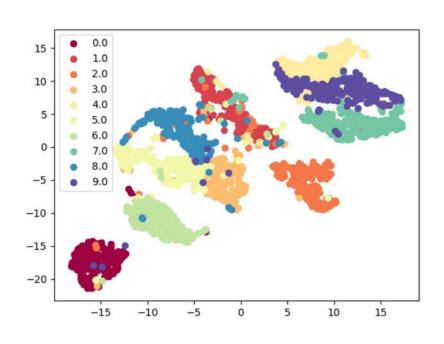


# Python编程与人工智能实践

算法篇: 数据降维-UMAP (Uniform Manifold Approximation and Projection)

# 均匀流形逼近与投影



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# **UMAP** (Uniform Manifold Approximation and Projection)

UMAP 是新近提出的一种新型的数据降维(数据可视化)方法。 其算法原理以及降维效果与t-sne类似,但有以下改进:

- (1) 比t-sne 可以得到更好的数据聚拢效果,能能够表达更好的局部结构。
- (2) 运算效率以及运算速度比t-sne好的多,可以适用于大规模数据降维
  - (3) 可以实现任意维度的降维

参考文献: [1] Mcinnes L, Healy J. UMAP: Uniform Manifold Approximation and Projection for Dimension Reduction[J]. The Journal of Open Source Software, 2018, 3(29):861.

论文代码: https://github.com/lmcinnes/umap

参考文案: [译]理解 UMAP(1): UMAP是如何工作的 & UMAP 与 tSNE的原理对比 - 知乎 (zhihu.com)

2021/10/16 https://zhuanlan.zhihu.com/p/150788883

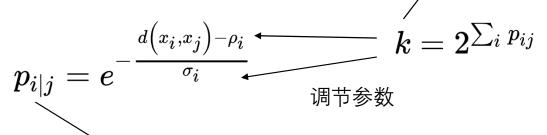


- •UMAP算法本身的理论推导比较复杂,涉及到黎曼几何、 拓扑代数等复杂的数学理论,但具体实现过程和t-sne算 法类似:
- (1) 设计一个函数 (**概率**) 来构建高维样本点,两两之间的关系 (联合概率)
- (2) 构建另一个函数 (**概率**) 来构建低维样本点两两之间的关系
- (3) 构造一个损失函数,通过学习的方法(梯度下降)令高维样本点之间的关系和低维样本点之前的关系尽可能相似。





条件概率



只考虑k个近邻点

联合概率 
$$p_{ij}=p_{i|j}+p_{j|i}-p_{i|j}p_{j|i}$$
 保证对称性

(2) 低维点之间的关系

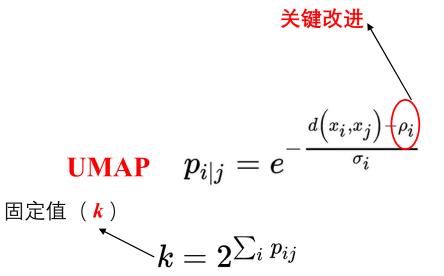
$$q_{ij} = \left(1 + a(y_i - y_j)^{2b}
ight)^{-1}$$
 通过调节 a,b 可以调整映射后低维数据的聚拢情况



# 与t-sen的比较

# (1) 高维点关系:

t-sne 
$$p_{j|i} = rac{\exp\left(-||x_i-x_j||^2/2\sigma_i^2
ight)}{\sum_{k 
eq i} \exp\left(-||x_i-x_k||^2/2\sigma_i^2
ight)}$$
 固定的 松弛系数  $\log(\operatorname{Per}) = -\sum_j p_{j|i} \log(p_{j|i})$ 



在具体应用中  $dig(x_i,x_jig)$  主要决定了  $p_{i|j}$  的输出

t-sne: 如果有一个点i距离所有的点都很远,那么所有的  $p_{i|j}$  都接近0,会造成图的不连接

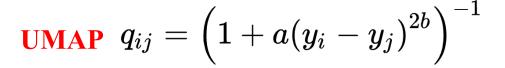
UMAP: 引入 $\rho_i$  (距离点i最近的点的距离) 保证至少有一个  $p_{i|j}=1$  , 保证图的连通性

去掉正则项,减少计算复杂度

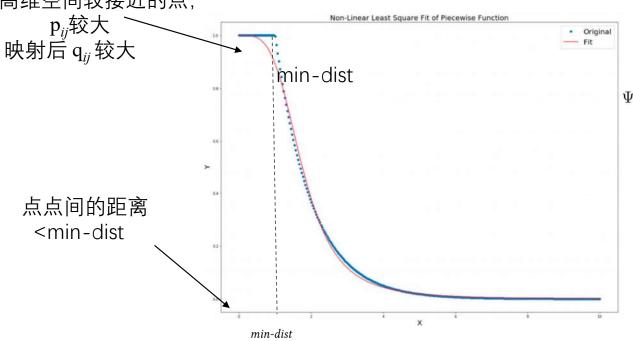


# (2) 低维点的关系

**t-sne** 
$$q_{ij} = \frac{\left(1 + \|y_i - y_j\|^2\right)^{-1}}{\sum_{k \neq l} \left(1 + \|y_k - y_l\|^2\right)^{-1}}.$$



高维空间较接近的点,



去掉正则项,增加了超参数a.b

a,b的设置的目的是为了拟合分段函数:

$$\Psi(\mathbf{x}, \mathbf{y}) = \begin{cases} 1 & \text{if } \|\mathbf{x} - \mathbf{y}\|_2 \leq \text{min-dist} \\ \exp(-(\|\mathbf{x} - \mathbf{y}\|_2 - \text{min-dist})) & \text{otherwise} \end{cases}$$

min-dist 越小,投影后相似的点越聚集 min-dist 越大、投影后相似的点越稀疏

在实际应用中 min-dist 为超参数 a,b通过曲线拟合的方式获取



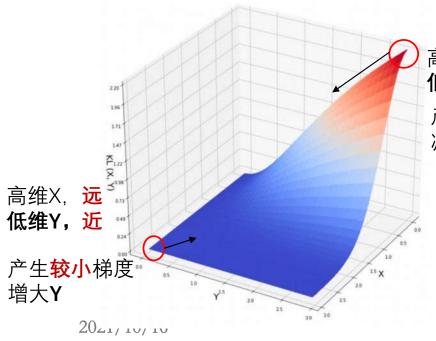
(3) 损失函数方面

$$X$$
 高维点  $Y$  低维点 间距离

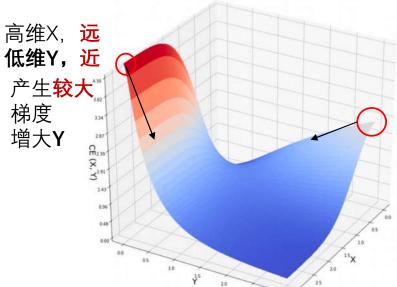
**t-sne** 
$$C = KL(P||Q) = \sum_{i} \sum_{i} p_{ij} \log \frac{p_{ij}}{q_{ij}}.$$

$$egin{aligned} \mathbf{UMAP} \quad CE(X,Y) &= \sum_i \sum_j \left[ p_{ij}(X) \log \left( rac{p_{ij}(X)}{q_{ij}(Y)} 
ight) + (1-p_{ij}(X)) \log \left( rac{1-p_{ij}(X)}{1-q_{ij}(Y)} 
ight) 
ight] \end{aligned}$$

t-sne



高维X, **近 低维Y, 远** 产生<mark>较大</mark>梯度 减少**Y** 



高维X, 近 低维Y, 远 产生<mark>较大</mark>梯度 减少Y

UMAP比tsne 更适合令高维空间较远的 点在低维空间也远

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## UMAP 算法流程:

- (1) 给定 min-dist , 利用曲线拟合的方法求超参数 a,b
- (2) 给定高维数据 X, [N,D],对每个样本点计算k个近邻点 求每个点的参数  $ho_i$  : 距离点i最近的点的距离  $\sigma_i$  利用  $k=2^{\sum_i p_{ij}}$  通过二值搜索得到

计算条件概率  $p_{i|j}=e^{-rac{d\left(x_i,x_j
ight)ho_i}{\sigma_i}}$  并得到联合概率  $p_{ij}=p_{i|j}+p_{j|i}-p_{i|j}p_{j|i}$ 

(3) 低维映射部分

将  $p_{ij}$  看做一个图,采用图割的方法,利用谱聚类,实现低维数据初始化

正则化 拉普拉斯矩阵

对L进行特征值分解,取特征值较小的d个特征值所对应的特征向量



训练部分:

$$CE(X,Y) = \sum_i \sum_j \left[ p_{ij}(X) \log \left(rac{p_{ij}(X)}{q_{ij}(Y)}
ight) + (1-p_{ij}(X)) \log \left(rac{1-p_{ij}(X)}{1-q_{ij}(Y)}
ight) 
ight]$$

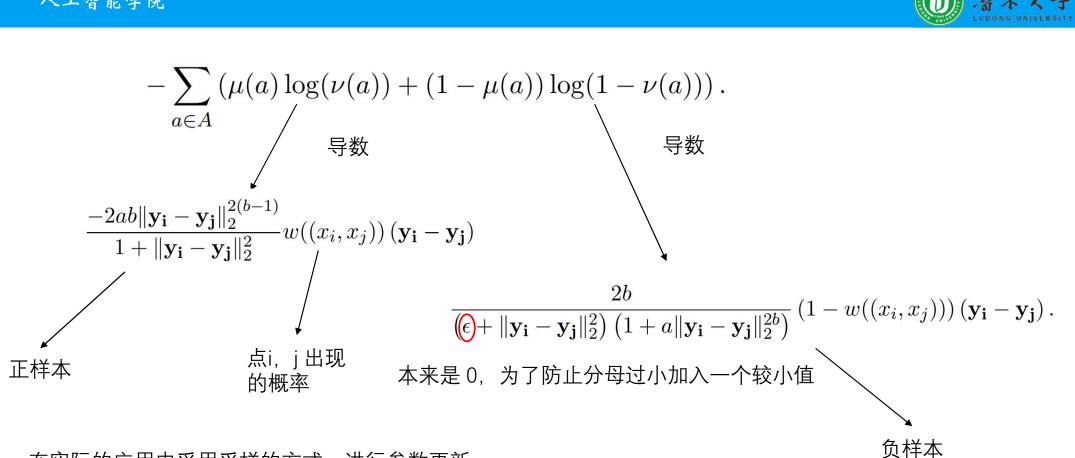
$$C((A,\mu),(A,\nu)) = \sum_{a \in A} \mu(a) \log \left(\frac{\mu(a)}{\nu(a)}\right) + (1-\mu(a)) \log \left(\frac{1-\mu(a)}{1-\nu(a)}\right)$$

$$= \sum_{a \in A} (\mu(a) \log(\mu(a)) + (1-\mu(a)) \log(1-\mu(a)))$$

$$- \sum_{a \in A} (\mu(a) \log(\nu(a)) + (1-\mu(a)) \log(1-\nu(a))).$$
与y相关

最小化: 
$$-\sum_{a\in A} (\mu(a)\log(\nu(a)) + (1-\mu(a))\log(1-\nu(a))).$$





在实际的应用中采用采样的方式,进行参数更新 概率大, 多更新, 概率小, 少更新



**if** Random()  $\leq p$  **then** # Sample simplex with probability p

$$y_a \leftarrow y_a + \alpha \cdot \nabla(\log(\Phi))(y_a, y_b)$$

 $\textbf{for} \ i \leftarrow 1, \dots, \textbf{n-neg-samples} \ \textbf{do}$ 

 $c \leftarrow \text{random sample from Y}$ 

$$y_a \leftarrow y_a + \alpha \cdot \nabla(\log(1 - \Phi))(y_a, y_c)$$

$$\alpha \leftarrow 1.0 - e/\text{n-epochs}$$

## return Y

```
人工智能学院
```

## 代码实现:

# 第一步 计算高维空间点之间的距离 (概率)

```
adef get graph Inputs(X,n neighbors,local connectivity=1):
    n samples = X.shape[0]
                                                                    计算K近邻
    # 计算每个样本点的N个临近点的位置和距离
    NN index, NN dists = get n neighbors(X, n neighbors)
    # 计算每个样本的 sigm 与 rho 为后边的图计算提供参数
    sigmas, rhos = compute sigmas and rhos (NN dists, n neighbors, local connectivity)
    # 计算两点间的 连接强度 即计算条件概率 Pili
    rows, cols, vals = compute membership strengths (NN index, NN dists, sigmas, rhos)
    # 构造稀疏矩阵
    result = scipy.sparse.coo matrix((vals, (rows, cols)), shape=(X.shape[0], X.shape[0]))
    result.eliminate zeros() # 去掉0
    # 计算联合概率 Pij
    transpose = result.transpose()
    prod matrix = result.multiply(transpose)
    \# Pij = Pj|i + Pi|j - Pj|i* Pi|j
    result = result + transpose - prod matrix
    return result
```

```
# x 维度 [N,D]

def cal_pairwise_dist(x):
    print("compute distance")
    N,D = np.shape(x)

dist = np.zeros([N,N])

for i in tqdm(range(N)):
    for j in range(N):
        dist[i,j] = np.sqrt(np.dot((x[i]-x[j]),(x[i]-x[j]).T))

#返回任意两个点之间距离
return dist
```

```
# 获取每个样本点的 n_neighbors个临近点的位置以及距离

def get_n_neighbors(data, n_neighbors = 15):
    dist = cal_pairwise_dist(data)
    dist[dist < 0] = 0
    N = dist.shape[0]
    NN_index = np.argsort(dist,axis=1)[:,0:n_neighbors]
    NN_dist = np.sort(dist,axis=1)[:,0:n_neighbors]
    return NN index,NN dist
```



```
求每个点的参数 
ho_i : 距离点i最近的点的距离 \sigma_i 利用 k=2^{\sum_i p_{ij}} 通过二值搜索得到
```

```
# 计算每个样本点的参数 sigmas 以及 rhos
def compute sigmas and rhos (distances, k,
                          local connectivity=1, n iter=64,
                          tol = 1.0e-5, min k dis scale=1e-3):
   print("computing sigmas and rhos")
    # 获取样本数目
   N= distances.shape[0]
    # 定义变量存储每个样本的 sigma 和 rho
    rhos = np.zeros(N, dtype=np.float32)
    sigmas = np.zeros(N, dtype=np.float32)
   mean distances = np.mean(distances)
    target = np.log2(k)
    for i in tqdm(range(N)):
       10 = 0.0
       hi = np.inf
       mid = 1.0
       # rho i 为距离第i个样本最近的第local connectivity个距离
       ith distances = distances[i]
       non zero dists = ith distances[ith distances > 0.0]
       rhos[i] = non zero dists[local connectivity - 1]
```

```
# 通过2值搜索的方法计算sigma i
for n in range(n iter):
    psum = 0.0
    for j in range(1, distances.shape[1]):
        d = distances[i, j] - rhos[i]
        if d > 0:
            psum += np.exp(-(d / mid))
        else:
            psum += 1.0
    if np.fabs(psum - target) < tol:</pre>
        break
    if psum > target:
       hi = mid
       mid = (lo + hi) / 2.0
    else:
        lo = mid
        if hi == np.inf:
           mid *= 2
       else:
            mid = (lo + hi) / 2.0
sigmas[i] = mid
# 进一步处理 防止 sigma i 过小
if rhos[i] > 0.0:
    mean ith distances = np.mean(ith distances)
    if sigmas[i] < min k dis scale * mean ith distances:</pre>
        sigmas[i] = min k dis scale * mean ith distances
 # rhos[i]<=0 N个近邻点距离过近
else:
    if sigmas[i] < min k dis scale * mean distances:</pre>
         sigmas[i] = min k dis scale * mean distances
```



```
# 计算两点间的连接强度
                                                                                p_{i|j} = e^{-rac{dig(x_i,x_jig)-
ho_i}{\sigma_i}}
def compute membership strengths(NN index,NN dists,sigmas,rhos):
    print("compute membership strengths")
    n samples, n neighbors = np.shape(NN index)
    rows = np.zeros(n samples*n neighbors, dtype=np.int32)
    cols = np.zeros(n samples*n neighbors, dtype=np.int32)
    vals = np.zeros(n samples*n neighbors, dtype=np.float32)
    for i in tqdm(range(n samples)):
       for j in range(n neighbors):
            if NN index[i, j] == i:
                val = 0.0
            elif NN dists[i, j] - rhos[i] \leq 0.0 or sigmas[i] == 0.0:
                val = 1.0
            else:
                val = np.exp(-((NN dists[i, j] - rhos[i]) / (sigmas[i])))
            rows[i * n neighbors + j] = i
            cols[i * n neighbors + j] = NN index[i, j]
            vals[i * n neighbors + j] = val
    return rows, cols, vals
```



```
∃def get graph Inputs (X, n neighbors, local connectivity=1):
    n \text{ samples} = X.\text{shape}[0]
    # 计算每个样本点的N个临近点的位置和距离
    NN index, NN dists = get n neighbors (X, n neighbors)
    # 计算每个样本的 sigm 与 rho 为后边的图计算提供参数
    sigmas, rhos = compute sigmas and rhos (NN dists, n neighbors, local connectivity)
    # 计算两点间的 连接强度 即计算条件概率 Pili
    rows, cols, vals = compute membership strengths(NN index,NN dists,sigmas,rhos)
    # 构造稀疏矩阵
    result = scipy.sparse.coo matrix((vals, (rows, cols)), shape=(X.shape[0], X.shape[0]))
    result.eliminate zeros() # 去掉0
                                                                                                    构造稀疏矩阵
    # 计算联合概率 Pij
                                                                                                    返回联合概率
    transpose = result.transpose()
    prod matrix = result.multiply(transpose)
    \# Pi\overline{j} = Pj|i + Pi|j - Pj|i* Pi|j
    result = result + transpose - prod matrix
    return result
```



```
def get embedding(graph,
                                                                    # 利用谱分析的方法,借助graph,对低维数据进行初始化
                dim,a,b,
                                                                    initialisation = init embedding spectral (graph, dim)
                negative sample rate,
                n epochs=None,
                                                                    # 加入一些随机数据增加随机性
                initial alpha=1.0):
                                                                    expansion = 10.0 / np.abs(initialisation).max()
                                                                    embedding = (initialisation * expansion).astype(
   # 行列交换
                                                                        np.float32
   graph = graph.tocoo()
                                                                    ) + np.random.normal(
   graph.sum duplicates()
                                                                        scale=0.0001, size=[graph.shape[0], dim]
   # 顶点数目
                                                                    ).astype(
   n vertices = graph.shape[1]
                                                                        np.float32
                                                                    )
   # 计算迭代轮次 数据越少迭代轮次越多
   if n epochs is None:
                                                                    # 计算图中每条边,每隔多少个epoch 更新一次
       if graph.shape[0] <= 10000:
                                                                    epochs per sample = make epochs per sample (graph.data, n epochs)
           n = 500
                                                                    # 负样本,每隔多少个epoch 更新一次
       else:
                                                                    epochs per negative sample = epochs per sample/negative sample rate
           n = 200
   # 边的权重过低,无法采样,将权重设置为0
   if n epochs > 10:
       graph.data[graph.data < (graph.data.max() / float(n epochs))] = 0.0</pre>
                                                                    # 开始进行训练, 获取 embedding
   graph.eliminate zeros()
                                                                    head = graph.row
                                                                    tail = graph.col
                                                                    # 训练获取降维数据
                                                                    embedding =train embedding(embedding,embedding,
                                                                                            head, tail,
                                                                                            epochs per sample, epochs per negative sample,
                                                                                            a,b,init alpha, n epochs, n vertices)
                                                                    return embedding
```



```
warn(
# 谱分析法进行初始化
def init_embedding_spectral(graph,dim):
    n samples = graph.shape[0]
    k = dim
    diag data = np.asarray(graph.sum(axis=0))
                                                                      return np.random.uniform(low=-10.0, high=10.0, size=(graph.shape[0], dim))
    # Normalized Laplacian
    I = scipy.sparse.identity(graph.shape[0], dtype=np.float64)
    D = scipy.sparse.spdiags(
        1.0 / np.sqrt(diag data), 0, graph.shape[0], graph.shape[0]
    )
    L = I - D * graph * D
    num lanczos vectors = max(2 * k + 1, int(np.sqrt(graph.shape[0])))
    try:
        if L.shape[0] < 2000000:
           eigenvalues, eigenvectors = scipy.sparse.linalg.eigsh(
               L,
               k,
               which="SM",
               ncv=num lanczos vectors,
               tol=1e-4,
               v0=np.ones(L.shape[0]),
               maxiter=graph.shape[0] * 5,
        else:
           print("-----")
           eigenvalues, eigenvectors = scipy.sparse.linalg.lobpcg(
               L, np.random.normal(size=(L.shape[0], k)), largest=False, t
        order = np.argsort(eigenvalues)[1:k] ____
        return eigenvectors[:, order]
                                                            最小特征值是0
```

图割的方法, 较小特征值映射权重较小的边

except scipy.sparse.linalg.ArpackError:

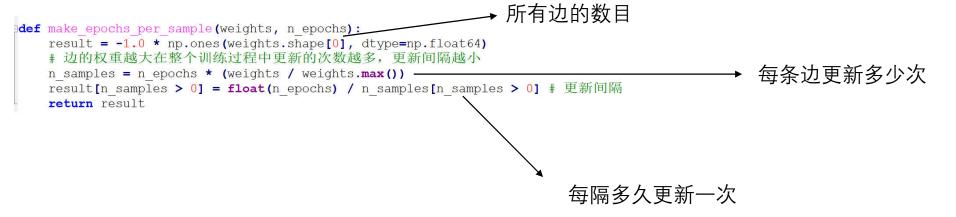
"WARNING: spectral initialisation failed! The eigenvector solver\n"

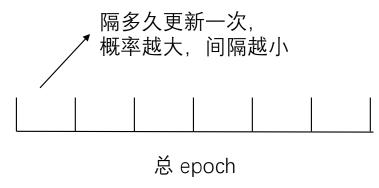
"failed. This is likely due to too small an eigengap. Consider\n"

"adding some noise or jitter to your data.\n\n"

"Falling back to random initialisation!"









```
# 通过训练获得embedding
def train embedding (head embedding, #头结点 向量
                 tail embedding, #尾结点 向量
                 head, # 头结点 编号
                                                                      for n in tqdm(range(n epochs)):
                 tail, #尾结点编号
                 epochs per sample, # 正样本采样控制
                                                                          # 进行1轮更新
                 epochs per negative sample, # 负样本采样控制
                 a,b, #
                 initial alpha, # 初始化学习率
                                                                                    head,
                 n epochs, # 训练轮次
                                                                                    tail,
                 n vertices # 顶点数目
                                                                                    n vertices,
                 ):
   dim = head embedding.shape[1]
   alpha = initial alpha
   epoch of next negative sample = epochs per negative sample.copy()
                                                                                    a,
   epoch of next sample = epochs per sample.copy()
                                                                                    b,
                                                                                    alpha,
   optimize fn = numba.njit(train one epoch, fastmath=True, parallel=False)
                                                                                    n,
                                                                                    dim)
                                                                          # 更新学习率
下次更新的epoch
                                    利用numba 提高
                                                                      return head embedding
                                    运行速度
```



```
def train one epoch (head embedding,
                    tail embedding,
                    head,
                    tail,
                    n vertices,
                    epochs per sample,
                    epochs per negative sample,
                    epoch of next sample,
                    epoch of next negative sample,
                    a,
                    b,
                    alpha,
                    n,
                    dim):
    for i in range(epochs per sample.shape[0]):
        #对正样本进行采样
        if epoch of next sample[i] <= n:</pre>
            j = head[i]
            k = tail[i]
            current = head embedding[j]
            other = tail embedding[k]
            # 计算两点间距离
            dist squared = np.dot((current-other),(current-other))
            # 计算正样本梯度
            if dist squared > 0.0:
                grad coeff = -2.0 * a * b * pow(dist squared, b - 1.0)
                grad coeff /= a * pow(dist squared, b) + 1.0
            else:
                grad coeff = 0.0
```

```
# 进行更新
for d in range(dim):
    # 梯度裁剪
    grad_d = clip(grad_coeff * (current[d] - other[d]))
    # 梯度
    current[d] += grad_d * alpha

# 下次更新的轮次
epoch_of_next_sample[i] += epochs_per_sample[i]
```

$$\frac{-2ab\|\mathbf{y_i} - \mathbf{y_j}\|_2^{2(b-1)}}{1 + \|\mathbf{y_i} - \mathbf{y_j}\|_2^2} w((x_i, x_j)) (\mathbf{y_i} - \mathbf{y_j})$$

正样本更新

2021/10/16



```
# 计算负样本的数目
n neg samples = int(
     (n - epoch of next negative sample[i]) / epochs per negative sample[i]
)
# 进行负样本采样
for p in range(n neg samples):
     k = np.random.randint(n vertices)
    other = tail embedding[k]
    dist squared = np.dot((current-other), (current-other))
    if dist squared > 0.0:
         grad coeff = 2.0 * b
         grad coeff \neq (0.001 + dist squared) * (
              a * pow(dist squared, b) + 1
                                                                    \frac{2\sigma}{\left(\epsilon + \|\mathbf{y_i} - \mathbf{y_j}\|_2^2\right) \left(1 + a\|\mathbf{y_i} - \mathbf{y_j}\|_2^{2b}\right)} \left(1 - w((x_i, x_j))\right) \left(\mathbf{y_i} - \mathbf{y_j}\right).
    elif j == k:
         continue
    else:
         grad coeff = 0.0
    for d in range(dim):
         if grad coeff > 0.0:
              grad d = clip(grad coeff * (current[d] - other[d]))
         else:
              grad d = 4.0
         current[d] += grad d * alpha
    # 计算下次负样本更新轮次
    epoch of next negative sample[i] += (
         n neg samples * epochs per negative sample[i]
```

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```
def UAMP (X,
       dim=2, # 降维后的维度
       n neighbors=15, # N近邻
       min dist = 0.1, # 控制投影后, 相似点的聚拢程度
       spread = 1,
       negative sample rate=5, # 负样本采样是正样本采样的多少倍
       n epochs=None, # 训练轮次
       __initial alpha= 1.0 # 初始化学习率
       ):
   # 估算参数 a,b
   a,b = find ab params (min dist, spread)
   # 根据高维数据 计算点与点之间的连接关系
   graph = get graph Inputs(X, n neighbors, local connectivity=1)
   print(graph)
   embedding = get embedding (graph, dim, a, b, negative sample rate, n epochs, initial alpha)
   return embedding
```

```
 \frac{\text{def curve}(\mathbf{x}, \mathbf{a}, \mathbf{b}):}{\text{return 1.0 / (1.0 + a * x ** (2 * b))}} 
 \frac{\text{def curve}(\mathbf{x}, \mathbf{a}, \mathbf{b}):}{\text{return 1.0 / (1.0 + a * x ** (2 * b))}} 
 \frac{\mathbf{y}(\mathbf{x}, \mathbf{y}) = \begin{cases} 1 & \text{if } ||\mathbf{x} - \mathbf{y}||_2 \leq \text{min-dist} \\ \exp(-(||\mathbf{x} - \mathbf{y}||_2 - \text{min-dist})) & \text{otherwise} \end{cases} 
 \frac{\mathbf{y}(\mathbf{x}, \mathbf{y}) = \begin{cases} 1 & \text{if } ||\mathbf{x} - \mathbf{y}||_2 \leq \text{min-dist} \\ \exp(-(||\mathbf{x} - \mathbf{y}||_2 - \text{min-dist})) & \text{otherwise} \end{cases} 
 \frac{\mathbf{y}(\mathbf{x}, \mathbf{y}) = \begin{cases} 1 & \text{if } ||\mathbf{x} - \mathbf{y}||_2 \leq \text{min-dist} \\ \exp(-(||\mathbf{x} - \mathbf{y}||_2 - \text{min-dist})) & \text{otherwise} \end{cases} 
 \frac{\mathbf{y}(\mathbf{x}, \mathbf{y}) = \begin{cases} 1 & \text{if } ||\mathbf{x} - \mathbf{y}||_2 \leq \text{min-dist} \\ \exp(-(||\mathbf{x} - \mathbf{y}||_2 - \text{min-dist})) & \text{otherwise} \end{cases} 
 \frac{\mathbf{y}(\mathbf{x}, \mathbf{y}) = \begin{cases} 1 & \text{if } ||\mathbf{x} - \mathbf{y}||_2 \leq \text{min-dist} \\ \exp(-(||\mathbf{x} - \mathbf{y}||_2 - \text{min-dist})) & \text{otherwise} \end{cases}
```

2021/10/16

params, covar = curve fit (curve, xv, yv)

return params[0], params[1]



```
def draw pic(datas,labs,name = '1.jpg'):
    plt.cla()
    unque labs = np.unique(labs)
    colors = [plt.cm.Spectral(each)
      for each in np.linspace(0, 1,len(unque labs))]
    []=q
    legends = []
    for i in range(len(unque labs)):
        index = np.where(labs==unque labs[i])
        pi = plt.scatter(datas[index, 0], datas[index, 1], c =[colors[i]] )
        p.append(pi)
        legends.append(unque labs[i])
    plt.legend(p, legends)
    plt.savefig(name)
if name == " main ":
    mnist datas = np.loadtxt("mnist2500 X.txt")
    mnist labs = np.loadtxt("mnist2500 labels.txt")
    print(mnist datas.shape)
    # mnist datas = mnist datas[:500,:]
    embedding = UAMP(mnist datas,dim=2,min dist=0.3,spread=2)
    print(embedding.shape)
    draw pic(embedding,mnist labs,name = "final-d0.01.jpg")
```

