

Introduction to Machine Learning

Homework 5: Gradient Calculations and Nonlinear Optimization

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[Solution]

1.

1. Suppose we want to fit a model,

$$\hat{y} = \frac{1}{w_0 + \sum_{j=1}^d w_j x_j},$$

for parameters \mathbf{w} . Given training data (\mathbf{x}_i, y_i) , $i = 1, \dots, n$, a nonlinear least squares fit could use the loss function,

$$J(\mathbf{w}) = \sum_{i=1}^n \left[y_i - \frac{1}{w_0 + \sum_{j=1}^d w_j x_{ij}} \right]^2$$

(a) Find a function $g(\mathbf{z})$ and matrix \mathbf{A} such that the loss function is given by,

$$J(\mathbf{w}) = g(\mathbf{z}), \quad \mathbf{z} = \mathbf{A}\mathbf{w},$$

and $g(\mathbf{z})$ is factorizable, meaning $g(\mathbf{z}) = \sum_i g_i(z_i)$ for some functions $g_i(z_i)$.

(b) What is the gradient $\nabla J(\mathbf{w})$?

(c) What is the gradient descent update for \mathbf{w} ?

(d) Write a few lines of python code to compute the loss function $J(\mathbf{w})$ and $\nabla J(\mathbf{w})$.

$$(a) \quad g(\mathbf{z}) = \sum_{k=1}^n [y_k - z_k^{-1}]^2 = \sum_{k=1}^n g(z_k)$$

$$\mathbf{A} = \begin{bmatrix} A_{11} & A_{12} & \dots & A_{1d} \end{bmatrix}$$

$$\dots \quad \dots \quad \dots \quad \dots$$

$$\begin{bmatrix} A_{n1} & A_{n2} & \dots & A_{nd} \end{bmatrix}$$

(b)

$$c_2) = \nabla_{\vec{w}} J(\vec{w}) = \begin{bmatrix} \frac{\partial J(\vec{w})}{\partial w_0} \\ \frac{\partial J(\vec{w})}{\partial w_1} \\ \vdots \\ \frac{\partial J(\vec{w})}{\partial w_d} \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^n 2(y_i - \frac{1}{w_0 + \sum_{j=1}^d w_j x_{ij}}) \cdot \frac{1}{(w_0 + \sum_{j=1}^d w_j x_{ij})^2} \\ \sum_{i=1}^n 2(y_i - \frac{1}{w_0 + \sum_{j=1}^d w_j x_{ij}}) \cdot \frac{x_{i1}}{(w_0 + \sum_{j=1}^d w_j x_{ij})^2} \\ \vdots \\ \sum_{i=1}^n 2(y_i - \frac{1}{w_0 + \sum_{j=1}^d w_j x_{id}}) \cdot \frac{x_{id}}{(w_0 + \sum_{j=1}^d w_j x_{id})^2} \end{bmatrix}$$

That is the gradient

(C)

□ Gradient descent algorithm:

- Start with initial w^0
- $w^{k+1} = w^k - \alpha_k \nabla f(w^k)$
- Repeat until some stopping criteria

□ α_k is called the **step size**

- In machine learning, this is called the **learning rate**

$\nabla f(w^k)$ is known, we can choose α_k as learning rate

(D)

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: y = # yi known from data
  tmp = 1 / ( w[0] + x.dot(w[1:]))

J = np.sum ( (y- tmp)**2 )
Jgrad = (y-tmp)* ( (x).dot(tmp**2) )

```

Use broadcasting

3.

3. *Matrix minimization.* Consider the problem of finding a matrix $\mathbf{P} \in \mathbb{R}^{m \times m}$ to minimize the loss function,

$$J(\mathbf{P}) = \sum_{i=1}^n \left[\frac{z_i}{y_i} - \ln(z_i) \right], \quad z_i = \mathbf{x}_i^T \mathbf{P} \mathbf{x}_i.$$

The problem arises in wireless communications where an m -antenna receiver wishes to estimate a spatial covariance matrix \mathbf{P} from n power measurements. In this setting, $y_i > 0$ is the i -th receive power measurement and \mathbf{x}_i is the beamforming direction for that measurement. In reality, the quantities would be complex, but for simplicity we will just look at the real-valued case. See the following article for more details:

Eliasi, Parisa A., Sundeep Rangan, and Theodore S. Rappaport. "Low-rank spatial channel estimation for millimeter wave cellular systems," *IEEE Transactions on Wireless Communications* 16.5 (2017): 2748-2759.

- What is the gradient $\nabla_{\mathbf{P}} z_i$?
- What is the gradient $\nabla_{\mathbf{P}} J(\mathbf{P})$?
- Write a few lines of python code to evaluate $J(\mathbf{P})$ and $\nabla_{\mathbf{P}} J(\mathbf{P})$ given data \mathbf{x}_i and y_i . You can use a for loop.
- See if you can rewrite (c) without a for loop. You will need Python broadcasting.

(a) $\text{ZGrad}[i] = \mathbf{x}[i].\text{dot}(\mathbf{P}.\text{dot}(\mathbf{x}[i].\text{T}))$

(b)
$$\mathbf{Jgrad} = \sum_{i=1}^n \left[\frac{\text{ZGrad}[i]}{y[i]} - \frac{\text{ZGrad}[i]}{z[i]} \right]$$

(n,n)

```

# x y known
for i in range(n):
    z[i] = x[i].T.dot(P.dot(x[i]))
    zgrad[i] = x[i].dot(P.dot(x[i].T)) # (n,n)
    J = J + (z[i]/y[i] - ln(z[i]))      # (n,)
    Jgrad += zgrad[i]/y[i] - zgrad[i]/z[i] # (n,n)

```

(c)

(d) broadcasting:

```
J = z[:,]/y[:,] - ln(z[:,])      # (n,)
Jgrad = zgrad[:,]/y.reshape(n,-1) - zgrad[:,]/z.reshape(n,-1)  # (n,n)
```

Let it be n x n

4.

4. *Nested optimization.* Suppose we are given a loss function $J(\mathbf{w}_1, \mathbf{w}_2)$ with two parameter vectors \mathbf{w}_1 and \mathbf{w}_2 . In some cases, it is easy to minimize over one of the sets of parameters, say \mathbf{w}_2 , while holding the other parameter vector (say, \mathbf{w}_1) constant. In this case, one could perform the following *nested* minimization: Define

$$J_1(\mathbf{w}_1) := \min_{\mathbf{w}_2} J(\mathbf{w}_1, \mathbf{w}_2), \quad \hat{\mathbf{w}}_2(\mathbf{w}_1) := \arg \min_{\mathbf{w}_2} J(\mathbf{w}_1, \mathbf{w}_2),$$

which represent the minimum and argument of the loss function over \mathbf{w}_2 holding \mathbf{w}_1 constant. Then,

$$\hat{\mathbf{w}}_1 = \arg \min_{\mathbf{w}_1} J_1(\mathbf{w}_1) = \arg \min_{\mathbf{w}_1} \min_{\mathbf{w}_2} J(\mathbf{w}_1, \mathbf{w}_2).$$

Hence, we can find the optimal \mathbf{w}_1 by minimizing $J_1(\mathbf{w}_1)$ instead of minimizing $J(\mathbf{w}_1, \mathbf{w}_2)$ over \mathbf{w}_1 and \mathbf{w}_2 .

(b) Suppose we want to minimize a nonlinear least squares,

$$J(\mathbf{a}, \mathbf{b}) := \sum_{i=1}^n \left(y_i - \sum_{j=1}^d b_j e^{-a_j x_i} \right)^2,$$

over two parameters \mathbf{a} and \mathbf{b} . Given parameters \mathbf{a} , describe how we can minimize over \mathbf{b} . That is, how can we compute,

$$\hat{\mathbf{b}} := \arg \min_{\mathbf{b}} J(\mathbf{a}, \mathbf{b}).$$

(c) In the above example, how would we compute the gradients,

$$\nabla_{\mathbf{a}} J(\mathbf{a}, \mathbf{b}).$$

(b) Given \mathbf{a} ,

let $J_{\text{grad}}(\mathbf{b}) = \nabla_{\mathbf{a}} J(\mathbf{a}, \mathbf{b}) \cdot 0$, solve the related \mathbf{b}

That is local minima, compare these solutions and get global minima

(c)

a known, b unknown

$$\nabla_a J(a, b) = \begin{bmatrix} \frac{\partial J}{\partial b_1} \\ \frac{\partial J}{\partial b_2} \\ \vdots \\ \frac{\partial J}{\partial b_n} \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^n (y_i - \sum_{j=1}^d b_j e^{-a_j x_i}) (-b_1 e^{-a_1 x_i}) \\ \vdots \\ \sum_{i=1}^n (y_i - \sum_{j=1}^d b_j e^{-a_j x_i}) (-b_n e^{-a_n x_i}) \end{bmatrix}$$

Let it be = 0