Softmax Optimizations for Intel® Xeon® Processor-based Platforms

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Abstract

This article presents our methodology of optimization and its results applied to softmax function. Scope of this work includes: algorithmic improvements (reduce general implementation so it is tailored for inference), profiling (identifying most time consuming fragments of code), using efficient computational libraries (Intel® MKL and Intel® MKL-DNN) as well as improving vectorization (analysis of applicability of OpenMP and manually crafted assembly code for vectorization improvement). By presenting this methodology, we hope to increase an interest in Deep Learning optimizations for CPUs.

1 Introduction

Softmax is a function used in classification problems in machine learning, and it has been widely used in deep learning for implementing image classification models, such as AlexNet [10], GoogleNet [14], or ResNet [7], where its execution time is small compared to convolution functions. However, natural language processing (NLP) models published recently use softmax more intensively [17], and its high computation cost triggered research towards equivalent but computationally cheaper methods, such as hierarchical softmax [11].

This article presents optimizations and performance improvements of the softmax operation for x86-64 architectures (in particular Intel® Xeon® processors). We focused on inference with deep attention matching (DAM) model, and for our experiments we used Baidu’s PaddlePaddle* deep learning platform [2]. We limited our efforts to single-thread execution as the usual optimization process starts with exploiting all the capabilities of a single core. Multithread performance improvements are not the topic of the paper and were explored in [9]. We believe that the optimization process presented here could be transferred to other deep learning frameworks such as Tensorflow or PyTorch.

1.1 Softmax theory

Softmax function is an extension of logistic regression to work with multiple classification categories.

\[ \text{softmax}(z_j) = \frac{e^{z_j}}{\sum_{i} e^{z_i}} \]  

(1)

It is often used as a tool to normalize data. Softmax calculates a probability vector \( z \) for classification tasks where values \( z_j \) of vector \( z \) are probability distribution over a set of categories.

1.2 Softmax as implemented in PaddlePaddle

Our starting point was PaddlePaddle’s softmax implementation using the popular Eigen [6] computation library to implement its deep learning operators. Mentioned implementation is presented at Figure[1]

PaddlePaddle does offer a functionality to check the time of execution of operators that were executed. The target CPU used for our work to get performance results of softmax execution was
template<typename DeviceContext, typename T>
void SoftmaxFunctor<DeviceContext, T>::operator()(
    const DeviceContext& context,
    const framework::Tensor* X,
    framework::Tensor* Y) {
auto logits = EigenMatrices<T>::Promo<X>;
auto softmax = EigenMatrices<T>::Promo<Y>;

const int kBatchDim = 0;
const int kClassDim = 1;
const int batch_size = logits.dimension(kBatchDim);
const int num_classes = logits.dimension(kClassDim);

Eigen::DSizes<int, 1> along_class(kClassDim);
Eigen::DSizes<int, 2> batch_by_one(batch_size, 1);
Eigen::DSizes<int, 2> one_by_class(1, num_classes);

auto shifted_logits = logits
    - logits.maximum(along_class);

    eval();
    reshape(batch_by_one);
    broadcast(one_by_class));

    unaryExpr(ValueClip<T>());

softmax.device(context) = shifted_logits.exp();
softmax.device(context) = (softmax -
    softmax.sum(along_class)
    .inverse());

    eval();
    reshape(batch_by_one);
    broadcast(one_by_class));

Figure 1: Reference implementation (introduced in PaddlePaddle PR#14337)

Intel® Xeon® Platinum 8180 Processor. We referred to PaddlePaddle profiling to get the performance status of both softmax and overall DAM model, while optimizing softmax. The exemplary profiler report from PaddlePaddle for DAM model execution is presented at figure 2:

-------------------------> Profiling Report <--------- --------------
Place: CPU
Time unit: ms
Sorted by total time in descending order in the same thread

| Event                  | Calls | Total | Min. | Max. | Ave. | Ratio. |
|------------------------|-------|-------|------|------|------|--------|
| thread0::layer_norm    | 316000| 68958 | 0.21599 | 18.1111 | 0.218222 | 0.396 |
| thread0::softmax       | 158000| 32188.1| 0.193633 | 0.882732 | 0.203722 | 0.185 |
| thread0::stack         | 19000 | 19002.9| 0.926812 | 2.51014 | 1.00015 | 0.09 |
| thread0::conv3d        | 2000  | 16806.6| 1.25346 | 19.4991 | 8.40328 | 0.096 |
| thread0::mul           | 317000| 13812.1| 0.009354 | 69.8051 | 0.0435712 | 0.079 |

Figure 2: Exemplary PaddlePaddle’s DAM profiling report

2 Optimization process
2.1 Algorithmic modifications
By inspecting the implementation code we can see that there is a functionality of ValueClip. When ValueClip is used, softmax does not produce zero values by assigning very small floating point constant eg. $10^{-60}$ to a variable that holds zero. This is needed in a situation when there is some logarithmic operation following softmax eg. cross-entropy loss. A logarithm of 0 is -inf which will later on produce NAN in a training. However as we are optimizing(speeding up) inference adding this minimal threshold is not needed. After removing mentioned functionality execution time is reduced by 5%.

2.2 Profiling
Once we analyzed softmax implementation and removed unnecessary elements, we can do profile operations in the softmax operator to find operations that are the most time consuming. Hotspots are the operations on which we focus our attention because their successful optimization can potentially give the highest performance gains.

\footnote{For details of our experiments that included profiling please refer to appendix: Notices and Disclaimers}
We used timestamp counter (TSC), which is very precise time measuring device for CPUs. Instruction \_\_rdtsc returns the current value of this CPU clock. Idea is that we measure the time of entire execution of operator as well as selected parts of it, so we know which part takes the most time relatively. When we begin modification/optimization the absolute value will also be useful to see if we are making progress. One note is that profiling is done on more than one executions of function for more reliable results. The rough idea of profiling is presented in listing 3. After finished execution, profiling told us that: over 50% of time of softmax execution is spent in exp part of function and sum\&div took around 30%. Hence optimization of \(e^t\) followed by summing and elementwise division would be our targets.

### 2.3 Performance improvements with Intel\textsuperscript{®} Math Kernel Library (Intel\textsuperscript{®} MKL)

To spare developers the effort of low level optimizations for the most common mathematical algorithms, a number of libraries have been created that provide optimized implementations of such operations: OpenBLAS\textsuperscript{11}, Eigen\textsuperscript{6} and Intel\textsuperscript{®} MKL. PaddlePaddle baseline code does use Eigen which is fast and elegant library, but we use Intel\textsuperscript{®} MKL as it provides implementations optimized for x86_64 architectures (in particular Intel\textsuperscript{®} Xeon\textsuperscript{8} processors). We replaced exponential computations and elementwise division with BLAS functions provided by Intel\textsuperscript{®} MKL and the remaining Eigen code was replaced with a manually hand crafted implementation[see figure\textsuperscript{2}]. Performance improvement was around 2X.

### 2.4 Auto-vectorization with OpenMP

Our next step was to improve the code that was not too be replaced with Intel\textsuperscript{®} MKL. We optimized the following operations:

- Subtracting value from all elements of vector (elementwise subtraction)
- Summing up vector elements
- Finding the maximal value within elements of vector
We took advantage of OpenMP simd reduction clause [12] that was introduced in OpenMP 4.0 and is available in ICC and GCC (from version 4.9). OpenMP simd can be seen as a way to provide additional details on a implementation and reduction mechanism so a compiler can more effectively vectorize the code. More detailed information on OpenMP vectorization can be found [3].

2.4.1 Elementwise subtraction

We inspected generated assembly of the already mentioned three operations and found that elementwise subtraction is already vectorized. So no further hints to the compiler were needed.

2.4.2 Summing Up Elements

We found that OpenMP simd by itself (hints to loops vectorization) did not provide much of a performance boost. It may result in code size reduction as the compiler did not have to generate multiple implementations of code, when some hints were provided. On the other hand OpenMP simd followed by reduction clause decreased execution time significantly.

Figure 5 presents original assembly of summing procedure, as generated by the compiler. It can be seen that although the Intel® AVX instruction set is used (eg. vaddss is used) it does not operate on 128/256 bit words, it just adds sequentially 32-bit words.

The highlighted line of code in figure 5 contains modification we introduced. By marking the loop in the line below with pragma omp simd reduction, we gave a hint to the compiler that reduction on variable sum can be safely vectorized, and each partial sum can be computed in parallel
using Intel® AVX instructions. We inspected the generated assembly (see Figure[10] to check that introduced modification brought expected vectorization[4]

```cpp
template <typename DeviceContext>
class SoftmaxFunctor<DeviceContext, float, true>
{
  void operator () (const DeviceContext& context, const framework::Tensor& X,
                   framework::Tensor& Y)
  {
    auto in_dims = X.dims();
    auto out_dims = Y.dims();
    const float in_data = X.data<float>();
    float* out_data = Y.data<float>();
    const int batchSizeDim = 0;
    const int kClassDim = 1;
    // 2D data Batch x C
    const int batchSize = in_dims[kBatchDim];
    const int num_classes = in_dims[kClassDim];
    for (int n = 0; n < batchSize; ++n) {
      float sum = out_data[num_classes];
      for (int c = 0; c < num_classes; ++c) {
        out_data[num_classes + c] = in_data[num_classes + c] - max;
      }
      vmax(num_classes + batch_size, out_data, out_data);
      for (int n = 0; n < batchSize; ++n) {
        float sum = out_data[num_classes];
        #pragma omp simd reduction(+ : sum)
        for (int c = 0; c < num_classes; ++c) {
          sum += out_data[num_classes + c];
        }
        cblas_vsExp(num_classes, 1.0f / sum, &out_data[num_classes], 1);
      }
    }
  }
};
```

Figure 6: MKL and openmp simd based implementation

This optimization brought an additional 5% reduction in time execution.

Although there was a performance improvement, we did not use it in PaddlePaddle. Summing `e^x` is an operation that sums positive values, and Intel® MKL already provides such operation, `cblas_sasum`, that sums absolute values of elements. The advantage of using MKL’s `sasum` is that OpenMP pragmas support is present in the recent generation of compilers, but in production environments some old compilers like MSVC and GCC 4.8 are still used so when using Intel® MKL we speed up also those older configurations. Fortunately our OpenMP vectorization effort was not discarded, as we upstreamed it into the Intel® MKL-DNN project[3] softmax implementation.

```asm
Figure 7: Fragment of Assembly code of vectorized reduction(summing up) of vector
```

2.4.3 Finding maximal value in an array of elements

We applied openmp simd reduction(max:) for searching maximal value in softmax operator, but despite asking the compiler for max reduction, the generated code was not vectorized. Hence we implemented max value search directly using assembly language (see[2.5]).

2.5 Vectorization with SIMD instructions

As we have showed here, compiler auto-vectorization capabilities, when used carefully, can bring visible performance improvements. However, that is not always the case because code generated by the compiler’s auto-vectorizer can turn out to be suboptimal, and the only option is to implement an algorithm manually with SIMD instructions (AVX, AVX2 and AVX512). So performance critical functionality may benefit significantly when implemented manually in assembly, in particular when vector instructions need to be used.

[4] Extract of generated assembly shows packed vector AVX instructions that implement sum reduction, that perform computations on 128 bit memory chunks e.g. `vaddps`

[5] MKL-DNN can be build either with Intel MKL as well as without
Assembly implementation of max value search was implemented with a help of Xbyak project. Xbyak is a JIT assembler that generates assembly code at runtime. JIT functionality suits deep learning use cases very well, as declared models (description of neural network) are usually not modified during their execution (inference, training). Hence, we can generate assembly after the model was defined and we can have assembly code suited for a neural network model. In particular, we can have different assembly code for different batch sizes.

The manually crafted assembly code for finding maximal value in an array is presented at figure 12. Due to the introduction of a manually crafted assembler, the max finding function is around three times faster than our reference code. As the percentage of time spent executing max function is small compared to the computation of exponential function \( e^x \), its performance impact on softmax is small. Softmax after implementing max finding value in Xbyak is on average 3% faster. It may seem small, but for data centers that are constantly executing deep learning workloads, even 3% improvement can account for a significant savings in energy and time.

Portability and maintainability problems are the main disadvantages of using assembly language for performance optimizations. Assembly code is not portable among different architectures, and it is more difficult to maintain than the implementations written in higher-level languages. In general, if possible, we recommend using existing softmax implementations like those provided by MKL-DNN, and implementing critical operations with assembly language only when they are not available in Intel® MKL-DNN or other fast computational libraries.

2.6 Limits of optimizations

When working on optimizing the code we would like to know if there is any room for improvement of its execution time. We need a measure of how close is actual performance of softmax to platform maximal capabilities. There are two limitations to improving performance on given hardware platform eg.

- memory bound limit
- computation bound limit

Those two limitations and kernel’s operational intensity are foundation for Roofline model, which is often used for estimation if further performance optimizations are possible. The application of Roofline model is out of scope of this document and was not used during the work discussed here. When working on softmax optimization in the context of a DAM model, we experimented by replacing softmax computation with memory copying routine eg. memcpy. Memcpy is usually well optimized (often written manually using vector instructions) so the speed of execution of memcpy is limited by memory throughput. Softmax takes some input buffer and writes its result to output buffer, but both buffers are of the same size hence memcpy can be used to replace softmax computation. The comparison of both execution times (actual softmax implementation and memcpy) can give us an idea of whether it is worth to invest more time into the optimization of softmax implementation. If the softmax execution time is close to memcpy then it is likely that the algorithm is bound by maximal memory throughput and we won’t get better performance in a given execution environment. We initially verified (using memcpy) that baseline (not fully vectorized) implementation is far from being memory bound (see Figure 8) and based on that result we concluded that performance can be increased by better utilisation of computing resources of processor eg. Introducing effective Intel® MKL implementations and more effective vectorization.

3 Performance Evaluation

Figure 8 shows that the softmax execution in DAM model is 2X faster than the original implementation. This optimization impacts performance of the entire DAM model and improves it by over 15% (figure 9).

4 Conclusion and Further Work

We presented the methods we used to optimize softmax as well as demonstrated the performance gain as a result of this methodology.

From profiling information, we observed that exponential functions execution take up significant amount of time. This could be further improved by using cheaper in execution approximation functions which can provide a performance boost in exchange for little computational inaccuracy. Another idea could be applying a roofline model to softmax implementations to get an estimation of
how much more performance could potentially be improved. Also, knowing that optimized imple-
mentation is far away from memory throughput limitation, it would be beneficial to use the Intel®
AVX512 instruction set to manually implement the entire Softmax operator. As softmax is a popular
deep learning primitive, we upstreamed our optimizations to the Intel® MKL-DNN library.

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6Sum reduction using both OpenMP vectorization MKL was merged to MKL-DNN codebase
Appendix: Inspecting generated assembly code

For the purpose of a work presented here generated assembly code was inspected using compiler switches (relevant to GCC):

```
-S -masm=intel
```

As well as injecting markers into code to easily locate section of code that we are interested in. For example following C++ code (Figure 10), after applying mentioned compiler switches results in generated assembly as presented on Figure 11.
```c
#define GENERATE_ASSEMBLY
asm volatile ("BEGIN SIMD SOFTMAX SUM! \n- - -");
#endif
asm volatile ("END SIMD SOFTMAX SUM! \n- - -");
#endif

float tmpptr = &out_data[n * num_classes];
#pragma omp simd reduction(+: result) aligned(tmpptr)
for (int i = 0; i < num_classes; ++i) {
    result += tmpptr[i];
}
entities[n] = result;
#endif

float tmpptr = &out_data[n * num_classes];
#pragma omp simd reduction(+: result) aligned(tmpptr)
for (int i = 0; i < num_classes; ++i) {
    result += tmpptr[i];
}
entities[n] = result;
#endif
```

Figure 10: Assembly code of vectorized reduction (summing up) of vector

### Appendix: Notices and Disclaimers

Intel® technologies features and benefits depend on system configuration and may require enabled hardware, software or service activation. Performance varies depending on system configuration.

Most of our work was upstreamed into PaddlePaddle and MKL-DNN projects. And can be accessed respectively at:

[https://github.com/PaddlePaddle/Paddle](https://github.com/PaddlePaddle/Paddle)

and

[https://github.com/intel/mkl-dnn](https://github.com/intel/mkl-dnn)

However, optimizations of softmax using direct implementation in assembly language (section 2.5) at the moment of writing this article are not part of PaddlePaddle and MKL-DNN repositories. Hence for taking performance measures we created an integration branch located at:

[https://github.com/tpatejko/Paddle/commits/tpatejko/jit-max-in-softmax](https://github.com/tpatejko/Paddle/commits/tpatejko/jit-max-in-softmax)

The experiments were executed using following commands:

```
OMP_NUM_THREADS=1 ./paddle/fluid/inference/tests/api/test_analyzer_dam \
    --infer_model=third_party/inference_demo/dam/model/ \
    --infer_data=third_party/inference_demo/dam/data.txt \
    --test_filter=Analyzer_dam.profile --batch_size=1 \
    --test_all_data=true --num_threads=1 --use_analysis=false --profile
echo "===> Batch 8"
OMP_NUM_THREADS=1 ./paddle/fluid/inference/tests/api/test_analyzer_dam \
    --infer_model=third_party/inference_demo/dam/model/ \
    --infer_data=third_party/inference_demo/dam/data.txt \
    --test_filter=Analyzer_dam.profile --batch_size=8 \
    --test_all_data=true --num_threads=1 --use_analysis=false --profile
echo "===> Batch 32"
OMP_NUM_THREADS=1 ./paddle/fluid/inference/tests/api/test_analyzer_dam \
    --infer_model=third_party/inference_demo/dam/model/ \
    --infer_data=third_party/inference_demo/dam/data.txt \
    --test_filter=Analyzer_dam.profile --batch_size=32 \
    --test_all_data=true --num_threads=1 --use_analysis=false --profile
echo "===> Batch 128"
OMP_NUM_THREADS=1 ./paddle/fluid/inference/tests/api/test_analyzer_dam \
    --infer_model=third_party/inference_demo/dam/model/ \
    --infer_data=third_party/inference_demo/dam/data.txt \
    --test_filter=Analyzer_dam.profile --batch_size=128 \
    --test_all_data=true --num_threads=1 --use_analysis=false --profile
```

---

7 All quoted Pull Requests within this article, are related to this repository
8 using commit 28bba75d9108026f236c312813ca5b5a72a6aabe from integration branch
BEGIN SIMD SUM!

MOV D WORD PTR [rdi], 0x00000000
MOV Q WORD PTR [rbp-48], 0
MOV Q WORD PTR [rbp-40], 0
MOV Q WORD PTR [rbp-32], 0
MOV Q WORD PTR [rbp-24], 0
JLE .L9
LEA ECX, [rdi-8]
SHR ECX, 3
ADD ECX, 1
CMP EDX, 7
JLE .L15
VMOVAP YMM0, YMMWORD PTR [rbp-48] XOR R8D, R8D
.L11:
MOV R9, R8
ADD R8, 1
SAL R9, 1
CMP ECX, R8D
JALE .L1
ADD EAX, 6
VADECDQ RAX, [RSI+ECX*8]
CMP EDX, ECX
JALE .L19
MOV R9, ECX
ADD R8, 1
SAL R9, 5
CMP ECX, R8D
JAL EAX, [RAX+2*8]
VADDPQ RAX, [RDI], RAX
CMPS EAX, EDX
JAE .L20
VADDPQ YMM0, YMM1, YMMWORD PTR [RDI]
VZEROUPPER
.L10:
MOV SXZ RCX, ECX
VMOVAP YMM0, DWORD PTR [RSI+ECX*4]
LEA ECX, [RAX+1]
VADXPQ RAX, [RBP-48], RAX
JLE .L9
VMOVAP YMM0, YMMWORD PTR [RDI]
VZEROUPPER
.L9:
VXORPS RAX, RAX, RAX
VADDPQ RAX, [RBP-48]
VADDPQ RAX, [RBP-44]
VADDPQ RAX, [RBP-40]
VADDPQ RAX, [RBP-36]
VADDPQ RAX, [RBP-32]
VADDPQ RAX, [RBP-28]
VADDPQ RAX, [RBP-24]
VADDPQ RAX, [RBP-20]
VADDPQ RAX, [RBP-16]
VADDPQ RAX, [RBP-12]
VADDPQ RAX, [RBP-8]
VADDPQ RAX, [RBP-4]
VADDPQ RAX, [RBP-0]
VMOVAP DWORD PTR [RDI], RAX
END SIMD SUM!

Figure 11: Assembly code of vectorized reduction (summing up) of vector
```cpp
struct maxUFunc
  public Xbyak::CodeGenerator {
    maxUFunc()
    {
      #ifdef (__x86_64__)
        // calling convention RDI, RSI, RDX, RCX, R8, R9
        // XMM = Reference to Result
        // RDI = PTR to Array
        // RSI = Num of Output elements * size of float (4)
        // RDX = Num of Output elements
        // Registers that need to be preserved: RBX, RBP, R12-R15
        // AVX2 support
        if (current_cpu.has(Xbyak::util::Cpu::tAVX2)) {
          printf("AVX2 supported\n");
        } else {
          printf("AVX2 not detected\n");
        }
      mov (rcx, rdx);
      push(rbx);
      shr (rcx, 3); // Divide by 8 (eight floats)
      shl (rdx, 2); // Use of Output elements * size of float (4)
      shl (rcx, 5); // Trunc to 32 bytes
      // Compute partial maximums
      vpbroadcastd(ymm0, ptr[rsi]); // Move offset for next 8 floating point values
      xor (rax, rax);
      jz("tail");
      vapuqmm2(ymm2, ptr[rsi + rax]); // A
      add(rax, 32); // Move offset for next 8 floating point values
      vmulp(ymm0, ymm0, ymm2);
      jmp("for_i");
    }
  
    // Tail execution
    L("for_i"),
    cmp(rdx, rdx);
    jl("seq");
    vmulp(ymm2, ptr[rsi + rax]); // A
    add(rax, 16); // Move offset for next 4 floating point values
    sub(rdx, 16);
    vpbroadcastd(ymm2, ptr[rsi + rax]); // Move offset for next 4 floating point values
    vmulp(ymm0, ymm0, ymm0);
    vpermilylps(xmm1, xmm0, 0x1B);
    vmaxps(ymm0, ymm0, ymm1);
    vpermilylps(xmm1, xmm0, 1);
    vmaxps(ymm0, ymm0, ymm1);
    // ymm0[0:31] contains global maximum
    vmovq(ptr[rdi], ymm0); // Result < Max(X)
    jz("done");
    vpbroadcastd(ymm2, ptr[rsi + rax]); // Move offset for next 4 floating point values
    vmulp(ymm0, ymm0, ymm2);
    // partial maxes in ymm0
    vpermilps(ymm1, ymm0, 0x0A1B);
    vmulp(ymm0, ymm0, ymm0); // partial maxes in ymm0
    vpermilps(ymm1, ymm0, 1);
    vpermilps(ymm2, ymm0, ymm0); // ymm0[0:31] contains global maximum
    vmovq(ptr[rdi], ymm0); // Result < Max(X)
    jz("done");
    #else
    printf("%2hi not supported\n");
    #endif
    ret();
  
};

Figure 12: JIT Assembly code of maximal value finding in an array
```