Action constrained quasi-Newton methods

Robert Gower

EUROPT 2014 Workshop on Advances in Continuous Optimization

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What and why quasi-Newton?

Classic quasi-Newton

New Action Constrained quasi-Newton

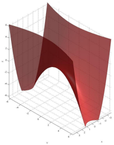
Implementing a Preconditioned Newton-CG with new metric

What's new

- A few Hessian-vector products are cheap $\Rightarrow$ use a handful to build Hessian approximation [1]
- Framework for "tracking" inverses of matrix fields
- General purpose Newton-CG preconditioners
- Good results on regularized logistic regression (compared to BFGS or Newton-CG)

[1] Walther, A. (2008). Computing sparse Hessians with automatic differentiation. ACM Trans. Math. Software, 34(1), Art. 3, 15.

Solving sequences of linear systems

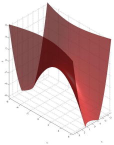


$$\min \quad f(x) \quad (C^2 - \text{diffeomorphism})$$

$$f(x_k + d) \approx f_k + \nabla f_k^T d + \tfrac{1}{2} d^T \nabla^2 f_k d$$

x_0

Solving sequences of linear systems



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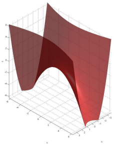

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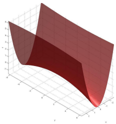
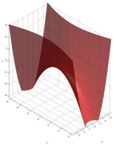


x_0

$d_0 = -\nabla^2 f_0^{-1} \nabla f_0$

x_1

Solving sequences of linear systems



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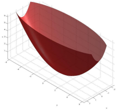

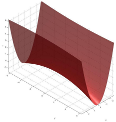

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x_1

x_2

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The quadratic model "slowly" changes; how to take advantage?

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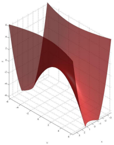

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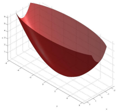

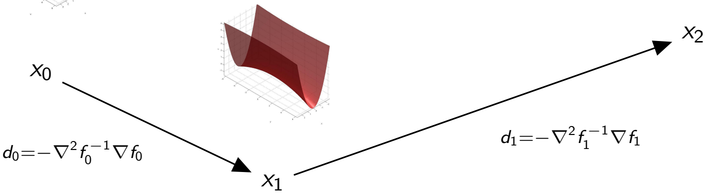

The quadratic model "slowly" changes; how to take advantage?

Maintain an approximation of the inverse: $H_{k+1} \approx \nabla^2 f_{k+1}^{-1}$.

"Slowly" update with cheap low rank matrices: $H_{k+1} = H_k + E_k$.

H_k is a *metric* matrix.

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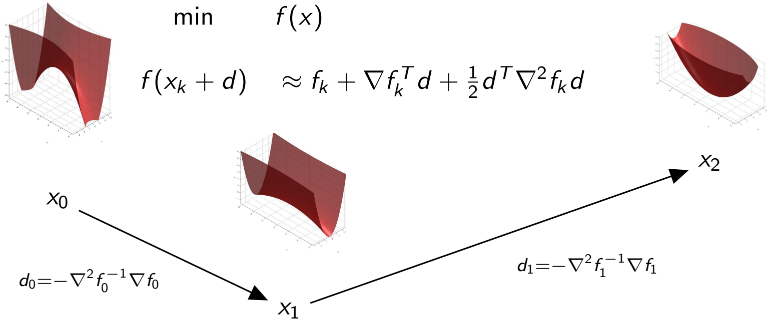

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Classic approach: imitating action of Hessian with the secant equation

$$\mathcal{A}\nabla^2 f_{k+1} = \int_0^1 \nabla^2 f(x_k + td_k)dt, \quad \gamma_k = (\nabla f_{k+1} - \nabla f_k).$$

Fundamental Theorem of Calculus says

$$\mathcal{A}\nabla^2 f_{k+1} \cdot d_k = \gamma_k \Rightarrow$$
$$d_k = (\mathcal{A}\nabla^2 f_{k+1})^{-1}\gamma_k \approx \left(\nabla^2 f_{k+1}\right)^{-1}\gamma_k$$

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The Secant Equation

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Still under-determined. Least squares idea + slowly changing [2]

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Build metric H that captures $D = [d_1, \ldots, d_p]$ directions of positive curvature

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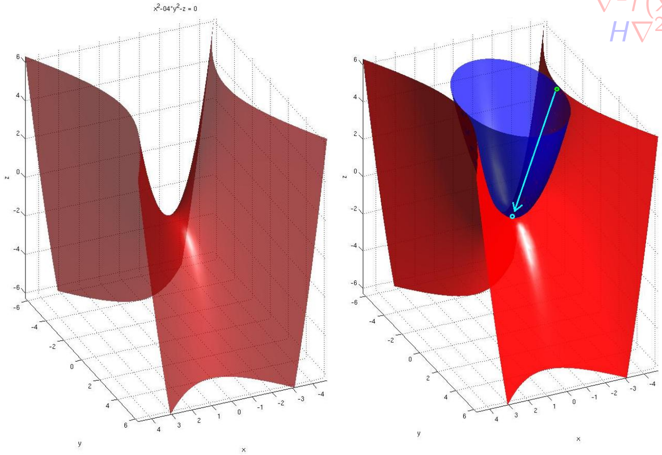
$$H \nabla^2 f(x) D = D$$



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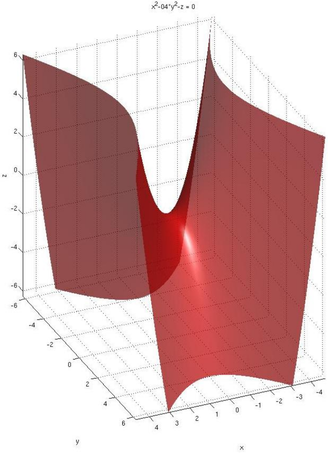

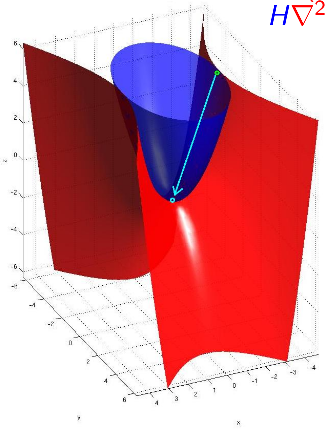

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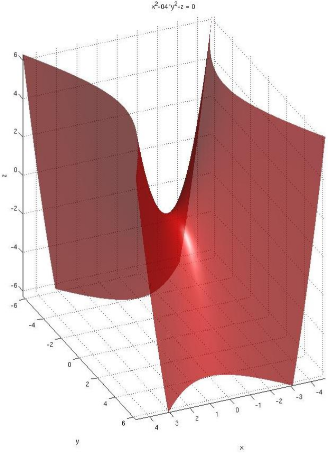
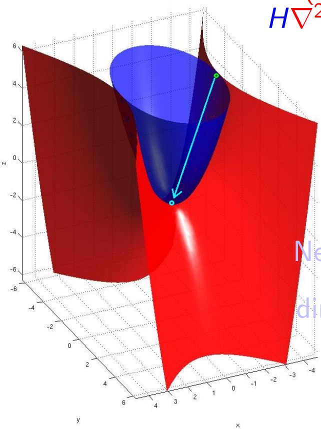
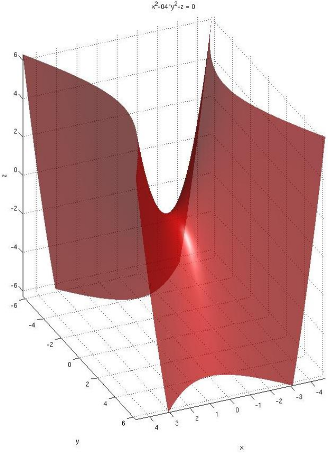


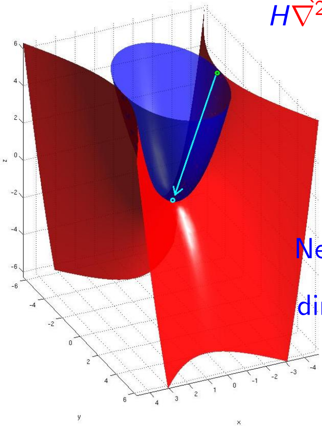


Newton-CG produces directions of positive curvature!

Overall idea of D_k

Build metric H that captures $D = [d_1, \ldots, d_p]$ directions of positive curvature





$$\nabla^2 f(x) D = H^{-1} D$$
$$H \nabla^2 f(x) D = D$$

Newton-CG produces directions of positive curvature!

Choosing D_k and W

Analogous to BFGS by choosing $W = \nabla^2 f_k$

quNac: quasi-Newton action constrained

$$H_{k+1} = \mathrm{proj}_{D_k}^{\nabla^2 f_{k+1}} + (I - \mathrm{proj}_{D_k}^{\nabla^2 f_{k+1}} \nabla^2 f_{k+1}) H_k (I - \nabla^2 f_{k+1} \mathrm{proj}_{D_k}^{\nabla^2 f_{k+1}}).$$

- A rank$-2p$ update
- Only need to calculate the p columns $\nabla^2 f_{k+1}(D_k)$.
- $\mathrm{proj}_{D_k}^{\nabla^2 f_{k+1}} = D_k(D_k^T \nabla^2 f_{k+1} D_k)^{-1} D_k^T$ is expensive?

Choose D_k according to

- **Hereditary** property $\Rightarrow$ for local convergence
- **Descent property** $\Rightarrow$ for Global stability

Quadratic Hereditary $\nabla^2 f(x) \equiv Q$ property

If $[D_1, \ldots, D_k] \in \mathbb{R}^{n \times n}$ and $D_i^T Q D_j = 0$ for $1 \leq j < i \leq k$ then

$$H_{k+1} Q D_i = D_i, \quad \text{for } i = 1, \ldots, k.$$

Lemma: $H_{k+1} Q = I \Rightarrow H_{k+1} = Q^{-1}$.

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proof:

$$\begin{aligned} H_{k+1} &= H_k + E_k \\ &= H_i + E_i + \cdots + E_k. \end{aligned}$$

If $D_i^T Q D_j = 0$ for $j < i$ then

$$\begin{aligned} &\left(\text{proj}_{D_j}^{Q} Q D_i = 0\right) \Rightarrow \left(E_j Q D_i = 0\right). \\ &\Rightarrow H_{k+1} Q D_i = H_{i+1} Q D_i = D_i. \quad \square \end{aligned}$$

Choose D_k conjugate to $\nabla^2 f_{k+1}$ as an approximation!

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Descent and Positive Definiteness

Descent: $d_k = -H_k \nabla f_k$ is less then 90^o with $-\nabla f_k$.

Sufficient Descent condition

If $H_k \succ 0$ then $-d_k^T \nabla f_k = \nabla f_k^T H_k \nabla f_k > 0$.

Classic quasi-Newton

If $H_k \succ 0$ and $\gamma_k^T d_k = d_k^T \mathcal{A} \nabla^2 f_{k+1} d_k > 0$ then $H_{k+1} \succ 0$.

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Implementing a Preconditioned Newton-CG with quNac

- Call Conjugate gradients on $\nabla^2 f_{k+1} d = -\nabla f_{k+1}$ to get D_k directions of positive curvature
- $\text{proj}_{D_k}^{\nabla^2 f_{k+1}} = D_k (D_k^T \nabla^2 f_{k+1} D_k)^{-1} D_k^T$ is $O\left(p^2\right)$ because $D_k^T \nabla^2 f_{k+1} D_k =$diagonal !

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quNac quasi-Newton action Constrained

- $H_0, x_0 \in \mathbb{R}, \; k = 0$

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- While $|\nabla f_k|/|\nabla f_0| > \epsilon$

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- While $|\nabla f_k|/|\nabla f_0| > \epsilon$
  - If $k = 0$

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  - **If** $k = 0$
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  - $H_{k+1} = H_k + E_k\left(D, \nabla^2 f_{k+1}(D)\right)$

LquNac quasi-Newton action Constrained

- $H_0, x_0 \in \mathbb{R},\ k = 0$
- While $|\nabla f_k|/|\nabla f_0| > \epsilon$
  - **If** $k = 0$
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  - **Else**
    - $s_0 = d_{CG}$
  - Select step-size a_k
  - $x_{k+1} = x_k + a_k s_k$
  - Calculate d_{CG} by applying CG to preconditioned system
    - $H_k \nabla^2 f_{k+1} d = -H_k \nabla f_{k+1}$.
    - Store conjugate directions in D and store $\nabla^2 f_{k+1} D$.
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LquNac Limited quasi-Newton action Constrained

- $H_0, x_0 \in \mathbb{R},\ k = 0$
- While $|\nabla f_k|/|\nabla f_0| > \epsilon$
  - **If** $k = 0$
    - $s_0 = -H_0 \nabla f_0$
  - **Else**
    - $s_0 = d_{CG}$
  - Select step-size a_k
  - $x_{k+1} = x_k + a_k s_k$
  - Calculate d_{CG} by applying CG to preconditioned system
    - $OpH_k \nabla^2 f_{k+1} d = -OpH_k \nabla f_{k+1}$.
    - Store conjugate directions in D and store $\nabla^2 f_{k+1} D$.
  - $OpH_{k+1} = H_0^k + E_k \left(D, \nabla^2 f_{k+1}(D)\right)$

Logistic L2 Regression tests:

$\min_w L_w(y,X) + \|w\|_2^2$

$$L_w(y,X) = \sum_{i=1}^{m} \ln\left(1 + \exp(-y_i \left\langle x^i, w \right\rangle)\right).$$

quNac	vs	BFGS
41		3
quNac	vs	Newton_CG
31		12
LquNac	vs	LBFGS
27		17
LquNac	vs	Newton_CG
14		29

Table: # fastest runs on 44 binary classifications problems from LibSVM

Logistic pseudo-Huber Regression tests:

$$\min_{w} L_w(y, X) + R_\mu(w) := \mu \sum_{i=1}^{n} \left(\sqrt{1 + x_i^2/\mu^2} - 1 \right).$$ [4]

quNac	vs	BFGS
32		10
quNac	vs	Newton_CG
37		4
LquNac	vs	LBFGS
18		25
LquNac	vs	Newton_CG
24		16

Table: # fastest runs on 44 binary classifications problems from LibSVM

[4] Fountoulakis, K., & Gondzio, J. (2013). A Second-Order Method for Strongly Convex l1-regularization Problems.

Conclusion

- Framework for approximating a changing inverse Hessian.
- Has good properties: **Hereditary** and **Descent**.
- Variable amount of curvature information at each iteration (depends on CG error).
- Developed Newton-CG Preconditioner for smooth functions.

In the works:

- Full and limited memory implementations for non-convex unconstrained.
- How does extra flexibility help mesh into globalization strategies: Interior point, Trust region, Sequential Quadratic?
- Connections to other problems: Matrix completion?

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Underlying Matrix Optimization Problem

$$\begin{aligned} &\min_E \|E\|^2_{Frobenius(W)} \\ \text{s.t.} \quad & ED = RD \\ & E = E^T \end{aligned}$$

Which has a low rank$-3p$ solution.

$$E = W^{-1}\text{proj}_D^{W^{-1}} R \left(I - \text{proj}_D^{W^{-1}} W^{-1} \right) + R\text{proj}_D^{W^{-1}} W^{-1}.$$

This is a matrix completion problem where one knows the desired matrix is symmetric and can only observe its action on a small subspace.