Computing the determinant

Group 12

Catterwell, A. Smith, M. Wang, R. Watson, K.

University of Edinburgh

April 1, 2019

Overview

1. Why calculate determinants?
   - Invertibility of matrices
   - Cramer's Rule
   - Eigenvalues and Eigenvectors
   - Jacobian determinant
2. Algorithms for computing determinants
   - Leibniz formula
   - Laplace expansion
   - LU decomposition
   - Bird's algorithm
3. Epilogue
   - Summary of determinant algorithms
   - How fast is Maple's implementation?

Invertibililty of matrices

Theorem

An $n \times n$ square matrix A is invertible if and only if

$$\det(A) \neq 0.$$

Cramer's Rule

Theorem

Given an equation $A\mathbf{x} = \mathbf{b}$ The solutions for $\mathbf{x}$ are given by

$$x_i = \frac{\det(A_i)}{\det(A)}$$

with A_i being the matrix formed by replacing the ith column of A by $\mathbf{b}$.

It turns out this method has the same runtime complexity as Gaussian elimination for solving systems of linear equations.

Eigenvalues and Eigenvectors

Definition

The Eigenvalues λ of a matrix A are the roots of the characteristic polynomial as defined

$$\chi_A = \det(A - \lambda I) = \mathbf{0}.$$

Eigenvalues and Eigenvectors

Definition

The Eigenvalues λ of a matrix A are the roots of the characteristic polynomial as defined

$$\chi_A = \det(A - \lambda I) = \mathbf{0}.$$

Definition

The Eigenvectors of A are the vectors $\mathbf{v}$ such that

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

Eigenvalues and Eigenvectors (cont.)

The absolute value of the determinant of real vectors is equal to the volume of the parallelepiped spanned by those vectors.
$f : \mathbb{R}^n \to \mathbb{R}^n$: the linear map represented by the A. S: any measurable subset of $\mathbb{R}^n$.

$$\text{volume}(f(S)) = |\det(A^T A)| \times \text{volume}(S).$$

Jacobian determinant

For $f : \mathbb{R}^n \to \mathbb{R}^n$, the Jacobian matrix is the $n \times n$ matrix whose entries are defined as

$$D(f) = \left(\frac{\partial f_i}{\partial x_j}\right)_{1 \leq i,j \leq n.}$$

Its determinant is known as the *Jacobian determinant*.

If the determinant of a continuously differentiable function f at a point p is. . .

- Non-zero, f is invertible near a point p in $\mathbb{R}^n$.
- Positive, then f preserves orientation near p.
- Negative, then f reverses orientation near p.

Big-O notation

We'll be looking at the runtime of algorithms, so this is useful.

Definition

A function f is said to be $\mathcal{O}(g)$, with g a function iff

$$\exists k \in \mathbb{R} \ni f(n) < k \cdot g(n)$$

for sufficiently large n.

Leibniz formula

Definition

The Leibniz formula defines the determinant of $A \in \mathbb{M}(n)$ as

$$\det(A) = \sum_{\sigma \in \mathfrak{S}_n} \left(\operatorname{sgn}(\sigma) \cdot \prod_{i=1}^{n} a_{i,\sigma(i)} \right)$$

where $\mathfrak{S}_n$ is the set of permutations length n.

Leibniz formula

Definition

The Leibniz formula defines the determinant of $A \in \mathbb{M}(n)$ as

$$\det(A) = \sum_{\sigma \in \mathfrak{S}_n} \left(\operatorname{sgn}(\sigma) \cdot \prod_{i=1}^{n} a_{i,\sigma(i)} \right)$$

where $\mathfrak{S}_n$ is the set of permutations length n.

Computing the determinant using this method is slow with runtime $\mathcal{O}(n \cdot n!)$.

Laplace expansion

The Laplace (1st row) expansion for computing determinants is usually the first method taught for computing determinants of 3×3 matrices and larger.

Laplace expansion

The Laplace (1st row) expansion for computing determinants is usually the first method taught for computing determinants of 3×3 matrices and larger.

Theorem

The formula for the (1st row) Laplace expansion of $A \in \mathbb{M}(n)$ is given as:

$$\det(A) = \sum_{j=1}^{n} a_{1,j}\, C_{1,j}$$

where $C_{i,j} = (-1)^{i+j} \det\left(A\langle i,j\rangle\right)$ is the (i,j) cofactor of A.

Laplace expansion

The Laplace (1st row) expansion for computing determinants is usually the first method taught for computing determinants of 3×3 matrices and larger.

Theorem

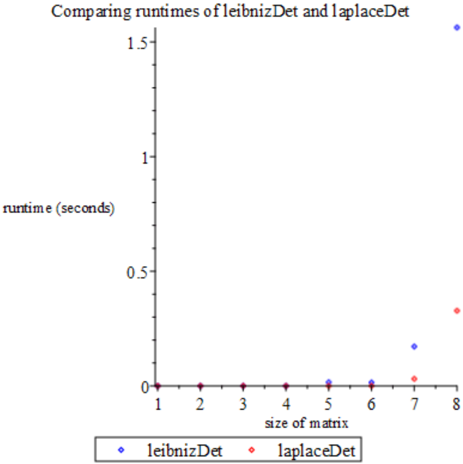
The formula for the (1st row) Laplace expansion of $A \in \mathbb{M}(n)$ is given as:

$$\det(A) = \sum_{j=1}^{n} a_{1,j}\, C_{1,j}$$

where $C_{i,j} = (-1)^{i+j} \det\left(A\langle i,j\rangle\right)$ is the (i,j) cofactor of A.

Its runtime complexity of $\mathcal{O}(n!)$ is poor.

Laplace expansion vs Leibniz formula



Runtimes are similar — both run in exponential time.

What is LU decomposition?

Definition

An LU decomposition of an invertible matrix A is a factorization

$$A = LU$$

where L and U are lower and upper triangular matrices, respectively.

Is there always an LU decomposition?

No.

An LU decomposition of A exists if and only if each of its *leading principle minors* (contiguous square submatrices in the top-left corner of A), are also invertible.

Is there always an LU decomposition?

No.

An LU decomposition of A exists if and only if each of its *leading principle minors* (contiguous square submatrices in the top-left corner of A), are also invertible.

Example

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

This matrix is invertible but has no LU decomposition.

Is there always an LU decomposition?

No.

An LU decomposition of A exists if and only if each of its *leading principle minors* (contiguous square submatrices in the top-left corner of A), are also invertible.

Example

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

This matrix is invertible but has no LU decomposition.

What can we do?

PLU decomposition

Partial pivoting.
We can pivot the matrix into the correct form by multiplication with an orthogonal, permutation matrix P (representing a permutation σ_P) which gives us the PLU decomposition:

$$\sigma_P(A) = PA = LU$$

PLU decomposition

Partial pivoting.
We can pivot the matrix into the correct form by multiplication with an orthogonal, permutation matrix P (representing a permutation σ_P) which gives us the PLU decomposition:

$$\sigma_P(A) = PA = LU$$

This technique works on *any* matrix.

How it helps us compute determinants

Now that we have $PA = LU$, it follows that

$$
\begin{aligned}
A &= P^{-1}LU \\
&= P^{T}LU
\end{aligned}
$$

since $P^{-1} = P^{T}$ by the definition of orthogonal matrices.

How it helps us compute determinants (cont.)

Now that we have $A = P^T LU$, it follows that

$$\begin{aligned}
\det(A) &= \det(P^T LU) \\
&= \det(P^T) \cdot \det(L) \cdot \det(U) && \text{(Thm. 4.4.1)} \\
&= \det(P) \cdot \det(L) \cdot \det(U) && \text{(Lem. 4.4.4)}
\end{aligned}$$

Given that

- the determinant of a triangular matrix is the product of its diagonal elements
- the determinant of a permutation matrix (P) is the parity of the permutation it represents (σ_P)

it follows that

$$\det(A) = \operatorname{sgn}(\sigma_P) \cdot \left(\prod_{i=1}^{n} l_{i,i} \right) \cdot \left(\prod_{i=1}^{n} u_{i,i} \right)$$

How do we find the PLU decomposition?

Input: $\mathbf{A} \in \mathbb{R}^{n\times n}$

Output: $\mathbf{L}, \mathbf{U}, \mathbf{P} \in \mathbb{R}^{n\times n}$, with $\mathbf{PA} = \mathbf{LU}$, $\mathbf{L}$ unit lower triangular, $\mathbf{U}$ non-singular upper triangular, and $\mathbf{P}$ a permutation matrix

1: $\mathbf{U} \leftarrow \mathbf{A}, \mathbf{L} \leftarrow \mathbf{I}, \mathbf{P} \leftarrow \mathbf{I}$
2: **for** $k \leftarrow 1, \dots, n-1$ **do** ▷ Loop over columns
3: Choose $i \in \{k, \dots, n\}$ which maximises $|u_{ik}|$
4: Exchange row $(u_{kk}, \dots, u_{kn})$ with $(u_{ik}, \dots, u_{in})$ ▷ Col. 1 to k have zeros below the diagonal
5: Exchange row $(l_{k1}, \dots, l_{k,k-1})$ with $(l_{i1}, \dots, l_{ik-1})$ ▷ $\mathbf{L}$ has unit diagonal, zeros above and below the diagonal in columns $k+1$ to n
6: Exchange row $(p_{k1}, \dots, p_{kn})$ with $(p_{i1}, \dots, p_{in})$
7: **for** $j \leftarrow k+1, \dots, n$ **do**
8: $l_{jk} \leftarrow u_{jk}/u_{kk}$ ▷ u_{kk} now largest possible
9: $(u_{jk}, \dots, u_{jn}) \leftarrow (u_{jk}, \dots, u_{jn}) - l_{jk}(u_{kk}, \dots, u_{kn})$
10: **end for**
11: **end for**

This algorithm only works on invertible matrices (line 8 division).

How do we find the PLU decomposition? (cont.)

$$A = \begin{pmatrix} 2 & 1 & 1 \\ 4 & 3 & 3 \\ 8 & 7 & 9 \end{pmatrix}$$

$$PA = LU$$

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 2 & 1 & 1 \\ 4 & 3 & 3 \\ 8 & 7 & 9 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 2 & 1 & 1 \\ 4 & 3 & 3 \\ 8 & 7 & 9 \end{pmatrix}$$

How do we find the PLU decomposition? (cont.)

$$A = \begin{pmatrix} 2 & 1 & 1 \\ 4 & 3 & 3 \\ 8 & 7 & 9 \end{pmatrix}$$

$$PA = LU$$

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 2 & 1 & 1 \\ 4 & 3 & 3 \\ 8 & 7 & 9 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 2 & 1 & 1 \\ 4 & 3 & 3 \\ 8 & 7 & 9 \end{pmatrix}$$

$$\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 2 & 1 & 1 \\ 4 & 3 & 3 \\ 8 & 7 & 9 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 8 & 7 & 9 \\ 4 & 3 & 3 \\ 2 & 1 & 1 \end{pmatrix}$$

How do we find the PLU decomposition? (cont.)

$$A = \begin{pmatrix} 2 & 1 & 1 \\ 4 & 3 & 3 \\ 8 & 7 & 9 \end{pmatrix}$$

$$PA = LU$$

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 2 & 1 & 1 \\ 4 & 3 & 3 \\ 8 & 7 & 9 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 2 & 1 & 1 \\ 4 & 3 & 3 \\ 8 & 7 & 9 \end{pmatrix}$$

$$\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 2 & 1 & 1 \\ 4 & 3 & 3 \\ 8 & 7 & 9 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 8 & 7 & 9 \\ 4 & 3 & 3 \\ 2 & 1 & 1 \end{pmatrix}$$

$$\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 2 & 1 & 1 \\ 4 & 3 & 3 \\ 8 & 7 & 9 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ \frac{1}{2} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 8 & 7 & 9 \\ 0 & -\frac{1}{2} & -\frac{3}{2} \\ 2 & 1 & 1 \end{pmatrix}$$

How do we find the PLU decomposition? (cont.)

$$\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 2 & 1 & 1 \\ 4 & 3 & 3 \\ 8 & 7 & 9 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ \frac{1}{2} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 8 & 7 & 9 \\ 0 & -\frac{1}{2} & -\frac{3}{2} \\ 2 & 1 & 1 \end{pmatrix}$$

How do we find the PLU decomposition? (cont.)

$$\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 2 & 1 & 1 \\ 4 & 3 & 3 \\ 8 & 7 & 9 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ \frac{1}{2} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 8 & 7 & 9 \\ 0 & -\frac{1}{2} & -\frac{3}{2} \\ 2 & 1 & 1 \end{pmatrix}$$

$$\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 2 & 1 & 1 \\ 4 & 3 & 3 \\ 8 & 7 & 9 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ \frac{1}{2} & 1 & 0 \\ \frac{1}{4} & 0 & 1 \end{pmatrix} \begin{pmatrix} 8 & 7 & 9 \\ 0 & -\frac{1}{2} & -\frac{3}{2} \\ 0 & -\frac{3}{4} & -\frac{5}{4} \end{pmatrix}$$

How do we find the PLU decomposition? (cont.)

$$\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 2 & 1 & 1 \\ 4 & 3 & 3 \\ 8 & 7 & 9 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ \frac{1}{2} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 8 & 7 & 9 \\ 0 & -\frac{1}{2} & -\frac{3}{2} \\ 2 & 1 & 1 \end{pmatrix}$$

$$\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 2 & 1 & 1 \\ 4 & 3 & 3 \\ 8 & 7 & 9 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ \frac{1}{2} & 1 & 0 \\ \frac{1}{4} & 0 & 1 \end{pmatrix} \begin{pmatrix} 8 & 7 & 9 \\ 0 & -\frac{1}{2} & -\frac{3}{2} \\ 0 & -\frac{3}{4} & -\frac{5}{4} \end{pmatrix}$$

$$\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 2 & 1 & 1 \\ 4 & 3 & 3 \\ 8 & 7 & 9 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ \frac{1}{2} & 1 & 0 \\ \frac{1}{4} & \frac{3}{2} & 1 \end{pmatrix} \begin{pmatrix} 8 & 7 & 9 \\ 0 & -\frac{1}{2} & -\frac{3}{2} \\ 0 & 0 & 1 \end{pmatrix}$$

How do we find the PLU decomposition? (cont.)

So we have

$$L = \begin{pmatrix} 1 & 0 & 0 \\ \frac{1}{2} & 1 & 0 \\ \frac{1}{4} & \frac{3}{2} & 1 \end{pmatrix}, U = \begin{pmatrix} 8 & 7 & 9 \\ 0 & -\frac{1}{2} & -\frac{3}{2} \\ 0 & 0 & 1 \end{pmatrix} \text{ and } \operatorname{sgn}(\sigma_P) = -1.$$

How do we find the PLU decomposition? (cont.)

So we have

$$L = \begin{pmatrix} 1 & 0 & 0 \\ \frac{1}{2} & 1 & 0 \\ \frac{1}{4} & \frac{3}{2} & 1 \end{pmatrix}, U = \begin{pmatrix} 8 & 7 & 9 \\ 0 & -\frac{1}{2} & -\frac{3}{2} \\ 0 & 0 & 1 \end{pmatrix} \text{ and } \operatorname{sgn}(\sigma_P) = -1.$$

Thus we have

$$\det(A) = \det \begin{pmatrix} 2 & 1 & 1 \\ 4 & 3 & 3 \\ 8 & 7 & 9 \end{pmatrix} = \operatorname{sgn}(\sigma_P) \cdot \left(\prod_{i=1}^{n} l_{i,i} \right) \cdot \left(\prod_{i=1}^{n} u_{i,i} \right)$$

$$= -1 \cdot 8 \cdot -\frac{1}{2} = 4.$$

Runtime analysis

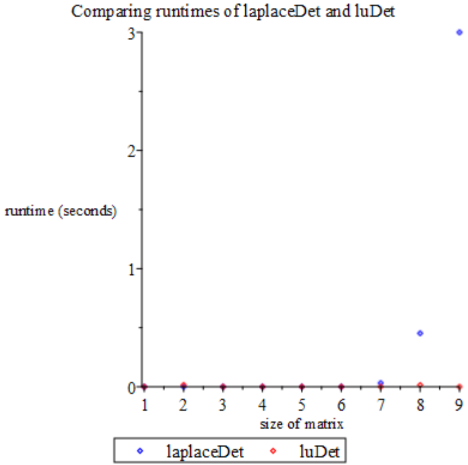
How quick is it?

- The PLU decomposition can be computed in $\mathcal{O}(n^3)$ time.
- The determinants of the triangular matrices computed in $\mathcal{O}(n)$ time.
- The parity of the permutation matrix in $\mathcal{O}(n^2)$ time.

Therefore the total runtime for computing the determinant using the method is

$$\mathcal{O}(n^3) + \mathcal{O}(n^2) + \mathcal{O}(n) = \mathcal{O}(n^3).$$

Laplace expansion vs LU decomposition



The difference between the exponential and polynomial-time function is clear.

Limitations of LU decomposition

The main problem with the LU decomposition algorithm used is that it often requires division.

Limitations of LU decomposition

The main problem with the LU decomposition algorithm used is that it often requires division.

- Division is not a ring operation, so it won't work on matrices over rings.

Limitations of LU decomposition

The main problem with the LU decomposition algorithm used is that it often requires division.

- Division is not a ring operation, so it won't work on matrices over rings.
- Unless we compute exactly (difficult on a computer), precision may be lost.

Limitations of LU decomposition

The main problem with the LU decomposition algorithm used is that it often requires division.

- Division is not a ring operation, so it won't work on matrices over rings.
- Unless we compute exactly (difficult on a computer), precision may be lost.

Let's try something else...

Bird's algorithm

Define $\mu : \mathbb{M}(n) \to \mathbb{M}(n)$:

$$\mu(X) = \begin{pmatrix} \mu_{2,2} - x_{2,2} & x_{1,2} & \cdots & x_{1,n-1} & x_{1,n} \\ 0 & \mu_{3,3} - x_{3,3} & \cdots & x_{2,n-1} & x_{2,n} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & \mu_{n,n} - x_{n,n} & x_{n-1,n} \\ 0 & 0 & \cdots & 0 & 0 \end{pmatrix}$$

Bird's algorithm

Define $\mu : \mathbb{M}(n) \to \mathbb{M}(n)$:

$$\mu(X) = \begin{pmatrix} \mu_{2,2} - x_{2,2} & x_{1,2} & \cdots & x_{1,n-1} & x_{1,n} \\ 0 & \mu_{3,3} - x_{3,3} & \cdots & x_{2,n-1} & x_{2,n} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & \mu_{n,n} - x_{n,n} & x_{n-1,n} \\ 0 & 0 & \cdots & 0 & 0 \end{pmatrix}$$

and $F_A : \mathbb{M}(n) \to \mathbb{M}(n)$, with $A \in \mathbb{M}(n)$

$$F_A(X) = \mu(X) \cdot A$$
$$F_A^2(X) = \mu(F_A(X)) \cdot A$$
$$\vdots$$
$$F_A^n(X) = \mu(F_A^{n-1}(X)) \cdot A.$$

Bird's algorithm (cont.)

Bird's Theorem

$$F_A^{n-1}(A) = \begin{pmatrix} d & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 \end{pmatrix} \text{ with } d = \begin{cases} \det(A) & \text{odd } n \\ -\det(A) & \text{even } n. \end{cases}$$

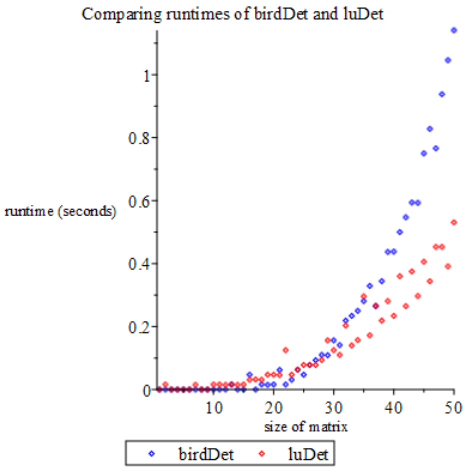
Bird's algorithm (cont.)

Bird's Theorem

$$F_A^{n-1}(A) = \begin{pmatrix} d & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 \end{pmatrix} \text{ with } d = \begin{cases} \det(A) & \text{odd } n \\ -\det(A) & \text{even } n. \end{cases}$$

- Enables the *division-free* computation of determinants in $\mathcal{O}(n \cdot M(n))$ where $M(n)$ is the runtime complexity of the matrix multiplication algorithm used.
- If the conventional $\mathcal{O}(n^3)$ matrix multiplication algorithm is used, then Bird's algorithm will run in $\mathcal{O}(n^4)$ time.
- But this can be reduced to $\mathcal{O}(n^{3.8})$ by using a faster (e.g. *Strassen*) algorithm for matrix multiplication.

Bird's algorithm vs LU decomposition

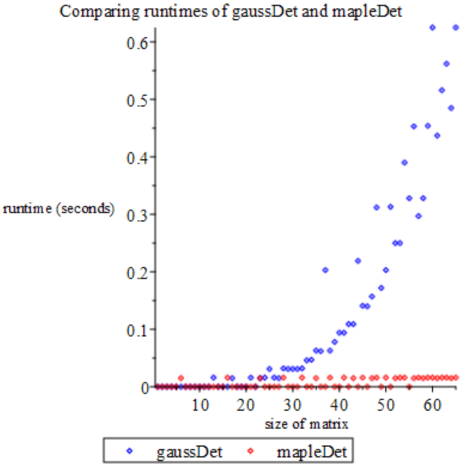


Bird's runtimes increase noticeably more rapidly than LU decomposition, but it's still polynomial.

Summary of determinant algorithms

Algorithm	*Runtime*	*Exact?*
Leibniz formula	$\mathcal{O}(n \cdot n!)$	Yes
Laplace expansion	$\mathcal{O}(n!)$	Yes
LU decomposition	$\mathcal{O}(n^3)$	No
Bird's algorithm	$\mathcal{O}(n^{3.8})$	Yes

How fast is Maple's built-in determinant function?



Very. Maple's optimisation means a fair comparison cannot be made.

Thanks!