Why “AD” in ADModel Builder?

ADMB

Automatic Differentiation Model Builder

ADMB Foundation

sibert@hawaii.edu

Outline

- Why are we interested in differentation?
- What is “automatic” about it?
- Automatic differentiation versus finite difference approximation
- What the AUTODIF library does

Differentiation finds maxima

Maximum Likelihood

Simple Example — Quadratic Regression

$$L(a,b) = f(x_1, x_2, x_3, \ldots, x_n | a, b) = \sum_{i=1}^{n} \left[y_i - (a + b x_i^2) \right]^2$$

$$\widehat{(a,b)} = \frac{\text{arg max}}{(a,b)} L(a,b)$$

$$\begin{aligned} \frac{\partial L}{\partial a} &= 2 \sum_{i=1}^{n} \left(a + b x_i^2 - y_i \right) \\ \frac{\partial L}{\partial b} &= 2 \sum_{i=1}^{n} x_i^2 \left(a + b x_i^2 - y_i \right) \end{aligned}$$

Automatic Differentiation

$$L_i(a,b) = \left[y_i - (a + bx_i^2)\right]^2$$

```
L(i) = pow(y(i)-(a+b*pow(x(i),2)),2);
```

1	$t_1 = x_i^2$	x_i^2
2	$t_2 = bt_1$	bx_i^2
3	$t_3 = a + t_2$	$a + bx_i^2$
4	$t_4 = y_i - t_3$	$y_i - (a + bx_i^2)$
5	$t_5 = t_4^2$	L_i

Derivative Chains

$$\frac{dL}{da} = \frac{dL}{dt_5} \cdot \frac{dt_5}{dt_4} \cdot \frac{dt_4}{dt_3} \cdot \frac{dt_3}{da} = 2(a + bx^2 - y)$$

$$\frac{dL}{db} = \frac{dL}{dt_5} \cdot \frac{dt_5}{dt_4} \cdot \frac{dt_4}{dt_3} \cdot \frac{dt_3}{dt_2} \cdot \frac{dt_2}{db} = 2x^2(a + bx^2 - y)$$

AUTODIF Algorithm — Reverse Mode AD

$$L_i(a,b) = \left[y_i - (a + bx_i^2)\right]^2$$

```
L(i) = pow(y(i)-pow(a+b*x(i),2),2);
```

1	$t_1 = x_i^2$	x_i^2
2	$t_2 = bt_1$	bx_i^2
3	$t_3 = a + t_2$	$a + bx_i^2$
4	$t_4 = y_i - t_3$	$y_i - (a + bx_i^2)$
5	$t_5 = t_4^2$	L_i

Derivative computation, $\tau_k = \frac{dt_{k+1}}{dt_k}$

	$\tau_5 = 1$	$\frac{\partial L}{\partial L}$
5	$\tau_4 = 2t_4\tau_5$	$2[y_i - (a + bx_i^2)]$
4	$\tau_3 = -\tau_4$	$2(a + bx_i^2 - y_i)$
	$\dot{y}_i = t_4$	
3	$\tau_2 = \tau_3$	$2(a + bx_i^2 - y_i)$
	$\dot{a} = \tau_3$	$2(a + bx_i^2 - y_i)$
2	$\tau_1 = b\tau_2$	
	$\dot{b} = t_1\tau_2$	$2x_i^2(a + bx_i^2 - y_i)$
1	$\dot{x}_i = 2x_i\tau_1$	

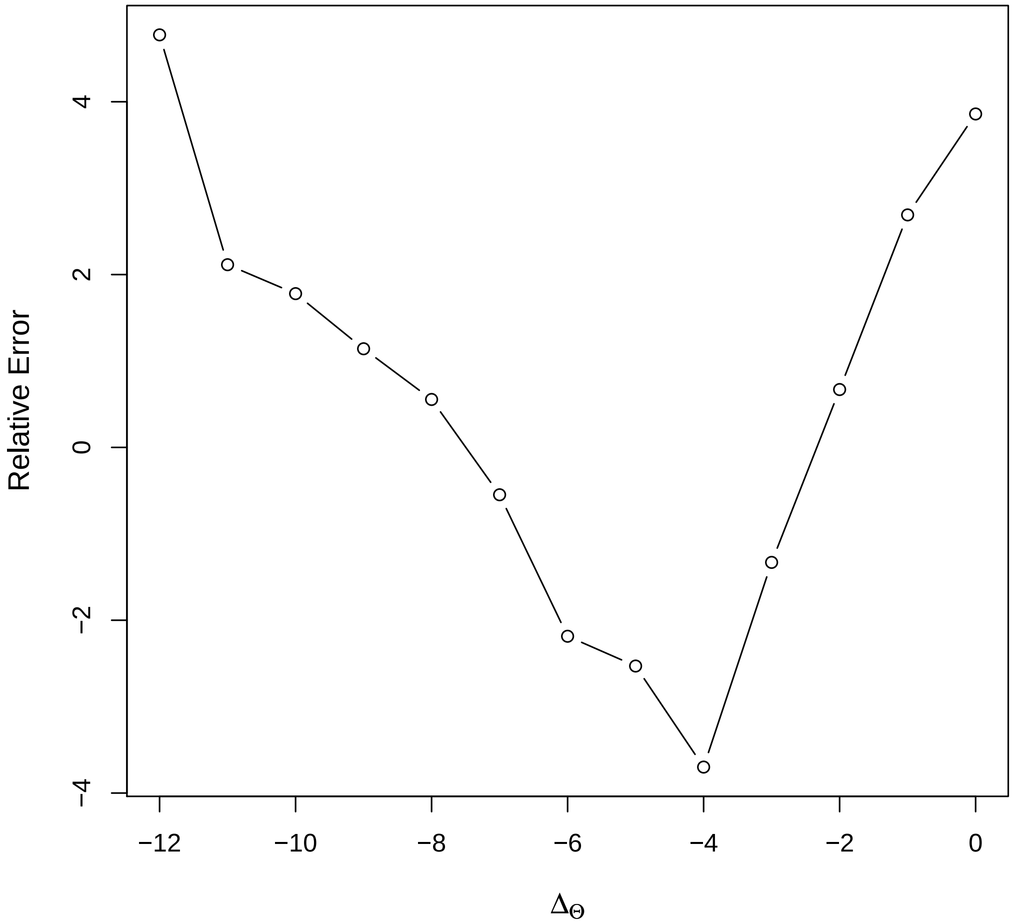
Finite difference approximations

- Expensive; cost proportional to number of parameters:

$$
\begin{aligned}
L = &\quad f(x_1, x_2, x_3, \ldots, x_n | \theta_1, \theta_2, \theta_3, \ldots, \theta_p) = &\quad f(X|\Theta) \\
\frac{\partial L}{\partial \theta_j} \approx &\quad \frac{f(X|\theta_j) - f(X|\theta_j - \Delta_\theta)}{\Delta_\theta} &\quad p+1 \text{ function evaluations} \\
\approx &\quad \frac{f(X|\theta_j + \Delta_\theta) - f(X|\theta_j - \Delta_\theta)}{2\Delta_\theta} &\quad 2p \text{ function evaluations}
\end{aligned}
$$

- Inaccurate, at best an approximation.
- Requires computation of differences between numbers of the same order of magnitude; accumulates large round-off errors.

Finite Difference Errors



AUTODIF Library

- Analytically correct derivatives computed to same precision as objective function using the Chain Rule and “reverse mode” automatic differentiation
- C++ Library
- Classes for differentiable objects: scalars, vectors, matrices, higher dimensional arrays with flexible dimensions and optional subscript checking
- **All** operators $(+, -, \times, \div, \ldots)$ **and** mathematical functions (`sqrt()`, `exp()`, `log()`, `sin()`, `...`) overloaded
- Built-in derivative checker
- Efficient, stable quasi-Newton function minimizer; flexible convergence criteria
- Vector and matrix operations
- Built-in derivative checker

The AUTODIF derivative checker

- Compares AUTODIF chain rule derivatives with central finite-difference approximation.
- Invoke by:
  - Typing `-dd n` on the command line to start derivative checker after function evaluation `n`, or
  - by pressing `Ctrl C` during execution after the first function evaluation
- Specify which variable(s) you want checked.
- Specify the finite difference step size, 10^{-4} is a good place to start.

Exercise – invoking the derivative checker

- Run the simple example and note how many functions evaluations are used before convergance
- Run the example again by typing `simple -dd XX` where XX is one less then the number of function evaluations you noted
- When you see the prompt
  `Enter index (1 ... 2) of derivative to check.  To check all derivatives, enter 0:   To quit enter -1:` , enter 0.
- When you see the prompt
  `Enter step size (to quit derivative checker, enter 0):`, enter `1e-4`
- When you see the prompt `Else enter 0`, enter `0`
- Compare the analytical computation and finite difference approximation. They should agree to 5 significant figures.
- How small can you make the step size? Try to make a plot of relative error as a function of step size.

Exercise – bigeye thermoregulation example

- Compile and run `qb.tpl` and observe its behavior.
- Does the model converge?
- What is the gradient when the function minimizer gives up?
- Check the derivatives.
- Find the error and try to fix it.

Don't break the chain!

$$k = \begin{cases} k_1 & \Delta Q < Q_T \\ k_2 & \Delta Q \geq Q_T \end{cases}$$

Where Q_T, k_1, and k_2 are model parameters, and $\Delta Q = f(k, \ldots)$ is state variable predicted by the model. Straightforward implementation of this assumption as

```
if (Q < QT)
  k = k1;
else
  k = k2;
```

breaks the derivative chain.

What to do about it?

References

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