# Approximated PCA

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July 30, 2017

# 1 PCA

## 1.1 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. The main steps of PCA can be summarized as follows:

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

Computing the eigenvectors is the principal step of PCA, and different methods can be used.

## 1.2 Algorithms

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 $S$ is obtained, the eigenvalues and eigenvectors need to be computed. One fast and estable method consists in transform the covariance matrix in a tridiagonal matrix, and then in a diagonal matrix, as follows:

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.

### 1.2.1 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.

### 1.2.2 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 $A$.

The proposed algorithms for the task are the Householder followed by a QL algorithm, which is a variation of the QR algorithm.

### 1.3 Householder

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 previous $A$. 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.

### 1.4 QL

The QL algorithm completes the process of diagonalization of the matrix, by iteratively approaching to the solution. There are $n-1$ stages in a matrix of $n \times n$. At each stage $i$, the elements of the offdiagonals $o_i$ are iteratively decreased, until they reach 0. At this moment, the algorithm steps to the next stage. A step is defined as one update of $o_i$ and $d_i$ in each iteration.

## 2 Experiments with Householder algorithm

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.

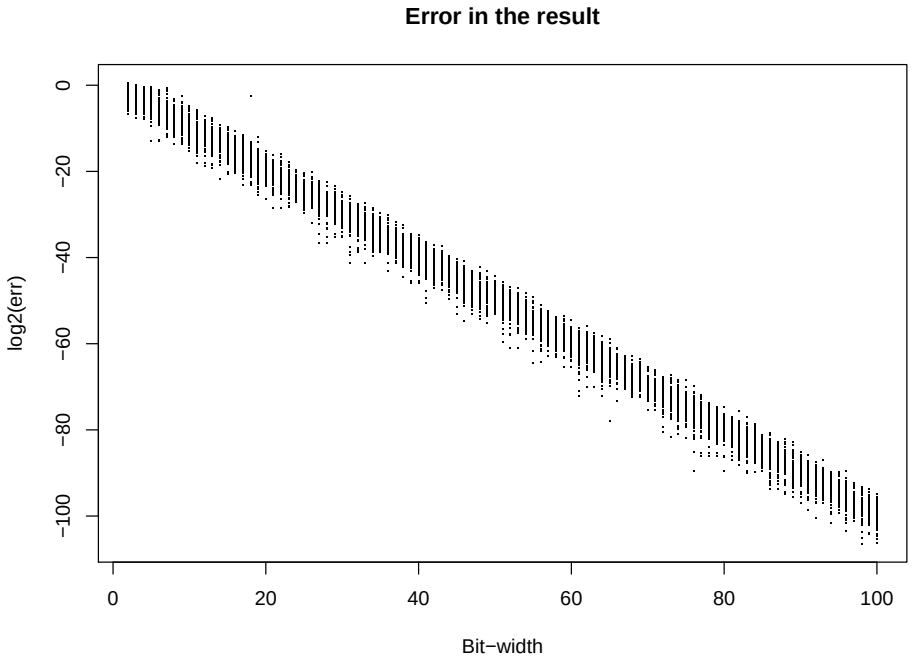
The aim of this set of experiments is to reduce the storage size needed while keeping a reasonable error.

## 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.

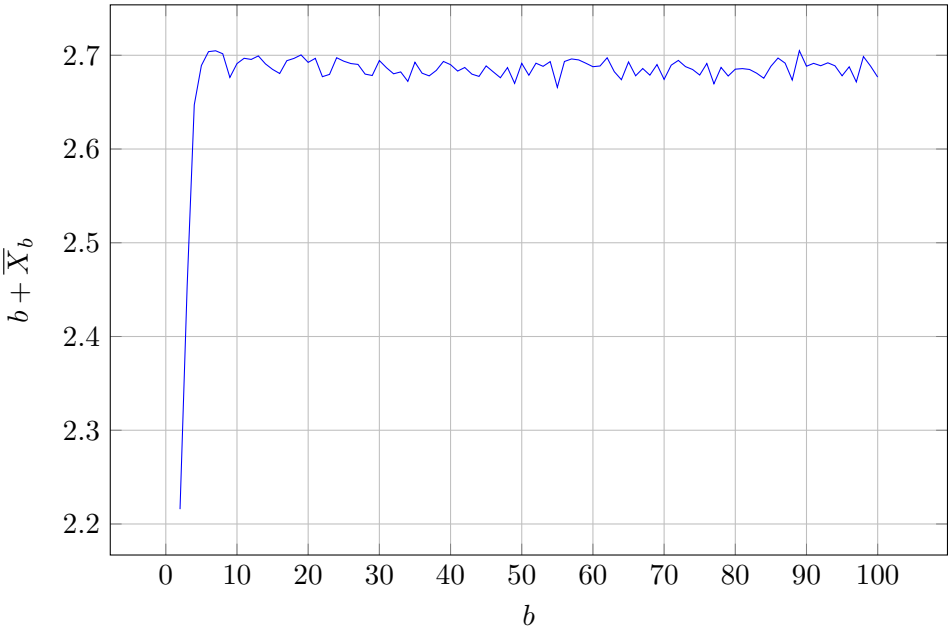



Figure 1: Plot of $b + \overline{X}_b$ as the number of bits $b$ increases.

**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.

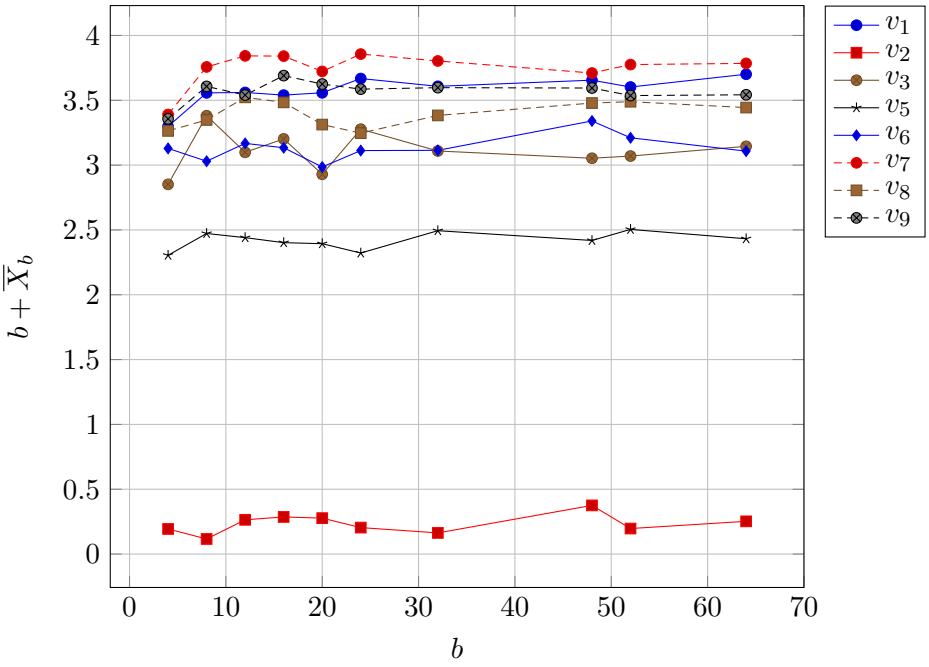



Figure 2: Different error mean for each variable.

**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 $Y$.

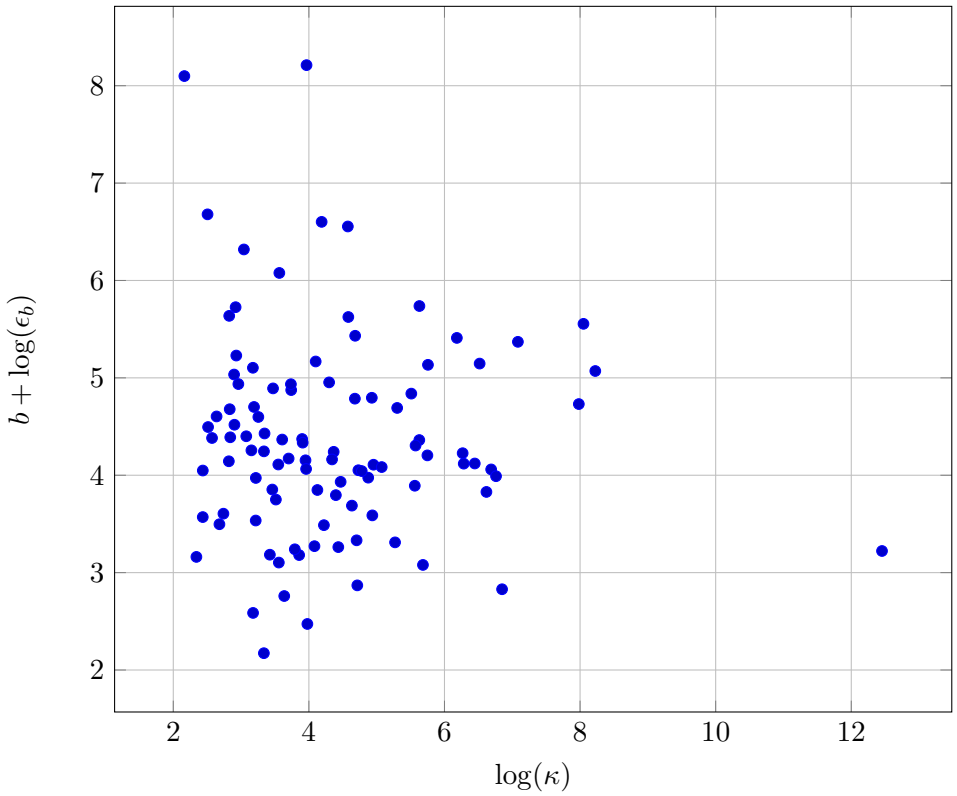



Figure 3: Using a fixed bit-width $b = 50$ the error is plotted against the condition number.

**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 $n$.

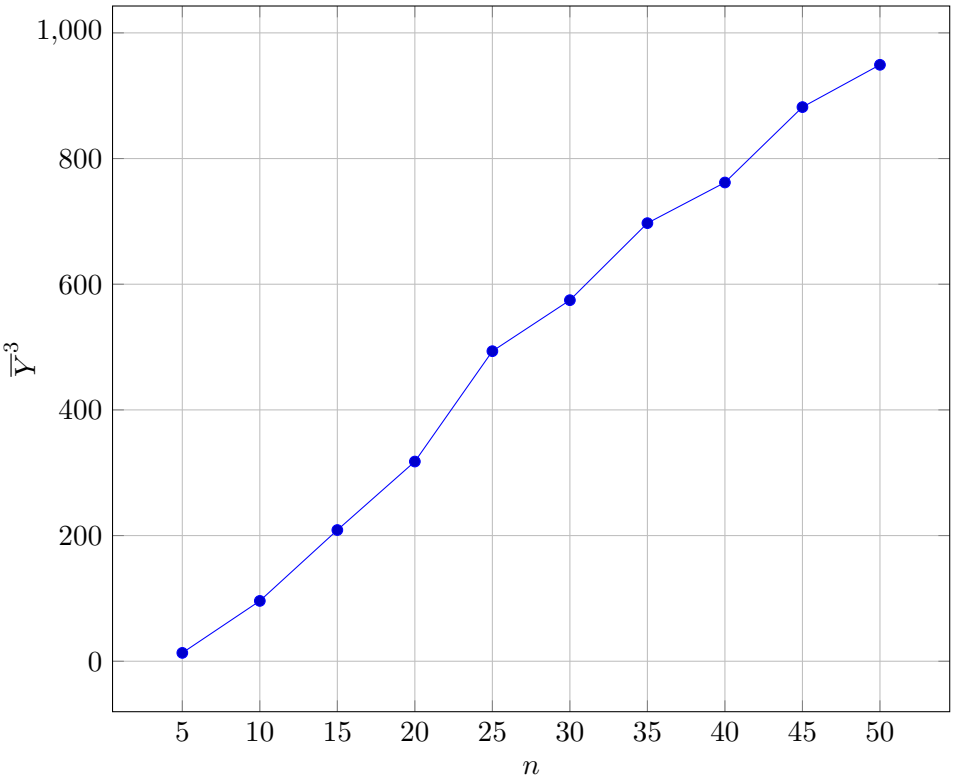



Figure 4: The error $\overline{Y}^3$ is computed with varying matrix sizes $n$.

**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.

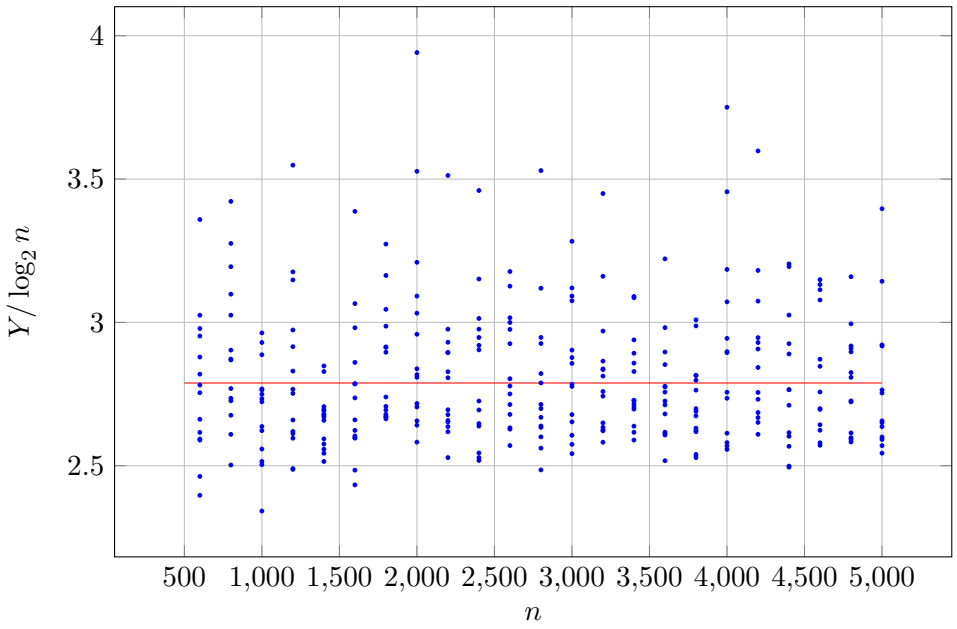



Figure 5: The error $\overline{Y}$ with varying matrix sizes $n$.

**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 6 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.

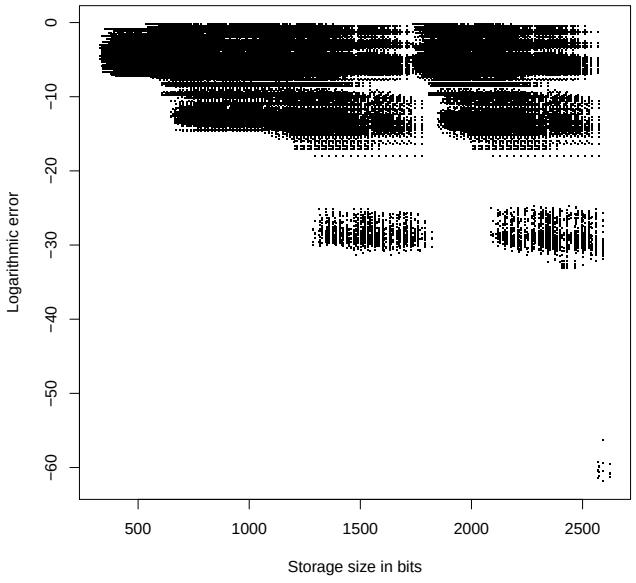



Figure 6: The error $\overline{Y}$ with varying matrix sizes $n$.

**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.

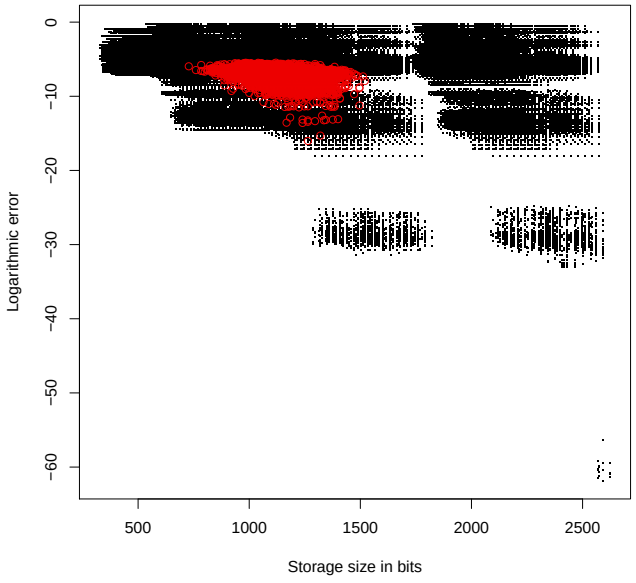



Figure 7: The error $\overline{Y}$ with varying matrix sizes $n$.

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

# 3 Experiments with QL

Some experiments were designed to reduce the number of steps required. The input matrices used in the experiments were generated using random elements uniformly distributed in $[-1, 1]$. The experiments A, B, C and D were executed using single precision (float), while the experiment E is executed using variable precision with the MPFR library.

The errors are measured by comparing the diagonal $d'$ after the QL algorithm (which should contain the eigenvalues), with the diagonal $d$ of the modified QL. The values of diagonals are first sorted, and the relative error $\delta$ is then measured as:

$$\delta = \frac{\|d - d'\|_2}{\|d'\|_2}$$

## Experiment A

**Objective** Determine if we can reduce the number of steps in QL, while keeping the relative error low.

**Description** First an estimation is used to compute the relative error at each step of the QL algortihm. Then the algorithm is stopped when the estimation measures a error below a threshold. The estimation is computed over the offdiagonal elements $o_i = a_{i,i+1}$ and the diagonal elements $d_i = a_{ii}$ as

$$s = \frac{\sum_{i=1}^{N-1} |o_i|}{\sum_{i=1}^{N} |d_i|}$$

**Result** In the figure 8 there can be seen 3 executions with random matrices of size $n \times n$ with $n \in \{50, 100, 200\}$. The relative error is compared with the ratio of completion of the QL algorithm. The error decreases more quickly in the last steps, and the slope becomes sharper as the size of the matrix increases. The 2 lines in red mark a interesting region, where the error is below 1% and the ratio is less than 90%.

**Conclusion** There is no enough reduction of the number of steps to consider this technique useful.

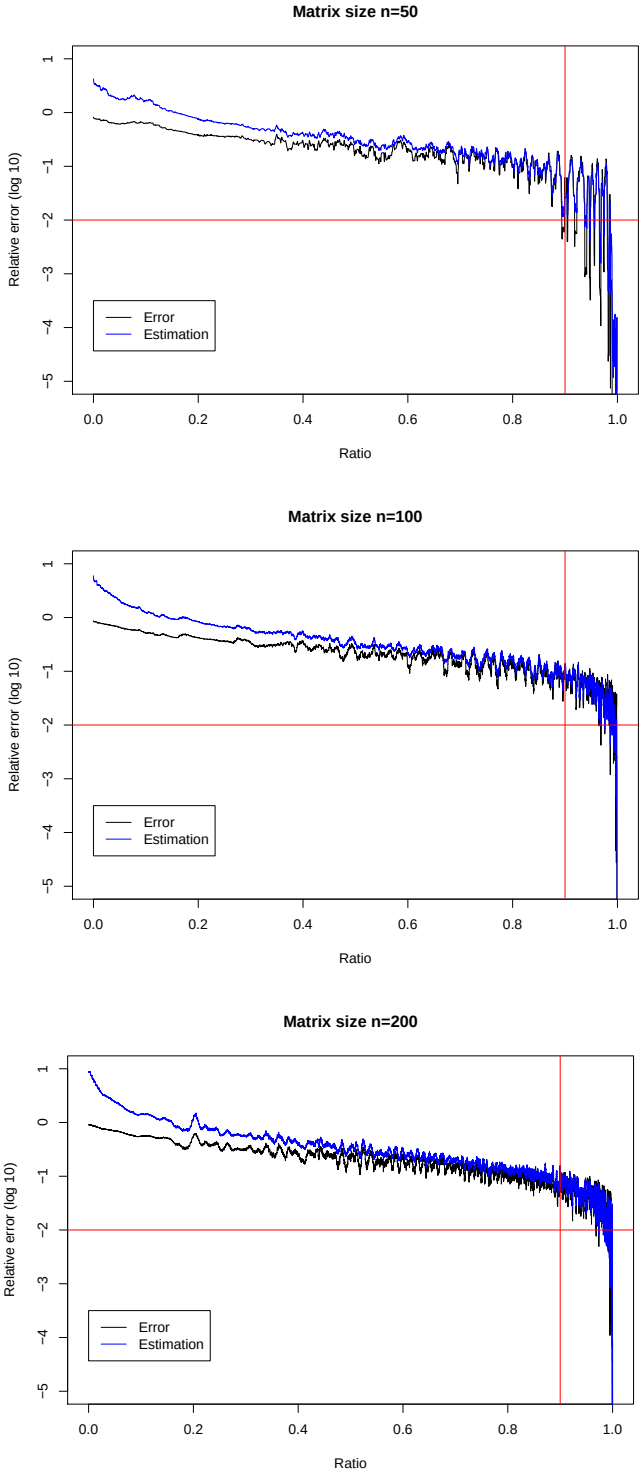



Figure 8: The logarithmic relative error as the number of steps grow.

## Experiment B

**Objective** Determine if we can reduce the number of steps in QL, while keeping the relative error low.

**Description** The QL algorithm iterates over the elements in the diagonal and subdiagonal, until the first non-zero subdiagonal element becomes zero. Then it moves to the next non-zero element. The number of iterations can vary, but a maximum of $m = 30$ is considered enough for any case. In this experiment, the maximum number of iterations $m$ is set to lower value, and if is reached, the execution moves to the next non-zero element.

**Result** In the figure 9 the error is measured against the ratio, with different values for $m$. Again a region of interest is represented in red lines, with less than 1% of relative error and less than 90% of steps. The red points have $m = 2$, and they are almost all in the interesting region.

More runs are tested in figure 10 with a fixed value of $m = 2$, with input matrix sizes of $n \times n$ with $n \in \{50, 100, 200\}$ an respective number of runs $r \in \{10^5, 10^4, 10^3\}$. The mean ratio seems to grow slowly with $n$, but stays close to 65%.

**Conclusion** By using this technique, the number of steps can be reduced down to 65%, while the relative error is mostly below 1%.

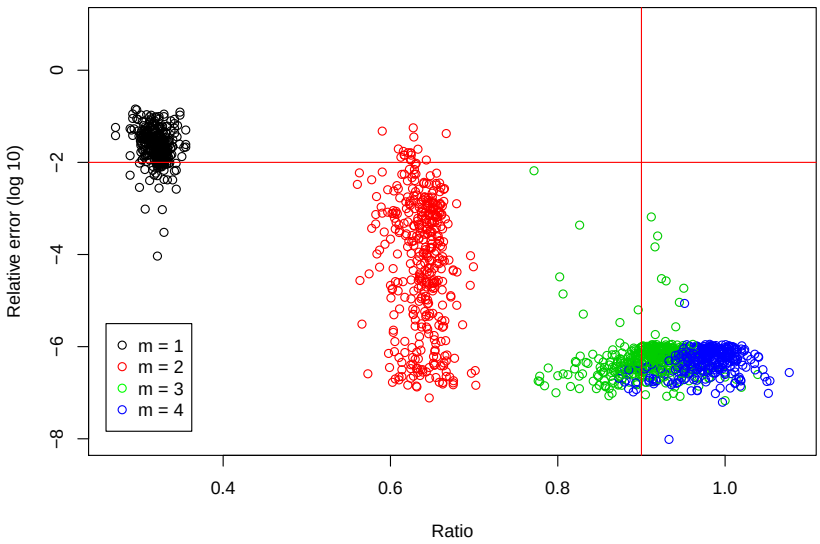



Figure 9: The logarithmic relative error with different values of $m$.

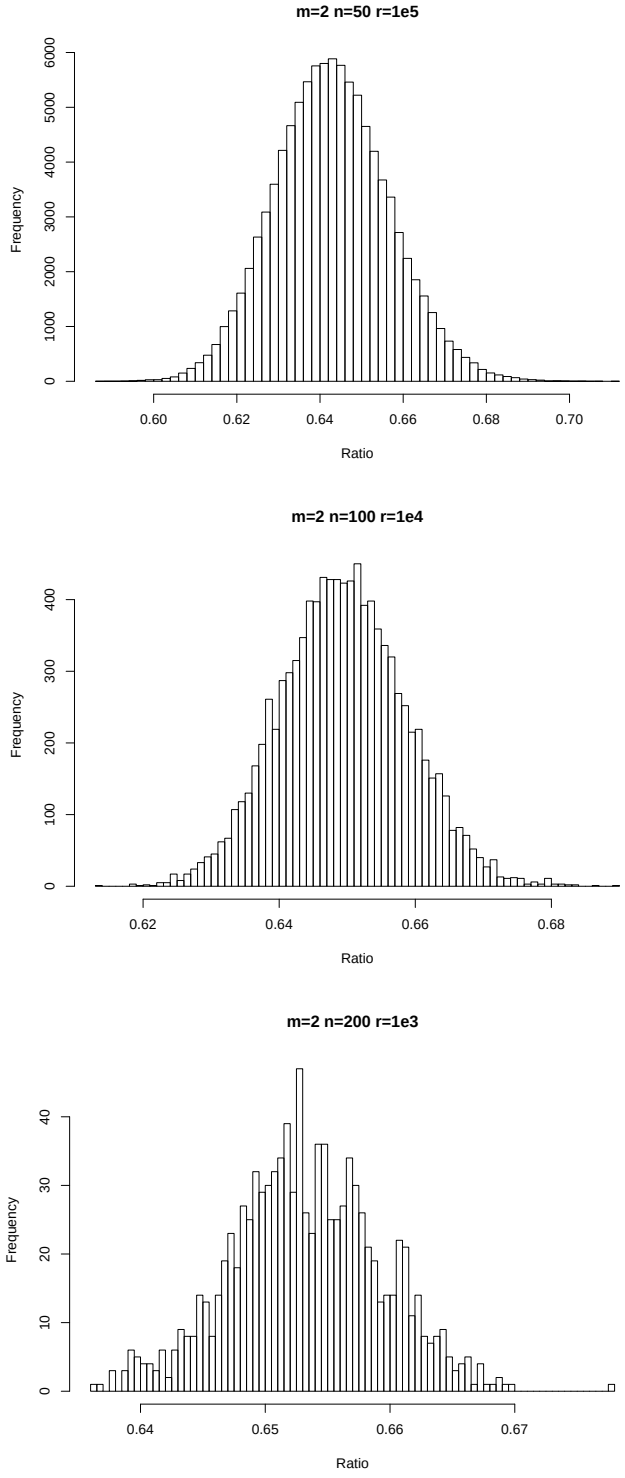



Figure 10: The histogram of the ratio as $n$ grows, with $m = 2$, using $r$ simulations.

## Experiment C

**Objective** Determine if we can reduce the number of steps in QL, while keeping the relative error low.

**Description** In this experiment, the comparison of the subdiagonal elements with 0 is relaxed by introducing a small tolerance $t$. So that a subdiagonal element $o_i$ is considered 0 if $|d_i| + |d_{i+1}| + |o_i| \leq (1+t)(|d_i| + |d_{i+1}|)$.

Different values of $t$ are tested while recording the ratio of steps and the relative error.

**Result** In the figure 11 different tolerances are tested for random input matrices of size $50 \times 50$, while the ratio and logarithmic relative error are measured. Each color represents a different tolerance, as can be seen in the figure 12. A horizontal red line corresponds to 1% of relative error, and it can be seen that there are some values in the interesting region, below this line.

**Conclusion** The experiment shows a interesting result, with a ratio of 30% and 50% we have relative errors between $10^{-2}$ and $10^{-6}$. The number of steps can be reduced down to 30% while keeping a relative error close to 1%.

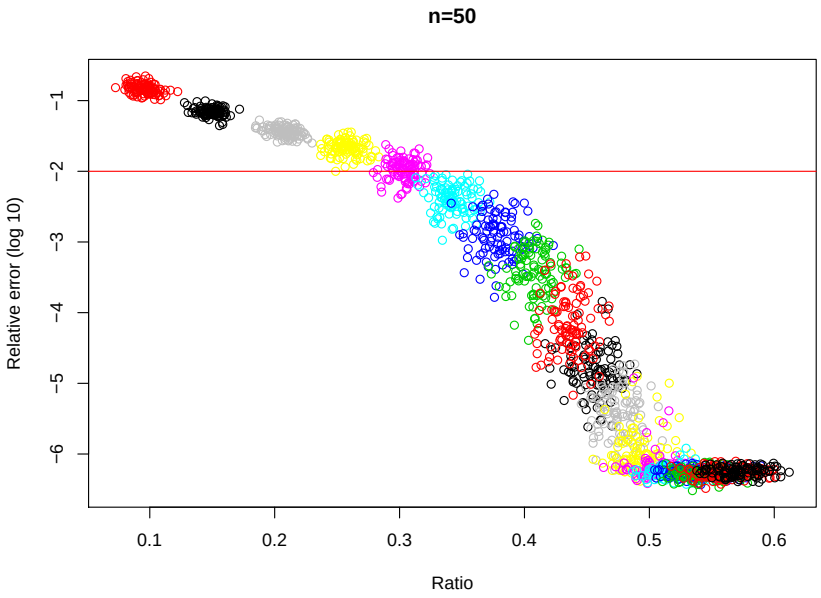



Figure 11: The logarithmic relative error and ratio with different tolerances.

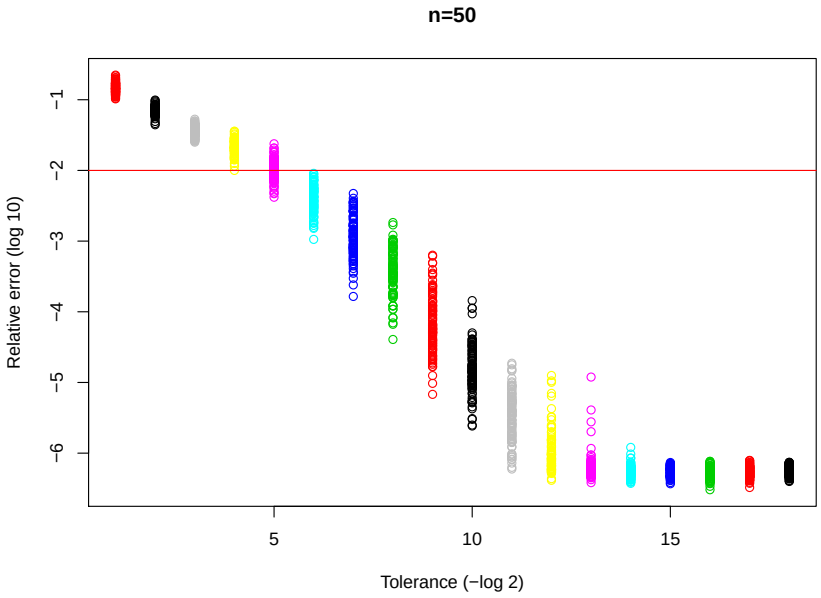



Figure 12: The logarithmic relative error with different tolerances.

## Experiment D

**Objective** Determine if we can reduce the number of steps in QL, while keeping the relative error low.

**Description** The technique of loop perforation is tested in the following way: we skip each step with probability $p$. Different values of $p$ are tested with $\log_{10} p \in [-7, -1]$. The size $n \times n$ of the random input matrices is also tested with $n \in \{10, 20, 50, 100\}$. The relative error and the ratio are finally measured.

**Result** In the figure 13 the relative error is plotted against the ratio, each color represent a different value of $p$. Points in the interesting region, below 1% of relative error and less than 90% of ratio, are never achieved. In the figure 14 it can be seen which is the effect of the probability $p$ on the error. Same colors are used in both figures.

**Conclusion** This technique doesn't seem to provide interesting results, it even introduces more error and more required steps than the original method.

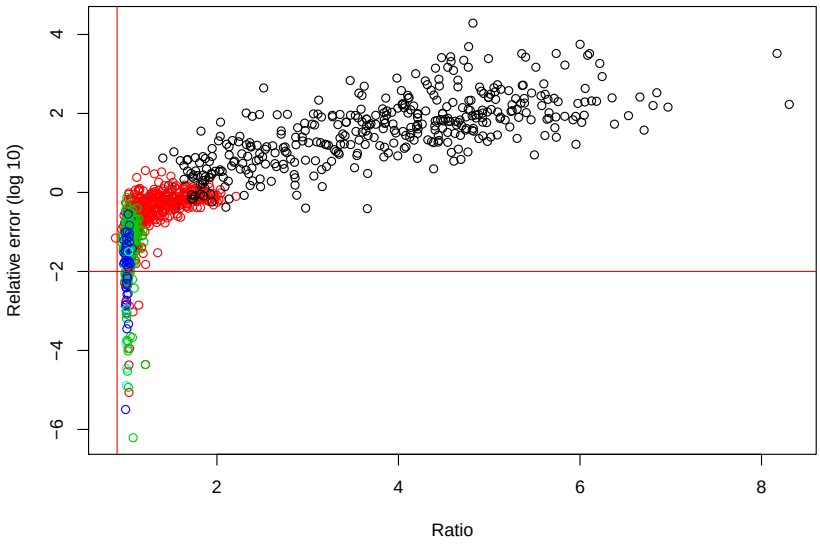



Figure 13: The logarithmic relative error and ratio with different probabilities.

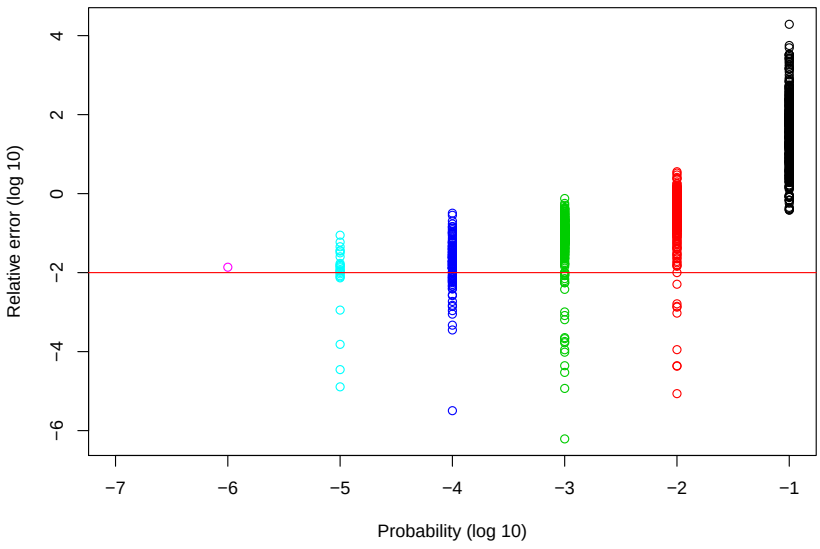



Figure 14: The logarithmic relative error with different probabilities.

## Experiment E

**Objective** Determine if the relative error can be reduced while the precision of the variables in the QL algorithm are changed.

**Description** The significant is set to $b$ bits of precision with $b \in \{2, 6, \ldots, 98\}$, then the results are compared with a reference result, with $b = 500$. The relative error and the ratio are measured. The ratio is computed based on the current execution steps over the steps with $b = 98$. Different matrix sizes of $n \times n$ with $n \in \{10, 20, 50, 100\}$ are also tested.

**Result** In the figure 15 the error is shown as the number of bits $b$ increases. The error decreases almost linearly with $b$, the same happened with Householder. To see the effect of the different sizes, let $Y = b + \log_2 \delta$, as shown in the figure 16. It can be seen that as the size $n$ grows, the variable $Y$ increases. Finally, in the figure 17 the ratio and logarithmic relative error are ploted, as $b$ grows. In the interesting region, delimited by a 1% relative error, and a 90% ratio, there are some interesting points. However, as the size increases, the points move outside the interesting region.

**Conclusion** For relative small sized matrices, this technique can reduce the number of steps up to 60%, while keeping an relative error lower than 1%. However as the matrices grow, the ratio increases, as well as the error.

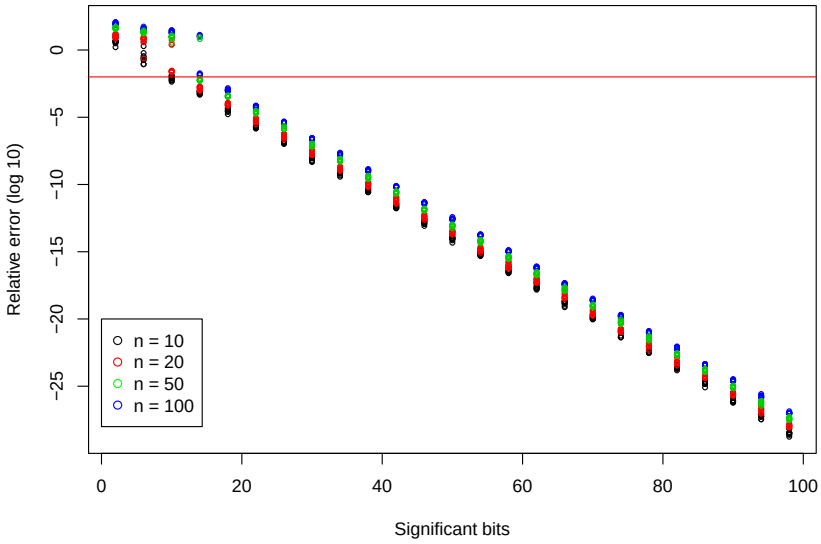



Figure 15: The logarithmic relative error as $b$ grows.

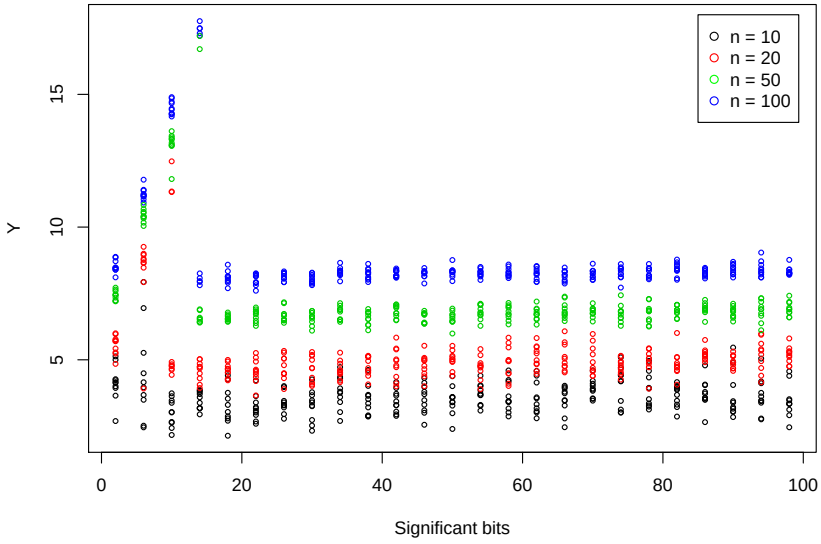



Figure 16: The difference $b + \log_2 \delta$ as $b$ grows.

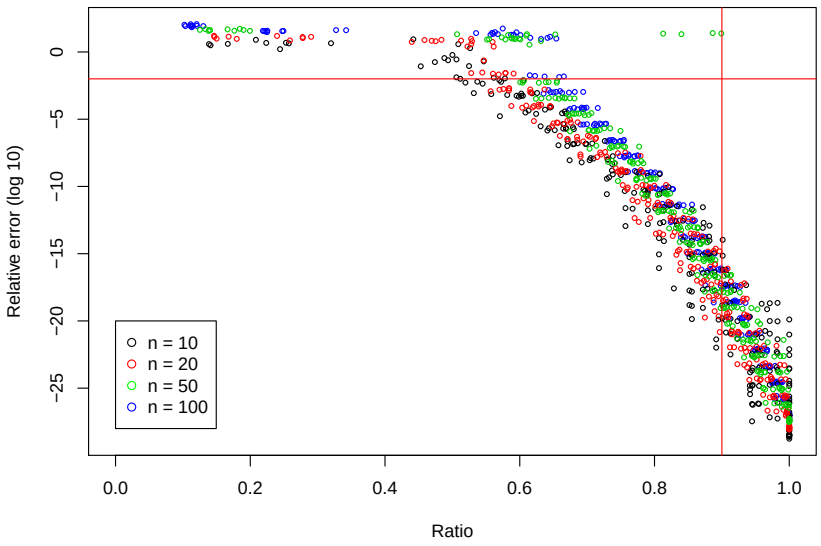



Figure 17: The $\log_{10} \delta$ and ratio as $b$ grows.

# 4 Discussion

The experiments in the Householder algorithm reveal that the relation between $\log_2 \Delta$ and $b$ is linear, and we can estimate the error by $\Delta \approx \epsilon n^{\alpha}$. A reduction in the storage size can be achieved with a reduction in $b$. The best configuration is to keep all the variables at the same precision. The reduction of size is proportional to $b$ and $n$.

In the other hand, by allowing a relative error of 1% in the QL algorithm, different techniques can be used to reduce the number of steps. The best ones are: The introduction of a tolerance in the measurement of the subdiagonal elements, which can reduce the number of steps down to 35%. The reduction of $b$, to around $50\% - 70\%$. And the limit in the maximum iterations, which at $m = 2$ reduces the steps to $60\% - 65\%$.