COMPSCI 590N
Lecture 8: Numerical Linear Algebra 2

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Outline

Matrix Inversion

Review: An $n \times n$ square matrix A is said to be **invertible** if there exists an $n \times n$ matrix B such that:

$$AB = BA = I$$

where I is the identity matrix. If B exists it is called the **inverse** and is denoted A^{-1}. Matrix inversion is the process of finding A^{-1} for a given matrix A.

Matrix Inversion: Applications

- Matrix inverses appear in statistics frequently. Part of the reason for this is because of the appearance of a matrix inverse in the PDF of the multivariate normal distribution.

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- The analytical solution for least-squares linear regression involves a matrix inverse.
- Matrix inversion plays a fundamental role in many computer graphics routines.
- Matrix inversion is a subroutine for many more complex linear algebra computations.

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- **Gaussian Elimination** is a method for solving equations of the form $Ax = b$ where A is a matrix, b is a vector, and we are solving for the vector b.
- Gaussian elimination can be thought of as a systematic application of simple substitution rules.
- Gauss-Jordan elimination is the application of this idea to the equation $AX = I$ where now X is a matrix rather than a vector.

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- Scaling a row by a non-zero constant.
- Adding a scaled row to another row.
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If we are able to do this without getting a row of all zeros on the left, then the right side will be A^{-1}. If at any point we get a row with all zeros, then the matrix has no inverse.

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  - This eliminates all entries below the diagonal and sets the diagonal to ones.
- Repeat this process from the bottom up, this time eliminating entries above the diagonal.

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  - We add row i to all rows below row i, so $n - i$ times.

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&= 2\left[n^2+2n^3-n^3+n^2\right] \\
&= 4n^2+2n^3 = \mathcal{O}(n^3)
\end{aligned}$$

Advanced Matrix Inverse Algorithms

As with matrix multiplication, more sophisticated algorithms exist the have complexity between n^2 and n^3.

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Solution:

1. Run a bunch of tests for different n and record the run times.
2. Fit a line to the log run times. The slope will be the degree of the polynomial and the intercept will be the logged constant.

Estimating the complexity of NumPy Matrix Inverse

Demo

Eigenreview

Let A be a square $n \times n$ matrix, then the $\mathbf{v}$ is an **eigenvector** of A if

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

for some constant λ known as an **eigenvalue**. **Eigen decomposition** is the process of finding the eigenvalue/eigenvector pairs of a matrix.

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  - Principal Components Analysis (PCA) is used in many data analysis settings to reduce the dimensionality of a dataset and reduce collinearity.
  - Spectral clustering is used in machine learning and computer vision for clustering data points and parts of images. Spectral clustering requires calculating the Eigen decomposition of a similarity matrix.

Eigen Decomposition: Eigenfaces

- One of the seminal early pieces of work in computer vision worked by compressing images into eigenvectors.

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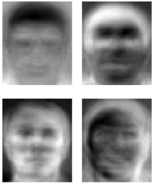

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The Power Method

1. Given an $n \times n$ matrix A, choose a random initial vector b_0.
2. Then, under some mild assumptions, the following sequence will converge to the dominant eigenvector:

$$\frac{Ab_0}{\|Ab_0\|}, \frac{A^2b_0}{\|A^2b_0\|}, \frac{A^3b_0}{\|A^3b_0\|}, \dots$$

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Fortunately, there is a better way. We can use the following interative algorithm:

$$b_k = \frac{A^k b_0}{\|A^k b_0\|} = \frac{A(A^{k-1}b_0)}{\|A(A^{k-1}b_0)\|} = \frac{Ab_{k-1}}{\|Ab_{k-1}\|}$$

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- The power method has complexity $\mathcal{O}(n^2)$ **per iteration**.

Inversion and Decomposition in Action: Linear Regression

Let $X \in \mathbb{R}^{n\times m}$ be a $n \times m$ matrix of data cases (i.e. design matrix) and let $y \in \mathbb{R}^n$ be a length n vector of real values. Then in ordinary least squares linear regression, we have the following model:

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where ϵ is a normally distributed vector of noise. Then using Maximum Likelihood Estimation, we estimate $\hat{\beta}$ as

$$\hat{\beta} = \arg\min_{\beta} (\beta X - y)^T (\beta X - y)$$

Inversion and Decomposition in Action: Linear Regression

The solution to this minimization problem can be found by taking the gradient with respect to β, setting it to zero, and solving. The results is:

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- The advanced linear algebraist may have noticed that $(X^T X)^{-1} X^T$ is called the **Moore-Penrose pseudoinverse**.
- There are specialized algorithms for computing the Moore-Penrose pseudoinverse.
- Part of Assignment 4 will be implementing and comparing linear regression using straight inversion vs. pseudoinversion.

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- Plus a few more...

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  - For example: Directly solving linear regression with 1,000 instances is feasible, but 1,000,000 might not be. In this case you should consider a different method.
- As a rule of thumb, assume $\mathcal{O}(n^3)$ runtime.
- Approximations for many of these computations exist that are good enough in many cases.