LBFGS

John Langford, Large Scale Machine Learning Class, February 5

(post presentation version)

We are still doing Linear Learning

Features: a vector $x \in \mathbb{R}^n$

Label: $y \in \mathbb{R}$

Goal: Learn $w \in \mathbb{R}^n$ such that $\hat{y}_w(x) = \sum_i w_i x_i$ is close to y.

But, this time in a batch fashion

Initialize w

Repeatedly:

1. Let $\hat{y}_w(x) = \sum_i w_i x_i$
2. Let $g_i = \sum_{(x,y)} \frac{\partial L(\hat{y}_w(x), y)}{\partial w_i}$
3. Compute update direction $d(g)$
4. Update weights $w_i \leftarrow w_i + d_i(g)$

The BFGS Update

$d(g) = Dg$ for some Direction matrix D
What is D?

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What is D?

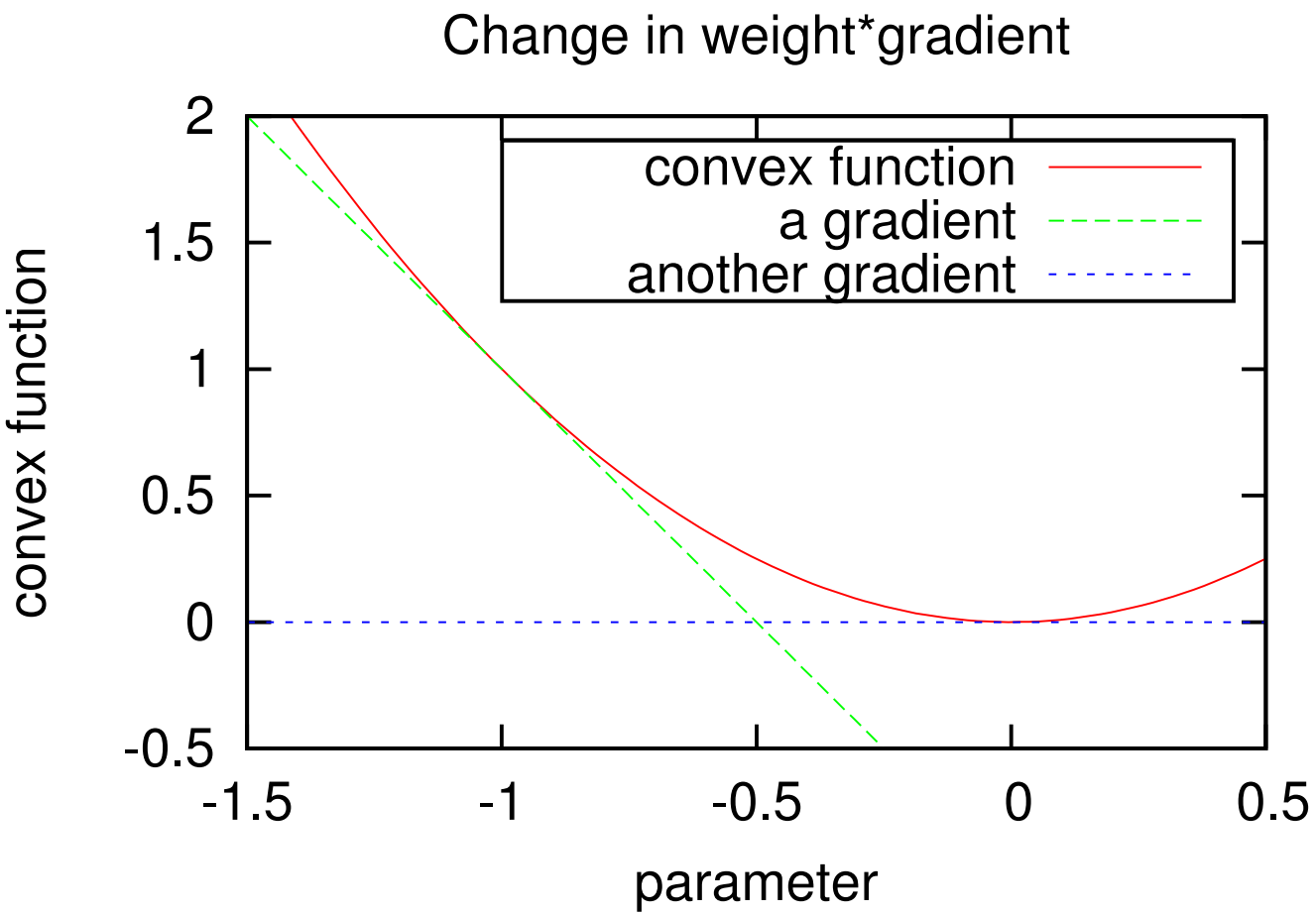
D is defined purely in terms of two empirical observations:

$g' = g_{\text{new}} - g_{\text{prev}}$

$w' = w_{\text{new}} - w_{\text{prev}}$

Assertion 1

$\sum_i g'_i w'_i = g'^{\top} w'$ should be positive for convex functions.



Assertion 2

$T_{kj} = \frac{g'_k w'_j}{\sum_i g'_i w'_i} = \frac{g' w'^{\top}}{g'^{\top} w'}$ Transforms direction g' to direction w' and vice versa.

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A matrix is a linear function which transforms one vector into another.

$$\sum_j T_{kj} v_j = \frac{\sum_j g'_k w'_j v_j}{\sum_i g'_i w'_i} = g'_k \frac{\sum_j v_j w'_j}{\sum_i g'_i w'_i}$$

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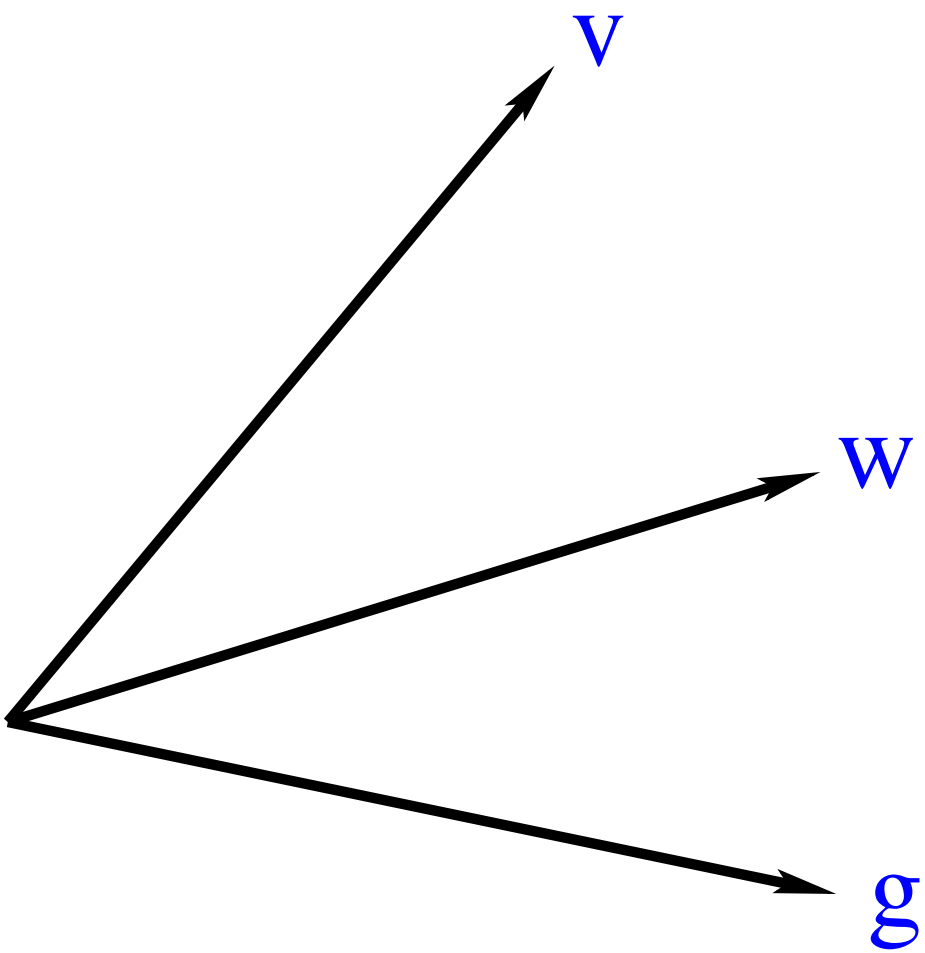
3 vectors, v, w, g



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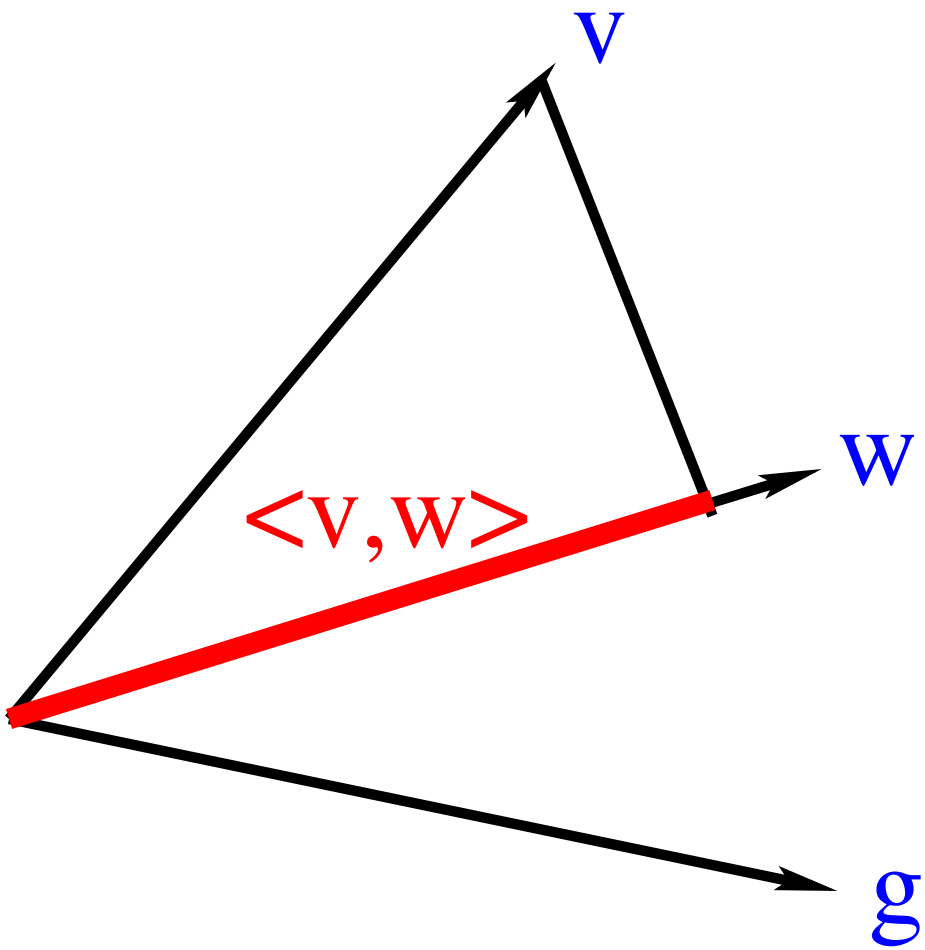

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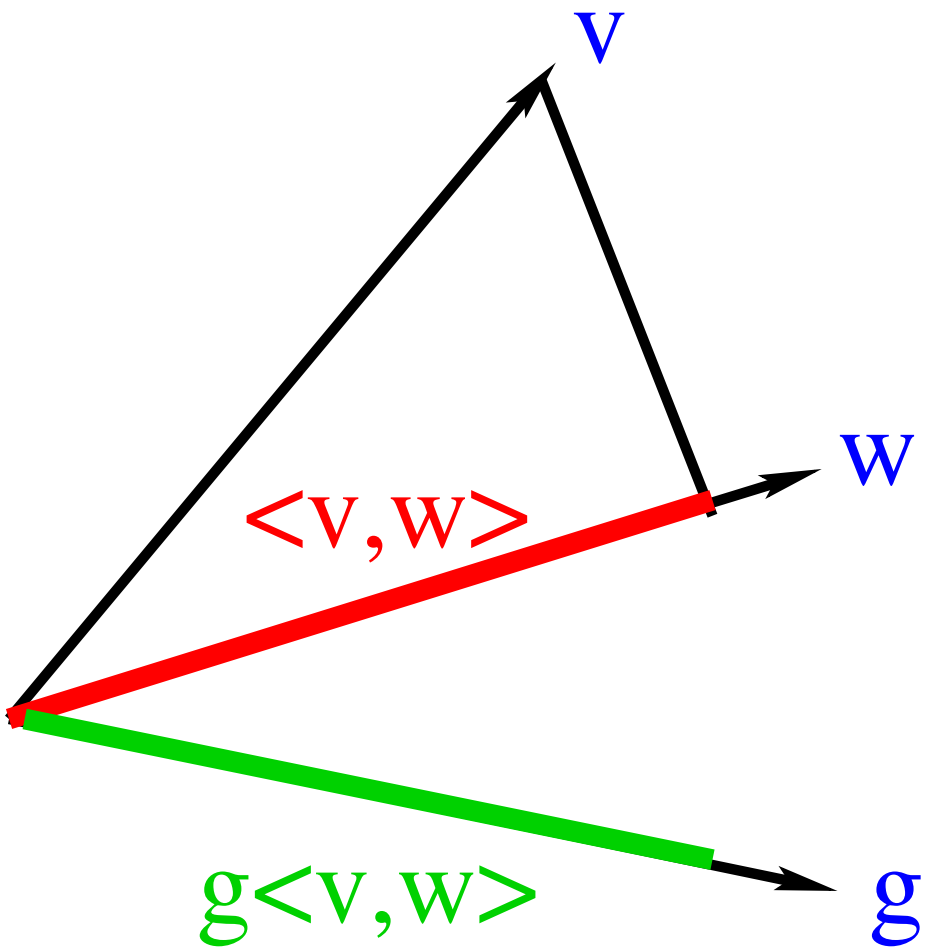

Assertion 3

Let $\delta_{kj} = I(k = j)$. if $k = j$ then 1 and 0 otherwise $S_{kj} = \delta_{kj} - T_{kj}$ Subtracts transform T_{kj} while keeping everything else.

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So an inverse should satisfy $Fg' \simeq w'$.

The BFGS direction

$D_{kj} \leftarrow \sum_{il} S_{ik} D_{il} S_{lj} + F_{kj}$

Or in recursive matrix form:

$D^t = S^{t\top} D^{t-1} S^t + F^t$

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LBFGS is the low rank approximation.

$$L^t = {S^t}^\top \ldots {S^{t-m}}^\top D^0 S^{t-m} \ldots S^t + {S^t}^\top \ldots {S^{t-m+1}}^\top F^{t-m} S^{t-m+1} \ldots S^t + \ldots + {S^t}^\top F^{t-1} S^t + F^t$$

Questions

What is D^0?

How do you make it fast?

How do you start?

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How do you regularize? Regularized loss has the form: $L'(\hat{y}, y) = L(\hat{y}, y) + \frac{c}{2} \sum_i w_i^2$. Imposing regularization is a once-per-pass dense operation.

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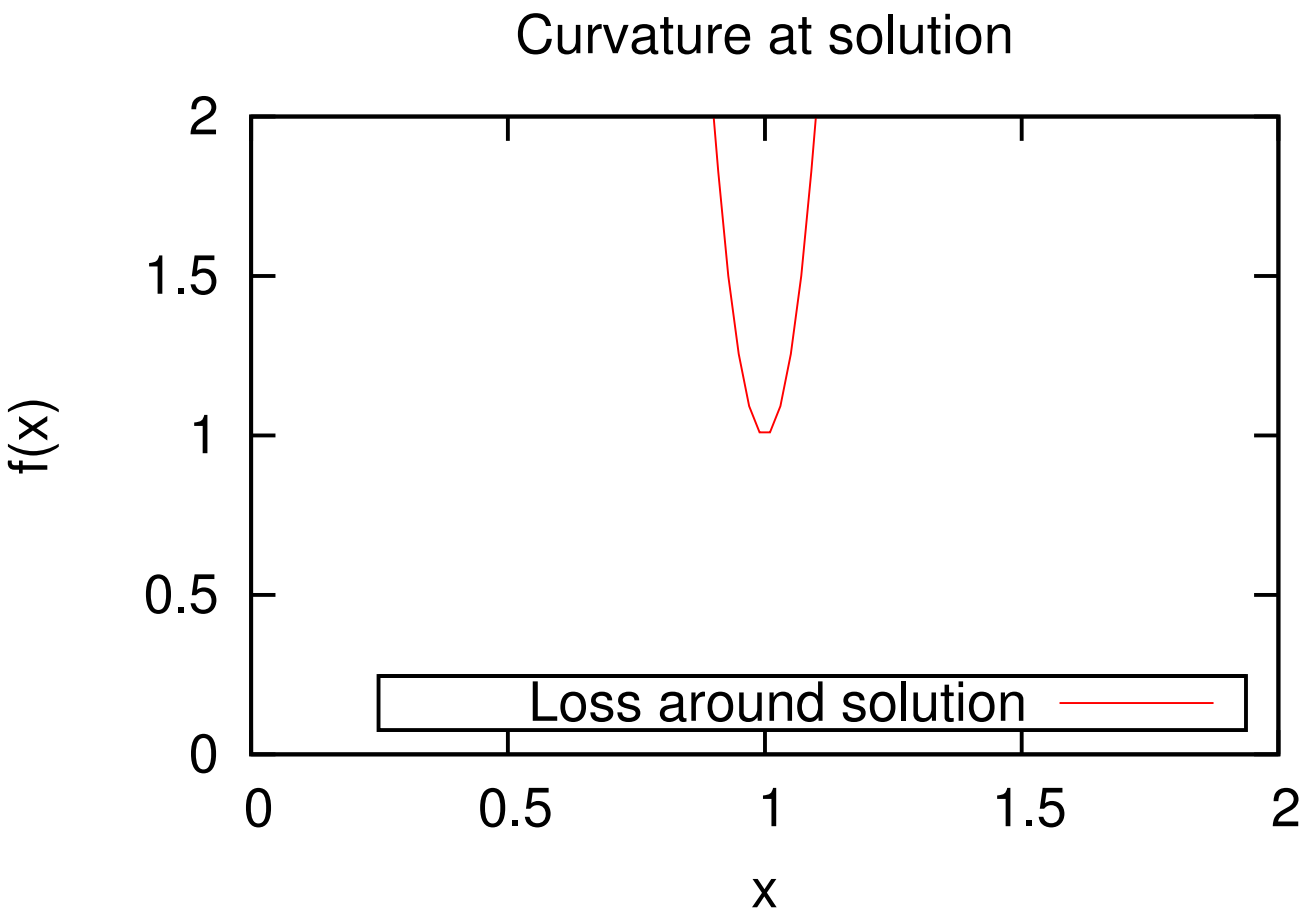

Compute and store: $r_i = \frac{\partial^2 L}{\partial w_i \partial w_i}$

On resumption, regularize by $\sum_i r_i (w_i - o_i)^2$ where o_i is the old weight value.

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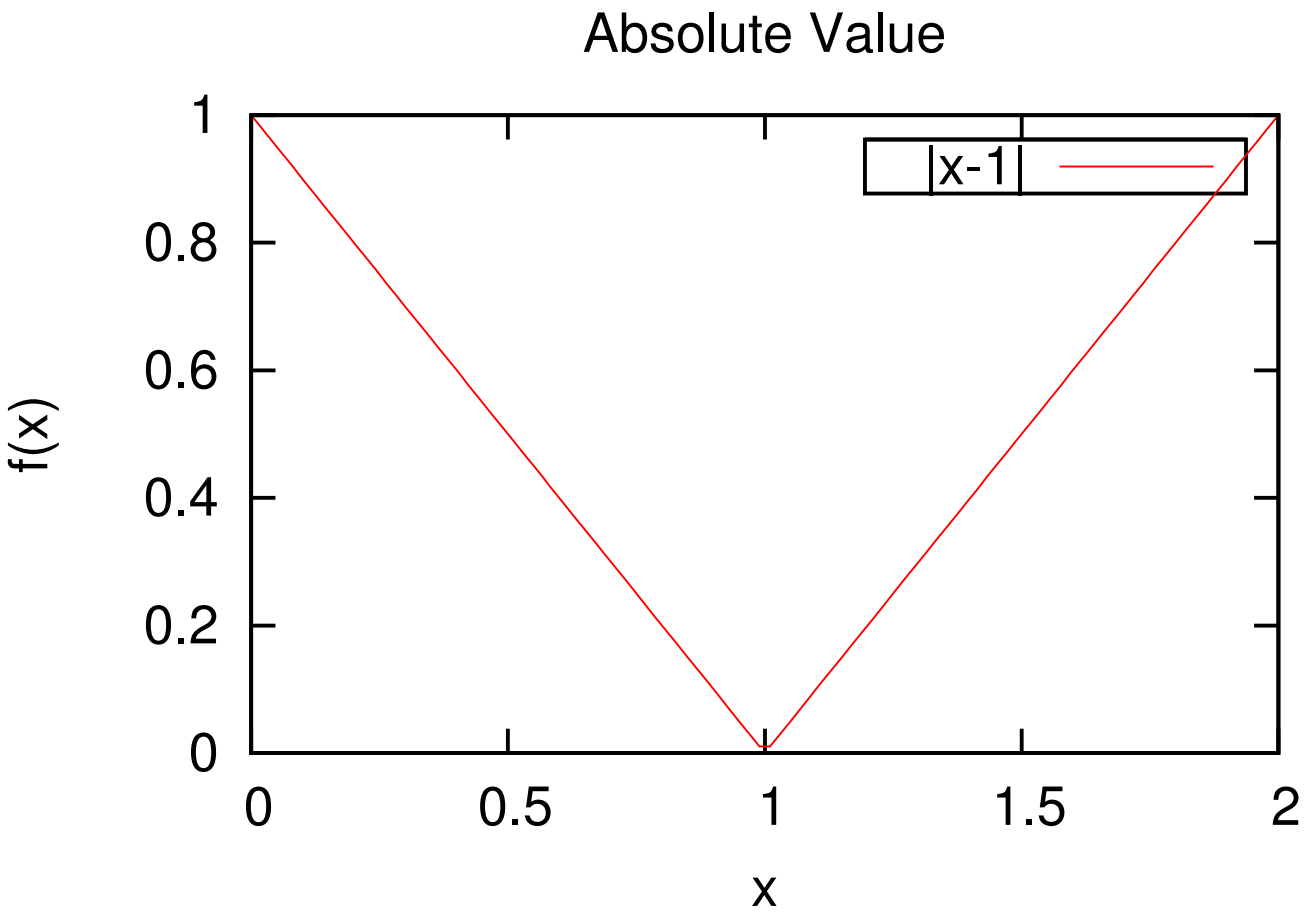
for some C.
Of course, it's rarely quadratic and you never perform exact line search.

What happens here?



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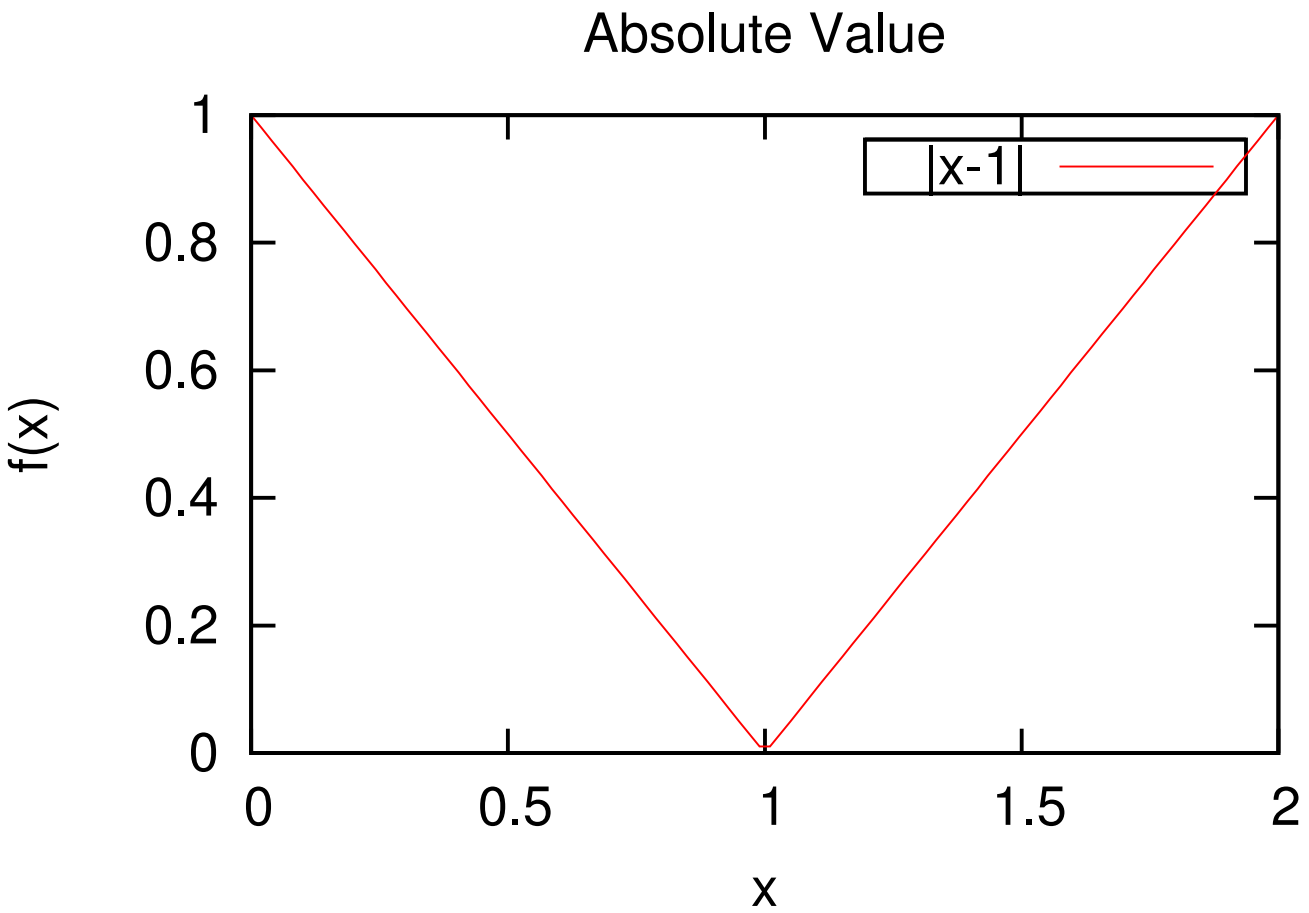

What happens to a true Newton step here?

References

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[G] Goldfarb, D., "A Family of Variable Metric Updates Derived by Variational Means", Math. of Comp. 24 (109):23-26.
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More References

Incremental LBFGS Olivier Chapelle