A new solution for computing quick and accurate numerical derivatives

Results from the working paper:
Kostyrka, A. V. (2025). What are you doing, step size:
Fast computation of accurate numerical derivatives with finite precision.

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DEM internal seminar series
Faculty of Law, Economics, and Finance (FDEF)
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Presentation structure

Motivation and empirical applications

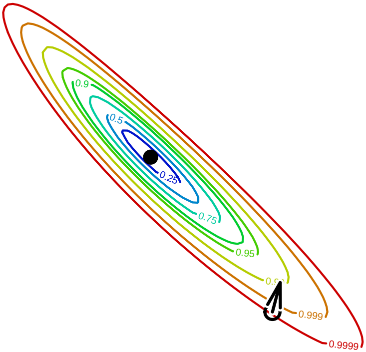
Contribution

I extend the existing numerical-methods literature and software ecosystem by:

1. Creating the open-source R package **pnd** for fast, parallelised numerical differentiation
   - First open-source parallel Jacobians, Hessians and higher-order-accurate gradients
2. Deriving analytical error bounds and optimal step-size rules for higher-order-accurate derivatives and second-order-accurate Hessians
3. Implementing previously proposed algorithms of step-size estimation, benchmarking their relative performance, and suggesting improved modifications

Which step size are we talking about?

Gradient-based optimisation



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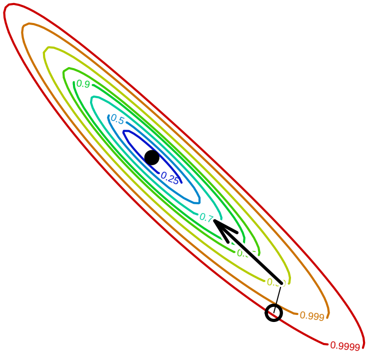

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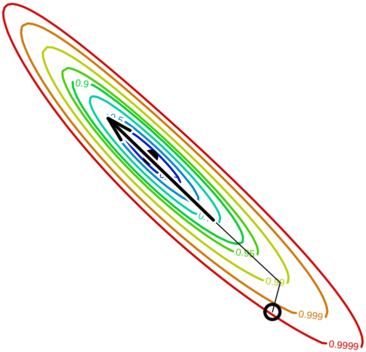

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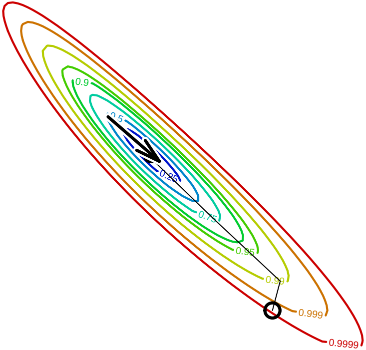

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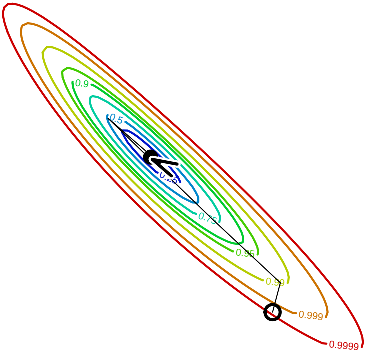

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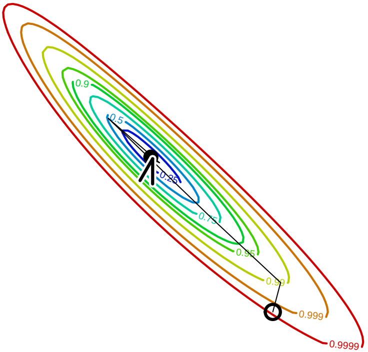

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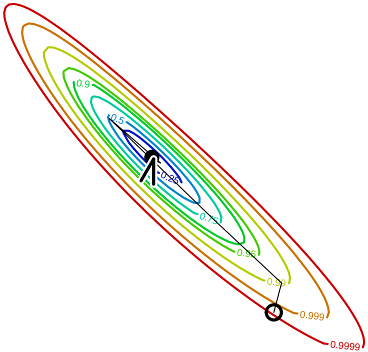

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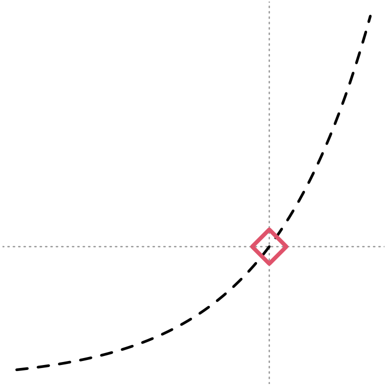

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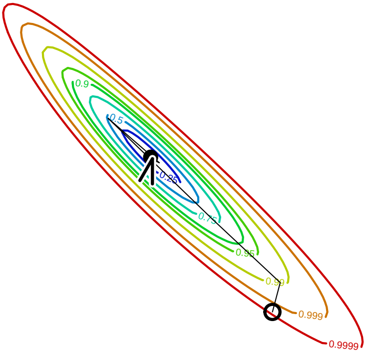

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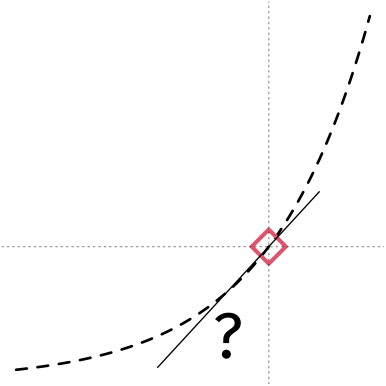

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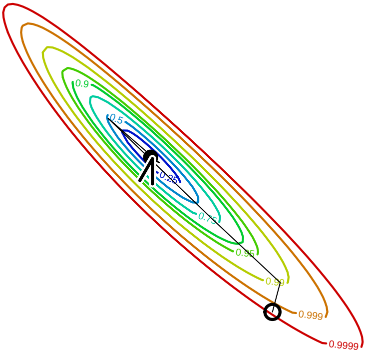

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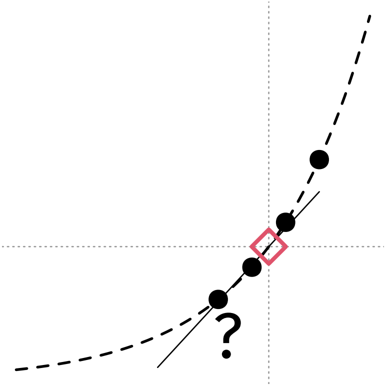

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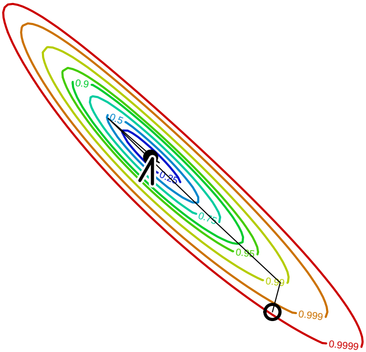

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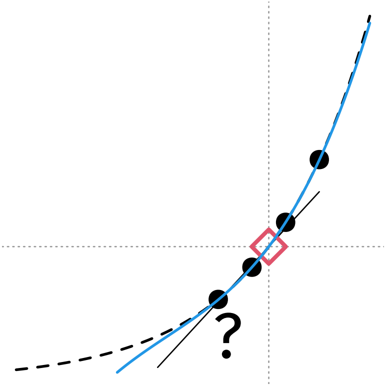

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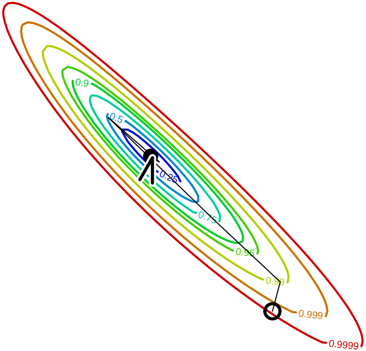

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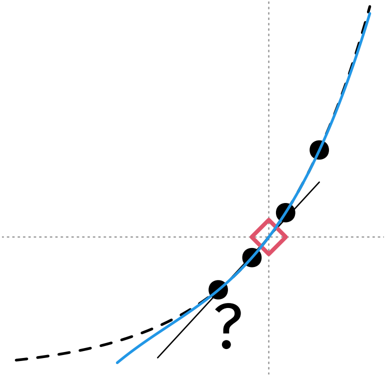


This one.

Which efficiency are we talking about?

- Huge data sets, billions of parameters, approximate solutions
- Big data sets, 1–1000 parameters, exact solutions $\Leftarrow$ **This one.**

Efficiency: parallelisation and full user control to reduce the guesswork carried out by the computer.

Accuracy: crucial for inference in science (inaccurate numerical Hessians $\Rightarrow$ wrong standard errors $\Rightarrow$ wrong conclusions about significance)

pnd *can* handle large Hessians, but the user should probably *avoid* inverting them (there could exist dedicated stable procedures).

Motivation and research question

- Researchers rely on optimisers, algorithms, black boxes etc. to ‘solve’ their models and carry out inference
- The end result is highly dependent on the solver quality
- Most popular modern optimisation techniques use numerical gradients for minimisation or maximisation

However, most software implementations yield **inaccurate** and **slow** numerical derivatives.

How can we attain the hardware-dependent accuracy bound for numerical derivatives?

Consequences of inaccurate derivatives

- Inexact solutions, values not at the optimum
- Wrong asymptotic-approximation-based inference
  - No causal interpretation or specification testing
  - Wrong standard errors and p values in non-linear models
- Worst case: negative Hessian-based variances
  - Methods based on empirical likelihood (EL) forego Hessians for inference, but converting a model into an EL-based one is non-trivial

Example from a financial application

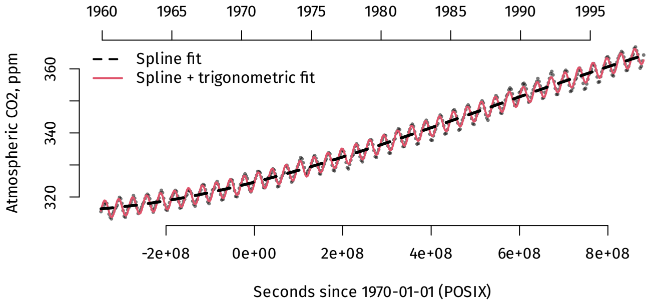
Simple AR(1)-GARCH(1, 1) model for NASDAQ log-returns, 1990–1994:

$$r_t = \mu + \rho r_{t-1} + \sigma_t U_t, \quad \sigma_t^2 = \omega + \alpha U_{t-1}^2 + \beta \sigma_{t-1}^2$$

Coefficient	Est.	t-stat (rugarch)	t-stat (fGarch)	t-stat (manual)
μ	0.0007	2.34	2.31	2.33
ρ	0.24	7.77	7.73	7.73
$\omega \times 10^3$	0.0098	NaN (default) or 65 (fallback)	3.09	3.08
α	0.13	11.1	4.27	4.26
β	0.73	39.6	10.9	11.0

Example from seasonal adjustment

Goal: estimate the slope of the seasonal component in CO_2 levels via the model $CO_2 = \beta' \mathrm{Spline}_3(x) + \gamma \sin(\frac{2\pi}{365.25 \cdot 86\,400} t - \delta)$.



Caveat: the time in the data based is encoded as POSIX time (seconds since 1970). Range of t: $-347155200 \ldots 880934400$.

Relative error: $\approx$100% (nonsensical dCO_2/dx within the range)!

Gradients, Jacobians, Hessians in economics

- **Gradient:** marginal effects and causal interpretation
    - It is common to numerically estimate the response of *Y* to a small change *X* in large systems of interdependent equations
- **Hessian:** standard errors in semi-parametric and parametric models (non-linear least squares, GMM, maximum likelihood: probit, logit, heckit…)
- **Jacobian:** must be supplied in constrained-optimisation problems (optimisation subject to $g(\theta) = 0$, $h(\theta) \geq 0$)
- Numerical optimisation with steepest-descent / hill-climbing methods

Necessary in any model that is not linear in parameters.

You have encountered numerical algorithms

12 heckman — Heckman selection model

```
. use https://www.stata-press.com/data/r18/twopart

. heckman yt x1 x2 x3, select(z1 z2) nonrtol

Iteration 0:  Log likelihood = -111.94996
Iteration 1:  Log likelihood = -110.82258
Iteration 2:  Log likelihood = -110.17707
Iteration 3:  Log likelihood = -107.70663  (not concave)
Iteration 4:  Log likelihood = -107.07729  (not concave)
  (output omitted)
Iteration 36: Log likelihood =  -104.0825

Heckman selection model                         Number of obs     =        150
(regression model with sample selection)              Selected    =         63
                                                      Nonselected =         87

                                                Wald chi2(3)      =   8.84e+08
Log likelihood = -104.0825                      Prob > chi2       =     0.0000
```

yt	Coefficient	Std. err.	z	P>|z|	[95% conf.	interval]
yt						
x1	.8974192	.0002164	4146.52	0.000	.896995	.8978434
x2	-2.525303	.0001244	-2.0e+04	0.000	-2.525546	-2.525059
x3	2.855786	.0002695	1.1e+04	0.000	2.855258	2.856314
_cons	.6975003	.0907873	7.68	0.000	.5195604	.8754402

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Gradient #1: quasi-Newton optimisation direction

yt	Coefficient	Std. err.	z	P>|z|	[95% conf. interval]	
yt						
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_cons	.6975003	.0907873	7.68	0.000	.5195604	.8754402

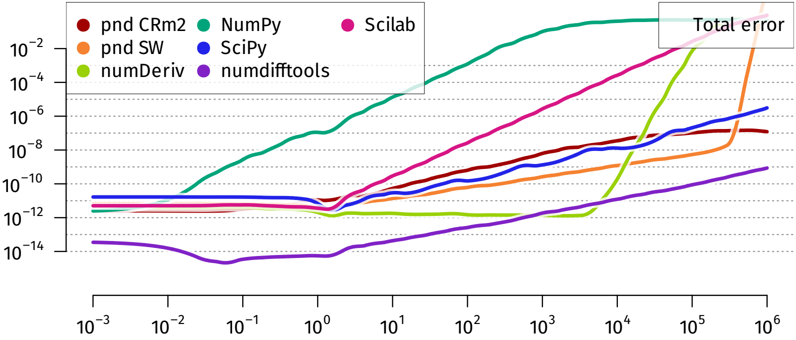
Gradient #2: Hessian-based SE from this at this

Existing literature / software

- Gilbert & Varadhan (2019). `numDeriv`: Accurate Numerical Derivatives. `cran.r-project.org/package=numDeriv`
  - Non-parallel version without vignettes or derivations
- Gerber & Furrer (2019). `optimParallel`: An R Package Providing a Parallel Version of the L-BFGS-B Optimization Method. *The R Journal* 11 (1). `cran.r-project.org/package=optimParallel`
  - Limited to the built-in `optim(method = "L-BFGS-B")`
- Papers on computer algorithms from the 1970s
- Hong, Mahajan & Nekipelov, (2015, *JoE*). Extremum estimation and numerical derivatives.

Selling pnd

Compare the software: numerical derivative error for $f(x) = \sin x$ on the evaluation grid $\log_{10} x \sim \mathrm{Unif}[-3, 6]$.



* Some entries are cheating and do better by being slower and computing more derivatives – impractical for heavy-duty applications.

pnd = numDeriv + optimParallel (+ tweaks)

Approximations of analytical derivatives

Derivative of a function

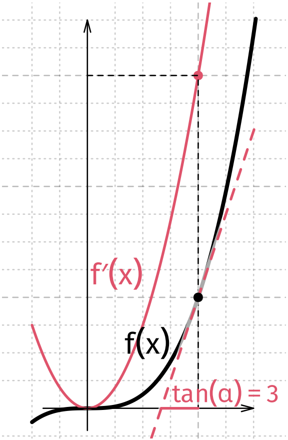
Derivative: The instantaneous rate of change of a function.

$$f'(x) = \frac{df}{dx} := \lim_{h\to 0} \frac{f(x+h) - f(x)}{h}$$

Assume that f is differentiable and therefore continuous.

$f'(x)$ is the slope of the tangent line to the graph at x.

Illustration: $f(x) := x^3, f'(x) = 3x^2$. $f(1) = 1, f'(1) = 3$. The tangent equation at $x = 1$ is $3x - 2$.



Naïve numerical derivatives

In the definition

$$f'(x) := \lim_{h \to 0} \frac{f(x+h) - f(x)}{h},$$

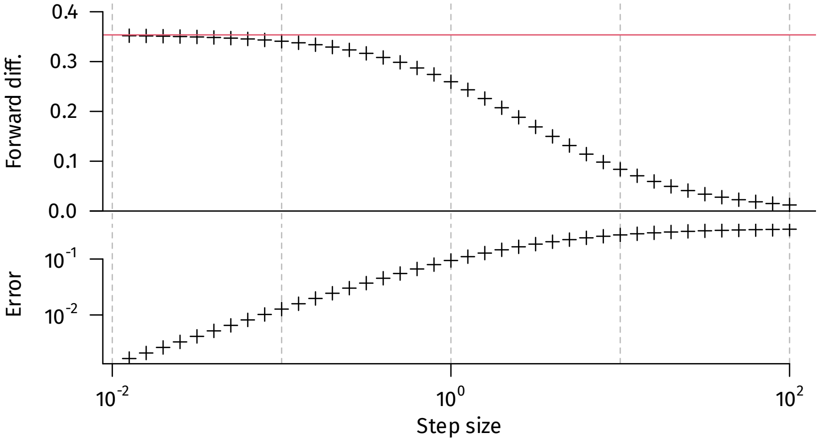
remove the limit to obtain a **forward difference**:

$$f'_{\mathrm{FD}}(x, h) := \frac{f(x+h) - f(x)}{h}$$

Choose a sequence of decreasing step sizes h_i (e. g. $\{0.1, 0.01, 0.001, \ldots\}$), observe the sequence $f'_{\mathrm{FD}}(x, 0.1), f'_{\mathrm{FD}}(x, 0.01), f'_{\mathrm{FD}}(x, 0.001), \ldots$ converge to f'.

Naïve numerical derivatives in practice

Mathematically, $f'_{\mathrm{FD}}(x, 0.1), f'_{\mathrm{FD}}(x, 0.01), f'_{\mathrm{FD}}(x, 0.001), \ldots$ converges to $f'(x)$.



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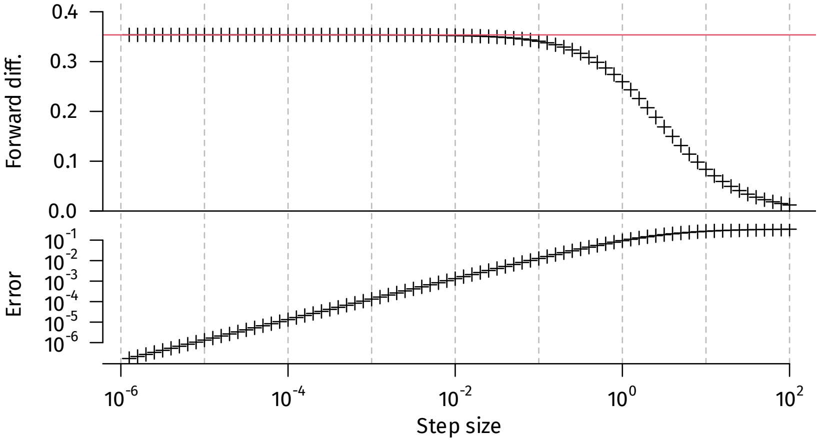
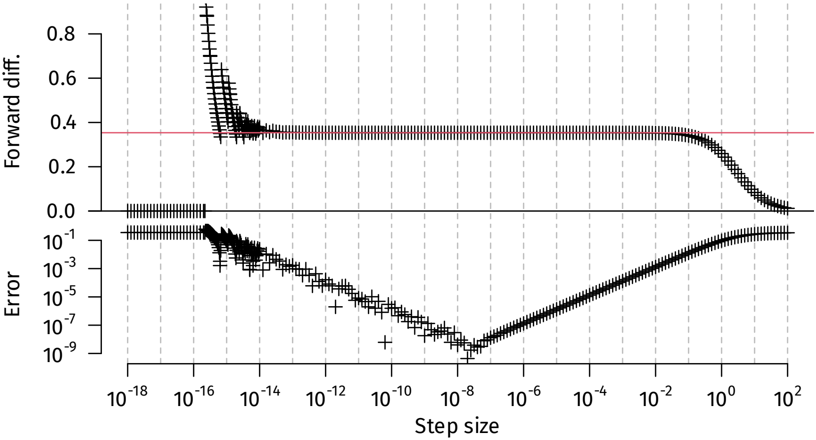
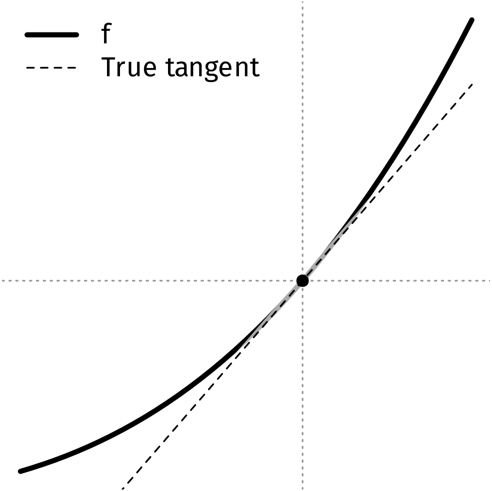


Naïve numerical derivatives in practice

Mathematically, $f'_{\mathrm{FD}}(x, 0.1), f'_{\mathrm{FD}}(x, 0.01), f'_{\mathrm{FD}}(x, 0.001), \ldots$ converges to $f'(x)$. **But not true in practice!**

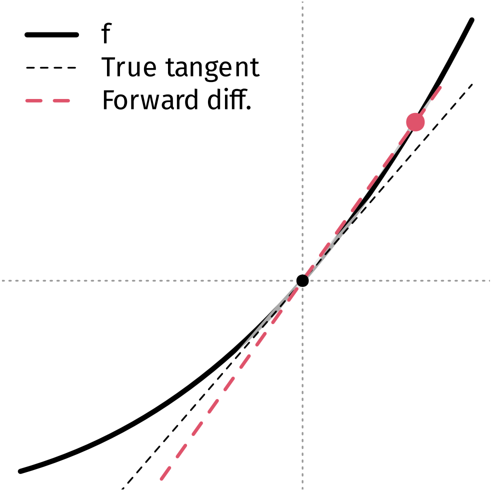


Graphical illustration of accuracy



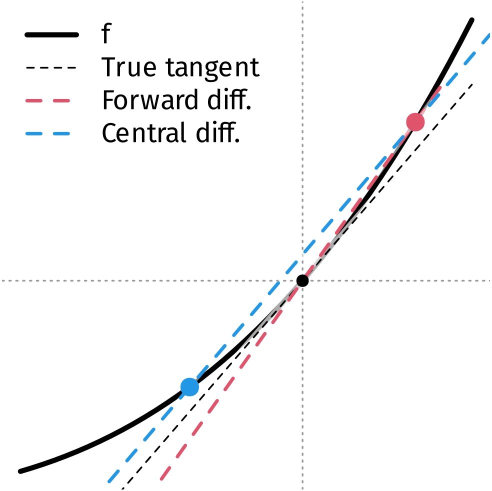
- $f(x) = x^3, x_0 = 1$
- $f'(x_0) = 3$

Graphical illustration of accuracy



- $f(x) = x^3, x_0 = 1$
- $f'(x_0) = 3$
- Step size $h = 0.2$
- $f'_{\text{FD}}(x_0, 0.2) = 3.64$
  Error $\approx 21\%$

Graphical illustration of accuracy



- $f(x) = x^3, x_0 = 1$
- $f'(x_0) = 3$
- Step size $h = 0.2$
- $f'_{FD}(x_0, 0.2) = 3.64$
  Error $\approx$ 21%
- $f'_{CD}(x_0, 0.2) = 3.04$
  Error $\approx$ 1.3%

Second-order accuracy of derivatives

Central differences are symmetrical around x:

$$f'_{\mathrm{CD}}(x, h) := \frac{f(x+h) - f(x-h)}{2h}$$

f'_{CD} is more accurate than f'_{FD}:*

- $f'(x) - f'_{\mathrm{FD}}(x, h) = -\frac{f''(x+\alpha h)}{2} h \approx -\frac{f''(x)}{2} h = O(h)$
- $f'(x) - f'_{\mathrm{CD}}(x, h) = -\frac{f'''(x+\beta h)}{6} h^2 \approx -\frac{f'''(x)}{6} h^2 = O(h^2)$

If $f(x)$ has not been evaluated, computing f'_{FD} and f'_{CD} takes the same amount of time – use f'_{CD}.

If $f(x)$ is already known, CD requires 1 more computation than f'_{FD}, which is 2 times slower – use f'_{FD} for costly f.

* Assuming f'' and f''' are uniformly bounded.

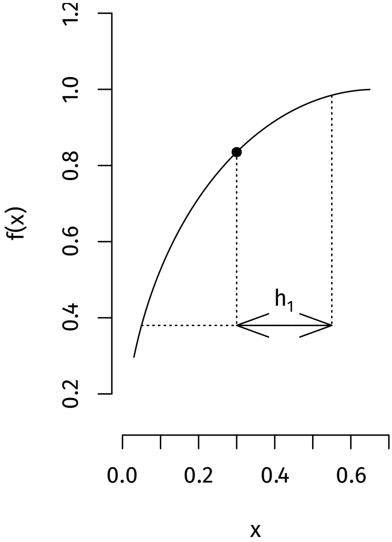
Improvements via Richardson extrapolation

Since numerical derivatives are based on polynomial approximations of functions, one can reduce the truncation error **iteratively**.

Romberg's method / Newton–Cotes formula:

1. Compute $f'_{\text{CD}}(x, h_1)$ and $f'_{\text{CD}}(x, h_2)$ for two different step sizes $h_1 > h_2$
2. Develop their Taylor expansions:
   $f'_{\text{CD}}(x, h_1) = f'(x) + c_1 h^2 + \ldots$
   $f'_{\text{CD}}(x, h_2) = f'(x) + c_2 h^2 + \ldots$
3. Find such weights $w_1 + w_2 = 1$ that $w_1 c_1 + w_2 c_2 = 0$ so that the $O(h^2)$ error term vanishes, yielding
   $c_1 f'_{\text{CD}}(x, h_1) + c_2 f'_{\text{CD}}(x, h_2) = f'(x) + O(h^4)$
4. Iterate further with $h_1 > h_2 > h_3 > \ldots$ and $h_i / h_{i+1} = r > 1$ to get a better approximation

Richardson-like extrapolation illustration



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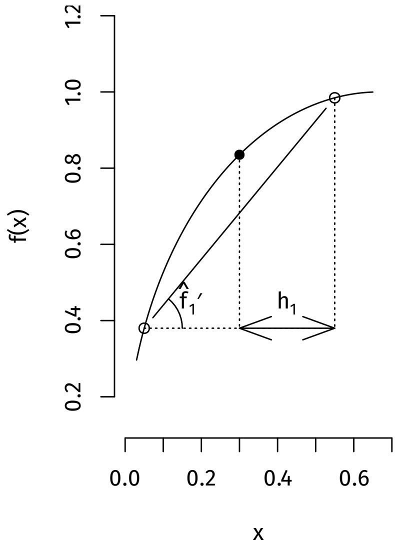

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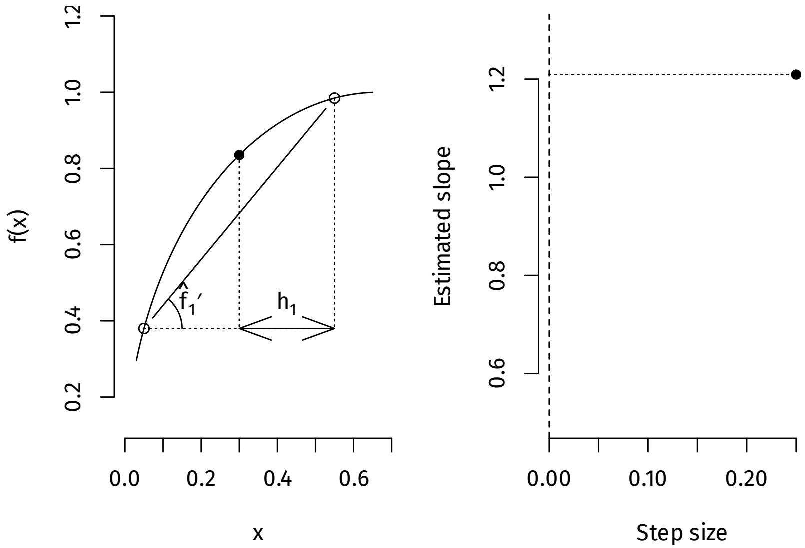

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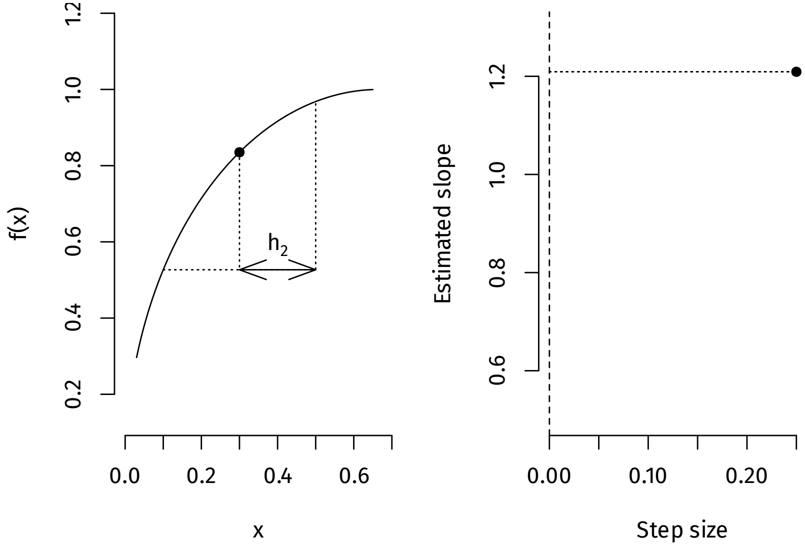

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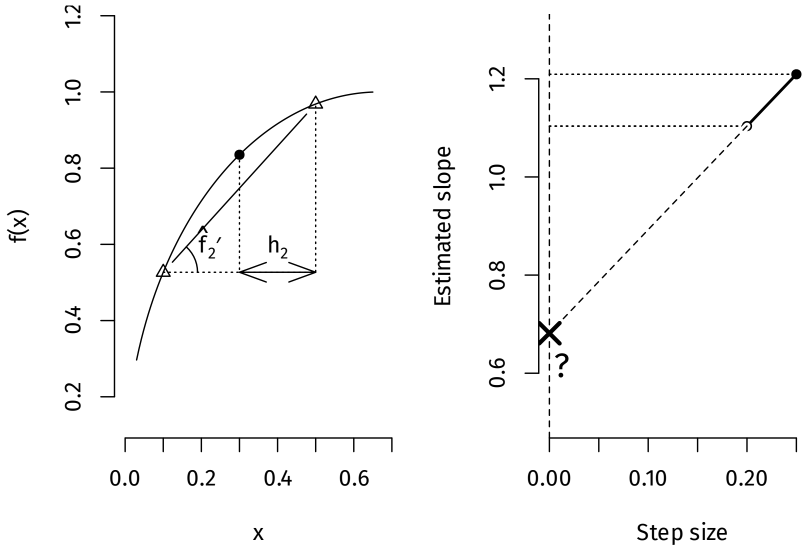

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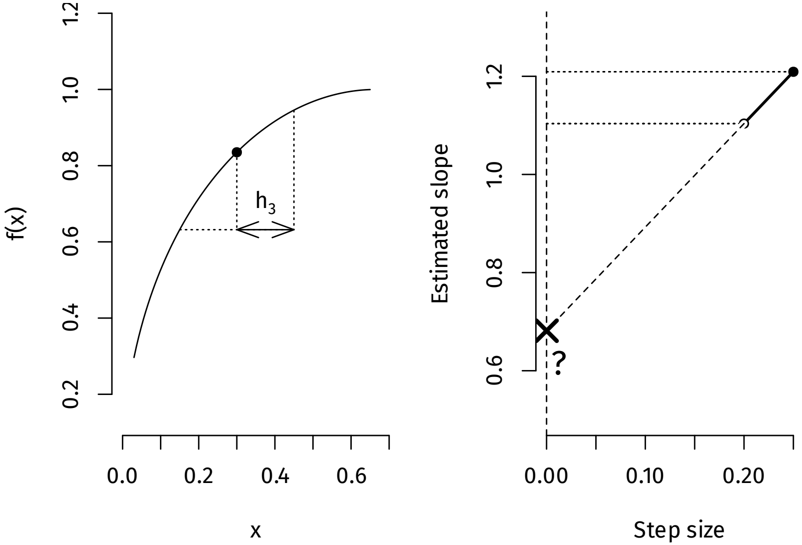

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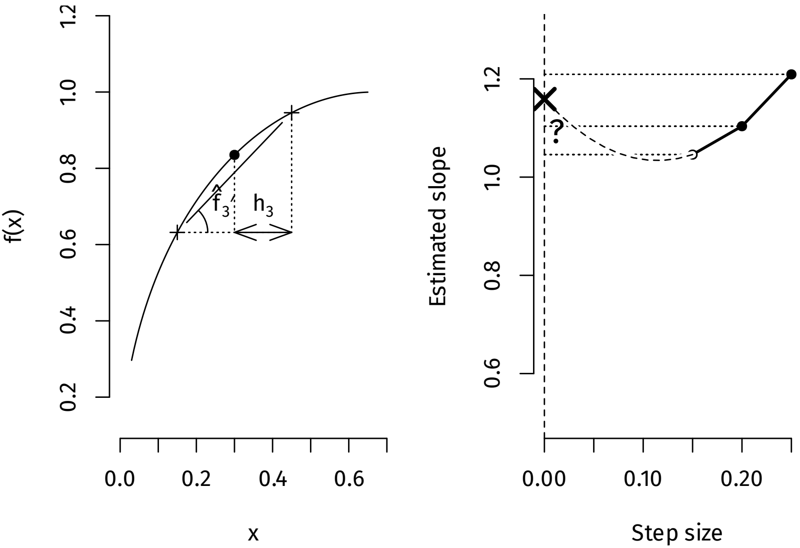

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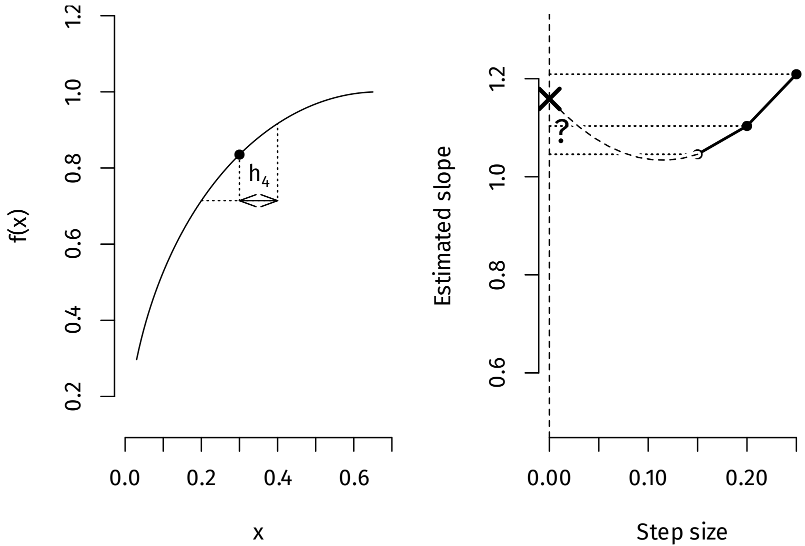

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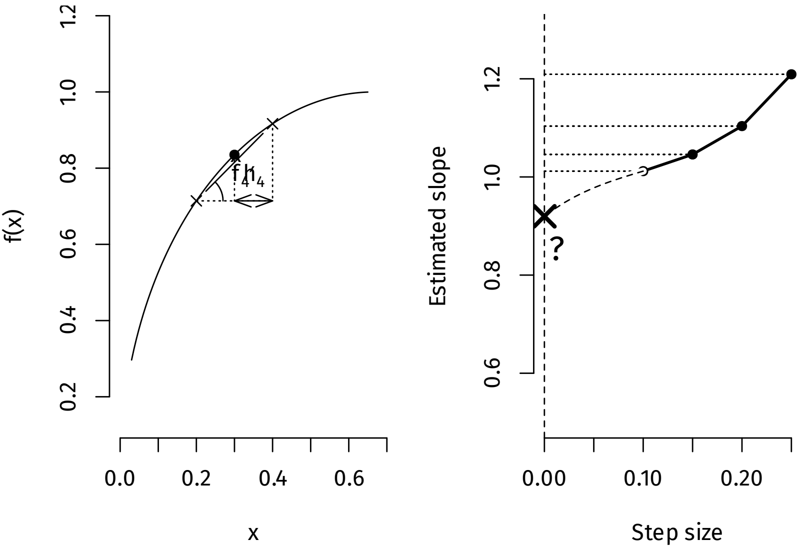

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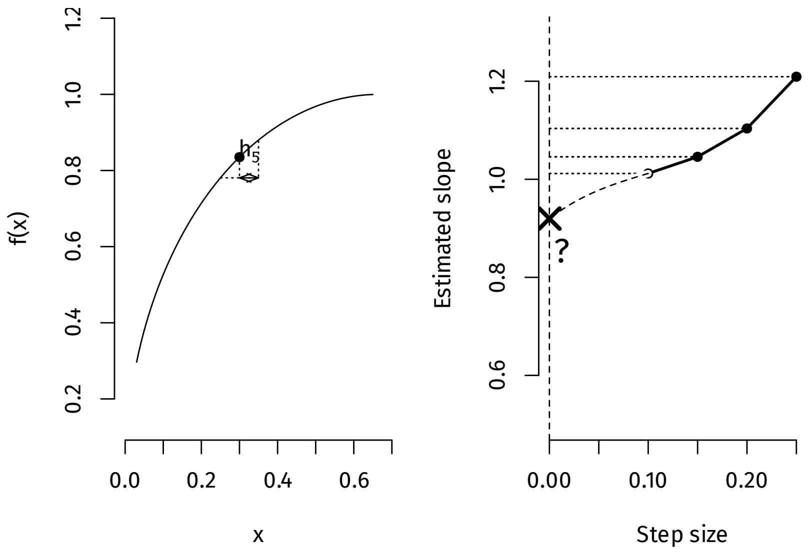

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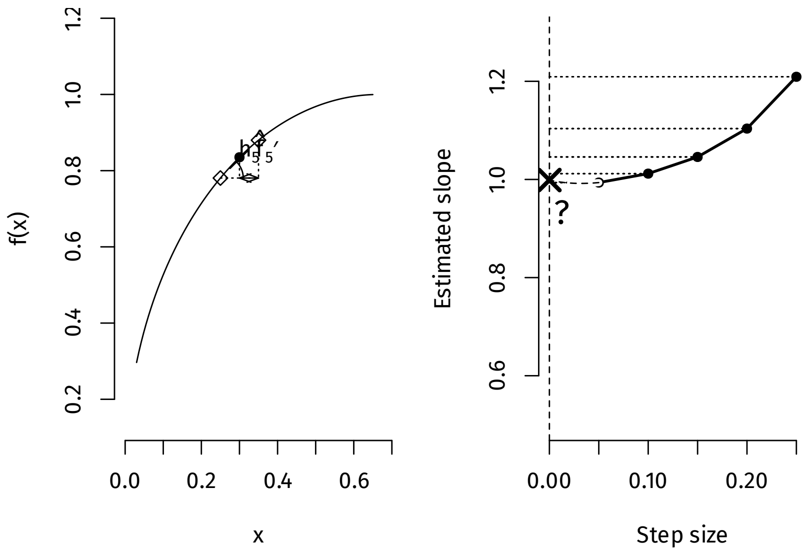


Higher-order accuracy of first derivatives

Better accuracy is achievable with more terms in the sum. Carefully choose the coefficients to eliminate the undesirable terms:

$$f' = \underbrace{\frac{-f(x-h) + f(x+h)}{2h}}_{f'_{\text{CD},2}} + O(h^2)$$

$$f' = \underbrace{\frac{f(x-2h) - 8f(x-h) + 8f(x+h) - f(x+2h)}{12h}}_{f'_{\text{CD},4}} + O(h^4)$$

For the same small h, the error of $f'_{\text{CD},4}$, $O(h^4)$, is generally smaller than that of $f'_{\text{CD},2}$, $O(h^2)$. **+ Parallelisation!**

Higher-order accuracy of m^{th}-order derivatives

Stencil: strictly increasing sequence of real numbers: $b_1 < \ldots < b_n$. (Preferably symmetric around 0 for the best accuracy.) Example: $b = (-2, -1, 1, 2)$.

Derivatives of any order m with error $O(h^a)$ may be approximated as weighted sums of f evaluated on the **evaluation grid** for that stencil: $x + b_1 h, \ldots, x + b_n h$.

With enough points ($n > m$), one can find such weights $\{w_i\}_{i=1}^n$ that yield the a^{th}-order-accurate approximation of $f^{(m)}$, where $a \leq n - m$:

$$\frac{\mathrm{d}^m f}{\mathrm{d}x^m}(x) = h^{-m} \sum_{i=1}^{n} w_i f(x + b_i h) + O(h^a)$$

Efficient parallelisation of gradients

Example: $\nabla f(x)$, $\dim x = 3$, stencil $b = (-2, -1, 1, 2)$ for 4th-order accuracy, same step size h. Total: 12 evaluations.

	$w_1 = \frac{1}{12}$	$w_2 = -\frac{8}{12}$	$w_3 = \frac{8}{12}$	$w_4 = -\frac{1}{12}$
$x^{(1)}$	$f(x - 2h_1)$	$f(x - h_1)$	$f(x + h_1)$	$f(x + 2h_1)$
$x^{(2)}$	$f(x - 2h_2)$	$f(x - h_2)$	$f(x + h_2)$	$f(x + 2h_2)$
$x^{(3)}$	$f(x - 2h_3)$	$f(x - h_3)$	$f(x + h_3)$	$f(x + 2h_3)$

- Create a list of length 12 containing $x + b_j h_i$
- Apply f **in parallel** to the list items, assemble $\left\{\{f(x + b_j h_i)\}_{i=1}^{3}\right\}_{j=1}^{4}$ in a matrix
- Compute weighted row sums

Step size effect on the approximation error

Real case #1: numerical derivative failure

- An economist is modelling some variable Y that is linear in the GDP: $Y := 1 \cdot GDP + g(\ldots) + U$
  - $\partial\mathbb{E}(Y \mid \ldots)/\partial GDP = 1$, but they use numerical derivatives
- Lux GDP is 80 bn € $\Rightarrow$ the gap between two representable numbers is $8 \cdot 10^{10}/2^{52} \approx 1.7 \cdot 10^{-5}$
- Step size: 10^{-8} (from the literature)

$$\nabla_{GDP} Y \Big|_{GDP_{\text{Lux}}} \approx \frac{[8 \cdot 10^{10} + 10^{-8}] - 8 \cdot 10^{10}}{10^{-8}}$$

- $[8 \cdot 10^{10} + 10^{-8}] = 8 \cdot 10^{10}$ because $10^{-8} < \frac{1}{2} \cdot 1.7 \cdot 10^{-5} \Rightarrow$ the numerator is zero (cf. Slide 14 plot)
  - Error: the computer returns $\widehat{\partial Y/\partial GDP} = 0$ instead of 1!

Total error in numerical derivatives

Step size selection is critical for accuracy:

- h too large $\to$ large **truncation error** from the truncated Taylor-series term (poor **mathematical** approximation)
- h too small $\to$ large **rounding error** (poor **numerical** approximation): catastrophic cancellation, division of something small by something small, machine accuracy always limited by ϵ_{mach}

Finding the optimal h^* to balance these two errors is possible.

Analytical error bounds for central diff.

Computing f results in a rounding error: $f(\ldots) := \hat{f}_{\text{FP64}}(\ldots) + e_{\text{round}}$.

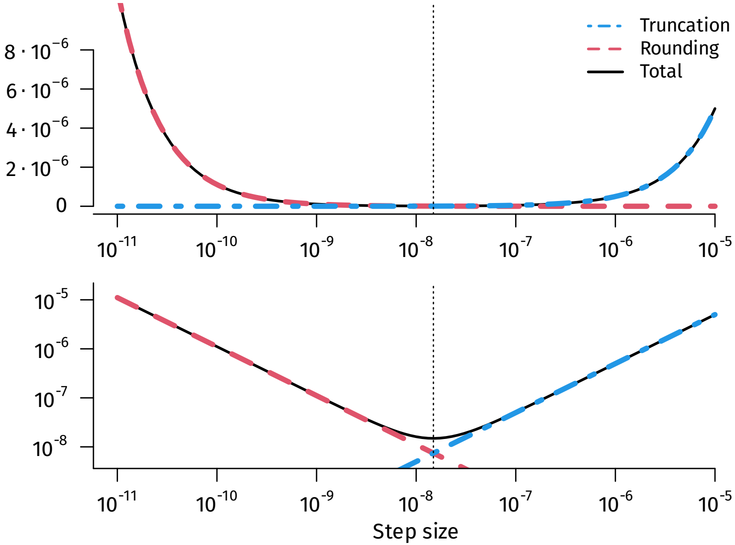
$$\underbrace{\left[f(x+h) - f(x-h)\right]}_{\text{true difference}} - \underbrace{\left[\hat{f}_{\text{FP64}}(x+h) - \hat{f}_{\text{FP64}}(x-h)\right]}_{\text{computer evaluation}} = e_+ - e_-$$

Rounding-error numerator bound:* $|e_+ - e_-| \le |f(x)|\epsilon_{\text{mach}}$.

$$\underbrace{f'(x) - \hat{f}'_{\text{CD}}(x,h)}_{\text{overall num. deriv. error}} \approx \underbrace{\frac{f'''(x)}{6}h^2}_{\text{truncation}} + \underbrace{\frac{0.5(e_+ - e_-)}{h}}_{\text{rounding}}$$

* $f(x+h), f(x-h)$ must have the same magnitude (binary exponent).

Total error composition



Optimal step size

Total-error function: conservative absolute bound (after several harmless simplifications).

$$E_{\mathrm{CD}}(x, h) := \frac{|f'''(x)|}{6} h^2 + 0.5|f(x)|\epsilon_{\mathrm{mach}} h^{-1}$$

$$E_{\mathrm{FD}}(x, h) := \frac{|f''(x)|}{2} h + |f(x)|\epsilon_{\mathrm{mach}} h^{-1}$$

Optimal step sizes that minimise it:

$$h^*_{\mathrm{CD}} = \sqrt[3]{\frac{1.5|f(x)|}{|f'''(x)|}\epsilon_{\mathrm{mach}}}, \qquad h^*_{\mathrm{FD}} = \sqrt{\frac{2|f(x)|}{|f''(x)|}\epsilon_{\mathrm{mach}}}$$

Therefore, $h^*_{\mathrm{CD}} \propto \epsilon_{\mathrm{mach}}^{1/3}$ and $h^*_{\mathrm{FD}} \propto \epsilon_{\mathrm{mach}}^{1/2}$ (machine-dependent).

Optimal step tips and tricks

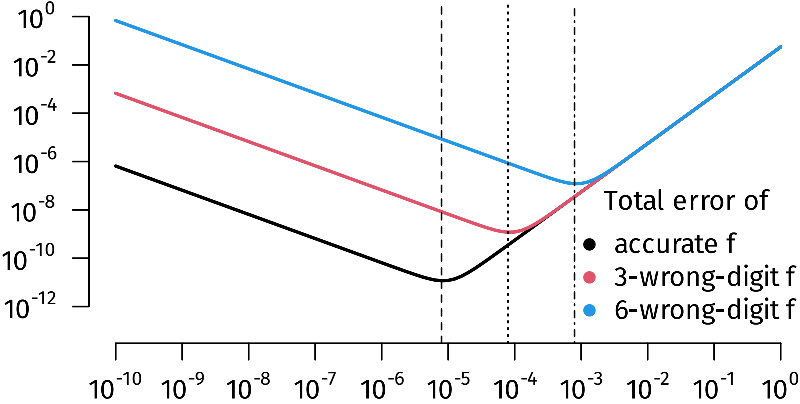
Rules of thumb to help one save time and obtain more useful quantities once they have determined $h^*_{\mathrm{CD},2}$"

- Since $h^{**}_{\mathrm{CD},2} \propto \epsilon_{\mathrm{mach}}^{1/4}$, $h^*_{\mathrm{CD},2}/h^{**}_{\mathrm{CD},4} \propto \epsilon_{\mathrm{mach}}^{1/12}$.
  Multiply $h^*_{\mathbf{CD},2}$ by ≈20 for a reasonable step size for **second derivatives** (f'')
  - Logic: higher derivation order ⇒ division by h^2 instead of h ⇒ higher rounding error ⇒ increasing h^* to reduce it
- Similarly, $h^*_{\mathrm{CD},4} =\propto \epsilon_{\mathrm{mach}}^{1/5}$, $h^*_{\mathrm{CD},2}/h^*_{\mathrm{CD},4} \propto \epsilon_{\mathrm{mach}}^{2/15}$.
  Multiply $h^*_{\mathbf{CD},2}$ by ≈100 for a reasonable step size for **4$^{\mathrm{th}}$-order-accurate first derivatives** (f' but better)
  - Logic: higher approximation order ⇒ more points ⇒ smaller truncation error at $h^*_{\mathrm{CD},2}$ ⇒ increasing h^* to reduce the rounding error

Optimal step troubleshooting

- If the function is quasi-quadratic, $f''' \approx 0, f'''' \approx 0, \dots$, then, the step-size search might be unreliable
  - Happens at the optima of likelihood functions in large samples
  - Solution: use the fixed step $\sqrt[3]{\epsilon_{\mathrm{mach}}} \max\{|x|, 1\}$ **after checking diagnostic messages**
  - Typical error: step size too large after dividing by f''', solution at the search range boundary, or solution greater than $|x| \dots$
- If the function is noisy / approximate, multiply $h^*_{\mathrm{CD},2}$ by 10 per 3 wrong digits of f
  - If $f(x)$ has numerical root search, optimisation, integration, differentiation, etc., $|f(x) - \hat{f}(x)|/|f(x)| \geq 0$ by more than ϵ_{mach}
  - In general, replace ϵ_{mach} in the total-error formula with the maximum expected relative error $\Rightarrow h$ becomes larger with more wrong decimal digits

Total error in noisy functions



Step-size selection algorithms

Using plug-in estimates of f'''

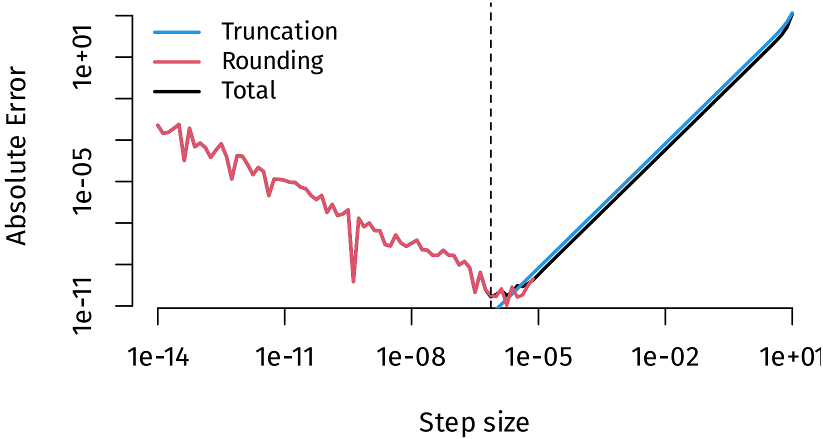
Since the optimal h^* for f'_{CD} depends on the true f''',

1. Compute $f'''_{\mathrm{CD}}(x, \tilde h)$ using any reasonable $\tilde h \propto \epsilon_{\mathrm{mach}}^{1/5}$ (e. g. naïve values like or $0.001 \max(1, |x|)$)
2. Compute $\hat h^*_{\mathrm{CD}} = \sqrt[3]{1.5|f(x)|\epsilon_{\mathrm{mach}}/|f'''_{\mathrm{CD}}(x, \tilde h)|}$
   - Dumontet–Vignes (1977) proposed an iterative search algorithm
   - Works for all differentiation and accuracy orders with appropriate changes
   - Reassemble the available values of $f(\{\pm h, \pm 2h\})$ into a 4^{th}-order-accurate $f'_{\mathrm{CD},4}$

```
Grad(FUN = f, x = x0, h = "plugin", h0 = 1e-5)
Grad(FUN = f, x = x0, h = "DV")
```

Objective function to minimise

$$f(x) := x^4 + \cos x + \exp(x-1), \quad x_0 = \pi/4, \quad f'(x_0) = ?$$



Controlling the error ratio

Observation: when the truncation error and the rounding error are similar, the total error is minimal.

Curtis & Reid (1974) proposed choosing such h that

$$\frac{\text{over-estimated truncation error } e_\mathrm{t}}{\text{rounding error } e_\mathrm{r}} \in [10, 1000] \qquad \text{(aim for 100)}$$

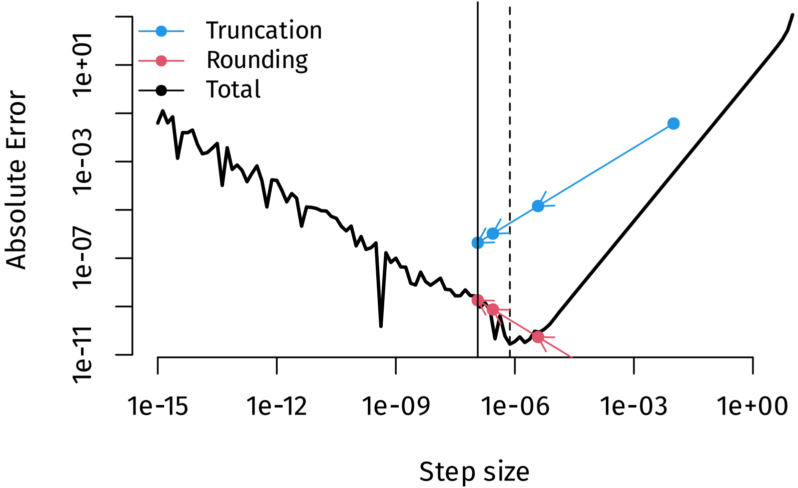
Estimate the truncation and rounding errors separately:

- $\hat{e}_\mathrm{t}(x, h) = |f'_\mathrm{CD}(x, h) - f'_\mathrm{FD}(x, h)|$ – too conservative
- $\hat{e}_\mathrm{r}(x, h) = 0.5|f(x)|\epsilon_\mathrm{mach}/h$

Since $\hat{e}_\mathrm{t}$ is over-estimated, this aim ensures that $e_\mathrm{t} \approx e_\mathrm{r}$.

```
Grad(func = f, x = x0, h = "CR")
```

Curtis–Reid algorithm visualisation

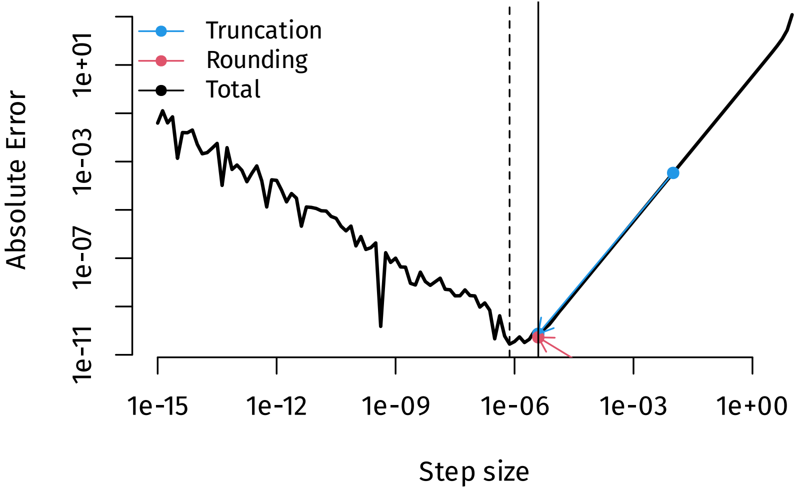


Error-ratio control improvement

- Larger stencil + parallelism = more accurate truncation estimate
- I correct the estimates and the target ratio
- With 4 evaluations, $f'_{\mathrm{CD},4}$ can be computed from existing values
  $\Rightarrow$ multiply the aim by $\epsilon_{\mathrm{mach}}^{-2/15} \approx 120$
  - Positive externality: the step search yields more than one asked for

```
Grad(f, x = x0, h = "CRm")
gradstep(f, x = x0, method = "CRm",
         control = list(acc.order = 4))
```

Curtis–Reid 2025 improvement visualisation



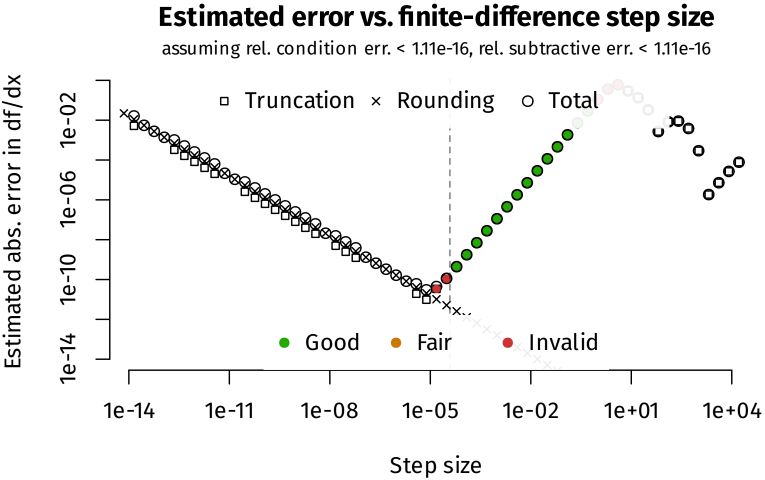
Controlling the truncation-branch slope

Stepleman & Winarsky (1979) and Mathur (2012) proposed similar algorithms based on the idea of descending down the right slope of the estimated truncation error:

- The slope of the right branch of the total error is a
- Choose a large enough h_0, set $h_1 = 0.5h_0$, get the truncation error estimate from $f'_{\mathrm{CD}}(x, h_1)$ and $f'_{\mathrm{CD}}(x, h_0)$
- Continue shrinking while the slope of $\hat{e}_t$ is ≈ 2 (accuracy order); stop when it deviates due to the substantial round-off error
  - Never deals with the indeterminable round-off

```
Grad(f, x = x0, h = "SW")
Grad(f, x = x0, method = "M")
```

Slope-control algorithm visualisation



Good: slope $\approx 2 \pm 1\%$, invalid: slope > 0, but slope $\not\approx 2$.

Showcase of pnd

Compatibility with `numDeriv`

`numDeriv` remains the most popular R package for non-parallel computation of accurate derivatives without step-size selection.

Simply replace the first lowercase letter with an uppercase one.

numDeriv	pnd
`grad(f, x)`	`Grad(f, x)`
`jacobian(fvector, x)`	`Jacobian(fvector, x)`
`hessian(fscalar, x)`	`Hessian(fscalar, x)`

Example #1: optimisation with gradients

$$f(x) := \sum_{i=1}^{\dim x} (x_i^2 + 2\sin x_i + 1.1^{x_i})$$

```r
library(pnd)
f <- function(x) sum(x^2 + 2*sin(x) + 1.1^x)
initval <- runif(10, -1, 1) # dim X = 10

optim(initval, f, method = "BFGS")

g <- function(x) Grad(f, x)  # length(g) = 10
optim(initval, f, gr = g, method = "BFGS")

# Custom step and higher accuracy
h  <- gradstep(f, initval, method = "plugin")$par
g2 <- function(x) Grad(f, x, acc.order = 4, h = h*10,
        elementwise = FALSE, vectorised = FALSE,
        multivalued = FALSE)
optim(initval, f, gr = g2, method = "BFGS")
```

Example #2: Jacobians and Hessians

$$f_2 := \sum_{i=1}^{\dim x} \begin{pmatrix} \sin x_i \\ \exp x_i \end{pmatrix}, \qquad f_3 := \prod_{i=1}^{\dim x} \sin x_i$$

```r
f2 <- function(x) c(sine = sum(sin(x)),
                    expo = sum(exp(x)))
Jacobian(x = 1:3, f2, report = 0)

# sine  0.5403023 -0.4161468 -0.9899925
# expo  2.7182818  7.3890561 20.0855369

f3 <- function(x) prod(sin(x))
Hessian(f3, x = 1:4, report = 0)

#  0.0817  0.0240  0.3681 -0.0453
#  0.0240  0.0817 -0.2624  0.0323
#  0.3681 -0.2624  0.0817  0.4951
# -0.0453  0.0323  0.4951  0.0817
```

User-friendliness and thoroughness of pnd

`pnd`

- 63 foreseen errors (so far)
- 26 foreseen warnings (as of today)
- 8 possible configurations of function properties and capabilities
  - Multi-stage input checks with error handling and possible parallelisation
- The user may supply arguments to ensure no run-time or silent error

`numDeriv`

- 19 foreseen errors
- Zero foreseen warnings
- Only 3 possible function configurations
  - One-stage input check only one error check
- Impossible to obtain Jacobians for certain functions (e. g. $f(x) := (\sin x, \cos x)'$)
  - No user controls

Example of error informativeness

pnd is more verbose and provides direct suggestions what to do in case the user has provided incompatible inputs.

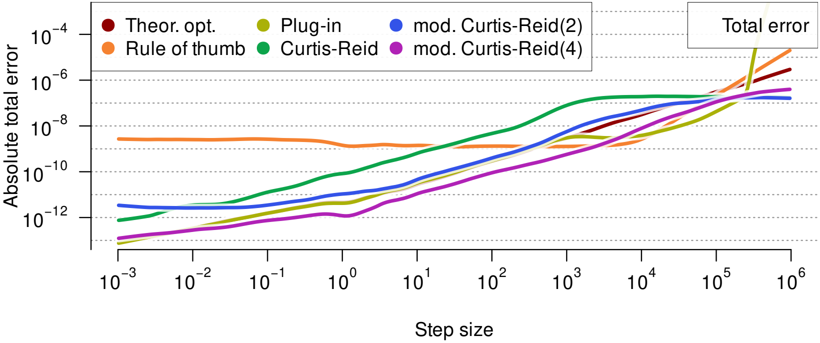
```
f2 <- function(x) c(sin(x), cos(x))
grad(f2, x = 1:4)
# Error: grad assumes a scalar valued function.

Grad(f2, x = 1:4)
# Use 'Jacobian()' instead of 'Grad()'
# for vector-valued functions to obtain
# a matrix of derivatives.
```

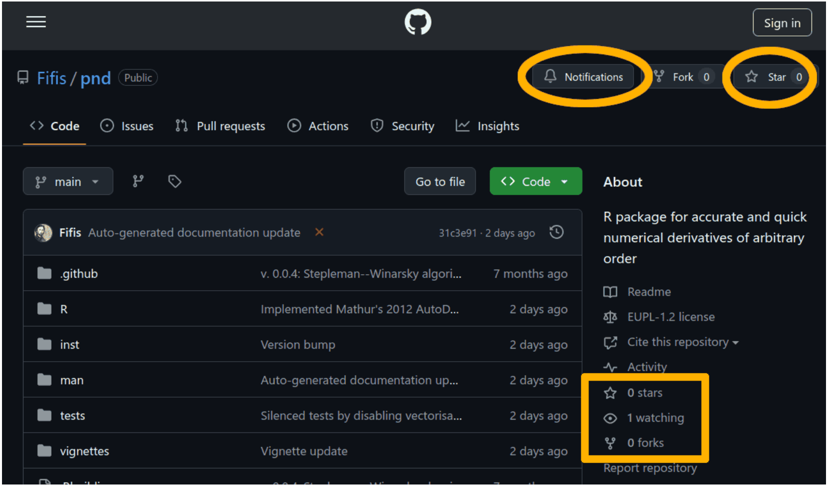
Error of step-selection methods for $f(x) := \sin x$

Theoretically optimal: $\sqrt[3]{\frac{1.5|f(x)|\epsilon_{\mathrm{mach}}}{|f'''(x)|}} = \sqrt[3]{1.5|\tan x|\epsilon_{\mathrm{mach}}}$

Rule of thumb: $\sqrt[3]{\epsilon_{\mathrm{mach}}} \cdot \min(1, |x|)$. Curtis–Reid: 1974 version + 2 modifications (2025). Evaluation grid: $x \in [10^{-3}, 10^{6}]$.



Project support



https://github.com/fifis/pnd

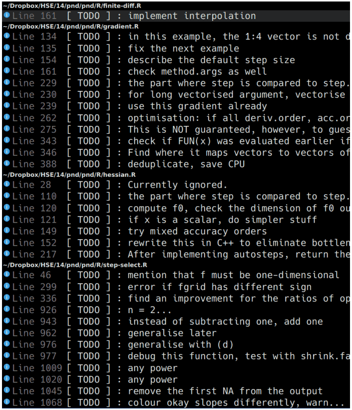
Demonstrations for another time

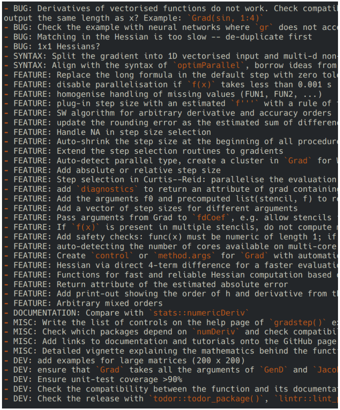
- Computing marginal effects in highly non-linear computationally heavy models with big data
- Computing accurate standard errors in conditional-volatility models (no more `NaN` in GARCH!)
- Choosing the optimal step size for complex multi-dimensional maximisation
- Handling f that is not accurate to the last digit

Further work – I

- Finish the formal part, test the suggested algorithm improvements
- Upload the R package to CRAN as `pnd` (currently tested on `github.com/Fifis/pnd`)
- Improve the Dumontet–Vignes and Mathur algorithm by returning higher-order-accurate derivatives from available calculations
  - Add facilities to compute higher-order-accurate derivatives from previous candidate step sizes
- Implement complex derivatives

Further work – II





- But most importantly… please send your failing examples!
- Unit tests $<$ user feedback and reproducible errors

Practical recommendations – I

Do not:

- Believe that computers cannot be arbitrarily wrong
  - Functions are lossy
- Trust the built-in numerical differences
  - Especially the step size
- Fix $h = 0.01$ because it ‘feels right’ / you interpret a 1-¢ change

Do:

- Benchmark evaluation time
- Use optimal-step search or simply $h = \epsilon_{\text{mach}}^{1/(a+m)}$
- For higher orders of derivatives and/or accuracy, increase h to keep the error low

Practical recommendations – II

Do not:

- Use FD when evaluating f is fast
- Request 20 cores for quick functions

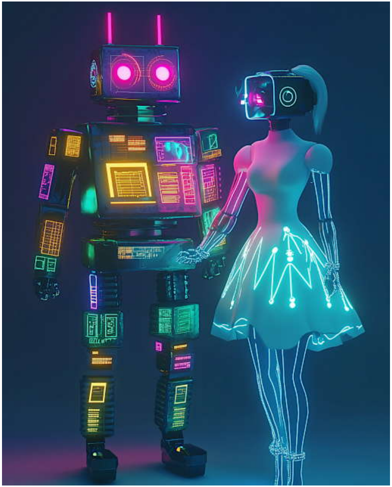
Do:

- Start costly optimisations with a parallel CD2 gradient, restart from the found optimum (or near it) with CD4
  - Use CD4 to measure $||\nabla f||$ for checking optima
- Use all CPU cores only if f is slower than 0.02 s
  - On Windows: create the cluster beforehand and pass it to `Grad()` / `Jacobian()`

Thank you for your attention and feedback!

github.com/Fifis/pnd

andrei.kostyrka@uni.lu



Function and its derivative accuracy comparison

- The vast majority of function evaluations on a computer are lossy due to finite memory, even linear transformations
  - Each operation typically adds a $\approx 10^{-16}$ relative error (at least)
- Numerical derivatives are **much less accurate** than function values
  - **...by a factor of $\approx$100 000** ***in the best case!***
  - Many software packages settle for a $\times$10 000 000 accuracy degradation
  - ...which is worse $\approx$100 times than it could have been

Non-existent literature / software

- Most modern articles focus on ultra-high-dimensional numerical gradients with much fewer evaluations
  - Only one (!) paper (Mathur 2012, Ph. D. thesis) with a comprehensive treatment of the classical case useful for low-dimensional models
- Existing algorithms (Curtis & Reid 1974, Dumontet & Vignes 1977, Stepleman & Winarsky 1979) lack open-source implementations
  - Popular software packages implement very rough rules and do not refer to any optimality results in the literature
- Most implementations of higher-order and cross-derivatives are through repeated differencing
  - Slower and less accurate than the best solution

Derivatives in linear models

$$
\begin{aligned}
FUELSALES = \beta_0 + \beta_1 P_{Lux} + \beta_2 P_{abroad} \\
+ \beta_3 COMMUTERS + \beta_4 LOCKDOWN + U
\end{aligned}
$$

- Exogeneity assumption: $\mathbb{E}(U \mid P_{Lux}, P_{abroad}, COMMUTERS, LOCKDOWN) = 0$
- $\frac{\partial}{\partial P_{abroad}} \mathbb{E}[FUELSALES \mid P_{Lux}, P_{abroad}, \ldots] = \beta_2$ by exogeneity
- **Causal interpretation:** if the foreign fuel price changes by 1 €, fuel sales will change by β_2 units *ceteris paribus* (including U)

Partial solutions

- R packages `numDeriv` and `optimParallel`
  - `numDeriv`: the most full-featured arsenal in terms of accuracy, but slow; `optimParallel`: speed gains but no focus on accuracy
- Python's `numdifftools`
  - Discusses Richardson extrapolation; no error analysis
- MATLAB's `Optimisation Toolbox`
  - Focuses on parallel evaluation, not accuracy
- Stata's `deriv`
  - Implements a step-size search to obtain 8 accurate digits

Derivatives in non-linear models

Economic vulnerability model for women over 50:

$$Y^* = \alpha_0 + \gamma_1 EducYears + \gamma_2 NonWhite + \gamma_3 EducYears \times NonWhite + X'\beta_0 + U := \tilde{X}'\theta_0 + U$$

$$Y := \begin{cases} 1, & Y^* > 0, \\ 0, & Y^* \le 0, \end{cases} \quad \mathbb{P}(Y = 1 \mid \tilde{X}) = F_U(\tilde{X}'\theta_0), \quad U \sim \mathcal{N}, \Lambda, \ldots$$

$$\frac{\partial \mathbb{P}(Y = 1 \mid \tilde{X})}{\partial EducYears} = f_U(\tilde{X}'\theta_0) \cdot (\gamma_1 + \gamma_3\, NonWhite)$$

$$\frac{\partial \mathbb{P}(Y = 1 \mid \tilde{X})}{\partial NonWhite} = f_U(\tilde{X}'\theta_0) \cdot (\gamma_2 + \gamma_3\, EducYears)$$

Inference on γ_3 is not intuitive.

Inference in non-linear models

Policy-makers are interested in the effects due to changes in *explanatory variables*, not parameters.

Average partial effect of the k^{th} variable: $\mathbb{E}\frac{\partial}{\partial X^{(k)}}\mathbb{P}(Y=1 \mid \tilde{X})$.

Its straightforward estimator is $\frac{1}{n}\sum_{i=1}^{n}\frac{\partial}{\partial X^{(k)}}\hat{\mathbb{P}}(Y_i=1 \mid \tilde{X}_i)$.

Embarrassingly parallel task: a problem that can be split into smaller problems that can be solved in parallel with no communication between the processes.

- Computing the n-dimensional derivative vector $\left\{\frac{\partial}{\partial X_i^{(k)}}\hat{\mathbb{P}}(Y_i=1 \mid \tilde{X}_i)\right\}_{i=1}^{n}$ is embarrassingly parallel
- Inference on θ_0 based on the Hessian of the log-likelihood is embarrassingly parallel

Complications in non-linear models

- F_U is often confined to a specific family (Poisson, exponential, Gaussian, logistic etc.)
  - This parametric assumption could be wrong
  - A more flexible approximation of the true distribution of U may not have a manageable closed-form derivative
- Most data-generating process in economics are highly non-linear and hard-to-formalise
  - Non-linear high-dimensional models tend to have a better explanatory power and yield more accurate forecasts
  - Loss of parameter interpretability
  - Numerical derivatives are often the only solution

Gradient of a function

Gradient: column vector of partial derivatives of a differentiable scalar function.

$$\nabla f(x) := \begin{pmatrix} \frac{\partial f}{\partial x^{(1)}}(x) \\ \vdots \\ \frac{\partial f}{\partial x^{(d)}}(x) \end{pmatrix}$$

- Vector input x + scalar output f = vector ∇
- At any point x, the gradient – the d-dimensional slope – is the **direction and rate of the steepest growth** of f

'A source of anxiety for non-mathematics students.'

J. Nash, 'Nonlinear Parameter Optimization' (2014).

[Visualisation of a gradient]

(3D clip)

Jacobian of a function

Jacobian: Matrix of gradients for a vector-valued function f.

If $\dim x = d, \dim f = k$,

$$\nabla f(x) := \begin{pmatrix} \frac{\partial f}{\partial x^{(1)}}(x) & \cdots & \frac{\partial f}{\partial x^{(d)}}(x) \end{pmatrix}_{k \times d} = \begin{pmatrix} \nabla^T f^{(1)}(x) \\ \vdots \\ \nabla^T f^{(k)}(x) \end{pmatrix}_{k \times d}$$

- Vector input x + vector output f = matrix ∇
- In constrained problems, most solvers (e. g. NLopt) for $\min_x f(x)$ s. t. $g(x) = 0$ require an explicit $\nabla g(x)$

Including incorrectly computed derivatives (mostly gradients or Jacobian matrices) <...> explains almost all the 'failures' of optimisation codes I see. *(Idem.)*

Hessian of a function

Hessian: Square matrix of second-order partial derivatives of a twice-differentiable scalar function.

$$\nabla^2 f(x) := \left\{ \frac{\partial^2 f}{\partial x^{(i)} \partial x^{(j)}} \right\}_{i,j=1}^{d} = \begin{pmatrix} \frac{\partial^2 f}{\partial x^{(1)} \partial x^{(1)}} & \cdots & \frac{\partial^2 f}{\partial x^{(1)} \partial x^{(d)}} \\ \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x^{(d)} \partial x^{(1)}} & \cdots & \frac{\partial^2 f}{\partial x^{(d)} \partial x^{(d)}} \end{pmatrix} (x)$$

The Hessian is the transpose Jacobian of the gradient:

$$\nabla^2 f(x) = \nabla^T [\nabla f(x)]$$

- Vector input x + scalar output f = matrix ∇^2
- If ∇f is differentiable, ∇_f^2 is symmetric

Taylor series

$$f(x \pm h) = \sum_{i=0}^{\infty} \frac{1}{i!} \frac{\mathrm{d}^i}{\mathrm{d}x^i} f(x) \cdot (\pm h)^i$$
$$= f(x) \pm \tfrac{f'(x)}{1!} h + \tfrac{f''(x)}{2!} h^2 \pm \tfrac{f'''(x)}{3!} h^3 + \ldots$$

The a^{th}-order approximation of f at x is a polynomial of degree a. The discrepancy between f and its approximation is the **remainder**. For some $\delta \in [0, 1]$,

$$f(x \pm h) - \sum_{i=0}^{a} \frac{1}{i!} \frac{\mathrm{d}^i f(x)}{\mathrm{d}x^i} (\pm h)^i = \frac{f^{(a+1)}(x \pm \delta h)}{(a+1)!} (\pm h)^{a+1}$$

For small h ($h < 1$, $h \to 0$), $h^{a+1} \xrightarrow{a \to \infty} 0$.

Example: Taylor series for CRRA utility

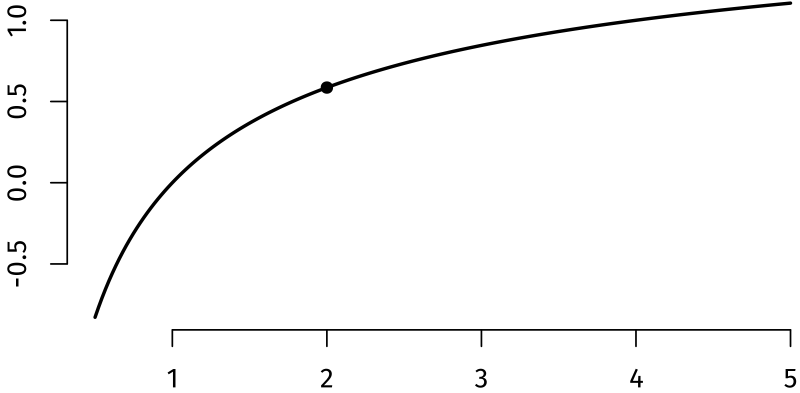
Linear approximation of CRRA utility with risk aversion η:

$$f(x) = \frac{x^{1-\eta}}{1-\eta}, \quad f'(x) = x^{-\eta}, \quad f''(x) = -\eta x^{-\eta-1}, \quad \ldots$$

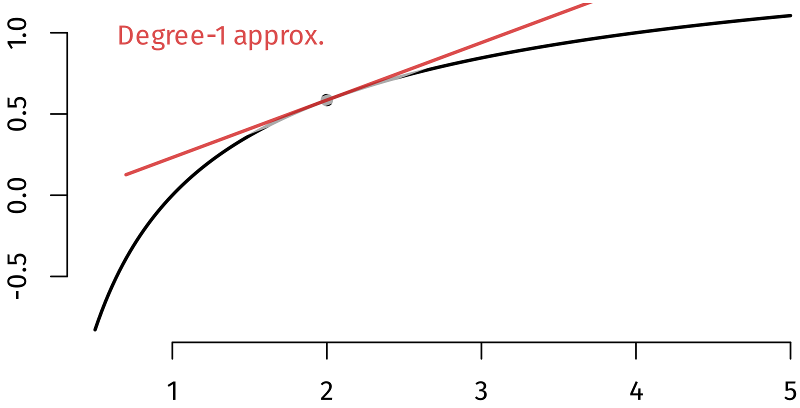
Assume $\eta = 1.5$, approximate f around $x_0 = 2$.

$$\begin{aligned} f(2+h) &\approx f(x_0) + f'(x_0)h = 0.59 + 0.35h = P_1(h) \\ &\approx P_1(h) + \tfrac{f''(x_0)}{2!}h^2 = 0.59 + 0.35h - 0.13h^2 = P_2(h) \\ &\approx P_2(h) + \tfrac{f'''(x_0)}{3!}h^3 = 0.59 + 0.35h - 0.27h^2 + 0.06h^3 \\ &\approx 0.59 + 0.35h - 0.27h^2 + 0.06h^3 - 0.02h^4 \approx \ldots \end{aligned}$$

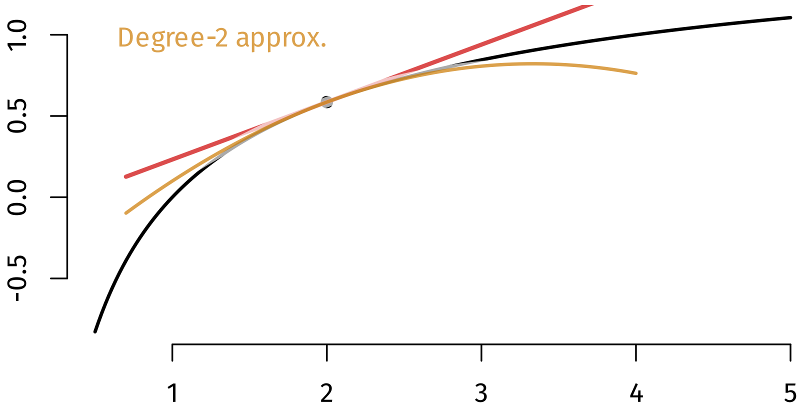
Example: CRRA utility visualisation



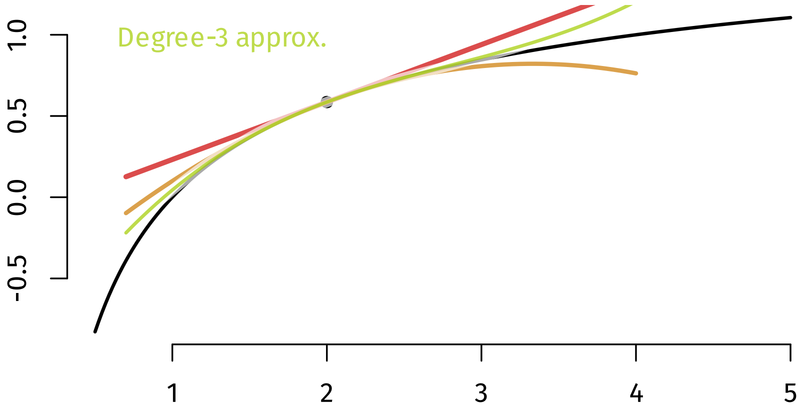
Example: CRRA utility visualisation



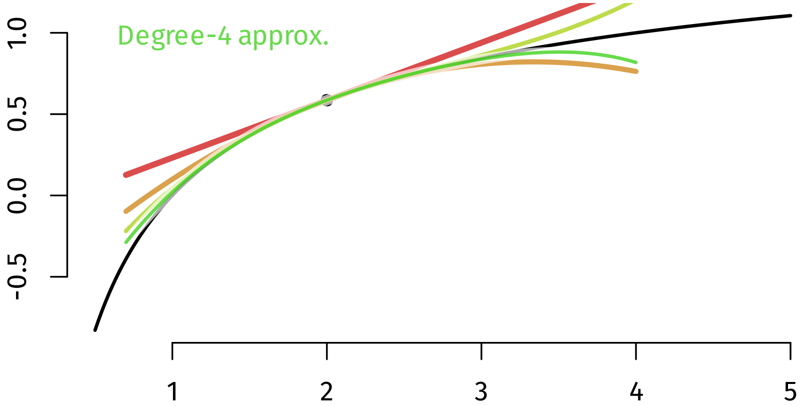
Example: CRRA utility visualisation



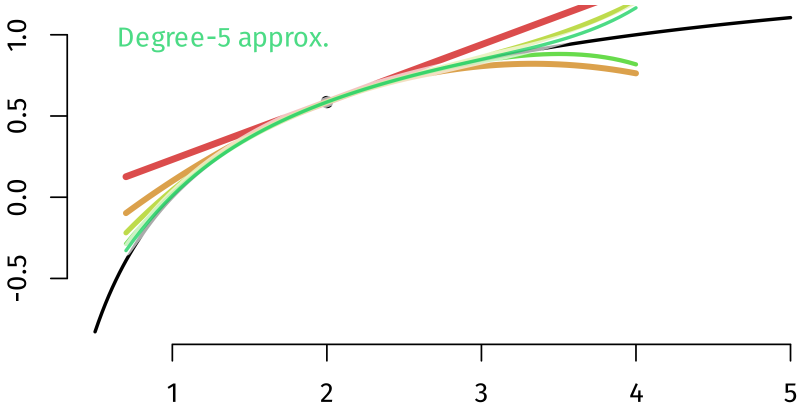
Example: CRRA utility visualisation



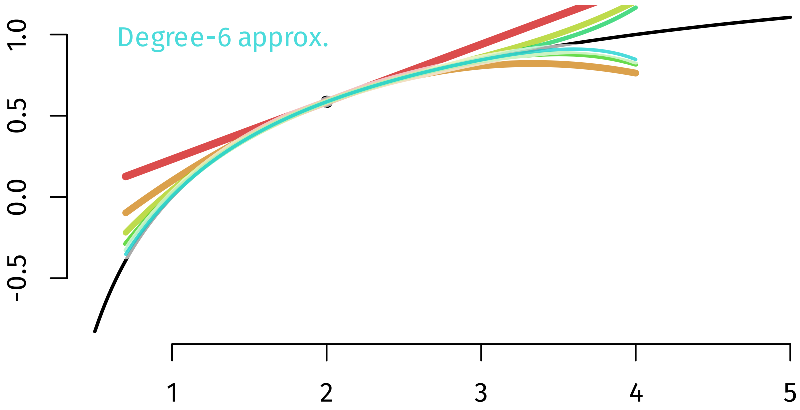
Example: CRRA utility visualisation



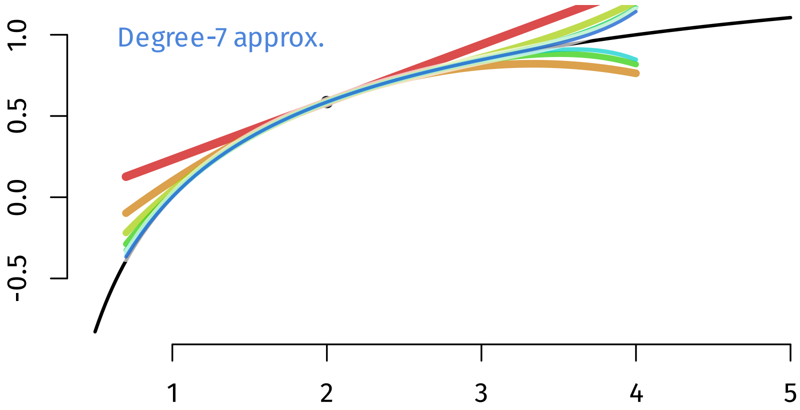
Example: CRRA utility visualisation



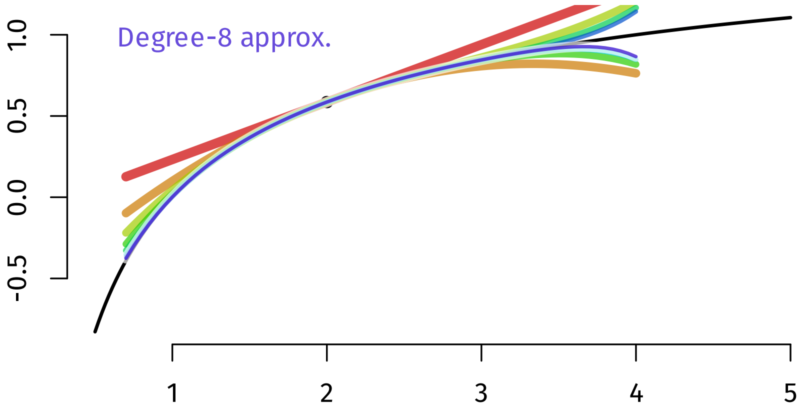
Example: CRRA utility visualisation



Example: CRRA utility visualisation



Example: CRRA utility visualisation



Reversing the Taylor series

- Taylor theorem: approximate $f(x)$ using $f(x_0),\ f'(x_0),\ f''(x_0)$ ('derivatives $\Rightarrow$ function values')
- 'function values $\Rightarrow$ derivatives' is also possible
- Polynomials are extremely easy to differentiate analytically: $\frac{\mathrm{d}}{\mathrm{d}x} x^n = n x^{n-1}$
  - Potentially up to n non-zero derivatives
- Use multiple values $f(x_0), \dots, f(x_n)$ to construct a degree-n polynomial approximation and calculate the derivative of the latter

Derivatives through Taylor series

$$f(x+h) = f(x) + f'(x)h + \frac{f''(x+\alpha h)}{2}h^2, \quad \alpha \in [0,1]$$

Subtract $f(x)$ and divide by h:

$$\frac{f(x+h) - f(x)}{h} = f'(x) + \frac{f''(x+\alpha h)}{2}h = f'(x) + O(h)$$

Therefore, assuming that $f''(x)$ is uniformly bounded*, $f'(x) = f'_{\mathrm{FD}}(x,h) + O(h) \approx f'_{\mathrm{FD}}(x,h) + \frac{f''(x)}{2}h$ (for small h), and $f'_{\mathrm{FD}}(x,h)$ is **first-order-accurate**.

This is the naïve approximation from Slide 13!

* $\exists M > 0\colon\ \sup_x |f''(x+\alpha h)| \le M < \infty$.

Symmetrical differences

To improve the accuracy, consider expansions at $x \pm h$:

$$f(x+h) = f(x) + f'(x)h + \frac{f''(x)}{2}h^2 + \frac{f'''(x+\beta_1 h)}{6}h^3, \ \beta_1 \in [0,1]$$

$$f(x-h) = f(x) - f'(x)h + \frac{f''(x)}{2}h^2 - \frac{f'''(x-\beta_2 h)}{6}h^3, \ \beta_2 \in [0,1]$$

Subtract (2) from (1):

$$f(x+h) - f(x-h) = 2f'(x)h + \frac{f'''(x+\beta_1 h) + f'''(x+\beta_2 h)}{6}h^3$$

Divide by $2h$ + generalised intermediate value theorem:

$$\frac{f(x+h) - f(x-h)}{2h} = f'(x) + \frac{f'''(x+\beta h)}{3}h^2, \quad \beta \in [-1,1]$$

Equivalence of extrapolation and weighted sums

The following is algebraically identical for higher-order accuracy:

- Extrapolating sequences of central differences at $(x \pm h_1)$, $(x \pm h_2), \ldots$
- Evaluating the function on the grid $x + (-h_1, -h_2, h_2, h_1)$ and combining the values with specific coefficients $w_1, \ldots, w_4$

This opens opportunities for **parallel evaluation**!

Accuracy: finding w_i requires inverting a numerically unstable Vandermonde matrix $\Rightarrow$ we use (and benchmark!) a reliable Björck–Pereyra (1970) algorithm.

Second derivatives via central differences

$$f''(x) := \frac{\mathrm{d}}{\mathrm{d}x} f'(x)$$

Find such a linear combination of $f(x-h), f(x), f(x+h)$ that the coloured terms should cancel out:

$$f(x+h) = f(x) + f'(x)h + \frac{f''(x)}{2}h^2 + \frac{f'''(x)}{6}h^3 + \frac{f''''(x+\gamma_1 h)}{24}h^4$$

$$f(x-h) = f(x) - f'(x)h + \frac{f''(x)}{2}h^2 - \frac{f'''(x)}{6}h^3 + \frac{f''''(x-\gamma_2 h)}{24}h^4$$

This weighted sum is the solution:

$$f''_{\mathrm{CD}}(x,h) := \frac{f(x-h) - 2f(x) + f(x+h)}{h^2}$$

Accuracy of second derivatives

The error order is the same as with f'_{CD}:

$$f''(x) - f''_{\mathrm{CD}}(x, h) \approx -\frac{f''''(x)}{12} h^2 = O(h^2)$$

However, the default implementation in many software products is **repeated differences**:

$$f''(x) \approx \frac{f'(x+h) + f'(x-h)}{2h} \approx \frac{f'_{\mathrm{CD}}(x+h) + f'_{\mathrm{CD}}(x-h)}{2h}$$

- Approximating $f''(x)$ via a 3-term f''_{CD} is **faster**: each f'_{CD} takes 2 evaluations
- **More accurate** with the optimal step size: the h^* that is optimal for f'_{CD} is too small for f''_{CD} (Slide 84)

Examples of stencils and weights

- $f'_{\text{FD}} = \frac{f(x+h)-f(x)}{h} = h^{-1}[-1 \cdot f(x + 0h) + 1 \cdot f(x + 1h)]$
  - Stencil: $b = (0, 1)$, weights: $w = (-1, 1)$
- $f'_{\text{CD}} = \frac{f(x+h)-f(x-h)}{2h} = h^{-1}[-\frac{1}{2}f(x - h) + \frac{1}{2}f(x + h)]$
  - Stencil: $b = (-1, 1)$ *(symmetric)*, weights: $w = \left(-\frac{1}{2}, \frac{1}{2}\right)$
- $f''_{\text{CD}} = \frac{f(x-h)-2f(x)+f(x+h)}{h^2}$
  - Stencil: $b = (-1, 0, 1)$, weights: $w = \left(1, -2, 1\right)$
- $f'_{\text{CD},4} = \frac{f(x-2h)-8f(x-h)+8f(x+h)-f(x+2h)}{12h}$
  - Stencil: $b = (-2, -1, 1, 2)$, weights: $w = \left(-\frac{1}{12}, \frac{8}{12}, -\frac{8}{12}, \frac{1}{12}\right)$

Numerical Hessians via central differences

Let $h_i := (0 \ \ldots \ 0 \underbrace{h}_{i^{\text{th}} \text{ position}} 0 \ \ldots \ 0)'$ and $x_{+-} := x + h_i - h_j$.

4 evaluations of f are required to approximate $\nabla^2_{ij} f$ via CD:

$$\nabla^2_{ij} f(x) := \left[\nabla^T \left(\nabla f(x)\right)\right]_{ij} := \nabla^2_{ij,\mathrm{CD}} f(x) + O(h^2) =$$
$$= \frac{f(x_{++}) - f(x_{-+}) - f(x_{+-}) + f(x_{--})}{4h^2} + O(h^2)$$

- The 4-term sum is as **fast** as the 4-term $\frac{\nabla_i f(x+h_j) - \nabla_i f(x-h_j)}{2h_j}$, but guaranteed to be **symmetric**: $\hat{\nabla}^2_{ij,\mathrm{CD}} = \hat{\nabla}^2_{ji,\mathrm{CD}}$
  - Symmetric repeated differences require 8 terms
- Accuracy implications are being investigated

Floating-point arithmetic

Computers convert inputs into **1**'s and **0**'s for processing.

Real numbers can be written with an **integer** mantissa (=significant digits) and an **integer** exponent (=magnitude):

$$1.8125 = \underbrace{18\,125}_{\text{integer mantissa}} \cdot \underbrace{10}_{\text{base}}{}^{\overbrace{-4}^{\text{integer exponent}}}$$

The number 18.125 has the same mantissa and a different exponent (-3). To multiply by 10 (the base), move the decimal point: $1.8125 \cdot 10 = 18.125$.

Such numbers are called **floating-point numbers**.

Available precision on 64-bit machines

1 bit sign	11 bits exponent	52 bits significant digits
0	10000001101	1100000011010001100110011001100110011001100110011001

Computing the number from bits:

$$(-1)^{\text{sign}} \cdot (1.\text{significand}) \cdot 2^{\text{exponent}-2^{10}+1} =$$

$$= 1.753198 \cdot 2^{1037-1023} = 28\,724.4$$

- 64-bit FP numbers represent $5 \cdot 10^{-324} \ \ldots \ 2 \cdot 10^{308}$
- Are 64-bit calculations relatively accurate up to 10^{-323}?
  No, only to $1/2^{52} = 2.2 \cdot 10^{-16}$**!**
- Precision beyond $\approx$16 decimal significant digits is lost

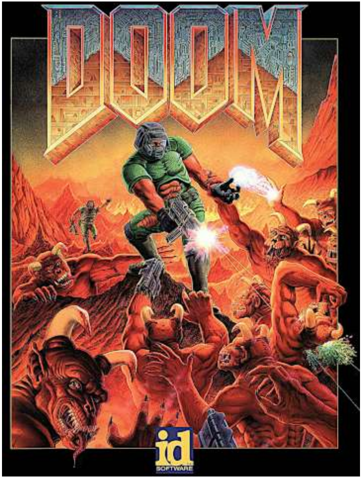
Computers have terrible precision

- **Machine epsilon** (ϵ_{mach}): maximum relative step between two representable numbers, or $\epsilon_{\mathrm{mach}} := 2^{-52} \approx 2.2 \cdot 10^{-16}$
  - If $x = 2^i$ for integer i, the mantissa is 52 zeros: 000...000; when the least significant bit is flipped from 0 to 1, the mantissa becomes 000...00**1**, and $x \mapsto (1 + \epsilon_{\mathrm{mach}})x$

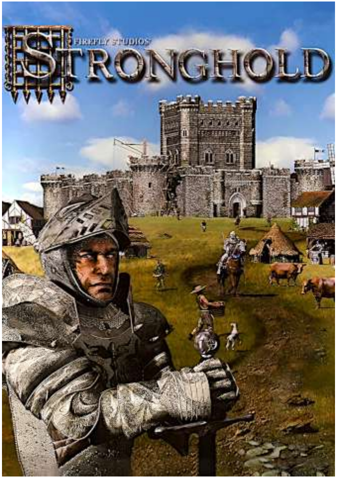
```
lm(formula = mpg ~ disp, data = mtcars)
Coef:         Estimate Std. Error t value Pr(>|t|)
(Intercept) 29.599855   1.229720  24.070  < 2e-16 ***
disp        -0.041215   0.004712  -8.747 9.38e-10 ***
```

- Rounding errors (e. g. if numbers have different orders of magnitude), catastrophic cancellation, ill conditioning (high sensitivity to small input errors)
- Input errors, user mistakes, programmer and hardware bugs – *purgamenta intrant, purgamenta exeunt*

Example: low bit rates in early software

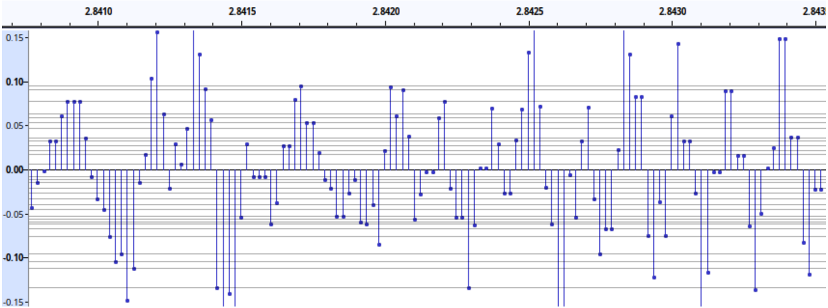


1993, **8-bit** audio,
11 025 Hz sampling



2001, **4-bit** audio,
44 100 Hz sampling

Example: 8-bit audio in the 1990s



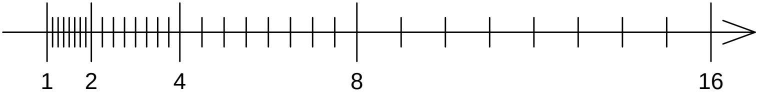
The vertical position of the wave can take any of the $2^8 = 256$ values; 1 point = 1 byte.

11 025 Hz = 11 kilobytes per second of audio.

Finite precision in digital data

- The vertical position of the sound wave intensity is digitally encoded as a number on a fixed grid:
  - 4 bits $\Rightarrow 2^4 = 16$ positions (very coarse)
  - 8 bits $\Rightarrow 2^8 = 256$ positions (coarse)
  - 16 bits $\Rightarrow 2^{16} = 65\,536$ positions (CD quality)
- 64-bit FP numbers use a similar grid to allow $\Rightarrow 2^{64} \approx 1.8 \cdot 10^{19}$ numbers **on the entire real line**
  - The amount of annual Internet traffic is $> 10^{21}$ bytes – already not enough even with positive integers
  - One is limited to 64 bits per number unless they use special libraries for arbitrary-precision arithmetic at the cost of extra memory and speed: GMP, MPFR…

Graphical representation of FP accuracy



- Intervals [1, 2], [2, 4], [4, 8], ... are cut into $2^{52} \approx 4.5 \cdot 10^{15}$ equal intervals; all numbers are snapped to the edges
- The gap between two representable numbers is proportional to the number magnitude
  - The rounding error is **proportional** to the number
  - Relative rounding error range: $[0 \ldots 1.1 \cdot 10^{-16}]$
- Caution: `round(3.5) = 4`, but `round(4.5) = 4` due to rounding towards the nearest *even* number
  - **Worst case:** the 1992 precision loss in the Patriot missile control system ⇒ 28 soldiers died to a Scud missile

Insufficient precision example

```
a = 2^52     # 4 503 599 627 370 496, 1/macheps
b = a + 0.4
c = b + 0.3
d = c + 0.3
d - a        # Question: is equal to what?
```

Answer: **zero**. (At least in FP64 precision.)

- The next number after 2^{52} representable by the machine is $2^{52} + 1$
- Everything less than $2^{52} + 0.5$ is rounded down to 2^{52}
  - Sort the inputs or use Kahan's compensated summation to extend the precision
  - But `2^52+0.3+0.3+0.3+0.3+0.3+0.3+... = 2^52`!
- **Max. rel. error:** $\epsilon_{\text{mach}}/2$, **max. abs. error:** $|y| \cdot \epsilon_{\text{mach}}/2$

Base-conversion precision loss example

Only finite sums of integer powers of 2 up to 2^{52} are stored losslessly in computer memory:

$1/2 = 0.5_{10} = 0.1_2$ – fine.

$4/5 = 0.8_{10} = 0.1100\,1100\ldots_2 = 0.\overline{1100}_2$ – infinite period.

With 52 bits, one can represent only $0.\underbrace{[1100]}_{\times 12}1100 = 0.8 - 2\cdot 10^{-16}$

or

$$0.\underbrace{[1100]}_{\times 12}1101 = 0.8 + 4\cdot 10^{-17}.$$

If 0.8 is saved as a number, it is read back as a **different** one:

```
print(0.8, 20) # 0.80000000000000004441.
```

Real case #2: catastrophic cancellation

The causal effect of a 1-euro debt change on the probability of self-reported good health condition (GH) in the probit model $\mathbb{P}(GH = 1 \mid Debt, \ldots) = \Phi(\gamma_0 Debt + \ldots)$:

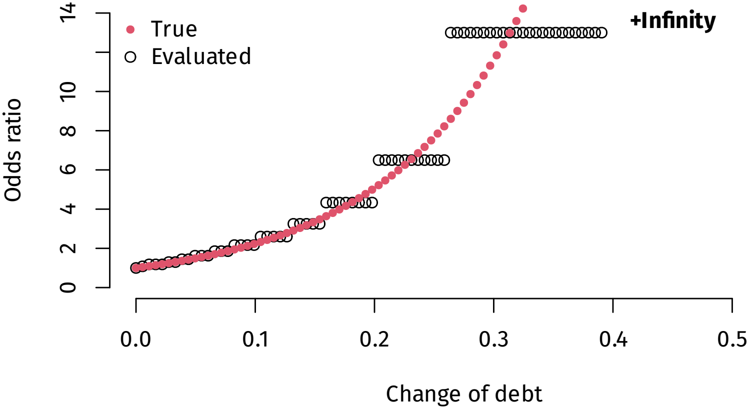
$$\frac{\partial \mathbb{P}(GH_i = 1)}{\partial Debt_i} \approx \frac{\Phi\big(\hat{\gamma}(Debt_i + 0.001) + \ldots\big) - \Phi(\hat{\gamma} Debt_i + \ldots)}{0.001}$$

If the argument of $\Phi(\cdot)$ is too large, probabilities close to 1 are predicted. If $\hat{\gamma} \cdot Debt_i + \ldots = 8.3$, the relative error of $\frac{\partial \mathbb{P}(GH_i = 0)}{\partial Debt_i}$ can be $\approx 17\%$.

Consequence: the error of the odds ratio is unbounded.

Illustration of catastrophic cancellation

Evaluated odds ratio $\frac{\mathbb{P}(GoodHealth_i = 0 | Debt_i)}{\mathbb{P}(GoodHealth_i = 0 | Debt_i + \text{change})}$.



Probit breaks at $X'\beta = 8.3$; logit breaks at $X'\beta = 36.8$.

Total error function properties

On the log-log scale,

- The slope of the left branch is the differentiation order m (times -1)
  - The rounding error of the difference is divided by h^m
- The slope of the right branch is the accuracy order a
  - The truncation error is approximately $f''^{\cdots}/a!$ times h^a

General step-size selection

Result: a^{th}-order-accurate m^{th} numerical derivatives have:

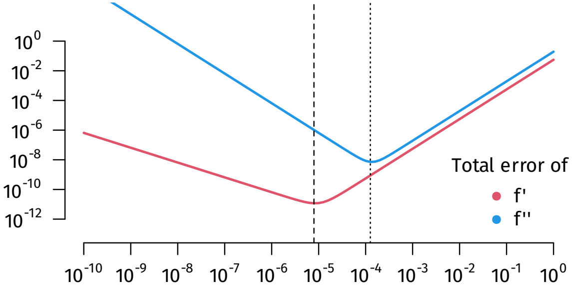
- Optimal step size $h_* \propto \sqrt[a+m]{\epsilon_{\text{mach}}}$
- Approximation error $\propto \epsilon_{\text{mach}}^{a/(a+m)} \propto h_*^a \propto \epsilon_{\text{mach}}/h_*^m$ with equal order of truncation and rounding components
  - The total error at the optimal h^* is $O(\epsilon_{\text{mach}}^{1/2})$ for one-sided and $O(\epsilon_{\text{mach}}^{2/3})$ for central differences
  - In 64-bit precision, f'_{FD} is accurate only to ≈7–8 decimal digits, and f'_{CD} to ≈10–11 digits **at most**
  - Second derivatives and Hessians: $h^{**}_{\text{CD}} \propto \epsilon_{\text{mach}}^{1/4}$
  - 4^{th}-order-accurate CD: $h^*_{\text{CD},4} \propto \epsilon_{\text{mach}}^{1/5}$ (≈12–13 digits)
- Hard limit: impossible to have > 16 accurate decimal places on 64-bit machines without extra effort

Is repeated differencing dangerous?

Options for $f''(x)$: $\frac{f(x-h)-2x+f(x+h)}{h^2}$ or $\frac{f'_{\mathrm{CD}}(x+h)-f'_{\mathrm{CD}}(x-h)}{2h}$.

Surprisingly, both have the same maximum attainable accuracy, $O(\epsilon_{\mathrm{mach}}^{1/2})$ (7–8 digits), with $h^{**}_{\mathrm{CD}} \propto \epsilon_{\mathrm{mach}}^{1/4}$. However, using $h^{*}_{\mathrm{CD}} \propto \epsilon_{\mathrm{mach}}^{1/3}$ results in an $O(\epsilon_{\mathrm{mach}}^{1/3})$ error, i. e. only 5–6 accurate digits!

Recall the **tip:** multiply h^{*}_{CD} by $\epsilon_{\mathrm{mach}}^{-1/12} \approx 20$.



Paradigms for step-size search

1. Theoretical (plug-in expressions)
2. Empirical (finding the minimum of the total error)

My package, `pnd`, provides multiple algorithms **(currently under active feature implementation and testing)**.

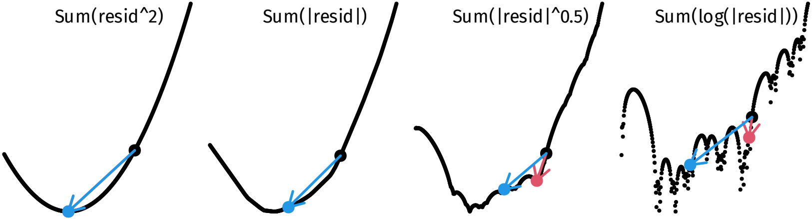
Analogy: Silverman's rule-of-thumb bandwidth vs. data-driven cross-validated bandwidth in non-parametric econometrics.

Naturally noisy functions

Noisy function: many local optima and strong abrupt changes of curvature.

In optimisation, accurate derivatives of noisy function are useless (local features obscure global optima).

Although $h^*_{\mathrm{CD}} = \sqrt[3]{1.5|f/f'''|\epsilon_{\mathrm{mach}}} \propto 1/f'''$, use **larger** step sizes to guess a better trend.



Relative or absolute step?

- The optimal step size, $h^*_{\text{CD}} = \sqrt[3]{\epsilon_{\text{mach}} \cdot 1.5|f(x)/f'''(x)|}$, depends on the value of x only through $f(x)/f'''(x)$
- However, **relative step** $x \cdot h^*_{\text{CD}}$ is often used to eliminate the problems of **units of measurement** for large $|x|$
  - If $x = 10^{12}$ and $\tilde h = 10^{-4}$, **argument-representation errors** appear: $|[x + \tilde h]_{\text{FP64}} - (x + \tilde h)| = 2 \cdot 10^{-5} \neq 0$ (Slide 78)
  - If $x = 10^{-5}$ and $\tilde h = 10^{-4}$, $x - \tilde h < 0$; bad if $\operatorname{dom} f = \mathbb{R}^{++}$: $\log x$, $\sqrt{x}\ldots$ (Slide 6)
- The magnitude of x may be informative of the curvature change, $f'''(x)$
- Common practice: choose $x_{\min} = 10^{-5}$; for $|x| < x_{\min}$, use step size $\tilde h$ and for $|x| \ge x_{\min}$, use step size $|x|\tilde h$
  - Helps only with large x, not small x such that $|f'''(x)| \gg 0$

Finite-difference stencils and weighs

Use `fdCoef()` to obtain the coefficients that yield an approximation of the m^{th} derivative with error $O(h^a)$ on the **smallest sufficient stencil**.

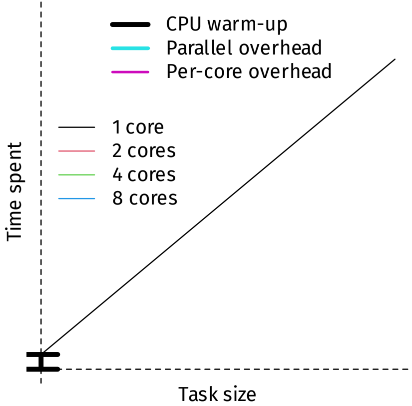
```
fdCoef(deriv.order = 2, acc.order = 4)
# $stencil:   -2        -1          0        1         2
# $weights:  x-2h      x-1h         x      x+1h      x+2h
#         -0.08333  1.33333 -2.50000  1.33333 -0.08333
```

Arbitrary stencils are supported; the resulting coefficients yield the **maximum attainable accuracy**:

```
fdCoef(deriv.order = 1, stencil = c(-1, 0, 4))$weights
#  x-1h     x  x+4h
# -0.80  0.75  0.05  # Second-order accuracy
```

Overhead in theory

Using mores cores requires spawning processes and copying memory pages – there are fixed costs.



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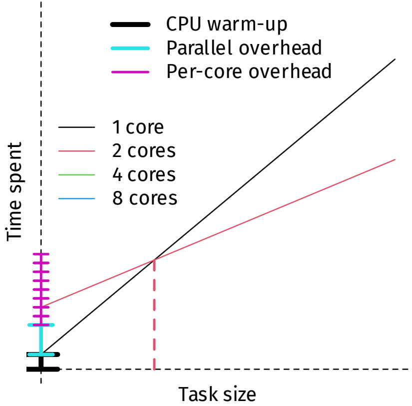

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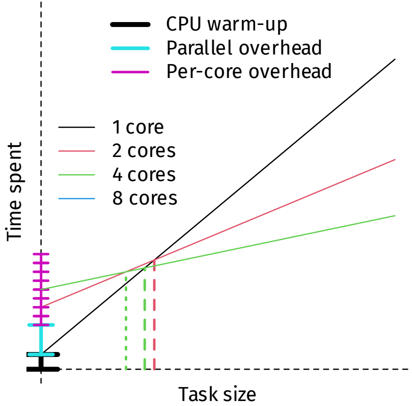

Overhead in theory

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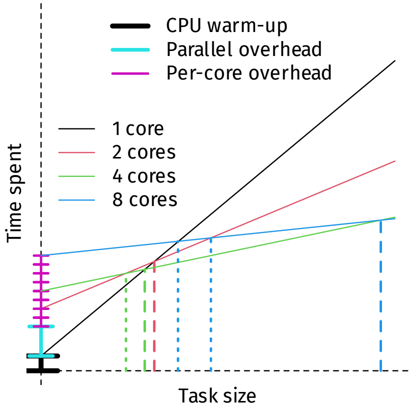


Overhead magnitude

- Requesting 2 cores for a parallel job: $\approx$0.01 s
  - 0.3–0.4 s on Windows due to its inability to fork effectively!
- Extra per-core time with pre-scheduling: $\approx$0.005 s
  - Plus extra time losses for communication between cores
- If one evaluation of f takes <0.01 s, compare the gains: reduction of the number of tasks vs. overhead per core
- If one evaluation of f takes 0.005–0.010 s, compare the gains: reduction of the number of tasks vs. overhead per core

Time per f	0.002	0.005	0.01	0.02	0.05	0.1	> 0.2
Use cores	1	2–3	4	8	12	16	≥ 24

Long gradients $\Rightarrow$ always parallelise! And **always benchmark**!

Overhead of pnd

How faster is calculating $\frac{f(x+h)-f(x-h)}{2h}$ by hand than running dozens of checks for user inputs?

Each call of `Grad()` adds 0.5 ms of overhead due to the infrastructure; it increases with $\dim x$. *(To be improved!)*

Compare the overhead of computing $\nabla f'_{\mathrm{CD},2}$ for $f(x) := \sum_{i=1}^{\dim x} x^2 + 4 \sin x + 1.1^x$ in seconds:

$\dim X$	1	10	100
Overhead	0.0005–0.0010	0.0008–0.0010	0.0038–0.0041

Is it acceptable in your practical application?

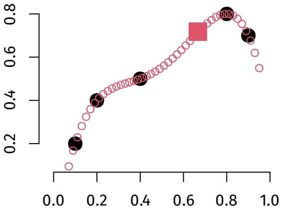
Finding approximations via interpolation

To calibrate η, you run thousands of simulations and compute the goodness of fit $f(\eta)$. You get $\eta = (0.1, 0.2, 0.4, 0.8, 0.9)$, $f(\eta) = (0.2, 0.4, 0.5, 0.8, 0.7)$, but you want to guess f and f' around $\eta_0 = 2/3$.

```
fdCoef(0, stencil = (n - n0))$weights %*% f
fdCoef(1, stencil = (n - n0))$weights %*% f
```

Weights for f: $(0.23, -0.56, 0.69, 0.98, -0.34) \Rightarrow f(2/3) \approx 0.71$.

Weights for f': $(-1.36, 3.51, -5.40, 3.30, -0.05) \Rightarrow f'(2/3) \approx 1.04$.



Parallel step-size selection: light functions

If there are no memory-heavy operations (cloning pages, passing data to child processes), the run time is roughly proportional to the number of cores.

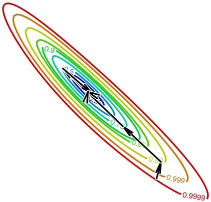
```
f(x) <- {Sys.sleep(s); sin(x)}
```

Times for the Stepleman–Winarsky algorithm to terminate in 7 evaluations / 3 iterations. Ideally, 3 iterations = 3 parallel calls = thrice the time of one call.

s	0.001	0.01	0.1	1
1 core	0.008	0.072	0.702	7.003
2 cores	0.038	0.091	0.456	4.061
3 cores	0.043	0.092	0.368	3.071

Parallel step-size selection: heavy functions

Smoothed empirical likelihood with missing endogenous variables (Cosma, Kostyrka, Tripathi, 2025). Maximising SEL + computing ∇^2-based std. errors via BFGS on 4 cores.




```
g4 <- function(x) Grad(SEL, x = x,
                       acc.order = 4, cores = 4)
optim(par = c(1, 1), SEL, gr = g4, method = "BFGS")
```

Method	Ord.	Time, s	$\|\nabla \mathrm{SEL}\|$	Evals	Iters
built-in	2	21+3.8	$3.6 \cdot 10^{-4}$	46	10
pnd	2	13+1.5	$2.1 \cdot 10^{-7}$	37	10
pnd	4	16+2.9	$3.3 \cdot 10^{-8}$	32	10

Available algorithms

1. Plug-in
2. Curtis–Reid (1974) and its modification (2025)
3. Dumontet–Vignes (1977)
4. Stepleman–Winarsky (1979)
5. Mathur (2012)

Improvements for the CR algorithm

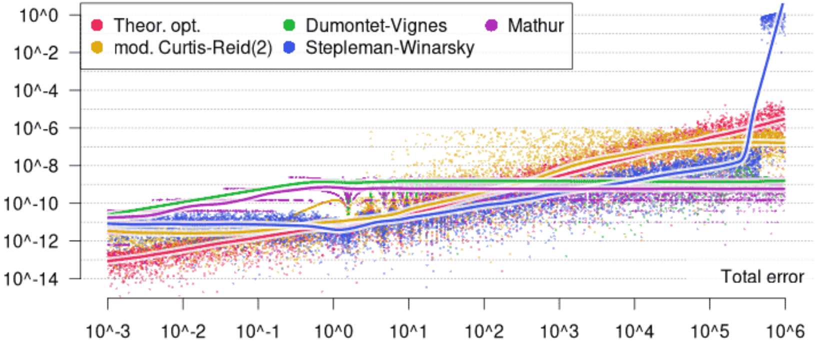
1. Estimate the correct truncation error order with 4 parallel evaluations and use the theoretically correct target ratio
   - Instead of ‘truncation error = rounding error’, use the optimal ‘truncation error = rounding error **halved**’ rule
2. Obtain $f'_{\mathrm{CD},4}$ with algorithmically chosen $h^*_{\mathrm{CD},2}$ times 120
   - $\approx$ 3 times more accurate than theoretical

Improvements to the AutoDX algorithm

Developed by Ravishankar Mathur (2012, Ph .D. thesis).

- The finite differences may be evaluated on the entire grid on a multi-core machine
- The user may plot the behaviour of the approximated total error as an added bonus

Are data-driven steps good for sin x?



- At different values of x, the rankings of methods change
- For other functions, the rankings are different

Sensitivity of the error to the step size

Choosing a *slightly* sub-optimal step size is not as scary. For $f = \sin$, $h^*_{\mathrm{CD},2} = \sqrt[3]{1.5|\tan x|\epsilon_{\mathrm{mach}}}$ is unbounded – a fixed h can work better.

Safest option: invoke Mathur's method with a plot.

Example: diagnosing $f(x) = \exp x$ at $x = 1$.

Comparison of median run times

Grid: 9000 exponentially spaced points between 10^{-3} and 10^{6} (exception: 3000 points in $[10^{-2} \dots 10^{1}]$ for $\exp x$).

Unit: millisecond per step size per grid point + derivative estimation.

Func.	$h^*_{\mathrm{CD},2}$	$\lvert x \rvert \sqrt{\epsilon_{\mathrm{mach}}}$	CR	CRm2	CRm4	DV	SW	M
$\sin x$	<0.01	<0.01	0.18	0.16	0.20	0.46	0.33	1.70
$\exp x$	<0.01	0.02	0.15	0.15	0.15	0.26	0.18	1.72
$\log x$	<0.01	0.01	0.15	0.11	0.15	0.17	0.27	2.09
$\sqrt{x}$	<0.01	<0.01	0.16	0.11	0.15	0.16	0.14	2.13
$\tan^{-1} x$	<0.01	<0.01	0.14	0.11	0.17	0.19	0.42	1.69

Comparison of median absolute errors

Error: $|f'(x) - f'_{\mathrm{CD},2}|$ for 9000 exponentially spaced points between 10^{-3} and 10^{6} (exception: 3000 points in $[10^{-2} \ldots 10^{1}]$ for $\exp x$).

Short exponential notation: `5.6e-9` $= 5.6 \cdot 10^{-9}$.

Func.	$h^*_{\mathrm{CD},2}$	$\lvert x\rvert\sqrt{\epsilon_{\mathrm{mach}}}$	CR	CRm2	**CRm4**	DV	*SW*	M
$\sin x$	5.7e-11	2.6e-09	1.2e-09	1.2e-10	**2.3e-11**	1.1e-09	*3.0e-11*	5.1e-10
$\exp x$	1.5e-11	2.6e-08	2.2e-10	5.7e-11	**1.3e-11**	3.7e-09	*1.4e-11*	2.7e-09
$\log x$	1.3e-12	0.0e+00	5.6e-12	1.7e-12	**1.6e-13**	1.3e-11	*5.3e-13*	1.0e-10
$\sqrt{x}$	2.1e-12	2.7e-10	9.3e-12	2.4e-12	**2.4e-13**	3.7e-11	*8.2e-13*	1.5e-10
$\tan^{-1} x$	6.8e-13	5.9e-11	3.5e-13	2.2e-13	**2.7e-14**	7.8e-13	*1.6e-13*	9.6e-12

Logic behind the best methods

- **Curtis–Reid (1974) + my modification #2:** use 4 available intermediate points and function values from truncation and rounding error estimation to obtain a 4th-order-accurate estimate (unlike 2)
- *Stepleman–Winarsky:* the truncation error should be quartered if the step size is halved ⇒ start at a step size larger than the best guess and halve it until the decrease is substantially different from 2 due to rounding errors
    - I added a safety step for checking finiteness and extra warnings for edge cases
- Mathur: SW-like evaluation for many points simultaneously + diagnostic plots available