Cache Models
and
Program Transformations

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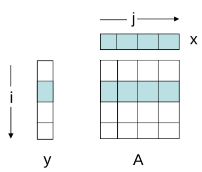
Goal of lecture

- Develop abstractions of real caches for understanding program performance
- Study the cache performance of matrix-vector multiplication (MVM)
  – simple but important computational science kernel
- Understand MVM program transformations for improving performance

Matrix-vector product

- Code:
```
for i = 1,N
  for j = 1,N
    y(i) = y(i) + A(i,j)*x(j)
```
- Total number of references = $4N^2$
  – This assumes that all elements of A,x,y are stored in memory
  – Smart compilers nowadays can register-allocate y(i) in the inner loop
  – You can get this effect manually
```
for i = 1,N
  temp = y(i)
  for j = 1,N
     temp = temp + A(i,j)*x(j)
  y(i) = temp
```
  – To keep things simple, we will not do this but our approach applies to this optimized code as well



Cache abstractions

- Real caches are very complex
- Science is all about tractable and useful abstractions (models) of complex phenomena
  – models are usually approximations
- Can we come up with cache abstractions that are both tractable and useful?
- Focus:
  – two-level memory model: cache + memory

Stack distance

Address stream from processor

- r_1 , r_2 : two memory references
  - r_1 occurs earlier than r_2
- stackDistance(r_1,r_2): number of distinct cache lines referenced between r_1 and r_2
- Stack distance was defined by defined by Mattson et al (IBM Systems Journal paper)
  - arguably the most important paper in locality

Modeling approach

- First approximation:
  - ignore conflict misses
  - only cold and capacity misses
- Most problems have some notion of “problem size”
  - (eg) in MVM, the size of the matrix (N) is a natural measure of problem size
- Question: how does the miss ratio change as we increase the problem size?
- Even this is hard, but we can often estimate miss ratios at two extremes
  - large cache model: problem size is small compared to cache capacity
  - small cache model: problem size is large compared to cache capacity
  - we will define these more precisely in the next slide.

Large and small cache models

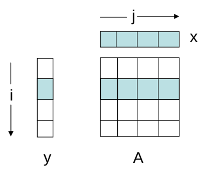
- Large cache model
  - no capacity misses
  - only cold misses
- Small cache model
  - cold misses: first reference to a line
  - capacity misses: possible for succeeding references to a line
    - let r_1 and r_2 be two successive references to a line
    - assume r_2 will be a capacity miss if stackDistance(r_1,r_2) is some function of problem size
    - argument: as we increase problem size, the second reference will become a miss sooner or later
- For many problems, we can compute
  - miss ratios for small and large cache models
  - problem size transition point from large cache model to small cache model

MVM study

- We will study five scenarios
  - Scenario I
    - i,j loop order, line size = 1 number
  - Scenario II
    - j,i loop order, line size = 1 number
  - Scenario III
    - i,j loop order, line size = b numbers
  - Scenario IV
    - j,i loop order, line size = b numbers
  - Scenario V
    - blocked code, line size = b numbers

Scenario I

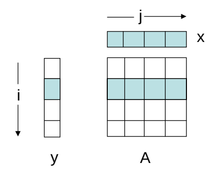
- Code:
  ```
  for i = 1,N
    for j = 1,N
      y(i) = y(i) + A(i,j)*x(j)
  ```
- Inner loop is known as DDOT in NA literature if working on doubles:
  - Double-precision DOT product
- Cache line size
  - 1 number
- Large cache model:
  - Misses:
    - A: N^2 misses
    - x: N misses
    - y: N misses
    - Total = N^2+2N
    - Miss ratio = $(N^2+2N)/4N^2$
      ~ 0.25 + 0.5/N



Scenario I (contd.)

Address stream: y(1) A(1,1) x(1) y(1) | y(1) A(1,2) x(2) y(1) ..... y(1) A(1,N) x(N) y(1) | y(2) A(2,1) x(1) y(2)

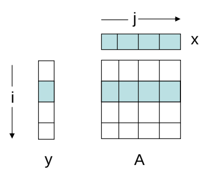
- Small cache model:
  - A: N^2 misses
  - x: N + N(N-1) misses (reuse distance=O(N))
  - y: N misses (reuse distance=O(1))
  - Total = $2N^2+N$
  - Miss ratio = $(2N^2+N)/4N^2$
    ~ 0.5 + 0.25/N
- Transition from large cache model to small cache model
  - As problem size increases, when do capacity misses begin to occur?
  - Subtle issue: depends on replacement policy (see next slide)



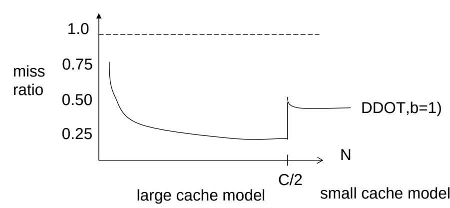
Scenario I (contd.)

Address stream: y(1) A(1,1) x(1) y(1) | y(1) A(1,2) x(2) y(1) ..... y(1) A(1,N) x(N) y(1) | y(2) A(2,1) x(1) y(2)

- Question: as problem size increases, when do capacity misses begin to occur?
- Depends on replacement policy:
  - Optimal replacement:
    - do the best job you can, knowing everything about the computation
    - only x needs to be cache-resident
    - elements of A can be "streamed in" and tossed out of cache after use
    - So we need room for (N+2) numbers
    - Transition: N+2 > C ➔ N ~C
  - LRU replacement
    - by the time we get to end of a row of A, first few elements of x are "cold" but we do not want them to be replaced
    - Transition: (2N+2) > C ➔ N ~ C/2
- Note:
  - optimal replacement requires perfect knowledge about future
  - most real caches use LRU or something close to it
  - some architectures support "streaming"
    - in hardware
    - in software: hints to tell processor not to cache certain references



Miss ratio graph



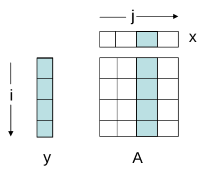
- Jump from large cache model to small cache model will be more gradual in reality because of conflict misses

Scenario II

- Code:

```
for j = 1,N
  for i = 1,N
    y(i) = y(i) + A(i,j)*x(j)
```

- Inner loop is known as AXPY in NA literature
  $$\mathbf{y} = \alpha \cdot \mathbf{x} + \mathbf{y}$$
- Miss ratio picture exactly the same as Scenario I
  – roles of x and y are interchanged

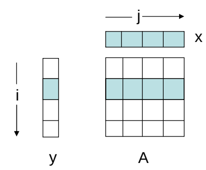


Scenario III

- Code:

```
for i = 1,N
  for j = 1,N
    y(i) = y(i) + A(i,j)*x(j)
```

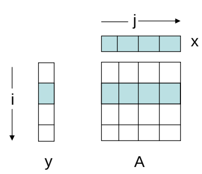
- Cache line size
  – b numbers
- Large cache model:
  – Misses:
    - A: N^2/b misses
    - x: N/b misses
    - y: N/b misses
    - Total = $(N^2+2N)/b$
    - Miss ratio = $(N^2+2N)/4bN^2$
      ~ 0.25/b + 0.5/bN



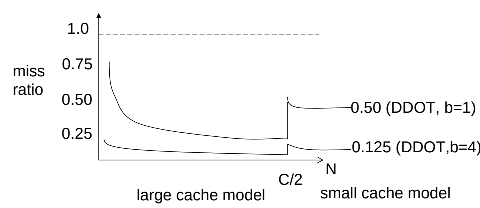
Scenario III (contd.)

Address stream: y(1) A(1,1) x(1) y(1) | y(1) A(1,2) x(2) y(1) …. | y(1) A(1,N) x(N) y(1) | y(2) A(2,1) x(1) y(2)

- Small cache model:
  – A: N^2/b misses
  – x: N/b + N(N-1)/b misses (reuse distance=O(N))
  – y: N/b misses (reuse distance=O(1))
  – Total = $(2N^2+N)/b$
  – Miss ratio = $(2N^2+N)/4bN^2$
    ~ 0.5/b + 0.25/bN
- Transition from large cache model to small cache model
  – As problem size increases, when do capacity misses begin to occur?
  – LRU: roughly when (2N+2b) = C
    - N ~ C/2
  – Optimal: roughly when (N+2b) ~ C ➔ N ~ C
- So miss ratio picture for Scenario III is similar to that of Scenario I but the y-axis is scaled down by b
- Typical value of b = 4 (SGI Octane)



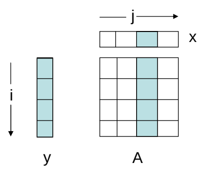
Miss ratio graph



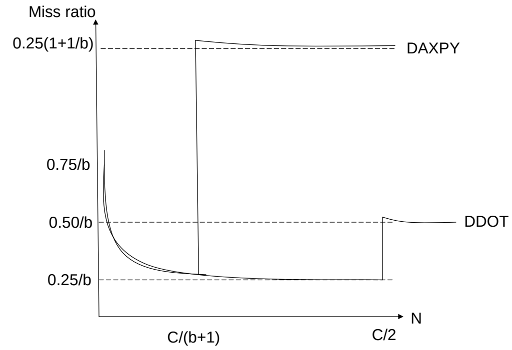
- Jump from large cache model to small cache model will be more gradual in reality because of conflict misses

Scenario IV

- Code:
```
for j = 1,N
  for i = 1,N
    y(i) = y(i) + A(i,j)*x(j)
```
- Large cache model:
  - Same as Scenario III
- Small cache model:
  - Misses:
    - A: N^2
    - x: N/b
    - y: N/b + N(N-1)/b = N^2/b
    - Total: N^2(1+1/b) + N/b
    - Miss ratio = 0.25(1+1/b) + 0.25/bN
- Transition from large cache to small cache model
  - LRU: Nb + N +b = C ➔ N ~ C/(b+1)
  - optimal: N + 2b ~ C ➔ N ~ C
- Transition happens much sooner than in Scenario III (with LRU replacement)

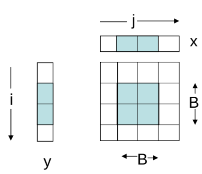


Miss ratios



Scenario V

- Intuition: perform blocked MVM so that data for each blocked MVM fits in cache
  - One estimate for B: all data for block MVM must fit in cache
    - ➔ B2 + 2B ~ C
    - ➔ B ~sqrt(C)
  - Actually we can do better than this
- Code: blocked code
```
for bi = 1,N,B
  for bj = 1,N,B
    for i = bi,min(bi+B-1,N)
      for j = bj,min(bj+B-1,N)
        y(i)=y(i)+A(i,j)*x(j)
```
- Choose block size B so
  - you have large cache model while executing block
  - B is as large as possible (to reduce loop overhead)
  - for our example, this means B~c/2 for row-major order of storage and LRU replacement
- Since entire MVM computation is a sequence of block MVMs, this means miss ratio will be 0.25/b independent of N!

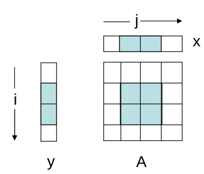


Scenario V (contd.)

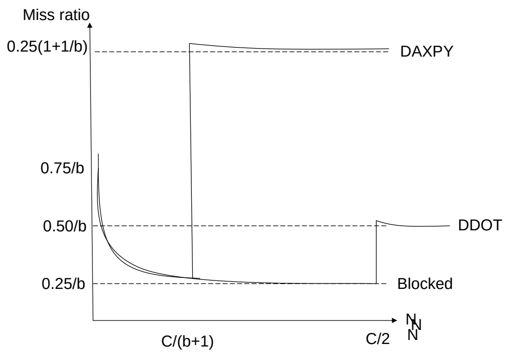
- Code: blocked code
```
for bi = 1,N,B
  for bj = 1,N,B
    for i = bi,min(bi+B-1,N)
      for j = bj,min(bj+B-1,N)
        y(i)=y(i)+A(i,j)*x(j)
```

Better code: interchange the two outermost loops and fuse bi and i loops
```
for bj = 1,N,B
  for i = 1,N
    for j = bj,min(bi+B-1,N)
      y(i)=y(i)+A(I,j)*x(j)
```

This has the same memory behavior as doubly-blocked loop but less loop overhead.



Miss ratios



Key transformations

- Loop permutation

```
for i = 1,N                for j = 1,N
  for j = 1,N       →        for i = 1,N
    S                          S
```

- Strip-mining

```
for i = 1,N         →      for bi = 1,N,B
  S                          for i = bi, min(bi+B-1,N)
                               S
```

- Loop tiling = strip-mine and interchange

```
for i = 1,N         →      for bi = 1,N,B
  for j = 1,N                for j = 1,N
    S                          for i = bj,min(bj+B-1,N)
                                 S
```

Notes

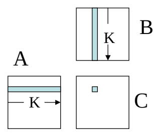
- Strip-mining does not change the order in which loop body instances are executed
  - so it is always legal
- Loop permutation and tiling do change the order in which loop body instances are executed
  - so they are not always legal
- For MVM and MMM, they are legal, so there are many variations of these kernels that can be generated by using these transformations
  - different versions have different memory behavior as we have seen

Matrix multiplication

- We have studied MVM in detail.
- In dense linear algebra, matrix-matrix multiplication is more important.
- Everything we have learnt about MVM carries over to MMM fortunately, but there are more variations to consider since there are three matrices and three loops.

MMM

```
DO I = 1, N//row-major storage
  DO J = 1, N
    DO K = 1, N
      C(I,J) = C(I,J) + A(I,K)*B(K,J)
```

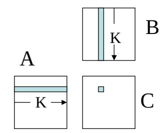


IJK version of matrix multiplication

- Three loops: I,J,K
- You can show that all six permutations of these three loops compute the same values.
- As in MVM, the cache behavior of the six versions is different

MMM

```
DO I = 1, N//row-major storage
  DO J = 1, N
    DO K = 1, N
      C(I,J) = C(I,J) + A(I,K)*B(K,J)
```

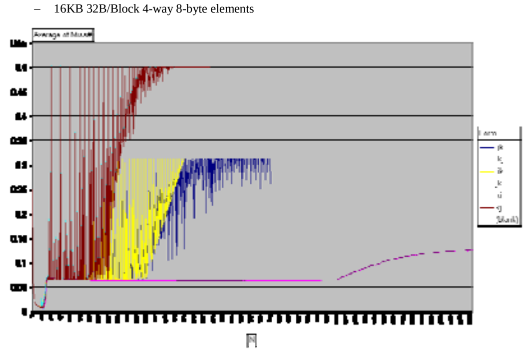


IJK version of matrix multiplication

- K loop innermost
  – A: good spatial locality
  – C: good temporal locality
- I loop innermost
  – B: good temporal locality
- J loop innermost
  – B,C: good spatial locality
  – A: good temporal locality
- So we would expect IKJ/KIJ versions to perform best, followed by IJK/JIK, followed by JKI/KJI

MMM miss ratios (simulated)

L1 Cache Miss Ratio for Intel Pentium III
- MMM with N = 1…1300
- 16KB 32B/Block 4-way 8-byte elements

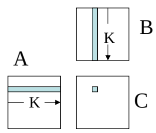


Observations

- Miss ratios depend on which loop is in innermost position
  – so there are three distinct miss ratio graphs
- Large cache behavior can be seen very clearly and all six version perform similarly in that region
- Big spikes are due to conflict misses for particular matrix sizes
  – notice that versions with J loop innermost have few conflict misses (why?)

IJK version

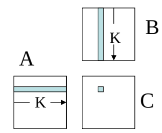
```
DO I = 1, N//row-major storage
  DO J = 1, N
    DO K = 1, N
      C(I,J) = C(I,J) + A(I,K)*B(K,J)
```



- Large cache scenario:
  - Matrices are small enough to fit into cache
  - Only cold misses, no capacity misses
  - Miss ratio:
    - Data size = 3 N^2
    - Each miss brings in b floating-point numbers
    - Miss ratio = 3 N^2 /b*4N^3 = 0.75/bN (eg) 0.019 (b = 4,N=10)

IJK version (large cache)

```
DO I = 1, N//row-major storage
  DO J = 1, N
    DO K = 1, N
      C(I,J) = C(I,J) + A(I,K)*B(K,J)
```



- Large cache scenario:
  - Matrices are small enough to fit into cache
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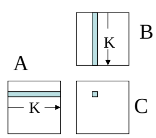
  - Miss ratio:
    - Data size = 3 N^2
    - Each miss brings in b floating-point numbers
    - Miss ratio = 3 N^2 /b*4N^3 = 0.75/bN = 0.019 (b = 4,N=10)

IJK version (small cache)

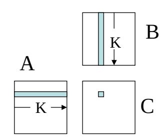
```
DO I = 1, N
  DO J = 1, N
    DO K = 1, N
      C(I,J) = C(I,J) + A(I,K)*B(K,J)
```



- Small cache scenario:
  - Matrices are large compared to cache
    - stack distance is not O(1) => miss
  - Cold and capacity misses
  - Miss ratio:
    - C: N^2/b misses (good temporal locality)
    - A: N^3 /b misses (good spatial locality)
    - B: N^3 misses (poor temporal and spatial locality)
    - Miss ratio → 0.25 (b+1)/b = 0.3125 (for b = 4)

Miss ratios for other versions

```
DO I = 1, N//row-major storage
  DO J = 1, N
    DO K = 1, N
      C(I,J) = C(I,J) + A(I,K)*B(K,J)
```



IJK version of matrix multiplication

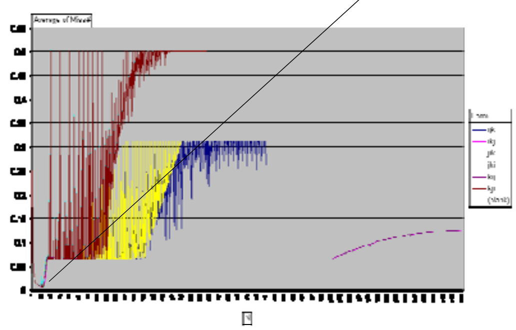
- K loop innermost
  - A: good spatial locality
  - C: good temporal locality 0.25(b+1)/b
- I loop innermost
  - B: good temporal locality (N^2/b + N^3 +N^3)/4N^3 → 0.5
- J loop innermost
  - B,C: good spatial locality (N^3/b + N^3/b + N^2/b)/4N^3 → 0.5/b
  - A: good temporal locality
- So we would expect IKJ/KIJ versions to perform best, followed by IJK/JIK, followed by JKI/KJI

MMM experiments

L1 Cache Miss Ratio for Intel Pentium III

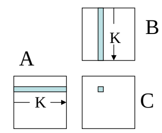
- MMM with N = 1…1300
- 16KB 32B/Block 4-way 8-byte elements

Can we predict this?



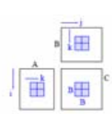
Transition out of large cache

```
DO I = 1, N//row-major storage
  DO J = 1, N
    DO K = 1, N
      C(I,J) = C(I,J) + A(I,K)*B(K,J)
```



- Find the data element(s) that are reused with the largest stack distance
- Determine the condition on N for that to be less than C
- For our problem:
  - $N^2 + N + b < C$ (with optimal replacement)
  - $N^2 + 2N < C$ (with LRU replacement)
  - In either case, we get N ~ sqrt(C)
  - For our cache, we get N ~ 45 which agrees quite well with data

Blocked code



```
for bi = 1,N,B
 for bj = 1,N,B
  for bk = 1,N,B
   for i = bi, min(bi+B-1,N)
     for j = bj, min(bj+B-1,N)
      for k = bk, min(bk+B-1,N)
          y(i) = y(i) + A(i,j)*x(j)
```

As in blocked MVM, we actually need to stripmine only two loops

Notes

- So far, we have considered a two-level memory hierarchy
- Real machines have multiple level memory hierarchies
- In principle, we need to block for all levels of the memory hierarchy
- In practice, matrix multiplication with really large matrices is very rare
  - MMM shows up mainly in blocked matrix factorizations
  - therefore, it is enough to block for registers, and L1/L2 cache levels
- How do we organize such a code?
  - We will study the code produced by ATLAS.
  - ATLAS also introduces us to self-optimizing programs.