Fundamental Algorithms
Chapter 8: Matrices and Scientific Computing

Sevag Gharibian

Universität Paderborn
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Outline

1. Introduction to matrices (review)
2. Matrix multiplication algorithms
   - Strassen's algorithm (1967)
   - Drineas-Kannan-Mahoney randomized algorithm (2006)
3. Random walks
   - Gambler's ruin
   - Google's PageRank algorithm (1999)
4. Polynomial multiplication
   - Complex numbers
   - Polynomials
   - $O(N \log N)$-time polynomial multiplication via Fourier Transform

References

- CLRS Chapters 28.1, 28.2, 30.1, 30.2
- M. Mahoney lecture notes: `https://www.stat.berkeley.edu/~mmahoney/f13-stat260-cs294/Lectures/lecture02.pdf`
- T. Leighton and T. Rubinfeld lecture notes: `http://web.mit.edu/neboat/Public/6.042/randomwalks.pdf`
- O. Levin: `http://discrete.openmathbooks.org/dmoi2/sec_recurrence.html`
- M. Nielsen lectures on Google technology: http://michaelnielsen.org/blog/lectures-on-the-google-technology-stack-1-introduction-to-pagerank/
- History of complex numbers https://www.cut-the-knot.org/arithmetic/algebra/HistoricalRemarks.shtml

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Matrices

Motivation - why matrices?

- Applications in most technical fields
- Physics: Classical mechanics, optics, electromagnetism, quantum mechanics
- Computer Science: Graphics, randomized algorithms, big data (e.g. Google's PageRank algorithm), quantum computing
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Note:

- Throughout these notes, we assume all operations are done over the field of real numbers, $\mathbb{R}$.
- We ignore issues of precision (which is an important topic).

Basics

Recall a 2×3 matrix M is given (e.g.) by:

$$M = \begin{pmatrix} 0 & 3 & -1 \\ 2 & 2 & 1 \end{pmatrix}.$$

The *transpose* of M is

$$M^T = \begin{pmatrix} 0 & 2 \\ 3 & 2 \\ -1 & 1 \end{pmatrix}.$$

The set of all $m \times n$ matrices over $\mathbb{R}$ is denoted $\mathbb{R}^{m\times n}$.

The *entry at position* (i, j) of M is denoted $M(i, j)$ or M_{ij}.

Basics

Recall: The set of all $m \times n$ matrices over $\mathbb{R}$ is denoted $\mathbb{R}^{m\times n}$.

Special cases of matrices:

- (Vectors) For $n = 1$ (resp. $m = 1$), have *column* (resp. *row*) vector:

$$\mathbf{v} = \begin{pmatrix} 3 \\ 5 \end{pmatrix}, \qquad \mathbf{v}^T = \begin{pmatrix} 5 & 3 \end{pmatrix}.$$

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- (Square matrix) Set $m = n$.
- (Diagonal matrix) A square matrix M with $M_{ij} = 0$ if $i \neq j$.
- (Identity matrix) The $n \times n$ (diagonal) matrix ($n = 2$ below)

$$I_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

Matrix operations

- (Matrix addition) For any $M, N \in \mathbb{R}^{m \times n}$, $(M + N)_{ij} = M_{ij} + N_{ij}$.

  Ex. What is $\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} 2 & 2 \\ 2 & 2 \end{pmatrix}$?

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- (Scalar multiplication) For any $c \in \mathbb{R}$, $(cM)_{ij} = c \cdot M_{ij}$.
- (Vector inner product) For any column vectors $\mathbf{v}, \mathbf{w} \in \mathbb{R}^n$,

$$\mathbf{v} \cdot \mathbf{w} = \sum_{i=1}^{n} v_i w_i \in \mathbb{R}.$$

  The inner product "measures" the overlap between **v** and **w**. When $\mathbf{v} \cdot \mathbf{w} = 0$, we say **v** and **w** are *orthogonal*.

  Ex. For $\mathbf{v} = (1 \;\; 0)^T$, $\mathbf{w} = (0 \;\; 1)^T$, what is $\mathbf{v} \cdot \mathbf{w}$? $\mathbf{v} \cdot \mathbf{v}$? Draw **v** and **w** on the 2D Euclidean plane to visualize the dot product.

Matrix Multiplication

- Since we are working over $\mathbb{R}$, can be defined using inner product[1].
- For any $M \in \mathbb{R}^{m\times n}$, $N \in \mathbb{R}^{n\times p}$:

$$(MN)_{ij} = M_{(i)}^T \cdot N^{(j)} = \sum_{k=1}^{n} M_{i,k}N_{k,j},$$

  where $M_{(i)}$ (resp. $M^{(i)}$) is the ith row of M (resp. ith column) of M.

  Ex. What is dimension of MN, i.e. what values are allowed for i, j?

- Examples:

$$\begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 2 & 1 \\ 4 & 3 \end{pmatrix}$$

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$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} b \\ a \end{pmatrix}.$$

Q: In 2D plane, what operation does last equation encode?

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Matrix Multiplication

More properties:

- For all $M \in \mathbb{R}^{m \times n}$, $I_m M = M I_n = M$.
- For any triple A, B, C (with appropriate dimensions):
  - (associativity) $A(BC) = (AB)C$
  - (distributivity) $A(B + C) = AB + AC$ and $(B + C)D = BD + CD$.
  - (commutativity) Does $AB = BA$ necessarily?

Ex. Let $M = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $N = \begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix}$. Does MN equal NM?

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Life lesson

That matrix multiplication is non-commutative is *not* just an academic question! The structure of the world around us depends on this property — it gives rise to the *uncertainty principle* in quantum mechanics, which in turn is used[2] to explain why matter is stable (i.e. why doesn't an electron just crash into the nucleus of the atom?).

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Can also do "low-level" analysis by factoring in cost of each field op:

- E.g. How many steps to actually implement n-bit addition of integers on a Turing machine? (Answer: $O(n)$.)
- This cost model is called *bit complexity*.

Here, we focus on operation complexity, i.e. we will not worry about the low-level details of implementing addition, multiplication etc over $\mathbb{R}$.

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Strassen's Algorithm

- Strassen, Volker. Gaussian Elimination is not Optimal, *Numer. Math.* 13, p. 354–356, 1969.
- Requires $O(n^{2.808})$ operations.
- Recursive, divide-and-conquer approach.
- Quite a surprise to the research community!

Outline

Goals of section

- Practice working with matrices
- Practice working with randomization
- Study a mix of classic and modern algorithms

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Warmup

Note: For simplicity, we assume n is a power of 2, where $M, N \in \mathbb{R}^{n \times n}$.

Write M, N, MN in block form. For $a, b, c, d, e, f, g, h, r, s, t, u \in \mathbb{R}^{\frac{n}{2} \times \frac{n}{2}}$:

$$M = \begin{pmatrix} a & b \\ c & d \end{pmatrix}, \quad N = \begin{pmatrix} e & f \\ g & h \end{pmatrix}, \quad MN = \begin{pmatrix} r & s \\ t & u \end{pmatrix}.$$

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Naive algorithm:

- Compute each block of MN independently as follows.

$$r = ae + bg \qquad s = af + bh \qquad t = ce + dg \qquad u = cf + dh.$$

- Recursively compute each $n/2 \times n/2$ product ae, bg, etc. . .

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Cost: For $M, N \in \mathbb{R}^{n\times n}$, recurrence relation for multiplication costs $T(n)$:

$$T(n) = 8T(n/2) + \Theta(n^2) \in \Theta(n^{\log_2 8}) \in \Theta(n^3) \ldots \text{ (why?)}$$

. . . no improvement!

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This cost was too large because we needed 8 recursive calls per level...

Q: Can we do it with 7 recursive calls?

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Q: Can we do it with 7 recursive calls?

- Remarkably, yes!
- We hence get runtime $\Theta(n^{\log_2 7}) \in \Theta(n^{2.808})$, as claimed.
- Ok, so how do we do it?

Strassen's algorithm - a bit of magic

1. Compute the following 7 products (recursively):

$$
\begin{array}{lll}
P_1 = a(f-h) & P_2 = (a+b)h & P_3 = (c+d)e \\
P_4 = d(g-e) & P_5 = (a+d)(e+h) & P_6 = (b-d)(g+h) \\
P_7 = (a-c)(e+f) & &
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2. Recall we wish to compute each block of MN, i.e.:

$$r = ae + bg \qquad s = af + bh \qquad t = ce + dg \qquad u = cf + dh.$$

Magically, we have:

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\begin{array}{ll}
r = P_5 + P_4 - P_2 + P_6 & s = P_1 + P_2 \\
t = P_3 + P_4 & u = P_5 + P_1 - P_3 - P_7.
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$$T(n) = 7T(n/2) + \Theta(n^2) \in \Theta(n^{\log_2 7}) \in \Theta(n^{2.808})!$$

Two questions you should always ask yourself:

1. Is this asymptotic improvement useful in practice?

[3] The precise definition of "numerically stable" depends on context. Roughly, it means one wants the algorithm to "behave well" even on "bad inputs/edge cases".

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2. Can we do better?

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Lower bounds

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- Embarrassingly, unknown whether optimal is $\omega(n^2)$ (after 50 years!)
- If we restrict the type of circuit computing the matrix product, then a lower bound of $\Omega(n^2 \log n)$ can be shown [Raz, 2003]

Can we do better?

Upper bounds

- Strassen (1969): $O(n^{2.808})$.
- Pan (1978): $o(n^{2.796})$
- Bini, Capovani, Romani, Lotti using *border rank* (1979): $o(n^{2.78})$
- Schönhage via τ*-theorem* (1981): $o(n^{2.548})$
- Romani (1982): $o(n^{2.517})$
- Coppersmith, Winograd (1981): $o(n^{2.496})$
- Strassen via *laser method* (1986): $o(n^{2.479})$
- Coppersmith, Winograd (1989): $o(n^{2.376})$
- V. V. Williams (2013): $O(n^{2.3729})$
- Le Gall (2014): $O(n^{2.3728639})$

The more advanced these algorithms get, the less useful they tend to be in practice. . .

What if we want something more useful in practice? Say for machine learning or big data?

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What if we want something more useful in practice? Say for machine learning or big data?

Common tool: Randomization

Tradeoff: Time/space versus accuracy

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Organizers:

Petros Drineas (Purdue University; chair), Ken Clarkson (IBM Almaden), Prateek Jain (Microsoft Research India), Michael Mahoney (International Computer Science Institute and UC Berkeley)

The focus of this workshop will be on recent developments in randomized linear algebra, with an emphasis on how algorithmic improvements from the theory of algorithms interact with statistical, optimization, inference, and related perspectives. One focus area of the workshop will be the broad use of sketching techniques developed in the data stream literature for solving optimization problems in linear and multi-linear algebra. The workshop will also consider the impact of theoretical developments in randomized linear algebra on (i) numerical analysis as a method for constructing preconditioners; (ii) applications as a principled feature selection method; and (iii) implementations as a way to avoid communication rather than computation. Another goal of this workshop is thus to bridge the theory-practice gap by trying to understand the needs of practitioners when working on real datasets.

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Basic probability theory

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Note: Expected value is a *linear* function, i.e. $E[X + Y] = E[X] + E[Y]$.

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Ex. Let $X \in \{1, -1\}$ be a random variable corresponding to a sampling experiment in which a fair coin is flipped, and if the coin lands HEADS (resp. TAILS), you gain (resp. lose) 1 EUR. What is $E[X]$? What is $\mathrm{Var}[X]$?

Back to matrix multiplication

Recall: Over $\mathbb{R}$, matrix multiplication can be viewed as *inner products* over rows of M and columns of N.

For any $M \in \mathbb{R}^{m\times n}$, $N \in \mathbb{R}^{n\times p}$:

$$(MN)_{ij} = M_{(i)}^T \cdot N^{(j)} = \sum_{k=1}^{n} M_{i,k} N_{k,j},$$

where $M_{(i)}$ (resp. $M^{(i)}$) is the ith row of M (resp. ith column) of M.

Outer products

Inner product of $\mathbf{v} \in \mathbb{R}^n$ and $\mathbf{w} \in \mathbb{R}^n$ multiplies row vector by column vector:

$$\mathbf{v} \cdot \mathbf{w} = \mathbf{v}^T \mathbf{w} = \begin{pmatrix} v_1 & v_2 & \cdots & v_n \end{pmatrix} \begin{pmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \end{pmatrix} \in \mathbb{R}.$$

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Q: What dimensions does the outer product of $\mathbf{v} \in \mathbb{R}^m$ and $\mathbf{w} \in \mathbb{R}^n$ have?

Ex: Let $\mathbf{v} = (1 \;\; 0)^T$, $\mathbf{w} = (0 \;\; 1)^T$. What are inner/outer products of $\mathbf{v}$ and $\mathbf{w}$?

Back to matrix multiplication

Inner product view: For any $M \in \mathbb{R}^{m \times n}$, $N \in \mathbb{R}^{n \times p}$:

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Q: What differences can you spot between the inner and outer product views?

Ex: Prove that the outer product view is correct.

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Suppose wish to approximate sum $\sum_{k=1}^{n} a_i$ over $a_i \in \mathbb{R}$ *without* adding all a_i.

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Sampling Lemma (Arora, Karger, Karpinski, 1999)

Suppose $\forall i$, $|a_i| \leq M$ for fixed M. If $s = g \log n$ samples are drawn, then

$$\sum_{i=1}^{n} a_i - nM\sqrt{\frac{f}{g}} \leq \alpha q \leq \sum_{i=1}^{n} a_i + nM\sqrt{\frac{f}{g}}$$

with probability at least $1 - n^{-f}$, for $\alpha = \frac{n}{s}$ and $f, g > 0$.

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Obvious question: Can we do something similar for matrix multiplication?

Drineas-Kannan-Mahoney algorithm

Recall:

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Q: How "close" is C to MN? Specifically, how do we define an "absolute value function" $|C - MN|$ for matrices C, M, N?

Norms

What properties does absolute value function (on $\mathbb{R}$) have? $\forall a, b \in \mathbb{R}$:

1. (Non-negativity) $|a| \geq 0$.
2. (Subadditivity) $|a+b| \leq |a| + |b|$.
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A *norm* $\|\cdot\| : V \mapsto \mathbb{R}_{\geq 0}$ generalizes this to vector spaces V over a field $F = \mathbb{R}$.

Any norm, by definition, satisfies that for all $c \in F$, $\mathbf{v}, \mathbf{w} \in V$:

1. (Non-negativity) $\|v\| \geq 0$.
2. (Subadditivity) $\|\mathbf{v} + \mathbf{w}\| \leq \|\mathbf{v}\| + \|\mathbf{w}\|$.
3. (Absolute scalability) $\|c\mathbf{v}\| = |c|\,\|\mathbf{v}\|$.
4. (Positive definiteness) $\|\mathbf{v}\| = 0$ iff $\mathbf{v} = 0$ (i.e. $\mathbf{v}$ is zero vector).

Recall: A vector space can refer to a space of *vectors* or *matrices*.

Constructing norms

Like absolute value function, a norm should "measure the size" of its input.

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But you already know one way...let's use that.

Euclidean norm for "vectors"

Let $V = \mathbb{R}^n$. Then, Euclidean norm of $\mathbf{v} \in V$ is $\|\mathbf{v}\|_2 = \sqrt{\sum_{i=1}^{n} v_i^2}$.

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Note: These two are actually the same thing if you “reshape” M into a vector $\mathbf{v}$ by concatenating its columns.

Exercises on norms

1. Define $\mathbf{v} = \begin{pmatrix} 1 \\ -1 \end{pmatrix}$. What is $\|\mathbf{v}\|_2$?
2. Draw $\mathbf{v}$ in the 2D Euclidean plane. What does $\|\mathbf{v}\|_2$ represent?
3. What does the subadditivity property represent in the 2D plane?
4. Prove that the Euclidean norm is indeed a norm.
5. Let's consider a different norm, the *Taxicab norm* or 1*-norm*:

   $$\|\mathbf{v}\|_1 = \sum_{i=1}^{n} |v_i| .$$

   What is $\|\mathbf{v}\|_1$ for $\mathbf{v}$ from the first exercise above? What does the Taxicab norm represent on the Euclidean plane?
6. Define $M = \begin{pmatrix} -1 & 1 \\ 2 & -4 \end{pmatrix}$. What is $\|M\|_{\mathrm{F}}$?
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Note: There is more than one way to generalize the 1-norm to matrices.

Returning to our question

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Quality of approximation

Lemma (Drineas-Kannan-Mahoney, 2006)

For input matrices M and N, suppose the DKM algorithm makes s samples and outputs matrix C. Then for all indices i, j:

$$E[C_{ij}] = (MN)_{ij} \quad \text{and} \quad \mathrm{Var}[C_{ij}] = \frac{1}{s}\left(n\sum_{k=1}^{n} M_{ik}^2 N_{kj}^2 - (MN)_{ij}^2\right).$$

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Proof. For iteration t, define $X_t = (\frac{n}{s} M^{(k_t)} N_{(k_t)})_{ij}$ //(i,j)th entry of sample t.

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$$E[C_{ij}] = E\left[\sum_{t=1}^{s} X_t\right] = \sum_{t=1}^{s} E[X_t] = (MN)_{ij}$$

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Q: Why do red equalities hold?

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We know how each *individual entry* of C deviates from its value in MN.

Q: How “far” then is the full matrix C from MN?

Quality of approximation

Theorem (Drineas-Kannan-Mahoney, 2006)

$$E\left[\|MN - C\|_{\mathrm{F}}^2\right] = \frac{1}{s}\left(n\sum_{k=1}^{n}\left\|M^{(k)}\right\|_2^2\left\|N_{(k)}\right\|_2^2 - \|MN\|_{\mathrm{F}}^2\right).$$

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Plugging in the bounds on $\mathrm{Var}[C_{ij}]$ from previous lemma:

$$\begin{aligned} E\left[\|MN - C\|_{\mathrm{F}}^2\right] &= \sum_{i=1}^{m}\sum_{j=1}^{p}\left(\frac{1}{s}\left(n\sum_{k=1}^{n} M_{ik}^2 N_{kj}^2 - (MN)_{ij}^2\right)\right) \\ &= \frac{1}{s}\left(n\sum_{k=1}^{n}\left(\sum_{i=1}^{m} M_{ik}^2\right)\left(\sum_{j=1}^{p} N_{kj}^2\right) - \|MN\|_{\mathrm{F}}^2\right) \end{aligned}$$

from which claim follows.

Optimizing further

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Q: In iteration t, we *uniformly* sample column/row pair $M^{(k_t)}$ and $N_{(k_t)}$.

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Obs: But if a column/row has large norm, it has more "impact" on MN.

Idea: Sample columns/rows with larger norm with larger probability. Set:

Optimizing further

Theorem (Drineas-Kannan-Mahoney, 2006)

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This distribution turns out to be *optimal*, i.e. minimizes $E\left[\|MN - C\|_{\mathrm{F}}^2\right]$:

$$E\left[\|MN - C\|_{\mathrm{F}}^2\right] = \frac{1}{s}\left(\sum_{k=1}^{n}\left\|M^{(k)}\right\|_2 \left\|N_{(k)}\right\|_2\right)^2 - \frac{1}{s}\|MN\|_{\mathrm{F}}^2 \qquad (***).$$

Ex. Prove $(***) \leq (**)$. (Hint: Use Cauchy-Schwarz inequality.)

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3. Random walks
   - Gambler's ruin
   - Google's PageRank algorithm (1999)
4. Polynomial multiplication
   - Complex numbers
   - Polynomials
   - $O(N \log N)$-time polynomial multiplication via Fourier Transform

Goals of section

- More practice with randomization (life lesson: don't gamble)
- Practice solving recurrence relations
- Real world applications of matrices (life lesson: get rich)

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- Can bet 1€ per turn on a color, either red or black.
- If ball lands on your color in that turn, win 1€; else, lose 1€.
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Let's formalize this

Gambler's ruin

- Start with n€, and make sequence of bets.
- For each bet, win 1€ w.p. p, lose €1 w.p. $1 - p$.
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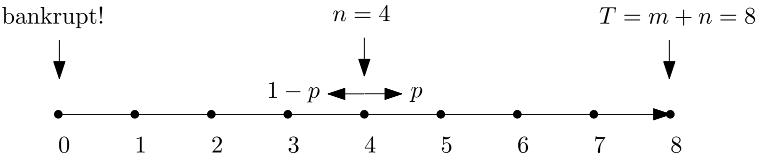

- Can be viewed as a 1-dimensional *random walk*.
- Move right 1 step with probability p, left 1 step with probability $1 - p$.

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More basic probability theory

A *sample space* Ω is an arbitrary set, the subsets of which are *events*.

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Law of total probability

Let $B_1, \ldots, B_n$ partition a sample space Ω. Then for any event A,

$$\Pr(A) = \sum_{i=1}^{n} \Pr(A \mid B_i)\Pr(B_i).$$

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So if we start with n€, we win with probability $P_n = pP_{n+1} + (1-p)P_{n-1}$, or

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This is a *linear homogeneous recurrence* with $P_0 = 0$ and $P_T = 1$.

Let's solve to get closed form for P_n, and determine odds of winning Roulette.

Idea: Use *characteristic root* technique.

Characteristic root technique

Consider recurrence relation $a_n + \alpha a_{n-1} + \beta a_{n-2} = 0$.

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- Case 1: $p \neq 1/2$, i.e. distinct roots. By Fact 1, $\exists$ constants a, b s.t.

$$P_n = a\left(\frac{1-p}{p}\right)^n + b \leq \left(\frac{p}{1-p}\right)^m.$$

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  Conclusion: For Roulette, $p = \frac{18}{38} \neq \frac{1}{2}$. Thus, $P_n \leq \left(\frac{p}{1-p}\right)^m \leq \frac{9}{10}^m$.

  - Probability of winning just 100€ (i.e. $m = 100$) is less than $\frac{1}{37648}$!
  - Note: P_n is *independent* of how much money, n, start with.

  Ex. For what range of p is $\lim_{m\to\infty} P_n = 0$?

(Google's disappointed face emoji)

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- Case 2: $p = 1/2$, i.e. same root. By Fact 1,

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Conclusion: When the game is fair ($p = 1/2$), odds of winning are what you expect — the closer you start (n) to your goal ($T = n + m$), the more likely you are to win an additional m€!

(Google's thinking face emoji)

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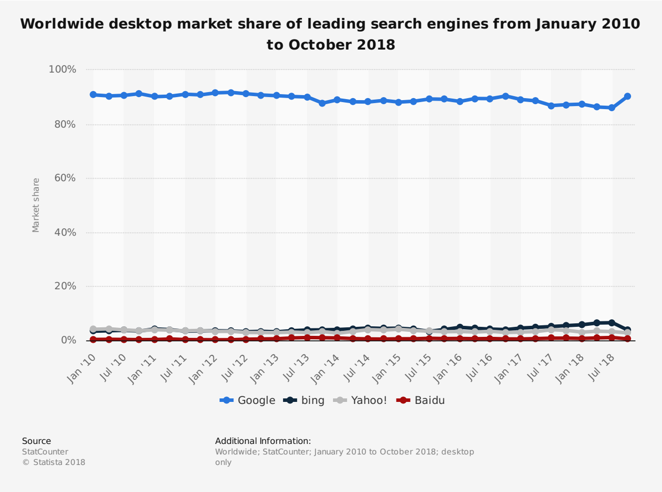
Now let's take random walks beyond 1D and throw in matrices.

Google search



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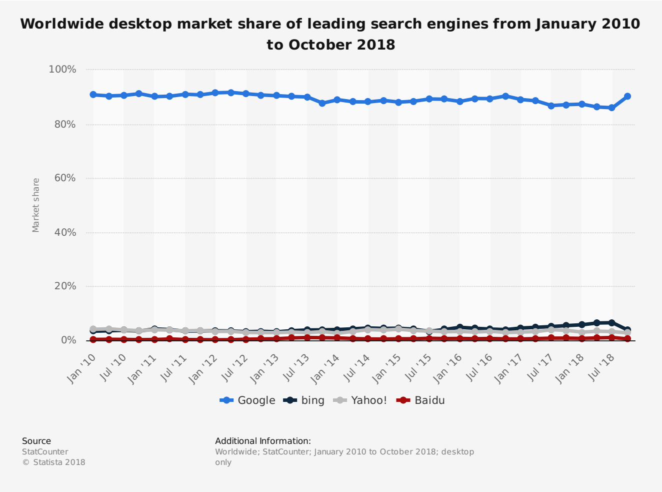

Conclusion: Google has strong impact on which information is accessed.

With great power comes great responsibility. . .

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Q: How does Google decide which websites are more important than others?

PageRank algorithm

- Named after Larry Page (together with Sergey Brin, founded Google)
- Ranks webpages by importance
- Assumption: Pages with more links to them are "more important"
- L. Page, S. Brin, R. Motwani, T. Winograd. "The PageRank citation ranking: Bringing order to the Web", 1999.

Idea sketch (simplified)

Suppose internet consists of N webpages.

Imagine a random websurfer, who repeatedly does the following:

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Observation: Websurfer is doing a random walk on the world wide web!

Encoding random walks into matrices

Visualize the world wide web as a directed graph $G(V, E)$:

- Each vertex $v \in V$ represents a webpage. Recall $|V| = N$.
- $(u, v) \in E$ if there is a link from page u to page v.

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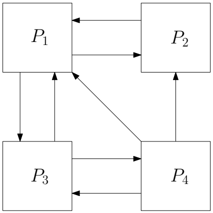
Ex. Consider directed graph $G = (V, E)$ with $V = \{A, B, C, D\}$:



The adjacency matrix A for G is

$$A = \begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix}.$$

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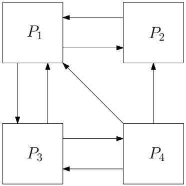

The adjacency matrix W for G is

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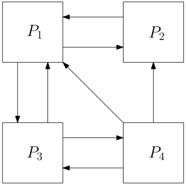

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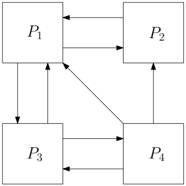

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- After 1 step, moves to P_2 or P_3, with prob. $1/2$ each. New state $\mathbf{p_1} = \begin{pmatrix} 0 \\ 0.5 \\ 0.5 \\ 0 \end{pmatrix}$.

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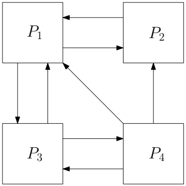

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View $\mathbf{p_i}$ as a *distribution* encoding probability that surfer at particular page after step i.

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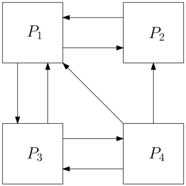

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View $\mathbf{p_i}$ as a *distribution* encoding probability that surfer at particular page after step i.

Q: Can we encode change in probabilities in each step by matrix multiplication?

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- Could $A\mathbf{p}_0 = \mathbf{p}_1$? Ex. Work this out.

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- Normalize each row of A by its out-degree (i.e. number of neighbors):

$$\widehat{A} = \begin{pmatrix} 0 & 1/2 & 1/2 & 0 \\ 1 & 0 & 0 & 0 \\ 1/2 & 0 & 0 & 1/2 \\ 1/3 & 1/3 & 1/3 & 0 \end{pmatrix}, \quad M := \widehat{A}^T = \begin{pmatrix} 0 & 1 & 1/2 & 1/3 \\ 1/2 & 0 & 0 & 1/3 \\ 1/2 & 0 & 0 & 1/3 \\ 0 & 0 & 1/2 & 0 \end{pmatrix}$$

Now $\widehat{A}^T\mathbf{p}_0 = M\mathbf{p}_0 = \mathbf{p}_1$!

Multiplying by M updates surfer's current distribution via 1 step of random walk!

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Thus, after k steps, surfer's distribution is $\mathbf{p_k} = M^k\mathbf{p_0}$.

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Observation: Note that $M\mathbf{p}_i = \mathbf{p}_i$ is just an eigenvalue equation!

Aside: Eigenvalues and eigenvectors

The PageRank vector is a distribution $\mathbf{p}_i$ satisfying $M^k \mathbf{p}_i = \mathbf{p}_i$.

Thus, want to find eigenvector $\mathbf{p}_i$ of M with eigenvalue 1.

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For $A \in \mathbb{R}^{n\times n}$ and $\mathbf{v} \in \mathbb{R}^n$, say $\mathbf{v}$ is an *eigenvector* of A with *eigenvalue* $\lambda \in \mathbb{R}$ if

$$A\mathbf{v} = \lambda\mathbf{v}. \tag{1}$$

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How to find eigenvectors and eigenvalues?

- "Traditional" method:
  - Solve for roots of characteristic equation $\det(A - \lambda I) = 0$ to obtain eigenvalues λ.
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PageRank implements Power method (with $\|\cdot\|$ the 1-norm/Taxicab norm (why?)).

Test case 1

Recall: $M = \begin{pmatrix} 0 & 1 & 1/2 & 1/3 \\ 1/2 & 0 & 0 & 1/3 \\ 1/2 & 0 & 0 & 1/3 \\ 0 & 0 & 1/2 & 0 \end{pmatrix}$ $\mathbf{p_0} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$ $\mathbf{p}_k = M^k \mathbf{p}_0.$

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Results (via Mathematica):

$\mathbf{p}_0$	(1., 0., 0., 0.)
$\mathbf{p}_1$	(0., 0.5, 0.5, 0.)
$\mathbf{p}_2$	(0.75, 0., 0., 0.25)
$\mathbf{p}_3$	(0.0833333, 0.458333, 0.458333, 0.)
$\mathbf{p}_4$	(0.6875, 0.0416667, 0.0416667, 0.229167)
$\mathbf{p}_5$	(0.138889, 0.420139, 0.420139, 0.0208333)
$\mathbf{p}_6$	(0.637153, 0.0763889, 0.0763889, 0.210069)
$\mathbf{p}_7$	(0.184606, 0.3886, 0.3886, 0.0381944)
$\mathbf{p}_8$	(0.595631, 0.105035, 0.105035, 0.1943)
$\mathbf{p}_9$	(0.222319, 0.362582, 0.362582, 0.0525174)
$\mathbf{p}_{10}$	(0.561379, 0.128665, 0.128665, 0.181291)
$\mathbf{p}_{11}$	(0.253428, 0.34112, 0.34112, 0.0643326)
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Seems to be converging, but slowly... No unique most important page yet...

Test case 2

Recall: $M = \begin{pmatrix} 0 & 1 & 1/2 & 1/3 \\ 1/2 & 0 & 0 & 1/3 \\ 1/2 & 0 & 0 & 1/3 \\ 0 & 0 & 1/2 & 0 \end{pmatrix}$ $\mathbf{p_0} = \begin{pmatrix} 1/4 \\ 1/4 \\ 1/4 \\ 1/4 \end{pmatrix}$ $\mathbf{p}_k = M^k \mathbf{p}_0.$

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Results (via Mathematica):

$\mathbf{p}_0$	(0.25, 0.25, 0.25, 0.25)
$\mathbf{p}_1$	(0.458333, 0.208333, 0.208333, 0.125)
$\mathbf{p}_2$	(0.354167, 0.270833, 0.270833, 0.104167)
$\mathbf{p}_3$	(0.440972, 0.211806, 0.211806, 0.135417)
$\mathbf{p}_4$	(0.362847, 0.265625, 0.265625, 0.105903)
$\mathbf{p}_5$	(0.433738, 0.216725, 0.216725, 0.132813)
$\mathbf{p}_6$	(0.369358, 0.26114, 0.26114, 0.108362)
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$\mathbf{p}_8$	(0.374723, 0.257439, 0.257439, 0.1104)
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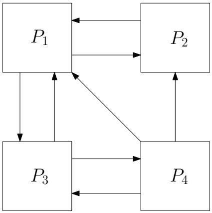
Much better! Singled out P_1 as having largest PageRank.

$\mathbf{p}_{12} = (0.382799, 0.251867, 0.251867, 0.113467)$

Much better! Singled out *A* as having largest PageRank.

Indeed, P_1 had the largest in-degree:



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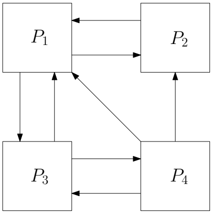

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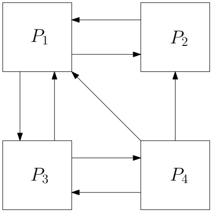

Rate of convergence:

- Seems to depend on starting vector, which is not really surprising.
- Can we hope to prove rigorous upper bound on number of required iterations to get “close” to PageRank vector?
- Yes, but I’ve sort of been lying to you so far...

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Steps:

1. Define more “realistic” model.
2. Define what we mean by being “close” to the target distribution.
3. “Show” that random walk algorithm converges exponentially quickly to PageRank vector.

More “realistic” model

Suppose internet consists of N webpages.

Fix $0 \leq s \leq 1$. Imagine random websurfer, who repeatedly does following:

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So our new transition matrix is $M(s) = sM + \frac{1-s}{N}J$ (why?).

Quantifying "closeness" of distributions

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Total variation distance

The *total variation distance* between distributions $\mathbf{p}, \mathbf{q} \in \mathbb{R}^n$ is

$$\|\mathbf{p} - \mathbf{q}\|_1 = \sum_{i=1}^{N} |p_i - q_i|.$$

Note this is just the Taxicab norm or 1-norm from earlier in slides.

Ex. What is the total variation distance between $\mathbf{p} = (1, 0, 0, 0)^T$ and $\mathbf{q} = (1/4, 1/4, 1/4, 1/4)$?

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It turns out that your optimal probability of guessing correctly is

$$\frac{1}{2} + \frac{1}{4} \|\mathbf{p} - \mathbf{q}\|_1 .$$

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Convergence bounds

Can now bound how quickly we converge to PageRank vector.

Suppose start with arbitrary distribution $\mathbf{p} \in \mathbb{R}^N$ over webpages.

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Ok, so remains to prove Claim 2.

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&= \sum_{k=1}^{n}\left|v_k\right| && \text{(sum of column entries of } A \text{ is 1)}\\
&= \|\mathbf{v}\|_1 .
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Done! We conclude PageRank converges exponentially quickly (in number of iterations, k), to its stationary distribution ($\mathbf{q}$), irrespective of size of the internet (N).

(Google's happy face emoji)

Outline

Goals of section

- Practice working with complex numbers
- Practice working with polynomials
- Introduce Fourier transform and its applications

Outline

Complex numbers

Question: What are the roots of $x^2 + 1 = 0$?

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"The shortest path between two truths in the real domain passes through the complex domain." – Hadamard

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  e.g. $x^2 + 1$ is degree 2, and has two complex roots: i, and $-i$.
- Moral: You should care about complex numbers!

Two views

Any complex number $z \in \mathbb{C}$ can be viewed in two equivalent ways:

- $z = x + yi$, for $x, y \in \mathbb{R}$, $i = \sqrt{-1}$.
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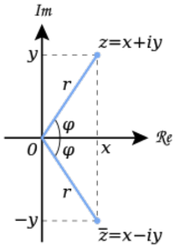
  - $\phi \in [\pi, -\pi)$ is the angle of z (in radians):



Exercises with complex numbers

1. Is $\mathbb{R} \subseteq \mathbb{C}$?
2. Compute sum $(a + bi) + (c + di)$.
3. Compute product $(a + bi)(c + di)$.
4. Recall for $z = x + iy$ that $|z| = \sqrt{x^2 + y^2}$. Observe that this reduces to the usual absolute value when $z \in \mathbb{R}$.
5. Show that for any $z \in \mathbb{C}$, $z + z^* \in \mathbb{R}$.
6. Rewrite the formula $|z| = \sqrt{x^2 + y^2}$ in terms of the product of zz^*.
7. What are $\pm 1, \pm i$ in polar form?
8. Using the 2D complex plane, derive the formula $|z| = \sqrt{x^2 + y^2}$.
9. If we allow angles $\phi \in \mathbb{R}$, is the representation of a given $z \in \mathbb{C}$ unique?
10. Use the 2D complex plane to derive the two square roots of 1. (Q: Why are we guaranteed that 1 has precisely 2 square roots?)

With $\mathbb{C}$ in hand, can now define polynomials with coefficients from $\mathbb{C}$.

Later, we will use $\mathbb{C}$ for the Fourier transform as well.

Outline

Polynomials (brief review)

Univariate polynomial

A univariate polynomial is a function $f : \mathbb{C} \mapsto \mathbb{C}$ of form

$$f(x) = a_n x^n + a_{n-1} x^{n-1} + \cdots + a_1 x + a_0 = \sum_{j=0}^{n} a_j x^j,$$

for all $a_j \in \mathbb{C}$. *Degree* of f is $\deg(f) = n$ (i.e. index of largest non-zero coefficient a_n). The set of univariate polynomials over $\mathbb{C}$ is denoted $\mathbb{C}[x]$.

Polynomials (brief review)

Univariate polynomial

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Sum and product of polynomials

For $f, g \in \mathbb{C}[x]$ with $f(x) = \sum_{j=0}^{n} a_j x^j$ and $g(x) = \sum_{j=0}^{n} b_j x^j$,

$$f(x) + g(x) = \sum_{j=0}^{n} (a_j + b_j) x^j, \quad \text{and} \quad f(x)g(x) = \sum_{j=0}^{2n} \left(\sum_{k=0}^{j} a_k b_{j-k} \right) x^j.$$

Ex. Prove the multiplication formula for $f(x)g(x)$ holds.

Exercises with polynomials

1. What is the degree of $f(x) = -7x^3 + 4x + \sqrt{2}$? $f(x) = 4$?
2. Are non-positive-integer exponents on x allowed in our definition of polynomials?
3. Compute the sum of $f(x) = 3x^2 - 4x - 9$ and $g(x) = x^3 + 4$.
4. For $f, g \in \mathbb{C}[x]$ of degree n_f and n_g, resp., what is $\deg(f(x) + g(x))$?
5. Compute the product of $f(x) = 3x^2 - 4x - 9$ and $g(x) = x^3 + 4$.
6. For $f, g \in \mathbb{C}[x]$ of degree n_f and n_g, resp., what is $\deg(f(x)g(x))$?
7. Recall the Fundamental Theorem of Algebra says that any $f \in \mathbb{C}[x]$ with $\deg(f) = n$ has precisely n roots over $\mathbb{C}$. What are the roots of $3x^2 - 1$? $x^3 - 1$? $x^4 - 1$? More generally, $x^n - 1$?
8. Is there a real-numbered analogue of the Fundamental Theorem of Algebra? i.e. true that any $f \in \mathbb{R}[x]$ with $\deg(f) = n$ has n roots over $\mathbb{R}$?

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How many field operations over $\mathbb{C}$ does the naive algorithm take to multiply two degree-n polynomials $f, g \in \mathbb{C}[x]$?

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3. Convert back from point-value representation to coefficient representation (i.e. *interpolate*) to recover final answer.

Two representations of polynomials

Coefficient representation

Polynomial $f \in \mathbb{C}[x]$ of degree n written as $f(x) = \sum_{j=0}^{n} a_j x^n$, or in vector form:

$$\mathbf{a} = \begin{pmatrix} a_0 & a_1 & \cdots & a_{n-1} & a_n \end{pmatrix}^T \in \mathbb{C}^n.$$

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Observation: Given $f \in \mathbb{C}[x]$ in coefficient form, can evaluate f at any point $x \in \mathbb{C}$ in $\Theta(n)$ time using *Horner's rule*:

$$f(x) = a_0 + x(a_1 + x(a_2 + \cdots + x(a_{n-1} + x(a_n))\cdots)).$$

Ex. Use Horner's rule to evaluate $f(x) = 5x^3 - 2x^2 - x + 1$ at $x = e^{i\pi}$.

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(Aside: What is $e^{i\pi}$?)

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Point-value rep. of $f \in \mathbb{C}[x]$ of degree n is a set of $n+1$ *point-value pairs* $(x_0, y_0), (x_1, y_1), \ldots, (x_n, y_n)$, such that:

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Conclusion: Unique solution for $\mathbf{a}$ given by $\mathbf{a} = V(x_0, \ldots, x_n)^{-1}\mathbf{y}$.

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Solution: Start with point-value representations for f and g which have $2n+1$ points (i.e. before multiplying).

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(Facebook relieved emoji)

Outline

1. Introduction to matrices (review)
2. Matrix multiplication algorithms
   - Strassen's algorithm (1967)
   - Drineas-Kannan-Mahoney randomized algorithm (2006)
3. Random walks
   - Gambler's ruin
   - Google's PageRank algorithm (1999)
4. Polynomial multiplication
   - Complex numbers
   - Polynomials
   - $O(N \log N)$-time polynomial multiplication via Fourier Transform

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More concisely, define principal *n*th root of unity as $\omega_n = e^{2\pi i/n}$.

Then, *n*th roots of unity are: $\omega_n^0, \omega_n^1, \omega_n^2, \ldots, \omega_n^{n-1}$.

Roots of unity

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Recall: What are the roots of $f(x) = x^n - 1$?

Nth roots of unity

The nth roots of unity are the roots of $f(x) = x^n - 1$, namely

$$1, e^{2\pi i/n}, e^{2\cdot 2\pi i/n}, e^{3\cdot 2\pi i/n}, \ldots, e^{(n-1)\cdot 2\pi i/n}.$$ (Why?)

More concisely, define principal nth root of unity as $\omega_n = e^{2\pi i/n}$.

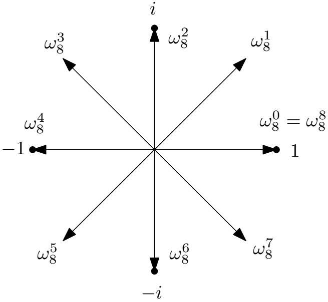
Then, nth roots of unity are: $\omega_n^0, \omega_n^1, \omega_n^2, \ldots, \omega_n^{n-1}$.

Ex. What is the magnitude of any root of unity, i.e. $\left|e^{2j\pi i/n}\right|$ for $j \in \mathbb{Z}$?

Ex. What are the 4th roots of unity?

Properties

Recall: $\omega_n = e^{2\pi i/n}$. Below are the 8th roots of unity:



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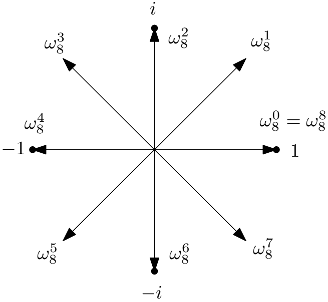

- **Cancellation Lemma:** For any integers $n, k \geq 0$, and $d > 0$, $\omega_{dn}^{dk} = \omega_n^k$.

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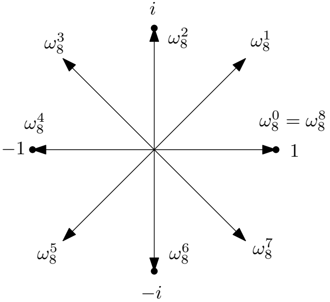

- Cancellation Lemma: For any integers $n, k \geq 0$, and $d > 0$, $\omega_{dn}^{dk} = \omega_n^k$.
- Summation Lemma: For any integer $n \geq 1$ and integer $k \neq 0$ not divisible by n,

$$\sum_{j=0}^{n-1} (\omega_n^k)^j = 0.$$

Q: What if $k = 0$?

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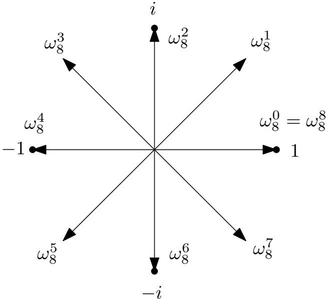

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Ex. Prove both lemmas above (Hint: Use closed form for geometric series). Can you visualize proofs on 2D plane?

Let $f = \sum_{j=0}^{n} a_j x^j \in \mathbb{C}[x]$, and recall $\omega_n = e^{2\pi i/n}$.

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- Hope: If could convert f to and from point-value form "quickly", could instead do point-wise multiplication, which takes $O(n)$ time.
- Key observation: Evaluating f at *arbitrary* points $x_0, \ldots, x_{2n}$ takes $O(n^2)$, but if we choose the x_j "carefully", can do it in $O(n \log n)$ time!

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- The *Discrete Fourier Transform (DFT)* evaluates f at n "carefully" chosen points x_j. Can you guess which ones?

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- A: The nth roots of unity, ω_n^k!
- For succinctness, let $N := n + 1$. Then, DFT maps coefficient vector $\mathbf{a}$ to:

$$\mathbf{a} = \begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_n \end{pmatrix} \quad \mapsto \quad \mathbf{y} = \begin{pmatrix} f(\omega_N^0) \\ f(\omega_N^1) \\ \vdots \\ f(\omega_N^{N-1}) \end{pmatrix},$$

i.e. $y_k = f(\omega_N^k) = \sum_{j=0} a_j \left(\omega_N^k\right)^j$.

Discrete Fourier Transform (DFT)

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Q: Can you guess the matrix now? (Hint: Vandermonde matrix.)

Interpolation Theorem

Any set of $n+1$ point-value pairs $\{(x_0, y_0), (x_1, y_1), \ldots, (x_n, y_n)\}$ with distinct x_i defines a unique polynomial f such that:

- $\deg(f) \leq n$,
- $f(x_j) = y_j$ for $j \in \{0, \ldots, n\}$.

Proof. Looking for $f(x) = \sum_{j=0}^{n} a_j x^n$ s.t. $f(x_i) = y_i$. Encode as matrix mult.:

$$\begin{pmatrix} 1 & x_0 & x_0^2 & \cdots & x_0^n \\ 1 & x_1 & x_1^2 & \cdots & x_1^n \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_n & x_n^2 & \cdots & x_n^n \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_n \end{pmatrix} = \begin{pmatrix} y_0 \\ y_1 \\ \vdots \\ y_n \end{pmatrix}$$

Write as $V(x_0, \ldots, x_n)\mathbf{a} = \mathbf{y}$, for $V \in \mathbb{C}^{n+1 \times n+1}$ a *Vandermonde matrix*.

Fact: Any Vandermonde matrix has an inverse if all x_j are distinct.
Conclusion: Unique solution for $\mathbf{a}$ given by $\mathbf{a} = V(x_0, \ldots, x_n)^{-1}\mathbf{y}$.

The DFT matrix

Moral: Evaluating a polynomial at a set of points is matrix multiplication.

Want to evaluate $f(x) = \sum_{j=0}^{n} a_j x^n$ at inputs $\omega_N^0, \omega_N^1, \ldots, \omega_N^{N-1}$:

$$\begin{pmatrix} 1 & ? & ? & \cdots & ? \\ 1 & ? & ? & \cdots & ? \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & ? & ? & \cdots & ? \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_n \end{pmatrix} = \begin{pmatrix} f(\omega_N^0) \\ f(\omega_N^1) \\ \vdots \\ f(\omega_N^{N-1}) \end{pmatrix}.$$

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The $N \times N$ complex matrix encoding the DFT of order N is thus:

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- A: $O(N^2) \in O(n^2)\ldots$ (Recall $N = n + 1$.) #$&%&$%!

This makes me feel. . .


?

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?

?

This makes me feel...

?

?

?

Breathe in, breathe out

We can't stop now…Let's remind ourselves why it really is important to find a clever implementation of the DFT.

`http://nautil.us/blog/`
`the-math-trick-behind-mp3s-jpegs-and-homer-simpsons-f`
Math Trick Behind MP3s, JPEGs, and Homer Simpson's Face

(Click on link in pdf to follow link)

Warning: Must read. I *will* test you on this on exam.

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Can implement DFT_N in time $O(N \log N)$:

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Halving Lemma

Suppose N is even. Then, for any $k \in \mathbb{Z}^+$, $(\omega_N^k)^2 = \omega_{N/2}^k$.

Proof.

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Idea: Halving Lemma allows us to recurse by simulating order-N DFT by a pair of order-$(N/2)$ DFTs.

Recursive breakdown of polynomials

Assume (WLOG) that $N = n + 1$ is a power of 2.

$$f(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3 + \cdots + a_{n-1} x^{n-1} + a_n x^n$$

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&=: f_0(x^2) + x f_1(x^2),
\end{aligned}
$$

for $f_0(x) := a_0 + a_2 x + \cdots a_{n-1} x^{(n-1)/2}$ and $f_1(x) := a_1 + a_3 x + \cdots a_n x^{(n-1)/2}$.

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&\quad \left(a_1x + a_3x^3 + a_5x^5 + \cdots + a_nx^n\right) \quad \text{(odd)} \\
&= \left(a_0 + a_2x^2 + a_4x^4 + \cdots + a_{n-1}x^{n-1}\right) + \quad \text{(even)} \\
&\quad x\left(a_1 + a_3x^2 + a_5x^4 + \cdots + a_nx^{n-1}\right) \quad \text{(odd)} \\
&= \left(a_0 + a_2(x^2)^1 + a_4(x^2)^2 + \cdots + a_{n-1}(x^2)^{\frac{n-1}{2}}\right) + \quad \text{(even)} \\
&\quad x\left(a_1 + a_3(x^2)^1 + a_5(x^2)^2 + \cdots + a_n(x^2)^{\frac{n-1}{2}}\right) \quad \text{(odd)} \\
&=: f_0(x^2) + xf_1(x^2),
\end{aligned}$$

for $f_0(x) := a_0 + a_2x + \cdots a_{n-1}x^{(n-1)/2}$ and $f_1(x) := a_1 + a_3x + \cdots a_nx^{(n-1)/2}$.

Observe:

- f_0 and f_1 have degree $(n-1)/2$!
- "Feels like" we've cut our problem into a pair of smaller problems of half the size.

The key step

Assume (WLOG) that $N = n + 1$ is a power of 2.

$$\begin{aligned} f(x) &= a_0 + a_1 x + a_2 x^2 + a_3 x^3 + \cdots + a_{n-1} x^{n-1} + a_n x^n \\ &= f_0(x^2) + x f_1(x^2), \end{aligned} \tag{3}$$

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- DFT_N evaluates degree-$(N-1)$ polynomial at Nth roots of unity.
- By Halving Lemma: Letting $x = \omega_N^k$ in Eqn. (3),

$$f_0(x^2) = f_0((\omega_N^k)^2) = f_0(\omega_{N/2}^k).$$

- Thus, roots of unity are very special — allow us to recursively simulate order-N DFT via order-$(N/2)$ DFTs.

FFT Algorithm

Preconditions: $N = n + 1$ is a power of 2.

Input: Coefficient vector $\mathbf{a} = (a_0, a_1, \ldots, a_n)^T$ representing polynomial $f \in \mathbb{C}[x]$.
Output: $\mathrm{DFT}_N\,\mathbf{a} = (f(\omega_N^0), f(\omega_N^1), \ldots, f(\omega_N^{N-1}))^T$.

FFT($\mathbf{a}$,N):

1. (Base case) if $N = 1$, return $\mathbf{a}$ (why?)
2. Set $\omega = 1$
3. Set $\mathbf{y}^{[0]} = \mathrm{FFT}((a_0, a_2, \ldots, a_{n-1}), N/2)$
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Let $f^{[j]}$ denote polynomial with coefficients $\mathbf{y}^{[j]}$ below.

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Runtime

- Each call to FFT takes $O(N)$ time, and makes two recursive calls of size $N/2$.
- Thus, runtime $T(N) = 2T(N/2) + \Theta(N) \in \Theta(N \log N)$.
- Conclusion: Evaluate degree-$(N-1)$ polynomial at Nth roots of unity in subquadratic time.

The big picture

Recall our battle plan for polynomial multiplication:

1. Convert $f, g \in \mathbb{C}[x]$ from *coefficient representation* to *point-value representation* by evaluating f, g at cleverly chosen points.
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Can now fill in details:

1. Convert $f, g \in \mathbb{C}[x]$ from *coefficient representation* to *point-value representation* by evaluating f, g at Nth roots of unity.
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Conclusion: Polynomial multiplication takes $O(N \log N)$ time.

Final exercises

1. Why does interpolation correspond to inverse DFT? (Hint: Recall proof of Interpolation Theorem.)
2. What is the matrix representation of the inverse of DFT_N?
3. We cheated slightly in our algorithm — where did we bend the rules? (Hint: How many data points did we need to evaluate a polynomial at in order to recover a unique inverse via interpolation?)

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- Shameless advertisements:
  - See upcoming Masters lecture on Introduction to Quantum Computation (SS2020)
  - Interested in undergraduate research in quantum computation? Come talk to me! Required background is Linear Algebra.

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