

Optimizing random walks

Victor Eijkhout, Susan Lindsey

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1. Malaria

- A mosquito flies in a straight line for some unit time,
- then it turns in a random direction.
- How far does it get in N time intervals?
- Answer: about \sqrt{N} .

2.

Code:

```
float avg_dist{0.f};  
for ( int x=0; x<experiments; x++ ) {  
    Mosquito m(dim);  
    for (int step=0; step<steps; step++)  
        m.step();  
    avg_dist += m.distance();  
}  
avg_dist /= experiments;
```

Output

[rand] vec:

```
D=3 after 10000  
      steps, distance=  
      83.7997  
D=3 after 100000  
      steps, distance=  
      224.372  
D=3 after 1000000  
      steps, distance=  
      922.599  
product took: 2776  
      milliseconds
```

3.

```
class Mosquito {  
private:  
    vector<float> pos;  
public:  
    Mosquito( int d )  
        : pos( vector<float>(d,0.f) ) { };
```

4.

```
void step() {  
    int d = pos.size();  
    auto incr = random_step(d);  
    for (int id=0; id<d; id++)  
        pos.at(id) += incr.at(id);  
};
```

5.

```
vector<float> random_coordinate( int d ) {  
    auto v = vector<float>(d);  
    for ( auto& e : v )  
        e = random_float();  
    return v;  
};
```

6.

```
vector<float> random_step(int d) {  
    for (;;) {  
        auto step = random_coordinate(d);  
        if ( auto l=length(step); l<=1.f ) {  
            if ( l==0.f ) {  
                /*  
                 * Zero lengths can conceivably happen for d==1  
                 * but should not for higher d.  
                 */  
                assert(d==1);  
            } else {  
                normalize(step,l);  
                return step;  
            }  
        }  
    }  
};
```

7. exercise

Take the basic code, and make a version based on

```
template<int d>  
class Mosquito { /* ... */
```

How much does this simplify your code? Do you get any performance improvement?

You can base this off the file `walk_vec.cxx` in the repository

8.

So we move the creation of the vectors outside of the computational routines. The random coordinates are now written into an array passed as parameter:

```
void random_coordinate( vector<float>& v ) {  
    for ( auto& e : v )  
        e = random_float();  
};
```

9.

Likewise the random step:

```
void random_step( vector<float>& step ) {  
    for (;;) {  
        random_coordinate(step);  
    }
```

10.

This process of passing the arrays in stops at the *step* method, which we want to keep parameterless. So we add an option *cache* to the constructor to store the step vector as well as the position:

Code:

```
class Mosquito {  
private:  
    vector<float> pos;  
    vector<float> inc;  
    bool cache;  
public:  
    Mosquito( int d,bool cache=false )  
        : pos( vector<float>(d,0.f)  
            ),cache(cache) {  
        if (cache) inc =  
            vector<float>(d,0.f);  
    };
```

Output

[rand] pass:

D=3 after 10000
steps, distance=
76.7711

D=3 after 100000
steps, distance=
257.19

D=3 after 1000000
steps, distance=
956.122

run took: 2852
milliseconds

D=3 after 10000
steps, distance=
87.034

11.

```
void step() {  
    int d = pos.size();  
    if (cache) {  
        random_step(inc);  
        step( inc );  
    } else {  
        vector<float> incr(d);  
        random_step(incr);  
        step( incr );  
    }  
};
```

12. Sum of squares

There is still a problem with the *length* calculation. Since there is no reduction operator for 'sum of squares', we need to create a temporary vector for the squares,
(or do we?)
so that we can do a plus-reduction on it.

13. Exercise

Explore options for this temporary. Discuss what's most elegant, and measure performance improvement.

- This temporary can be passed in as a parameter;
- it can be stored in a global variable;
- or we can declare it `static`.
- With the C++20 standard, you could also use the `ranges` header.

14.

```
float length( const vector<float>& step ) {  
    vector<float> square;  
    int s = step.size();  
    if (square.size() != s) square.resize(s);  
    for ( int i=0; i<s; i++) square[i] = step[i];  
    for_each( square.begin(), square.end(),  
              [] (float& x) { x *= x; } );  
    auto l = sqrt  
        ( accumulate( square.begin(), square.end(), 0.f ) );  
    return l;  
};
```

15.

```
template<int d>
float length( const array<float,d>& step ) {
    array<float,d> square = step;
    for_each( square.begin(),square.end(),
              [] (float& x) { x *= x; } );
    auto l = sqrt
        ( std::accumulate( square.begin(),square.end(),0.f ) );
    return l;
};
```


16. Optimization

While above we have removed all unnecessary allocation, we get an extra performance boost from optimizations from the compiler knowing the length of the array. Thus, instead of a loop of length two, the compiler will probably replace this by two explicit instructions.

17.

Code:

```
float avg_dist{0.f};  
for ( int x=0; x<experiments; x++ ) {  
    Mosquito<dim> m;  
    for (int step=0; step<steps; step++)  
        m.step();  
    avg_dist += m.distance();  
}  
avg_dist /= experiments;
```

Output

[rand] arr:

```
D=3 after 10000  
      steps, distance=  
      76.3221  
D=3 after 100000  
      steps, distance=  
      247.5  
D=3 after 1000000  
      steps, distance=  
      959.735  
product took: 358  
      milliseconds
```