2 Linear Systems

Lab Objective: *The fundamental problem of linear algebra is solving the linear system $A\mathbf{x} = \mathbf{b}$, given that a solution exists. There are many approaches to solving this problem, each with different pros and cons. In this lab we implement the LU decomposition and use it to solve square linear systems. We also introduce SciPy, together with its libraries for linear algebra and working with sparse matrices.*

Gaussian Elimination

The standard approach for solving the linear system $A\mathbf{x} = \mathbf{b}$ on paper is reducing the augmented matrix $[A \mid \mathbf{b}]$ to row-echelon form (REF) via *Gaussian elimination*, then using back substitution. The matrix is in REF when the leading non-zero term in each row is the diagonal term, so the matrix is upper triangular.

At each step of Gaussian elimination, there are three possible operations: swapping two rows, multiplying one row by a scalar value, or adding a scalar multiple of one row to another. Many systems, like the one displayed below, can be reduced to REF using only the third type of operation. First, use multiples of the first row to get zeros below the diagonal in the first column, then use a multiple of the second row to get zeros below the diagonal in the second column.

$$\left[\begin{array}{ccc|c} 1 & 1 & 1 & 1 \\ 1 & 4 & 2 & 3 \\ 4 & 7 & 8 & 9 \end{array}\right] \longrightarrow \left[\begin{array}{ccc|c} 1 & 1 & 1 & 1 \\ 0 & 3 & 1 & 2 \\ 4 & 7 & 8 & 9 \end{array}\right] \longrightarrow \left[\begin{array}{ccc|c} 1 & 1 & 1 & 1 \\ 0 & 3 & 1 & 2 \\ 0 & 3 & 4 & 5 \end{array}\right] \longrightarrow \left[\begin{array}{ccc|c} 1 & 1 & 1 & 1 \\ 0 & 3 & 1 & 2 \\ 0 & 0 & 3 & 3 \end{array}\right]$$

Each of these operations is equivalent to left-multiplying by a *type III elementary matrix*, the identity with one non-diagonal non-zero term. If row operation k corresponds to matrix E_k, the following equation is $E_3E_2E_1A = U$.

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -4 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \left[\begin{array}{ccc|c} 1 & 1 & 1 & 1 \\ 1 & 4 & 2 & 3 \\ 4 & 7 & 8 & 9 \end{array}\right] = \left[\begin{array}{ccc|c} 1 & 1 & 1 & 1 \\ 0 & 3 & 1 & 2 \\ 0 & 0 & 3 & 3 \end{array}\right]$$

However, matrix multiplication is an inefficient way to implement row reduction. Instead, modify the matrix in place (without making a copy), changing only those entries that are affected by each row operation.

```
>>> import numpy as np

>>> A = np.array([[1, 1, 1, 1],
...               [1, 4, 2, 3],
...               [4, 7, 8, 9]], dtype=np.float)

# Reduce the 0th column to zeros below the diagonal.
>>> A[1,0:] -= (A[1,0] / A[0,0]) * A[0]
>>> A[2,0:] -= (A[2,0] / A[0,0]) * A[0]

# Reduce the 1st column to zeros below the diagonal.
>>> A[2,1:] -= (A[2,1] / A[1,1]) * A[1,1:]
>>> print(A)
[[ 1.  1.  1.  1.]
 [ 0.  3.  1.  2.]
 [ 0.  0.  3.  3.]]
```

Note that the final row operation modifies only part of the third row to avoid spending the computation time of adding 0 to 0.

If a 0 appears on the main diagonal during any part of row reduction, the approach given above tries to divide by 0. Swapping the current row with one below it that does not have a 0 in the same column solves this problem. This is equivalent to left-multiplying by a type II elementary matrix, also called a *permutation matrix*.

Achtung!

Gaussian elimination is not always numerically stable. In other words, it is susceptible to rounding error that may result in an incorrect final matrix. Suppose that, due to roundoff error, the matrix A has a very small entry on the diagonal.

$$A = \begin{bmatrix} 10^{-15} & 1 \\ -1 & 0 \end{bmatrix}$$

Though 10^{-15} is essentially zero, instead of swapping the first and second rows to put A in REF, a computer might multiply the first row by 10^{15} and add it to the second row to eliminate the -1. The resulting matrix is far from what it would be if the 10^{-15} were actually 0.

$$\begin{bmatrix} 10^{-15} & 1 \\ -1 & 0 \end{bmatrix} \longrightarrow \begin{bmatrix} 10^{-15} & 1 \\ 0 & 10^{15} \end{bmatrix}$$

Round-off error can propagate through many steps in a calculation. The NumPy routines that employ row reduction use several tricks to minimize the impact of round-off error, but these tricks cannot fix every matrix.

Problem 1. Write a function that reduces an arbitrary square matrix A to REF. You may assume that A is invertible and that a 0 will never appear on the main diagonal (so only use type III row reductions, not type II). Avoid operating on entries that you know will be 0 before and after a row operation. Use at most two nested loops.

Test your function with small test cases that you can check by hand. Consider using `np.random.randint()` to generate a few manageable tests cases.

The LU Decomposition

The *LU decomposition* of a square matrix A is a factorization $A = LU$ where U is the **upper** triangular REF of A and L is the **lower** triangular product of the type III elementary matrices whose inverses reduce A to U. The LU decomposition of A exists when A can be reduced to REF using only type III elementary matrices (without any row swaps). However, the rows of A can always be permuted in a way such that the decomposition exists. If P is a permutation matrix encoding the appropriate row swaps, then the decomposition $PA = LU$ always exists.

Suppose A has an LU decomposition (not requiring row swaps). Then A can be reduced to REF with k row operations, corresponding to left-multiplying the type III elementary matrices $E_1, \dots, E_k$. Because there were no row swaps, each E_i is lower triangular, so each inverse E_i^{-1} is also lower triangular. Furthermore, since the product of lower triangular matrices is lower triangular, L is lower triangular.

$$\begin{aligned} E_k \dots E_2 E_1 A = U \quad \longrightarrow \quad A &= (E_k \dots E_2 E_1)^{-1} U \\ &= E_1^{-1} E_2^{-1} \dots E_k^{-1} U \\ &= LU \end{aligned}$$

Thus L can be computed by right-multiplying the identity by the matrices used to reduce U. However, in this special situation, each right-multiplication only changes one entry of L, matrix multiplication can be avoided altogether. The entire process, only slightly different than row reduction, is summarized below.

Algorithm 2.1

```
procedure LU Decomposition(A)
    m, n ← shape(A)                    ▷ Store the dimensions of A.
    U ← copy(A)                        ▷ Make a copy of A with np.copy().
    L ← I_m                            ▷ The m × m identity matrix.
    for j = 0 ... n − 1 do
        for i = j + 1 ... m − 1 do
            L_{i,j} ← U_{i,j} / U_{j,j}
            U_{i,j:} ← U_{i,j:} − L_{i,j} U_{j,j:}
    return L, U
```

Problem 2. Write a function that finds the LU decomposition of a square matrix. You may assume that the decomposition exists and requires no row swaps.

Forward and Backward Substitution

If $PA = LU$ and $A\mathbf{x} = \mathbf{b}$, then $LU\mathbf{x} = PA\mathbf{x} = P\mathbf{b}$. This system can be solved by first solving $L\mathbf{y} = P\mathbf{b}$, then $U\mathbf{x} = \mathbf{y}$. Since L and U are both triangular, these systems can be solved with backward and forward substitution. We can thus compute the LU factorization of A once, then use substitution to efficiently solve $A\mathbf{x} = \mathbf{b}$ for various values of $\mathbf{b}$.

Since the diagonal entries of L are all 1, the triangular system $L\mathbf{y} = \mathbf{b}$ has the following form.

$$\begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ l_{21} & 1 & 0 & \cdots & 0 \\ l_{31} & l_{32} & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ l_{n1} & l_{n2} & l_{n3} & \cdots & 1 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_n \end{bmatrix}.$$

Matrix multiplication yields the following equations.

$$\begin{aligned} y_1 &= b_1 & y_1 &= b_1 \\ l_{21}y_1 + y_2 &= b_2 & y_2 &= b_2 - l_{21}y_1 \\ &\vdots & &\vdots \\ \sum_{j=1}^{k-1} l_{kj}y_j + y_k &= b_k & y_k &= b_k - \sum_{j=1}^{k-1} l_{kj}y_j \end{aligned} \tag{2.1}$$

The triangular system $U\mathbf{x} = \mathbf{y}$ yields similar equations, but in reverse order.

$$\begin{bmatrix} u_{11} & u_{12} & u_{13} & \cdots & u_{1n} \\ 0 & u_{22} & u_{23} & \cdots & u_{2n} \\ 0 & 0 & u_{33} & \cdots & u_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & u_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_n \end{bmatrix}$$

$$\begin{aligned} u_{nn}x_n &= y_n & x_n &= \frac{1}{u_{nn}}y_n \\ u_{n-1,n-1}x_{n-1} + u_{n-1,n}x_n &= y_{n-1} & x_{n-1} &= \frac{1}{u_{n-1,n-1}}\left(y_{n-1} - u_{n-1,n}x_n\right) \\ &\vdots & &\vdots \\ \sum_{j=k}^{n} u_{kj}x_j &= y_k & x_k &= \frac{1}{u_{kk}}\left(y_k - \sum_{j=k+1}^{n} u_{kj}x_j\right) \end{aligned} \tag{2.2}$$

Problem 3. Write a function that, given A and $\mathbf{b}$, solves the square linear system $A\mathbf{x} = \mathbf{b}$. Use the function from Problem 2 to compute L and U, then use (2.1) and (2.2) to solve for $\mathbf{y}$, then $\mathbf{x}$. You may again assume that no row swaps are required ($P = I$ in this case).

SciPy

SciPy is a powerful scientific computing library built upon NumPy. It includes high-level tools for linear algebra, statistics, signal processing, integration, optimization, machine learning, and more.

SciPy is typically imported with the convention `import scipy as sp`. However, SciPy is set up in a way that requires its submodules to be imported individually.[1]

```
>>> import scipy as sp
>>> hasattr(sp, "stats")            # The stats module isn't loaded yet.
False

>>> from scipy import stats         # Import stats explicitly. Access it
>>> hasattr(sp, "stats")            # with 'stats' or 'sp.stats'.
True
```

Linear Algebra

NumPy and SciPy both have a linear algebra module, each called `linalg`, but SciPy's module is the larger of the two. Some of SciPy's common `linalg` functions are listed below.

Function	Returns
`det()`	The determinant of a square matrix.
`eig()`	The eigenvalues and eigenvectors of a square matrix.
`inv()`	The inverse of an invertible matrix.
`norm()`	The norm of a vector or matrix norm of a matrix.
`solve()`	The solution to $A\mathbf{x} = \mathbf{b}$ (the system need not be square).

This library also includes routines for computing matrix decompositions.

```
>>> from scipy import linalg as la

# Make a random matrix and a random vector.
>>> A = np.random.random((1000,1000))
>>> b = np.random.random(1000)

# Compute the LU decomposition of A, including pivots.
>>> L, P = la.lu_factor(A)

# Use the LU decomposition to solve Ax = b.
>>> x = la.lu_solve((L,P), b)

# Check that the solution is legitimate.
>>> np.allclose(A @ x, b)
True
```

[1] SciPy modules like `linalg` are really *packages*, which need to be initialized separately. For example, to import SciPy's `linalg` package use `from scipy import linalg as la`.

As with NumPy, SciPy's routines are all highly optimized. However, some algorithms are, by nature, faster than others.

Problem 4. Write a function that times different `scipy.linalg` functions for solving square linear systems.

For various values of n, generate a random $n \times n$ matrix A and a random n-vector $\mathbf{b}$ using `np.random.random()`. Time how long it takes to solve the system $A\mathbf{x} = \mathbf{b}$ with each of the following approaches:

1. Invert A with `la.inv()` and left-multiply the inverse to $\mathbf{b}$.
2. Use `la.solve()`.
3. Use `la.lu_factor()` and `la.lu_solve()` to solve the system with the LU decomposition.
4. Use `la.lu_factor()` and `la.lu_solve()`, but only time `la.lu_solve()` (not the time it takes to do the factorization with `la.lu_factor()`).

Plot the system size n versus the execution times. Use log scales if needed.

ACHTUNG!

Problem 4 demonstrates that computing a matrix inverse is computationally expensive. In fact, numerically inverting matrices is so costly that there is hardly ever a good reason to do it. Use a specific solver like `la.lu_solve()` whenever possible instead of using `la.inv()`.

Sparse Matrices

Large linear systems can have tens of thousands of entries. Storing the corresponding matrices in memory can be difficult: a $10^5 \times 10^5$ system requires around 40 GB to store in a NumPy array (4 bytes per entry $\times$ 10^{10} entries). This is well beyond the amount of RAM in a normal laptop.

In applications where systems of this size arise, it is often the case that the system is *sparse*, meaning that most of the entries of the matrix are 0. SciPy's `sparse` module provides tools for efficiently constructing and manipulating 1- and 2-D sparse matrices. A `sparse` matrix only stores the nonzero values and the positions of these values. For sufficiently sparse matrices, storing the matrix as a `sparse` matrix may only take megabytes, rather than gigabytes.

For example, diagonal matrices are sparse. Storing an $n \times n$ diagonal matrix in the naïve way means storing n^2 values in memory. It is more efficient to instead store the diagonal entries in a 1-D array of n values. In addition to using less storage space, this allows for much faster matrix operations: the standard algorithm to multiply a matrix by a diagonal matrix involves n^3 steps, but most of these are multiplying by or adding 0. A smarter algorithm can accomplish the same task much faster.

SciPy has seven sparse matrix types. Each type is optimized either for storing sparse matrices whose nonzero entries follow certain patterns, or for performing certain computations.

Name	Description	Advantages
`bsr_matrix`	Block Sparse Row	Specialized structure.
`coo_matrix`	Coordinate Format	Conversion among sparse formats.
`csc_matrix`	Compressed Sparse Column	Column-based operations and slicing.
`csr_matrix`	Compressed Sparse Row	Row-based operations and slicing.
`dia_matrix`	Diagonal Storage	Specialized structure.
`dok_matrix`	Dictionary of Keys	Element access, incremental construction.
`lil_matrix`	Row-based Linked List	Incremental construction.

Creating Sparse Matrices

A regular, non-sparse matrix is called *full* or *dense*. Full matrices can be converted to each of the sparse matrix formats listed above. However, it is more memory efficient to never create the full matrix in the first place. There are three main approaches for creating sparse matrices from scratch.

- **Coordinate Format**: When all of the nonzero values and their positions are known, create the entire sparse matrix at once as a `coo_matrix`. All nonzero values are stored as a coordinate and a value. This format also converts quickly to other sparse matrix types.

```
>>> from scipy import sparse

# Define the rows, columns, and values separately.
>>> rows = np.array([0, 1, 0])
>>> cols = np.array([0, 1, 1])
>>> vals = np.array([3, 5, 2])
>>> A = sparse.coo_matrix((vals, (rows,cols)), shape=(3,3))
>>> print(A)
  (0, 0)    3
  (1, 1)    5
  (0, 1)    2

# The toarray() method casts the sparse matrix as a NumPy array.
>>> print(A.toarray())              # Note that this method forfeits
[[3 2 0]                            # all sparsity-related optimizations.
 [0 5 0]
 [0 0 0]]
```

- **DOK and LIL Formats**: If the matrix values and their locations are not known beforehand, construct the matrix incrementally with a `dok_matrix` or a `lil_matrix`. Indicate the size of the matrix, then change individual values with regular slicing syntax.

```
>>> B = sparse.lil_matrix((2,6))
>>> B[0,2] = 4
>>> B[1,3:] = 9

>>> print(B.toarray())
[[ 0.  0.  4.  0.  0.  0.]
 [ 0.  0.  0.  9.  9.  9.]]
```

- **DIA Format**: Use a `dia_matrix` to store matrices that have nonzero entries on only certain diagonals. The function `sparse.diags()` is one convenient way to create a `dia_matrix` from scratch. Additionally, every sparse matrix has a `setdiags()` method for modifying specified diagonals.

```
# Use sparse.diags() to create a matrix with diagonal entries.
>>> diagonals = [[1,2],[3,4,5],[6]]     # List the diagonal entries.
>>> offsets = [-1,0,3]                  # Specify the diagonal they go on.
>>> print(sparse.diags(diagonals, offsets, shape=(3,4)).toarray())
[[ 3.  0.  0.  6.]
 [ 1.  4.  0.  0.]
 [ 0.  2.  5.  0.]]

# If all of the diagonals have the same entry, specify the entry alone.
>>> A = sparse.diags([1,3,6], offsets, shape=(3,4))
>>> print(A.toarray())
[[ 3.  0.  0.  6.]
 [ 1.  3.  0.  0.]
 [ 0.  1.  3.  0.]]

# Modify a diagonal with the setdiag() method.
>>> A.setdiag([4,4,4], 0)
>>> print(A.toarray())
[[ 4.  0.  0.  6.]
 [ 1.  4.  0.  0.]
 [ 0.  1.  4.  0.]]
```

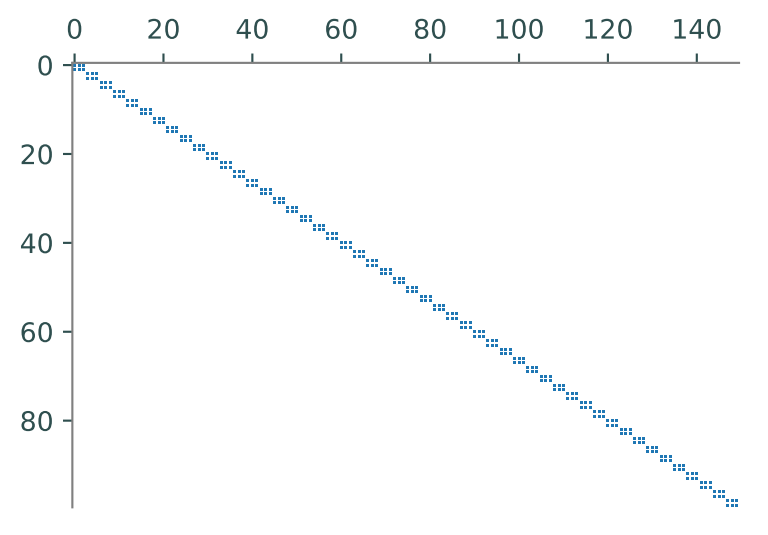
- **BSR Format**: Many sparse matrices can be formulated as block matrices, and a block matrix can be stored efficiently as a `bsr_matrix`. Use `sparse.bmat()` or `sparse.block_diag()` to create a block matrix quickly.

```
# Use sparse.bmat() to create a block matrix. Use 'None' for zero blocks.
>>> A = sparse.coo_matrix(np.ones((2,2)))
>>> B = sparse.coo_matrix(np.full((2,2), 2.))
>>> print(sparse.bmat([[  A , None,  A  ],
                       [None,  B  , None]], format='bsr').toarray())
[[ 1.  1.  0.  0.  1.  1.]
 [ 1.  1.  0.  0.  1.  1.]
 [ 0.  0.  2.  2.  0.  0.]
 [ 0.  0.  2.  2.  0.  0.]]

 # Use sparse.block_diag() to construct a block diagonal matrix.
 >>> print(sparse.block_diag((A,B)).toarray())
[[ 1.  1.  0.  0.]
 [ 1.  1.  0.  0.]
 [ 0.  0.  2.  2.]
 [ 0.  0.  2.  2.]]
```

Note

If a sparse matrix is too large to fit in memory as an array, it can still be visualized with Matplotlib's `plt.spy()`, which colors in the locations of the non-zero entries of the matrix.

```
>>> from matplotlib import pyplot as plt

# Construct and show a matrix with 50 2x3 diagonal blocks.
>>> B = sparse.coo_matrix([[1,3,5],[7,9,11]])
>>> A = sparse.block_diag([B]*50)
>>> plt.spy(A, markersize=1)
>>> plt.show()
```



Problem 5. Let I be the $n \times n$ identity matrix, and define

$$A = \begin{bmatrix} B & I & & & \\ I & B & I & & \\ & I & \ddots & \ddots & \\ & & \ddots & \ddots & I \\ & & & I & B \end{bmatrix}, \qquad B = \begin{bmatrix} -4 & 1 & & & \\ 1 & -4 & 1 & & \\ & 1 & \ddots & \ddots & \\ & & \ddots & \ddots & 1 \\ & & & 1 & -4 \end{bmatrix},$$

where A is $n^2 \times n^2$ and each block B is $n \times n$. The large matrix A is used in finite difference methods for solving Laplace's equation in two dimensions, $\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0$.

Write a function that accepts an integer n and constructs and returns A as a sparse matrix. Use `plt.spy()` to check that your matrix has nonzero values in the correct places.

Sparse Matrix Operations

Once a sparse matrix has been constructed, it should be converted to a `csr_matrix` or a `csc_matrix` with the matrix's `tocsr()` or `tocsc()` method. The CSR and CSC formats are optimized for row or column operations, respectively. To choose the correct format to use, determine what direction the matrix will be traversed.

For example, in the matrix-matrix multiplication AB, A is traversed row-wise, but B is traversed column-wise. Thus A should be converted to a `csr_matrix` and B should be converted to a `csc_matrix`.

```
# Initialize a sparse matrix incrementally as a lil_matrix.
>>> A = sparse.lil_matrix((10000,10000))
>>> for k in range(10000):
...     A[np.random.randint(0,9999), np.random.randint(0,9999)] = k
...
>>> A
<10000x10000 sparse matrix of type '<type 'numpy.float64'>'
    with 9999 stored elements in LInked List format>

# Convert A to CSR and CSC formats to compute the matrix product AA.
>>> Acsr = A.tocsr()
>>> Acsc = A.tocsc()
>>> Acsr.dot(Acsc)
<10000x10000 sparse matrix of type '<type 'numpy.float64'>'
    with 10142 stored elements in Compressed Sparse Row format>
```

Beware that row-based operations on a `csc_matrix` are very slow, and similarly, column-based operations on a `csr_matrix` are very slow.

Achtung!

Many familiar NumPy operations have analogous routines in the `sparse` module. These methods take advantage of the sparse structure of the matrices and are, therefore, usually significantly faster. However, SciPy's `sparse` matrices behave a little differently than NumPy arrays.

Operation	`numpy`	`scipy.sparse`
Component-wise Addition	`A + B`	`A + B`
Scalar Multiplication	`2 * A`	`2 * A`
Component-wise Multiplication	`A * B`	`A.multiply(B)`
Matrix Multiplication	`A.dot(B)`, `A @ B`	`A * B`, `A.dot(B)`, `A @ B`

Note in particular the difference between `A * B` for NumPy arrays and SciPy sparse matrices. Do **not** use `np.dot()` to try to multiply sparse matrices, as it may treat the inputs incorrectly. The syntax `A.dot(B)` is safest in most cases.

SciPy's sparse module has its own linear algebra library, `scipy.sparse.linalg`, designed for operating on sparse matrices. Like other SciPy modules, it must be imported explicitly.

```
>>> from scipy.sparse import linalg as spla
```

Problem 6. Write a function that times regular and sparse linear system solvers.

For various values of n, generate the $n^2 \times n^2$ matrix A described in Problem 5 and a random vector $\mathbf{b}$ with n^2 entries. Time how long it takes to solve the system $A\mathbf{x} = \mathbf{b}$ with each of the following approaches:

1. Convert A to CSR format and use `scipy.sparse.linalg.spsolve()` (`spla.spsolve()`).
2. Convert A to a NumPy array and use `scipy.linalg.solve()` (`la.solve()`).

In each experiment, only time how long it takes to solve the system (not how long it takes to convert A to the appropriate format).

Plot the system size n^2 versus the execution times. As always, use log scales where appropriate and use a legend to label each line.

Achtung!

Even though there are fast algorithms for solving certain sparse linear system, it is still very computationally difficult to invert sparse matrices. In fact, the inverse of a sparse matrix is usually not sparse. There is rarely a good reason to invert a matrix, sparse or dense.

See `http://docs.scipy.org/doc/scipy/reference/sparse.html` for additional details on SciPy's `sparse` module.

Additional Material

Improvements on the LU Decomposition

Vectorization

Algorithm 2.1 uses two loops to compute the LU decomposition. With a little vectorization, the process can be reduced to a single loop.

Algorithm 2.2

procedure FAST LU DECOMPOSITION(A)
  $m, n \leftarrow \text{shape}(A)$
  $U \leftarrow \text{copy}(A)$
  $L \leftarrow I_m$
  for $k = 0 \dots n-1$ **do**
    $L_{k+1:,k} \leftarrow U_{k+1:,k} / U_{k,k}$
    $U_{k+1:,k:} \leftarrow U_{k+1:,k:} - L_{k+1:,k} U_{k,k:}^{\mathsf{T}}$
  return L, U

Note that step 7 is an *outer product*, not the regular dot product ($\mathbf{x}\mathbf{y}^{\mathsf{T}}$ instead of the usual $\mathbf{x}^{\mathsf{T}}\mathbf{y}$). Use `np.outer()` instead of `np.dot()` or `@` to get the desired result.

Pivoting

Gaussian elimination iterates through the rows of a matrix, using the diagonal entry $x_{k,k}$ of the matrix at the kth iteration to zero out all of the entries in the column below $x_{k,k}$ ($x_{i,k}$ for $i \geq k$). This diagonal entry is called the *pivot*. Unfortunately, Gaussian elimination, and hence the LU decomposition, can be very numerically unstable if at any step the pivot is a very small number. Most professional row reduction algorithms avoid this problem via *partial pivoting*.

The idea is to choose the largest number (in magnitude) possible to be the pivot by swapping the pivot row[2] with another row before operating on the matrix. For example, the second and fourth rows of the following matrix are exchanged so that the pivot is -6 instead of 2.

$$\begin{bmatrix} \times & \times & \times & \times \\ 0 & 2 & \times & \times \\ 0 & 4 & \times & \times \\ 0 & -6 & \times & \times \end{bmatrix} \longrightarrow \begin{bmatrix} \times & \times & \times & \times \\ 0 & -6 & \times & \times \\ 0 & 4 & \times & \times \\ 0 & 2 & \times & \times \end{bmatrix} \longrightarrow \begin{bmatrix} \times & \times & \times & \times \\ 0 & -6 & \times & \times \\ 0 & 0 & \times & \times \\ 0 & 0 & \times & \times \end{bmatrix}$$

A row swap is equivalent to left-multiplying by a type II elementary matrix, also called a *permutation matrix*.

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} \times & \times & \times & \times \\ 0 & 2 & \times & \times \\ 0 & 4 & \times & \times \\ 0 & -6 & \times & \times \end{bmatrix} = \begin{bmatrix} \times & \times & \times & \times \\ 0 & -6 & \times & \times \\ 0 & 4 & \times & \times \\ 0 & 2 & \times & \times \end{bmatrix}$$

For the LU decomposition, if the permutation matrix at step k is P_k, then $P = P_k \dots P_2 P_1$ yields $PA = LU$. The complete algorithm is given below.

[2] *Complete pivoting* involves row and column swaps, but doing both operations is usually considered overkill.

Algorithm 2.3

procedure LU Decomposition with Partial Pivoting(A)
  $m, n \leftarrow \text{shape}(A)$
  $U \leftarrow \text{copy}(A)$
  $L \leftarrow I_m$
  $P \leftarrow [0,\ 1,\ \ldots,\ n-1]$ ▷ See tip 2 below.
  for $k = 0 \ldots n-1$ **do**
    Select $i \geq k$ that maximizes $|U_{i,k}|$
    $U_{k,k:} \leftrightarrow U_{i,k:}$ ▷ Swap the two rows.
    $L_{k,:k} \leftrightarrow L_{i,:k}$ ▷ Swap the two rows.
    $P_k \leftrightarrow P_i$ ▷ Swap the two entries.
    $L_{k+1:,k} \leftarrow U_{k+1:,k}/U_{k,k}$
    $U_{k+1:,k:} \leftarrow U_{k+1:,k:} - L_{k+1:,k}U_{k,k:}^{\mathsf{T}}$
  return L, U, P

The following tips may be helpful for implementing this algorithm:

1. Since NumPy arrays are mutable, use `np.copy()` to reassign the rows of an array simultaneously.
2. Instead of storing P as an $n \times n$ array, fancy indexing allows us to encode row swaps in a 1-D array of length n. Initialize P as the array $[0, 1, \ldots, n]$. After performing a row swap on A, perform the same operations on P. Then the matrix product PA will be the same as `A[P]`.

```
>>> A = np.zeros(3) + np.vstack(np.arange(3))
>>> P = np.arange(3)
>>> print(A)
[[ 0.  0.  0.]
 [ 1.  1.  1.]
 [ 2.  2.  2.]]

# Swap rows 1 and 2.
>>> A[1], A[2] = np.copy(A[2]), np.copy(A[1])
>>> P[1], P[2] = P[2], P[1]
>>> print(A)                        # A with the new row arrangement.
[[ 0.  0.  0.]
 [ 2.  2.  2.]
 [ 1.  1.  1.]]
>>> print(P)                        # The permutation of the rows.
[0 2 1]
>>> print(A[P])                     # A with the original row arrangement.
[[ 0.  0.  0.]
 [ 1.  1.  1.]
 [ 2.  2.  2.]]
```

There are potential cases where even partial pivoting does not eliminate catastrophic numerical errors in Gaussian elimination, but the odds of having such an amazingly poor matrix are essentially zero. The numerical analyst J.H. Wilkinson captured the likelihood of encountering such a matrix in a natural application when he said, "Anyone that unlucky has already been run over by a bus!"

In Place

The LU decomposition can be performed in place (overwriting the original matrix A) by storing U on and above the main diagonal of the array and storing L below it. The main diagonal of L does not need to be stored since all of its entries are 1. This format saves an entire array of memory, and is how `scipy.linalg.lu_factor()` returns the factorization.

More Applications of the LU Decomposition

The LU decomposition can also be used to compute inverses and determinants.

- **Inverse**: $(PA)^{-1} = (LU)^{-1} \longrightarrow A^{-1}P^{-1} = U^{-1}L^{-1} \longrightarrow LUA^{-1} = P$. Solve $LU\mathbf{a}_i = \mathbf{p}_i$ with forward and backward substitution (as in Problem 3) for every column $\mathbf{p}_i$ of P. Then

$$A^{-1} = \left[\begin{array}{c|c|c|c} & & & \\ \mathbf{a}_1 & \mathbf{a}_2 & \cdots & \mathbf{a}_n \\ & & & \end{array}\right],$$

  the matrix where $\mathbf{a}_k$ is the kth column.

- **Determinant**: $\det(A) = \det(P^{-1}LU) = \frac{\det(L)\det(U)}{\det(P)}$. The determinant of a triangular matrix is the product of its diagonal entries. Since every diagonal entry of L is 1, $\det(L) = 1$. Also, P is just a row permutation of the identity matrix (which has determinant 1), and a single row swap negates the determinant. Then if S is the number of row swaps, the determinant is given by the following equation.

$$\det(A) = (-1)^S \prod_{i=1}^{n} u_{ii}$$

The Cholesky Decomposition

A square matrix A is called *positive definite* if $\mathbf{z}^\mathsf{T}A\mathbf{z} > 0$ for all nonzero vectors $\mathbf{z}$. In addition, A is called *Hermitian* if $A = A^\mathsf{H} = \overline{A^\mathsf{T}}$. If A is Hermitian positive definite, it has a *Cholesky Decomposition* $A = U^\mathsf{H}U$ where U is upper triangular with real, positive entries on the diagonal. This is the matrix equivalent to taking the square root of a positive real number.

The Cholesky decomposition takes advantage of the conjugate symmetry of A to simultaneously reduce the columns *and* rows of A to zeros (except for the diagonal). It thus requires only half of the calculations and memory of the LU decomposition. Furthermore, the algorithm is *numerically stable*, which means that round-off errors do not propagate throughout the computation. This decomposition is used when possible to solve least squares, optimization, and state estimation problems.

Algorithm 2.4

```
procedure CHOLESKY DECOMPOSITION(A)
    U ← A                                   ▷ Copy A if desired.
    for i = 0 ... n − 1 do
        for j = i + 1 ... n − 1 do
            U_{j,j:} ← U_{j,j:} − U_{i,j:} conj(U_{ij}) / U_{ii}
        U_{i,i:} ← U_{i,i:} / sqrt(U_{ii})
    return U
```

As with the LU decomposition, SciPy's `linalg` module has optimized routines, `la.cho_factor()` and `la.cho_solve()`, for using the Cholesky decomposition.