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pyaudi: A truncated Taylor polynomial algebra toolbox for differentiable intelligence, automatic differentiation, and verified integration applications.

Dario Izzo [1], **Francesco Biscani**[2], **and Sean Cowan** [1]

1 Advanced Concepts Team, European Space Research and Technology Center (Noordwijk, NL) **2** Max Planck Institute for Astronomy (Heidelberg, DE)

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Summary

pyaudi is a Python toolbox developed at the European Space Agency that implements the algebra of Taylor truncated polynomials to achieve high-order order, forward mode, automatic differentiation in a multivarate setting. The forward mode automatic differentiation is implemented via C++ class templates exposed to python using pybind11. This allows the generalized dual number type to behave like a drop-in replacement for floats (or other scalar types), while operator overloading propagates derivatives automatically.

All standard mathematical functions are all implemented exploiting the nihilpotency property of truncated polynomials lacking the constant term.

On top of the algebra of Taylor truncated polynomials, pyaudi also offers an implementation of Taylor models (Makino, 1998), which combine truncated Taylor polynomials with an interval bounding its truncation error as well as a number of miscellaneous algorithms useful for applications in differential intelligence, automatic differentiation, verified integration and more.

Statement of need

pyaudi enables researchers to compute and manipulate order n Taylor expansions of generic computational trees as well as bound precisely the truncation error introduced using its corresponding Taylor model. The resulting polynomial representations of the program outputs can be used to perform fast Monte Carlo simulations, rigorous uncertainty analyses local inversions of output-input relations as well as high-order sensitivity analysis. The package implements the approach to high-order automated differentiation by (Berz et al., 2014) and (Makino, 1998) introducing original implementation details aimed at increased efficiency in the polynomial multiplication routines and bounding of Taylor models.

Key aspects

The main features of pyaudi are:

- Efficient truncated polynomial arithmetic in arbitrary dimensions, built on top of Obake, a C++ library for symbolic manipulation of sparse multivariate polynomials, truncated power series, and Poisson series. Unlike other packages, which often face severe memory bottlenecks as the polynomial order or number of variables grows, pyaudi avoids large static memory allocations and keeps computations memory-efficient.
- Vectorized generalized dual numbers, enabling simultaneous evaluation of identical computational graphs at multiple expansion points. This makes it possible to compute

high-order tensors efficiently while amortizing the overhead of graph bookkeeping.

- Taylor models implemented using Bernstein polynomials for bounding the range of multivariate polynomials. The only other comparable open-source package, called TaylorModels.jl, calculates bounds using Horner's scheme combined with interval arithmetic. A quick test in the next section shows significant speedup for even a relatively simple trivariate polynomial.
- Map inversion algorithm, implementing the algorithm described in (Berz et al., 2014), thus allowing local inversion of the input–output relation of generic computational graphs.

Comparison with TaylorModels.jl

We test the performance of the implementation of Taylor models in `pyaudi` against the Julia package TaylorModels.jl. To perform the comparison we use three functions f, g, h: one univariate, one bivariate and one trivariate defined below. We then construct Taylor models of all the variables separately and time the evaluation of the corresponding Taylor model. The comparison is made on a single CPU machine.

$$
\begin{aligned}
f(x,y,z) = &\frac{4\tan(3y)}{3x + x\sqrt{\frac{6x}{-7(x-8)}}} - 120 - 2x - 7z(1+2y) \\
&- \sinh\left(0.5 + \frac{6y}{8y+7}\right) + \frac{(3y+13)^2}{3z} - 20z(2z-5) \\
&+ \frac{5x\tanh(0.9z)}{\sqrt{5y}} - 20y\sin(3z) \\
g(x,y) = &\sin(1.7x + 0.5)(y+2)\sin(1.5y) \\
h(x) = &\, x(x-1.1)(x+2)(x+2.2)(x+2.5)(x+3)\sin(1.7x+0.5)
\end{aligned}
$$

Dimension	Package	Remainder Bound (Order 1)	Remainder Bound (Order 15)	Speed Comparison
h(x)	TaylorModels.jl	1e-15	1e-15	~1.5–2× faster than pyaudi
	pyaudi	1e+2	1e-5	~1.5–2× slower than TaylorModels.jl
g(x, y)	TaylorModels.jl	1e+1	1e-6	Slower: pyaudi is 5× faster (order 3), 15× faster (order 15), 7800× faster (order 1, edge case)
	pyaudi	1e+1	1e-6	Faster (see above)
f(x, y, z)	TaylorModels.jl	1e+0	1e-11	Slower: pyaudi is 8× faster (order 3), 155× faster (order 15), 13000× faster (order 1, edge case)
	pyaudi	1e-1	1e-17	Faster (see above)

In the table above, a clear trend can be seen both in terms of speed and accuracy. For univariate Taylor models, TaylorModels.jl is both faster and produces tighter bounds. At two dimensions, the remainder bounds are already of equal size, but `pyaudi` is significantly faster, with the speedup increasing with the order of the polynomial. At three dimensions, `pyaudi` produces significantly tighter bounds and is again significantly faster, with the speedup increasing with the order of the polynomial.

References

A number of references to relevant work and algorithms implemented in `pyaudi` are:

- (Biscani, 2020)
- (Makino, 1998)
- (Titi & Garloff, 2019)

Other software packages that do similar things are:

- JAX (Bradbury et al., 2018)
- TensorFlow (Abadi et al., 2015)
- PyTorch (Paszke et al., 2019)
- COSY INFINITY (Makino & Berz, 2006)
- DACE (Massari et al., 2018)
- TaylorSeries.jl/TaylorModels.jl (Benet et al., 2019)
- CORA (Althoff, 2015)

Ongoing research

- EclipseNET (Acciarini, Biscani, et al., 2024) (Acciarini et al., 2025)
- CR3BP stochastic continuation (Acciarini, Baresi, et al., 2024)
- Long-term propagation (Caleb & Lizy-Destrez, 2020)
- Rapid nonlinear convex guidance (Burnett & Topputo, 2025)
- Differentiable genetic programming (Izzo et al., 2017)

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