Matrix Correlation Optimization

Assignment Group 2

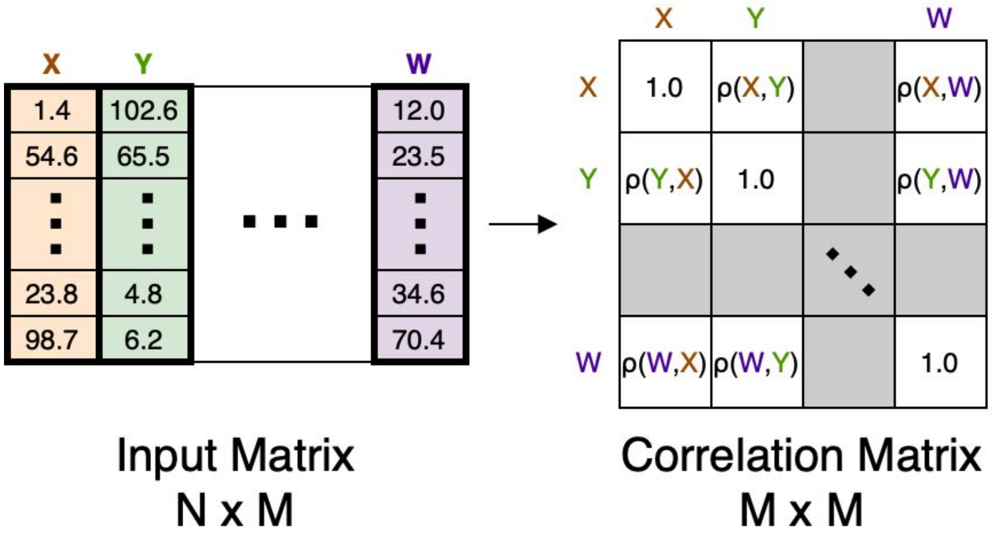
Denny Ciccia, Francesco Mecatti, Nicola Morelli

Problem: Compute the Correlation Matrix

Calculation of the **correlation matrix** of a given sequence of column vectors, denoted X, Y, ..., W in the below image.

Correlation matrix = **square** matrix that contains the **correlation coefficient** between column X and Y at the **intersection** of row X and column Y.

The correlation matrix is an **upper triangular** matrix, the lower triangle (or vice versa) carries **duplicate information**.

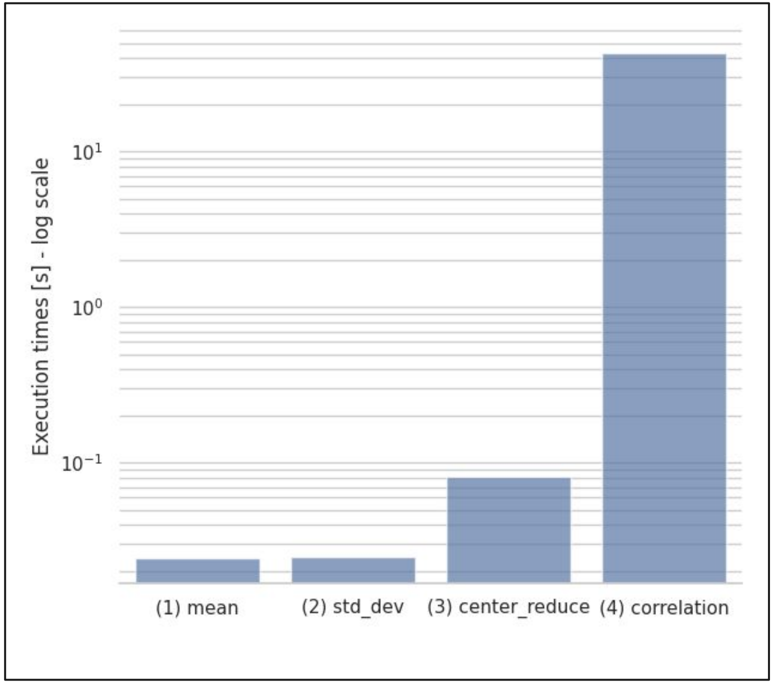


Starting Point

$$\rho_{X,Y} = \frac{\mathrm{cov}(X,Y)}{\sigma_X \sigma_Y} = \sum_{i=1}^{N} \frac{(X_i - \bar{X})}{\sigma_X \sqrt{N}} \frac{(Y_i - \bar{Y})}{\sigma_Y \sqrt{N}}$$

The formula is implemented according to this algorithm:

1. compute **mean** for each column vector
2. compute **std. dev.** for each column vector
3. **center and reduce** each column vector
4. compute **correlation** coefficients between each pair of column vectors



Data collected with `gprof` on **large** dataset

Loop Interchange

```
for (size_t j1 = 0; j1 < _PB_M - 1; j1++) {
  symmat[j1][j1] = 1.0;

  for (size_t j2 = j1 + 1; j2 < _PB_M; j2++) {
    symmat[j1][j2] = 0.0;

    for (size_t i = 0; i < _PB_N; i++)
      symmat[j1][j2] += (data[i][j1] * data[i][j2]);

    symmat[j2][j1] = symmat[j1][j2];
  }
}
```

```
for (size_t j1 = 0; j1 < _PB_M - 1; j1++)
  for (size_t j2 = j1 + 1; j2 < _PB_M; j2++)
    symmat[j1][j2] = 0.0;

for (size_t i = 0; i < _PB_N; i++) {
  for (size_t j1 = 0; j1 < _PB_M - 1; j1++) {
    symmat[j1][j1] = 1.0;

    for (size_t j2 = j1 + 1; j2 < _PB_M; j2++)
      symmat[j1][j2] += (data[i][j1] * data[i][j2]);
  }
}

for (size_t j1 = 0; j1 < _PB_M - 1; j1++)
  for (size_t j2 = j1 + 1; j2 < _PB_M; j2++)
    symmat[j2][j1] = symmat[j1][j2];
```

```
Performance counter stats for './correlation_acc':

    7.494.184.899      cycles
    3.706.045.620      instructions              #    0,49  insn per cycle
      999.027.913      cache-misses

      5,003132178 seconds time elapsed
```

```
Performance counter stats for './correlation_acc':

    2.287.939.837      cycles
    4.200.460.190      instructions              #    1,84  insn per cycle
       39.891.848      cache-misses

      1,482564826 seconds time elapsed
```

Improved **spatial locality** by turning column-major order into a **row-major order** according to the cache layout, which resulted in **25 times less** cache **misses**.

Parallel for

Parallelization on **host cores** combined with **SIMD** instructions showed to be the best-performing approach.

Code organized in such a way that **race conditions** are **prevented** without synchronization mechanisms.

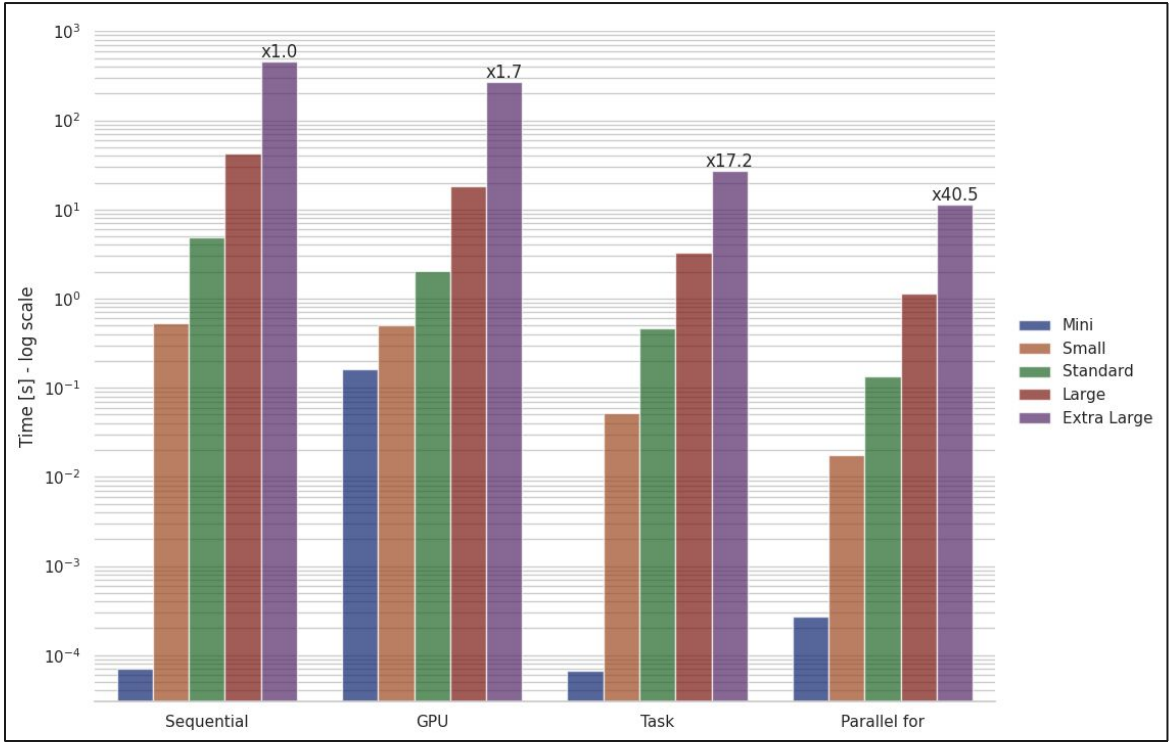
Explicit **loop unrolling** increases work for each iteration, **amortizing** thread **activation cost**.

```
#pragma omp parallel for
for (size_t j1 = 0; j1 < _PB_M - 1; j1++) {
  symmat[j1][j1] = 1.0;

  for (size_t j2 = j1 + 1; j2 < _PB_M; j2++)
    symmat[j1][j2] = 0.0;
}

int unroll_size_ = 4;
int blocks = _PB_N / unroll_size_;

for (size_t i = 0; i < blocks; i += 1) {

  #pragma omp parallel for schedule(dynamic)
  for (size_t j1 = 0; j1 < _PB_M - 1; j1++) {

    #pragma omp simd
    for (size_t j2 = j1 + 1; j2 < _PB_M; j2++) {
      size_t idx = i * unroll_size_;
      symmat[j1][j2] += (data[idx][j1] * data[idx][j2]);
      symmat[j1][j2] += (data[idx + 1][j1] * data[idx + 1][j2]);
      symmat[j1][j2] += (data[idx + 2][j1] * data[idx + 2][j2]);
      symmat[j1][j2] += (data[idx + 3][j1] * data[idx + 3][j2]);
    }
  }
}

for (size_t i = unroll_size_ * blocks; i < _PB_N; i++)
  for (size_t j1 = 0; j1 < _PB_M - 1; j1++)
    for (size_t j2 = j1 + 1; j2 < _PB_M; j2++)
      symmat[j1][j2] += (data[i][j1] * data[i][j2]);

#pragma omp parallel for
for (size_t j1 = 0; j1 < _PB_M - 1; j1++) {
  #pragma omp simd
  for (size_t j2 = j1 + 1; j2 < _PB_M; j2++) {
    symmat[j2][j1] = symmat[j1][j2];
  }
}
```

Execution times and speedups

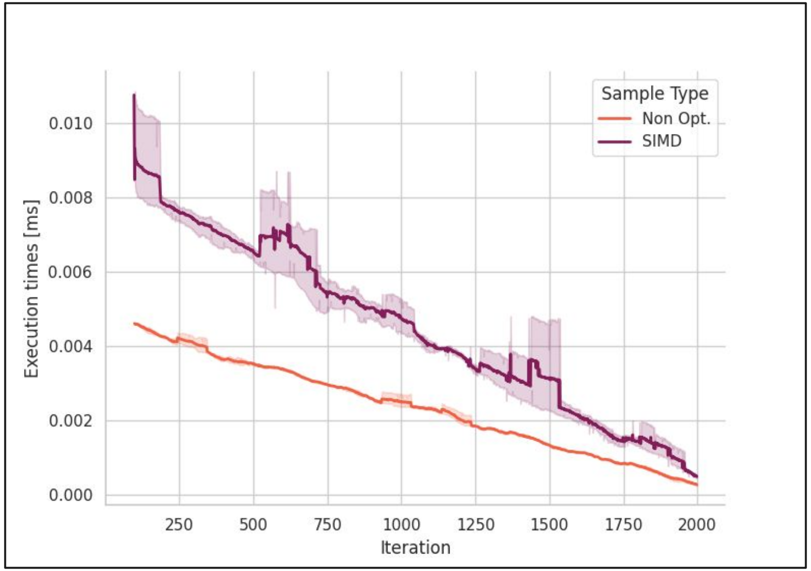
Alternative **approaches** based on **tasks** and **GPU offloading** tested but led to minor speedups.

The baseline on the graph refers to a **sequential** execution with **loop interchange** transformation applied, which is **4.5 times faster** than **original** sequential code.



Execution times of **four** different **approaches** have been profiled for **each dataset size**.

Final Considerations



Innermost loops exec. time vs outermost iteration @ large dataset

(1) **Dynamic scheduling** works better than static one since **workload varies** across **iterations**.
(2) **GPU** offloading **underperforms** due to the **memory copyin/copyout** between host and target, given than **OpenMP** does **not exploit** Ampere's **unified memory** architecture. In our case, memory copy is a huge overhead compared to the much smaller computation time.