FYS3150 Computational Physics - Project 2

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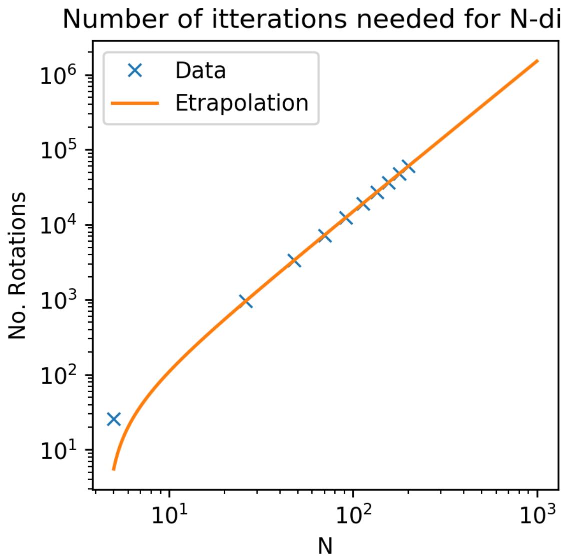
This is an abstract



Jacobi Eigenvalue Algorithm

```
τ = (a_ll − a_kk) / (2 a_kl)

if τ ≥ 0:
    t = 1 / (τ + sqrt(1 + τ^2))
else:
    t = −1 / (−τ + sqrt(1 + τ^2))

c = 1 / sqrt(1 + t^2)
s = tc

a'_kk = a_kk
a'_ll = a_ll

a_kk = c^2 * a'_kk − 2cs * a_kl + s^2 * a'_ll
a_ll = s^2 * a'_kk + 2cs * a_kl + c^2 * a'_ll
a_kl = 0.0
a_lk = 0.0

for i = 1, 2, ... N:
    if i ≠ k and i ≠ l:
        a_ik = a_ik
        a_il = a_il
        a_ik = c * a_ik − s * a_il
        a_ki = a_ik
        a_il = c * a_il + s * a_ik
        a_li = a_il
```

INTRODUCTION

Preservation of scalar product & orthogonality in unitary transformations

Consider an orthonormal set of basis vectors $\mathbf{v}_i$ such that $\mathbf{v}_j^T\mathbf{v}_i = \delta_{ij}$. Let unitary matrix U where $U^TU = I_N$, where I_N denotes the $N \times N$ identity matrix, operate on $\mathbf{v}_i$ to get $\mathbf{w}_i$

$$\mathbf{w}_i = U\mathbf{v}_i \tag{1}$$

Then

$$\mathbf{w}_j^T\mathbf{w}_i = (U\mathbf{v}_j)^T U\mathbf{v}_i = \mathbf{v}_j^T U^T U\mathbf{v}_i = \mathbf{v}_j^T\mathbf{v}_i = \delta_{ij} \tag{2}$$

In the unitary transformation of $\mathbf{v}_i$ both the scalar product and orthogonality has been preserved.

THEORY, ALGORITHMS AND METHODS

RESULTS AND DISCUSSIONS

CONCLUSIONS

[1] M. Hjorth-Jensen, Computational Physics - Lecture Notes 2015, (2015).