CS368 MATLAB Programming

Lecture 12

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Numerical Differentiation

Math

- Derivatives can be approximated using Newton's formula,

$$\frac{df}{dx} \approx \frac{f(x+h) - f(x)}{h},$$

for some small h close to 0.

- The derivative of f at x is usually approximated by,

$$\frac{df}{dx} \approx \frac{f(x+h) - f(x-h)}{2h}.$$

Numerical Differentiation Diagram

Math

Finite Differences

Math

- There are more accurate approximations using finite differences, for example,

$$\frac{df}{dx} \approx \frac{-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x-2h)}{12h},$$

for some small h close to 0.

Partial Derivatives

Math

- Partial derivatives of a multivariate function are derivatives with respect to one of the variables holding the other variables constant.

$$\frac{\partial f(x,y)}{\partial x} \approx \frac{f(x+h,y) - f(x-h,y)}{2h}.$$

$$\frac{\partial f(x,y)}{\partial y} \approx \frac{f(x,y+h) - f(x,y-h)}{2h}.$$

Partial Derivatives Too

Math

- Higher order derivatives can be approximated in a similar way,

$$\frac{\partial^2 f(x,y)}{\partial x^2} \approx \frac{f(x+h,y) - 2f(x,y) + f(x-h,y)}{h^2}.$$
$$\frac{\partial^2 f(x,y)}{\partial y^2} \approx \frac{f(x,y+h) - 2f(x,y) + f(x,y-h)}{h^2}.$$

and,

$$\frac{\partial f(x,y)}{\partial x \partial y} \approx \frac{f(x+h,y+h) + f(x-h,y-h)}{4h^2} - \frac{f(x+h,y-h) + f(x-h,y+h)}{4h^2}.$$

Gradient

Math

- The gradient of a multivariate function is the vector of (partial) derivatives, one for each variable.

$$\nabla f(x, y) = \begin{bmatrix} \frac{\partial f}{\partial x} \\ \frac{\partial f}{\partial y} \end{bmatrix}.$$

Gradient Quiz Question

Quiz

Derivative as a Function

Code

- It is possible to compute the numerical derivative as a function (a MATLAB function, not a closed form expression of the function).

```
function d = df(f)
   h = 0.0001;
   d = @(x)((f(x + h) - f(x - h)) / (2 * h));
end
```

Automatic Differentiation

Code

- *diff* (y) computes the difference between consecutive elements of y and returns $(y_2 - y_1, y_3 - y_2, \ldots, y_n - y_{n-1})$ and can be used to approximate the derivative of the discretized function $y = f(x)$.
- *diff* (f) computes the derivative of f and returns a function. It requires MATLAB's Symbolic Math Toolbox.

Numerical Integration or Quadrature

Math

- Definite integrals can be approximated using finite Riemann sums.
- If the right Riemann sum is used, then,

$$\int_{x_0}^{x_1} f(x)\,dx \approx \sum_{i=1}^{n} f(x_0 + i \cdot h)\,h,$$

for $h = \dfrac{x_1 - x_0}{n}$, for some large n.

- If the left Riemann sum is used, then,

$$\int_{x_0}^{x_1} f(x)\,dx \approx \sum_{i=1}^{n} f(x_0 + (i-1) \cdot h)\,h,$$

for $h = \dfrac{x_1 - x_0}{n}$, for some large n.

Numerical Integration Diagram

Math

Midpoint Rule

- If the midpoint rule is used, then,

$$\int_{x_0}^{x_1} f(x)\,dx \approx \sum_{i=1}^{n} f(x_0 + (i - 0.5) \cdot h)\, h,$$

for $h = \dfrac{x_1 - x_0}{n}$, for some large n.

- If the trapezoidal rule is used, then,

$$\int_{x_0}^{x_1} f(x)\,dx \approx \sum_{i=1}^{n} \frac{1}{2} \left(f(x_0 + i \cdot h) + f(x_0 + (i - 1) \cdot h)\right) h,$$

for $h = \dfrac{x_1 - x_0}{n}$, for some large n.

Adaptive and Monte Carlo

Math

- The points at which the function is evaluated can be chosen adaptively or randomly.
- For example, smaller h can be used when $f'(x)$ is large and larger h can be used when $f'(x)$ is small.

Double Integral

Math

- Finite Riemann sums can be used to approximate multiple integrals too.

$$\int_{x_0}^{x_1} \int_{y_0}^{y_1} f(x, y)\, dxdy$$
$$\approx \sum_{i=1}^{n} \sum_{j=1}^{m} f\left(x_0 + (i - 0.5) \cdot h, y_0 + (j - 0.5) \cdot k\right) \cdot hk,$$

for $h = \dfrac{x_1 - x_0}{n}, k = \dfrac{y_1 - y_0}{m}$, for some large n, m.

- If $n \times m$ is too large, sometimes, Monte Carlo methods are used instead.

Indefinite Integral as a Function

Code

- It is possible to compute the numerical integral as a function (a MATLAB function, not a closed form expression of the function). Instead of having the $+C$ at the end, an arbitrary constant is used.

```
function d = df(f)
   h = 0.01;
   d = @(x)(sum(f(h:h:x)) * h);
end
```

- This approximation uses the right Riemann sum and it does not work on improper integrals.

Integration

Code

- *integral (f, x0, x1)* finds the numerical definite integral $\int_{x_0}^{x_1} f(x)\,dx$.
- *int (f)* finds the indefinite integral of f and returns a function. It requires MATLAB's Symbolic Math Toolbox.

Integral Quiz Questions

Quiz

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