Hunting Inverse Hessian Matrices

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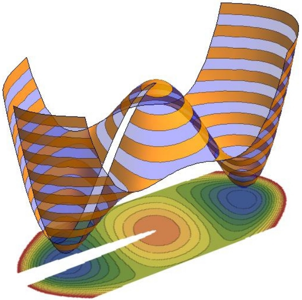
and Jacek Gondzio

Irish Applied Mathematics Research Students' Meeting 2014, Galway.

December 11, 2014

Nonlinear optimization is where I hunt

$$\min_x f(x)$$
with $g(x) \leq 0$.



"Nothing in the world takes place without optimization, and there is no doubt that all aspects of the world that have a rational basis can be explained by optimization methods", Leonhard Euler (1744).

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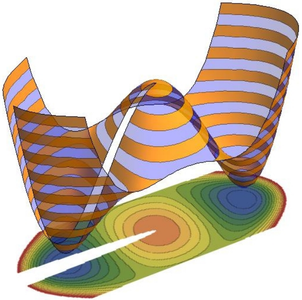

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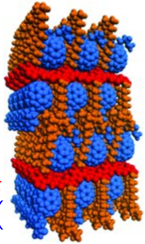

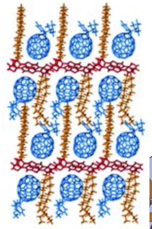

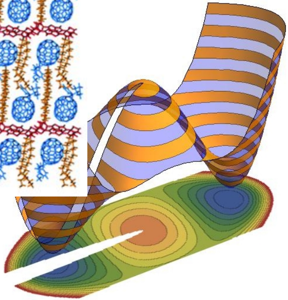

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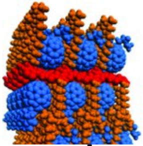
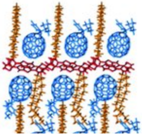
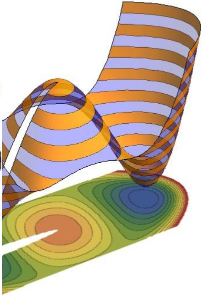
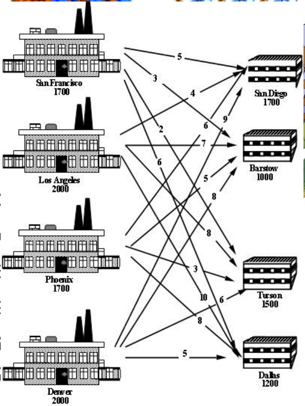






$\color{red}{\min_x}$
with $\color{blue}{g(}$



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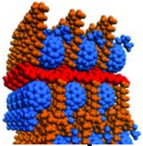

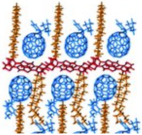

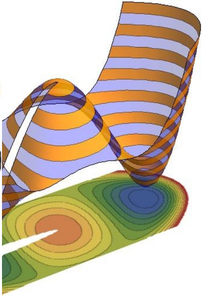

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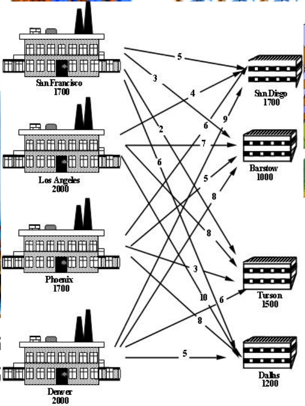

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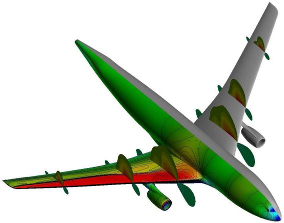

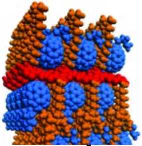

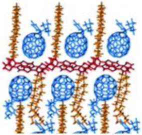

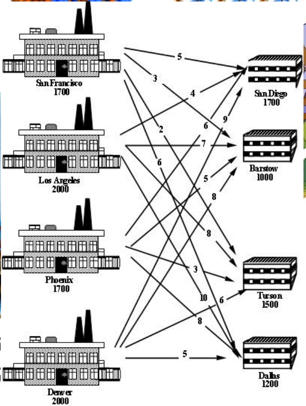

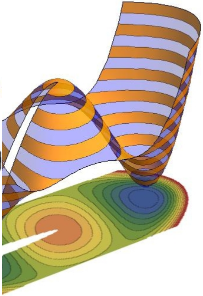

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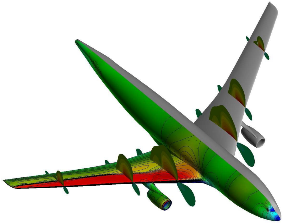

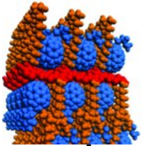

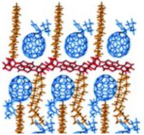

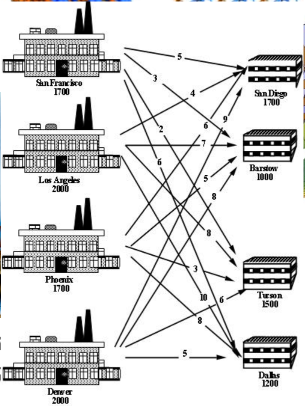

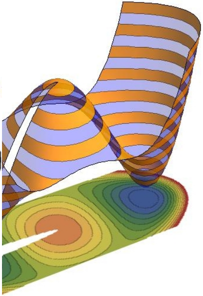

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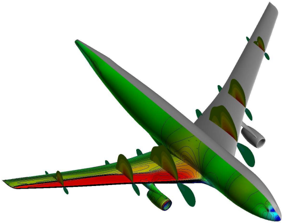

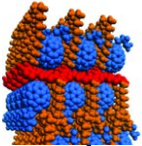

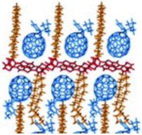

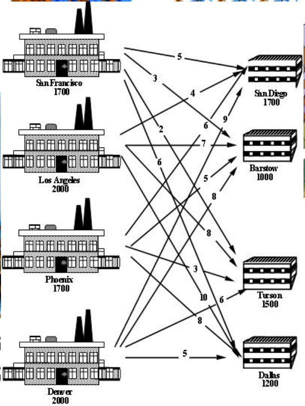

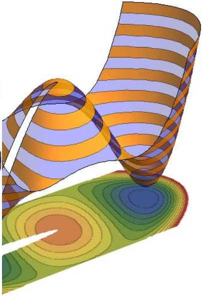

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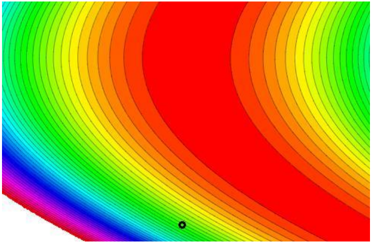
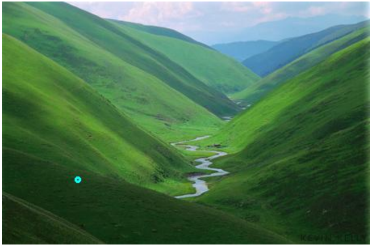
$\min_x f(x) = 100(x - y^2)^2 + (y-1)^2$





Difficult global problem. Use a local information.

Input: $x_0 \in \mathbb{R}^n$
for $k = 0, 1, 2, \ldots$ **do**
  $x_{k+1} = x_k - \nabla f(x_k)$
end

Zigzags 4'000 iterations!

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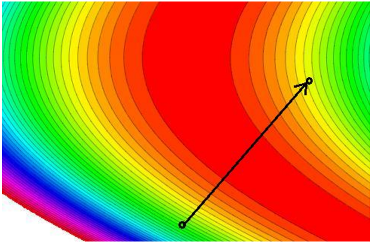

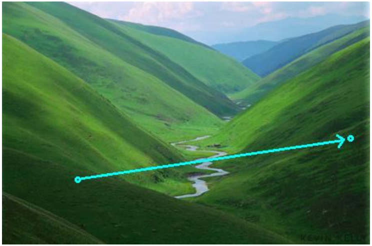

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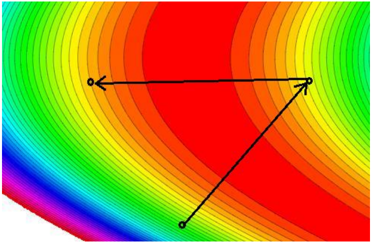

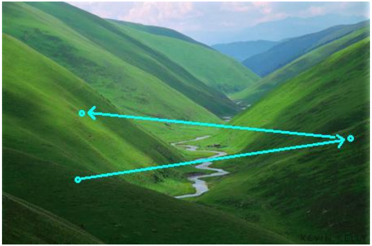

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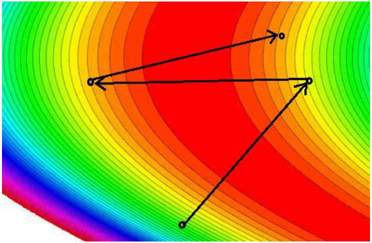

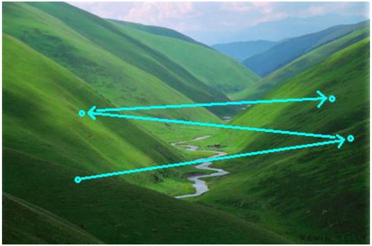

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Using Second-order information

Search for stationary point

$$\nabla f(x) = 0, \quad \text{Fermat 1646}$$

linearize around x_k

$$\nabla f(x_k + d) \approx \nabla^2 f(x_k) d + \nabla f(x_k)$$

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Solve a linear system

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Solving one Newton system

Proxy solve $\nabla^2 f(x_k) d_k = -\nabla f(x_k)$

$$d_k = \min_{d \in \mathcal{S}_k} \|\nabla^2 f(x_k) d + \nabla f(x_k)\|$$

where $\mathcal{S}_k \subset \mathbb{R}^n$ is a subspace.
Requires calculating $\nabla^2 f_k \mathcal{S}_k$

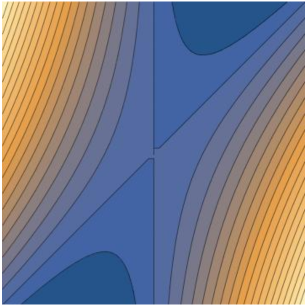

Figure: Contour $d^T \nabla^2 f_k d$

Problem: Solving linears system expensive. What can be done?

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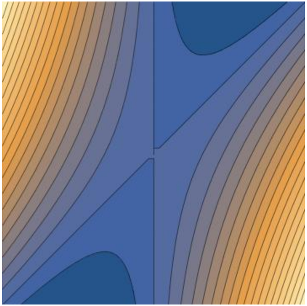

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$$f(x_k + d) \approx f(x_k) + \langle \nabla f(x_k), d \rangle + \frac{1}{2} d^T \nabla^2 f(x_k) d.$$

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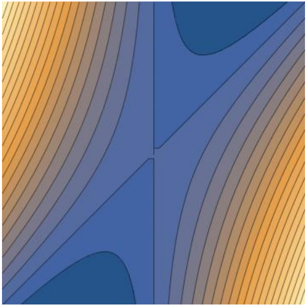

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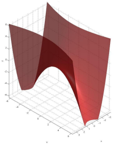
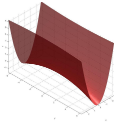


x_0



d_0

x_1

The Hessian "slowly" changes $\nabla^2 f(x_{k+1}) \approx \nabla^2 f(x_k)$.

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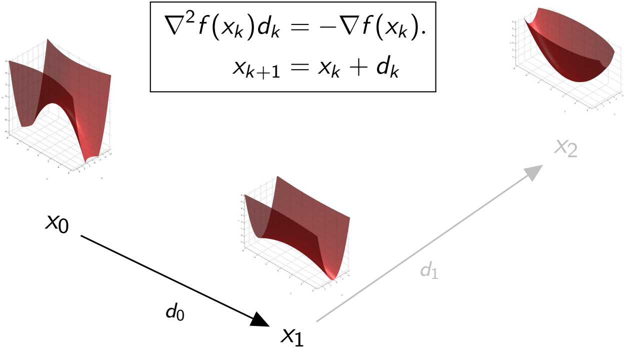

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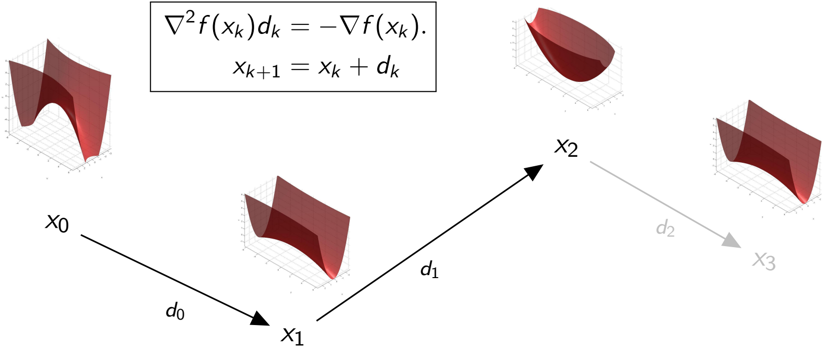

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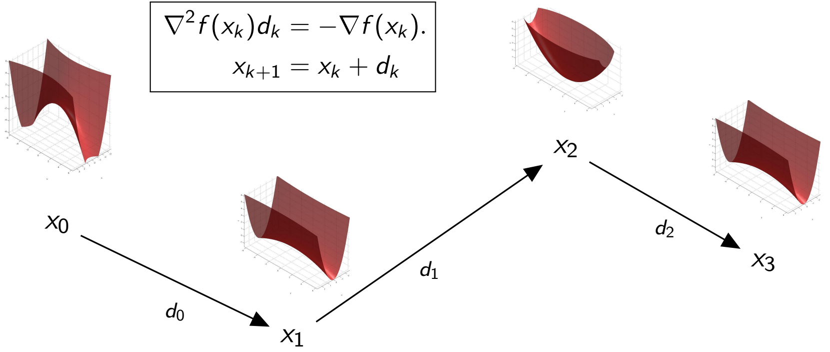

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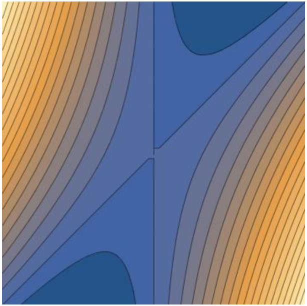

Figure: $d^T \nabla^2 f_k d$

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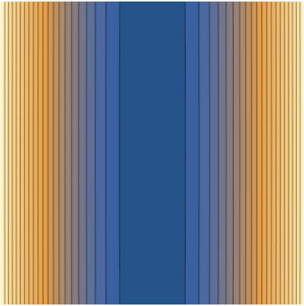

Figure: $y^T P^T \nabla^2 f_k P y$

Changing Coordinates $d = Py$ can help when
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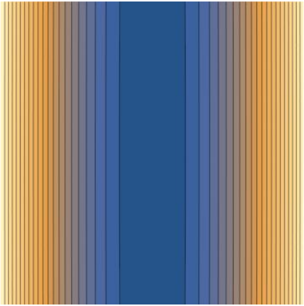

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Objective: $P_{k-1} \approx \nabla^2 f(x_{k-1})^{-1}$ from available information to precondition $\|\nabla^2 f(x_k) P_{k-1} y + \nabla f(x_k)\|$.

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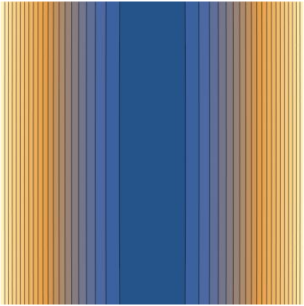

Figure: $y^T P^T \nabla^2 f_k P y$

Changing Coordinates $d = Py$ can help when $P \approx \nabla^2 f_k^{-1}$ then $\nabla^2 f_k P \approx I$, easy.

$\boxed{\text{Objective: } P_{k-1} \approx \nabla^2 f(x_{k-1})^{-1} \text{ from available information to precondition } \|\nabla^2 f(x_k) P_{k-1} y + \nabla f(x_k)\|.}$

Solving one Newton system **using the previous**

Proxy solve $\nabla^2 f(x_k) d_k = -\nabla f(x_k)$

$$d_k = \arg \min_{Py \in \mathcal{S}_k} \|\nabla^2 f(x_k) P y + \nabla f(x_k)\|$$

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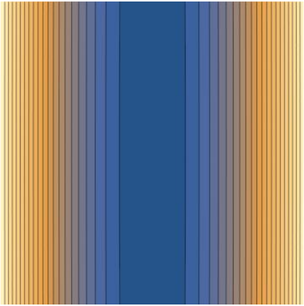

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Preconditioned Newton's Method

Input: $P_0 = I$

for $k = 1, 2, \ldots$ **do**

`Proxy solve` $\nabla^2 f(x_k) P_{k-1} d_k = -\nabla f(x_k)$

Preconditioned Newton's Method

Input: $P_0 = I$
for $k = 1, 2, \ldots$ **do**
    `Proxy solve` $\nabla^2 f(x_k) P_{k-1} d_k = -\nabla f(x_k)$;
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Calculate P_k from P_{k-1} and $\nabla^2 f(x_k) \mathcal{S}_k$.

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Just the Facts for calculating P_k

- $\|\nabla^2 f(x_k)^{-1} - \nabla^2 f(x_{k-1})^{-1}\|$ small $\Rightarrow$ make $\|P_k - P_{k-1}\|$ small

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- Has the action $\nabla^2 f(x_k)^{-1} \left(\nabla^2 f(x_k)\mathcal{S}_k\right) = \mathcal{S}_k \Rightarrow$ make $P_k \left(\nabla^2 f(x_k)\mathcal{S}_k\right) = \mathcal{S}_k$

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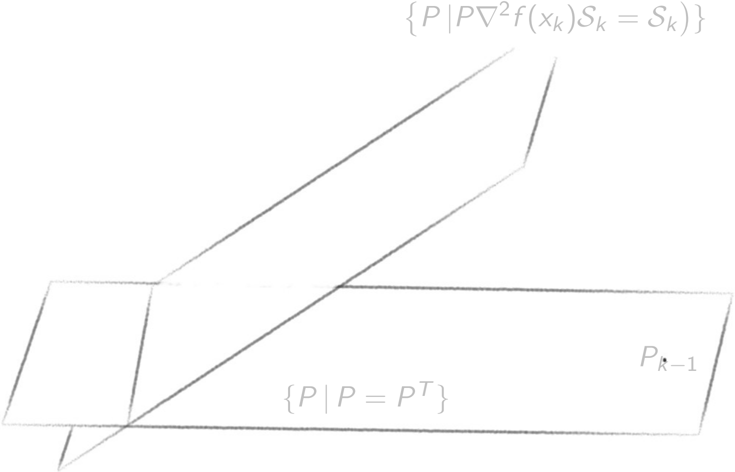
Problem: We have $P_{k-1} \approx \nabla^2 f(x_{k-1})$ we observe $\nabla^2 f(x_k)\mathcal{S}_k$ how to estimate $\nabla^2 f(x_k)^{-1}$



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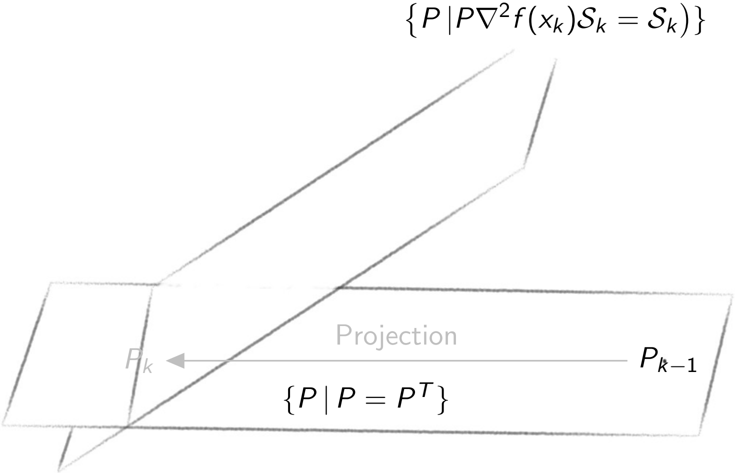

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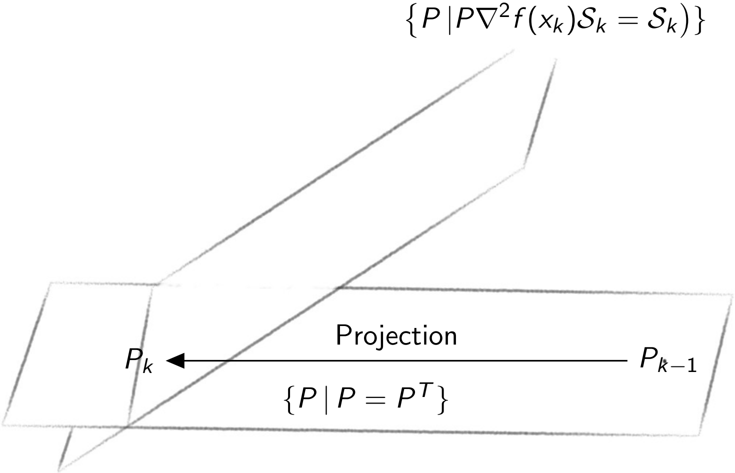

Hunting the Inverse

$$
\begin{aligned}
\min_{P_k} \quad & \|P_k - P_{k-1}\|^2_{Frobenius(\mathcal{W}_k)} \\
& P_k \nabla^2 f_k \mathcal{S}_k = \mathcal{S}_k \\
& P_k = P_k^T.
\end{aligned}
$$

- Iteratively updating metric; changes “slowly”
- Same action of $\nabla^2 f(x_k)^{-1}$ and P_k over $\nabla^2 f(x_k)\mathcal{S}_k$.

Hunting the Inverse

$$\min_{P_k} \quad \|P_k - P_{k-1}\|^2_{Frobenius(\mathcal{W}_k)}$$

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$$P_k = \nabla^2 f(x_k) + \left(I - \mathcal{W}_k \mathrm{proj}_{\mathcal{S}_k}^{\mathcal{W}_k}\right)\left(P_{k-1} - \nabla^2 f(x_k)\right)\left(I - \mathrm{proj}_{\mathcal{S}_k}^{\mathcal{W}_k} \mathcal{W}_k\right)$$

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Hunting the Inverse

$$\min_{P_k} \quad \boxed{\|P_k - P_{k-1}\|^2_{Frobenius(\mathcal{W}_k)}}$$
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$\mathrm{proj}_{\mathcal{S}}^{A} A := \mathcal{S}(\mathcal{S}^T A \mathcal{S})^{-1}\mathcal{S}^T A = A-$projection onto $\mathrm{span}(\mathcal{S})$.

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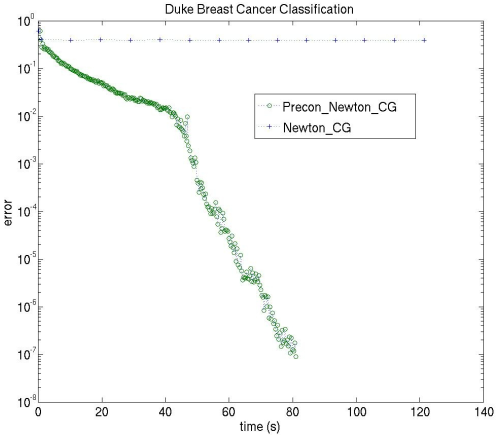
Testing on Duke-Breast-Cancer Classification



7129 features and 44 data

Preconditioning can make all the difference

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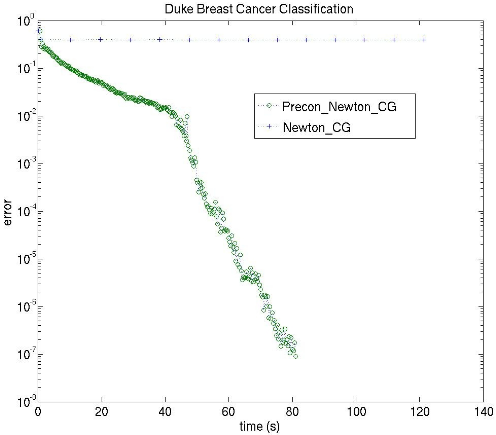

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