Automatic modeling along search directions for high dimensional optimization

Abstract Optimization and machine learning must tune models to fit data. Large-scale problems are typically optimized using a variant of gradient descent, where the gradient is calculated automatically, but the lack of higher-order information about function behavior slows progress. This poster explores the possibility of using unconventional number types to collect more "intelligence" about function behavior along a chosen search direction. By extracting a richer model of its behavior, it becomes easier to build robust and effective optimization routines.

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Automatic modeling, an extension of automatic differentiation

Traditional approach: compute gradients (and possibly Hessians) by automatic differentiation and build a model of the objective. Use model to predict next trial point. (But how far can you trust the model?)

Concept behind automatic differentiation

Dual numbers $a + b\epsilon$ where ϵ is an infinitesimal obeying $\epsilon^2 = 0$. Evaluate $f(x + w\epsilon) = f(x) + wf'(x)\epsilon$. **Julia packages**: ForwardDiff, Zygote (reverse mode).

Alternative approach: automatically model function with guaranteed limits.
Julia packages: IntervalArithmetic, TaylorSeries, *Bound3Numbers* (tentative name).

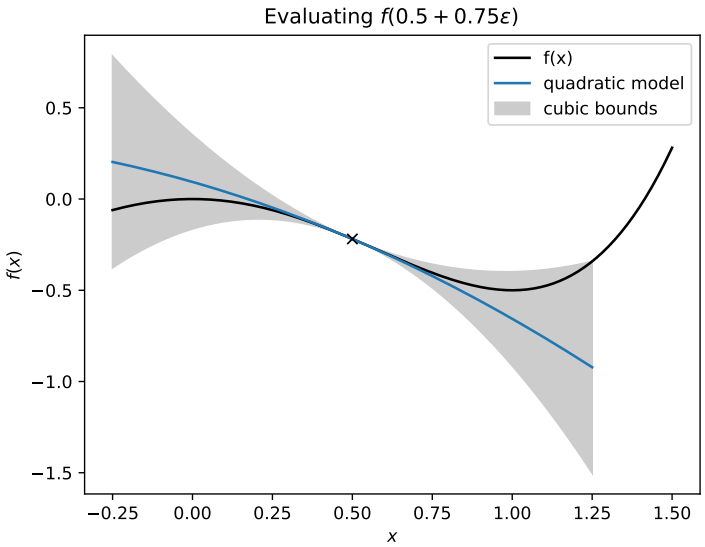
Concept behind automatic bounding

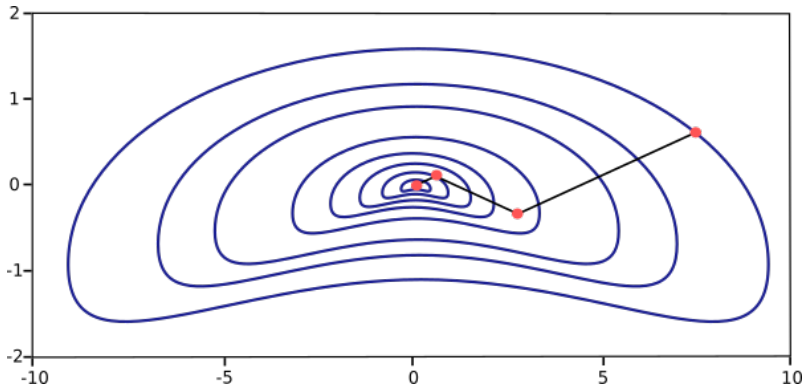
Model $f(y)$ for $y \in [x - w, x + w]$ as a second-order polynomial with third-order remainder, $|f(x + \alpha w) - f(x) - \alpha w f'(x) - \frac{1}{2}\alpha^2 w^2 f''(x)| \le r|\alpha|^3$, by evaluating $f(x + w\epsilon)$. Requires *Bound3 numbers* $v + s\epsilon + c\epsilon^2 + r\rho$, where

$$a\epsilon + b\epsilon = (a + b)\epsilon \qquad a\epsilon^2 + b\epsilon^2 = (a + b)\epsilon^2 \qquad a\rho + b\rho = (|a| + |b|)\rho$$

$$\epsilon^3 = \epsilon\rho = \rho^2 = \rho \quad (\text{models } |\alpha|^n \le |\alpha|^3 \text{ for } |\alpha| \le 1)$$

Using automatic bounding for optimization





Computing $f(\mathbf{x} + \omega\mathbf{p}\epsilon)$ enables simple & effective line searches:

Features:

- You have slope and curvature
- You have a guaranteed interval for improvement (no checking needed)
- $\Rightarrow$ Globally-convergent Newton's method in 1d with just polynomial computations.

$$\alpha = \begin{cases} \frac{-s}{c+\sqrt{c^2+3r|s|}} & c > 0; \\ -\operatorname{sign}(s)\frac{|c|+\sqrt{c^2+3r|s|}}{3r} & \end{cases}$$

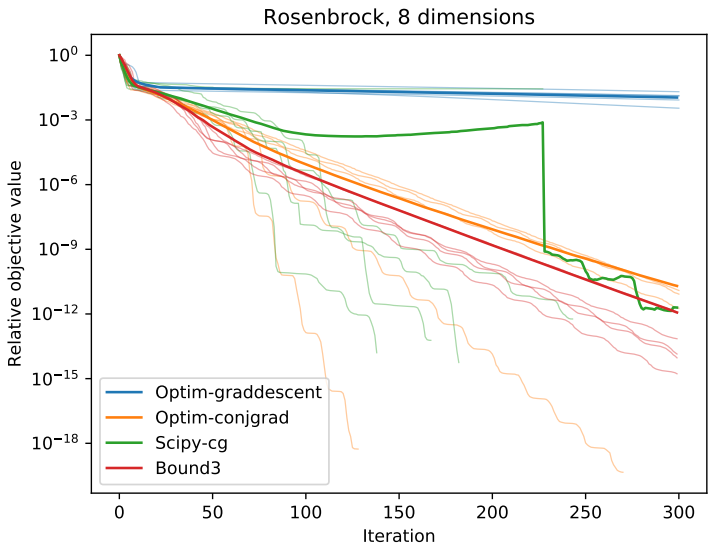
$$\mathbf{x} \to \mathbf{x} + \omega \operatorname{clamp}(\alpha, -1, 1)\mathbf{p}$$

$$\alpha_t = \frac{c^2\delta + 3r|s|/2}{c^2 + 3r|s|} \qquad (\delta \approx 10^{-5})$$

$$\omega \to \alpha/\alpha_t$$

Results & conclusions

The (multidimensional) Rosenbrock function can be defined as $f(\mathbf{x}) = \sum_i 100(x_{i+1} - x_i^2)^2 + (1 - x_i)^2$
Results from gradient descent and three different conjugate-direction methods:



200 different starting points `rand(8)`, average across all runs, a few individual traces shown in faint colors. Note that `scipy.fmin_cg` hops to wrong basin $\sim 0.5\%$ of the time.

Optimization with ϵ, ϵ^2, ρ numbers shares many features with more conventional methods. We trade increased complexity in the "automodeler" against decreased complexity in the algorithm.
Future directions:

- Stochastic descent: using the bounds to detect the impact of batches on updates
- Hybrid first- and second-order methods: extracting gradient and "scale"

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