# Lecture 2 and 3: Algorithms for Linear Algebra

STAT 545: Introduction to computational statistics

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Preliminaries: cost of standard matrix algebra operations

# Solving a system of linear equations

Preliminaries: cost of standard matrix algebra operations

Consider $AX = b$, where $A$ is $N \times N$, and $X$ and $b$ are $N \times k$.

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Calculate the inverse of $A$ and multiply? No!

- Directly solving for $X$ is faster, and more stable numerically
- $A^{-1}$ need not even exist

```
> solve(A,b)         # Directly solve for b
> solve(A) %*% b     # Return inverse and multiply
```

http://www.johndcook.com/blog/2010/01/19/dont-invert-that-matrix/

# Gauss-Jordan elimination

$$A \cdot X = b$$

$$A \cdot \left[\, X \,,\; A^{-1} \,\right] = [\, b \,,\; I \,]$$

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$$\begin{bmatrix} 1 & 0 & 1 \\ 2 & 0 & 1 \\ 1 & -2 & -1 \end{bmatrix} \begin{bmatrix} x_1 & v_{11} & v_{12} & v_{13} \\ x_2 & v_{21} & v_{22} & v_{23} \\ x_3 & v_{31} & v_{32} & v_{33} \end{bmatrix} = \begin{bmatrix} 4 & 1 & 0 & 0 \\ 10 & 0 & 1 & 0 \\ 3 & 0 & 0 & 1 \end{bmatrix}$$

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At step $i$:

- Make element $a_{ii} = 1$ (by scaling or pivoting)
- Set other elements in column $i$ to 0 by multiplying and subtracting that row

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Multiply row 1 by 2 and subtract

$$\begin{bmatrix} 1 & 0 & 1 \\ 0 & 0 & -1 \\ 1 & -2 & -1 \end{bmatrix} \begin{bmatrix} x_1 & v_{11} & v_{12} & v_{13} \\ x_2 & v_{21} & v_{22} & v_{23} \\ x_3 & v_{31} & v_{32} & v_{33} \end{bmatrix} = \begin{bmatrix} 4 & 1 & 0 & 0 \\ 2 & -2 & 1 & 0 \\ 3 & 0 & 0 & 1 \end{bmatrix}$$

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Subtract row 1

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Pivot

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 & v_{11} & v_{12} & v_{13} \\ x_2 & v_{21} & v_{22} & v_{23} \\ x_3 & v_{31} & v_{32} & v_{33} \end{bmatrix} = \begin{bmatrix} 6 & -1 & 1 & 0 \\ 2.5 & -1.5 & 1 & 0.5 \\ -2 & 2 & -1 & 0 \end{bmatrix}$$

Continue till we get an identity matrix

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 & v_{11} & v_{12} & v_{13} \\ x_2 & v_{21} & v_{22} & v_{23} \\ x_3 & v_{31} & v_{32} & v_{33} \end{bmatrix} = \begin{bmatrix} 6 & -1 & 1 & 0 \\ 2.5 & -1.5 & 1 & 0.5 \\ -2 & 2 & -1 & 0 \end{bmatrix}$$

What is the cost of this algorithm?

$$A \cdot \left[ X \, , \; A^{-1} \right] = [\, b \, , \; I \,]$$

# Gauss elimination with back-substitution

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$O(N^3)$ manipulation to get:

$$U \cdot \left[\, X \,,\; A^{-1} \,\right] = [\, \hat{c}_1 \,,\; \hat{C}_2 \,]$$

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Here, $U$ is an upper-triangular matrix.

Cannot just read off solution. Need to backsolve.

What are we actually doing?

$$A = LU$$

Here $L$ and $U$ are lower and upper triangular matrices.

$$L = \begin{bmatrix} 1 & 0 & 0 \\ l_{21} & 1 & 0 \\ l_{31} & l_{32} & 1 \end{bmatrix}, U = \begin{bmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{bmatrix}$$

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Is this always possible?

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

$$PA = LU, \quad P \text{ is a permutation matrix}$$

Crout's algorithm, $O(N^3)$, stable, $L, U$ can be computed in place.

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Then solve $X$ by back substitution

$$UX = Y$$

# Comments

- LU-decomposition can be reused for different $b$'s.
- Calculating LU decomposition: $O(N^3)$.
- Given LU decomposition, solving for $X$: $O(N^2)$.
- $|A| = |P^{-1}LU| = (-1)^S \prod_{i=1}^{N} u_{ii}$ ($S$: num. of exchanges)
- $LUA^{-1} = PI$, can solve for $A^{-1}$. (back to Gauss-Jordan)

# Cholesky decomposition

If $A$ is symmetric positive-definite:

$$A = LL^T \quad \text{(but now } L \text{ need not have a diagonal of ones)}$$

- 'Square-root' of $A$
- More stable.
- Twice as efficient.
- Related: $A = LDL^T$ (but now $L$ has a unit diagonal).

# Eigenvalue decomposition

An $N \times N$ matrix $A$: a map from $\mathbb{R}^N \to \mathbb{R}^N$.
An eigenvector $v$ undergoes no rotation:

$$Av = \lambda v$$

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Let $\Lambda = \mathrm{diag}(\lambda_1, \cdots, \lambda_N)$ with $\lambda_1 \geq \lambda_2, \ldots, \lambda_N$, and
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Real Symmetric matrices have

- real eigenvalues
- different eigenvalues have orthogonal eigenvectors

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Let $A$ be any real symmetric matrix.

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- Adjust $A$ so eigenvalue corresponding to $\mathbf{v}_1$ equals 0

$$\begin{bmatrix} 10 & 7 & 8 & 7 \\ 7 & 5 & 6 & 5 \\ 8 & 6 & 10 & 9 \\ 7 & 5 & 9 & 10 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 32 \\ 23 \\ 33 \\ 31 \end{bmatrix}$$

What is the solution? How about for $b = [32.1, 22.9, 33.1, 30.9]^T$?

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Why the difference?

- the determinant?
- the inverse?
- the condition number?

An *ill-conditioned* problem can strongly amplify errors.

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- Even without any rounding error

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For a general, real matrix, $\|A\| = \sqrt{\lambda_{\max}(A^T A)}$ (why?)

# Stability analysis

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If $A = BC$, and all matrices are in $\mathbb{R}^{N\times N}$,

$$\|A\| \leq \|B\|\|C\| \qquad \text{(why?)}$$

# Stability analysis

For a perturbation, $\delta b$ let $\delta x$ be the change in solution to $Ax = b$

$$A(x + \delta x) = b + \delta b$$

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Condition number of a matrix $A$ is given by

$$\kappa(A) = \|A\|\|A^{-1}\|$$

Large condition number implies unstable solution

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Condition number is a property of a problem

Stability is a property of an algorithm

A bad algorithm can mess up a simple problem

Consider reducing to upper triangular

$$\begin{bmatrix} v_{11} & v_{12} & v_{13} \\ v_{21} & v_{22} & v_{23} \\ v_{31} & v_{32} & v_{33} \end{bmatrix}$$

Gaussian elimination: divide row 1 by $v_{11}$

# Gaussian elimination with partial pivoting

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Why does it work?

Recall Gaussian elimination decomposes $A = LU$ and solves two intermediate problems.

What are the condition numbers of $L$ and $U$?

Try

$$\begin{bmatrix} 1e-4 & 1 \\ 1 & 1 \end{bmatrix}$$

Note: `R` does pivoting for you automatically! (see the function `lu` in package `Matrix`)

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Does this mean we should use QR decomposition?

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$$\tilde{\mathbf{u}}_i = \mathbf{x}_i - \sum_{j=1}^{i-1} (\mathbf{x}_i^T \mathbf{u}_j) \mathbf{u}_i, \quad \mathbf{u}_i = \tilde{\mathbf{u}}_i / \|\tilde{\mathbf{u}}_i\| \quad i = 2 \ldots, N$$

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Modified Gram-Schmidt

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- $\tilde{\mathbf{u}}_i = \mathbf{x}_i - (\mathbf{x}_i^T \mathbf{u}_1)\mathbf{u}_1,$
- $\tilde{\mathbf{u}}_i = \mathbf{x}_i - (\mathbf{u}_2^T \mathbf{u}_1)\mathbf{u}_2,$
- $\ldots$
- $\mathbf{u}_i = \tilde{\mathbf{u}}_i / \|\tilde{\mathbf{u}}_i\|$

$\ldots$

# QR decomposition

$$A \quad = \quad Q \quad R$$

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = \begin{bmatrix} q_{11} & q_{12} & q_{13} \\ q_{21} & q_{22} & q_{23} \\ q_{31} & q_{32} & q_{33} \end{bmatrix} \begin{bmatrix} r_{11} & r_{12} & r_{13} \\ 0 & r_{22} & r_{23} \\ 0 & 0 & r_{33} \end{bmatrix}$$

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\begin{array}{ccccc}
A & = & Q & & R
\end{array}
$$

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QR decomposition: Gram-Schmidt on columns of $A$
(can you see why?)

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QR decomposition: Gram-Schmidt on columns of $A$
(can you see why?)

Of course, there are more stable/efficient ways of doing this
(Householder rotation/Givens rotation)

$O(N^3)$ algorithms (though about twice as slow as LU)

# QR algorithm

Algorithm to calculate all eigenvalues/eigenvectors of a (not too-large) matrix

Start with $A_0 = A$. At iteration $i$:

- $A_i = Q_i R_i$
- $A_{i+1} = R_i Q_i$

Then $A_i$ and $A_{i+1}$ have the same eigenvalues (why?), and the diagonal contains the eigenvalues.

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Then $A_i$ and $A_{i+1}$ have the same eigenvalues (why?), and the diagonal contains the eigenvalues. Can be made this more stable/efficient.

One of Dongarra & Sullivan (2000)'s list of top 10 algoirithms.

`https://www.siam.org/pdf/news/637.pdf`

See also number 4, ”decompositional approach to matrix computations”

$$\log(p(X|\mu, \Sigma)) = -\frac{1}{2}(X-\mu)^T\Sigma^{-1}(X-\mu) - \frac{N}{2}\log 2\pi - \frac{1}{2}\log|\Sigma|$$

# Multivariate normal

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Can also just forward solve for $L^{-1}$: $LL^{-1} = I$
(Inverted triangular matrix isn't too bad)

Sampling a univariate normal:

- Inversion method (default for `rnorm`?).
- Box-Muller transform: $(Z_1, Z_2)$ : independent standard normals.

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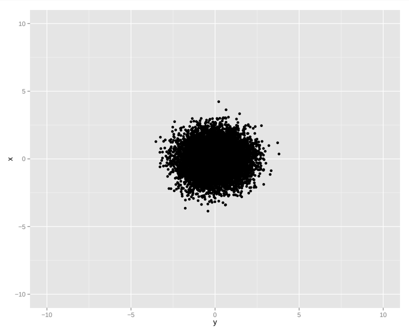
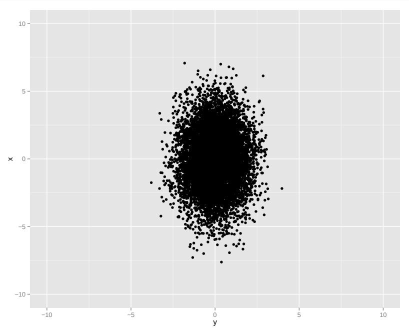
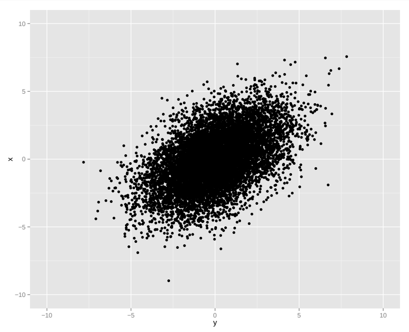
- Box-Muller transform: $(Z_1, Z_2)$ : independent standard normals.
- Let $Z \sim \mathcal{N}(0, I)$
- $X = \mu + LZ$
- $Z = \mathcal{N}(\mu, L^T L)$



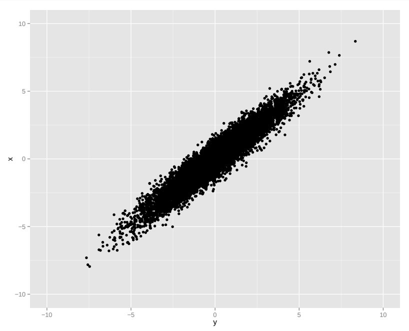

$$\Sigma = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$




$$\Sigma = \begin{bmatrix} 4 & 0 \\ 0 & 1 \end{bmatrix}$$




$$\Sigma = \begin{bmatrix} 4 & 2 \\ 2 & 4 \end{bmatrix}$$




$$\Sigma = \begin{bmatrix} 4 & 3.8 \\ 3.8 & 4 \end{bmatrix}$$