Object-Oriented Programming for Scientific Computing

Dynamic Polymorphism

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Objects of Derived Classes as Function Arguments

Objects of a derived class can be used in functions that expect objects of the base class, as was shown before, but

- only the part belonging to the base class is copied if the argument is passed call-by-value (slicing).
- only the part belonging to the base class will be accessible when the argument is passed by reference.

In particular: even if a function has been redefined in the derived class, it is always the function of the base class that will be called.

Problems with Inheritance

```cpp
#include <iostream>

class A
{
    public:
        int work(int a)
        {
            return(a);
        }
};

class B : public A
{
    public:
        int work(int a)
        {
            return(a*a);
        }
};

int doWork(A& object)
{
    return(object.work(2));
}
```

```cpp
int main()
{
    A objectA;
    B objectB;
    std::cout << objectA.work(2) << ", ";
    std::cout << objectB.work(2) << ", ";
    std::cout << doWork(objectA) << ", ";
    std::cout << doWork(objectB) << std::endl;
}
```

Output:

```
2, 4, 2, 2
```

Virtual Functions

```
#include <iostream>

class A
{
    public:
        virtual int work(int a)
        {
            return(a);
        }
};

class B : public A
{
    public:
        int work(int a)
        {
            return(a*a);
        }
};

int doWork(A& object)
{
    return(object.work(2));
}
```

```
int main()
{
    A objectA;
    B objectB;
    std::cout << objectA.work(2) << ", ";
    std::cout << objectB.work(2) << ", ";
    std::cout << doWork(objectA) << ", ";
    std::cout << doWork(objectB) << std::endl;
}
```

Output:
2, 4, 2, 4

Virtual Functions

This is known as polymorphism ("many shapes", "many forms"):

- When a function is declared as `virtual` in the base class, then the function of the derived class will be called for objects of the derived class, even if the method is called via a reference or a pointer with the type of the base class.
- Declaring the function as `virtual` in the derived class has no effect, but can serve as a reminder that polymorphism is used.
- The function definition in the derived class has to match that of the base class, otherwise the function is overloaded as usual.
- The return value of the method may differ if it is a class derived from the base class, e.g. for correct behavior of "virtual constructors" (later in lecture).

C++11: Override

- As mentioned above, if the function definition in the derived class doesn't exactly match the one of the base class, the function is simply overloaded.
- This is often the result of a typing error and not what was intended.
- Also writing `virtual` before the function in the derived class only has the consequence that this overloaded function is also virtual.
- C++11 provides the additional keyword `override`. If this is written after the function header in a derived class, then a compiler error will occur if the function doesn't redefine a virtual method of the base class.
- It's advised to use this keyword whenever possible.

```
class B : public A
{
    public:
        int work(int a) override
        {
            return(a*a);
        }
};
```

Virtual Functions and Scoping

When a method is selected by explicit specification of the namespace (scoping), then the corresponding variant is directly invoked without polymorphism.

```
int doWork(A& object)
{
    return(object.A::work(2));
}
```

creates the output

```
2, 4, 2, 2
```

This way, the behavior without `virtual` remains accessible for methods that have been defined `virtual`.

Typical Implementation of Dynamic Polymorphism

- To implement this kind of polymorphism, the compiler adds a *hidden pointer* to each object (the "virtual table pointer" or "vpointer"). This "vpointer" points to a global table (the "virtual table" or "vtable").
- The compiler generates a vtable for each class that contains at least one virtual function. The vtable itself has a pointer for each virtual function of the class.
- During a call to a virtual function, the runtime system accesses the code of the method using the vpointer of the object and then the function pointer in the vtable.
- The overhead in terms of memory consumption is therefore a pointer per object containing virtual methods, plus a pointer for each virtual method. The runtime overhead are two additional memory accesses (for the vpointer and the address of the method).
- Inlining is not possible with virtual methods (because the lines that would replace the function call depend on context).

Example: Typical Implementation

```cpp
class B1
{
public:
  void f0() {}
  virtual void f1() {}
  int int_in_b1;
};

class B2
{
public:
  virtual void f2() {}
  int int_in_b2;
};

class D : public B1, public B2
{
public:
  void d() {}
  void f2() {} // override B2::f2()
  int int_in_d;
};
```

Example memory layout for an object of type `D`:

```
d:
  +0: pointer to virtual method table
      of D (for B1)
  +4: value of int_in_b1
  +8: pointer to virtual method table
      of D (for B2)
 +12: value of int_in_b2
 +16: value of int_in_d

virtual method table of D (for B1):
  +0: B1::f1()  // B1::f1() is not overridden

virtual method table of D (for B2):
  +0: D::f2()   // B2::f2() is overridden
                   by D::f2()
```

Interface Base Classes

- The purpose of an interface base class (abstract base class, ABC) is to provide a common interface for derived classes.
- Interface base classes usually have no attributes (and contain no data).
- Methods of interface base classes are typically purely virtual, which means their functionality is only implemented in the derived classes. This is indicated by adding `= 0` after the function declaration.
- Classes that contain at least one purely virtual function are called abstract base classes. There is no way to create objects of such an ABC, but there may be references and pointers of this type (which then point to objects of a derived class).
- Objects of a derived class can only be created if *all* purely virtual functions of the base class have been implemented. This ensures that the class complies with the complete interface.

Interface Base Classes

Example for abstract base classes:

```
class AbstractBaseClass
{
    public:
        virtual int  functionA(double x) = 0;
        virtual void functionB(int y)    = 0;
        virtual ~AbstractBaseClass() // will be explained later
        {};
}

class DerivedClass : public AbstractBaseClass
{
    public:
        int  functionA(double x); // has to exist
        void functionB(int y);    // has to exist
}
```

Function Objects (Functors)

Definition:
A *function object* (functor) is an object which can be called like a function.[1]

- In C++ a function is of the form

  ```
  ReturnType foo(Type1 arg1, Type2 arg2);
  ```

- An object which defines the parenthesis operator `operator()` can be used as a function, e.g.

  ```
  class Foo
  {
    public:
      ReturnType operator()(Type1 arg1, Type2 arg2);
  };
  ```

[1] D. Vandevoorde, N. M. Josuttis: C++ Templates — The Complete Guide, p. 417

Benefits of Functors

Functors are more than just simple functions:

- Functors are “intelligent functions”, they can
  - provide other methods in addition to `operator()`
  - have an internal state
  - be pre-initialized
- Every functor has its own type
  - The functions (or function pointers to) `bool less(int,int)` and `bool greater(int,int)` would have the same type
  - The functors `class less` and `class greater` have different type

Internal state: can e.g. be used for caching of results or statistics

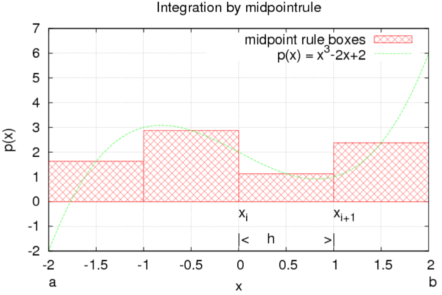
Type: simplifies function dispatch and treatment of special cases

Numerical Integration (Quadrature)

As an example of these concepts (dynamic polymorphism and functors) we want to implement a class for numerical integration of arbitrary functions with the composite midpoint rule.

$$\int_a^b f(x)dx \approx \sum_{i=0}^{n-1} f((i+\frac{1}{2})\cdot h)\cdot h$$

$$\text{with } h = \frac{b-a}{n}$$



Application of midpoint rule with $n = 4$ for $p(x) = x^3 - 2x + 2$.

Example: Numerical Integration of $\cos(x-1)$

The example program integrates $\cos(x-1)$ with the composite midpoint rule. The files used are:

- `functor.h`: contains the interface base class for a functor.
- `cosine.h`: contains the definition of a concrete functor: $\cos(ax+b)$
- `midpoint.h`: contains the definition of a function that takes a functor as argument and integrates it with the composite midpoint rule.
- `integration.cc`: contains the main program that uses the integrator to integrate $\cos(x-1)$ over the interval $[1 : \frac{\pi}{2}+1]$.

functor.h

```
#ifndef FUNCTORCLASS_H
#define FUNCTORCLASS_H

// Base class for arbitrary functions with one double parameter

class Functor
{
  public:
    virtual double operator()(double x) = 0;
    virtual ~Functor() // will be explained later
    {}

};

#endif
```

cosine.h

```
#ifndef COSINECLASS_H
#define COSINECLASS_H

#include <cmath>
#include "functor.h"

// realization of a function cos(a*x + b)
class Cosine : public Functor
{
  public:
    Cosine(double a_ = 1., double b_ = 0.) : a(a_), b(b_)
    {}

    double operator()(double x) override
    {
        return cos(a*x + b);
    }

  private:
    double a, b;
};

#endif
```

midpoint.h

```
#include "functor.h"

double MidpointRule(Functor& f, double a = 0.,
                    double b = 1., size_t n = 1000)
{
    double h = (b-a)/n; // length of a single interval

    // compute the integral boxes and sum them
    double result = 0.;
    for (size_t i = 0; i < n; ++i)
    {
        // evaluate function at midpoint and sum integral value
        result += f(a + (i + 0.5)*h);
    }

    return h*result;
}
```

integration.cc

```
// include system headers
#include <iostream>
// own headers
#include "midpoint.h"
#include "cosine.h"

int main()
{
  Cosine cosine(1.,-1.);
  std::cout << "Integral of cos(x-1) in "
            << "the interval [1 : pi/2+1] is "
            << MidpointRule(cosine,1.,M_PI_2+1.) << std::endl;

  return 0;
}
```

integrator.h

In an alternative implementation, it is also possible to generalize the integrator:

```
#ifndef INTEGRATORCLASS_H
#define INTEGRATORCLASS_H

#include "functor.h"

class Integrator
{
  public:
    virtual double operator()(Functor& f) = 0;
    virtual ~Integrator() // will be explained later
    {}
};

#endif
```

midpoint_class.h

```
#include "integrator.h"

class MidpointRule : public Integrator
{
    double a, b;
    size_t n;
  public:
    MidpointRule(double a_, double b_, size_t n_) : a(a_), b(b_), n(n_)
    {}
    double operator()(Functor& f) override
    {
        double h = (b-a)/n; // length of a single interval

        // compute the integral boxes and sum them
        double result = 0.;
        for (size_t i = 0; i < n; ++i)
        {
            // evaluate function at midpoint and sum integral value
            result += f(a + (i + 0.5)*h);
        }

        return h*result;
    }
};
```

simpson_class.h

```
#include "integrator.h"

class SimpsonRule : public Integrator
{
    double a, b;
    size_t n;
  public:
    SimpsonRule(double a_, double b_, size_t n_) : a(a_), b(b_), n(n_)
    {}
    double operator()(Functor& f) override
    {
        double h = (b-a)/n; // length of a single interval

        // compute the integral boxes and sum them
        double result = f(a) + f(b);
        for (size_t i = 1; i < n; i += 2)
            result += 4. * f(a + i*h);
        for (size_t i = 2; i < n; i += 2)
            result += 2. * f(a + i*h);

        return (h*result)/3.;
    }
};
```

integration_class.cc

```
#include <iostream>
#include <memory>
#include "midpoint_class.h"
#include "simpson_class.h"
#include "cosine.h"

int main()
{
  Cosine cosine(1.,-1.);
  std::unique_ptr<Integrator>
    integrate(new MidpointRule(1.,M_PI_2+1.,10));
  std::cout << "Integral of cos(x-1) in "
            << "the interval [1 : pi/2+1] is "
            << (*integrate)(cosine) << std::endl;
  SimpsonRule simpson(1.,M_PI_2+1.,10);
  std::cout << "Integral of cos(x-1) in "
            << "the interval [1 : pi/2+1] is "
  << simpson(cosine) << std::endl;
  return 0;
}
```

Arrays of Objects

- It is often necessary to create an array of objects of a common interface base class, e.g. the parameter functions for various materials which are used in a simulation.
- Since references must be initialized when they are created, only an array of base class pointers may be used, with the pointers pointing to the various objects.
- The pointer should be initialized with 0 or in C++11 with `nullptr`, or (even better) `std::unique_ptr` or `std::shared_ptr` should be used.

```
std::vector<std::unique_ptr<Functor> > Function(4);
Function[0] = std::unique_ptr<Functor>(new Cosine(1.,-1.));
// alternative
Function[0].reset(new Cosine(1.,-1.));
...
```

Virtual Destructors

- If only base class pointers are available to objects of the derived class, then only the destructor of the base class can be called.
- Since derived classes could use allocated resources that must be released in the destructor, it makes sense to give the base class a (typically empty) virtual destructor.
- This has the consequence that the correct destructor is called for each derived class object even when using a base class pointer.
- The destructor can not be purely virtual.

```
class Functor
{
  public:
    virtual double operator()(double x) = 0;
    virtual ~Functor() // allows correct deletion of anonymous
    {};                // Functor pointers in arrays
};
```

- In C++11 and above this is done via the keyword `default`:

```
    virtual ~Functor() = default;
```

Dynamic Cast

In a running program it may be desirable to find out whether a pointer to an object can be converted into a pointer to another class (e.g. because it actually points to an object of a derived class).

- This can be achieved using `dynamic_cast`:

  ```
  Functor* func = dynamic_cast<Functor*>(f);
  ```

  converts the pointer `f` into a pointer to a functor if this is allowed.
- This also works the other way around in the class hierarchy:

  ```
  Cosine* cos = dynamic_cast<Cosine*>(func);
  ```

- A `dynamic_cast` returns either a converted pointer or a null pointer if the conversion is not possible (e.g. missing type hierarchy).

Dynamic Cast

- `dynamic_cast` also works with references:

  ```
  Cosine& cos = dynamic_cast<Cosine&>(f);
  ```

  An invalid conversion will throw an exception of the type `std::bad_cast`.
- C++11 and above have the free function `std::dynamic_pointer_cast` that provides this functionality for `std::shared_ptr`s:

  ```
  std::shared_ptr<Functor> func
      = std::dynamic_pointer_cast<Functor>(f);
  ```

  A direct conversion as above is not possible, since `shared_ptr<Derived>` is not derived from `shared_ptr<Base>`, even if that is the case for `Derived` and `Base`.

Dynamic Cast

The following code detects the actual type behind the base class reference, and treats Cosine functors in a special way:

```
#include <cstdlib>
#include "midpoint.h"
#include "simpson.h"
#include "cosine.h"

double Integrate(Functor& f, double a, double b)
{
    // try to convert address of f to Cosine pointer
    Cosine* cos = dynamic_cast<Cosine*>(&f);
    if (cos == nullptr)
        // not Cosine, use midpoint rule
        return MidpointRule(f,a,b);
    else
        // Cosine, use Simpson rule
        return SimpsonRule(f,a,b);
}
```

Virtual Constructors

If you only have a base class pointer to an object, then it is usually impossible to create an object of the same type (i.e. the derived class) or to copy the entire object (only the base class part is copied).

Using so-called "virtual constructors" this can be done anyway:

```
class Functor
{
  public:
    ...
    virtual Functor* create() = 0;
    virtual Functor* clone()  = 0;
}
```

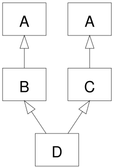
```
class Cosine : public Functor
{
  public:
    ...
    Cosine* create()
    {
        return new Cosine();
    }

    Cosine* clone()
    {
        return new Cosine(*this);
    }
}
```

This is an application of covariant return types of virtual functions. Note that this, again, does not work with smart pointers (missing type hierarchy).

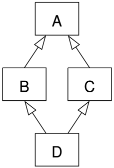
Virtual Base Classes

- Sometimes it is useful to derive a class from several other classes that are derived from the same base class.
- One possible application is to let the derived classes execute various aspects of a problem that can be implemented in different ways in each case, but need to access the same data in the base class.
- A class derived from these classes using multiple inheritance then combines their functionality into a certain complete process.
- Normally each class has its own copy of the base class, but this would mean that the data exists multiple times. This can be prevented using *virtual inheritance*.

Deadly Diamond of Death



no virtual inheritance



virtual inheritance

Source: RokerHRO, Wikipedia

Non-virtual (i.e. standard) multiple inheritance:

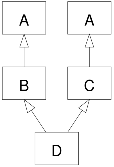
```
class A {};
class B : public A {};
class C : public A {};
class D : public B, public C {};
```

Virtual multiple inheritance:

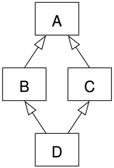
```
class A {};
class B : virtual public A {};
class C : virtual public A {};
class D : public B, public C {};
```

Note that the keyword `virtual` has to be placed in the definitions of `B` and `C`, despite these classes not being directly involved with multiple inheritance!

Deadly Diamond of Death



no virtual inheritance



virtual inheritance

Source: RokerHRO, Wikipedia

- If the inheritance is not declared `virtual`, then each intermediate class has a copy of the base class. `D` therefore contains two copies of `A` (these can be accessed via `D::B::A` and `D::C::A`).
- If the inheritance is declared `virtual`, then there is *one* copy of the base class that is shared, i.e. `D::B::A` and `D::C::A` refer to the same namespace.
- Forgetting the keyword `virtual` for one of the classes results in *two* copies of `A`:
  - one for the class missing `virtual`
  - one for the other class (es)

  This can quickly lead to inconsistencies and unintended consequences.

Rule of thumb: not using `virtual` is likely result of a misconception about inheritance, using `virtual` is indication of an overly complex design choice.

Example: Newton Method from DUNE-PDELab

Example: the Newton method is used to solve a nonlinear system of equations.

A Newton method consists of:

- a basic algorithm
- steps that must be performed at the start of each Newton iteration (e.g. reassembly of the Jacobi matrix)
- a test whether the process has converged
- optionally a linesearch to enlarge the convergence area

Each of these intermediate steps is outsourced to a separate class, so you can replace all the components independently.

The common data and virtual methods are placed in a base class.

```
// data to operate on, iteration count, etc.
class NewtonBase
{...};

// perform linear solve, compute step direction
class NewtonSolver : public virtual NewtonBase
{...};

// check termination criterion
class NewtonTerminate : public virtual NewtonBase
{...};

// perform line search strategy
class NewtonLineSearch : public virtual NewtonBase
{...};

// local linearization (jacobian), thresholds, etc.
class NewtonPrepareStep : public virtual NewtonBase
{...};

// combine above classes into one complete class
class Newton : public NewtonSolver, public NewtonTerminate,
               public NewtonLineSearch, public NewtonPrepareStep
{...};
```

Actual implementation combines this with templatization on all levels (later)

Summary

If there are several objects that embody a fundamental principle (such as circle, triangle, rectangle etc. are special realizations of a geometric object) or a specific functionality (such as the trapezoidal rule and Simpson's rule being a special variant of the integration process), then it is good style in C++ to define a common interface that is implemented by each specific realization in its own way.

Dynamic polymorphism

- uses abstract base classes (ABCs) and virtual functions for this
- employs special language constructs to ensure that each class actually implements the full interface functionality (pure virtual functions)
- allows variant selection at runtime
- requires additional work (virtual function table)
- prevents some optimizations (inlining, loop unrolling)