# Iterators and ranges for numerical problems


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# Outline

# Motivation

Problem: Find the root of a function $\quad 0 = f(x)$

Newtons algorithm: $\quad x_{n+1} = x_n - f(x)/f'(x)$

```
auto newton( auto x , auto f , auto df ) {
    while( std::abs( f(x) ) > 1.0e-12 )
        x = x - f(x) / df( x );
    return x;
}
// ...
double root = newton( x , f , df );
```

# Motivation

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    while( std::abs( f(x) ) > 1.0e-12 )
        x = x - f(x) / df( x );
    return x;
}
// ...
double root = newton( x , f , df );
```

Idea: Return a range

```
auto newton( auto x , auto f , auto df ) { ... }
// ...
auto range = newton( x , f , df );
for( auto x : range ) cout << x << endl;
cout << "Final value: " << range.value() << endl;
```

# Motivation

Use iterators and ranges for three problems:

- Numerical Sequences
- Dynamical systems
- Convergence algorithms

The range is here a proxy for the algorithm!

The user can look inside the algorithm!
$\longrightarrow$ Debugging, logging, combine with other algorithms, ...

# Iterators – Overview

Operations

- Increment, dereference, assign, copy, decrement, ...

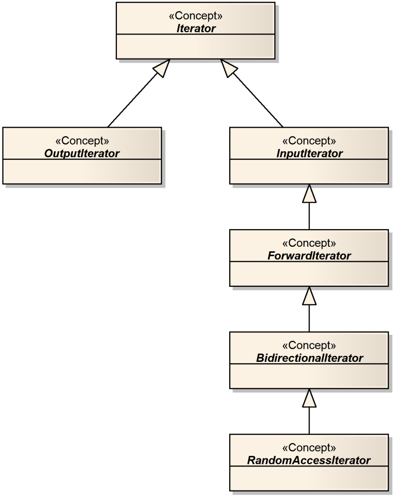
Use cases

- Traverse containers, IO, expressing algorithms

Special iterators

- `zip_iterator`, `transform_iterator`, ...

# Iterator concepts



# Ranges

- Simplification and generalization of iterators
- Ranges in boost:
  - Ranges are pairs of iterators.
  - Ranges can be adapted/decorated.

```
vector< double > values;
// fill values
boost::for_each( values , []( auto x ) {
    cout << x << endl; } );
```

Operations on ranges:

```
range_t r;
using iterator = boost::range_iterator< range_t >::type;
auto begin = boost::begin( r ); // begin iterator
auto end = boost::end( r );     // end iterator
```

# Ranges for the C++ standard library

Eric Niebler: N4128: Ranges for the Standard Library.

- Ranges are based on iterators
- New concepts:
  - Iterable – Container, holding the elements
  - Range – Lightweight adapters (decorators)
- Three kinds of ranges
  - Iterator pairs, Iterator and a count, Iterator and a predicate
- Variants of each algorithm
  - sort( in.begin() , in.end() );
  - sort( in );
  - in | view::transform( op );
  - in | cont::sort( op );

# Numerical sequences

# Numerical sequences

In numerical algorithms one needs often sequences of numerical values

- As part of an algorithm
- Reference data
- Test data

Example: Sampled function $f(x)$

$$t_n = 0.1n \qquad \text{(Sampling)}$$

$$x_n = \sin(2t_n) + 0.1 \qquad \text{(Numerical sequence – sampled function)}$$

# Numerical sequences

## Range of integers

```
int n = 1024;
auto seq = boost::counting_range( 0 , n );
for( auto x : seq )
    cout << x << " ";
```

## Output

```
0 1 2 3 ...
```

# Numerical sequences

## Sampling

```
using namespace boost::adaptors;

auto seq = boost::counting_range( 0 , n );
auto seq2 = seq | transformed( []( auto x ) {
    return 0.1 * static_cast< double >( x ); } );

for( auto x : seq2 )
    cout << x << " ";
```

## Output

```
0 0.1 0.2 0.3 ...
```

# Numerical sequences

## Sampled function

```
auto seq = boost::counting_range( 0 , n );
auto seq2 = seq | transformed( []( auto x ) {
    return 0.01 * static_cast< double >( x ); } );
auto seq3 = seq2 | transformed( []( auto x ) {
    return sin( 2.0 * x ) + 0.1; } );

for( auto x : seq3 )
    cout << x << " ";
```

## Output

```
0.1 0.298669 0.489418 0.664642 ...
```

# Numerical sequences

## Use a function

```
auto sequence( int n , double sampling , auto f ) {
    auto seq = boost::counting_range( 0 , n );
    return seq | transformed( [sampling,f]( auto x ) {
        return f(sampling*static_cast<double>( x ) ); } );
}

auto seq = sequence(1024 ,0.1 ,[]( auto x ) {
    return sin(2.0*x)+0.1;} );
for( auto x : seq )
    cout << x << " ";
```

## Output

```
0.1 0.298669 0.489418 0.664642 ...
```

# Numerical ranges and standard C++ ranges

## Infinite sequences:

```
using std::view;
auto sequence( double sampling , auto f ) {
    return iota(0) | transform( [sampling,f]( auto x ) {
        return f( sampling * x ); } );
}

for( auto x : take( sequence( 0.1 , f ) , 10 ) )
    cout << x << endl;
```

## Custom break conditions:

```
auto seq = take_while( sequence( 0.1 , f ) , []( auto x ) {
    return x < 1.0; } );
for( auto x : seq )
    cout << x << endl;
```

# Numerical Ranges and standard C++ ranges

Zipped sequences:

```
using std::view;
auto seq1 = sequence( 1024 , 0.01 , f1 );
auto seq2 = sequence( 1024 , 0.01 , f2 );
auto seq3 = zip( seq1 , seq2 );
for( auto x : seq3 )
    cout << std::get<0>(x) << " "<< std::get<1>(x) << "\n";
```

Joined sequences:

```
auto seq3 = join( seq1 , seq2 );
```

Cartesian sequences – missing yet

# Dynamical systems

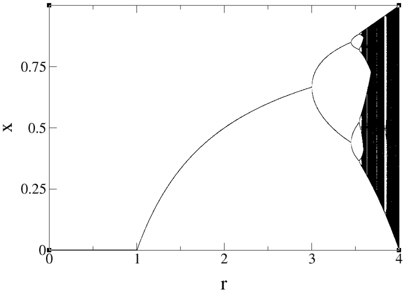
# Dynamical systems – Maps

Map – time discrete dynamical system:

$$x_{n+1} = f(x_n)$$

Example: Logistic map

$$x_{n+1} = r\, x_n(1 - x_n)$$



# Map range

Abstraction for $x_{n+1} = f(x_n)$

Two versions:

1. `map_range` - stop predicate
2. `counted_map_range` - iterates *n*-times

# Map range

```
template< typename T , typename F , typename C >
class map_range
{
    struct iterator { ... };

  public:
    map_range( T value , F func , C condition )
    : m_value { std::move( value ) }
    , m_func { std::move( func ) }
    , m_condition( condition )
    {}

    iterator begin() const { return iterator( this ); }
    iterator end() const { return iterator( nullptr ); }

private:
    mutable T m_value;
    mutable F m_func;
    C m_condition;
};
```

# Map range

```
struct iterator {
    iterator( map_range const* _r ) : r( _r ) {}

    iterator& operator++() {
        r->m_value = r->m_func( r->m_value );
        if( r->m_condition( r->m_value ) ) {
            r = nullptr;
        }
        return *this;
    }

    T& operator*() const {
        return r->m_value; }
    bool operator==( iterator const& o ) const {
        return ( r == o.r ); }
    bool operator!=( iterator const& o ) const {
        return ! ( *this == o );
    }

    map_range const* r;
};
```

# Factory functions

```
template< typename T , typename F , typename C >
auto make_map_range( T t , F f , C condition )
{
    return map_range< T , F , C >(
        std::move( t ) ,
        std::move( f ) ,
        std::move( condition ) );
}
```

```
template< typename T , typename F >
auto make_counted_map_range( T t , F f , size_t
    max_iterations )
{
    return counted_map_range< T , F >(
        std::move( t ) ,
        std::move( f ) ,
        max_iterations );
}
```

# Example - logistic map

```
double r = 3.2;
auto l = [r]( auto x ) {return r * x * ( 1.0 - x ); };

auto range = make_counted_map_range( 0.5 , l , 1000 );
for( auto x : range )
{
    cout << x << endl;
}
```

# Dynamical system – cellular automaton

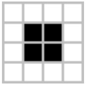
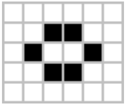
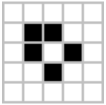
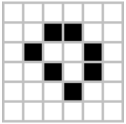
Cellular automaton: Time-discrete and value-discrete

Conway's Game of Life

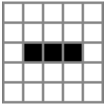
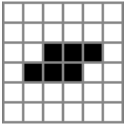
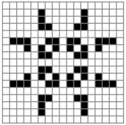
- Each cell has two states: *alive* or *dead*
- Transition rules
  - Less then two neighbors -> dead (under-population)
  - Two or three neighbors -> alive
  - More then three neighbors -> dead (over-population)
  - Dead cell with three neighbors -> alive (reproduction)

# Game of life – patterns

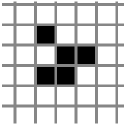
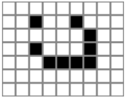
Still lifes:

Oscillators:

Spaceships:

Game of life can implement a Touring machine :)

# Conway’s game of life

```
using board = vector< vector< bool > >;

auto show_board = []( board const& b ) { ... }
auto next_board = []( board const& b ) -> board { ... }

board b;
// initialize b

auto r = make_counted_map_range( b , next_board , 1000 );
for( auto b : r )
{
    show_board( b );
}
```

# Map range for time discrete dynamical systems

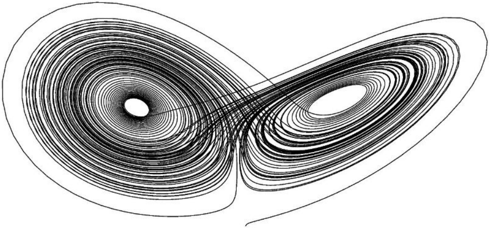
- The range is a proxy for the dynamical system
  - Customizable iteration body
  - Custom stopping criterions
  - *N*-times iteration
- Not optimized - a custom range could be optimized

# Dynamical systems – ODEs

$$\frac{\mathrm{d}x}{\mathrm{d}t} = f(x, t)$$

Example: Lorenz attractor

$$\dot{x} = \sigma(y - x) \quad , \quad \dot{y} = x(\rho - z) - y \quad , \quad \dot{z} = xy - \beta z$$



Numerical solution: $x(t + \Delta t) = F(x(t))$

# Example – ODE solver

Solve $\dot{x} = f(x,t)$, Solver $F : x(t+\delta t) = F(x(t))$
Example Boost.Odeint:

```
namespace odeint = boost::numeric::odeint;

auto lorenz = []( auto const& x , auto& dxdt , auto t )
{
    dxdt[0] = 10.0 * ( x[1] - x[0] );
    dxdt[1] = 28.0 * x[0] - x[1] - x[0] * x[2];
    dxdt[2] = -8.0 / 3.0 * x[2] + x[0] * x[1];
};

using state_type = std::array< double , 3 >;
odeint::runge_kutta4< state_type > stepper;

state_type x {{ 10.0 , 10.0 , 10.0 }};
double t = 0.0 , dt = 0.01;
stepper.do_step( lorenz , x , t , dt );
t += dt;
```

Integrate functions:

```
auto obs = []( auto x , auto t ) { std::cout << t << " " << x[0] << "\n"; };
odeint::integrate_const( stepper , lorenz , x , 0.0 , 10.0 , dt , obs );
```

# Example – ODE solver

```
auto make_ode_range( auto sys , auto stepper , auto x ,
    auto t0 , auto dt , auto t1 )
{
    auto solve = [sys,stepper,dt]( auto x ) mutable {
        stepper.do_step( sys , x.first , x.second , dt );
        x.second += dt;
        return x; };
    auto cond = [t1]( auto const& x ) { return x.second > t1; };
    auto range = make_map_range( std::make_pair(x,t0) , solver , cond );
    return range;
}
```

Can be used as

```
state_type x {{ 10.0 , 10.0 , 10.0 }};
stepper_type stepper;
auto range = make_ode_range( lorenz , stepper , x , 0.0 , 0.1 , 100.0 );

for( auto r : range )
    std::cout << r.second << " " << r.first[0] << " " << r.first[1] << "\n";
```

# ODE ranges

Superior to integrate functions:

- Break conditions are easy
- ODE-Ranges can be used in a natural C++ way, `find`, `transform` , etc.

Map implementation has drawbacks -> custom implementation

- Better performance.
- Step size control – complicated iteration.
- Break condition can use the last two values.

# Convergence methods

# Newton method

Find the root: $0 = f(x)$

Newtons method

- Choose $x_0$
- Iterate $x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$

# Newton method – Implementation

```
auto newton_range(
    auto x , auto f , auto df ,
    auto break_condition )
{
    return make_map_range(
        x ,
        [f,df]( auto x ) { return x - f( x ) / df( x ); } ,
        break_condition );
}
```

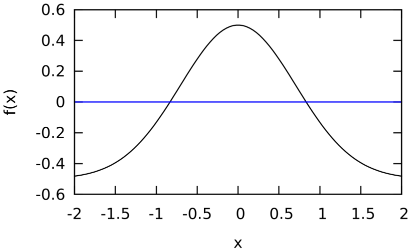
# Newton method – Example

Solve $\exp(-x^2) - 0.5 = 0$

```
auto f = []( auto x ) { return exp(-x*x) - 0.5; };
auto df = []( auto x ) { return -2.0*x * exp(-x*x); };
auto cond  = [f]( auto x ) {
    return std::abs(f(x)) < 1.0e-12; };

auto range = newton_range( 1.0 , f , df , cond );

for( auto r : range )
    std::cout << r << " : " << f( r ) << std::endl;
```



# Similar problems

- Optimizations methods
  - Broyden-Fletcher-Goldfarb-Shanno algorithm (BFGS)
  - Simulated annealing
  - Genetic algorithms
  - Genetic programming
  - ...
- Approximation of functions
- ...

# Conclusion

- Iterators and ranges can be used for numerical problems
  - Numerical sequences, dynamical systems, optimization methods, ...
- Range is a proxy for the algorithm
- Custom range implementation needed for optimal performance

Outlook – open points

- Break condition on last two values, e.g. $|v_k - v_{k-1}| < \epsilon$
- More complicated break condition,
  e.g. count and predicate

# References

- www.odeint.com
- github.com/headmyshoulder/iterator-talks
- github.com/headmyshoulder/map_iterator

# Backup

# Example – basic use

```
for( auto iter = values.begin() ;
     iter != values.end() ;
     ++iter )
{
    cout << *iter << endl;
}
```

# Example – basic use

```
for( auto iter = values.begin() ;
     iter != values.end() ;
     ++iter )
{
    cout << *iter << endl;
}
```

## C++11 - use range based for

```
for( auto v : values )
{
    cout << v << endl;
}
```

# Example – Container traversal

```
list< double > values;
list< double > values2( values.size() );
```

Can be used in

```
transform( values.begin() , values.end() ,
           values2.begin() ,
           []( double x ) {
               return x * 2.0; } );
```

# Example – Container traversal

```
vector< double > values;
vector< double > values2( values.size() );
```

Can be used in

```
transform( values.begin() , values.end() ,
           values2.begin() ,
           []( double x ) {
               return x * 2.0; } );
```

# Examples – IO

## Input

```
vector< double > values;
copy_if( istream_iterator< double >( cout ) ,
         istream_iterator< double >() ,
         back_inserter( values ) ,
         []( double x ) { return x > 0.0; } );
```

## Output

```
vector< double > values;
// fill values
copy_if( values.begin() , values.end() ,
         ostream_iterator< double >( std::cout , "\n" ) ,
         []( double x ) { return x > 0.0; } );
```

# Algorithms

I all_of
I any_of
I none_of
I for_each
I count
I count_if
I mismatch
I equal
I find
I find_if
I find_if_not
F find_end
I,F find_first_if
F adjacent_find
F search
F search_n
I,O copy
I,O copy_if
I,O copy_n
B,O copy_backward
I,O move
B,O move_backward
F fill
F fill_n
I,O transform
F generate
I generate_n

F remove
F remove_if
I,O remove_copy
I,O remove_copy_if
F replace
F replace_if
I,O replace_copy
I,O replace_copy_if
F swap_ranges
F iter_swap
B reverse
B,O reverse_copy
F rotate
F,O rotate_copy
R random_shuffle
R shuffle
F unique
I,O unique_copy

I is_partitioned
F,B partition
I,O partition_copy
B stable_partition
F partition_point
F is_sorted
F is_sorted_until
R sort
R partial_sort
I,R partial_sort_copy
R stable_sort
R nth_element

F lower_bound
F upper_bound
F binary_search
F equal_range
I,O merge
B inplace_merge
I includes
I,O set_difference
I,O set_intersection
I,O set_symmetric_difference
I,O set_unition

R is_heap
R is_heap_until
R make_heap
R push_heap
R pop_heap
R sort_heap

F max_element
F min_element
F minmax_element
I lexicographical_compare
F is_permutation
B next_permutation
B prev_permutation

F iota
I accumulate
I inner_product
I,O adjacent_difference
I,O partial_sum

# Examples – generalized iota

Generalized Iota:

```
size_t n = 10;
auto iota = make_counted_map_range( 1 , []( auto x ) {
    return x * 2; } , 10 );

std::vector< int > values;
boost::copy( iota_range , std::back_inserter( values ) );
for( auto i : values ) { cout << i << endl; }
```

# Examples – generalized iota

**Problem:** We can not easily generate a square iota:
$1, 4, 9, 16, 25, 36, ...$

# Examples – generalized iota

**Problem:** We can not easily generate a square iota:
$1, 4, 9, 16, 25, 36, ...$
Introduce a projected map range.

```
auto iota_range = make_projected_counted_map_range(
    1
    , []( auto x ) { return x+1 ; }
    , 11
    , []( auto x ) { return x*x; }
    );
for( auto i : iota_range ) { std::cout << i << std::endl; }
```

# Map range - applications

- Generalized iota
- Ordinary differential equations
- Maps (dynamical maps)
- Functional random number generators
- Opmization methods
  - Genetic algorithms, Simulated annealing, ...

# Map range - applications

- Generalized iota
- Ordinary differential equations
- Maps (dynamical maps)
- Converging algorithms
- Functional random number generators

# Iterators for GPUs algorithms

# High-level libraries for GPUs

- Thrust
- VexCL
- Boost.Compute
- ViennaCL
- Cuda-MTL

# Thrust

Thrust is STL-like library for Cuda – Based on iterators.

```
thrust::host_vector<int> h_vec( 1024 );
std::generate(h_vec.begin(), h_vec.end(), rand);

thrust::device_vector<int> d_vec = h_vec;
thrust::sort(d_vec.begin(), d_vec.end());

thrust::copy(d_vec.begin(), d_vec.end(), h_vec.begin());
```

# Iterators in Thrust

- `device_vector< T >::iterator`
- `host_vector< T >::iterator`
- Special (fancy) iterator
  - `zip_iterator`
  - `transform_iterator`
  - `permutation_iterator`
  - `constant_iterator`, `counting_iterator`, `discard_iterator`, `reverse_iterator`

Custom algorithms

# Special iterators for Thrust

Calculate the norm of a vector

$$||x|| = \sum_{i=1}^{N} x_i^2$$

```
thrust::device_vector< double > x;
// fill x

double n = thrust::reduce(x.begin(), x.end(), 0.0); // ?
```

# Special iterators for Thrust

Calculate the norm of a vector

$$||x|| = \sum_{i=1}^{N} x_i^2$$

```
thrust::device_vector< double > x;
// fill x

auto op = []( auto x , auto y ) { return x + y*y; };
double n = thrust::reduce(x.begin() ,x.end() ,0.0 ,op); //
    ?
```

# Special iterators for Thrust

Calculate the norm of a vector

$$||x|| = \sum_{i=1}^{N} x_i^2$$

```
thrust::device_vector< double > x;
// fill x

op = []( auto x ) { return x*x; };
double n = thrust::reduce(
    thrust::make_transform_iterator(x.begin(), op) ,
    thrust::make_transform_iterator(x.end(), op), 0.0);
    // correct
```

# SAXPY

$s = ax + y \qquad s, x, y \in \mathbb{R}^N,\ a \in \mathbb{R}$

# Special problems - and solutions

Bucket sort

# Solving an ensemble of low-dimensional ODEs

Lorenz example and ODEs