16-745 Optimal Control Lecture 3

Reid Graves

January 22, 2025

1 Last Time

- Stability
- Discrete Time Simulation
- Forward/Backward Euler
- RK4 (should be your go-to)

2 Today

- Notation
- Root Finding
- Minimization

3 Some Notation

- Given $f(x) : \mathbb{R}^n \to \mathbb{R}$

  $$\frac{\partial f}{\partial x} \in \mathbb{R}^{1\times n} \text{ is a } \textbf{Row Vector}$$

  Because if you write it in this format, then the chain rule works.

- This is because $\frac{\partial f}{\partial x}$ is the linear operator mapping of Δx into Δf:

  $$f(x + \Delta x) \approx f(x) + \frac{\partial f}{\partial x}\Delta x$$

- Similarly $g(y) : \mathbb{R}^m \to \mathbb{R}^n$

  $$\frac{\partial g}{\partial y} \in \mathbb{R}^{n\times m} \text{ because:}$$

  $$g(y + \Delta y) \approx g(y) + \frac{\partial g}{\partial y}\Delta y$$

- These conventions make the chain rule work:

  $$f(g(y + \Delta y)) \approx f(g(y)) + \frac{\partial f}{\partial x}|_{g(y)}\frac{\partial g}{\partial y}|_{y}\Delta y$$

- For convenience, we will define:

$$\nabla f(x) = \left(\frac{\partial f}{\partial x}\right)^T \in \mathbb{R}^{n\times 1} \quad \textbf{Column Vector}$$
$$\nabla^2 f(x) = \frac{\partial}{\partial x}(\nabla f(x)) = \frac{\partial^2 f}{\partial x^2} \in \mathbb{R}^{n\times n}$$
$$f(x+\Delta x) = f(x) + \frac{\partial f}{\partial x}\Delta x + \frac{1}{2}\Delta x^T \frac{\partial^2 f}{\partial x^2}\Delta x$$

4 Root Finding

- Given $f(x)$, find x^* such that $f(x^*) = 0$

4.1 Example: Equilibrium of a continuous time dynamics system

- Closely related: fixed point:

$$f(x^*) = x^*$$

(equilibrium of discrete time dynamics)

4.2 Fixed-point Iteration

- Simplest solution method
- If fixed point is stable, just "iterate the dynamics" until convergence
- Only works if x^* is a stable equilibrium point and if initial guess is in the basin of attraction
- Can converge slowly (depends on f)

4.3 Newton's Method

- Fit a linear approximation to $f(x)$:

$$f(x+\Delta x) \approx f(x) + \frac{\partial f}{\partial x}|_x \Delta x$$

- Set the approximation to zero and solve for Δx:

$$f(x) + \frac{\partial f}{\partial x}\Delta x = 0 \rightarrow \Delta x = \left(\frac{\partial f}{\partial x}\right)^{-1} f(x)$$

- Apply correction:

$$x \leftarrow x + \Delta x$$

- Repeat until convergence

4.4 Example: Backward Euler

$$
\begin{aligned}
f(x_{n+1}, x_n, u_n) &= 0 \\
x_{n+1} &= x_n + hf(x_{n+1}) \text{ (Evaluate f at future time)} \\
\rightarrow f(x_{n+1}, x_n, u_n) &= x_{n+1} - x_n - hf(x_{n+1}) = 0
\end{aligned}
$$

- Very fast convergence with Newton (Quadratic)- Cancels out the first term in the Taylor expansion
- Can get machine precision
- Most expensive part is solving a linear system $\mathcal{O}(n^3)$ (why it isn't used in machine learning)
- Can improve complexity by taking advantage of problem structure/sparsity (more later)

5 Minimization

$$min_x f(x), \quad f(x) : \mathbb{R}^n \rightarrow \mathbb{R}$$

- If f is smooth, $\frac{\partial f}{\partial x}|_{x^*} = 0$ at a local minimum
- Now we have a root finding problem $gradf(x) = 0$

$$\Rightarrow \text{Apply Newton!}$$

$$
\begin{aligned}
\nabla f(x + \Delta x) \approx \nabla f(x) + \frac{\partial}{\partial x}(\nabla(f(x))\Delta x = 0 \\
\Rightarrow \Delta x = -(\nabla^2 f(x)^{-1} \nabla f(x) \\
x \leftarrow x + \Delta x
\end{aligned}
$$

Repeat until convergence

- Intuition:
  - Fit a quadratic approximation to $f(x)$
  - Exactly minimize approximation

5.1 Example

$$min_x f(x) = x^4 + x^3 - x^2 - x$$

- Start at $1.0, -1.5, 0$ (0 maximized!)
- Takeaway messages
  - Newton is a **local root finding** method
  - will converge to the closest fixed point to the initial guess (min, max, saddle)
- Sufficient conditions

- $\nabla f = 0$ "first order necessary condition" for a minimum, not a sufficient condition
- Let's look at scalar case:

$$\Delta x = -\left(\nabla^2 f\right)^{-1} \nabla f$$

- $\nabla^2 f$ is the "learning rate/step size"

$$\nabla^2 f > 0 \Rightarrow \text{ descent (minimization)}$$
$$\nabla^2 f < 0 \Rightarrow \text{ ascent (maximization)}$$

- In $\mathbb{R}^n$, $\nabla^2 f > 0$, $\nabla^2 f \in S^n_{++}$

$$\text{(Positive definite)} \Rightarrow \text{descent}$$

- if $\nabla^2 f > 0$ everywhere $(\forall x) \Rightarrow f(x)$ is strongly convex

$$\Rightarrow \text{Can always sove with Newton}$$

- Usually not the case for hard/non-linear problems

• Regularization:
  - Practical solution to make sure we always minimize:

$$\begin{aligned} H &\leftarrow \nabla^2 f \\ \text{while } H &\text{ not positive definite} \\ H \leftarrow H + \beta I \text{ Scalar hyperparameter } \beta &> 0 \\ \text{end} & \\ \Delta x &= -H^{-1} \nabla f \\ x &\leftarrow x + \Delta x \end{aligned}$$

  - Also called "damped newton" (shrinks steps)
  - Guarantees descent

• Example:
  - Regularizaiton makes sure we minimize
  - What about overshoot? (next time)