Implementation

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Outline

1. Introduction
2. Storage
3. Generation of $\phi(\text{pad}(Z^{m,i}))$
4. Evaluation of $(v^i)^T P^m_{\phi}$
5. Discussion
Outline

1. Introduction
2. Storage
3. Generation of $\phi(\text{pad}(Z^{m,i}))$
4. Evaluation of $(v^i)^T P^m_\phi$
5. Discussion
After checking formulations for gradient calculation we would like to get into implementation details.

Take the following operation as an example:

\[
\frac{\partial \xi_i}{\partial W^m} = \frac{\partial \xi_i}{\partial S_{m,i}} \phi(\text{pad}(Z^{m,i}))^T
\]

- It's a matrix-matrix product.
- We all know that a three-level for loop does the job.
- Does that mean we can then write an efficient implementation?
- The answer is no.
To explain this, we check some details of matrix-matrix products.

We also introduce optimized BLAS (Basic Linear Algebra Subprograms).
We know that \[ C = AB \]
is a mathematics operation with
\[ C_{ij} = \sum_{k=1}^{n} A_{ik} B_{kj} \]
Optimized BLAS: an Example by Using Block Algorithms I

- Let’s test the matrix multiplication
- A C program:
  ```c
  #define n 2000
  double a[n][n], b[n][n], c[n][n];

  int main()
  {
    int i, j, k;
    for (i=0; i<n; i++)
      for (j=0; j<n; j++)
        ...
Optimized BLAS: an Example by Using Block Algorithms II

\[
a[i][j]=1; \quad b[i][j]=1;
\]

\[
\text{for } (i=0; i<n; i++)
\]

\[
\text{for } (j=0; j<n; j++)
\]

\[
c[i][j]=0;
\]

\[
\text{for } (k=0; k<n; k++)
\]

\[
c[i][j] += a[i][k]*b[k][j];
\]
Optimized BLAS: an Example by Using Block Algorithms III

- The result
  
cjlin@linux6:~$ gcc -O3 mat.c  
cjlin@linux6:~$ time ./a.out  
real 0m59.251s  
user 0m58.994s  
sys 0m0.096s

- Let’s try another way:
#define n 2000
double a[n][n], b[n][n], c[n][n];

int main()
{
    int i, j, k;
    for (i=0; i<n; i++)
        for (j=0; j<n; j++)
            a[i][j] = 1; b[i][j] = 1;
            c[i][j] = 0;
for (j=0; j<n; j++) {
    for (k=0; k<n; k++)
        for (i=0; i<n; i++)
            c[i][j] += a[i][k]*b[k][j];
}

```c

for (j=0; j<n; j++) {
    for (k=0; k<n; k++)
        for (i=0; i<n; i++)
            c[i][j] += a[i][k]*b[k][j];
}
```

- The result
Optimized BLAS: an Example by Using Block Algorithms VI

cjlin@linux6:~$ gcc -O3 mat1.c
cjlin@linux6:~$ time ./a.out
real 2m13.199s
user 2m12.810s
sys 0m0.060s

- We see that first approach is faster. Why?
- For each of
  
  \[ c[i][j] \ a[i][k] \ b[k][j]; \]
  
  we do column-access
C is row-oriented rather than column-oriented
Now we sense that memory access can be an issue
Let’s try a Matlab program on the same computer

```matlab
n = 2000;
A = randn(n,n); B = randn(n,n);
t = cputime; C = A*B; t = cputime - t
```
To remove the effect of multi-threading, use
`matlab -singleCompThread`
Timing is an issue
Optimized BLAS: an Example by Using Block Algorithms VIII

Elapsed time versus CPU time

cjlin@linux6:~$ matlab -singleCompThread
>> n = 2000;
>> A = randn(n,n); B = randn(n,n);
>> tic; C = A*B; toc
Elapsed time is 1.139780 seconds.
>> t = cputime; C = A*B; t = cputime -t

1.1200

- If using multiple cores,
Optimized BLAS: an Example by Using Block Algorithms IX

cjlin@linux6:~$ matlab
>> tic; C = A*B; toc
Elapsed time is 0.227179 seconds.
>> t = cputime; C = A*B; t = cputime -t
1.6800

- Matlab is much faster than a code written by ourselves. Why?
- Optimized BLAS: data locality is exploited
- Use the highest level of memory as possible
Optimized BLAS: an Example by Using Block Algorithms X

- Block algorithms: transferring sub-matrices between different levels of storage
  They localize operations to achieve good performance
Memory Hierarchy I

CPU
↓
Registers
↓
Cache
↓
Main Memory
↓
Secondary storage (Disk)
Memory Hierarchy II

- ↑: increasing in speed
- ↓: increasing in capacity

When I studied computer architecture, I didn’t quite understand that this setting is so useful

But from optimized BLAS I realize that it is extremely powerful
Memory Management I

- Page fault: operand not available in main memory transported from secondary memory (usually) overwrites page least recently used
- I/O increases the total time
- An example: $C = AB + C$, $n = 1,024$
- Assumption: a page 65,536 doubles = 64 columns
- 16 pages for each matrix
- 48 pages for three matrices
Memory Management II

- Assumption: available memory 16 pages, matrices access: column oriented

\[ A = \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix} \]

column oriented: 1 3 2 4
row oriented: 1 2 3 4

- access each row of \( A \): 16 page faults, \( \frac{1024}{64} = 16 \)

- Assumption: each time a continuous segment of data into one page

- Approach 1: inner product
We use a matlab-like syntax here

- At each (i,j): each row \( a(i, 1:n) \) causes 16 page faults
Total: $1024^2 \times 16$ page faults

- at least 16 million page faults

- Approach 2:
  
  ```plaintext
  for j =1:n
    for k=1:n
      for i=1:n
        c(i,j) = a(i,k)*b(k,j)+c(i,j);
      end
    end
  end
  ```
For each \( j \), access all columns of \( A \)
\( A \) needs 16 pages, but \( B \) and \( C \) take spaces as well
So \( A \) must be read for every \( j \)

For each \( j \), 16 page faults for \( A \)
\( 1024 \times 16 \) page faults
\( C, B : 16 \) page faults

Approach 3: block algorithms (\( nb = 256 \))
for j =1:nb:n
    for k=1:nb:n
        for jj=j:j+nb-1
            for kk=k:k+nb-1
                c(:,jj) = a(:,kk)*b(kk,jj)+c(:,jj);
            end
        end
    end
end

In MATLAB, 1:256:1025 means 1, 257, 513, 769
Note that we calculate

\[
\begin{bmatrix}
A_{11} & \cdots & A_{14} \\
\vdots & & \vdots \\
A_{41} & \cdots & A_{44}
\end{bmatrix}
\begin{bmatrix}
B_{11} & \cdots & B_{14} \\
\vdots & & \vdots \\
B_{41} & \cdots & B_{44}
\end{bmatrix}
= \begin{bmatrix}
A_{11}B_{11} + \cdots + A_{14}B_{41} & \cdots \\
\vdots & & \vdots \\
\end{bmatrix}
\]
Memory Management VIII

- Each block: $256 \times 256$

\[
C_{11} = A_{11}B_{11} + \cdots + A_{14}B_{41} \\
C_{21} = A_{21}B_{11} + \cdots + A_{24}B_{41} \\
C_{31} = A_{31}B_{11} + \cdots + A_{34}B_{41} \\
C_{41} = A_{41}B_{11} + \cdots + A_{44}B_{41}
\]

- For each $(j, k)$, $B_{k,j}$ is used to add $A_{\cdot,k}B_{k,j}$ to $C_{\cdot,j}$
Example: when $j = 1, k = 1$

\[
C_{11} \leftarrow C_{11} + A_{11}B_{11} \\
\vdots \\
C_{41} \leftarrow C_{41} + A_{41}B_{11}
\]

Use Approach 2 for $A_{:,1}B_{11}$

- $A_{:,1}$: 256 columns, $1024 \times 256 / 65536 = 4$ pages.
- $A_{:,1}, \ldots, A_{:,4}$: $4 \times 4 = 16$ page faults in calculating $C_{:,1}$

For $A$: $16 \times 4$ page faults

- $B$: 16 page faults, $C$: 16 page faults
Optimized BLAS Implementations

- OpenBLAS
  http://www.openblas.net/
  It is an optimized BLAS library based on GotoBLAS2 (see the story in the next slide)
- Intel MKL (Math Kernel Library)
  https://software.intel.com/en-us/mkl
Some Past Stories about Optimized BLAS

- BLAS by Kazushige Goto
  https://www.tacc.utexas.edu/research-development/tacc-software/gotoblas2

- See the NY Times article: “Writing the fastest code, by hand, for fun: a human computer keeps speeding up chips”
Discussion 1

- This discussion roughly explains why GPU is used for deep learning.
- Somehow we can do fast matrix-matrix operations on GPU.
- Note that we did not touch multi-core implementations, though parallelization is possible.
- Anyway, the conclusion is that for some operations, using code written by experts is more efficient than our own implementation.
- How about other operations besides matrix-matrix products?
Discussion II

- If they can also be done by calling others’ efficient implementation, then a simple and efficient CNN implementation can be done.
- The MATLAB implementation in simpleNN is a good experimental environment for us to study this.
- We will explain details and use it in our subsequent projects.
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5. Discussion
In the earlier discussion, we check each individual data.

However, for practical implementations, all (or some) instances must be considered together for memory and computational efficiency.

Recall we do mini-batch stochastic gradient.

In our discussion we use $l$ to denote the number of data instances in calculating the gradient (or the sub-gradient).
In our implementation, we store $Z^{m,i}$, $\forall i = 1, \ldots, l$ as the following matrix.

$$
\begin{bmatrix}
Z^{m,1} & Z^{m,2} & \ldots & Z^{m,l}
\end{bmatrix} \in \mathbb{R}^{d_{m} \times a_{m} b_{m} l}.
$$

(1)

Similarly, we store

$$
\frac{\partial \xi_i}{\partial \text{vec}(S^{m,i})^T}, \quad \forall i
$$

as

$$
\begin{bmatrix}
\frac{\partial \xi_1}{\partial S^{m,1}} & \ldots & \frac{\partial \xi_l}{\partial S^{m,l}}
\end{bmatrix} \in \mathbb{R}^{d_{m+1} \times a_{\text{conv}} b_{\text{conv}} l}.
$$

(2)
Storage III

- We will explain our decision.
- Note that (1)-(2) are only the main setting to store these matrices because for some operations they may need to be re-shaped.
- For an easy description we may follow past discussion to let
  \[ Z^{\text{in},i} \text{ and } Z^{\text{out},i} \]
  be the input and output images of a layer, respectively.
Recall that we conduct the following operations

$$\frac{\partial \xi_i}{\partial \text{vec}(S^{m,i})^T} = \left( \frac{\partial \xi_i}{\partial \text{vec}(Z^{m+1,i})^T} \odot \text{vec}(I[Z^{m+1,i}])^T \right) P_{\text{pool}}^{m,i}$$  \hspace{1cm} (3)

$$\frac{\partial \xi_i}{\partial W^m} = \frac{\partial \xi_i}{\partial S^{m,i}} \phi(\text{pad}(Z^{m,i}))^T$$  \hspace{1cm} (4)

$$\frac{\partial \xi_i}{\partial \text{vec}(Z^{m,i})^T} = \text{vec} \left( (W^m)^T \frac{\partial \xi_i}{\partial S^{m,i}} \right)^T P_{\phi}^m P_{\text{pad}}^m$$  \hspace{1cm} (5)
Operations of a Convolutional Layer II

- Based on the way discussed to store variables, we will discuss two operations in detail
  - Generation of $\phi(\text{pad}(Z_{m,i}^m))$
  - Vector $\times P^m_{\phi}$
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im2col in Existing Packages I

- Due to the wide use of CNN, a subroutine for $\phi(\text{pad}(Z^{m,i}))$ has been available in some packages.
- For example, MATLAB has a built-in function `im2col` that can generate $\phi(\text{pad}(Z^{m,i}))$ for $s = 1$ and $s = h$ (width of filter).

- But this function cannot handle general $s$.
- Can we do a reasonably efficient implementation by ourselves?
For an easy description we consider

$$\text{pad}(Z^{m,i}) = Z^{\text{in},i} \rightarrow Z^{\text{out},i} = \phi(Z^{\text{in},i}).$$
Consider the following column-oriented linear indices (i.e., counting elements in a column-oriented way) of $Z^{in,i}$:

$$
\begin{bmatrix}
1 & d^{in} + 1 & \ldots & (b^{in}a^{in} - 1)d^{in} + 1 \\
2 & d^{in} + 2 & \ldots & (b^{in}a^{in} - 1)d^{in} + 2 \\
\vdots & \vdots & \ddots & \vdots \\
d^{in} & 2d^{in} & \ldots & (b^{in}a^{in})d^{in}
\end{bmatrix} \in \mathbb{R}^{d^{in} \times a^{in}b^{in}}.
$$

(6)
Linear Indices and an Example II

- Every element in

\[ \phi(Z_{in,i}) \in \mathbb{R}^{hhd_{in} \times a_{out} b_{out}}, \]

is extracted from \( Z_{in,i} \).

- The task is to find the mapping between each element in \( \phi(Z_{in,i}) \) and a linear index of \( Z_{in,i} \).

- Consider an example with

\[ a_{in} = 3, \quad b_{in} = 2, \quad d_{in} = 1. \]

Because \( d_{in} = 1 \), we omit the channel subscript.
In addition, we omit the instance index $i$, so the image is

$$\begin{bmatrix}
  z_{11} & z_{12} \\
  z_{21} & z_{22} \\
  z_{31} & z_{32}
\end{bmatrix}.$$ 

If $h = 2, s = 1$, two sub-images are

$$\begin{bmatrix}
  z_{11} & z_{12} \\
  z_{21} & z_{22}
\end{bmatrix}$$

and

$$\begin{bmatrix}
  z_{21} & z_{22} \\
  z_{31} & z_{32}
\end{bmatrix}.$$
Linear Indices and an Example IV

- By our earlier way of representing images,

\[ Z_{in,i} = \begin{bmatrix}
  z_{1,1,1}^i & z_{2,1,1}^i & \ldots & z_{a_{in},b_{in},1}^i \\
  \vdots & \vdots & \ddots & \vdots \\
  z_{1,1,d_{in}}^i & z_{2,1,d_{in}}^i & \ldots & z_{a_{in},b_{in},d_{in}}^i
\end{bmatrix} \]

the one we have is

\[ Z_{in} = \begin{bmatrix}
  z_{11} & z_{21} & z_{31} & z_{12} & z_{22} & z_{32}
\end{bmatrix} \]

- The linear indices from (6) are

\[ \begin{bmatrix}
  1 & 2 & 3 & 4 & 5 & 6
\end{bmatrix}. \]
Recall that

\[
\phi(Z^{\text{in},i}) =
\begin{bmatrix}
Z_1^{i,1,1} & Z_1^{i} & Z_1^{i}+(a^{\text{out}}-1)s,1+(b^{\text{out}}-1)s,1 \\
Z_2^{i,1,1} & Z_2^{i} & Z_2^{i}+(a^{\text{out}}-1)s,1+(b^{\text{out}}-1)s,1 \\
\vdots & \vdots & \vdots \\
Z_h^{i,1,1} & Z_h^{i} & Z_h^{i}+(a^{\text{out}}-1)s,h+(b^{\text{out}}-1)s,1 \\
Z_h^{i,1,d^{\text{in}}} & Z_h^{i} & Z_h^{i}+(a^{\text{out}}-1)s,h+(b^{\text{out}}-1)s,d^{\text{in}}
\end{bmatrix}
\]
Therefore,

\[
\phi(Z^{in}) = \begin{bmatrix}
  z_{11} & z_{21} \\
  z_{21} & z_{31} \\
  z_{12} & z_{22} \\
  z_{22} & z_{32}
\end{bmatrix}.
\]

Linear indices of \(Z^m\) to get elements of \(\phi(Z^m)\):

\[
\begin{align*}
Z^{m,i} & \quad [1 \ 2 \ 3 \ 4 \ 5 \ 6]^T \\
\phi(Z^{m,i}) & \quad [1 \ 2 \ 4 \ 5 \ 2 \ 3 \ 5 \ 6]^T.
\end{align*}
\]

Example of using Matlab/Octave
Linear Indices and an Example VII

octave:8> reshape((1:6)', 3, 2)
ans =
   1   4
   2   5
   3   6

octave:9>
octave:9> im2col(reshape((1:6)', 3, 2), [2,2], "sliding")
ans =
Linear Indices and an Example VIII

To handle all instances together, we store

$$Z_{\text{in},1}, \ldots, Z_{\text{in},l}$$

as

$$\begin{bmatrix}
\text{vec}(Z_{\text{in},1}) & \ldots & \text{vec}(Z_{\text{in},l})
\end{bmatrix}$$
Linear Indices and an Example IX

- Denote it as a MATLAB matrix $Z$
- Then

$$[\text{vec}(\phi(Z^{m,1})) \ldots \text{vec}(\phi(Z^{m,l}))]$$

is simply $Z(P,:)$
in MATLAB, where we store the mapping by

$$P = [1 \ 2 \ 4 \ 5 \ 2 \ 3 \ 5 \ 6]^T$$
Linear Indices and an Example $X$

- All instances handled in one line
- Moreover, we hope Matlab’s implementation on this operation is efficient
- But how to obtain $P$?
- Note that

$$\begin{bmatrix} 1 & 2 & 4 & 5 & 2 & 3 & 5 & 6 \end{bmatrix}^T.$$  

also corresponds to column indices of non-zero elements in $P^{m}_{\phi}$. 

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Generation of $\phi(\text{pad}(Z_{m,i}^j))$

Linear Indices and an Example XI

\[
\begin{pmatrix}
  z_{11} \\
  z_{21} \\
  z_{12} \\
  z_{22} \\
  z_{21} \\
  z_{31} \\
  z_{22} \\
  z_{32}
\end{pmatrix}
= 
\begin{pmatrix}
  1 & 1 & 1 \\
  1 & 1 & 1 \\
  1 & 1 & 1 \\
\end{pmatrix}
\begin{pmatrix}
  z_{11} \\
  z_{21} \\
  z_{31} \\
  z_{12} \\
  z_{22} \\
  z_{22} \\
  z_{32}
\end{pmatrix}
\]

(7)
A General Setting I

- We begin with checking how linear indices of $Z_{in,i}$ can be mapped to the first column of $\phi(Z_{in,i})$.
- For simplicity, we consider only channel $j$.
- From

$$Z_{in,i} = \begin{bmatrix} z_{1,1,1} & z_{2,1,1} & \ldots & z_{a_{in},1,1} & z_{1,2,1} & \ldots & z_{a_{in},b_{in},1} \\ \vdots & \vdots & \ddots & \vdots & \vdots & & \vdots \\ z_{1,1,j} & z_{2,1,j} & \ldots & z_{a_{in},1,j} & z_{1,2,j} & \ldots & z_{a_{in},b_{in},j} \\ \vdots & \vdots & \ddots & \vdots & \vdots & & \vdots \\ z_{1,1,d_{in}} & z_{2,1,d_{in}} & \ldots & z_{a_{in},1,d_{in}} & z_{1,2,d_{in}} & \ldots & z_{a_{in},b_{in},d_{in}} \end{bmatrix}$$
we have

<table>
<thead>
<tr>
<th>Linear indices in $z^{in}$</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>$j$</td>
<td>$z_{1,1,j}^{in}$</td>
</tr>
<tr>
<td>$d^{in} + j$</td>
<td>$z_{2,1,j}^{in}$</td>
</tr>
<tr>
<td>$...$</td>
<td>$...$</td>
</tr>
<tr>
<td>$(h - 1)d^{in} + j$</td>
<td>$z_{h,1,j}^{in}$</td>
</tr>
<tr>
<td>$a^{in}d^{in} + j$</td>
<td>$z_{1,2,j}^{in}$</td>
</tr>
<tr>
<td>$...$</td>
<td>$...$</td>
</tr>
<tr>
<td>$(((h - 1) + a^{in})d^{in} + j$</td>
<td>$z_{h,2,j}^{in}$</td>
</tr>
<tr>
<td>$...$</td>
<td>$...$</td>
</tr>
<tr>
<td>$(((h - 1) + (h - 1)a^{in})d^{in} + j$</td>
<td>$z_{h,h,j}^{in}$</td>
</tr>
</tbody>
</table>
A General Setting III

- We rewrite linear indices in the earlier table as

\[
\begin{pmatrix}
0 + 0a^{in} \\
\vdots \\
(h - 1) + 0a^{in} \\
0 + 1a^{in} \\
\vdots \\
(h - 1) + 1a^{in} \\
\vdots \\
0 + (h - 1)a^{in} \\
\vdots \\
(h - 1) + (h - 1)a^{in}
\end{pmatrix}
\]

\[d^{in} + j. \quad (8)\]
Every linear index in (8) can be represented as

$$(p + qa^{in})d^{in} + j,$$ \hspace{1cm} (9)

where

$$p, \ q \in \{0, \ldots, h - 1\}$$

Then \((p + 1, q + 1)\) correspond to the pixel position in the convolutional filter.

Next we consider other columns in \(\phi(Z^{in,i})\) by still fixing the channel to be \(j\).
A General Setting V

From

\[ \phi(Z^{in,i}) = \begin{bmatrix}
\vdots & \vdots \\
Z_{1,1,j}^{i} & Z_{1}^{i} + s_{1,1,j} \\
Z_{2,1,j}^{i} & Z_{2}^{i} + s_{1,1,j} \\
\vdots & \vdots & \ddots & \vdots \\
Z_{h,h,j}^{i} & Z_{h}^{i} + s_{h,h,j} \\
\vdots & \vdots & \ddots & \vdots \\
Z_{h,h,d^{in}}^{i} & Z_{h}^{i} + s_{h,h,d^{in}} \\
\end{bmatrix} \]

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each column contains the following elements from the $j$th channel of $Z_{in,i}^j$.

$$Z_{in,i}^{1+p+as,1+q+bs \cdot j}, \ a = 0, 1, \ldots, a^{out} - 1,$$

$$b = 0, 1, \ldots, b^{out} - 1, \quad (10)$$

where

$$(1 + as, 1 + bs)$$

is the top-left position of a sub-image in the channel $j$ of $Z_{in,i}^j$. 
From (6), the linear index of each element in (10) is

$$\left( (1 + p + as - 1) + (1 + q + bs - 1)a^{in} \right) d^{in} + j$$

(column index in $Z^{in,i}$)

$$= (a + ba^{in})sd^{in} + (p + qa^{in})d^{in} + j.$$  \hspace{1cm} (11)

Now we have known for each element of $\phi(Z^{in,i})$ what the corresponding linear index in $Z^{in,i}$ is.

Next we discuss the implementation details.
First, we compute elements in (8) with $j = 1$ by applying Matlab’s ‘+’ operator, which has the implicit expansion behavior, to compute the outer sum of the following two arrays.

$$
\begin{bmatrix}
1 \\
d^{in} + 1 \\
\vdots \\
(h - 1)d^{in} + 1
\end{bmatrix}
$$

and

$$
\begin{bmatrix}
0 \\
a^{in}d^{in} \\
\vdots \\
(h - 1)a^{in}d^{in}
\end{bmatrix}.
$$
The result is the following matrix

\[
\begin{bmatrix}
1 & a^{in}d^{in} + 1 & \ldots & (h - 1)a^{in}d^{in} + 1 \\
 d^{in} + 1 & (1 + a^{in})d^{in} + 1 & \ldots & (1 + (h - 1)a^{in})d^{in} + 1 \\
\vdots & \vdots & \ddots & \vdots \\
(h - 1)d^{in} + 1 & ((h - 1) + a^{in})d^{in} + 1 & \ldots & ((h - 1) + (h - 1)a^{in})d^{in} + 1
\end{bmatrix}
\] (12)

If columns are concatenated, we get (8) with \( j = 1 \)

To get (9) for all channels \( j = 1, \ldots, d^{in} \), we compute the outer sum:

\[
\text{vec}((12)) + \begin{bmatrix} 0 & 1 & \ldots & d^{in} - 1 \end{bmatrix}
\] (13)
A General Setting X

- Then we have the first column of $\phi(Z^{in,i})$
- Next, we obtain other columns in $\phi(Z^{in,i})$
- In the linear indices in (11), the second term corresponds to indices of the first column, while the first term is the following column offset

$$(a + ba^{in})sd^{in}, \quad \forall a = 0, 1, \ldots, a^{out} - 1,$$
$$b = 0, 1, \ldots, b^{out} - 1.$$
A General Setting XI

- This is the outer sum of the following two arrays.

\[
\begin{bmatrix}
0 \\
\vdots \\
a^{\text{out}} - 1
\end{bmatrix} \times sd^{\text{in}} \quad \text{and} \quad 
\begin{bmatrix}
0 & \ldots & b^{\text{out}} - 1
\end{bmatrix} \times a^{\text{in}}sd^{\text{in}}
\]

(14)

- Finally, we compute the outer sum of the column offset and the linear indices in the first column of \( \phi(Z^{\text{in},i}) \)

\[
\text{vec}((14))^T + \text{vec}((13))
\]

(15)
In the end we store

$$\text{vec}((15)) \in \mathbb{R}^{hhd^{\text{in}}a^{\text{out}}b^{\text{out}} \times 1}$$

It is a vector collecting column index of the non-zero in each row of $P^m_\phi$

Note that each row in the 0/1 matrix $P^m_\phi$ contains exactly only one non-zero element.

See the example in (7)

The obtained linear indices are independent of the values of $Z^{\text{in},i}$. 
Thus the above procedure only needs to be run once in the beginning.
function idx = find_index_phiZ(a,b,d,h,s)

  first_channel_idx = ([0:h-1]*d+1)' + [0:h-1]*a*d;
  first_col_idx = first_channel_idx(:) + [0:d-1];
  a_out = floor((a - h)/s) + 1;
  b_out = floor((b - h)/s) + 1;
  column_offset = ([0:a_out-1]' + [0:b_out-1]*a)*s*d;
  idx = column_offset(:)' + first_col_idx(:);
  idx = idx(:);
Discussion

- The code is simple and short
- We assume that Matlab operations used here are efficient and so is our resulting code
- But is that really the case?
- We will do experiments to check this
- Some works have tried to do similar things (e.g., https://github.com/wiseodd/hipsternet), though we don’t see complete documents and evaluation
Outline

1. Introduction
2. Storage
3. Generation of $\phi(\text{pad}(Z_{m,i}))$
4. Evaluation of $(v_i)^T P^m_\phi$
5. Discussion
In the backward process, the following operation is applied.

\[(\mathbf{v}^i)^T P^m_{\phi}, \quad (16)\]

where

\[\mathbf{v}^i = \text{vec} \left((W^m)^T \frac{\partial \xi_i}{\partial S_{m,i}}\right)\]

Consider the same example used for \(\phi(Z^{\text{in},i})\)
We have

$$P^m_\phi = \begin{bmatrix}
1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & & \\
1 & 1 & 1 & & \\
& 1 & 1 & & \\
& & & & 1
\end{bmatrix}$$
Thus

$$\left( P^m_\phi \right)^T \mathbf{v}^i = \left[ v_1 \ v_2 + v_5 \ v_6 \ v_3 \ v_4 + v_7 \ v_8 \right]^T,$$

which is a kind of “inverse” operation of $\phi(\text{pad}(Z^{m,i}))$

We accumulate elements in $\phi(\text{pad}(Z^{m,i}))$ back to their original positions in $\text{pad}(Z^{m,i})$. 

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Evaluation of $(\mathbf{v}^i)^T P^m_\phi$ IV

- In MATLAB, given indices

$$[1 \ 2 \ 4 \ 5 \ 2 \ 3 \ 5 \ 6]^T$$ (18)

and the vector $\mathbf{v}$, a function `accumarray` can directly generate the vector (17).

- Example:
$$\left(v^i\right)^T P^m_\phi V$$

```
octave:18> [v a]
an =

    1   0.406445
    2   0.067872
    4   0.036638
    5   0.279801
    2   0.490535
    3   0.369743
    5   0.429186
    6   0.054324
```
\begin{align*}
(v^i)^T P^m_\phi \mathbf{V}\mathbf{I}
\end{align*}

\begin{verbatim}
octave:19> accumarray(v,a)
ans =

0.406445
0.558407
0.369743
0.036638
0.708987
0.054324
\end{verbatim}
To do the calculation over a batch of instances, we aim to have
\[
\left[ (P^m)_{\phi}^T \mathbf{v}^1 \right]^T \\
\vdots \\
\left[ (P^m)_{\phi}^T \mathbf{v}^l \right] 
\]
(19)

We can apply MATLAB's `accumarray` on the vector
\[
\begin{bmatrix}
\mathbf{v}^1 \\
\vdots \\
\mathbf{v}^l
\end{bmatrix},
\]
(20)
by giving the following indices as the input.

\[
\begin{bmatrix}
(18) \\
(18) + a^m_{\text{pad}} b^m_{\text{pad}} d^m \mathbb{1}_{h^m h^m d^m a^m_{\text{conv}} b^m_{\text{conv}}} \\
(18) + 2a^m_{\text{pad}} b^m_{\text{pad}} d^m \mathbb{1}_{h^m h^m d^m a^m_{\text{conv}} b^m_{\text{conv}}} \\
\vdots \\
(18) + (l - 1)a^m_{\text{pad}} b^m_{\text{pad}} d^m \mathbb{1}_{h^m h^m d^m a^m_{\text{conv}} b^m_{\text{conv}}}
\end{bmatrix}, \quad (21)
\]

where

\[a^m_{\text{pad}} b^m_{\text{pad}} d^m\] is the size of \(\text{pad}(Z^{m,i})\)
and

$$h^m h^m d^m a^m_{\text{conv}} b^m_{\text{conv}}$$ is the size of $\phi(\text{pad}(Z^{m,i}))$ and $\mathbf{v}_i$.

That is, by using the offset $(i - 1)a^m_{\text{pad}} b^m_{\text{pad}} d^m$, accumarray accumulates $\mathbf{v}^i$ to the following positions:

$$(i - 1)a^m_{\text{pad}} b^m_{\text{pad}} d^m + 1, \ldots, i a^m_{\text{pad}} b^m_{\text{pad}} d^m. \quad (22)$$
(\mathbf{v}^i)^T P^m_\phi \mathbf{X}

- (21) can be easily obtained by the following outer sum

\[ \text{vec}((18) + [0 \ldots l - 1] a^m_{pad} b^m_{pad} d^m) \]

- To obtain

\[
\begin{bmatrix}
\mathbf{v}^1 \\
\vdots \\
\mathbf{v}^l
\end{bmatrix}
\]

we note that it is the same as

\[
\text{vec} \left( (W^m)^T \left[ \frac{\partial \xi_1}{\partial S^{m,1}} \ldots \frac{\partial \xi_l}{\partial S^{m,l}} \right] \right).
\]
Thus we do a matrix-matrix multiplication.

From (23), we can see why \( \partial \xi_i / \partial \text{vec}(S_{m,i})^T \) over a batch of instances are stored in the form of

\[
\left[ \frac{\partial \xi_1}{\partial S_{m,1}} \quad \cdots \quad \frac{\partial \xi_l}{\partial S_{m,l}} \right] \in \mathbb{R}^{d_{m+1}^a \times b_{conv}^m \cdot l}.
\]
A Simple Code I

\[
a_{\text{prev}} = \text{model.ht\_pad}(m);
b_{\text{prev}} = \text{model.wd\_pad}(m);
d_{\text{prev}} = \text{model.ch\_input}(m);
\]

\[
\text{idx} = \text{net.idx\_phiZm}(:) + [0:\text{num\_v}-1]\ast d_{\text{prev}}\ast a_{\text{prev}}\ast b_{\text{prev}};
\]

\[
vTP = \text{accumarray}(\text{idx}(::), V(::), [d_{\text{prev}}\ast a_{\text{prev}}\ast b_{\text{prev}}\ast \text{num\_v} 1])';
\]
A Simple Code II

Here we assume

$$V = \begin{bmatrix} v_1 & \cdots & v_l \end{bmatrix}$$

and \texttt{num_v} is the number of columns
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Efficient Implementation 1

- If a package provides efficient implementations of the following operations:
  - matrix-matrix products
  - matrix expansion for $\phi(\text{pad}(Z^{m,i}))$
  - outer sum
  - accumarray

then we can easily have a good CNN implementation.

- Unfortunately, the difficulty to optimize these operations may vary.
To work on instances together, it’s difficult to decide the best storage settings. Further, storage settings affect the implementations. Do you think our setting is already the best? How could we easily check the running time of using different storage settings? Is our code flexible enough for such experiments?
References I