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2018/19 Semester 2

Object Oriented Programming with Applications

Problem Sheet 4 - Wednesday 24th October 2018[1]

Exercise 4.1. Get a working implementation of the `CompositeIntegrator` class. Use the lecture material.

You will notice that the class, as presented in lectures is not *robust*. Consider and modify your code according for the following situations (i.e. throw appropriate exceptions).

1. What if `newtonCotesOrder` in the is a number other than $1, 2, 3, 4$?
2. What if `N` in the `Integrate` method is less than or equal to 0?
3. Does the code work if `a` $>$ `b` in the `Integrate` method?

Exercise 4.2. The Newton's method for approximating solutions x to $f(x) = 0$, where $f : \mathbb{R} \to \mathbb{R}$ is assumed to be differentiable is an iterative method where, given an initial guess for the solution x_0 the next entry in the sequence of approximations is calculated as:

$$x_n := x_{n-1} - \frac{f(x_{n-1})}{f'(x_{n-1})}\,, \quad n = 1, 2, \ldots\,.$$

Do the following:

1. To see that you understand how this works calculate the first three approximations to $0 = x^2 - 2 =: f(x)$ with $x_0 = 2$ (this is a nice way of approximating $\sqrt{2}$ if you ever have to do this by hand).
2. Create a method with the following "signature":

```
static double NewtonSolver(Func<double, double> f,
                           Func<double, double> fPrime,
                           double x0,
                           double maxError, int maxIter)
```

   It should have the following properties: the return value should be the approximation x_n of solution to $f(x) = 0$ such that $|f(x)| <$`maxError`. If the number of iterations has reached or exceeded `maxIter` then an exception should be thrown. If `fPrime != null` then it should be used, otherwise the derivative should be approximated using symmetric finite differences. That is, for a given $\delta > 0$ we say that

$$f'(x_0) \quad \text{is approximately} \quad \frac{1}{2\delta}\left(f(x_0 + \delta) - f(x_0 - \delta)\right).$$

3. Test it by approximating the solution to $0 = x^2 - 2$ with $x_0 = 2$.

[1]Last updated 9th October 2018

Exercise 4.3. Newton's method generalises to higher dimensions. Indeed consider a differentiable $F : \mathbb{R}^d \to \mathbb{R}^d$. Let $J_F(x)$ denote the Jacobian matrix of this function evaluated at x. That is:

$$J_F(x) = \begin{pmatrix} \frac{\partial F_1}{\partial x_1} & \frac{\partial F_1}{\partial x_2} & \cdots & \frac{\partial F_1}{\partial x_d} \\ \frac{\partial F_2}{\partial x_1} & \frac{\partial F_2}{\partial x_2} & \cdots & \frac{\partial F_2}{\partial x_d} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial F_d}{\partial x_1} & \frac{\partial F_d}{\partial x_2} & \cdots & \frac{\partial F_d}{\partial x_d} \end{pmatrix}.$$

Given an initial guess $x_0 \in \mathbb{R}^d$ we obtain successive approximations to x such that $F(x) = 0$ by solving

$$J_F(x_{n-1})(x_n - x_{n-1}) = -F(x_{n-1}), \;\; n = 1, 2, \dots .$$

Your task is to complete the class below:

```
public class NewtonSolver
{
    private const double delta = 1e-8; // for approximating partial derivatives

    private double tol;
    private int maxIt;

    public NewtonSolver(double tolerance, int maximumIterations)
    {
        tol = tolerance;
        maxIt = maximumIterations;
    }
    public Matrix<double> ApproximateJacobian(Func<Vector<double>,
                                  Vector<double>> F, Vector<double> x)
    {
    /* ... write the code ...*/
    }

    public Vector<double> Solve(Func<Vector<double>, Vector<double>> F,
              Func<Vector<double>, Matrix<double>> J_F, Vector<double> x_0)
    {
    /* ... write the code ...*/
    }
}
```

The Newton Method should stop if either `maxIt` is reached or if the l^2 norm (i.e. the usual Euclidean norm) of $F(x_n)$ is smaller than `tol`.
Now test it by approximating the solution to $F(x, y) = 0$ where

$$F(x, y) := \begin{pmatrix} x^2 + y^2 - 2xy - 1 \\ x^2 - y^2 - 7 \end{pmatrix}$$

with $x_0 = (1, -1)^T$. Note that it is easy to see that at least one solution is $x = 4, y = 3$.
Hints.

- To define something like $F : \mathbb{R}^d \to \mathbb{R}^d$ in C# use:

```
Func<Vector<double>, Vector<double>> F = (x) =>
{
    Vector<double> y = Vector<double>.Build.Dense(x.Count);
    y[0] = x[0]*x[0] + x[1]*x[1] - 2*x[0]*x[1] - 1;
    y[1] = x[0]*x[0] - x[1]*x[1] - 7;
    return y;
};
```

- To define something like the Jacobian Matrix use:

```
Func<Vector<double>,Matrix<double>> J_F = (x) => {
   int d = x.Count;
   Matrix<double> J_F_vals = Matrix<double>.Build.Dense (d, d);
   J_F_vals[0,0] = 2*x[0] -2*x[1];
   J_F_vals[0,1] = 2*x[1]-2*x[0];
   J_F_vals[1,0] = 2*x[0];
   J_F_vals[1,1] = -2*x[1];
   return J_F_vals;
};
```

- You can see above how to define an empty vector and matrix respectively.
- To fill in a whole jth column in a matrix you can use: `M.SetColumn(j,v)` assuming `M` is a matrix and `v` is a vector of appropriate length.
- To solve a linear system $Ax = b$ (with A a $d \times d$ matrix and b a vector in $\mathbb{R}^d$, x unknown) use: `Vector<double> x = A.Solve(b);`.
- To find a determinant of a matrix A use `double determinant = A.Determinat();` Note that `A.Solve(b)` might also fail when the determinant is very small rather than exactly 0.

Exercise 4.4. In fact our interest in the Newton's method is also for minimization problems. A differentiable function $f : \mathbb{R}^d \to \mathbb{R}$ will have a local minimum (or maximum or saddle point) at x if

$$\nabla f(x) := \begin{pmatrix} \frac{\partial f}{\partial x_1}(x) \\ \vdots \\ \frac{\partial f}{\partial x_d}(x) \end{pmatrix}$$

is equal to zero. If f is convex then this will be the global minimum.
So we are approximating solutions to $F(x) = \nabla f(x) = 0$ using Newton's method.
The Jacobian matrix of F is now

$$\begin{pmatrix} \frac{\partial F_1}{\partial x_1} & \frac{\partial F_1}{\partial x_2} & \cdots & \frac{\partial F_1}{\partial x_d} \\ \frac{\partial F_2}{\partial x_1} & \frac{\partial F_2}{\partial x_2} & \cdots & \frac{\partial F_2}{\partial x_d} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial F_d}{\partial x_1} & \frac{\partial F_d}{\partial x_2} & \cdots & \frac{\partial F_d}{\partial x_d} \end{pmatrix} = \begin{pmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_d} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_d} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_d \partial x_1} & \frac{\partial^2 f}{\partial x_d \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_d^2} \end{pmatrix}$$

which is the Hessian matrix of f.
In some cases one would have to approximate the Hessian using finite differences. Let us define $T_{\delta,i} y : \mathbb{R}^d \to \mathbb{R}^d$ as

$$T_{\delta,i} y = (y_1, \ldots, y_{i-1}, y_i + \delta, y_{i+1}, \ldots, y_d)^T.$$

Then

$$\begin{aligned} &\frac{\partial^2 f}{\partial x_i \partial x_j}(x) \\ &\approx \frac{1}{2h}\left(\frac{\partial f}{\partial x_j}(T_{i,h}x) - \frac{\partial f}{\partial x_j}(T_{i,-h}x)\right) \\ &\approx \frac{1}{2h}\left(\frac{1}{2h}\left(f(T_{j,h}T_{i,h}x) - f(T_{j,-h}T_{i,h}x)\right) - \frac{1}{2h}\left(f(T_{j,h}T_{i,-h}x) - f(T_{j,-h}T_{i,-h}x)\right)\right). \end{aligned}$$

Your task is to develop a Newton based minimizer by completing the class below

```
public class NewtonMnimizer
{
    private const double delta = 1e-7; // for approximating grad
    private NewtonSolver solver;

    public NewtonMnimizer(double tol, int maxIt)
    {
        solver= new NewtonSolver(tol, maxIt);
    }
    private Vector<double> ApproximateGrad(Func<Vector<double>, double> f,
                                          Vector<double> x)
    {
    /* ... write the code ... */
    }
    private Matrix<double> ApproximateHessian(Func<Vector<double>, double> f,
                                              Vector<double>> grad_f,
                                              Vector<double> x)
    {
    /* ... write the code, allow for grad_f == null ... */
    }
    public Vector<double> Minimize(Func<Vector<double>, double> f,
                            Func<Vector<double>, Vector<double>> grad_f,
                            Func<Vector<double>, Matrix<double>> hessian_f,
                            Vector<double> x_0)
    {
    /* ... write the code,
    allow for grad_f == null and also hessian_f == null ... */
    }
}
```

Test it by finding the global minimum of the function f given by $f(x, y) = x^2 + y^2$ by running the following code:

```
NewtonMnimizer minimizer = new NewtonMnimizer (1e-5, 100);
Func<Vector<double>, double> f = (x) => x [0] * x [0] + x [1] * x [1];

Vector<double> startPt = Vector<double>.Build.Dense (2);
startPt[0] = 1; startPt[1] = -1;

Console.WriteLine ("With approximate grad of f and hessian of f using f.d.");
Console.WriteLine(minimizer.Minimize(f, null, null, startPt));

Console.WriteLine ("With exact grad_f and approximate hessian f using f.d.");
Func<Vector<double>, Vector<double>> grad_f = (x) => {
    Vector<double> grad = Vector<double>.Build.Dense(x.Count);
    grad[0] = 2*x[0]; grad[1] = 2*x[1];
    return grad;
};
Console.WriteLine(minimizer.Minimize(f, grad_f, null, startPt));

Console.WriteLine ("With exact grad of f and hessian of f.");
Func<Vector<double>, Matrix<double>> hessian_f = (x) => {
    Matrix<double> hessian = Matrix<double>.Build.Dense(x.Count,x.Count);
    hessian[0,0] = 2; hessian[0,1] = 0;
    hessian[1,0] = 0; hessian[1,1] = 2;
    return hessian;
};
Console.WriteLine(minimizer.Minimize(f, grad_f, hessian_f, startPt));
Console.ReadKey ();
```