# Approximated PCA

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## 1 Introduction

The PCA method transforms a set of observations of possibly correlated variables into a set of values of linearly uncorrelated variables called principal components using an orthogonal transformation (rotations and reflections).

The transformation, projects the data in a new subspace, in which each new variable it's now uncorrelated. That means that the covariance of each pair of new variables is zero. To compute the transformation, different approaches can be taken. In a first attempt, the covariance matrix will be used. Let $x_{ij}$ be the observation $j$ of the variable $i$. Let $n$ be the number of variables and $m$ the number of observations. Each element $s_{ij}$ in the covariance matrix $S$ is computed by

$$s_{ij} = \frac{\sum x_{ik}x_{jk} - \sum x_{ij}x_{jk}}{n(n-1)}$$

Once the covariance matrix $S$ in computed, it can be used to find his eigenvalues and eigenvectors. One method to compute those values, is a combination of a Householder transformation, followed by the QR transformation. The first will transform $S$ in a product of two matrix $Q$ and $R$.

$$S = QR$$

Such that $R$ contains 3 diagonals (tridiagonal) with elements and zeros in the rest. The QR transformation then takes this two matrices, and computes iteratively a new diagonal matrix $A^{(i+1)} = R^{(i)}Q^{(i)}$. Finally, the eigenvalues are in the diagonal of $A$ and the eigenvectors are computed from these.

## 2 Householder tridiagonalization

The Householder tridiagonalization it's a process where a matrix $A$ is transformed by multiplying with an orthogonal matrix $P^{(k)}$: $P^{(k)} = I - 2ww^T$ Such matrix $P^{(k)}$ has been prepared, so that $P^{(k)}A$ is a new matrix, with zeros below the $k+1$ element in the $k$ column. This new matrix, has the same eigenvalues as the provious $A$. The step is repeated until the final matrix has only elements in the diagonal, and the two sub-diagonals. The process is similar to a Gaussian elimination.

# 3 Eigenvalue sensitivity

Corolary 8.1.6: If $A$ and $A + E$ are $n$-$by$-$n$ symmetric matrices, then

$$|\lambda_k(A + E) - \lambda_k(A)| \leq \|E\|_2$$

for $k = 1 : n$.

Then, the difference between the eigenvalue of a noisy matrix, and the original, can be bounded by the 2-norm of $E$, also the maximum eigenvalue of $E$.

# 4 First approach

The first experiment to be carried out consists in determining which parts of the algorithm can be suitable for approximate computing. The main steps of PCA can be summarized as follow:

1. Take a dataset $X$ of $n$ variables.
2. Scale and center the variables.
3. From $X$ compute the $n \times n$ covariance matrix $S$.
4. **Compute the eigenvalues and eigenvectors of $S$.**
5. *Optional: Ignore some eigenvectors.*
6. Generate a new basis from the selected eigenvectors.
7. Project $X$ into the new basis.

Computing the eigenvectors is the principal step of PCA.

## 4.1 Computing eigenvalues and eigenvectors

1. Take the $n \times n$ target matrix $A = S$.
2. Compute a tridiagonal matrix $T$: $A = PTP^T$.
3. From $T$ compute a diagonal matrix $D$: $T = QDQ^T$.
4. The eigenvalues of $A$ are in the diagonal of $D$.
5. Compute the eigenvectors from $D$.

Computing a tridiagonal matrix is called **tridiagonalization**. For the diagonal, **diagonalization**. Several algorithms exists for both steps.

### 4.2 Tridiagonalization algorithms

These algorithms transform a **symmetric** matrix $A$ into a new pair of matrices $P$ and $T$ such that $P$ is orthogonal, $T$ is tridiagonal, and $A = PTP^T$

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{pmatrix} = P \begin{pmatrix} t_{11} & t_{12} & & \\ t_{21} & t_{22} & t_{23} & \\ & t_{32} & t_{33} & t_{34} \\ & & t_{43} & t_{44} \end{pmatrix} P^T$$

Some algorithms can be used for this factorization:

| Algorithm | Complexity | Iterative | Stability |
|---|---|---|---|
| Householder | $O(4n^3/3)$ | No | Great |
| Givens | $O(kn^3)$ | No | Good |
| Lanczos | $O(kpn^2)$ | Yes | Bad |
| Others | | | |

Where $n \times n$ is the dimension of the matrix $A$, $k$ is some constant, and $p$ the number of iterations.

### 4.3 Diagonalization algorithms

These algorithms take a **tridiagonal** matrix $T$ into a new pair of matrices $Q$ and $D$ such that $Q$ is orthogonal, $D$ is diagonal, and $T = QDQ^T$

$$\begin{pmatrix} t_{11} & t_{12} & & \\ t_{21} & t_{22} & t_{23} & \\ & t_{32} & t_{33} & t_{34} \\ & & t_{43} & t_{44} \end{pmatrix} = Q \begin{pmatrix} d_{11} & & & \\ & d_{22} & & \\ & & d_{33} & \\ & & & d_{44} \end{pmatrix} Q^T$$

The matrix $D$ contains the **eigenvalues** in the diagonal. Some algorithms can be used to compute the diagonalization:

| Algorithm | Complexity | Convergence |
|---|---|---|
| QR | $O(6n^3)$ | Cubic |
| Divide and conquer | $O(8n^3/3)$ | Quadratic |
| Jacobi | $O(n^3)$ | Quadratic |
| Power iteration | $O(n^3)$ | Linear |
| Inverse iteration | $O(n^3)$ | Linear |
| Others | | |

All these algorithms are iterative and $n \times n$ is the dimension of the matrix $A$.

# 5 Experiments with the bit-width

The reduction of bits in the mantisa of the floating points used by the algorithm can lead to an acceleration in the ALU. However, the precision of the results can be affected by the number of bits used.

For this reason, a set of experiments are performed, to test how the error grows as the number of bits of the mantisa is reduced.

The library MPFR is designed to perform computations with an arbitrary mantissa length. After rewrite the Householder algorithm, the results can be compared with a golden execution. This golden execution is done with a very big mantissa, such that the error of the result is so low that can be ignored, compared with the errors produced in the experiments.

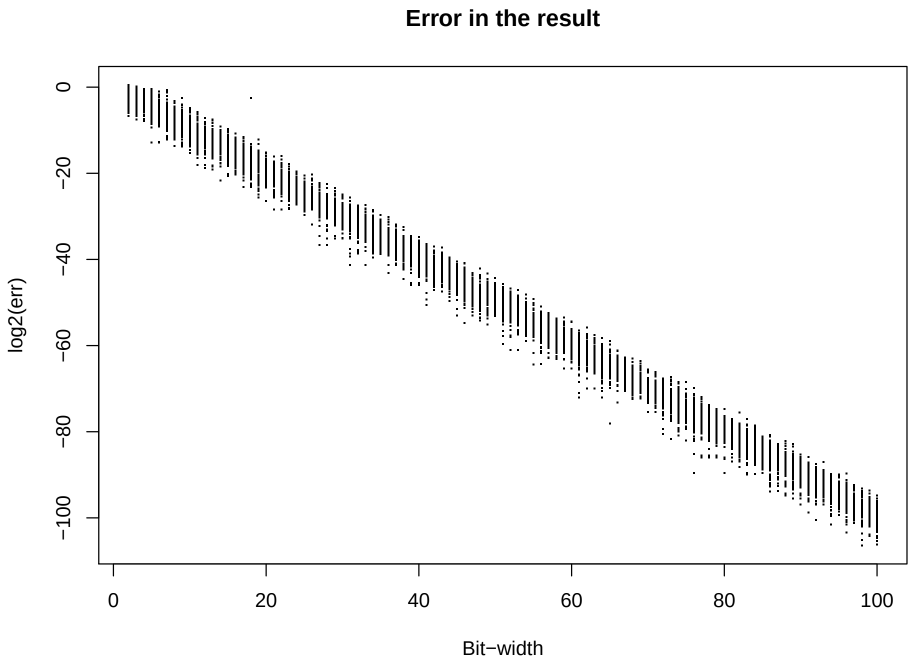
The aim of this set of experiments is to reduce the storage size needed while keeping a reasonable error.

### Experiment A

**Objective** Understand how the bit-width $b$ affects the error in the Householder algorithm.

**Description** For an input matrix $A$ symmetric and random, of size $n \times n$ with $n = 5$, a gold result is computed, using a high precision computation with $b = 500$. Then, in each run, the bit-width $b$ is set to a value in the range $[2, 100]$ and Householder runs again on the same input. The error $\Delta$ is measured compared as with the golden result.

**Result** The error is drawn as the bit-width $b$ grows.




**Conclusion** It can be observed that $\log_2 \Delta$ is close to $-b$. More experiments are needed to test this hypothesis.

### Experiment B

**Objective** Test if the relation between the $\log_2 \Delta$ and $b$ is linear.

**Description** Let $X_b = \log_2 \Delta$ and $Y = b + \overline{X}_b$. We can now plot $Y$ as $b$ grows. If $\overline{X}_b = -b$, then $Y$ should be 0. For each bit-width $b$ in the range $[2, 100]$, a set of 10000 simulations are performed with $n = 5$, and the sample mean $\overline{X}_b$ is computed.

**Result** The random variable $Y$ seems to be constant as the bit-width grows, as can be seen in the figure 1.

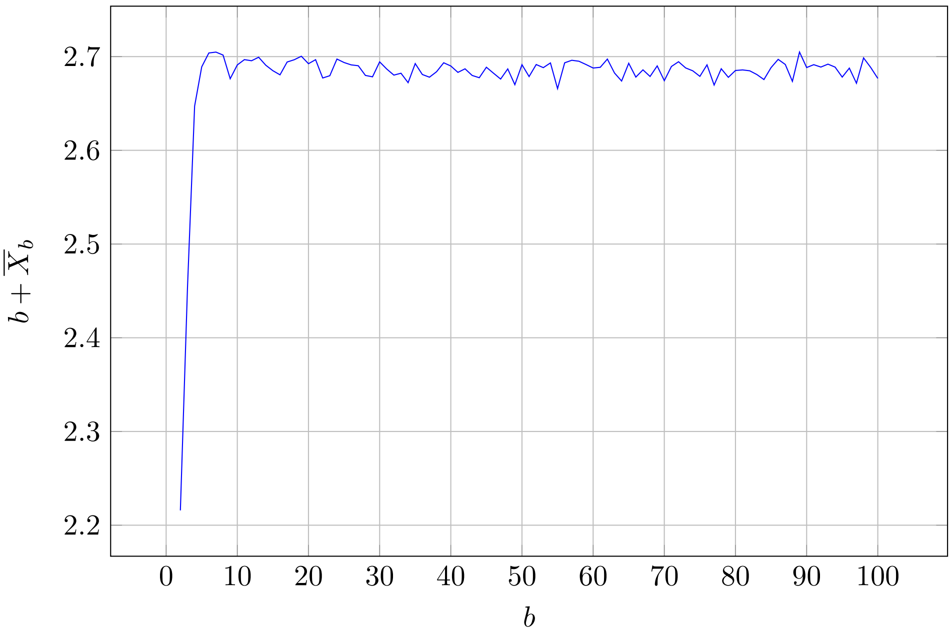



Figure 1: Plot of $b + \overline{X}_b$ as the number of bits $b$ increases.

**Conclusion** Further statistical analysis reveals that, if the values with $b < 5$ are not considered, $Y$ is independent of $b$, and has a mean in the interval $2.68691 \pm 0.00190$ at a confidence level of 0.95. Then, the relation between $\overline{X}_b$ and $b$ is linear. More experiments are needed to determine if the mean of $Y$ is always constant.

### Experiment C

**Objective** Test if there is any relation between $Y$ and the precision of each variable of the Householder algorithm.

**Description** The precision is now determined by a vector $\boldsymbol{b}$, so that each variable used in the Householder algorithm is assigned a own $b_i$. Let $\boldsymbol{v}$ be the set of variables. Then $v_1$ is the matrix A, $v_2$ the diagonal, $v_3$ the offdiagonal, and the others $v_i$ are the internal parameters of Householder algorithm. The variable $v_i$ is set a bit-width of $b_i$. The experiment is repeated as in the experiment B, but we only change one $b_i$ at the time, selecting a precision from [5,100], while the others are set at 500 bits.

**Result** The experiments show that the variable $v_4$ don't produce any error in the output. This variable is a internal scale variable of the Householder algorithm, and will be ignored, to show the other variables.

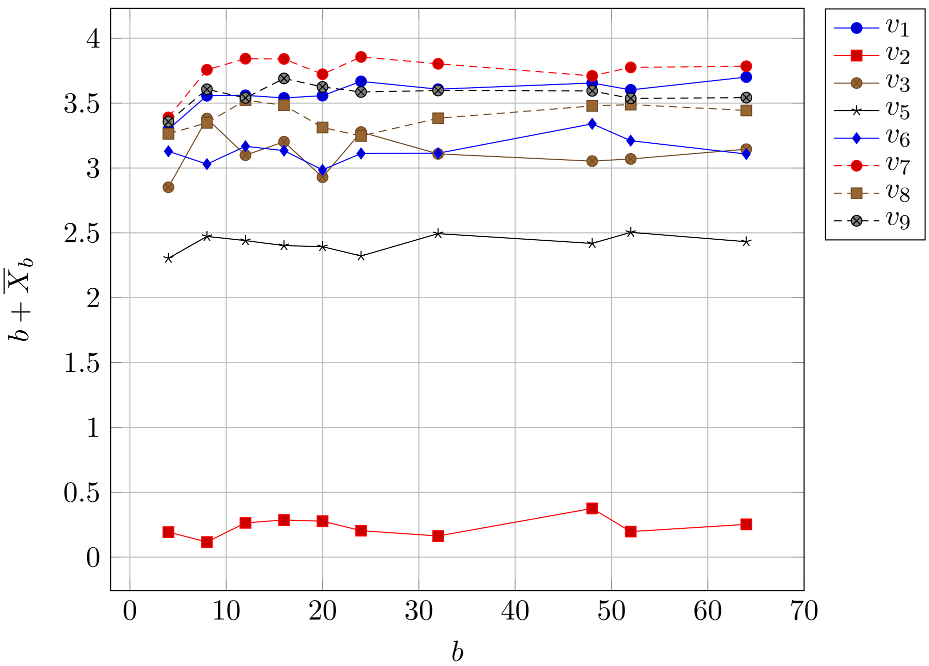



Figure 2: Different error mean for each variable.

**Conclusion** It can be shown that the precision of the variables affect the value of the $Y$, and also that is independent of the value of $b$.

### Experiment D

**Objective** Test if there is any relation between $Y$ and the condition number $\kappa$ of the input matrix.

**Description** The Householder algorithm is executed with a fixed bit-width $b = 50$ and compared with the gold result with $b = 500$. The error is plotted against the logarithmic condition number $\log \kappa$ computed from the input matrix.

**Result** In the figure 3 it can be seen that there is no clear relationship between the condition number and $Y$.

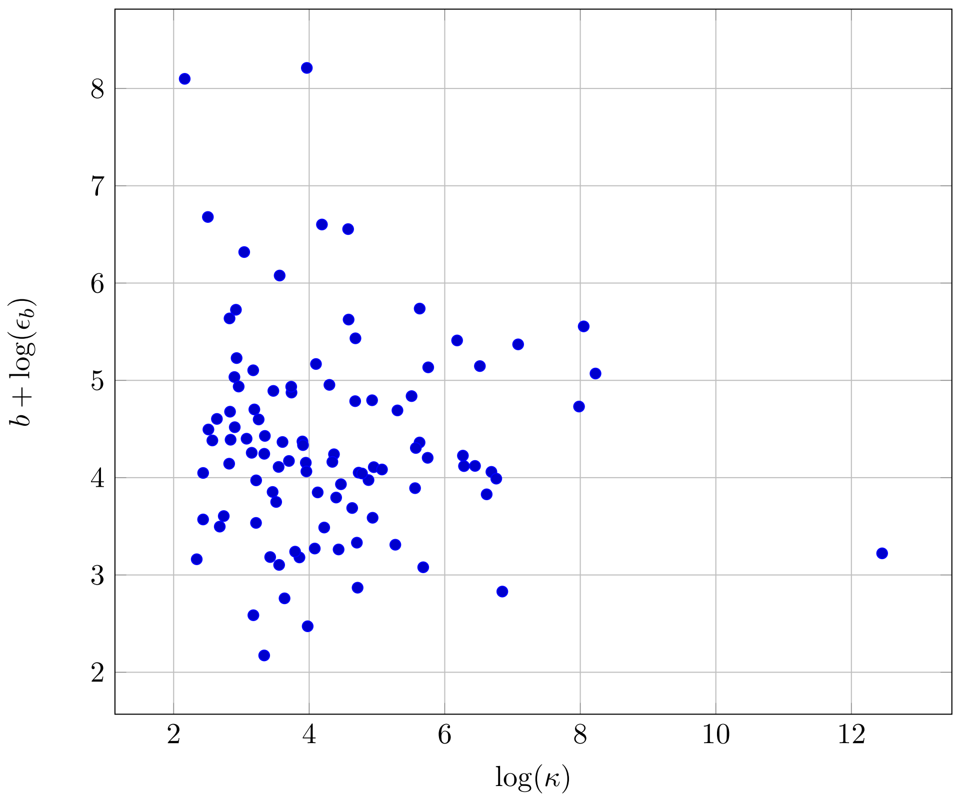



Figure 3: Using a fixed bit-width $b = 50$ the error is plotted against the condition number.

**Conclusion** The condition number doesn't affect the random variable $Y$ in a meaningful way.

### Experiment E

**Objective** Determine the relation between $Y$ and $n$.

**Description** The Householder algorithm is executed varying both the bit-width $b$ and the size of the $n \times n$ input matrix. The error is measured by computing the norm-2 of the difference between the output vectors of the gold result, and the current result.

**Result** The mean of the sample $Y$ is computed from the values with the same input size $n$. In the figure 4, the cubic mean $\overline{Y}^3$ is plotted against $n$.

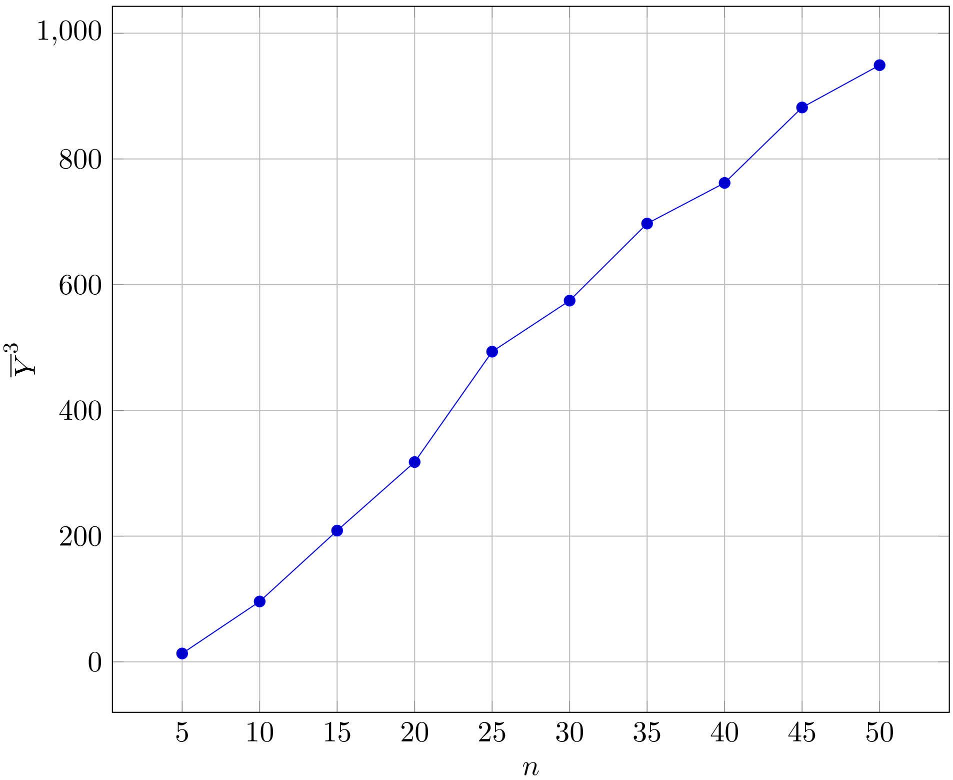



Figure 4: The error $\overline{Y}^3$ is computed with varying matrix sizes $n$.

**Conclusion** It can be seen that the relation between $\overline{Y}^3$ and $n$ seems linear, but more data is necessary. A new experiment should be designed to cope with bigger matrices.

## Experiment F

**Objective** Determine the relation between $Y$ and $n$ when $n$ is big.

**Description** The experiment E is now designed to deal with bigger matrices, and is executed with values of $n$ in the range of [500, 5000]. To compute the exact exponent, we plot the ratio $Y/\log_2 n$ as $n$ grows.

**Result** It can be seen that the ratio is almost constant, as $n$ grows, and the mean is 2.78857, represented as a red line in the figure 5.

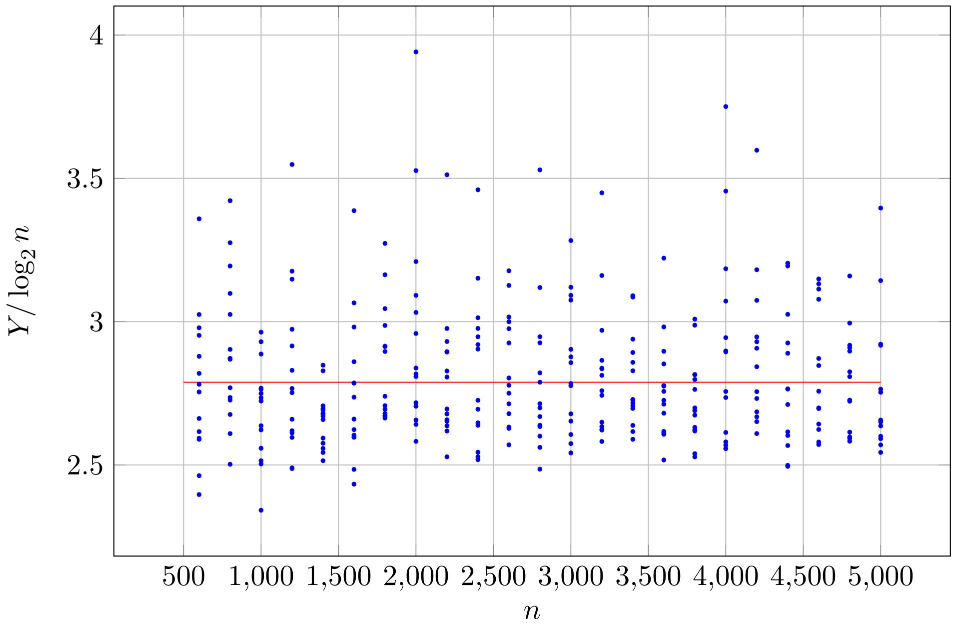



Figure 5: The error $\overline{Y}$ with varying matrix sizes $n$.

**Conclusion** The error $Y$ seems to grow with $n$, with a power of $\alpha =$ 2.78857,

$$Y/\log_2(n) \approx 2.78857 = \alpha$$

So, we can compute an approximation of the rounding error $\Delta$ as a function of $b$ and $n$, for bigger values of $n$.

$$X = \log_2(\Delta) \approx -b + Y = -b + \alpha \log_2(n)$$

And as $\epsilon = 2^{-b}$, we get:

$$\Delta \approx \epsilon \cdot n^{\alpha}$$

### Experiment G

**Objective** Determine if we can use less storage space while maintaining a low error, with different precisions in the variables of Householder algorithm, as well as the input matrix $A$, and the two vectors diagonal and offdiagonal.

**Description** In this experiment the variables used in the Householder algorithm are set with individual precisions. The input matrix A and the diagonal vectors diagonal and offdiagonal are set each with individual precisions. The golden result is computed using 500 bits of precision in all the variables. The storage size is plotted against the error.

**Result** It can be seen in the figure 7 the relation between the error and the storage size in bits. When the main variables like the input matrix $A$, or the diagonal and offdiagonal vectors are assigned a low precision, less space is needed, but the error increases. Also, by using a mix of high and low precision variables, the error keeps high.

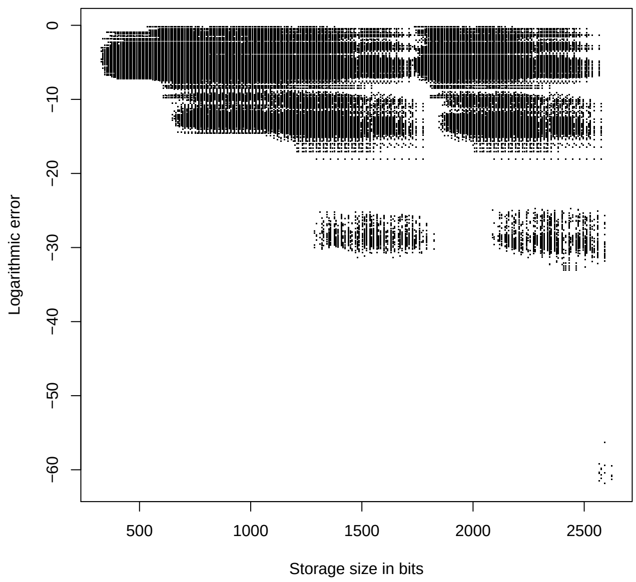



Figure 6: The error $\overline{Y}$ with varying matrix sizes $n$.

**Conclusion** It seems better to select all precision to the same value, in order to obtain the smallest error.

### Experiment H

**Objective** Determine the effect of the precision in the different elements in the input matrix $A$ and the vector diagonal and offdiagonal, as they change.

**Description** In each step, a random configuration of bits is assigned to each element in the matrix and in both vectors. The possible values are $\{8, 16, 32, 64\}$, and are selected randomly with a probability of $1/4$ each.

Once the configuration of bits for the data storage is completed, the Householder algorithm runs with the internal variables at 64 bits. Then, the error is computed from the gold result.

**Result** It can be seen, in red, the configurations now have a big error and use more space than the previous experiment.

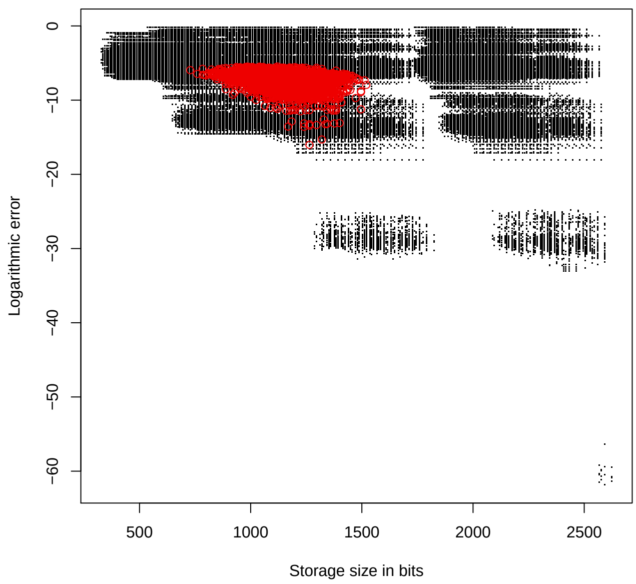



Figure 7: The error $\overline{Y}$ with varying matrix sizes $n$.

**Conclusion** Is better to left all the precisions inside the matrix or vectors to the same value.