
   print(betas_cov_)
   err = np.linalg.norm(cov_-betas_cov_,"fro")
   print(f"err:{err:.6f}, err_rel:{err/np.linalg.norm(cov_,'fro'):.6f}")
17
   data = generate_data(beta0, n=10000)
18
   X, probs = data["X"], data["probs"]
19
   betas = experiment(X, probs, num_tri=100)
   betas_mean = np.mean(betas, axis=0)
   betas_cov = np.cov(betas.T)
   W = sparse.diags(probs*(1-probs))
   Fisher = X.T a W a X
```

```
plt.figure(figsize=(12, 6))
   radius = 0.4
   plt.subplot(121)
   x0 = np.linspace(beta0[0]-radius, beta0[0]+radius, 50)
  x1 = np.linspace(beta0[1]-radius, beta0[1]+radius, 50)
   X0, X1 = np.meshgrid(x0, x1) # create x0-x1 meshgrid
   pos = np.dstack((X0, X1))
                               # shape-(num1,num2,d)
   binorm rv1 = stats.multivariate normal(beta0, cov )
10
   Z1 = binorm_rv1.pdf(pos)
   plt.plot(betas[:, 0], betas[:, 1], 'o', mfc='none')
                                                       # scatter
CS1 = plt.contour(X0, X1, Z1, cmap='cool')
                                                          # contour
   plt.clabel(CS1, inline=1)
   plt.title(r'Comparison ($n=10000$)')
   plt.savefig('./comparison_10000.pdf', bbox_inches='tight')
17
   plt.subplot(122)
   x2 = np.linspace(betas_mean[0]-radius, betas_mean[0]+radius, 50)
19
   x3 = np.linspace(betas_mean[1]-radius, betas_mean[1]+radius, 50)
   X2, X3 = np.meshgrid(x2, x3) # create x0-x1 meshgrid
   pos2 = np.dstack((X2, X3))
                                 # shape-(num1,num2,d)
23
binorm_rv2 = stats.multivariate_normal(betas_mean, betas_cov)
Z2 = binorm rv2.pdf(pos2)
CS1 = plt.contour(X0, X1, Z1, cmap='cool')
plt.clabel(CS1, inline=1)
cs2 = plt.contour(X2, X3, Z2, cmap='spring')
```

```
plt.clabel(CS2, inline=1)
plt.title(r'Comparison with asymptotical distribution')
plt.savefig('./Asymptotical distribution.pdf', bbox_inches='tight')

plt.show()
```

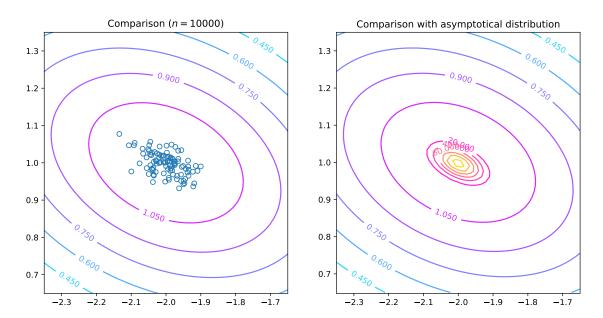


Figure 3.2: Comparison

The asymptotic distribution with the larger sample size, which has a more intense concentration and a lower error rate, suggests a better fit for the MLEs.

## 4 Problem 4

Consider the probit regression model

$$Y \mid X, \beta \sim \text{Bernoulli } (p), \quad p = \Phi(X\beta)$$

where  $\Phi$  is the cumulative distribution function of the standard normal distribution. Similarly as in Problem 3, generate a large covariate matrix X with 100000 instances and 100 features, and response Y with true parameter  $\beta_0$ 

```
import numpy as np
np.random.seed(1234)

n, d = 100000, 100

X = np.random.normal(size=(n, d))
beta_0 = np.random.normal(size=d)
```

(1). Compare gradient descent and Nesterov's accelerated gradient descent.

```
def GD(self,init,tol = 1e-6, step_size = 0.0001, maxit = 1000):
```

```
beta_old = np.zeros(shape = (np.shape(init)[0],)) + 1
            beta new = init
            likelihood = np.array([])
            l = 1000
            l_next = 1
            for i in range(1, maxit +1):
                l = l_next
                if i % 100 == 0 :
                    print(l)
10
                grad = self.gradient(beta_new)
11
                beta_old = beta_new
                beta_new = beta_old + step_size * grad
                l_next = self.loglikelihood(beta_new)
                likelihood = np.append(likelihood,l_next)
                if abs(l - l_next) / abs(l) < tol:</pre>
16
                    break
            return beta_new, likelihood
18
19
   def NAG(self, init, tol = 1e-6, step_size = 0.0001, maxit = 1000):
        beta_previous = init
        beta_now = init
        beta_new = init
       likelihood = np.array([])
24
       l = 1000
25
        l_next = 1
        for i in range(1, maxit +1):
            l = l_next
28
            beta_previous = beta_now
            beta now = beta new
30
            if i % 100 == 0 :
31
                print(l)
            y = beta_now + (i - 2) / (i + 1) * (beta_now - beta_previous)
            grad = self.gradient(y)
34
            beta_new = y + step_size * grad
            l_next = self.loglikelihood(beta_new)
            likelihood = np.append(likelihood,l_next)
37
            if abs(l - l_next) / abs(l) < tol:</pre>
                break
        return beta_new, likelihood
40
```

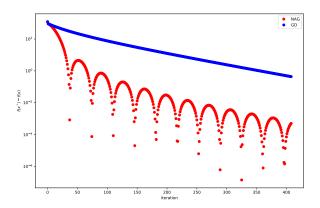


Figure 4.3: Comparison: SGD and NAG

Although the objective function is non-monotone decreasing when using nesterov's acceleration, it can reach a much optimal value in a fairly less amount of time.

(2). Compare vanilla stochastic gradient descent with different adaptive stochastic gradi- ent descent methods, including AdaGrad, RMSprop, and Adam. Using minibatch sizes 32,64,128.

```
def SGD(self, init, tol = 1e-6, step_size = 0.1, batch_size = 32, maxit = 2500):
        beta_old = np.zeros(shape = (np.shape(init)[0],)) + 1
        beta_new = init
       likelihood = np.array([])
        l = 1000
        l_next = 1
        for i in range(1, maxit +1):
            l = l_next
            if i % 100 == 0 :
                print(l)
10
            grad = self.stoch_grad(beta_new, batch = batch_size)
11
            beta_old = beta_new
            beta_new = beta_old + step_size * grad
            l_next = self.loglikelihood(beta_new)
14
            likelihood = np.append(likelihood,l_next)
            if abs(l - l_next) / abs(l) < tol:</pre>
16
                break
        return beta_new, likelihood
19
   def AdaGrad(self, init, tol = 1e-10, epsilon = 1e-8, step_size = 0.2, batch_size = 32,
20
21
                maxit = 2500):
        beta_new = init
        likelihood = np.array([])
        l = 1000
        l next = 1
        grad_sum = 0
26
        for i in range(1, maxit +1):
27
            l = l next
28
```

```
if i % 100 == 0 :
                print(l)
30
            grad = self.stoch_grad(beta_new, batch = batch_size)
31
            grad_sum = grad_sum + np.square(grad)
            beta_new = beta_new + step_size * grad / np.sqrt(grad_sum + epsilon)
            l_next = self.loglikelihood(beta_new)
34
            likelihood = np.append(likelihood,l_next)
            if abs(l - l_next) / abs(l) < tol:</pre>
                break
37
        return beta_new, likelihood
38
   def RMSprop(self, init, tol = 1e-10, epsilon = 1e-8, step_size = 0.01, batch_size = 32,
40
                maxit = 2500):
        beta new = init
42
        likelihood = np.array([])
43
        l = 1000
        l next = 1
45
        grad_sum = 0
46
        for i in range(1, maxit +1):
            l = l_next
            if i % 100 == 0 :
49
                print(l)
            grad = self.stoch_grad(beta_new, batch = batch_size)
            grad_sum = 0.9 * grad_sum + 0.1 * np.square(grad)
52
            beta_new = beta_new + step_size * grad / np.sqrt(grad_sum + epsilon)
            l_next = self.loglikelihood(beta_new)
            likelihood = np.append(likelihood,l_next)
55
            if abs(l - l_next) / abs(l) < tol:</pre>
        return beta_new, likelihood
58
   def Adam(self, init, tol = 1e-10, epsilon = 1e-8, step_size = 0.008, batch_size = 32,
60
             maxit = 2500):
61
        beta1 = 0.9
62
        beta2 = 0.999
63
       beta_new = init
64
       likelihood = np.array([])
        l = 1000
        l_next = 1
67
        grad_sum = 0
        grad_square = 0
        for i in range(1, maxit +1):
70
            l = l_next
71
            if i % 100 == 0 :
                print(l)
            grad = self.stoch_grad(beta_new, batch = batch_size)
74
            grad_sum = beta1 * grad_sum + (1 - beta1) * grad
```

```
grad_square = beta2 * grad_square + (1 - beta2) * np.square(grad)

beta1_power = beta1 ** (i + 1)

beta2_power = beta2 ** (i + 1)

mt = grad_sum / (1 - beta1_power)

vt = grad_square / (1 - beta2_power)

beta_new = beta_new + step_size * mt / np.sqrt(vt + epsilon)

l_next = self.loglikelihood(beta_new)

likelihood = np.append(likelihood,l_next)

if abs(l - l_next) / abs(l) < tol:

break

return beta_new, likelihood
```

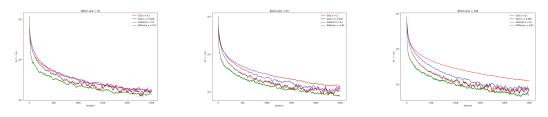


Figure 4.4: Comparison: batch size = 32, 64, 128

We can see that the adaptive learning rate methods can rapidly fall to a minimum value at the beginning of training, and this becomes more obvious when we enlarge batch size. Among the four, AdaGrad performs the best, while RMSProp fluctuates a lot. As the batch size enlarges, all of the adaptive learning rate methods can reach a lower value.

(3). Bonus question. Generate a random mask matrix M as follows and use it to sparsify the covariance matrix X

```
np.random.seed(1234)

sparse_rate = 0.3

M = np.random.uniform(size=(n,d)) < sparse_rate

X[M] = 0.</pre>
```

Repeat your experiments in (2), and compare with the results for the full covariance matrix

# Solution.

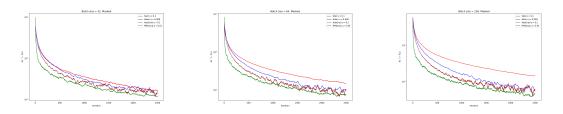


Figure 4.5: Comparison: batch size = 32, 64, 128

In this setting, the difference between SGD and its adaptive variants becomes more obvious, especially in the case of large batch size. Other observations are roughly the same as (2).