Computer Modeling and Simulation

Lecture 23-24

Simulation Techniques

- Numerical Methods for solving ODEs
  - Euler’s Method,
  - Runge-Kutta 2
  - Runge-Kutta 4

Euler's method

- Consider an unconstrained growth model where

  growth_rate = 0.10

  population(0) = 100

  growth(t) = growth_rate * population(t - Δt)

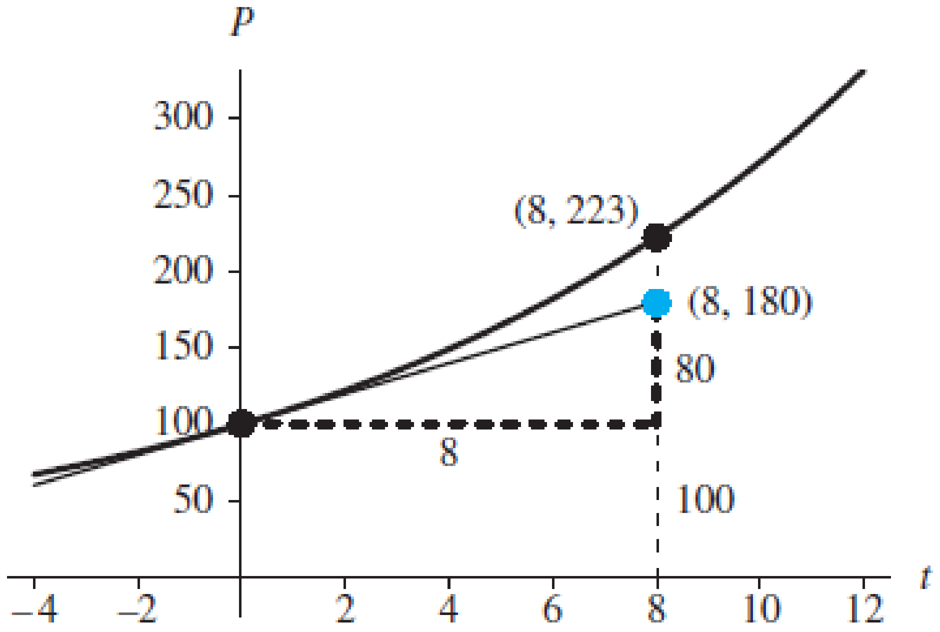
  population(t) = population(t - Δt) + growth(t) * Δt

- Starting with $P_0 = P(0) = 100$ and using $\Delta t = 8$. In the situation, $t = 8$, $t - \Delta t = 0$, growth(t) is the derivative at that time is $P'(0) = 0.1(100) = 10$, which is the slope of the tangent line to the curve $P(t)$ at (0,100).
- We multiply Δt, 8, by this derivative at the previous time step, 10, to obtain the estimated change in P, 80.
- Consequently, the estimate for P_1 is as follows:

$$\text{estimate for } P_1 = \text{previous value of } P + \text{estimated change in } P$$

$$= P_0 + P'(0)\Delta t$$

$$= 100 + 10(8)$$



Actual point, (8, 223), and point obtained by Euler’s method, (8, 180)

Euler’s Method Algorithm

Algorithm 1: Euler’s Method

$t \leftarrow t_0$
$P(t_0) \leftarrow P_0$
Initialize *SimulationLength*
while $t < SimulationLength$ do the following:

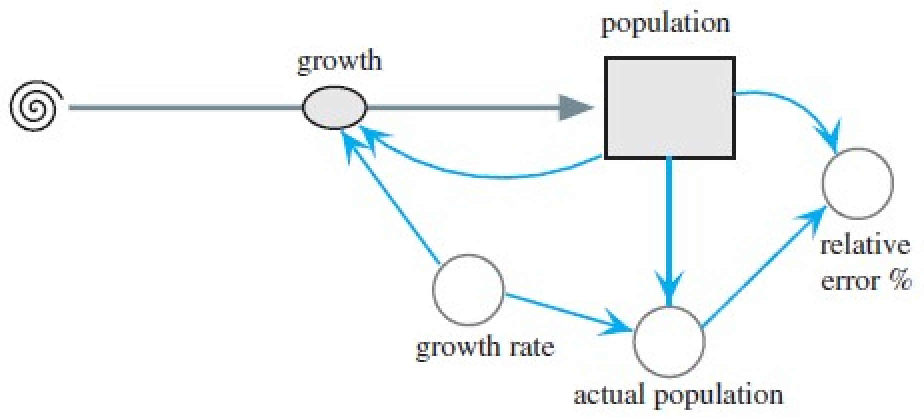
$t \leftarrow t + \Delta t$
$P(t) = P(t - \Delta t) + P'(t - \Delta t)\ \Delta t$

Algorithm 2 Revised Euler’s Method to minimize error accumulation of time with $f(t_{n-1}, P_{n-1})$ indicating the derivative dP/dt at step $n - 1$

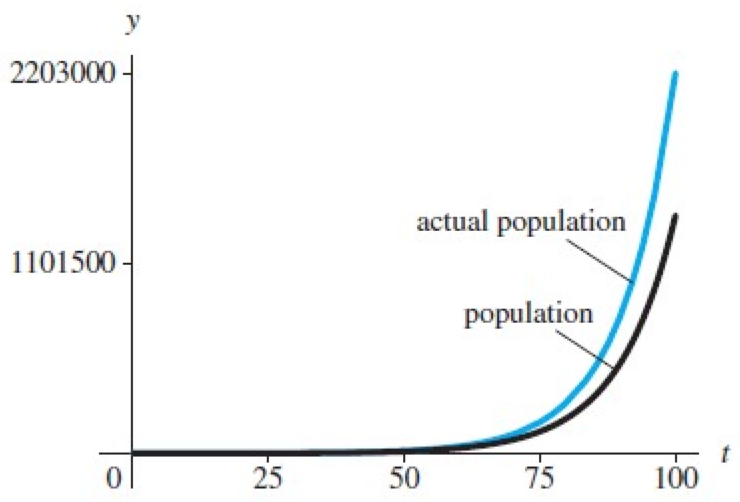
Initialize t_0 and P_0
Initialize *NumberOfSteps*
for n going from 1 to *NumberOfSteps* do the following:

$t_n = t_0 + n\ \Delta t$
$P_n = P_{n-1} + f(t_{n-1}, P_{n-1})\ \Delta t$

Error in Euler Method



Unconstrained growth model with monitoring



Graphs of analytical solution and Euler's Method solution with $\Delta t = 1$

Error in Euler Method

- At time 100, the analytical value for the population is 2,202,647, while the simulated solution using Euler's method produces 1,378,061, so that the relative error is more than 37.4%.
- For Δt being cut in half, the relative error is almost cut in half to 21.5% at time 100.
- If we cut the time step in half again so that Δt is 0.25, the relative also reduces by about half to 11.6% at time 100.
- Thus, the relative error is proportional to Δt. We say that the relative error is **on the order of $\boldsymbol{\Delta t}$, O($\boldsymbol{\Delta t}$)**

Runge-Kutta 2 Method

- **Also called Euler's predictor-corrector (EPC)**
- In the first step, Euler method is used to predict the value of the function whose differential equation we wish to solve.
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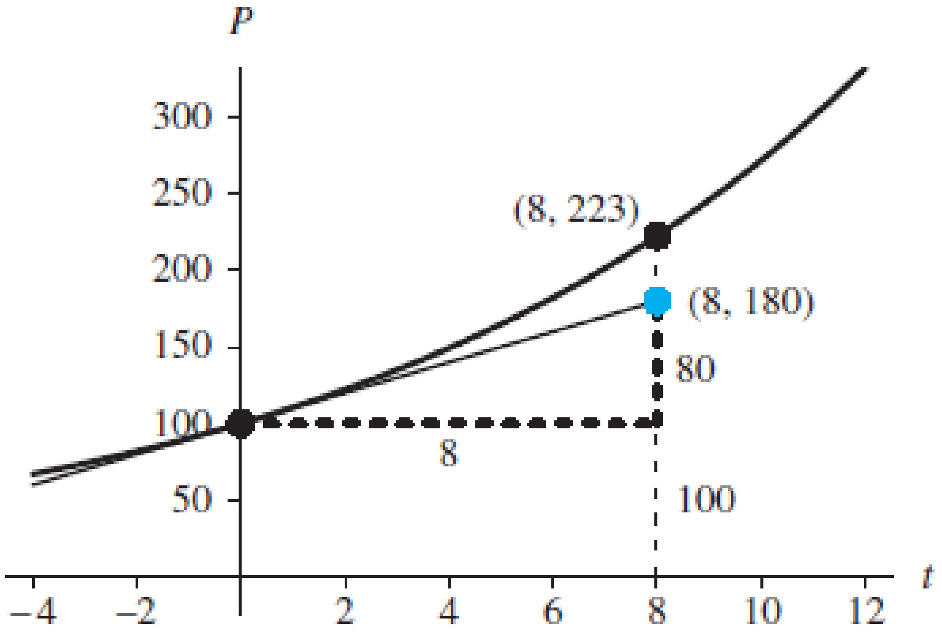
Euler's Estimate as a Predictor

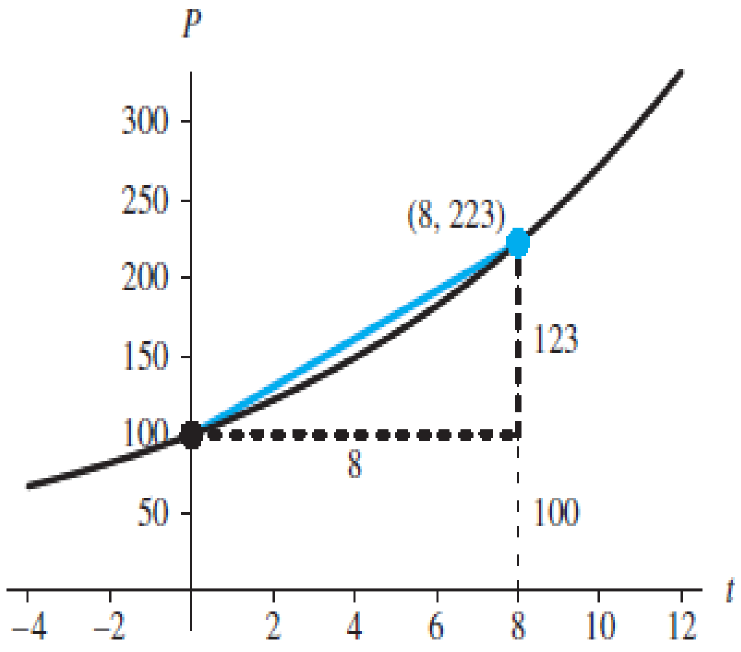
- $f(t_n, P_n)$ is sometimes a more convenient notation for the derivative dP/dt at Step n.
- Thus, at $(t, P) = (0, 100)$, the derivative is $f(0, 100) = 0.1(100) = 10$. According to that technique, using the derivative at (t_{n-1}, P_{n-1}), which is always equal to the slope of the tangent line there, we have the following computation for t_n and estimation of P_n:
- $t_n = t_0 + n\,\Delta t$
- $P_n = P_{n-1} + f(t_{n-1}, P_{n-1})\,\Delta t$



Actual point, (8, 223), and point obtained by Euler’s method, (8, 180)

Corrector

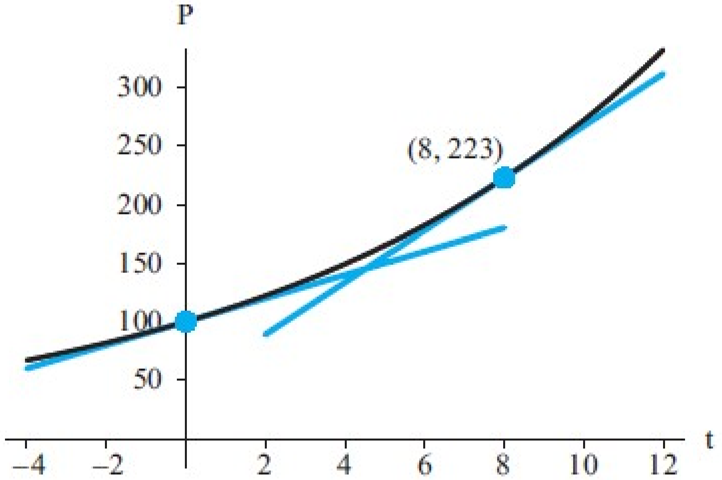
- To estimate (t_n, P_n), we would really like to use the slope of the chord from (t_{n-1}, P_{n-1}) to (t_n, P_n) instead of the slope of the tangent line at (t_{n-1}, P_{n-1}).



Actual point, $(8, P(8)) \approx (8, 223)$, along the chord between (0, 100) ar
223)

Corrector

- Although we do not know the slope of the chord between (0, *P*(0)) and (8, *P*(8)), we can estimate it as approximately the average of the slopes of the tangent lines at *P*(0) and *P*(8):
- slope of the chord b/w P(0) and P(8) = (slope of tan at *P*(0))+ ((slope of tan at *P*(8))/2

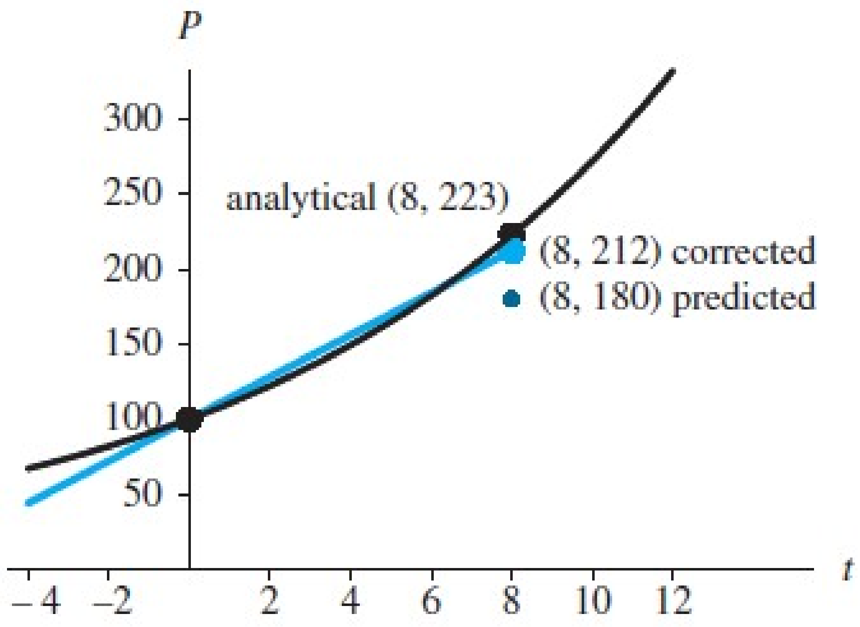


Tangent lines at (0, *P*(0)) and (8, *P*(8))

Corrector

- How can we find the slope of the tangent line at $P(8)$ when we do not know $P(8)$?
- Instead of using the exact value, which we do not know, we predict $P(8)$ as in Euler's
- method.
- As the computation in the first section, "Euler's Estimate as a Predictor," shows, in this case, the prediction is $Y = 180$. We use the point (8, 180) in derivative formula to obtain an estimate of slope at $t = 8$.
- In this case, the slope of the tangent line at (8, 180), or the derivative, is $f(8, 180) = 0.1(180) = 18$.
- Using 18 as the approximate slope of the tangent line at $(8, P(8))$, we estimate the slope of chord between $(0, P(0))$ and $(8, P(8))$ as the following average of tangent line slopes:
- slope of chord ≈ $(10 + 18)/2 = 0.5(10 + 18) = 14$
- Using 14, the corrected estimate is $P1 = 100 +$

RK-2 Method



Predicted and corrected estimation of (8, P(8))

RK-2 Algorithm

Algorithm for Euler's Predictor-Corrector (EPC) Method, or Runge-Kutta 2, with $f(t_{n-1}, P_{n-1})$ indicating the derivative dP/dt at step $n - 1$

Initialize t_0 and P_0
Initialize *NumberOfSteps*
for n going from 1 to *NumberOfSteps* do the following:

$t_n = t_0 + n\,\Delta t$
$Y_n = P_{n-1} + f(t_{n-1}, P_{n-1})\Delta t$, which is the Euler's method estimate
$P_n = P_{n-1} + 0.5\,(f(t_{n-1}, P_{n-1}) + f(t_n, Y_n))\Delta t$

Error in RK-2 Method

Estimates of $P(100)$ and Relative Errors for Various Changes in Time Using Runge-Kutta 2 Simulation Method, where $dP/dt = 0.10P$ with $P_0 = 100$

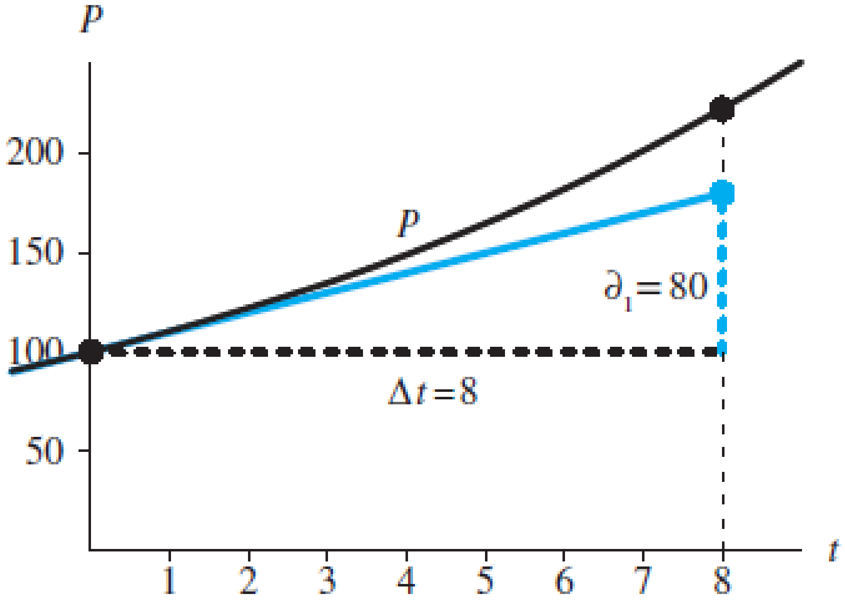
EPC Estimates at Time 100		
Δt	*Estimated* $P(100)$	*Relative Error*
1.00	2,168,841	1.53%
0.50	2,193,824	0.40%
0.25	2,200,396	0.10%

Runge-Kutta 4

- Of the three integration techniques —Euler's, Runge-Kutta 2, and Runge-Kutta 4 methods—the last is the most involved but the most accurate.
- The relative errors of the techniques are $O(\Delta t)$, $O(\Delta t^2)$, and $O(\Delta t^4)$, respectively, with the names Runge-Kutta 2 and 4 indicating the exponents of Δt. Thus, the latter technique improves the most as Δt gets smaller.
- To illustrate Runge-Kutta 4 method, we use the example $f(t, P) = dP/dt = 0.10P$, with $P_0 = 100$ and $\Delta t = 8$, to show the derivation of P_1 from P_0.
- To estimate P_n, the technique adds to P_{n-1} a weighted average of four estimates—$\partial 1$, $\partial 2$, $\partial 3$,and $\partial 4$—of the change in P

First Estimate, ∂1, Using Euler's Method

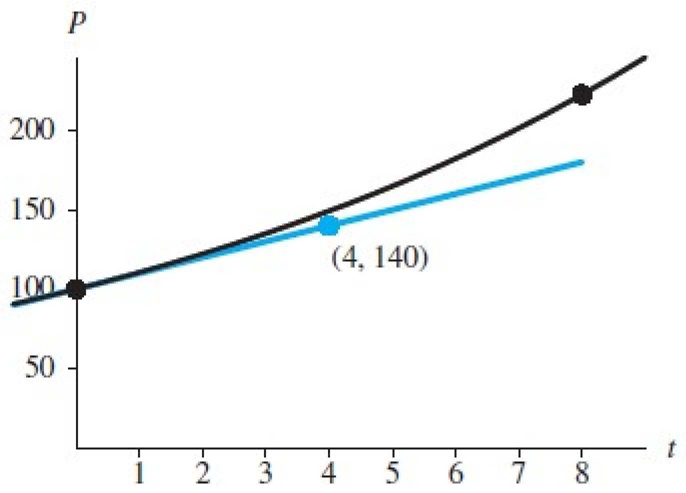
- In general, the **first estimate** of $\Delta P = P_n - P_{n\text{-}1}$ is as follows:
- $\boldsymbol{\partial 1 = f(t n\text{–}1,\ P n\text{–}1)\Delta t}$



First estimate of change in P, $\partial_1 = 80$

Second Estimate, ∂2

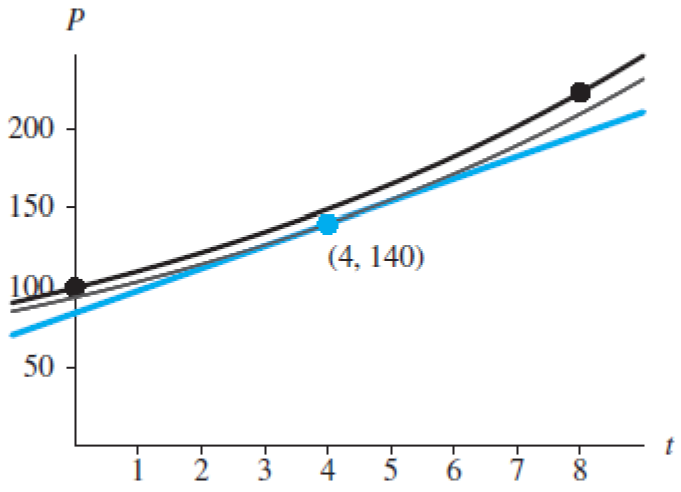
- To calculate the second estimate of ΔP for the previous example, we use the point halfway between the initial point $(t0, P0)$, and point from Euler's estimate, $(t_0 + \Delta t, P_0 + \partial 1)$, in the figure below.
- The midpoint is on the tangent line to the graph of the function P at $(t_0, P_0) = (0, 100)$. Its first coordinate is $t_0 + 0.5\Delta t = 0 + 0.5(8) = 4$, and its second coordinate is $P_0 + 0.5\partial 1 = 100 + 0.5(80) = 140$. Figure below depicts this point



Midpoint (4, 140) between $(t_0, P_0) = (0, 100)$ and $(t_0 + \Delta t, P_0 + \partial_1) = (8, 180)$

Second Estimate, ∂2

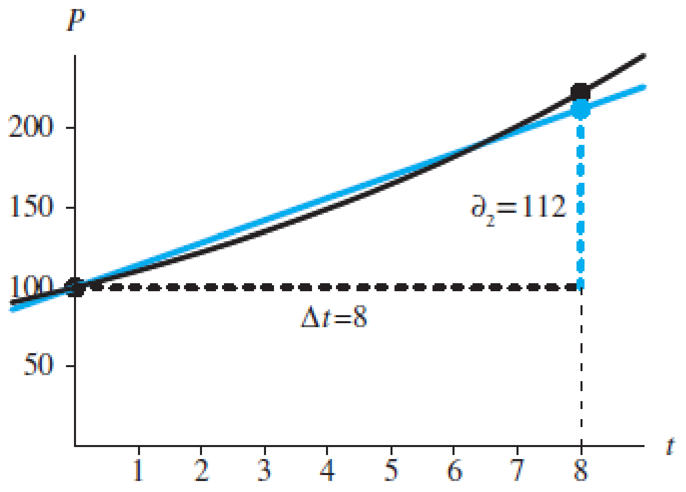
- We calculate the derivative, f, for this midpoint using the derivative formula $f(t,P) = 0.1P$, as follows:
- $f(4, 140) = 0.1(140) = 14$
- Figure below shows, with less thickness, the exponential function through (4, 140) that has derivative 14 at $t = 4$. Thus, at $t = 4$ the curve's tangent line, which is in color, has slope 14



Estimate slope at midpoint between (0, 100) and (8, 180)

Second Estimate, ∂2

- For the second estimate of the change in P, ∂2, we determine the change in the vertical direction for this line for $\Delta t = 8$, as follows:
- $\partial 2 = ((0.1)(140))\ (8) = 14\ (8) = 112$
- Figure below pictures a line of the same slope (14) that passes through the initial point (0, 100). After a change in t of 8 units, P



Second estimate of change in P, $\partial_2 = 112$

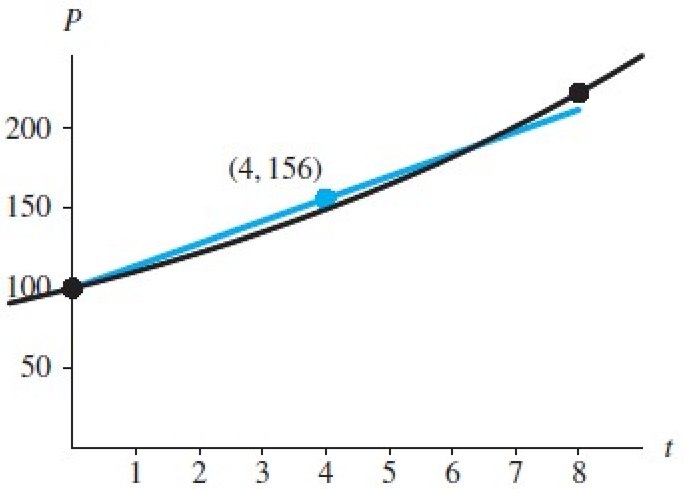
Second Estimate, ∂2

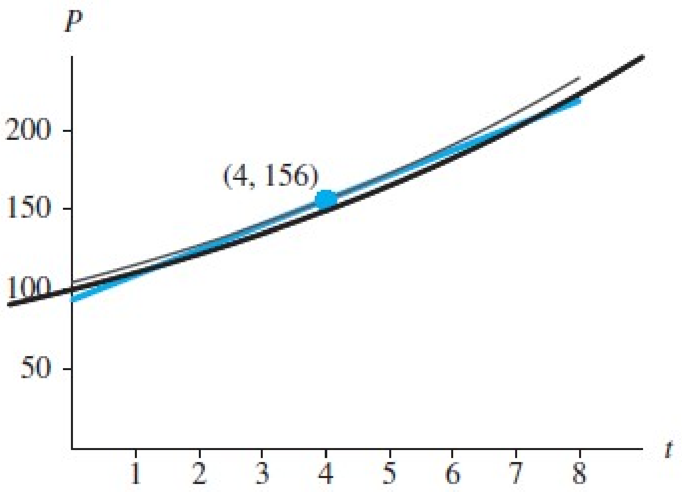
The second estimate for the change in P employs the estimated slope at the point $(t_{n-1} + 0.5\Delta t, P_{n-1} + 0.5\partial_1)$, as follows:

$$\partial_2 = f(t_{n-1} + 0.5\Delta t, P_{n-1} + 0.5\partial_1)\Delta t$$

Third Estimate, ∂3

- For the third estimate, ∂3, we use the same process as for the second estimate on the line that passes through the initial point (0, 100) and the second estimate point, $(t + \Delta t, P_0 + \partial 2) = (8, 212)$.
- First, we find the midpoint, (4, 156), between the endpoints.
- Using the derivative formula, $f(t, P) = 0.1P$, we estimate the slope of the curve at $t = 4$ as $f(4, 156) = 0.1(156) = 15.6$. The line through (4, 156) with slope 15.6 appears in color in



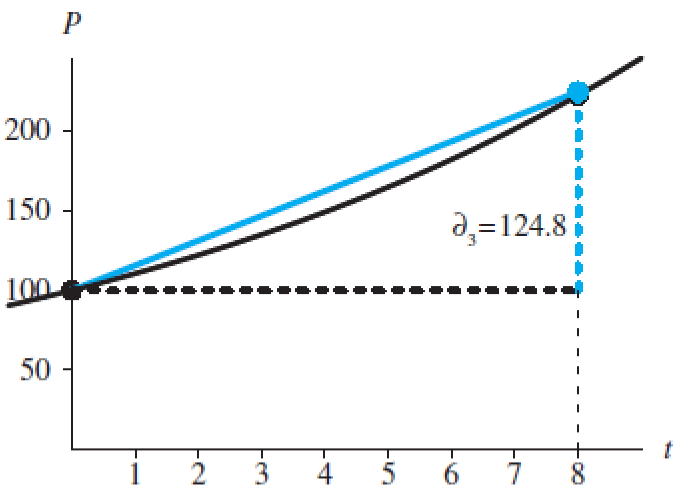


Midpoint (4, 156) between $(t0, P0) = (0, 100)$ and $(t0 + \Delta t, P0 + \partial 2) = (8, 212)$

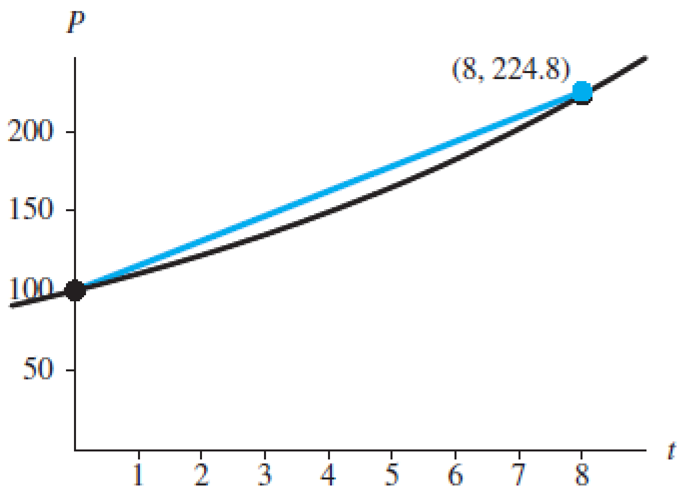
Estimate slope at midpoint between (0, 100) and (8, 212)

Third Estimate, ∂3

- Using the slope of this line, we determine the third estimated change in *P* over $\Delta t = 8$, ∂3, as follows:
- ∂3 = ((0.1)(156)) (8) = 15.6 (8) = 124.8
- Figure below displays this third estimate of ΔP, ∂3, as the length of the colored, vertical dashed line to the point, (8, 224.8), both of which are in color



Third estimate of change in P, $\partial_3 = 124.8$



Endpoint $(t_0 + \Delta t,\ P_0 + \partial_3) = (8, 224.8)$

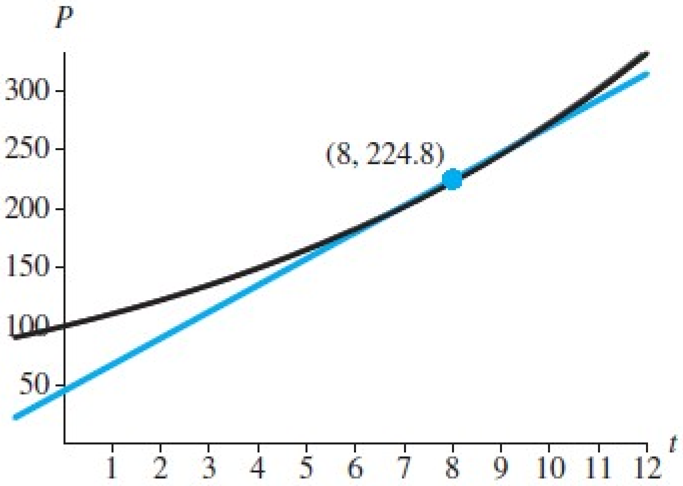
Third Estimate, ∂3

The third estimate for the change in P employs the estimated slope at the point $(t_{n-1} + 0.5\Delta t, P_{n-1} + 0.5\partial_2)$, as follows:

$$\partial_3 = f(t_{n-1} + 0.5\Delta t, P_{n-1} + 0.5\partial_2)\Delta t$$

Fourth Estimate, ∂4

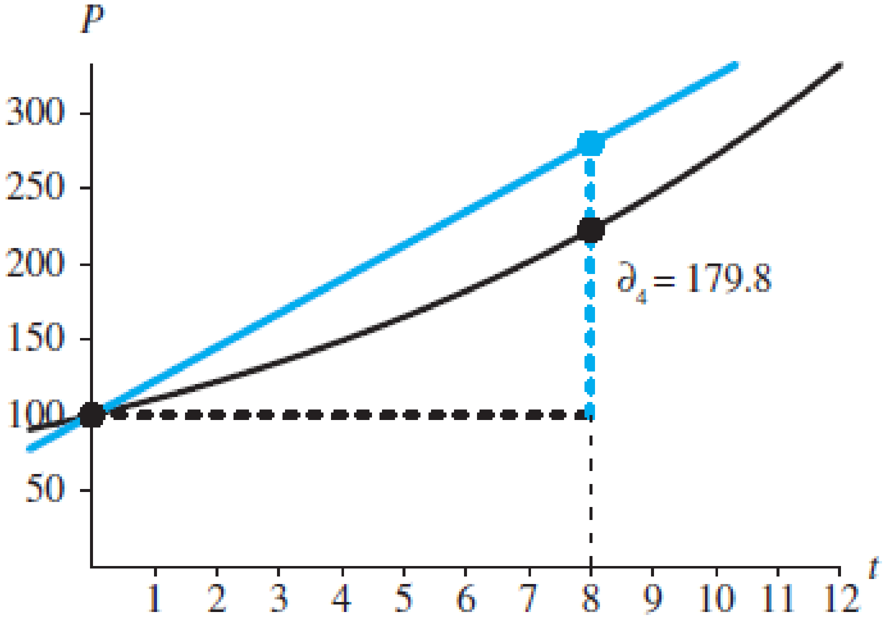
- The fourth estimate, ∂4, of the change in P over the interval of length Δt occurs at the end of the interval.
- Using the third estimate ∂3, the endpoint is ($t_0 + \Delta t$, P_0 + ∂3) = (8, 224.8) for the example under discussion.
- With $dP/dt = f(t, P) = 0.1P$, The following computation estimates the slope at the endpoint: $f(8, 224.8) = 0.1(224.8) = 22.48$
- Below figure shows the endpoint along with the exponential function and tangent line of slope 22.48 through that point.



Estimate slope at (8, 224.8)

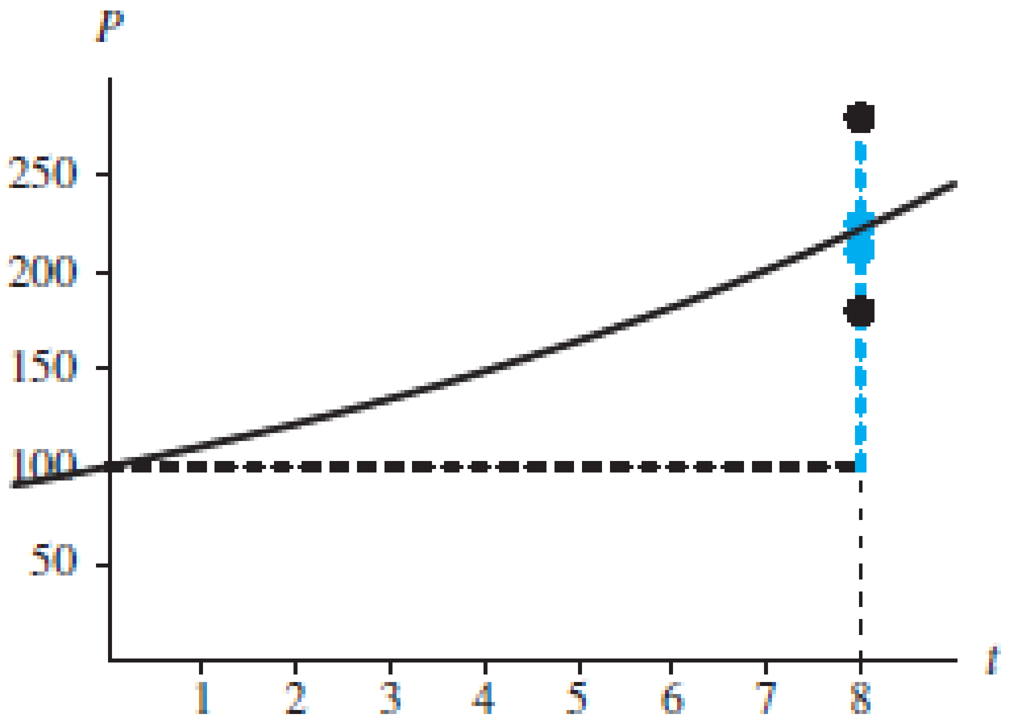
Fourth Estimate, ∂4

- With this slope, we estimate ∂4, the increase in *P* as *t* increases, by $\Delta t = 8$, as follows:
- $\partial 4 = ((0.1)(224.8))(8) = 22.48(8) = 179.84$
- This fourth estimate of ΔP is the length of the boldfaced, vertical dashed line to the point lor in the below figure. Using ∂4, 2



Fourth estimate of change in *P*, $\partial_4 = 179.84$

Four estimates of RK 4 method



Four estimates of ΔP

Using the four estimates

- To determine the Runge-Kutta 4 estimate of $P1$, we add to $P0 = 100$ a weighted average of ∂1, ∂2, ∂3, and ∂4. Giving twice the weight to the estimates at the midpoint, the computation is as follows:
- $P_1 = P_0 + (\partial 1 + 2\partial 2 + 2\partial 3 + \partial 4)/6$
- $= 100 + (80 + 2 \bullet 112 + 2 \bullet 124.8 + 179.84)/6$
- $= 100 + 122.24$
- $=$

The Runge-Kutta 4 estimate of P_n is as follows:

$$P_n = P_{n-1} + (\partial_1 + 2\partial_2 + 2\partial_3 + \partial_4)/6$$

Runge-Kutta 4 Algorithm

Runge-Kutta 4 Algorithm with $f(t_{n-1}, P_{n-1})$ indicating the derivative dP/dt at step $n - 1$

Initialize t_0 and P_0
Initialize *NumberOfSteps*
for n going from 1 to *NumberOfSteps* do the following:

$$t_n = t_0 + n\,\Delta t$$
$$\partial_1 = f(t_{n-1}, P_{n-1})\,\Delta t$$
$$\partial_2 = f(t_{n-1} + 0.5\Delta t, P_{n-1} + 0.5\partial_1)\Delta t$$
$$\partial_3 = f(t_{n-1} + 0.5\Delta t, P_{n-1} + 0.5\partial_2)\Delta t$$
$$\partial_4 = f(t_{n-1} + \Delta t, P_{n-1} + \partial_3)\Delta t$$
$$P_n = P_{n-1} + (\partial_1 + 2\partial_2 + 2\partial_3 + \partial_4)/6$$

Error

Relative Errors of $P(100)$ for Various Time Changes and Simulation Methods, where $dP/dt = 0.10P$ with $P_0 = 100$

Relative Errors at Time 100			
Δt	*Euler's*	*EPC*	*Runge-Kutta 4*
1.00	37.4%	1.53%	0.000767%
0.50	21.5%	0.40%	0.000050%
0.25	11.6%	0.10%	0.000003%