ITMO UNIVERSITY
Saint Petersburg, Russia

Квазиньютоновские методы нелинейной оптимизации без ограничений

С4113
Кошман Варвара
Самарин Антон
Гончаров Андрей

Общий алгоритм

$while\ ||g_k||\ > \varepsilon$

$argmin_{a>0} f(x_k\ +\ a * (-H_k *\ g_k))$

$x_{k+1} = x_k +\ a_k * (-H_k *\ g_k)$

$g_{k+1} = \nabla x_{k+1} f$

$H_{k+1} = \text{алгоритм}(H_k, x_k, x_{k+1}, g_k, g_{k+1})$

$k = k\ +\ 1$

NB

$$x_{n+1} = x_n - [H_{x_n} f]^{-1} \nabla a_n f$$

Методы

BHHH

$$\nabla_x^2 f(x) \cong N^{-1} \sum_{i=1}^{N} \nabla_x q(w_i, x)' \nabla_x q(w_i, x),$$

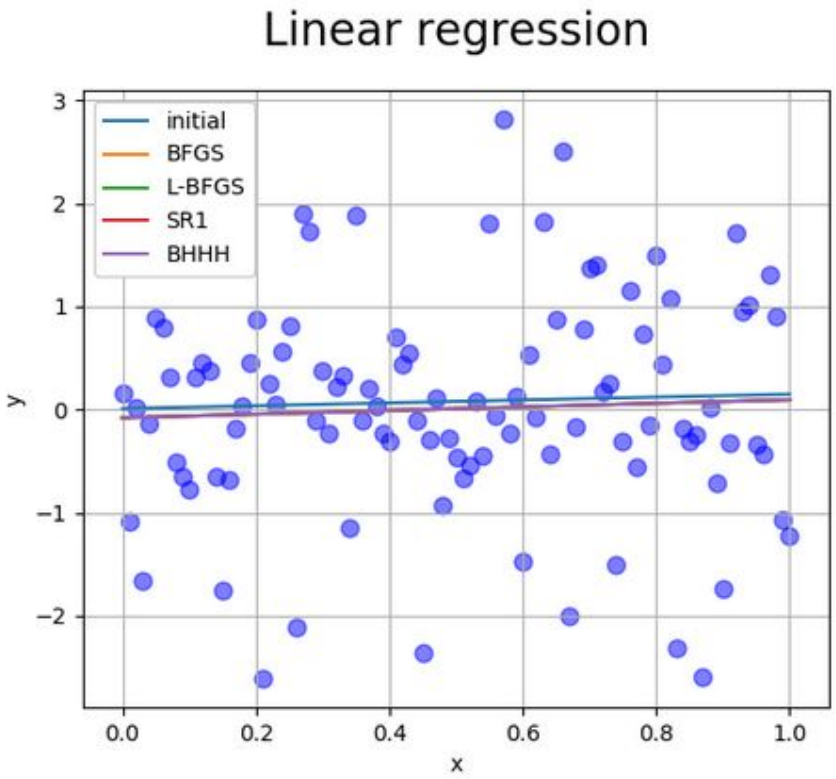
SR1

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

BFGS

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

Линейная модель



method	root (precision = 10e-3)	# of iterations
Newton	[0.17520752 -0.07967756]	4
BFGS	[0.17518778 -0.07966777]	2
L-BFGS	[0.17518773 -0.0796678]	5
SR1	[0.17499377 -0.07958188]	10
BHHH	[0.1751878 -0.07966781]	10

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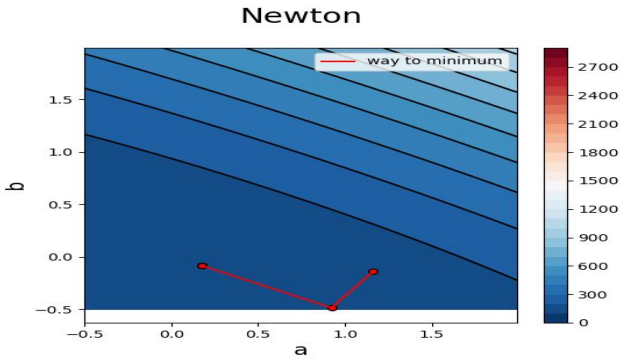
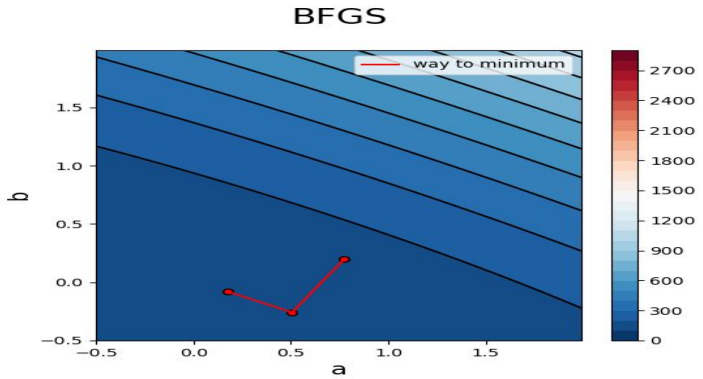
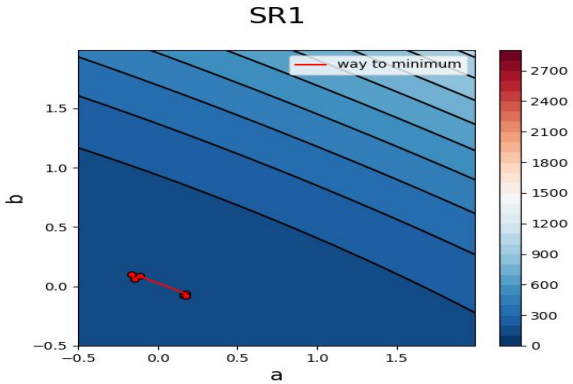
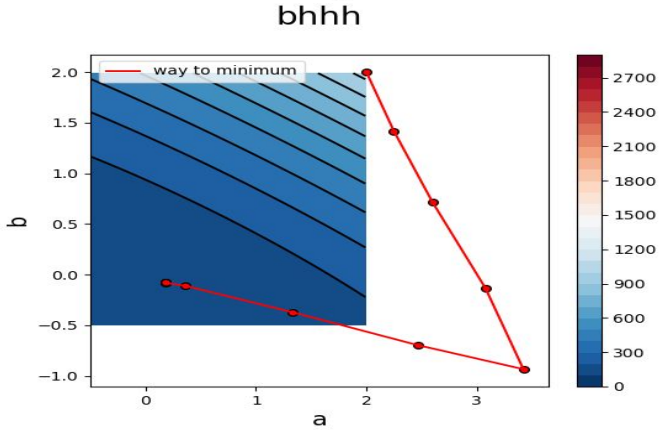
Линии уровня целевой функции и оптимизации алгоритмов









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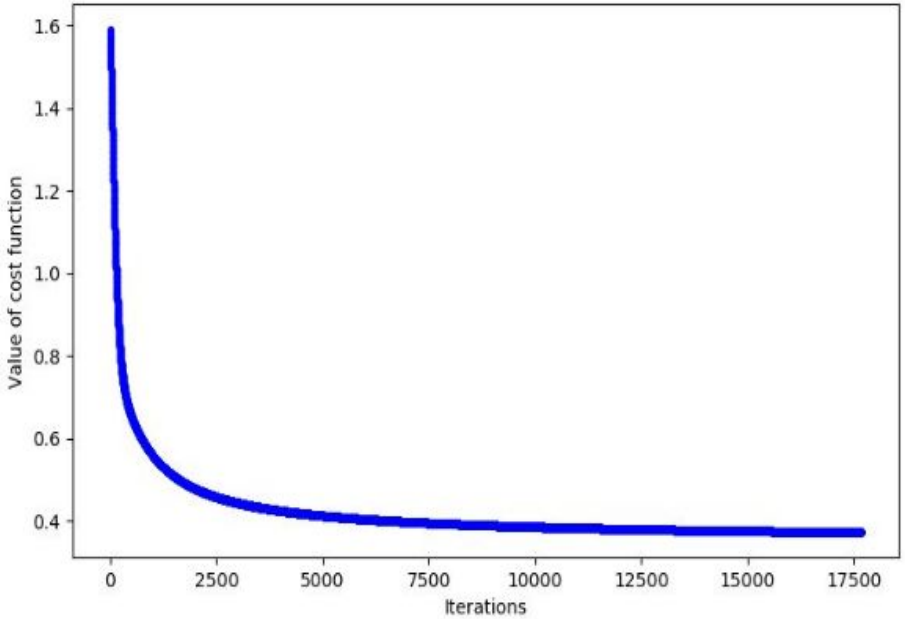
Результаты оптимизации на медицинских данных

method	accuracy	# of iterations
Gradient descent with fixed step	85.25%	17752
Newton	85.25%	9
BFGS	85.25%	79
Limited memory BFGS	85.25%	20



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Спасибо за внимание!

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