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1 backprop()

```
/** Calculate and set gradients for MultiLayerNetwork, based on OutputLayer and labels*/
protected void backprop() {

Pair<Gradient, INDArray> pair = calcBackpropGradients(null, true);
this.gradient = (pair == null ? null : pair.getFirst());
this.epsilon = (pair == null ? null : pair.getSecond());
}
```

根据注释可以看出是基于输出层和标签计算多层网络的梯度。之后跳进另外一个函数内。

1.1 calcBackpropGradients

这段代码提供的注释很多,这里直接翻译原有注释

```
    /** 计算梯度和偏差. 在一下的两个地方使用:
    * (a) backprop (用于标准的网络结构)
    * (b) backpropGradient (layer类方法,用于当MultiLayerNetwork类被用作layer的时候)
    * @param epsilon 偏差 (technically errors .* activations). 当withOutputLayer = true时,不被使用
    * @param withOutputLayer 如果为true:认为最后一层为输出层,并且根据标签计算偏差.在这种情况下输入的epsilon将不会被使用(可能为null)
    * 如果为false:计算反向传播的梯度
    * @return 输入的梯度和偏差 (epsilon)
    * /
    protected Pair<Gradient, INDArray> calcBackpropGradients (INDArray epsilon, boolean
```

```
withOutputLayer) {
10.     if (flattenedGradients == null)
11.         initGradientsView();
```

在刚开始运行的时候 flattenedGradients 字段为null。之后进入 initGradientsView() 方法。

1.1.1 initGradientsView()

1.1.1.1 numParams(NeuralNetConfiguration conf)

因为需要计算每一层的参数个数,所以需要调用如上的函数,每一个层参数的计算个数方法为 nin * nout + nout。 然后继续返回到上层函数继续执行。

1.1.1 initGradientsView()

```
//以上计算得出参数的总个数之后,创建ndarray。'f'代表数组的存储顺序,有兴趣可以查阅nd4j官网
flattenedGradients = Nd4j.zeros(new int[] {1, backpropParamLength}, 'f');

int backpropParamsSoFar = 0;
for (int i = 0; i < layers.length; i++) {
    //如果该层参数个数为0则跳过当前层
    if (nParamsPerLayer[i] == 0)
        continue; //This layer doesn't have any parameters...

//NDArrayIndex.point(0)用于指定是第几行,这里就是指定第0行
//NDArrayIndex.interval(backpropParamsSoFar, backpropParamsSoFar + nParamsPerLayer[i])用于获取列坐标索引

INDArray thisLayerGradView = flattenedGradients.get(NDArrayIndex.point(0),
```

```
NDArrayIndex.interval(backpropParamsSoFar, backpropParamsSoFar + nParamsPe
    rLayer[i]));
14.    layers[i].setBackpropGradientsViewArray(thisLayerGradView);
15.    backpropParamsSoFar += nParamsPerLayer[i];
16. }
```

刚开始看这段代码的时候,不懂很明白这是要做什么,这时候需要回看到这个函数的目的是什么。这个函数的目的

是 initializes the flattened gradients array (used in backprop) and sets the appropriate subset in all layers 这里的for loop主要是设置各个层的梯度数组。

1.1.1.2 flattenedGradients.get()

```
1.  /**
2.  * Returns a subset of this array based on the specified
3.  * indexes
4.  *
5.  * @param indexes the indexes in to the array
6.  * @return a view of the array with the specified indices
7.  */
8.  INDArray get(INDArrayIndex... indexes);
```

这个方法主要是根据给定的数组索引获取数组的子集。

1.1.1.3 point(int point)

```
1.  /**
2.  * Returns a point index
3.  * @param point the point index
4.  * @return the point index based
5.  * on the specified point
6.  */
7.  public static INDArrayIndex point(int point) {
8.     return new PointIndex(point);
9.  }
```

用户返回指定点的索引,在这里使用主要是指定行索引。

1.1.1.4 interval(int begin, int end)

```
1.  /**
2.  * Generates an interval from begin (inclusive) to end (exclusive)
3.  *
4.  * @param begin the begin
5.  * @param end the end index
6.  * @return the interval
7.  */
8.  public static INDArrayIndex interval(int begin, int end) {
9.   return interval(begin, 1, end, false);
10.  }
```

生成区间[begin, end)区间内数据的索引,用于获取列索引。

1.1 calcBackpropGradients

```
1. String multiGradientKey;
2. //使用初始化之后的flattenedGradients构造梯度类
```

```
3. Gradient gradient = new DefaultGradient(flattenedGradients);
4. Layer currLayer;
5.
6. //计算并应用每个图层的后向梯度
7. /**
8. * 跳过索引的输出层,只是向后循环更新每个层的系数。
9. * (当 withOutputLayer == true)
10. *
11. * 激活为每个图层应用激活函数,并将其设置为下一图层的输入。
12. *
13. * Typical literature contains most trivial case for the error calculation: wT * weights
14. * This interpretation transpose a few things to get mini batch because ND4J is rows vs colum ns organization for params
15. */
16. int numLayers = getnLayers();
17. //将梯度存储为列表; used to ensure iteration order in DefaultGradient linked hash map. i.e., layer 0 first instead of output layer
18. LinkedList<Triple<String, INDArray, Character>> gradientList = new LinkedList<>();
```

在构造梯度类,梯度列表以及获取网络结构的层数之后,继续执行以下语句:

```
    int layerFrom;

Pair<Gradient, INDArray> currPair;
    //判断是否使用输出层
   if (withOutputLayer) {
        //对输出层做类型检查
        if (!(getOutputLayer() instanceof IOutputLayer)) {
            log.warn("Warning: final layer isn't output layer. You cannot use backprop without an
    output layer.");
           return null;
       }
        //获取输出层
        IOutputLayer outputLayer = (IOutputLayer) getOutputLayer();
        //对标签进行检查
        if (labels == null)
            throw new IllegalStateException("No labels found");
        //设置输出层的标签,用于计算偏差
        outputLayer.setLabels(labels);
        //首先获取输出层的梯度
        currPair = outputLayer.backpropGradient(null);
```

接下来单步进入输出层反向传播梯度的的函数

1.2.1 outputLayer.backpropGradient(INDArray epsilon)

```
1. @Override
2. public Pair<Gradient, INDArray> backpropGradient(INDArray epsilon) {
3.    Pair<Gradient, INDArray> pair = getGradientsAndDelta(preOutput2d(true)); //Returns
    Gradient and delta^(this), not Gradient and epsilon^(this-1)
4.    INDArray delta = pair.getSecond();
5.
6.    INDArray epsilonNext =
    params.get(DefaultParamInitializer.WEIGHT_KEY).mmul(delta.transpose()).transpose();
7.    return new Pair<> (pair.getFirst(), epsilonNext);
8. }
```

1.2.1.1 preOutput2d(true)

```
protected INDArray preOutput2d(boolean training) {
     return preOutput(training);
public INDArray preOutput(boolean training) {
   applyDropOutIfNecessary(training);
    INDArray b = getParam(DefaultParamInitializer.BIAS KEY);
    INDArray W = getParam(DefaultParamInitializer.WEIGHT KEY);
    //Input validation:
     if (input.rank() != 2 || input.columns() != W.rows()) {
         if (input.rank() != 2) {
            throw new DL4JInvalidInputException("Input that is not a matrix; expected matrix
(rank 2), got rank "
                             + input.rank() + " array with shape " + Arrays.toString(input.shape
 ()));
        }
        throw new DL4JInvalidInputException("Input size (" + input.columns() + " columns; shap
                         + Arrays.toString(input.shape())
                         + ") is invalid: does not match layer input size (layer # inputs = " +
W.size(0) + ")");
   }
     if (conf.isUseDropConnect() && training && conf.getLayer().getDropOut() > 0) {
         W = Dropout.applyDropConnect(this, DefaultParamInitializer.WEIGHT_KEY);
     INDArray ret = input.mmul(W).addiRowVector(b);
     if (maskArray != null) {
        applyMask(ret);
     return ret;
}
```

因为这里是OutputLayer在调用,这里相当于使用 y = xw + b计算并得出输出层还未经过激活函数变换的输出。并将计算得出的结果传入到 getGradientsAndDelta(INDArray preOut)方法中

1.2.1.2 getGradientsAndDelta(INDArray preOut)

```
/** Returns tuple: {Gradient, Delta, Output} given preOut */
private Pair<Gradient, INDArray> getGradientsAndDelta(INDArray preOut) {
    //首先获取当前层的损失函数
    ILossFunction lossFunction = layerConf().getLossFn();
    //获取2维的列表。 (主要是针对RNN CNN这种网络, 因为他们的数据组成方式是3d或者4d,需要转化为2d之后才能残油矩阵运算)
    INDArray labels2d = getLabels2d();
    //判断两个矩阵的形状,进行一个检验
    if (labels2d.size(1) != preOut.size(1)) {
        throw new DL4JInvalidInputException("Labels array numColumns (size(1) = " + labels2d.size(1) + ") does not match output layer" + " number of outputs (nOut = " + preOut.size(1) + ") does not match output layer" + " number of outputs (nOut = " + preOut.size(1) + ")");

//传入标签,输出层的输出,激活函数和掩码,利用损失函数来计算偏差
INDArray delta = lossFunction.computeGradient(labels2d, preOut,
```

```
layerConf().getActivationFn(), maskArray);
```

1.2.1.2.1 lossFunction.computeGradient

```
    @Override
    public INDArray computeGradient(INDArray labels, INDArray preOutput, IActivation activationFn, INDArray mask) {
    INDArray gradients = super.computeGradient(labels, preOutput, activationFn, mask);
    return gradients.divi(labels.size(1));
    }
```

之后调用父类的 computeGradient () 方法来计算梯度

```
@Override
public INDArray computeGradient(INDArray labels, INDArray preOutput, IActivation activationFn
 , INDArray mask) {
     //因为前面获取的preOutput只是 y = xw + b部分,尚未经过激活函数的变化
     //所以这里先 复制一份preOutput, 然后经过激活函数的变换获得output
     INDArray output = activationFn.getActivation(preOutput.dup(), true);
     //这里先计算两个矩阵之间的差距, 然后再*2
     //这里是因为当前的损失函数类型为LossMSE(), 所以需要对
     INDArray dLda = output.subi(labels).muli(2);
     //损失函数的权重为null,为此不进行改步操作
     if (weights != null) {
         dLda.muliRowVector(weights);
     //如若使用掩码,则与掩码进行计算
     f(mask != null && LossUtil.isPerOutputMasking(dLda, mask)){
     //For *most* activation functions: we don't actually need to mask dL/da in addition t
 o masking dL/dz later
        //but: some, like softmax, require both (due to dL/dz_i being a function of dL/da_j,
        //We could add a special case for softmax (activationFn instanceof ActivationSoftmax)
but that would be
       // error prone - but buy us a tiny bit of performance
         LossUtil.applyMask(dLda, mask);
     //根据激活函数计算梯度
     INDArray gradients = activationFn.backprop(preOutput, dLda).getFirst();
```

这里会调用激活函数的backprop, 主要是用于求其在激活函数之后的梯度。

因为我这里最后一层的函数为IDENTITY,本身对输入不会做任何变换,所以直接返回本身。

```
    @Override
    public Pair<INDArray, INDArray> backprop(INDArray in, INDArray epsilon) {
    return new Pair<>(epsilon, null);
    }
```

之后调用Pair.getFirst(),就是为了获取激活函数求导之后的epsilon

```
//Loss function with masking
if (mask != null) {
```

```
3. LossUtil.applyMask(gradients, mask);
4. }
5.
6. return gradients;
7. }
```

在这个函数最后调用掩码进行计算,然后这个函数到这里执行完毕,返回上层函数。

1.2.1.2.1 lossFunction.computeGradient

```
1. INDArray gradients = super.computeGradient(labels, preOutput, activationFn, mask);
2. return gradients.divi(labels.size(1));
3. }
```

调用 gradients.divi(labels.size(1)) ,梯度除以labels的第二个维度。一般情况下为最后一层的神经元个数。然后返回到 getGradientsAndDelta(INDArray preOut)方法中。

1.2.1.2 getGradientsAndDelta(INDArray preOut)

```
//初始化新的梯度类
 Gradient gradient = new DefaultGradient();
//获取权重梯度视图
INDArray weightGradView = gradientViews.get(DefaultParamInitializer.WEIGHT KEY);
//获取偏重梯度视图
INDArray biasGradView = gradientViews.get(DefaultParamInitializer.BIAS KEY);
//Equivalent to: weightGradView.assign(input.transpose().mmul(delta));
//相当于更新权重的梯度
Nd4j.gemm(input, delta, weightGradView, true, false, 1.0, 0.0);
//对权重梯度进行赋值,初始值为 delta的第0行之和
biasGradView.assign(delta.sum(0));
//将权重的梯度放入到初始化之后的梯度类中
gradient.gradientForVariable().put(DefaultParamInitializer.WEIGHT KEY, weightGradView);
 gradient.gradientForVariable().put(DefaultParamInitializer.BIAS KEY, biasGradView);
 //返回梯度和delta
 return new Pair<> (gradient, delta);
```

返回到上层函数 backpropGradient (INDArray epsilon) 中

1.2.1 outputLayer.backpropGradient(INDArray epsilon)

1.1 calcBackpropGradients

```
//获取到了当前层的Pair<Gradient, INDArray>
    currPair = outputLayer.backpropGradient(null);
    //遍历梯度map里面的 权重梯度以及偏置梯度
    for (Map.Entry<String, INDArray> entry : currPair.getFirst().gradientForVariable().entrySe
 t()) {
        //获取原始的名称,基本为"W", "b"
        String origName = entry.getKey();
        //然后根据当前所在的层数进行拼装,比如变成"1 W", "1 b"
        multiGradientKey = String.valueOf(numLayers - 1) + " " + origName;
        //然后构建三元组, 字符串新名称, 梯度INDArray,以及展平之后的梯度INDArray
        //添加到链表的最后
        gradientList.addLast(new Triple<>(multiGradientKey, entry.getValue(),
                       currPair.getFirst().flatteningOrderForVariable(origName)));
    }
    //判断是否有输入预处理操作
    if (getLayerWiseConfigurations().getInputPreProcess(numLayers - 1) != null)
        currPair = new Pair<> (currPair.getFirst(),
                       this.layerWiseConfigurations.getInputPreProcess(numLayers - 1)
                                      .backprop(currPair.getSecond(), getInputMiniBatchSize()
));
     //numLayers - 1为输出层,且输出层的梯度和误差以及计算好了
    //所以layerFrom为 numLayers - 2
    layerFrom = numLayers - 2;
} else {
     //如果无输出层,则从numLayers - 1开始
    currPair = new Pair<>(null, epsilon);
    layerFrom = numLayers - 1;
}
//根据前面计算的梯度来进行反向传播
// Calculate gradients for previous layers & drops output layer in count
for (int j = layerFrom; j >= 0; j--) {
     //获取当前网络层
    currLayer = getLayer(j);
    //如果当前层是FrozenLayer,终止反向传播
    if (currLayer instanceof FrozenLayer)
        break;
    //根据上一层的误差来重新计算梯度和误差便于继续反向传播
    currPair = currLayer.backpropGradient(currPair.getSecond());
    //新建三元组子列表
    LinkedList<Triple<String, INDArray, Character>> tempList = new LinkedList<>();
    for (Map.Entry<String, INDArray> entry : currPair.getFirst().gradientForVariable().entrySe
t()) {
        String origName = entry.getKey();
        multiGradientKey = String.valueOf(j) + "_" + origName;
        tempList.addFirst(new Triple<> (multiGradientKey, entry.getValue(),
                       currPair.getFirst().flatteningOrderForVariable(origName)));
     }
```

1 backprop()

```
/** Calculate and set gradients for MultiLayerNetwork, based on OutputLayer and labels*/
protected void backprop() {
    Pair<Gradient, INDArray> pair = calcBackpropGradients(null, true);
    this.gradient = (pair == null ? null : pair.getFirst());
    this.epsilon = (pair == null ? null : pair.getSecond());
}
```

对于当前的 MultiLayerNetwork 类设置成员变量的值。

Pair数据结构源码解读

```
1. package org.deeplearning4j.berkeley;
2.
3. /**
4.    * A generic-typed pair of objects.
5.    * @author Dan Klein
6.    */
7. public class Pair<F, S> implements Serializable, Comparable<Pair<F, S>> {
8.    static final long serialVersionUID = 42;
9.
10.    F first;
11.    S second;
12.
13.    public F getFirst() {
14.         return first;
15.    }
16.
17.    public S getSecond() {
18.         return second;
19.    }
20.
21.    public void setFirst(F pFirst) {
22.         first = pFirst;
```

```
23.    }
24.
25.    public void setSecond(S pSecond) {
26.         second = pSecond;
27.    }
28.
29.    public Pair<S, F> reverse() {
30.         return new Pair<>(second, first);
31.    }
32. }
```

Gradient

```
    package org.deeplearning4j.nn.gradient;

 3. /**
 4. * Generic gradient
     * @author Adam Gibson
 8. public interface Gradient extends Serializable {
        * Gradient look up table *
         * @return the gradient look up table
        Map<String, INDArray> gradientForVariable();
        * The full gradient as one flat vector *
         * @return
          */
        INDArray gradient(List<String> order);
        * The full gradient as one flat vector *
         * @return
          */
         INDArray gradient();
          * Clear residual parameters (useful for returning a gradient and then clearing old objec
    ts)
          */
         void clear();
        /**
         * The gradient for the given variable
          * @param variable the variable to get the gradient for
          * @return the gradient for the given variable or null
          */
         INDArray getGradientFor(String variable);
* Update gradient for the given variable
```

```
* @param variable the variable to get the gradient for
     * @param gradient the gradient values
     * @return the gradient for the given variable or null
     INDArray setGradientFor(String variable, INDArray gradient);
     * Update gradient for the given variable; also (optionally) specify the order in which t
he array should be flattened
     * to a row vector
      * @param variable
                             the variable to get the gradient for
      * @param gradient
                             the gradient values
      ^{*} @param flatteningOrder the order in which gradients should be flattened (null ok - def
      * @return the gradient for the given variable or null
     INDArray setGradientFor(String variable, INDArray gradient, Character flatteningOrder);
     * Return the gradient flattening order for the specified variable, or null if it is not
explicitly set
      * @param variable Variable to return the gradient flattening order for
      * @return
                         Order in which the specified variable's gradient should be
flattened
      */
     Character flatteningOrderForVariable (String variable);
```

DefaultGradient

```
    package org.deeplearning4j.nn.gradient;

3. /**
      * Default gradient implementation. Basically lookup table
      * for ndarrays
      * @author Adam Gibson
      * /
10. public class DefaultGradient implements Gradient {
       public static final char DEFAULT_FLATTENING_ORDER = 'f';
        private Map<String, INDArray> gradients = new LinkedHashMap<>();
        private Map<String, Character> flatteningOrders;
        private INDArray flattenedGradient;
        public DefaultGradient() {}
         public DefaultGradient(INDArray flattenedGradient) {
            this.flattenedGradient = flattenedGradient;
        @Override
         public Map<String, INDArray> gradientForVariable() {
          return gradients;
```

```
27. @Override
          public INDArray gradient(List<String> order) {
              List<INDArray> toFlatten = new ArrayList<>();
              if (flatteningOrders == null) {
                  for (String s : order) {
                      if (!gradients.containsKey(s))
                          continue;
                      toFlatten.add(gradients.get(s));
                  }
              } else {
                  for (String s : order) {
                      if (!gradients.containsKey(s))
                          continue;
                      if (flatteningOrders.containsKey(s) && flatteningOrders.get(s) !=
      DEFAULT_FLATTENING_ORDER) {
                          //Arrays with non-default order get flattened to row vector first, then ev
      erything is flattened to f order
                          //TODO revisit this, and make more efficient
                          toFlatten.add(Nd4j.toFlattened(flatteningOrders.get(s), gradients.get(s)))
                      } else {
                          toFlatten.add(gradients.get(s));
              return Nd4j.toFlattened(DEFAULT FLATTENING ORDER, toFlatten);
          private void flattenGradient() {
              if (flatteningOrders != null) {
                  //Arrays with non-default order get flattened to row vector first, then
      everything is flattened to f order
                  //TODO revisit this, and make more efficient
                  List<INDArray> toFlatten = new ArrayList<>();
                   for (Map.Entry<String, INDArray> entry : gradients.entrySet()) {
                      if (flatteningOrders.containsKey(entry.getKey())
                                       && flatteningOrders.get(entry.getKey()) !=
      DEFAULT FLATTENING ORDER) {
                           //Specific flattening order for this array, that isn't the default
                           \verb|toFlatten.add| (\verb|Nd4j.toFlattened| (\verb|flatteningOrders.get| (entry.getKey|))|, entry| \\
      .getValue()));
                      } else {
                          //default flattening order for this array
                           toFlatten.add(entry.getValue());
                  flattenedGradient = Nd4j.toFlattened(DEFAULT_FLATTENING_ORDER, toFlatten);
              } else {
                  //Standard case: flatten all to f order
                  flattenedGradient = Nd4j.toFlattened(DEFAULT FLATTENING ORDER, gradients.values())
              }
          @Override
          public INDArray gradient() {
              if (flattenedGradient != null)
                  return flattenedGradient;
              flattenGradient();
              return flattenedGradient;
```

```
82. @Override
          public void clear() {
             gradients.clear();
          @Override
          public INDArray getGradientFor(String variable) {
             return gradients.get(variable);
          @Override
          public INDArray setGradientFor(String variable, INDArray newGradient) {
             INDArray last = gradients.put(variable, newGradient);
              // TODO revisit whether setGradientFor should update the gradient that can be pulled
     from this object in any form - currently does not update flattened
             // use of unitialized var for flattengradient in backprop is generating an error in g
      radient calc if bellow is used
                       flattenGradient();
             return last;
         public INDArray setGradientFor(String variable, INDArray gradient, Character
      flatteningOrder) {
             INDArray last = setGradientFor(variable, gradient);
              if (flatteningOrder != null) {
                  if (flatteningOrders == null)
                     flatteningOrders = new LinkedHashMap<>();
                  flatteningOrders.put(variable, flatteningOrder);
              return last;
         @Override
         public Character flatteningOrderForVariable (String variable) {
            if (flatteningOrders == null)
                 return null:
             return flatteningOrders.get(variable);
         @Override
          public String toString() {
            return "DefaultGradient{" + "gradients=" + gradients + (flatteningOrders != null ? fla
      tteningOrders : "") + '}';
          }
```

Nd4j.gemm

```
* @param b Second matrix
* @param c result matrix. Used in calculation (assuming beta != 0) and result is stored in t
his. f order,

* zero offset and length == data.length only

* @param transposeA if true: transpose matrix a before mmul

* @param transposeB if true: transpose matrix b before mmul

* @return result, i.e., matrix c is returned for convenience

*/

public static INDArray gemm(INDArray a, INDArray b, INDArray c, boolean transposeA, boolean t
ransposeB,

double alpha, double beta) {
    getBlasWrapper().level3().gemm(a, b, c, transposeA, transposeB, alpha, beta);
    return c;

}
```