Benchmarking of quasi-Newton methods

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Introduction

The most well-known minimization technique for unconstrained problems is Newtons Method. In each iteration, the step update is $x_{k+1} = x_k - \left(\nabla^2 f_k\right) \nabla f_k$. wever, the inverse of the Hessian has to be calculated in every iteration so it takes $O\left(n^3\right)$. Moreover, in some applications, the second derivatives may be unavailable. One fix to the problem is to use a finite difference approximation to the Hessian.
We consider solving the nonlinear unconstrained minimization problem

$$\min f(x), x \in \mathbb{R}$$

Let's consider the following quadratic model of the objective function
$m_k(p) = f_k + \nabla f_k^T p + \frac{1}{2} B_k p$, where $B_k = B_k^T, B_k \succ 0$ is an $n \times n$
The minimizer p_k of this convex quadratic model $p_k = -B_k^{-1} \nabla f_k$ is used as the search direction, and the new iterate is
$x_{k+1} = xk + \alpha p_k$, let $s_k = \alpha p_k$
The general structure of quasi-Newton method can be summarized as follows

- Given x_0, B_0(or H_0), $k \to 0$;
- **For** $k = 0, 1, 2, \dots$
  Evaluate gradient g_k.
  Calculate s_k by line search or trust region methods.
  $x_{k+1} \leftarrow x_k + s_k$
  $y_k \leftarrow g_{k+1} - g_k$
  Update B_{k+1} or H_{k+1} according to the quasi-Newton formulas.

  End(for)

Basic requirement in each iteration, i.e., $B_k s_k = y_k$ (or $H_k y_k = s_k$)

Quasi-Newton Formulas for Optimization

BFGS

$\min ||H - H_k||$,
s.t $H = H^T$, $Hy_k = s_k$

$H_{k+1} = (I - \rho s_k y_k^T) H_k (I - \rho y_k s_k^T) + \rho s_k s_k^T$
where $\rho = \frac{1}{y_k^T s_k}$

$B_{k+1} = B_k - \frac{B_k s_k s_k^T B_k}{s_k^T B_k s_k} + \frac{y_k y_k^T}{y_k^T s_k}$

DFP

$\min ||B - B_k||$,
s.t $B = B^T$, $Bs_k = y_k$

$B_{k+1} = (I - \gamma y_k s_k^T) H_k (I - \gamma s_k y_k^T) + \gamma y_k y_k^T$
where $\gamma = \frac{1}{y_k^T s_k}$

$H_{k+1} = H_k - \frac{H_k y_k y_k^T H_k}{y_k^T H_k y_k} + \frac{s_k s_k^T}{y_k^T s_k}$

PSB

$\min ||B - B_k||$,
s.t $(B - B_k) = (B - B_k)^T$,
$Bs_k = y_k$

$B_{k+1} = B_k - \frac{(y_k - B_k s_k) s_k^T + s_k (y_k - B_k s_k)^T}{s_k^T s_k} + \frac{s_k (y_k - B_k s_k) s_k s_k^T}{(s_k^T s_k)^2}$

$H_{k+1} = H_k - \frac{(s_k - H_k y_k) y_k^T + y_k (s_k - H_k y_k)^T}{y_k^T y_k} + \frac{s_k (s_k - H_k y_k) y_k y_k^T}{(y_k^T y_k)^2}$

SR1

$B_{k+1} = B_k + \sigma \nu \nu^T$,
s.t $B_{k+1} s_k = y_k$

$B_{k+1} = B_k + \frac{(y_k - B_k s_k)(y_k - B_k s_k)^T}{(y_k - B_k s_k)^T s_k}$,

$H_{k+1} = H_k + \frac{(s_k - H_k y_k)(s_k - H_k y_k)^T}{(s_k - H_k y_k)^T y_k}$

Method	Advantages	Disadvantages
BFGS	• $H_0 \succ 0$ hence if $H_0 \succ 0$ • self correcting property if Wolfe chosen • superlinear convergence	• $y_k^T s_k \approx 0$ formula produce bad results • sensitive to round-off error • sensitive to inaccurate bad line search • can get stuck on a saddle point for nonlinear problem
DFP	• can be highly inefficient at correcting large eigenvalues of matrices	• sensitive to round-off error • sensitive to inaccurate bad line search • can get stuck on a saddle point for nonlinear problem
PSB	• superlinear convergence	
SR1	• garantees to be $B_{k+1} \succ 0$ even if $s_k y_k > 0$ doesn't satisfied • very good approximations to the Hessian matrices, often better than BFGS	

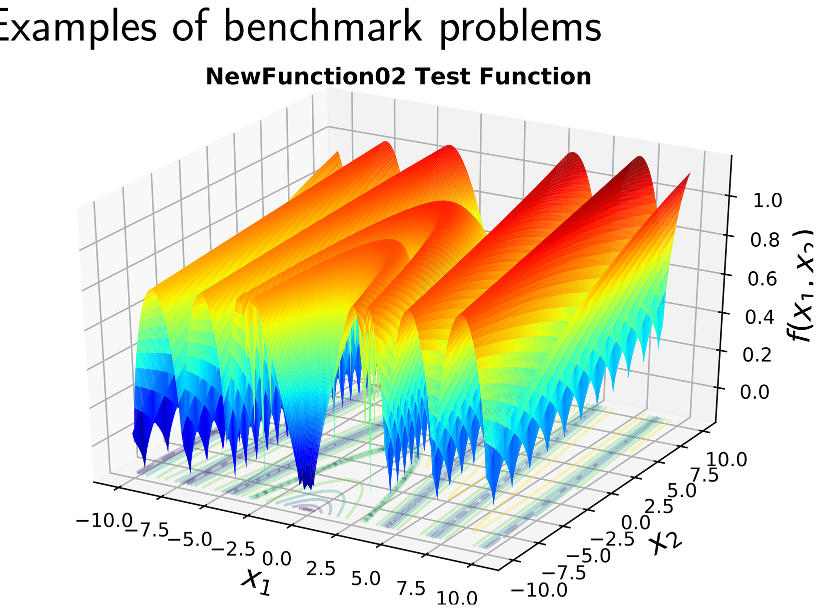
Line Search vs. Trust Region

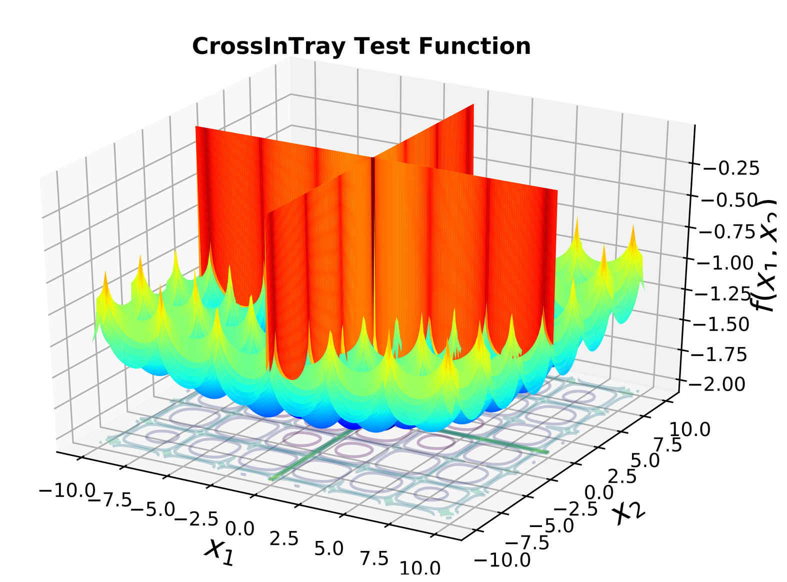
- Line search (strong Wolfe conditions)
  $f(x_k + \alpha_k p_k) \le f(x_k) + c_1 \alpha_k \nabla f_k^T p_k$
  $|f(x_k + \alpha_k p_k)^T p_k| \le c_2 |\nabla f_k^T p_k|$
- Trust region
  Both direction and step size find from solving
  $\min_{p \in \mathbb{R}^n} m_k(p) = f_k + \nabla f_k^T p + \frac{1}{2} B_k p$ s.t $||p|| \le \Delta_k$

Numerical Experiment

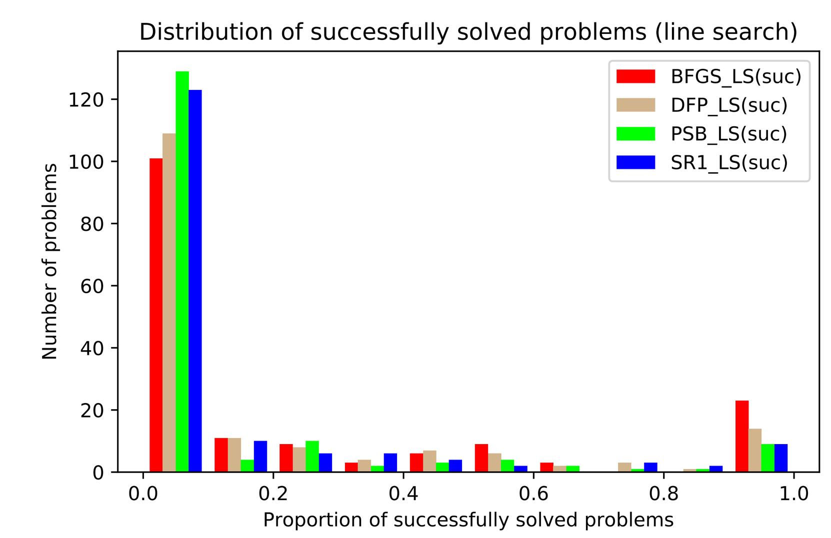
- All quasi-newton methods (BFGS,DFP, PSB, SR1) with two strategies (line search, trust region) were implemented in Python (overall 8 algorithms)
- 165 various N-$d(N \ge 2)$ strong benchmark problems
- For each algorithm all problems were launched from random point of domain 100 times and results were averaged

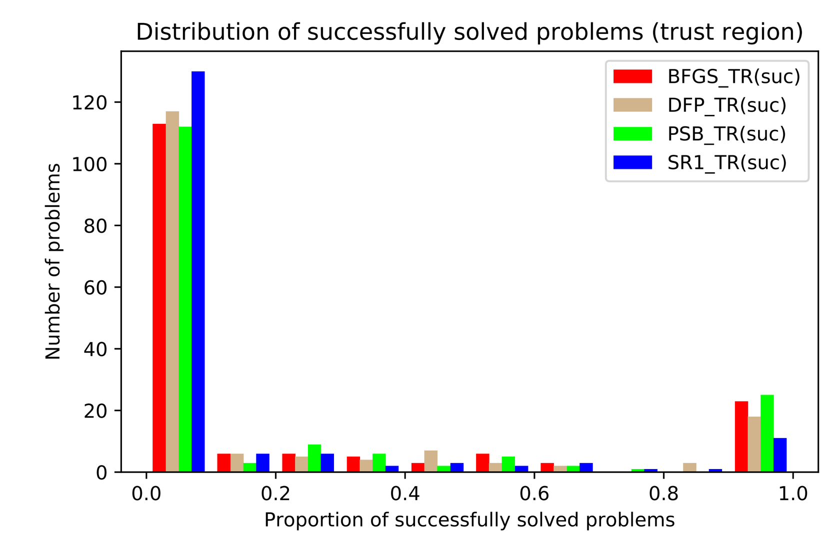
Examples of benchmark problems





Results

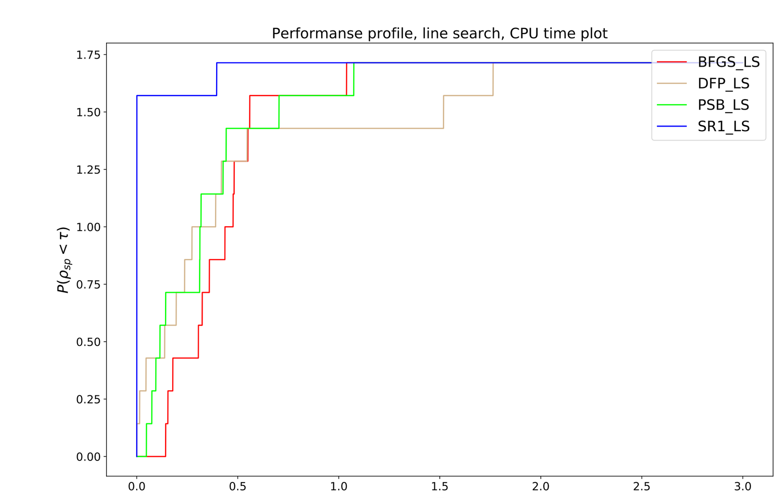


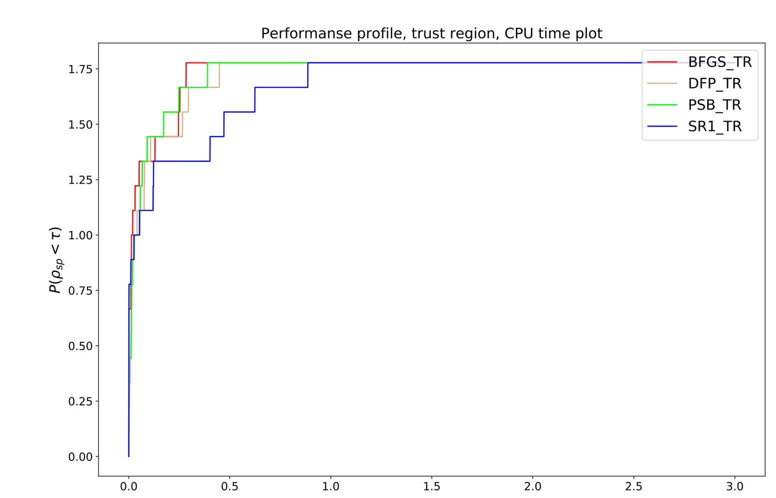


proportion of problems where have been successfully found global minimizer in more than half of all launches	in more than 0.99 launches	square under perforanse profile plot

Strategy	BFGS			DFP			PSB			SR1			Total	
LS	0.21	0.12	2.58	0.16	0.08	2.54	0.09	0.05	2.66	0.09	0.05	2.97	0.07	0.04
TR	0.18	0.12	2.93	0.16	0.1	2.91	0.19	0.14	2.93	0.11	0.06	2.83	0.1	0.05

Performance evaluation: n_s - number of solvers, n_p - number of problems, $t_{s,p}$ - time, $r_{s,p} = \frac{t_{s,p}}{\min\{t_{s,p} : s \in S\}}$ - performance profile function
$\rho_s(\tau) = \frac{1}{n_p} size\{p : 1 \le p \le n_p, \quad \log(r_{s,p} \le \tau)\}$ - defines the probability for solver s that the performance ratio $r_{s,p}$ is within a factor τ of the best possible ratio





Conclusions and Further Work

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Bibliography

[1] Ding, Yang, Enkeleida Lushi, and Qingguo Li. "Investigation of quasi-Newton methods for unconstrained optimization." Simon Fraser University, Canada (2004).

[2] Wright, Stephen, and Jorge Nocedal. Numerical optimization. Springer Science 35.67-68 (1999)

[3] Dolan, Elizabeth D., and Jorge J. Mor. "Benchmarking optimization software with performance profiles." Mathematical programming 91.2 (2002): 201-213.