Optimization for Machine Learning

Lecture 4: Quasi-Newton Methods

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The Story So Far

Two Different Philosophies

- **Online Algorithms:** Use a small subset of the data at a time and repeatedly cycle
- **Batch Optimization:** Use the entire dataset to compute gradients and function values

Gradient Based Approaches

- **Bundle Methods:** Lower bound the objective function using gradients
- **Quasi-Newton algorithms:** Use the gradients to estimate the Hessian (build a quadratic approximation of the objective)

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Outline

1. **Classical Quasi-Newton Algorithms**
2. Non-smooth Problems
3. BFGS with Subgradients
4. Experiments

Broyden, Fletcher, Goldfarb, Shanno

Standard BFGS - I

Locally Quadratic Approximation

- $\nabla J(w_t)$ is the gradient of J at w_t
- H_t is an $n \times n$ estimate of the Hessian of J

$$m_t(w) = J(w_t) + \langle \nabla J(w_t), w - w_t \rangle + \frac{1}{2}(w - w_t)^\top H_t (w - w_t)$$

Parameter Update

$$w_{t+1} = \operatorname*{argmin}_{w} J(w_t) + \langle \nabla J(w_t), w - w_t \rangle + \frac{1}{2}(w - w_t)^\top H_t (w - w_t)$$

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$$w_{t+1} = w_t - \eta_t B_t \nabla J(w_t)$$

- η_t is a step size usually found via a line search
- $B_t = H_t^{-1}$ is a symmetric PSD matrix

Standard BFGS - II

B Matrix Update

Update B by

$$B_{t+1} = \operatorname*{argmin}_{B} ||B - B_t||_w \text{ s.t. } s_t = By_t$$

- $y_t = \nabla J(w_{t+1}) - \nabla J(w_t)$ is the difference of gradients
- $s_t = w_{t+1} - w_t$ is the difference in parameters
- This yields the update formula

$$B_{t+1} = \left(I - \frac{s_t y_t^\top}{\langle s_t, y_t \rangle}\right) B_t \left(I - \frac{y_t s_t^\top}{\langle s_t, y_t \rangle}\right) + \frac{s_t s_t^\top}{\langle s_t, y_t \rangle}$$

Limited memory variant: use a low-rank approximation to B

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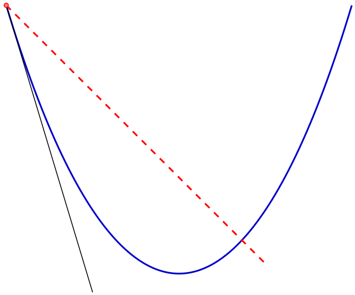
Line Search

Wolfe Conditions

Sufficient decrease: $J(w_t + \eta_t d_t) \leq J(w_t) + c_1 \eta_t \langle \nabla J(w_t), d_t \rangle$

Curvature condition: $\langle \nabla J(w_t + \eta_t d_t), d_t \rangle \geq c_2 \langle \nabla J(w_t), d_t \rangle$,

where $0 < c_1 < c_2 < 1$.



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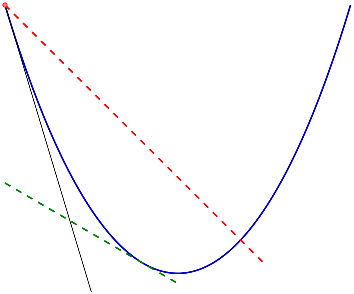

Outline

Non-smooth Convex Optimization

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- But, some of our losses look like this

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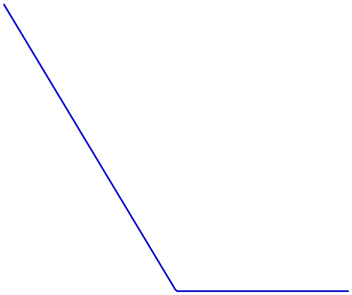

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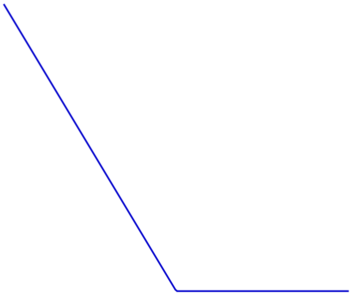
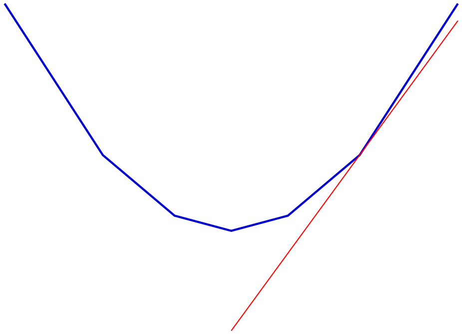


Houston we Have a Problem!

Subgradients

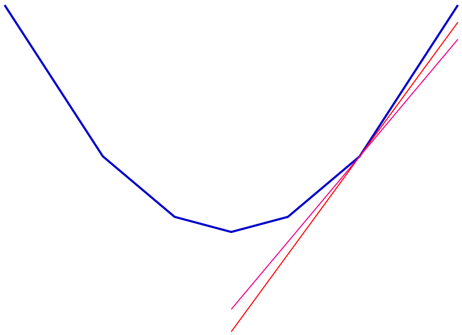


A subgradient at x' is any vector s which satisfies

$$f(x) \geq f(x') + \langle x - x', s \rangle \text{ for all } x$$

Set of all subgradients is denoted as $\partial f(w)$

Subgradients



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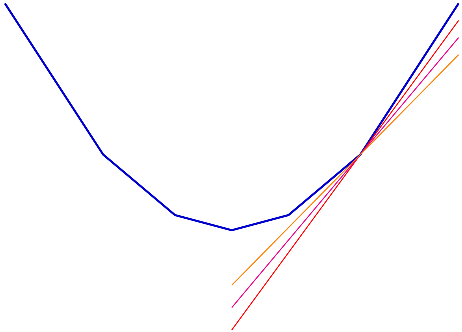

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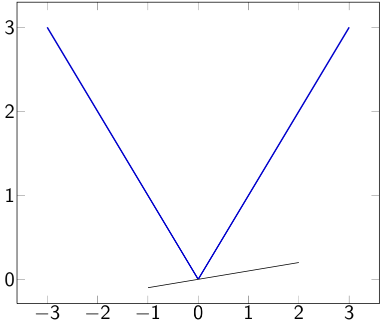
Why is Non-Smooth Optimization Hard?

The Key Difficulties

- A negative subgradient direction $\neq$ a descent direction
- Abrupt changes in function value can occur
- It is difficult to detect convergence



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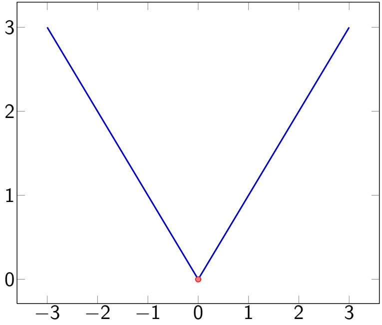

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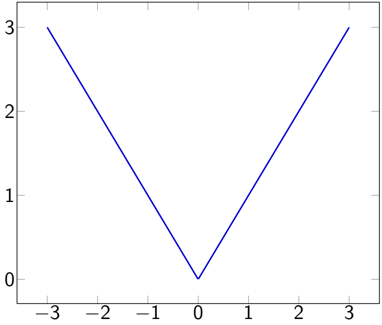

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Subgradients

The Good, the Bad, and the Ugly

The subdifferential is a convex set

Not every subgradient is a descent direction!

d is a descent direction if, and only if, $\langle d, s \rangle < 0$ for all $s \in \partial f(x)$

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When Working with Subgradients

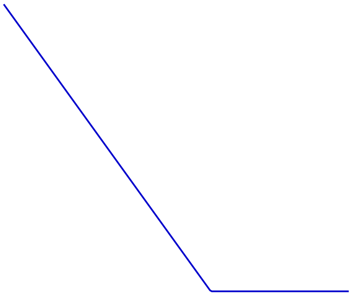
Three Things Break Down

- The locally quadratic approximation is no longer well defined
- The descent direction $-B_t \nabla J(w_t)$ is not well defined
- The line search to find η_t needs to be modified

Changing the Approximation

Locally Quadratic Approximation

$$m_t(w) = J(w_t) + \langle \nabla J(w_t), w - w_t \rangle + \frac{1}{2}(w - w_t)^\top H_t(w - w_t)$$



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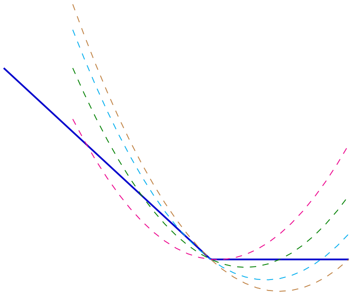

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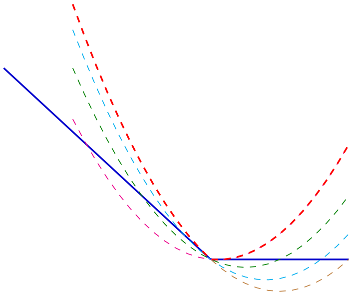

Descent Direction Finding

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Require: *maxitr*

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    if ⟨s_k, d_k⟩ < 0 then
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until k ≥ maxitr
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The Hinge Loss Revisited

The objective function $J(w) := \frac{\lambda}{2}||w||^2 + \frac{1}{m}\sum_{i=1}^{m} \max(0, 1 - y_i \langle x_i, w \rangle)$

The Hinge Loss Revisited

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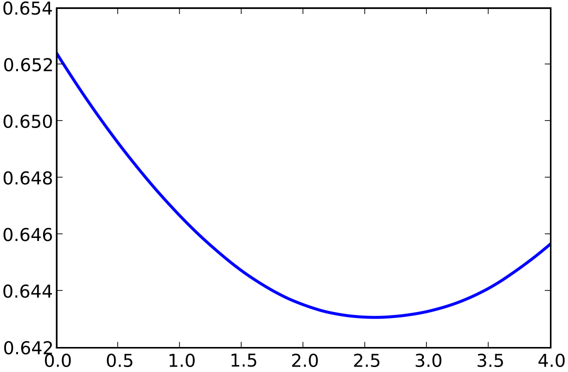
Plotted along any direction looks like this



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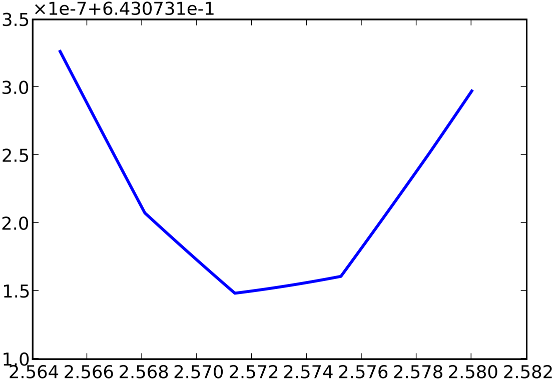

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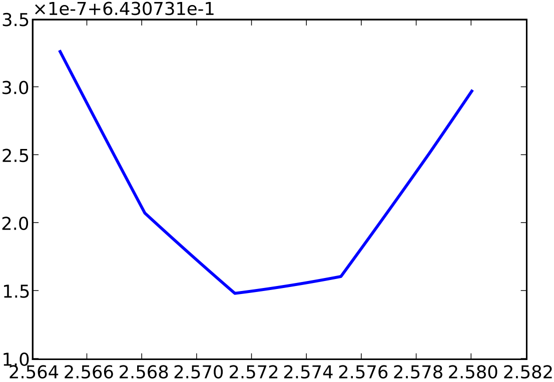


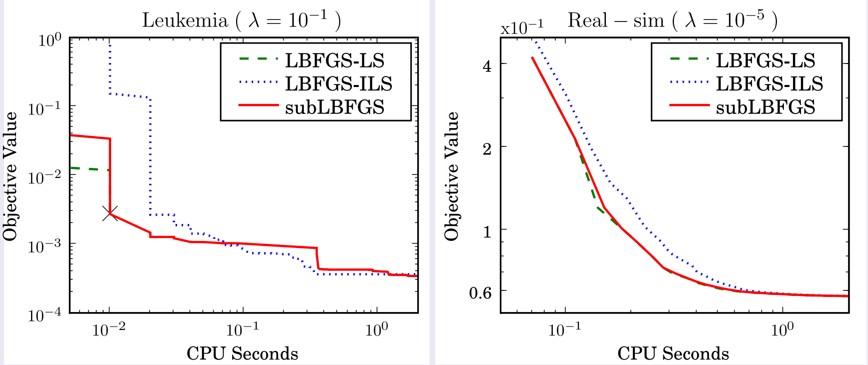
Piecewise quadratic $\implies$ exact line search in linear time.

Outline

Why Not Just Use BFGS?

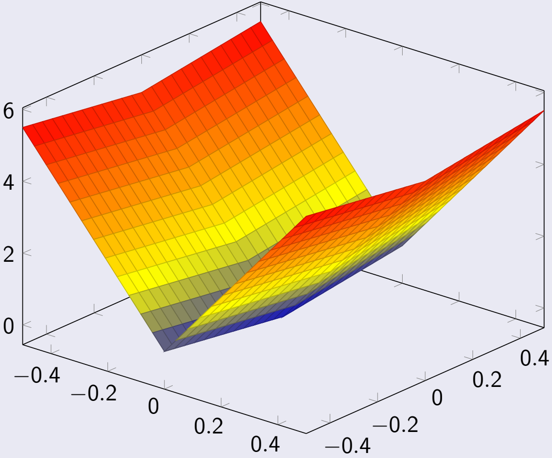
- Leukamia: 38 train, 34 test, 7129 dimensions
- real-sim: 57763 train, 14438 test, 20958 dimension

CPU Time vs Objective Function Value



subBFGS: Results on a Simple Problem

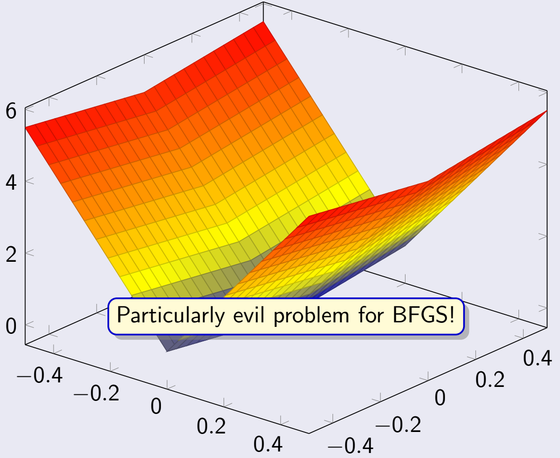
The Problem



$$J(w_1, w_2) = 10 * |w_1| + |w_2|$$

subBFGS: Results on a Simple Problem

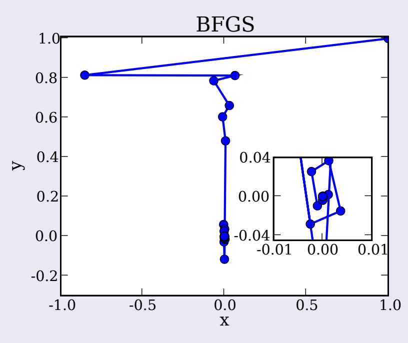
The Problem



$$J(w_1, w_2) = 10 * |w_1| + |w_2|$$

subBFGS: Results on a Simple Problem

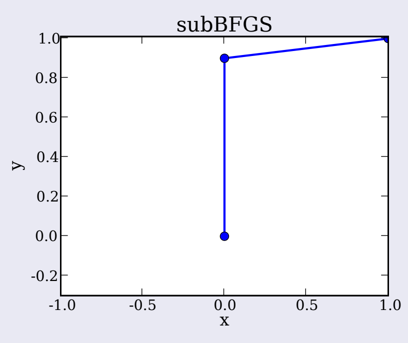
BFGS



- Hops from orthant to orthant
- Slow convergence :(

subBFGS: Results on a Simple Problem

subBFGS

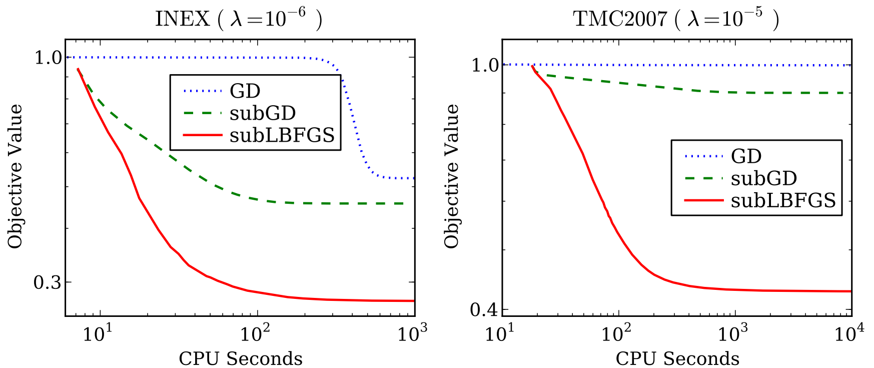


- Exact line search
- Converges in 2 iterations :)

Are Our Modifications Helpful?

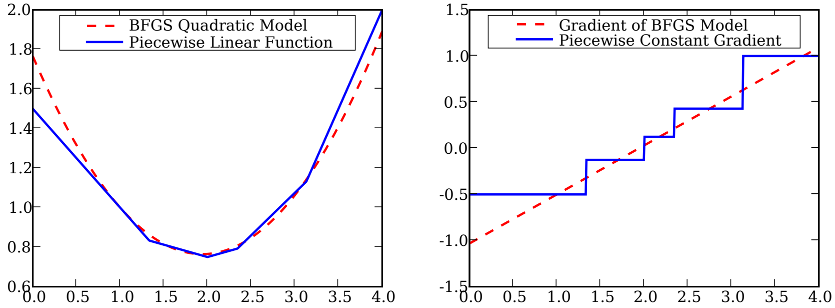
- INEX: 6053 train, 6054 test, 167295 dimensions, 18 classes.
- TMC2007: 21519 train, 7077 test, 30438 dimensions, 22 classes.

CPU Time vs Objective Function Value



On a Simple Toy Problem

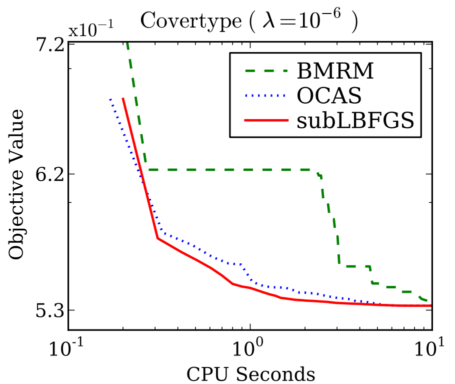
BFGS Approximation to the Objective Function and Gradient



Results on some standard datasets

- Covertype: 522911 train, 58101 test, 54 dimensions.

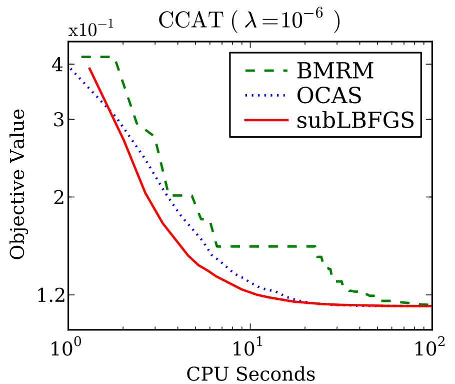
CPU Time vs Objective Function Value



Results on some standard datasets

- CCAT: 781265 train, 23149 test, 47236 dimensions.

CPU Time vs Objective Function Value



The Pros and Cons of subBFGS

Quasi-Newton Philosophy

- Use the gradients to build a quadratic approximation
- Initially this approximation is a good fit
  - Rapid initial progress
- Closer to the optimum the hinges matter
  - Progress slows down near the optimum

Line Search

- subBFGS requires a line search which fulfills Wolfe conditions
- For binary and multiclass hinge loss an exact line search is cheap
- Can we do a cheap line search for structured losses?

References

- J. Yu, S. V. N. Vishwanathan, S. Günter, and N. N. Schraudolph. *A quasi-Newton approach to nonsmooth convex optimization*. Submitted to JMLR (short version in ICML 2008).
- A. Smola, S. V. N. Vishwanathan, and Q. Le.*Bundle methods for machine learning*. submitted to JMLR (short version in NIPS 2007).
- C-H. Teo, Q. Le, A. Smola, and S. V. N. Vishwanathan. *A scalable modular convex solver for regularized risk minimization*. KDD 2007.