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Automatic Differentiation in ROOT

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In mathematics and computer algebra, automatic differentiation (AD) is a set of techniques to evaluate the derivative of a function specified by a computer program. AD exploits the fact that every computer program, no matter how complicated, executes a sequence of elementary arithmetic operations (addition, subtraction, multiplication, division, etc.) and elementary functions (exp, log, sin, cos, etc.) including control flow statements. AD takes source code of a function as input and produces source code of the derived function. By applying the chain rule repeatedly to these operations, derivatives of arbitrary order can be computed automatically, accurately to working precision, and using at most a small constant factor more arithmetic operations than the original program.

AD is an alternative technique to symbolic and numerical differentiation. These classical methods run into problems: symbolic differentiation leads to inefficient code (unless done carefully) and faces the difficulty of converting a computer program into a single expression, while numerical differentiation can introduce round-off errors in the discretization process and cancellation. Both classical methods have problems with calculating higher derivatives, where the complexity and errors increase. Finally, both classical methods are slow at computing the partial derivatives of a function with respect to many inputs, as is needed for gradient-based optimization algorithms. AD solves all of these problems, at the expense of introducing more software dependencies.

Our talk presents AD techniques available in ROOT, supported by Cling, to produce derivatives of arbitrary C/C++ functions through implementing source code transformation and employing the chain rule of differential calculus in both forward mode and reverse mode. We explain it's current integration for gradient computation in TFormula. We demonstrate the correctness and performance improvements in ROOT's fitting algorithms.

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