Lecture 3: Numerical Differentiation

Introduction to Data Analysis Techniques

1 Taylor Approximation

Convention 1.1 (Standing Smoothness Assumption). [conv:smoothness-assumption] Continuity, differentiability, and smooth function spaces; real-analysis
Unless stated otherwise, every function $f : \mathbb{R} \to \mathbb{R}$ considered in this lecture is assumed to satisfy $f \in C^{\infty}_{\mathbb{R}\to\mathbb{R}}$. This means that its derivatives of every order, including order zero, are continuous

Definition 1.1. [def:taylor-polynomial-generator]
Taylor terms; real-analysis, pending transfer
The Taylor term constructor takes f, then a centre a, then an order n, and returns the nth term as a polynomial function

$$\begin{aligned}\text{TaylorGen} &: C^{\infty}_{\mathbb{R}\to\mathbb{R}} \to \mathbb{R} \to \mathbb{N} \to (\mathbb{R} \to \mathbb{R}) \\ &\equiv f \mapsto \big(a \mapsto \big(n \mapsto \big(x \mapsto \frac{\mathrm{D}^n(f)(a)}{n!} \cdot (x-a)^n\big)\big)\big)\end{aligned}$$

Definition 1.2. [def:taylor-polynomial]
Taylor polynomials; real-analysis, pending transfer
The N-th order Taylor polynomial generator is defined as

$$\begin{aligned}\text{TaylorPoly} &: C^{\infty}_{\mathbb{R}\to\mathbb{R}} \to \mathbb{R} \to \mathbb{N} \to (\mathbb{R} \to \mathbb{R}) \\ &\equiv f \mapsto a \mapsto N \mapsto x \mapsto \sum_{0}^{N} (n \mapsto \text{TaylorGen}(f)(a)(n)(x))\end{aligned}$$

This uses the zero-based finite index ranges

Convention 1.2. [conv:taylor-polynomial-notation]
Taylor polynomial notation; real-analysis, pending transfer
Fix $f \in C^{\infty}_{\mathbb{R}\to\mathbb{R}}$ and $a \in \mathbb{R}$. Construct the term and polynomial families

$$\begin{aligned}T &: \mathbb{N} \to (\mathbb{R} \to \mathbb{R}) \equiv \text{TaylorGen}(f)(a), \\ P &: \mathbb{N} \to (\mathbb{R} \to \mathbb{R}) \equiv \text{TaylorPoly}(f)(a)\end{aligned}$$

Thus $T(n)$ is the nth term function, while $P(N)$ is the polynomial through order N. Their values satisfy

$$\forall N \in \mathbb{N},\ \forall x \in \mathbb{R}, \quad P(N)(x) = \sum_{0}^{N} \big(n \mapsto T(n)(x)\big)$$

The zeroth term is $T(0)(x) = f(a)$, so $P(0) = x \mapsto f(a)$. The names T and P are local to the chosen f and a; construct them before using them in a derivation

Definition 1.3. [def:taylor-remainder] Fix $f \in C^{\infty}_{\mathbb{R}\to\mathbb{R}}$ and $a \in \mathbb{R}$
Construct $P \equiv \text{TaylorPoly}(f)(a)$. The Taylor remainder family is

$$R : \mathbb{N} \to (\mathbb{R} \to \mathbb{R}) \equiv n \mapsto \big(x \mapsto f(x) - P(n)(x)\big)$$

Thus, for every $n \in \mathbb{N}$ and $x \in \mathbb{R}$,

$$f(x) = P(n)(x) + R(n)(x)$$

For fixed f, a, and n, different values of x may give different remainder values $R(n)(x)$

Theorem 1.1 (Finite Taylor Expansion). [thm:finite-taylor-expansion]
Taylor expansion with remainder; real-analysis, pending transfer
Let $f \in C^{\infty}_{\mathbb{R}\to\mathbb{R}}$, $n \in \mathbb{N}$, and $a \in I$, where $I \subseteq \mathbb{R}$ is an open interval. Construct the polynomial family

$$P : \mathbb{N} \to (\mathbb{R} \to \mathbb{R}) \equiv \mathrm{TaylorPoly}(f)(a)$$

Let R be the corresponding remainder family. Then

$$\forall x \in I \setminus \{a\},\ \exists \xi \in \big(\min(a,x), \max(a,x)\big) :$$
$$f(x) = P(n)(x) + \underbrace{\frac{\mathrm{D}^{n+1}(f)(\xi)}{(n+1)!} \cdot (x-a)^{n+1}}_{R(n)(x)}$$

At $x = a$, $f(a) = P(n)(a)$ and $R(n)(a) = 0$. The intermediate point ξ may depend on x and n; the quantifier order is $\forall x\, \exists \xi$

Definition 1.4 (Taylor Series). [def:taylor-series]
Taylor series and convergence; real-analysis, pending transfer
Let $f \in C^{\infty}_{\mathbb{R}\to\mathbb{R}}$ and $a \in \mathbb{R}$. Construct $P \equiv \mathrm{TaylorPoly}(f)(a)$ as in the polynomial-family notation. Its *Taylor-series sum* at x, when it exists, is

$$\lim\big(N \mapsto P(N)(x)\big)$$

Each partial sum includes Taylor terms indexed by $0, \ldots, N$. The displayed expression equals $f(x)$ precisely when $f(x) - P(N)(x) \to 0$ as $N \to \infty$

Remark 1.1 (Taylor Series Approximation). [rem:taylor-series-approx]
Taylor approximation and remainder control; real-analysis, pending transfer
We can truncate the Taylor series to obtain a finite approximation. The Taylor expansion with remainder expresses its error under suitable differentiability assumptions
Adding terms does not automatically improve the approximation. The remainder must be controlled; equality with the infinite series requires that the remainder tend to zero as the number of terms increases

Example 1.1 (Electric Field of a Dipole for $x \gg a$). [eg:dipole-field] Consider the electric field on the axis of a dipole with charges $+q$ at $x = a$ and $-q$ at $x = -a$, where $a > 0$ and $x > a$

$$E = \frac{q}{4\pi\varepsilon_0} \cdot \left[\frac{1}{(x-a)^2} - \frac{1}{(x+a)^2}\right]$$

Expanding in a/x using the Taylor series gives

$$E = \frac{q}{4\pi\varepsilon_0 \cdot x^2} \cdot \left[4\frac{a}{x} + 8\left(\frac{a}{x}\right)^3 + 12\left(\frac{a}{x}\right)^5 + \cdots\right]$$

Keeping the first two nonzero terms gives an approximation for $x \gg a$

$$E \approx \frac{q}{4\pi\varepsilon_0 \cdot x^2} \cdot \left[4\frac{a}{x} + 8\left(\frac{a}{x}\right)^3\right]$$

The leading term is proportional to x^{-3}

Taylor expansion in two variables through second order, including mixed derivatives; real-analysis

2 Error Orders

Convention 2.1 (Approximation Error)**.** [conv:approximation-error] Let X be a common input set, and let $u, v : X \to \mathbb{R}$ denote the computed and target functions, respectively. We write their error as

$$E : X \to \mathbb{R} \equiv t \mapsto \big(u(t) - v(t)\big)$$

Thus error means computed value minus target value; its magnitude is $|E(t)|$

Definition 2.1 (Big-O at Zero)**.** [def:big-o-at-zero]
Big-O as the argument tends to zero from above; real-analysis, pending transfer
Put $\mathcal{F} \equiv (\mathbb{R}_{>0} \to \mathbb{R})$. For $h \to 0^+$, define

$$\begin{aligned} &\mathrm{BigO} : \mathcal{F} \to \mathcal{P}(\mathcal{F}) \\ &\quad \equiv g \mapsto \{E \in \mathcal{F} \mid \exists C, \delta \in \mathbb{R}_{>0},\ \forall h \in (0, \delta),\ |E(h)| \le C \cdot |g(h)|\} \end{aligned}$$

The constants C and δ are independent of h

Convention 2.2 (Big-O Notation)**.** [conv:big-o-notation] Write $\mathcal{O}(g) \equiv \mathrm{BigO}(g)$ and use $E = \mathcal{O}(g)$ for $E \in \mathcal{O}(g)$. For $p \in \mathbb{N}$, the shorthand for a power bound is

$$E(h) = \mathcal{O}(h^p) \quad \iff \quad E \in \mathrm{BigO}\big(h \mapsto h^p\big)$$

Here the limit is $h \to 0^+$; functions on $\mathbb{R}$ are restricted to positive inputs. For $h \to +\infty$, the corresponding bound instead holds for all $h > H$, for some fixed $H > 0$

3 Numerical Differentiation

Derivative at a point and differentiability; real-analysis, pending transfer

Convention 3.1 (Forward Difference)**.** [conv:forward-difference] Fix $f \in C^\infty_{\mathbb{R}\to\mathbb{R}}$. Given $h > 0$, write

$$f'_{h,+} : \mathbb{R} \to \mathbb{R} \equiv x \mapsto \frac{f(x+h) - f(x)}{h}$$

For small h, this approximates the derivative pointwise:

$$\forall x \in \mathbb{R}, \quad f'_{h,+}(x) \approx \mathrm{D}(f)(x)$$

The required step size may depend on the chosen x

Convention 3.2 (Backward Difference)**.** [conv:backward-difference] Fix $f \in C^\infty_{\mathbb{R}\to\mathbb{R}}$. Given $h > 0$, write

$$f'_{h,-} : \mathbb{R} \to \mathbb{R} \equiv x \mapsto \frac{f(x) - f(x-h)}{h}$$

For small h, this approximates the derivative pointwise:

$$\forall x \in \mathbb{R}, \quad f'_{h,-}(x) \approx \mathrm{D}(f)(x)$$

The required step size may depend on the chosen x

Definition 3.1 (Numerical Derivative Error)**.** [def:numerical-derivative-error] Fix $f : \mathbb{R} \to \mathbb{R}$ under the standing smoothness assumption. For each $h > 0$, let $f'_h : \mathbb{R} \to \mathbb{R}$ denote a chosen numerical approximation to $\mathrm{D}(f)$. Applying the error convention, its error function is

$$E_h : \mathbb{R} \to \mathbb{R} \equiv x \mapsto \big(f'_h(x) - \mathrm{D}(f)(x)\big)$$

Here f'_h denotes the approximation, while $\mathrm{D}(f)$ denotes the exact derivative

Proposition 3.1 (First-Order Difference Errors). [prop:first-order-difference-errors] *Let $f : \mathbb{R} \to \mathbb{R}$ satisfy the standing smoothness assumption. Let E_h^+ and E_h^- be the error functions of the forward and backward approximations, respectively. Then*

$$\forall x \in \mathbb{R},\ \forall h \in \mathbb{R}_{>0},\ \exists \xi_+ \in (x, x+h),\ \exists \xi_- \in (x-h, x) :$$
$$E_h^+(x) = \frac{h}{2!} \cdot \mathrm{D}^2(f)(\xi_+),$$
$$E_h^-(x) = -\frac{h}{2!} \cdot \mathrm{D}^2(f)(\xi_-)$$

For each fixed x, the functions $h \mapsto E_h^+(x)$ and $h \mapsto E_h^-(x)$ belong to $\mathcal{O}(h \mapsto h)$ as $h \to 0^+$, meaning

$$\forall x \in \mathbb{R},\ \exists C, \delta \in \mathbb{R}_{>0},\ \forall h \in (0, \delta) :$$
$$|E_h^+(x)| \le C \cdot h, \qquad |E_h^-(x)| \le C \cdot h$$

The intermediate points and error bounds may depend on x; the intermediate points may also depend on h

Proof. Fix $x \in \mathbb{R}$ and $h > 0$. By the finite Taylor expansion, there exists $\xi_+ \in (x, x+h)$ such that

$$f(x+h) = f(x) + h \cdot \mathrm{D}(f)(x) + \frac{h^2}{2!} \cdot \mathrm{D}^2(f)(\xi_+)$$

Rearranging and dividing by h yields

$$\mathrm{D}(f)(x) = \frac{f(x+h) - f(x)}{h} - \frac{h}{2!} \cdot \mathrm{D}^2(f)(\xi_+)$$

For the forward approximation, substituting into the error function gives

$$\begin{aligned} E_h^+(x) &= f'_{h,+}(x) - \mathrm{D}(f)(x) \\ &= \frac{f(x+h) - f(x)}{h} - \mathrm{D}(f)(x) \\ &= \frac{f(x+h) - f(x)}{h} - \left(\frac{f(x+h) - f(x)}{h} - \frac{h}{2!} \cdot \mathrm{D}^2(f)(\xi_+) \right) \\ &= \frac{h}{2!} \cdot \mathrm{D}^2(f)(\xi_+) \end{aligned}$$

Since $\mathrm{D}^2(f)$ is continuous, there exist $M, \delta > 0$ such that $|\mathrm{D}^2(f)(y)| \le M$ whenever $|y - x| < \delta$. Hence, for $0 < h < \delta$,

$$|E_h^+(x)| = \frac{h}{2!} \cdot |\mathrm{D}^2(f)(\xi_+)| \le \frac{M}{2!} \cdot h$$

Thus $E_h^+(x) = \mathcal{O}(h)$ as $h \to 0^+$. The backward case follows analogously by expanding $f(x-h)$ about x □

Convention 3.3 (Central Difference). [conv:central-difference] Fix $f \in C^\infty_{\mathbb{R}\to\mathbb{R}}$ and $h > 0$. Averaging the forward and backward approximations gives

$$f'_{h,0} : \mathbb{R} \to \mathbb{R} \equiv x \mapsto \frac{f'_{h,+}(x) + f'_{h,-}(x)}{2}$$

Thus, pointwise for small h,

$$\forall x \in \mathbb{R}, \quad f'_{h,0}(x) = \frac{f(x+h) - f(x-h)}{2h} \approx \mathrm{D}(f)(x)$$

Proposition 3.2 (Central Difference Error). [prop:central-difference-error] *For the central approximation, construct*

$$E_h^0 : \mathbb{R} \to \mathbb{R} \equiv x \mapsto \left(f'_{h,0}(x) - \mathrm{D}(f)(x)\right)$$

The error is of second order pointwise as $h \to 0^+$*:*

$$\forall x \in \mathbb{R},\ \exists C, \delta \in \mathbb{R}_{>0},\ \forall h \in (0, \delta), \quad |E_h^0(x)| \leq C \cdot h^2$$

Equivalently, for each fixed x*,* $E_h^0(x) = \mathcal{O}(h^2)$

Proof. Fix $x \in \mathbb{R}$ and $h > 0$. Taylor expansion about x gives $\xi_+ \in (x, x+h)$ and $\xi_- \in (x-h, x)$ such that

$$f(x \pm h) = f(x) \pm h \cdot \mathrm{D}(f)(x) + \frac{h^2}{2!} \cdot \mathrm{D}^2(f)(x) \pm \frac{h^3}{3!} \cdot \mathrm{D}^3(f)(\xi_\pm)$$

Subtracting cancels the constant and quadratic terms. Hence

$$\begin{aligned} E_h^0(x) &= \frac{f(x+h) - f(x-h)}{2h} - \mathrm{D}(f)(x) \\ &= \frac{h^2}{2 \cdot 3!} \cdot \left(\mathrm{D}^3(f)(\xi_+) + \mathrm{D}^3(f)(\xi_-)\right) \end{aligned}$$

Continuity of $\mathrm{D}^3(f)$ gives $M, \delta > 0$ such that $|\mathrm{D}^3(f)(y)| \leq M$ whenever $|y - x| < \delta$. Thus, for $0 < h < \delta$,

$$|E_h^0(x)| \leq \frac{M}{3!} \cdot h^2$$

Taking $C = M/3!$ proves the stated bound □

Convention 3.4 (Central Second Derivative). [conv:central-second-derivative] Fix $f \in C^\infty_{\mathbb{R}\to\mathbb{R}}$ and $h > 0$. Write

$$f''_{h,0} : \mathbb{R} \to \mathbb{R} \equiv x \mapsto \frac{f(x+h) - 2 \cdot f(x) + f(x-h)}{h^2}$$

Pointwise for small h,

$$\forall x \in \mathbb{R}, \quad f''_{h,0}(x) \approx \mathrm{D}^2(f)(x)$$

Proposition 3.3. [prop:central-second-derivative-error] *The error is* $\mathcal{O}(h^2)$ *pointwise as* $h \to 0^+$

Proof. Fix $x \in \mathbb{R}$. Expand, add, and rearrange:

$$\begin{aligned} f(x+h) &= f(x) + h \cdot \mathrm{D}(f)(x) + \frac{h^2}{2!} \cdot \mathrm{D}^2(f)(x) + \frac{h^3}{3!} \cdot \mathrm{D}^3(f)(x) + \mathcal{O}\left(h^4\right), \\ f(x-h) &= f(x) - h \cdot \mathrm{D}(f)(x) + \frac{h^2}{2!} \cdot \mathrm{D}^2(f)(x) - \frac{h^3}{3!} \cdot \mathrm{D}^3(f)(x) + \mathcal{O}\left(h^4\right), \\ f(x+h) + f(x-h) &= 2 \cdot f(x) + h^2 \cdot \mathrm{D}^2(f)(x) + \mathcal{O}\left(h^4\right), \\ \frac{f(x+h) - 2 \cdot f(x) + f(x-h)}{h^2} &= \mathrm{D}^2(f)(x) + \mathcal{O}\left(h^2\right) \end{aligned}$$

□

TODO: Implement the difference formulas for sine at x=1; compare with the exact derivatives over several step sizes

4 Euler's Method

Convention 4.1 (Approximate Functions). [conv:approximate-function-notation] Fix $f \in C^\infty_{\mathbb{R}\to\mathbb{R}}$ and a set $X \subseteq \mathbb{R}$ of evaluation points. We use $f', f^\dagger : X \to \mathbb{R}$ for numerical approximations to the derivative and the original function, respectively:

$$\forall x \in X, \quad f'(x) \approx \mathrm{D}(f)(x), \qquad f^\dagger(x) \approx f(x)$$

The approximations depend on the chosen method and step size. For Euler's method, X is the time grid

Convention 4.2. [conv:forward-euler] For a small non-zero h, the forward Euler update is

$$f(x+h) = f(x) + h \cdot f'(x)$$

Proof. According to the definition of the forward deritive, ie

$$\mathrm{D}(f) \approx f' = \frac{f(x+h) - f(x)}{h}$$

Rearrange,

$$h \cdot f' = f(x+h) - f(x) \implies f(x+h) = f(x) + h \cdot f'(x)$$

□

Convention 4.3 (Procedure of Applying Forward Euler). [conv:procedure-forward-euler]

1. Start from the ODE $\forall x \in \mathbb{R}$, $\mathrm{D}(f)(x) = g(x, f(x))$, with known g and unknown f
2. Specify an initial point x_0 and a known value $y_0 = f(x_0)$
3. Choose a step size $h > 0$ and a number of steps $N \in \mathbb{N}_1$
4. Set $x_n \equiv x_0 + n \cdot h$ for $n \in \mathrm{Fin}(N+1)$, and define the grid $X \equiv \{x_n \mid n \in \mathrm{Fin}(N+1)\}$
5. Construct $f^\dagger : X \to \mathbb{R}$, starting with $f^\dagger(x_0) \equiv y_0$
6. For $n = 0, \ldots, N-1$, compute and store

$$f^\dagger(x_{n+1}) \equiv f^\dagger(x_n) + h \cdot g(x_n, f^\dagger(x_n))$$

7. Return $f^\dagger$, represented by the sampled pairs $(x_n, f^\dagger(x_n))$ for $n \in \mathrm{Fin}(N+1)$

Convention 4.4. [conv:backward-euler] For a small non-zero h, the backward Euler update is

$$f(x-h) = f(x) - h \cdot f'(x)$$

Proof. According to the definition of the backward difference, ie

$$\mathrm{D}(f) \approx f' = \frac{f(x) - f(x-h)}{h}$$

Rearrange,

$$h \cdot f' = f(x) - f(x-h) \implies f(x-h) = f(x) - h \cdot f'(x)$$

□

TODO: Derive the forward Euler update from the forward difference formula, then distinguish local and global errors
TODO: Solve x'=-x with x(0)=1 and compare with exp(-t) using several time steps

Convention 4.5 (Euler for Second-Order Dynamics). [conv:second-order-euler]

1. Start from the ODE $\forall x \in \mathbb{R}$, $\mathrm{D}^2(f)(x) = g(x, f(x), \mathrm{D}(f)(x))$, with known g and unknown f

2. Specify an initial point x_0 which has known values $y_0 = f(x_0)$ and $v_0 = \mathrm{D}(f)(x_0)$
3. Choose a step size $h > 0$ and a number of steps $N \in \mathbb{N}_1$
4. Set $x_n \equiv x_0 + n \cdot h$ for $n \in \mathrm{Fin}(N+1)$, and define the grid $X \equiv \{x_n \mid n \in \mathrm{Fin}(N+1)\}$
5. Construct $f^\dagger : X \to \mathbb{R}$, starting with $f^\dagger(x_0) \equiv y_0$
6. Construct $f' : X \to \mathbb{R}$, starting with $f'(x_0) \equiv v_0$
7. For $n = 0, \ldots, N-1$, compute and store

$$f'(x_{n+1}) \equiv f'(x_n) + h \cdot g(x_n, f^\dagger(x_n), f'(x_n))$$

$$f^\dagger(x_{n+1}) \equiv f^\dagger(x_n) + h \cdot f'(x_n)$$

   Both updates use values at x_n on their right-hand sides
8. Return $f^\dagger$, represented by the sampled pairs $(x_n, f^\dagger(x_n))$ for $n \in \mathrm{Fin}(N+1)$

Convention 4.6 (Euler for General-Order Dynamics)**.** [conv:general-order-euler]

1. Fix an order $m \in \mathbb{N}_1$ and a known function $g : \mathbb{R} \times \mathbb{R}^m \to \mathbb{R}$. Start from the ODE

$$\forall x \in \mathbb{R}, \quad \mathrm{D}^m(f)(x) = g\big(x, k \mapsto \mathrm{D}^k(f)(x)\big)$$

   The second input to g collects the derivatives of orders $0, \ldots, m-1$ into a vector
2. Specify an initial point x_0 and known initial values $a : \mathbb{R}^m$ satisfying

$$\forall k \in \mathrm{Fin}(m), \quad \mathrm{D}^k(f)(x_0) = a(k)$$

3. Choose $h > 0$ and $N \in \mathbb{N}_1$, and construct x_n and the grid X as in the forward Euler procedure
4. Construct a family $U : \mathrm{Fin}(m) \to (X \to \mathbb{R})$, where $U(k)$ approximates $\mathrm{D}^k(f)$, starting with

$$\forall k \in \mathrm{Fin}(m), \quad U(k)(x_0) \equiv a(k)$$

5. For $n = 0, \ldots, N-1$, collect the old state

$$s_n : \mathbb{R}^m \equiv k \mapsto U(k)(x_n)$$

   Compute and store

$$\forall k \in \mathrm{Fin}(m-1), \quad U(k)(x_{n+1}) \equiv U(k)(x_n) + h \cdot U(k+1)(x_n)$$

$$U(m-1)(x_{n+1}) \equiv U(m-1)(x_n) + h \cdot g(x_n, s_n)$$

   All right-hand sides use the old state at x_n
6. Return $f^\dagger \equiv U(0)$, or retain the full family U if approximations to the derivatives are also needed

For $m = 2$, $U(0) = f^\dagger$ and $U(1) = f'$, recovering the second-order procedure

TODO: Implement the pendulum model and compare results as the time step changes