13.8. **Predictor-corrector methods.** We consider the Adams methods, obtained from the formula

$$y(x_{n+1} - y(x_n) = \int_{x_n}^{x_{n+1}} y'(x)\,dx = \int_{x_n}^{x_{n+1}} f(x, y(x))\,dx$$

by replacing f by an interpolating polynomial. If we use the points $x_n, x_{n-1}, \ldots, x_{n-p}$, we get the Adams-Bashforth methods. If we use the points $x_{n+1}, x_n, \ldots, x_{n-p}$, we get the Adams-Moulton formulas.

In a $p+1$-step method, implicit methods have one additional parameter (b_{-1}) to specify. Hence, one can show that the highest attainable order of a zero-stable $p+1$-step method is less in the case of an explicit method than for an implicit method. If we compare methods of the same order, then explicit methods require an additional starting value, but we might still prefer an explicit method with a higher stepnumber to an implicit method of the same order, (but lower stepnumber). To see the advantages of implicit methods, consider the following table comparing explicit Adams-Bashforth methods to implicit Adams-Moulton methods.

TABLE 4. Adams-Bashforth explicit methods

stepnumber k	1	2	3	4
order r	1	2	3	4
error constant C_{r+1}	1/2	5/12	3/8	251/720
abs. stab. interval $(\alpha, 0)$	-2	-1	-6/11	-3/10

TABLE 5. Adams-Moulton implicit methods

stepnumber k	1	2	3	4
order r	2	3	4	5
error constant C_{r+1}	-1/12	-1/24	-19/720	-3/160
abs. stab. interval $(\alpha, 0)$	$-\infty$	-6	-3	-90/49

If we want a 4th order Adams method, then the choices are a 4-step explicit method or a 3-step implicit method. Note that the implicit method has an error constant smaller by a factor of $\approx 1/13$ and an absolute stability interval 10 times that of an explicit method. Hence for stability and accuracy, we would like to use the implicit method. To do so, we must solve at each step the nonlinear equation:

$$y_{n+1} = \sum_{i=0}^{p} a_i y_{n-i} + h \sum_{i=-1}^{p} b_i f(x_{n-i}, y_{n-i})$$

(note y_{n+1} also appears on the right hand side of the equation).

A simple iteration procedure for this is:

$$y_{n+1}^{j+1} = \sum_{i=0}^{p} [a_i y_{n-i} + h b_i f(x_{n-i}, y_{n-i})] + h b_{-1} f_{n+1}^j,$$

where $f_{n+1}^j = f(x_{n+1}, y_{n+1}^j)$. Hence, the error between y_{n+1} and the approximation y_{n+1}^{j+1} satisfies:

$$y_{n+1} - y_{n+1}^{j+1} = hb_{-1}[f_{n+1} - f_{n+1}^j].$$

Assuming f satisfies a Lipschitz condition with Lipschitz constant L, we get

$$|y_{n+1} - y_{n+1}^{j+1}| \le h|b_{-1}|L|y_{n+1} - y_{n+1}^j|.$$

It easily follows that

$$|y_{n+1} - y_{n+1}^j| \le [h|b_{-1}|L]^j|y_{n+1} - y_{n+1}^0|.$$

Hence, if $h|b_{-1}|L < 1$, the iteration converges.

Since each iteration involves an evaluation of the function f, we would like a good starting guess to minimize the number of iterations needed to meet a given error tolerance. We do this by using an explicit method (called a predictor) to produce the initial guess y_{n+1}^0. The iteration then consists of the following steps: PECECE ..., where P denotes the application of the predictor method, E denotes the evaluation of f at this value of y_{n+1}^j, and C denotes the application of the corrector method (the implicit method), using the evaluation of f just produced on the right hand side. There are two basic possibilities for stopping this iteration. The first is to iterate to convergence. In practice this would mean until $|y_{n+1}^{j+1} - y_{n+1}^j| < \epsilon$, where ϵ is a preassigned tolerance. The advantage of this is that the final result is independent of the starting guess and the local truncation error and stability properties are those of the corrector alone. The disadvantage is that we don't know how many function evaluations this may take and hence it may be time consuming. The second possibility is to specify in advance the number of times the corrector is applied. In this case, the number of function evaluations is known, but the local truncation error and stability properties now depend on the combination of the predictor and corrector. These methods are denoted by $P(EC)^m$ or $P(EC)^mE$, depending on whether a final evaluation is done. The common practice is to use $m = 1$ or $m = 2$.

The Adams-Bashforth, Adams-Moulton $p + 1$-step methods provide good combinations for predictor-corrector pairs. In that case, the order of the corrector will be one higher than the order of the predictor. A variable order, variable step-size code, written by Shampine and Gordon, (and implemented in *Matlab* as `ode113`) uses these methods and the iteration PECE. Changes in step-size and order are based on estimating the local error by comparing the difference between a k and $k + 1$ order corrector, both using a kth order predictor.

In using multistep methods, one needs a way of generating the additional starting values and also additional values when the step-size is changed. Starting values can be obtained by using Runge-Kutta or Taylor series methods. When the step-size is changed, additional values can be obtained by Runge-Kutta methods or by interpolation. In the Shampine-Gordon code, the codes are started with a 1-step Adam's method, then a 2-step method, and so on until all the starting values are generated. The step-size is changed using the divided difference form of the interpolating polynomial, which allows the method to be generalized to unequally spaced points.

13.9. **Generalization to first order systems.** We consider the first order system

$$Y' = F(x, Y), \qquad Y(a) = \eta,$$

where $Y = [y^1, \ldots, y^m]^T$ and $F(x, Y) = [f^1(x, y^1, \ldots, y^m), \ldots, f^m(x, y^1, \ldots, y^m)]^T$. We showed previously that Runge-Kutta methods are applicable to such systems. Multistep methods are also applicable, although we need to extend some of the theory. The stability theory previously developed was for the model problem $y' = \lambda y$, where λ was considered a local approximation of $\partial f / \partial y$. For systems, the analogous model problem is: $Y' = AY$, where A is a matrix with constant coefficients, considered a local approximation to the Jacobian matrix, i.e., $A_{ij} \approx (\partial f^i / \partial y^j)$. Applying the multistep method, we obtain

$$[I - hb_{-1}A]Y_{n+1} = \sum_{i=0}^{p}[a_i I + hb_i A]Y_{n-i}.$$

If A is diagonalizable, i.e., there exists a nonsingular matrix H and a diagonal matrix Λ such that $H^{-1}AH = \Lambda$, (where the eigenvalues of A lie on the diagonal of Λ), then multiplying the above on the left by H^{-1}, we get

$$[H^{-1} - hb_{-1}H^{-1}A]Y_{n+1} = \sum_{i=0}^{p}[a_i H^{-1} + hb_i H^{-1}A]Y_{n-i}.$$

Setting $HZ_n = Y_n$, we get

$$[I - hb_{-1}\Lambda]Z_{n+1} = \sum_{i=0}^{p}[a_i I + hb_i \Lambda]Z_{n-i}.$$

Since I and Λ are diagonal matrices, the system decouples and we get for each component z^j of Z,

$$[1 - hb_{-1}\lambda_j]z_{n+1}^j = \sum_{i=0}^{p}[a_i + hb_i\lambda_j]z_{n-i}^j.$$

The definition of absolute stability depended on the interval of $h\lambda$ for which all solutions of the multistep method applied to the model problem $y' = \lambda y$ remain bounded as $n \to \infty$. Since H is constant, the components of Y_n will remain bounded if the components of Z_n do. Now the difference equation obtained above is the same one obtained previously. Hence, the solutions remain bounded if all roots r of the characteristic polynomial $\rho(z) - h\lambda\sigma(z)$ satisfy $|r| \leq 1$ (and roots of magnitude one are simple). To be absolutely stable, we require these conditions to hold when λ is any eigenvalue of the matrix A. Although A is real, its eigenvalues might be complex. Hence, for first order systems, we modify our definition to read:

Definition: A linear multistep method is *absolutely stable in the region $\mathcal{R}$ of the complex plane* if for all $h\lambda \in \mathcal{R}$, all roots of the characteristic polynomial $\rho(z) - h\lambda\sigma(z)$ associated with the method satisfy $|r| \leq 1$ (and roots of magnitude one are simple).

A similar modification is made for the definition of relative stability.

Example: Euler's method: $Y_{n+1} = Y_n + hF_n$. We apply the method to $y' = \lambda y$ to get the difference equation $y_{n+1} = (1+h\lambda)y_n$. The characteristic polynomial has one root $r = 1+h\lambda$, so we want $|1 + h\lambda| \leq 1$. Now $\lambda = \lambda_1 + i\lambda_2$ may be complex, so our condition becomes $|1 + h\lambda| = \sqrt{(1 + h\lambda_1)^2 + (h\lambda_2)^2} \leq 1$, i.e., $(1 + h\lambda_1)^2 + (h\lambda_2)^2 \leq 1$. Thus $\mathcal{R}$ is a circle in the complex plane (with real axis $h\lambda_1$ and imaginary axis $h\lambda_2$) centered at $(-1, 0)$ and radius 1. The interval of absolute stability $(-2, 0)$ is the intersection of $\mathcal{R}$ with the $h\lambda_1$ axis.

Example: Trapezoidal rule: $Y_{n+1} = Y_n + (h/2)(F_{n+1} + F_n)$. There is only one root of the characteristic polynomial given by $r = (1 + h\lambda/2)/(1 - h\lambda/2)$. Hence, we require $|1 + h\lambda/2| \leq |1 - h\lambda/2|$, i.e.,

$$(1 + h\lambda_1/2)^2 + (h\lambda_2/2)^2 \leq (1 - h\lambda_1/2)^2 + (h\lambda_2/2)^2.$$

Clearly, this will hold for $h\lambda_1 \leq 0$, so the region of absolute stability is the entire left half-plane (the largest possible region of absolute stability).
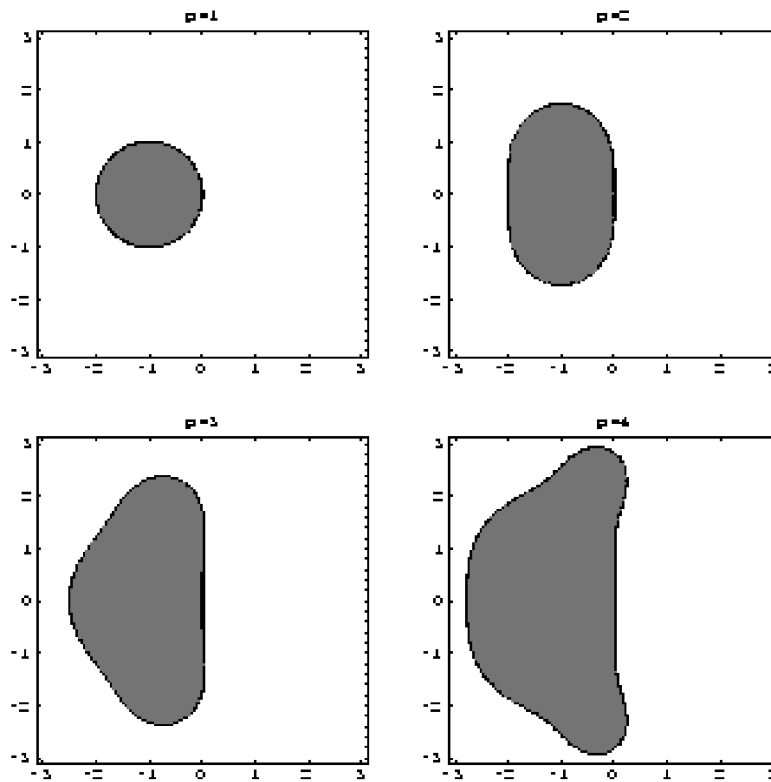

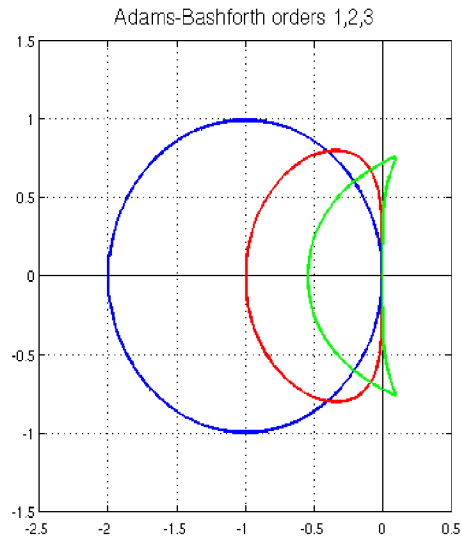FIGURE 4. Stability regions for Runge-Kutta methods
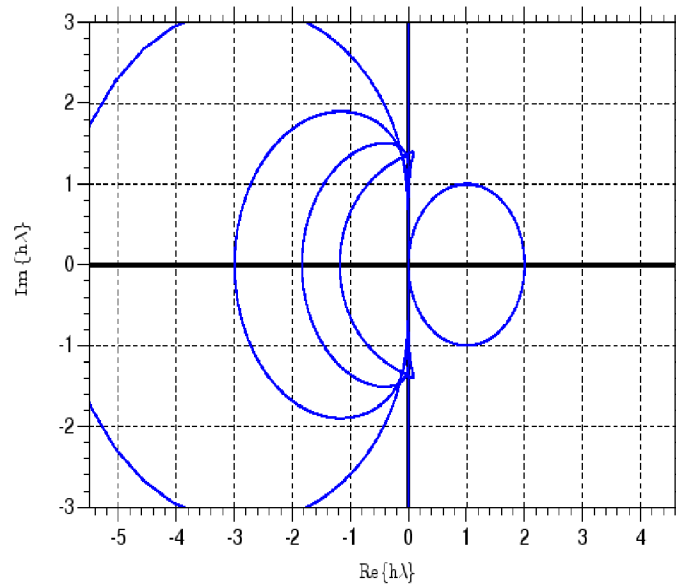
FIGURE 5. Stability regions for Adams-Bashforth methods

FIGURE 6. Stability regions for Adams-Moulton methods (1-6)