Whirlwind Tour of LA Part 1: Some Nitty-Gritty Stuff

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Logistics

- ▶ PS1/2 deferred to next Weds/Fri
 - ▶ Brandon has OH tonight 5-7
 - ▶ I will arrange extra OH early next week (TBA)
- Please keep up with the reading!
- Ask me questions!

Big picture: What's a matrix?

An array of numbers, or a representation of

- A tabular data set?
- A graph?
- A linear function between vector spaces?
- ▶ A bilinear function on two vectors?
- A pure quadratic function?

It's all the above, plus being an interesting object on its own!

Let's start concrete.

Basics: Constructing matrices and vectors

```
\begin{array}{lll} x = [1; \ 2]; & \% \ \textit{Column vector} \\ y = [1, \ 2]; & \% \ \textit{Row vector} \\ M = [1, \ 2; \ 3, \ 4]; & \% \ \textit{2-by-2 matrix} \\ M = [I, \ A]; & \% \ \textit{Horizontal matrix concatenation} \end{array}
```

Basics: Constructing matrices and vectors

```
I = eye(n); % Build n-by-n identity

Z = zeros(n); % n-by-n matrix of zeros

b = rand(n,1); % n-by-1 random matrix (uniform)

e = ones(n,1); % n-by-1 matrix of ones

D = diag(e); % Construct a diagonal matrix

e2 = diag(D); % Extract matrix diagonal
```

Basics: Transpose, rearrangements

```
% Reshape A to a vector, then back to a matrix
% Note: MATLAB is column—major
avec = reshape(A, prod(size(A)));
A = reshape(avec, n, n);
A = A'; % Conjugate transpose
A = A.'; % Simple transpose
idx = randperm(n); % Random permutation of indices
Ac = A(:,idx); % Permute columns of A
Ar = A(idx,:); % Permute rows of A
Ap = A(idx,idx); % Permute rows and columns
```

Basics: Submatrices, diagonals, triangles

```
A = \mathbf{randn}(6,6); \qquad \% 6 - by - 6 \ random \ matrix \\ A(1:3,1:3) \qquad \% \ Leading \ 3 - by - 3 \ submatrix \\ A(1:2:\mathbf{end},:) \qquad \% \ Rows \ 1, \ 3, \ 5 \\ A(:,3:\mathbf{end}) \qquad \% \ Columns \ 3 - 6 \\ Ad = \mathbf{diag}(A); \qquad \% \ Diagonal \ of \ A \ (as \ vector) \\ A1 = \mathbf{diag}(A,1); \qquad \% \ First \ superdiagonal \\ Au = \mathbf{triu}(A); \qquad \% \ Upper \ triangle \\ Al = \mathbf{tril}(A); \qquad \% \ Lower \ triangle
```

Basics: Matrix and vector operations

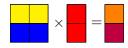
```
y = d.*x; % Elementwise multiplication of vectors/matrices
y = x./d; % Elementwise division
z = x + y; % Add vectors/matrices
z = x + 1; % Add scalar to every element of a vector/matrix
y = A*x; % Matrix times vector
y = x'*A; % Vector times matrix
C = A*B; % Matrix times matrix
% Don't use inv!
x = A \ b; % Solve Ax = b * or* least squares
y = b/A; % Solve yA = b or least squares
```

Two basic operations

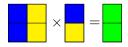
- ▶ Matrix-vector product (matvec): $O(n^2)$
- ▶ Matrix-matrix product (matmul): $O(n^3)$

Matvec

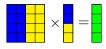
A matvec is a collection of dot products.



A matvec is a sum of scaled columns.



Can also think of *block* rows/columns.



Same (scalar) operations, different order!

Matvec: Diagonal

```
% Bad idea
D = diag(1:n); % O(n^2) setup
y = D*x; % O(n^2) matvec
% Good idea
d = (1:n)'; % O(n) setup
y = d.*x; % O(n) matvec
```

- Matrix-vector products are a basic op.
- Can you write the two nested loops?
- ► Obvious form: y = Ax
- Obvious isn't always best!

Matvec: Low rank

$$A = u*v'; % O(n^2)$$

 $y = A*x;$
 $a = v'*x; % O(n)$
 $y = u*a;$

Don't form low rank matrices explicitly!

Matvec: Low rank

Write an outer-product decomposition for

- A matrix of all ones
- \blacktriangleright A matrix of ± 1 in a checkerboard
- A matrix of ones and zeros in a checkerboard

Matvec: Sparse

```
% Sparse (O(n) = number nonzeros to form / multiply)

e = ones(n-1,1);

T = speye(n) - spdiags(e,-1,n,n) - spdiags(e,1,n,n);

% Dense (O(n^2))

T = eye(n) - diag(e,-1) - diag(e,1);
```

Will talk about this in more detail - keep it in mind!

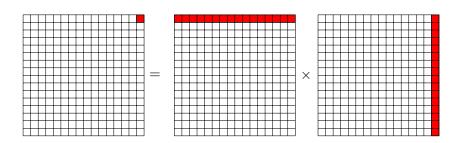
From matvec to matmul

Matrix-vector product is a key kernel in *sparse* NLA. Matrix-matrix product is a key kernel in *dense* NLA.

Surprisingly tricky to get fast – so let someone else write fast matmul, and use it to accelerate our codes!

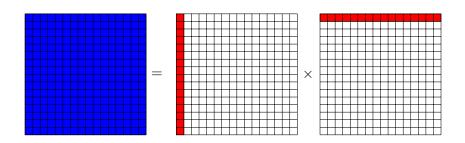
Matmul: Inner product version

An entry in C is a dot product of a row of A and column of B.



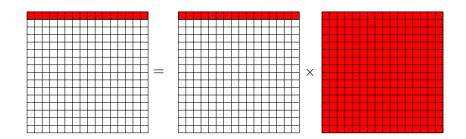
Matmul: Outer product version

C is a sum of outer products of columns of A and rows of B.



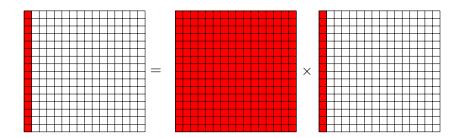
Matmul: Row-by-row

A row in C is a row of A multiplied by B.



Matmul: Col-by-col

A column in C is A multiplied by a column of B.

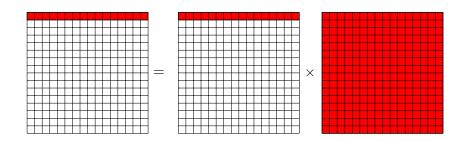


Reality intervenes

These arrangements of matmul are theoretically equivalent. What about in practice?

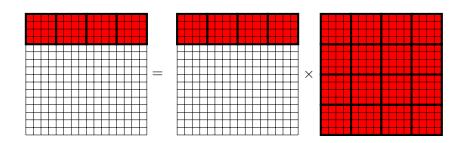
Answer: Big differences due to memory hierarchy.

One row in naive matmul



- ► Access A and C with stride of 8M bytes
- ▶ Access all $8M^2$ bytes of B before first re-use
- ► Poor *arithmetic intensity*

Engineering strategy: blocking/tiling



Simple model

Consider two types of memory (fast and slow) over which we have complete control.

- ▶ m = words read from slow memory
- $t_m = \text{slow memory op time}$
- ightharpoonup f = number of flops
- $ightharpoonup t_f = time per flop$
- ightharpoonup q = f/m = average flops / slow memory access

Time:

$$ft_f + mt_m = ft_f \left(1 + \frac{t_m/t_f}{q} \right)$$

Larger q means better time.

How big can q be?

- 1. Dot product: *n* data, 2*n* flops
- 2. Matrix-vector multiply: n^2 data, $2n^2$ flops
- 3. Matrix-matrix multiply: $2n^2$ data, $2n^3$ flops

These are examples of level 1, 2, and 3 routines in *Basic Linear Algebra Subroutines* (BLAS). We like building things on level 3 BLAS routines.

q for naive matrix multiply

 $q \approx 2$ (on board)

q for blocked matrix multiply

q pprox b (on board). If M_f words of fast memory, $b pprox \sqrt{M_f/3}$.

Th: (Hong/Kung 1984, Irony/Tishkin/Toledo 2004): Any reorganization of this algorithm that uses only associativity and commutativity of addition is limited to $q = O(\sqrt{M_f})$

Note: Strassen uses distributivity...

Concluding thoughts

- ▶ Will not focus on performance *details* here (see CS 5220!)
- ► Knowing "big picture" issues makes a big difference
 - Order-of-magnitude improvements through blocking ideas
 - ▶ Even more possible through appropriate use of structure
- Next time: More theoretical stuff!