Nonlinear Conjugate Gradients

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Nonlinear CG Intro

Conjugate Gradients approach can be formulated as follows:

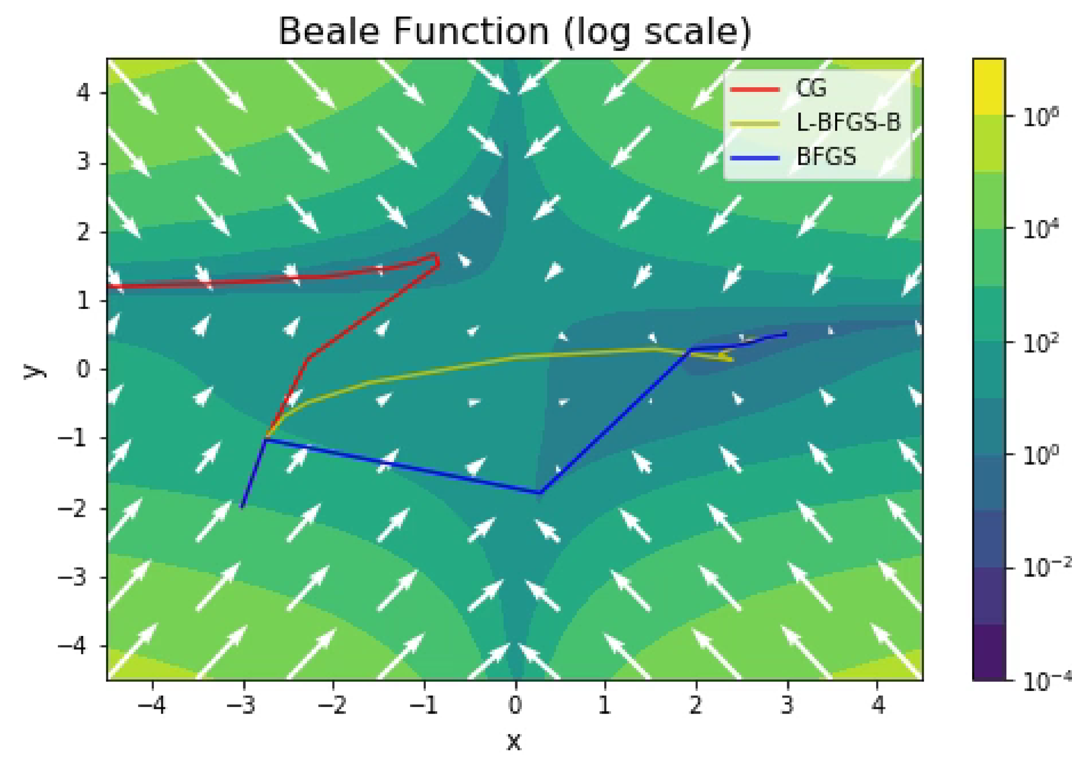
1. Direction generation rule
$$\mathbf{d_0} = -\nabla f(\mathbf{x_0})$$
$$\mathbf{d_k} = -\nabla f(\mathbf{x_k}) + \beta_k \mathbf{d_{k-1}}$$
2. Line search for an appropriate point:
   (a) Exact solution (usually too expensive)
   $$\mathbf{d_k}^T \nabla f(\mathbf{x_k} + \alpha_k \mathbf{d_k}) = 0$$
   (b) Strong Wolfe conditions
   $$f(\mathbf{x_k} + \alpha_k \mathbf{d_k}) \le f(\mathbf{x_k}) + c_1 \alpha_k \mathbf{d_k}^T \nabla f(\mathbf{x_k})$$
   $$|\mathbf{d_k}^T \nabla f(\mathbf{x_k} + \alpha_k \mathbf{d_k})| \le c_2 |\mathbf{d_k}^T \nabla f(\mathbf{x_k})|$$
   (c) Weak Wolfe conditions
   $$f(\mathbf{x_k} + \alpha_k \mathbf{d_k}) \le f(\mathbf{x_k}) + c_1 \alpha_k \mathbf{d_k}^T \nabla f(\mathbf{x_k})$$
   $$\mathbf{d_k}^T \nabla f(\mathbf{x_k} + \alpha_k \mathbf{d_k}) \ge c_2 \mathbf{d_k}^T \nabla f(\mathbf{x_k})$$

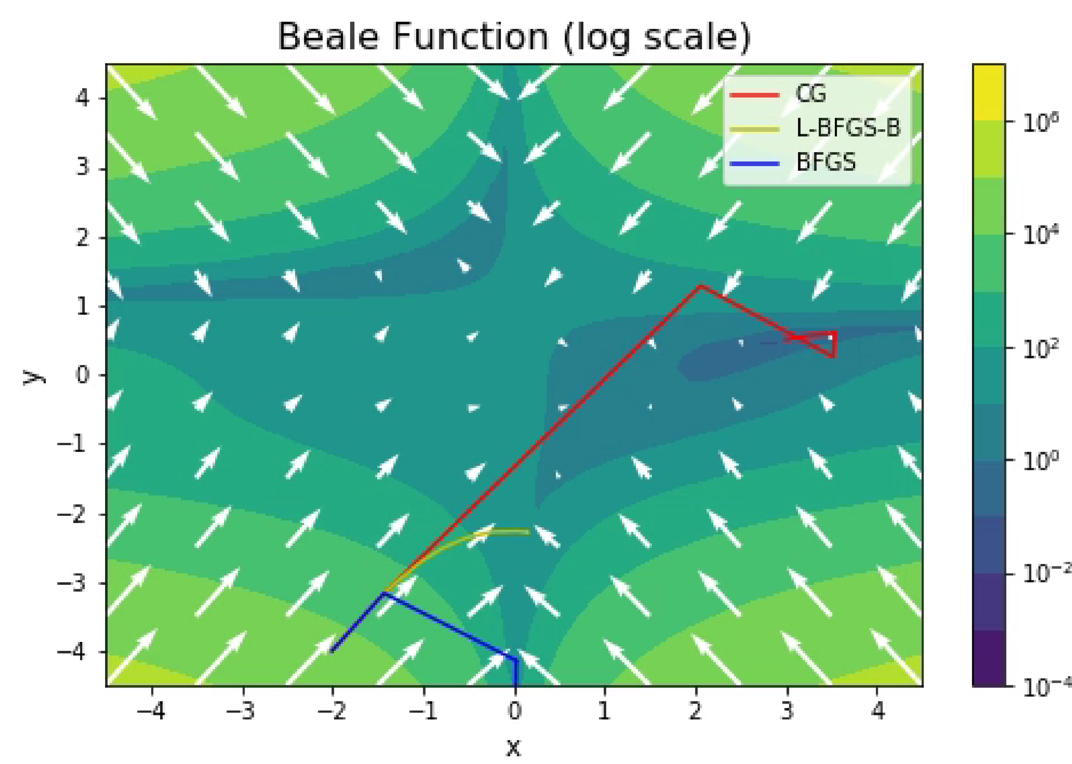
There are many possibilities for β_k selection and each of them is equivalent to **linear CG** in case of quadratic loss function with exact line search on each step:

1. Fletcher-Reeves [1]
$$\beta_k^{FR} = \frac{||\mathbf{g_k}||}{||\mathbf{g_{k-1}}||}$$
2. Polak-Ribiere-Polyak [2] (used in *SciPy* [6])
$$\beta_k^{PRP} = \frac{\mathbf{g_k}^T \mathbf{y_k}}{||\mathbf{g_{k-1}}||}, \quad \mathbf{y_k} = \mathbf{g_k} - \mathbf{g_{k-1}}$$
3. Hestenes-Stiefel [3]
$$\beta_k^{HS} = \frac{\mathbf{g_k}^T \mathbf{y_k}}{\mathbf{d_{k-1}}^T \mathbf{y_k}}, \quad \mathbf{y_k} = \mathbf{g_k} - \mathbf{g_{k-1}}$$
4. Dai-Yuan [4]
$$\beta_k^{DY} = \frac{||\mathbf{g_k}||}{\mathbf{d_{k-1}}^T \mathbf{y_k}}, \quad \mathbf{y_k} = \mathbf{g_k} - \mathbf{g_{k-1}}$$
5. Hager-Zhang [5]
$$\beta_k^{HZ} = \frac{1}{\mathbf{d_{k-1}}^T \mathbf{y_k}} \left(\mathbf{y_k} - 2\mathbf{d_{k-1}} \frac{||\mathbf{y_k}||}{\mathbf{d_{k-1}}^T \mathbf{y_k}} \right)^T \mathbf{g_k}$$

Competing BFGS and L-BFGS

The **BFGS** and **L-BFGS** methods are widely used in unconstrained optimization. Moreover, they are often thought to be better than **CG** in average case. It must be noted that initial point selection is crucial for the whole optimization process. Polak-Ribiere-Polyak version of CG is used below.



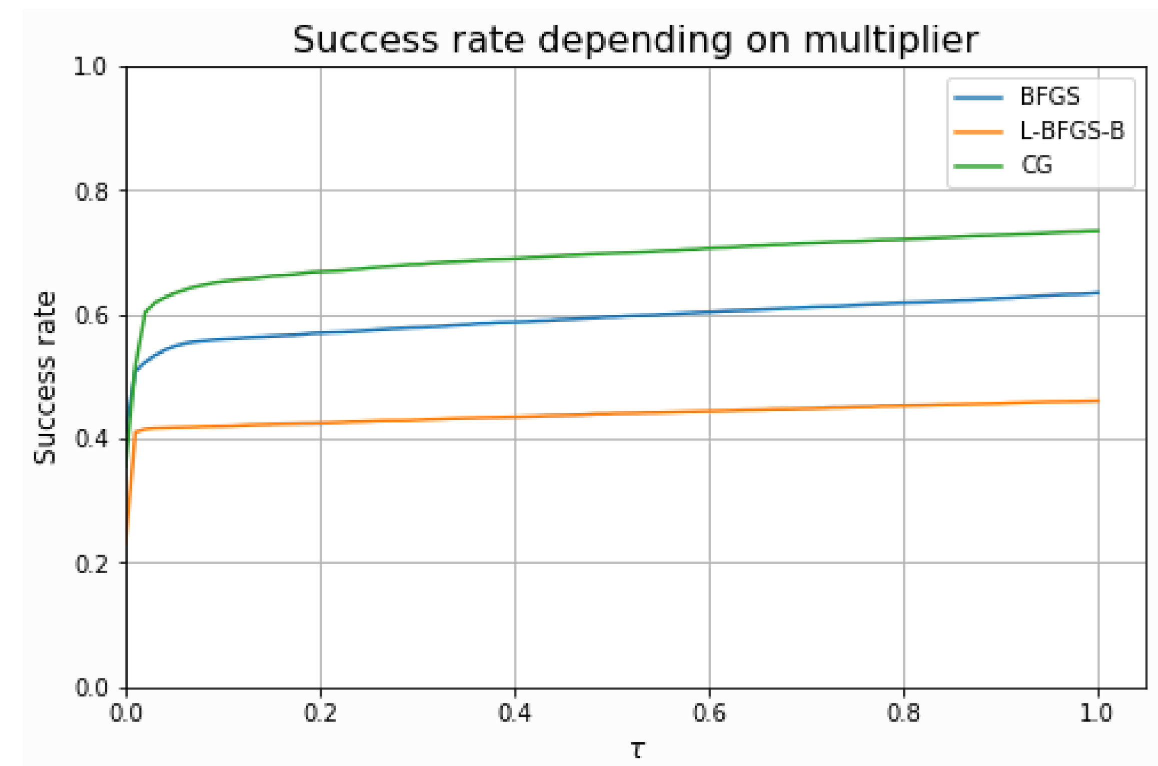


To compare robustness of the algorithms following method is suggested [7]:

1. Generate set of points uniformly distributed in $\mathbf{G} = [x_{min}, x_{max}] \times [y_{min}, y_{max}]$:
$$P = \{p_i\}_{i=1}^N \in unif([x_{min}, x_{max}] \times [y_{min}, y_{max}])$$
2. Take set $\mathcal{A} = \{A_1, A_2, \ldots\}$ of algorithms to be compared. Try to find the minimizer taking p_i as starting point and save the value obtained by algorithm A_k as $F_{A_k}(p_i)$. Denote $F_{min}(p_i) = \min_k F_{A_k}(p_i)$.
3. Take set of $\tau \in [0, +\infty]$ and compute [S]uccess rate as
$$S(A_k, \tau) = \frac{||\{p_i \mid F_{A_k}(p_i) \le \tau F_{min}(p_i)\}||}{||P||}$$
4. Plot $S(A_k, \tau)$ for each $A_k \in \mathcal{A}$ as function of τ.

Results

Numerical experimets were performed with $||P|| = 10000$ points from for Beale function [8] and $p_i \in unif([-4.5, -4.5] \times [-4.5, -4.5])$. The plot shows that the **CG** algorithm performs at least as well as **BFGS** and **L-BFGS** methods. Moreover, while offering lower memory consumption (as **L-BFGS** does), it also has higher reliability. So we can do an informal statement: while the family of **BFGS** methods collects information about the curvature during optimization process, they explicitly assume that the function doesn't change to much between the steps. This also means that we can't move too far each iteration. In contrast, **CG** searches for a minimum along given direction and can perform quite big steps, while keeping the search directions very 'unique' in the sense of conjugacy.



References

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[4] Dai, Y.H. and Yuan, Y., 2000, A nonlinear conjugate gradient method with a strong global convergence property. SIAM Journal on Optimization, 10, 177182.

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