Advanced Systems Lab - Part2

11740 characters in 1933 words on 356 lines

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June 10, 2020

1 sparse linear algebra

linear algebra usually memory bound hence for sparse matrixes, compression pays off for BLAS 1, only 18% performance in 8mb working set

1.1 sparse matrix vector multiplication (MVM)

core building block of sparse linear algebra y += A *x; execute many times for different x's

operational intensity

for K nonzero entries

W(n) = 2K (one add, one mul per entry)

Q(n) = K + 3n (load nonzeros; load y,x; store y)

hence upper bound $\leq 1/4$ for doubles (8*Q(n))

trivial storage format

many zeros stored; unnecessary operations & movements operational itensity very low hence need better storage formats

1.2 compressed sparse row format (CSR)

NM matrix A, K non-zero entries values with non-zero entries in row-major (K length) col_{idx} with column of respective value (K length) row_start with index where new row starts (m+1 length)

storage

2K (values & column array) + m+1 (row_start array)

. . . .

loop over m rows go to next row when $col_idx[i] \ge row_start[j]$

example

[a,0,b; 0,c,0; 0,0,0] values [a,b,c] col_{idx} [0,2,1] row_start [0,2,3]

advantages

only nonzero values stored all arrays accessed consecutively (good spatial locality) good temporal locality with y

disadvantages

insertion into A costly bad spatial & temporal locality with x of y = A*x

because columns (hence matching entry of x) unordered

comparison to dense MVM

2x slower compared to trivial loop performance is input dependent blocking requires change of data structure

1.3 blocked CSR (BCSR)

block for registers to reduce traffic with x NM matrix A, K non-zero entries, r*c blocksize store whole blocks including zero-values b_values with all blocks which have non-zero entries b_col_idx with block-based column of block b_row_start with index where block-based row starts

storage space

 $rcK (blocks) + K (values) + m/r+1 (row_start)$

code

loop over m/r+1 rows dense micro MMM in inner loop

example

[a,0,b,0;0,c,0,0;0,0,0,0;0,0,0,0]

for r=c=2 values [a,0,0,c,b,0,0,0,0] col_{idx} [0,1] row_start [0,2]

advantages;

temporal locality of x and y less index storage

disadvantages

need to store some 0s (storage, computational overhead) relevant bc problem already memory bound

1.4 choose CSR / BCSR

performance hard to predict, maschine dependent BCSR often better in well-known sparse matrix set but CSR also has winning scenarios

by extensive search

transformation cost CSR \to BCSR equals 10 SMVM hence extensive BCSR block size search too slow

by estimating gain/loss

estimate gain with dense performance of BCSR / CSR is machine dependent, hence could do at compile time estimate loss with matrix values of BCSR / CSR is data dependent, hence likely need to do at run time choose best gain / loss ratio $\,$

1.5 principles

optimize memory hierarchy

blocking for registers (same as ATLAS) change data structure of A optimizations are input dependent

fast basic blocks (micro MVM)

unrolling / scalar replacement

search for CSR, BCSR & block size

use performance model to choose best variant (versus mesuring runtime like in ATLAS)

1.6 other ideas

cache blocking

divide sparse matrix into smaller sparse matrixes only useful for very large matrixes

value compression

only store unique values replace values array with index to its unique value

pattern-based compression

extend BCSR with bit patterns defining non-zero entries choose different kernel for each bit pattern in values, no longer need to store 0s now like $0306 \rightarrow$ bit pattern 0101; values 142

${\bf multiple\ inputs\ szenario}$

block accross multiple MVM runs hence do A *yxz in single run

2 fast fourier transform (FFT)

used to do signal processing analog (with currents)

2.1 introduction

history

1805 Gauss discovered FFT for personal paper-interpolation $1965\ \mathrm{FFT}$ cooley tukey rediscovers; enables digital processing

purpose

change of basis by multiplying with fixed matrix is a linear transform (n-vector input/output) $y = Tx (y_k = sum_of(t_k *x_l))$

optimization potential

up to 35x faster

5x for locality, 3x for vectorization, 3x for threading

2.2 discrete fourier transform (DFT)

 $y_k = \text{sum_of(e^(-2*kl*pi*i / n) *x_l)}$ all n roots of unity (of one) w_n called primitive nth root of 1

notation

 $y = DFT_n*x, 2n^2$ operations

evaluate

get multiplicator using n (size) m = kl*2pi/n insert k/l (row/column; zero-based) then evaluate with cos(a) + i*sin(m) remember that sin(0) = 0, cos(0) = 1

 DFT_2 [[1 1], [1 -1]] no mults (bc all factors 1), 1 adds/sub $y_1 = x_1 + x.2$; $y_2 = x_1 - x_2$ called butterfly

DFT_4

in complex arithmetic, needs to be mapped to machine

further examples

DFT & RDFT universally used MPEG & JPEG uses own kind of DFT

2.3 cooley-tukey FFT

FFT transformation algorithm calculate T like T = T_1*T_2*.... * T_m only useful if T_i are sparse, and m low

2.3.1 FFT=4

essentially 4 DFT of size 2

matrix

 $\begin{array}{ll} {\rm for} \ . = 0 \ ({\rm better} \ {\rm readability}) \\ {\rm T1} = [1...,.1.,.1..,..1] \ ({\rm shift}; \ 0 \ {\rm ops}) \\ {\rm T2} = [1 \ 1...,1 \ -1...,.1 \ 1,..1 \ -1] \ ({\rm four} \ {\rm adds}) \\ {\rm T3} = [1...,1..,.1..,...i] \ ({\rm one} \ {\rm mul} \ {\rm by} \ i) \\ {\rm T4} = [1.1.,.1.1,1.-1..,1.-1] \ ({\rm four} \ {\rm adds}) \\ {\rm y} = {\rm T4}*{\rm T3}*{\rm T2}*{\rm T1}*{\rm x} \\ \Rightarrow {\rm reduced} \ {\rm FFT} \ {\rm opcount} \ {\rm to} \ 8 \ {\rm adds}, \ 1 \ {\rm mul} \end{array}$

algebra

(DFT-2 (x) I-2)diag(1,1,1,i)(I-2 (x) DFT-2)L-2^4 $I_2 = \text{diag}(1,1)$ is identity matrix of size 2 L-2^4 = permutation with stride 2 for (x) kroenecker product multiply entry on left with whole matrix right produces for 2*2 (x) n*n = 2n*2n result

dataflow representation

right x1,x2,x3,x4 flows to left y1y2y3y4 permutation of x2 and x3 (L.2^4) DFT_2 applied to x1,x2 and x3x4 (I.2 (x) DFT_2) scaling represented as black dots (diag(1,1,1,i)) DFT_2 applied to x1,x3 and x2x4 (DFT_2 (x) I.2)

2.3.2 generalization

(DFT_k (x) I_m)T_m^n(I_k (x) DFT_m)L_k^n choose radix k, select m to fit input DFT_k (x) (x) I_m results with DFT_k in the diagonal T_m^n as diagonal with m-1 1s, then an i, then repeat I_k (x) DFT_m results in m A's at stride m L_k^n permutation; read at stride k, write at stride 1 can reformulate to read at stride 1, write at stride m get n logn algorithm

variants

decimation-in-time decimation-in-frequency (transposed cooley-turkey)

factors

can choose radix k, but in the end k*m = n for factors of 2 trivial; for primes need different algorithm

cost

n log(n) complex adds; each needs 2 real adds n log(n)/2 complex mults; each needs 2 adds, 4 mults hence 3n log(n) adds, 2n log(n) mults = $5n \log(n)$ reduce op count depending on recusion because can simplify *i or *1

recursive vs iterative

calculation order different (DAG equivalent) iterative in stages (compute all of same kind of butterfly) recursive in recusion (compute butterfly as soon as dependency resolved) only order of operation changes, not count recursive better on caches be temporal locality

2.4 FFT variants

iterative

inital permutation step then bigger and bigger butterflies size of butterflies defined by radix

pease

permute result of butterflies to only operate on 2butterflies; good for CPUs

stockham

big butterflies and then permute permutations always in pairs of two good for 2-element cache lines

six-step FFT

optimized for parallelization three stages of communication, two parallel stages works for all sizes, any computation

multi-core FFT

similar to six-steps, but always two elements travel together well if block size 2; no false sharing hence two processes access elements in same cache line

2.5 complexity

use L_c as measure; defines cost add/mul = 1 for number <|c| used L_2 in proofs; L.infinity would be more real-worldly

upper bounds

for $n = 2^k \Rightarrow 3/2$ n log(n) other n \Rightarrow 8 n log(n)

lower bound

 $L_c(DFT) \ge 1/2 \text{ n log_c(n)}$

hence as n goes to infinity then constant c also goes to infinity current existing algorithm is close under $4n \log(n)$ for $n=2^k$

current usage

algorithm currently in use uses bit more than 4nlogn

2.6 optimizations

2.6.1 choice of algorithm

iterative used to be the best choice be easy to implement, fewer instructions recursive now better be caches (temporal locality)

2.6.2 locality improvement

trivially need 4 data passes (bc 4 steps)

DFTree

fuse T1,T2 (read stride k, DFT.m, write stride 1) introduce interface DFTrec(m, x, y, k, j) for m size, x/y vectors, k input stride, j output stride out-of-place (reads x, writes y) called recusively (just change stride)

DFTscaled

fuse T3,T4 (read stride m, prescale, DFT_k, write stride m) introduce interface DFTscaled(k, y, d, m) for k size, y input/output vector, d prescale, m input/output stride in-place (reads & writes y) base case (hence rewritten for each radix factor)

pseudocode

for n size, x/y input/output vector, t prescale lookup choose k (depends on n; ensure base case for DFTscaled exists) let m=n/k for (i until k) DFTrec(m, x+i, y + m*i, k, 1) for (i until m) DFTscaled(k, y+i, t[i], m)

2.6.3 constants

FFT needs multiplications by roots of unity expensive because needs sin/con to compute

precompute

DFT_init(n) for n input size to create lookup table then reuse result for all same-sized DFT computations prestore for small input sizes

2.6.4 optimized basic blocks

unroll recursions

bc hard for compiler to do it automatically function calls overhead negligible (bc base case reached fast)

base cases

to optimize specifically for small inputs empirically useful for n \leq 32 but then need 31 DFTrec & DFTscaled each can be generated (as its done by FFTW)

2.6.5 adaptivity

adapt recusion strategy to platform do search within init function (reuse $DFT_{init}(n)$) use dynamic programming (saves perf. compared to exhaustive)

valid recusions

generated droplet for base cases must exist DFTscaled as a basecase (hence always right-recusive)

2.7 FFTW (fastest fourier transform in the west)

generates codelets using SIMD with input n generates DFTrec, DFTscaled in three steps

2.7.1 DAG generator

create trees based on sum formula includes cooley-tukey, split-radix, fuse trees into DAG

2.7.2 simplifier

simplify DAG

algebraic transformations

mults $(0*x \Rightarrow 0$, similar cases for -1,1) distribution laws $(kx + ky \Rightarrow k(x+y))$ canonicalization $(x-y,y-x \Rightarrow x-y, -(y-x))$

common subexpression eliminiation (CSE) $\,$

use temporary variables to avoid double computation

reduce constants (DFT specific)

has many multiplications with many different constants each constant used positive & negative (bc $\sin(a) = -\sin(a)$) reduce register pressure by storing only positive constant and use subtraction where $-\sin(a)$ would be nedeed

2.7.3 scheduler

transform DAG to c under register spill minimization want to reach target $I = O(\log(C))$ for cache size C uses SSA style, scoping

approach

cut DAG in middle

then recurse on connected components (butterflies) to outside hence use minimal number of registers for "durchstich"

cut DAG middle

start from the outsides (left = input, right = output) color immediate next inner reachable nodes repeat recursively until nodes touch in the middle

2.8 comparison

MMMM (ATLAS) sparse MVM (Sparsity, Bebop) DFT (FFTW)

cache optimizations

blocking for MMM, SMVM recusive FFT & fusion of steps for FFTW

register optimizations

blocking for MMM, SMVM schedule small FFT for FFT

optimized basic blocks

unrolling

scalar replacement & SSA scheduling & simplifications for FFT

other optimizations

precompute constants for small DFT for large FFT the algorithm becomes memory bound hence avoid precomputation to save on storage

adaptivity

search blocking parameters for MMM search register block size for SMVM search recusion strategy for DFT

2.9 spiral

specifically to optimize FFT for specific input size applicable for locality, threading, ...

algorithm

use signal processing language (SPL) is mathematical, declarative, point-free (any input size) divide and conquer applied to transform algorithms

generate code

decompose DFT with SPL rules to algorithm optimize for parallelization/vectorization transform to structure with sums optimize for locality transform to C program optimize in basic blocks

vectorization optimization

some SPL expressions directly relate to SIMD code like DFT_2 (x) I_4 which can be transformed easily hence rewrite given SPL to vectorizable SPL expressions

generate base cases

express intrinsics as matrices then search for matrixes matching base cases

generalize for any input size

need many more codelets results in huge library size but faster than other approaches; including FFTW