Vectorized Code

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Code Vectorization

- R comes with many efficient operations that applies on vectors/matrices directly.
    - These operations will be translated into SIMD instructions to accelerate computation.
- Code using vector operations/functions instead of scalar operations and `for` loops is called **vectorized code**.
- Vectorized R code runs significantly faster than non-vectorized R code.

Different Levels of Vectorization

Vectorization can happen at different "levels". Let us demonstrate this using the matrix multiplication.

Different Levels of Vectorization

- Non-vectorized matrix multiplication in R using scalar operations only

```
matmul1 <- function(A,B){
    # Create a zero matrix C
    C <- matrix(0, nrow = dim(A)[1], ncol = dim(B)[2])
    # Loop over rows of A
    for (i in 1:dim(A)[1]){
        # Loop over cols of B
        for (j in 1:dim(B)[2]){
            # Loop over cols of A
            for (k in 1:dim(A)[2]){
            C[i,j] <- C[i,j] + A[i,k]*B[k,j]
            }
        }
    }
    return(C)
}
```

Different Levels of Vectorization

- Using vector ops to replace the inner most `for` loop.

```
matmul2 <- function(A,B){
    # Create a zero matrix C
    C <- matrix(0, nrow = dim(A)[1], ncol = dim(B)[2])
    # Loop over rows of A
    for (i in 1:dim(A)[1]){
        # Loop over rows of B
        for (j in 1:dim(B)[2]){
        C[i,j] <- A[i,] %*% B[, j]
        }
    }
    return(C)
}
```

  - $C_{i,j} = A_{[i,\cdot]} \cdot B_{[\cdot,j]}$

Different Levels of Vectorization

- Using vector ops to replace the **two** innermost `for` loop.

```
matmul3 <- function(A,B){
    # Create a zero matrix C
    C <- matrix(0, nrow = dim(A)[1], ncol = dim(B)[2])
    # Loop over rows of A
    for (i in 1:dim(A)[1]){
        C[i, ] <- A[i, ]%*%B
    }
    return(C)
}
```

  - $C_{[i,\cdot]} = A_{[i,\cdot]} \cdot B$

Different Levels of Vectorization

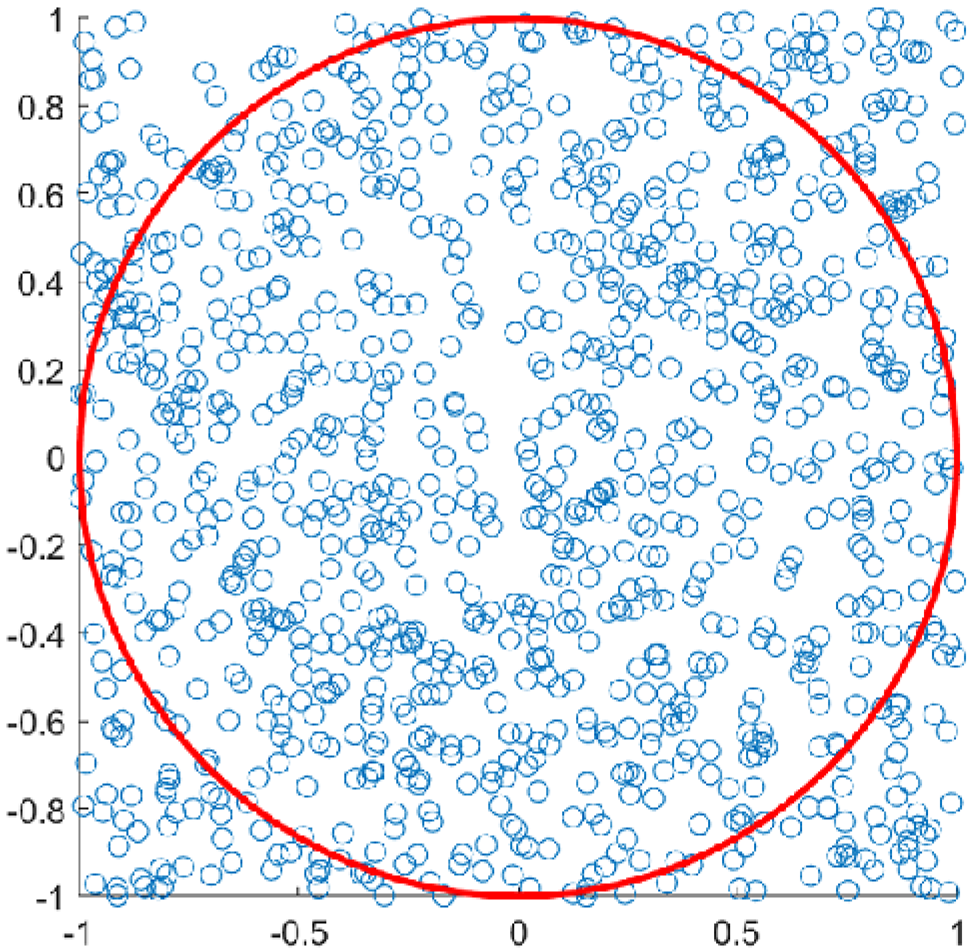
- Using built-in R `%*%` function with no `for` loop: `A%*%B`

Performance of Vectorized Code

- Let us test the performance of these implementations on 500 by 500 matrices.
    - 3 for loops: 15 sec.
    - 2 for loops: 2 sec.
    - 1 for loop: 0.2 sec.
    - no for loop: .08 sec.
- **Each time you eliminate a `for` loop in your code, your program gets a performance boost.**

Calculating π using Monte Carlo

- sample uniformly in the box $[-1, 1]^2$
- $\pi \approx$ #samples in circle/#samples * 4



Non-vectorized Code

```
dist <- function(a,b){
  return(sqrt(sum((a-b)^2)))
}

n <- 1000000
#generating n*2 samples from unif(-1,1)
x <- runif(n*2, -1, 1)
#create an n by 2 matrix from x
X <- matrix(x, nrow=n)

count <-0
for (i in 1:n){
  # using a for loop to count samples inside circle
  if (dist(X[i,],0) < 1){
    count <- count + 1
  }
}

print(count/n * 4) # print pi estimation
```

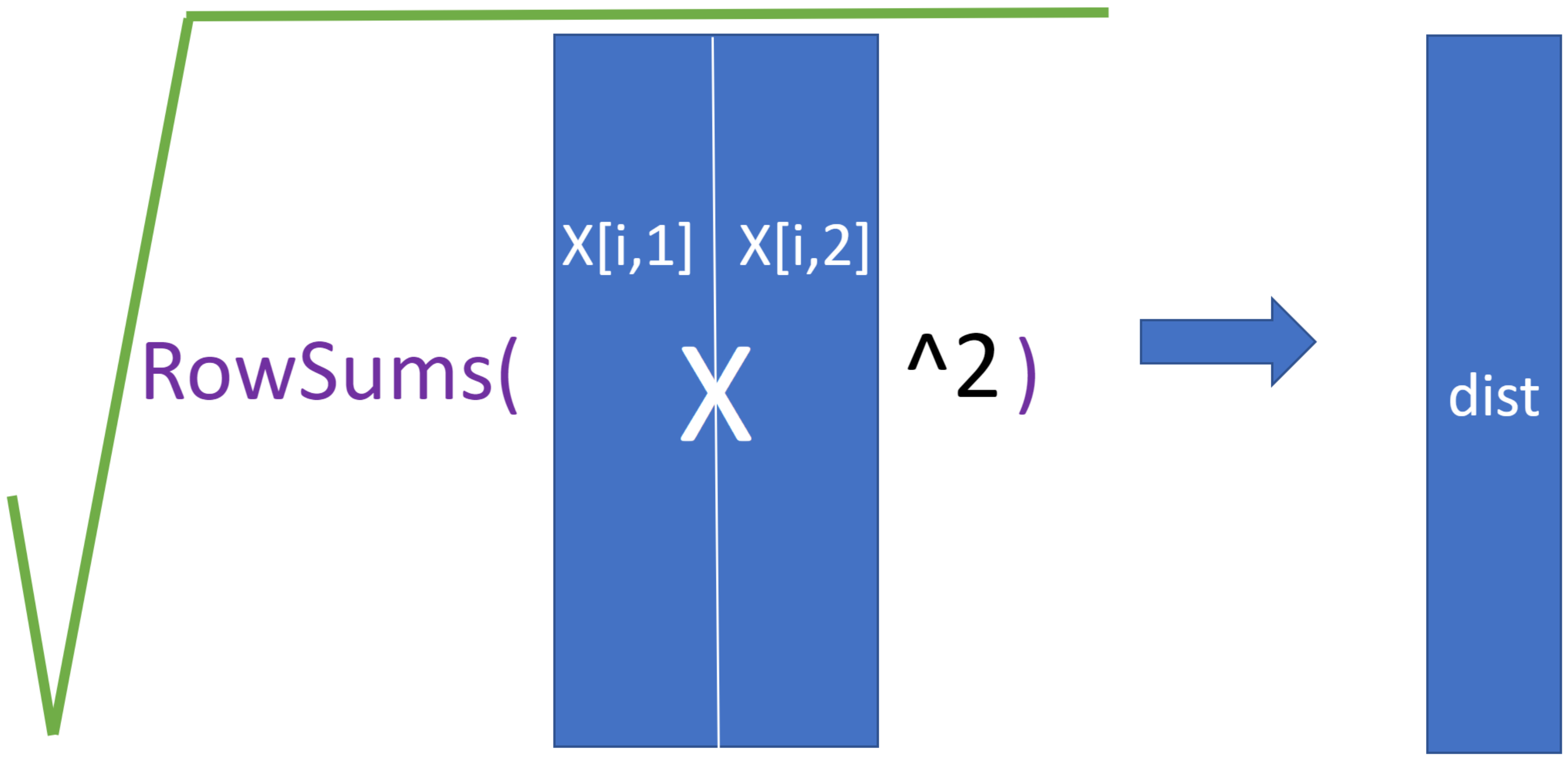
Vectorized Code

```
n <- 1000000
#generating n*2 samples from unif(-1,1)
x <- runif(n*2, -1, 1)
#create an n by 2 matrix from x
X <- matrix(x, nrow=n)

dist <- sqrt(rowSums((X - 0)^2))
count <- length(dist[dist < 1])

print(count/n * 4) # print pi estimation
```

- `rowSums` sums over rows of a matrix.

Vectorized Code

`dist <- sqrt(rowSums((X - 0)^2))` does the following



- The vectorized code is about 50 times faster than its non-vectorized counterpart.

Conclusion

- Using vector/matrix operators instead of scalar operators will significantly increase the efficiency of your R code.
- Do not use `for` loop in R unless you absolutely have to.
- In exams, pay attention to the question and see whether it permits vectorized code or not.

Homework 1: Generating Dummy Data

1. Create **two 500 by 784 matrices** filled with random observations from a **standard** normal distribution.
    - Hint: `rnorm(n,mean,std)` produces a **vector** of size `n` filled with samples from a normal distribution with `mean` as mean and `std` as standard deviation.

Homework 2: Scalar Compute

2. Write a function called `pdist1` takes two matrices A, B as inputs, and outputs a matrix D, where $D_{i,j} = \text{dist}(A_{[i,]}, B_{[j,]})$ and $\text{dist}(a, b)$ is the Euclidean distance between two vectors a, b.
   - This is the Part II of TB1 project.
   - Your code should have **3 for loops**, in other words, you should write non-vectorized code.
   - Test the function on matrices generated in step 1.

Homework 2 (submit): Vectorization

3. Write another function called `pdist2`, that does exactly the same thing, using only **two for loops**.
    - Hint, use the `dist` function you wrote in the last week's lab to help you.
4. Write another function called `pdist3`, that does exactly the same thing, using **only one for loop**.
    - Hint, to compute the i-th row in D, first compute three terms: `sum(A[i,]^2)`, `rowSums(B^2)` and `A[i,]%*%t(B)`.
    - Combine them to get the i-th row of D.

Homework 3 (Challenge): Vectoriz.

5. Write another function called `pdist4`, that does exactly the same thing **without using any for loop**.
    - Do not use any built-in function other than `sum` and `rowSums`.
    - Express D by matrix algebra using A and B.
        - $D = \sqrt{a\mathbf{1}_b^\top + \mathbf{1}_a b^\top - 2AB^\top}$,
        - where `a := rowsum(A^2)`, $\mathbf{1}_a$ is a all-one column vector with `dim(A)[1]` elements.
    - Hint: `matrix(k, nrow = M, ncol =N)` will create an `M` by `N` matrix filled with value `k`.
    - Hint: `rowSums` will convert your matrix into a vector. To perform matrix algebra, you need to convert it back to a matrix using `matrix` command.

Homework 3 (Challenge): Vectoriz.

6. Test all above functions using the matrices you generated in the first step. How long does it take them to run?