NTNU | Norwegian University of Science and Technology

TTK4135 – Lecture 15
Quasi-Newton

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Learning goal Ch. 2, 3 and 6: Understand this slide

Line-search unconstrained optimization

$$\min_{x} f(x)$$

```
1. Initial guess $x_0$
2. While termination criteria not fulfilled
    a) Find descent direction $p_k$ from $x_k$
    b) Find appropriate step length $\alpha_k$; set $x_{k+1} = x_k + \alpha_k p_k$
    c) $k = k+1$
3. $x_M = x^*$?  (possibly check sufficient conditions for optimality)
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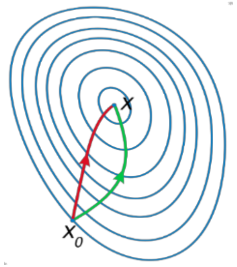


A comparison of steepest descent and Newton's method. Newton's method uses curvature information to take a more direct route. (wikipedia.org)

Termination criteria:

Stop when first of these become true:

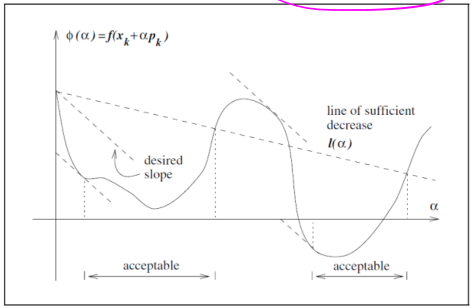
- $\|\nabla f(x_k)\| \le \epsilon$ (necessary condition)
- $\|x_k - x_{k-1}\| \le \epsilon$ (no progress)
- $\|f(x_k) - f(x_{k-1})\| \le \epsilon$ (no progress)
- $k \le k_{\max}$ (kept on too long)

Descent directions:

- Steepest descent
  $p_k = -\nabla f(x_k)$
- Newton
  $p_k = -(\nabla^2 f(x_k))^{-1} \nabla f(x_k)$
- Quasi-Newton
  $p_k = -B_k^{-1} \nabla f(x_k)$
  $B_k \approx \nabla^2 f(x_k)$

How to calculate derivatives – Ch. 8

Step length line search (Wolfe):



$\phi(\alpha) = f(x_k + \alpha p_k)$
desired slope
line of sufficient decrease
$l(\alpha)$
α
acceptable
acceptable

How many iterations? (Convergence rates)

Outline today: Quasi-Newton

- Q-N efficiently produce good search directions
  - Steepest descent: Need many iterations, but each iteration cheap (need only gradient)
  - Newton: Need few iterations, but each iteration expensive (need also Hessian)
  - Quasi-Newton: Few and cheap iterations by approximating the Hessian using only the gradient

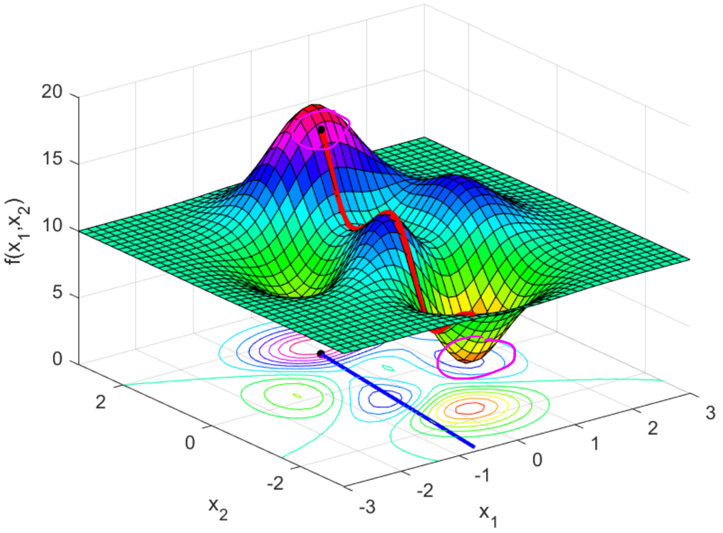
→
- Secant condition
- BFGS (and DFP) Hessian approximation update formulas

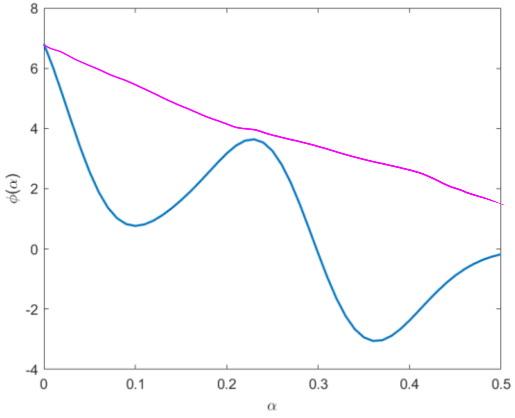
What is this used for? A lot!

Unconstrained and constrained optimization, nonlinear MPC, machine learning, image processing, …

Reference: N&W Ch.6-6.1 (Superficially 7.1)

Line search

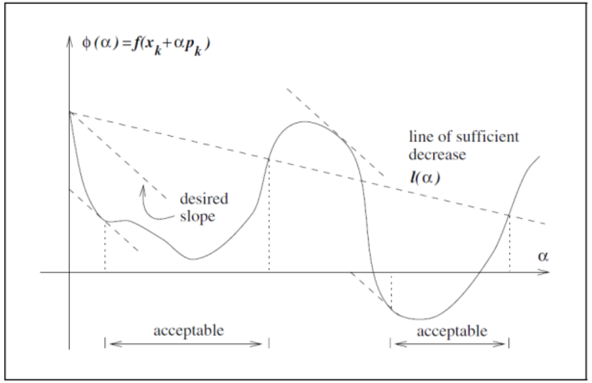




Conditions for a good step length: Wolfe conditions

$$f(x_k + \alpha p_k) \le f(x_k) + c_1 \alpha_k \nabla f_k^\top p_k \quad \text{Sufficient decrease (Armijo condition)}$$

$$\nabla f(x_k + \alpha_k p_k)^\top p_k \ge c_2 \nabla f_k^\top p_k \quad \text{Desired slope (Curvature condition)}$$



Newton's method

Approximate ("model") $f(x)$ at x_k

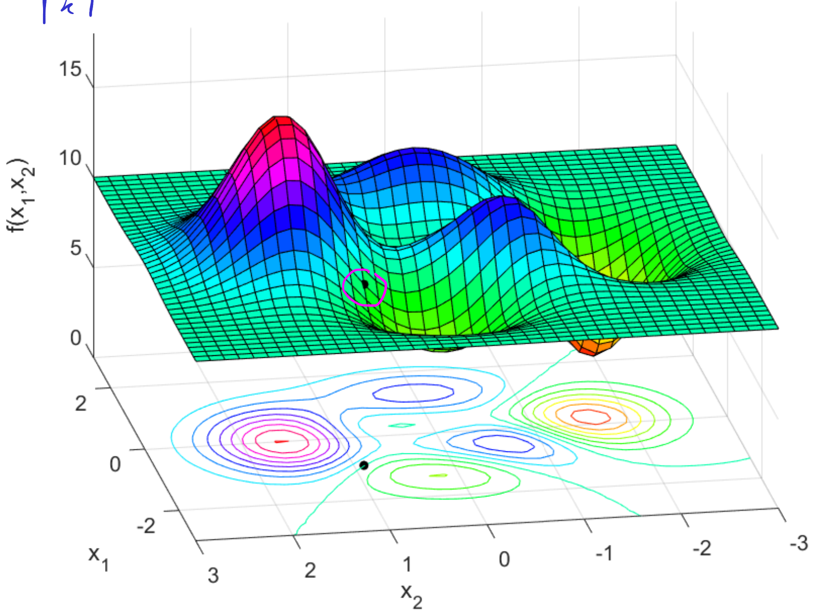
$$f(x_k+p) = m_k(p) = f_k + \nabla f_k^T p + \frac{1}{2} p^T \nabla^2 f_k p$$

$\hookrightarrow$ $f_k = f(x_k)$

$\nabla f_k = \nabla f(x_k)$

$\nabla^2 f_k = \nabla^2 f(x_k)$

$x_0 = (-0.9, 0.9)^\top$



Newton’s method

$$f(x_k + p) \approx m_k(p) = f_k + \nabla f_k^\top p + \tfrac{1}{2} p^\top \nabla^2 f_k p$$

Newton direction : $\boxed{p = \arg\min_p m_k(p)}$

Assume $\nabla^2 f_k > 0 \Rightarrow m_k(p)$ convex

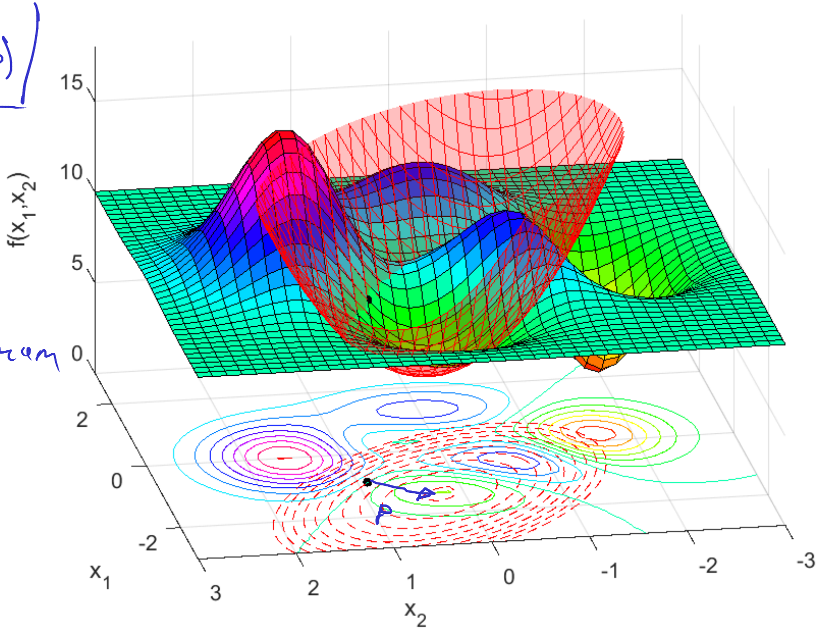
$\Rightarrow \nabla m_k(p) = 0$ nec & suff.

for p to be optimum

$$\nabla m_k(p) = \nabla f_k + \nabla^2 f_k p = 0$$

$$\Rightarrow p = -\left[\nabla^2 f_k\right]^{-1} \nabla f_k$$

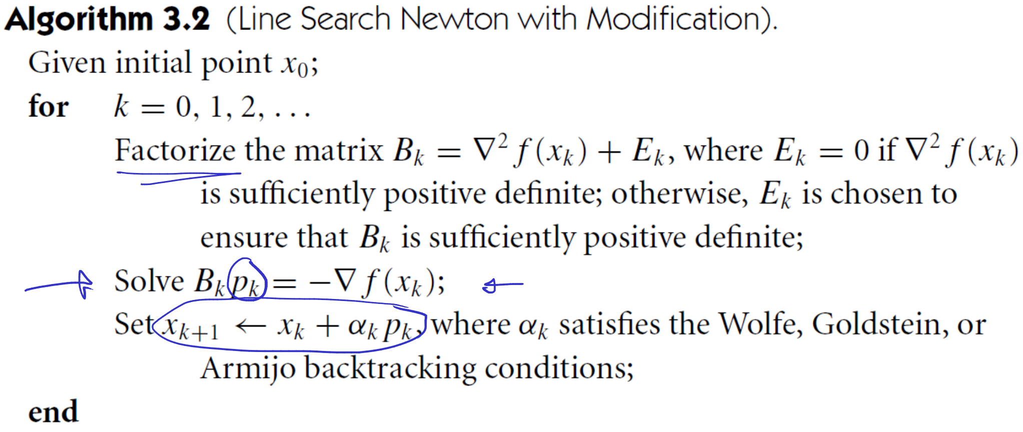
invertible since > 0



Hessian modification for Newton's method

- For $p_k = -B_k^{-1}\nabla f(x_k)$ to be a descent direction, we need $B_k > 0$

- In general, this does not hold true for Newton, $B_k = \nabla^2 f(x_k)$. We therefore modify the Hessian when it is not positive definite:



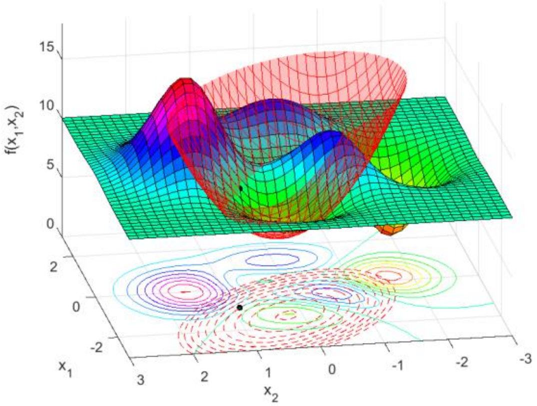
Algorithm 3.2 (Line Search Newton with Modification).

```
Given initial point $x_0$;
for $k = 0, 1, 2, \ldots$
    Factorize the matrix $B_k = \nabla^2 f(x_k) + E_k$, where $E_k = 0$ if $\nabla^2 f(x_k)$
        is sufficiently positive definite; otherwise, $E_k$ is chosen to
        ensure that $B_k$ is sufficiently positive definite;
    Solve $B_k p_k = -\nabla f(x_k)$;
    Set $x_{k+1} \leftarrow x_k + \alpha_k p_k$, where $\alpha_k$ satisfies the Wolfe, Goldstein, or
        Armijo backtracking conditions;
end
```

- A good, but inefficient method: $E_k = \tau_k I, \quad \tau_k = \max\left(0, \delta - \lambda_{\min}\left(\nabla^2 f(x_k)\right)\right)$
- More efficient to do "similar" changes during factorization process
  - E.g. "modified Cholesky" method

Newton’s method

$$\underline{x_{k+1} = x_k + \alpha_k p_k;} \qquad \boxed{\underline{p_k = -\left[\nabla^2 f_k\right]^{-1} \nabla f_k}}$$



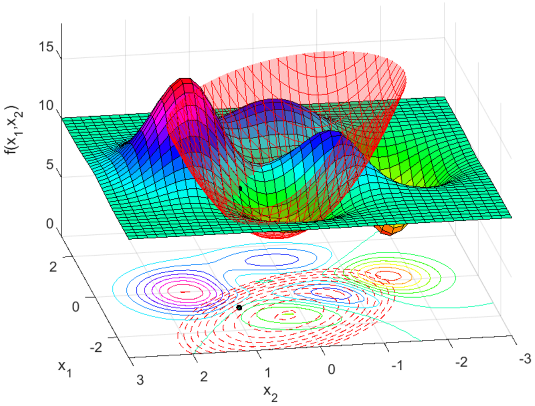
Advantage: $\underline{\text{Fast}}$ convergence

[close to optimum]

Drawback: Expensive

- to calculate (and store) $\nabla^2 f_k$
- to solve $\underline{\nabla^2 f_k p_k = -\nabla f_k}$

Quasi-Newton



Q-N approximation of $f(x)$

$$f(x_k+p) = f_k + \nabla f_k^T p + \frac{1}{2} p^T B_k p$$

How to choose B_k? We want:

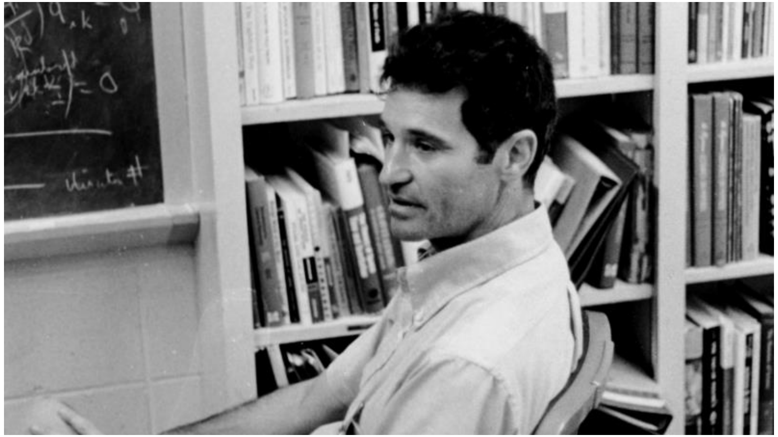
1) $B_k > 0$ → ensure descent direction

2) $B_k \approx \nabla^2 f_k$ → ensure fast convergence

3) Cheap computations → Only use gradients ∇f_k to compute B_k

Quasi-Newton

- Invented by Bill Davidon, physicist at Argonne National Labs, around mid 1950s
- “The Davidon-Fletcher-Powell (DFP) update formula”



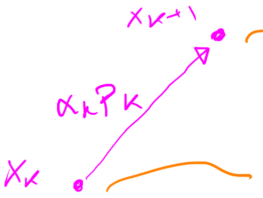
- “One of the most creative ideas in nonlinear optimization”, tremendous impact

Fun fact 1: His first paper on Q-N was not accepted for publication before 1991, over thirty years later

Fun fact 2: Bill Davidon was a peace activist, mastermind behind a break-in at an FBI office in 1971 (Movie: “1971”)

Secant condition

Consider $m_{k+1}(p) = f_{k+1} + \nabla f_{k+1}^T p + \frac{1}{2} p^T B_{k+1} p$



$$\nabla m_{k+1}(0) = \nabla f_{k+1}$$

$$\nabla m_{k+1}(-\alpha_k p_k) = \nabla f_{k+1} - \alpha_k B_{k+1} p_k \overset{\overset{\text{want!}}{\downarrow}}{=} \nabla f_k$$

$$B_{k+1} \underbrace{\alpha_k p_k}_{s_k = x_{k+1} - x_k} = \underbrace{\nabla f_{k+1} - \nabla f_k}_{y_k}$$

Secant condition: $\boxed{B_{k+1} s_k = y_k}$!

Secant condition

Also: Taylor expansion of $\nabla f(x_k)$

$$\nabla f_{k+1} = \nabla f_k + \nabla^2 f_k \, (x_{k+1} - x_k) + \dots$$

$$\underbrace{\nabla f_{k+1} - \nabla f_k}_{y_k} = \nabla^2 f_k \, \underbrace{(x_{k+1} - x_k)}_{s_k} + \dots$$

That is: $\boxed{B_{k+1} \approx \nabla^2 f_k}$ (Enforced by secant condition)

Positive definite requirement

Remember : We want $B_{k+1} > 0$

Note : $\underline{s_k^T y_k} = s_k^T B_{k+1} s_k \ \underline{\overset{\text{want}}{>}}\ 0$

That is : We must require that $\boxed{s_k^T y_k > 0}$

$(x_{k+1} - x_k)^T (\nabla f_{k+1} - \nabla f_k)$

This holds :

→ If α_k fulfills Wolfe conditions

(→ for any α_k if $f(x)$ is convex)

DFP update formula

Observation: Infinitely many B_{k+1} that fulfills $B_{k+1} s_k = y_k$

⇒ Let's choose the one closest to B_k!

$$B_{k+1} = \arg\min_{B} \| B - B_k \| \quad \text{s.t.} \quad B = B^T, \quad B s_k = y_k$$

which matrix norm?

Solution with "weighted Frobenius norm"

$$\boxed{B_{k+1} = (I - \rho_k \underline{y_k s_k^T}) B_k (I - \rho_k \underline{s_k y_k^T}) + \rho_k \underline{y_k y_k^T},}$$

$$\rho_k = \frac{1}{y_k^T s_k}$$

Inverse update formula

$p_k = -B_k^{-1} \nabla f_k$

DFP formula for updating B_k:

$$\rightarrow \quad B_{k+1} = \left(I - \rho_k y_k s_k^\top\right) B_k \left(I - \rho_k s_k y_k^\top\right) + \rho_k y_k y_k^\top, \quad \rho_k = \frac{1}{y_k^\top s_k}$$

→ **But: since we need B_k^{-1} in $p_k = -B_k^{-1}\nabla f_k$, can we update $\underline{H_k = B_k^{-1}}$ instead?**

Yes: Multiply out DFP as

$$\rightarrow \quad B_{k+1} = B_k + \begin{pmatrix} B_k s_k & y_k \end{pmatrix} \begin{pmatrix} 0 & -\rho_k \\ -\rho_k & \rho_k + s_k^\top B_k s_k \rho_k^2 \end{pmatrix} \begin{pmatrix} s_k^\top B_k \\ y_k^\top \end{pmatrix}, \quad \rho_k = \frac{1}{y_k^\top s_k},$$

use the *matrix inversion lemma* (Sherman-Morrison-Woodbury formula)

$$(A + UCV)^{-1} = A^{-1} - A^{-1}U(C^{-1} + VA^{-1}U)^{-1}VA^{-1}$$

to obtain the inverse DFP formula:

$$\boxed{H_{k+1} = H_k - \frac{H_k y_k y_k^\top H_k}{y_k^\top H_k y_k} + \frac{s_k s_k^\top}{y_k^\top s_k}} \quad \rightarrow \quad p_k = -H_k \nabla f_k$$

BFGS update formula

Alternatively: Choose H_{k+1} closest to H_k:

$$H_{k+1} = \arg\min_{H} \| H - H_k \| \quad \text{s.t.} \quad H = H^T, \; H y_k = s_k$$

weighted Frobenius norm

Solution: BFGS formula

$$\boxed{H_{k+1} = (I - \rho_k s_k \underline{y_k}^T) H_k (I - \rho_k y_k s_k^T) + \rho_k s_k s_k^T}$$

BFGS: Considered most effective Q-N formula!

BFGS update formula

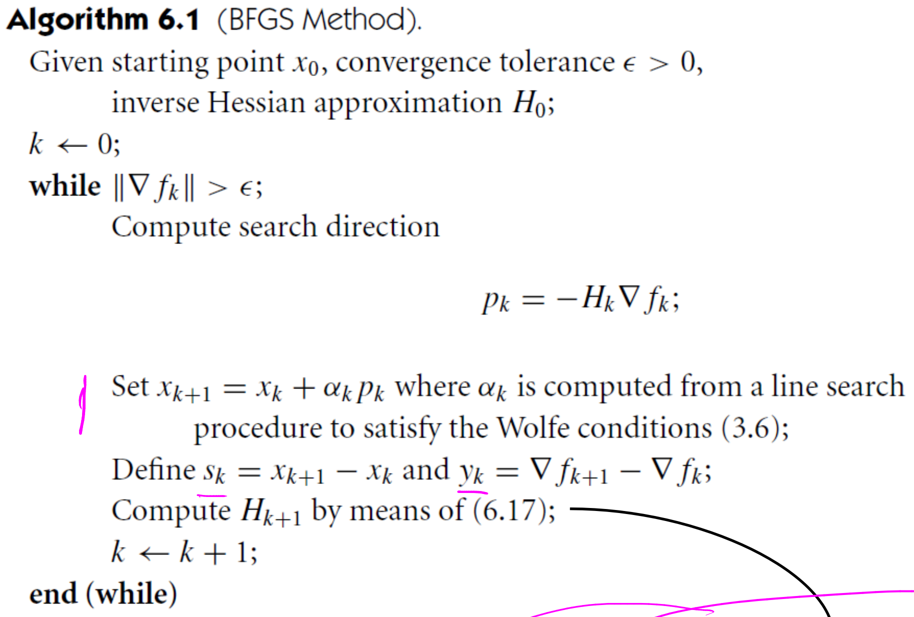
- How to choose H_0? Typically, $H_0 = I$
- Note: H_{k+1} pos. def. if $\boxed{y_k^T s_k > 0}$ ⇒ $\rho_k = \frac{1}{y_k^T s_k} > 0$

$$x^T H_{k+1} x = \underbrace{x^T (\dots)^T H_k (\dots) x}_{>0} + \underbrace{\rho_k \, x^T s_k s_k^T x}_{\substack{\rho_k \cdot \| s_k^T x \| \\ >0 \qquad\quad >0}} > 0$$

BFGS (1970)

Broyden, Fletcher, Goldfarb, Shanno

BFGS method



Algorithm 6.1 (BFGS Method).

```
Given starting point $x_0$, convergence tolerance $\epsilon > 0$,
        inverse Hessian approximation $H_0$;
$k \leftarrow 0$;
while $\|\nabla f_k\| > \epsilon$;
        Compute search direction
                $p_k = -H_k \nabla f_k$;
        Set $x_{k+1} = x_k + \alpha_k p_k$ where $\alpha_k$ is computed from a line search
                procedure to satisfy the Wolfe conditions (3.6);
        Define $s_k = x_{k+1} - x_k$ and $y_k = \nabla f_{k+1} - \nabla f_k$;
        Compute $H_{k+1}$ by means of (6.17);
        $k \leftarrow k + 1$;
end (while)
```

$$H_{k+1} = (I - \rho_k s_k y_k^T) H_k (I - \rho_k y_k s_k^T) + \rho_k s_k s_k^T$$

Local convergence rates (close to optimum)

Steepest descent:
Linear convergence

$$\frac{\|x_{k+1} - x^*\|}{\|x_k - x^*\|} \leq r \quad \text{for all } k \text{ sufficiently large, } r \in (0,1)$$

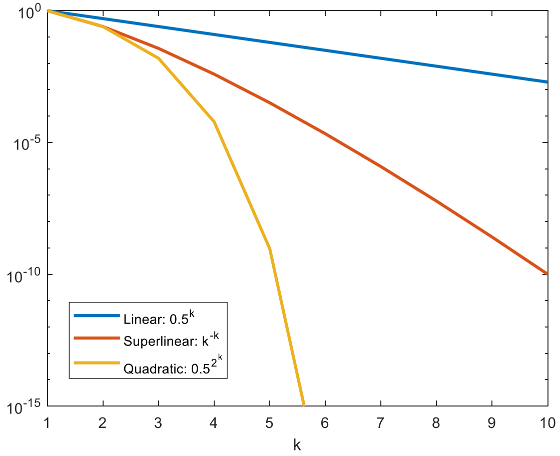
Newton:
Quadratic convergence

$$\frac{\|x_{k+1} - x^*\|}{\|x_k - x^*\|^2} \leq M \quad \text{for all } k \text{ sufficiently large, } M > 0$$

Quasi-Newton:
Superlinear convergence

$$\lim_{k \to \infty} \frac{\|x_{k+1} - x^*\|}{\|x_k - x^*\|} = 0$$

$$\frac{\|x_{k+1} - x^*\|}{\|x_0\|}$$

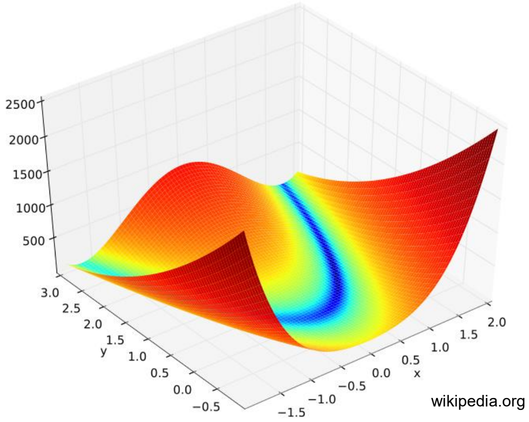


Example (from book)

- Using steepest descent, BFGS and inexact Newton on Rosenbrock function

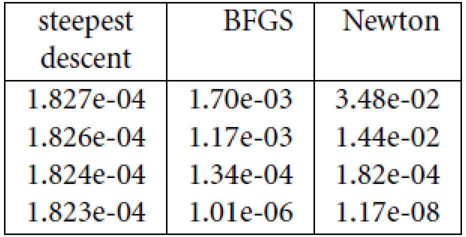
$$f(x) = 100(x_2 - x_1^2)^2 + (1 - x_1)^2$$

- Iterations from starting point (-1.2,1):
  - Steepest descent: 5264
  - BFGS: 34
  - Newton: 21



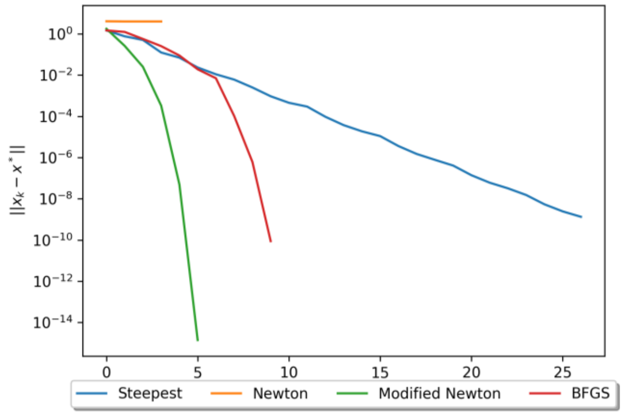
wikipedia.org

- Last iterations; value of $\|x_k - x^*\|$

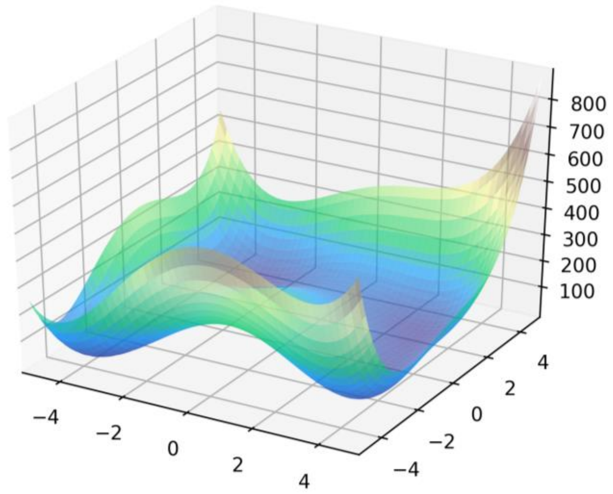


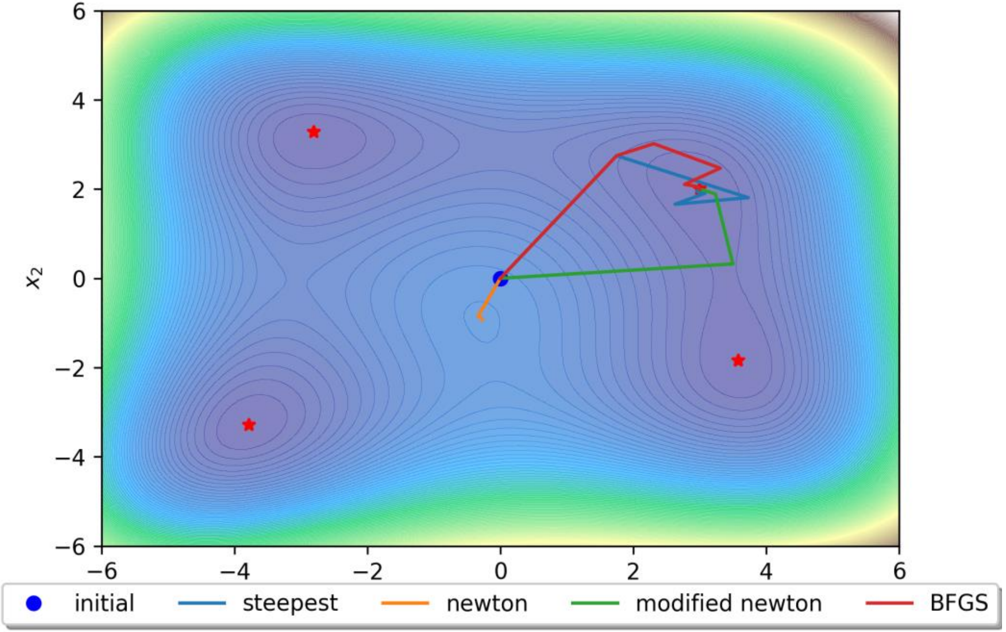
steepest descent	BFGS	Newton
1.827e-04	1.70e-03	3.48e-02
1.826e-04	1.17e-03	1.44e-02
1.824e-04	1.34e-04	1.82e-04
1.823e-04	1.01e-06	1.17e-08

Example: Himmelblau



$$f(x, y) = (x^2 + y - 11)^2 + (x + y^2 - 7)^2$$





Limited-memory BFGS (L-BFGS)

For $n = 1\,000\,000$, then H is $n \times n$ symmetric matrix

H has $\frac{n(n+1)}{2}$ elements

$5 \cdot 10^{11}$ elements $\sim$ 4000 GB

H becomes too large to store and manipulate!

Limited-memory BFGS (L-BFGS)

Remedy: Use L-BFGS.

- Store last m s_k, y_k (instead of H_k) $m = 5$
- Calculate $H_k \nabla f_k$ (Remember: $x_{k+1} = x_k + \alpha_k H_k \nabla f_k$

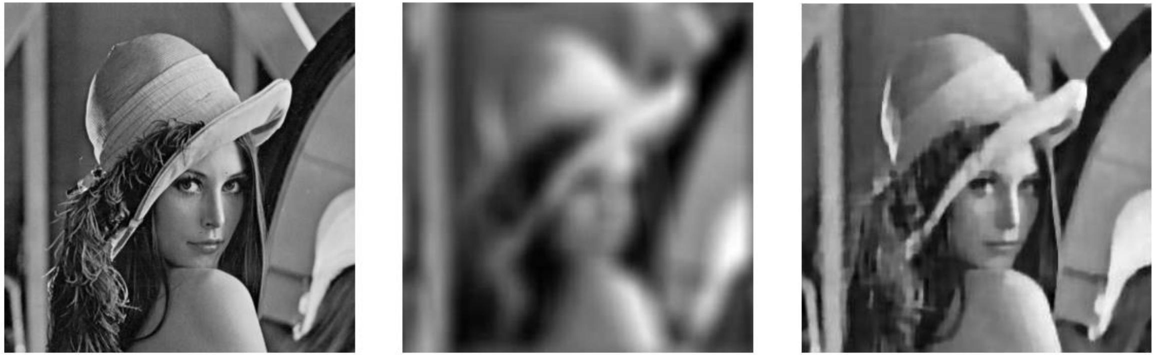
  Using

  $$H_{k+1} = (\ )^T H_k (\ ) + \rho_k s_k s_k^T, \quad H_{k-m} = I$$

  <u>without</u> actually forming H_k

  only using vector-vector products

Example: image deblurring



Original image **Blurred image** **Reconstruction**

Figures from (Wang et. al, 2009)

Given corrupted $m \times n$ image represented as vector $y \in \mathbb{R}^{m \cdot n}$, find $x \in \mathbb{R}^{m \cdot n}$ by solving the optimization problem

$$\underset{x}{\text{minimize}} \quad \|K * x - y\|_2^2 + \lambda \left(\sum_{i=1}^{n-1} |x_{mi} - x_{m(i+1)}| + \sum_{i=1}^{m-1} |x_{ni} - x_{n(i+1)}| \right)$$

where $K*$ denotes 2D convolution with some filter K

http://www.cs.cmu.edu/afs/cs/academic/class/15780-s16/www/slides/optimization.pdf

Example: machine learning

Virtually all machine learning algorithms can be expressed as minimizing a *loss function* over observed data

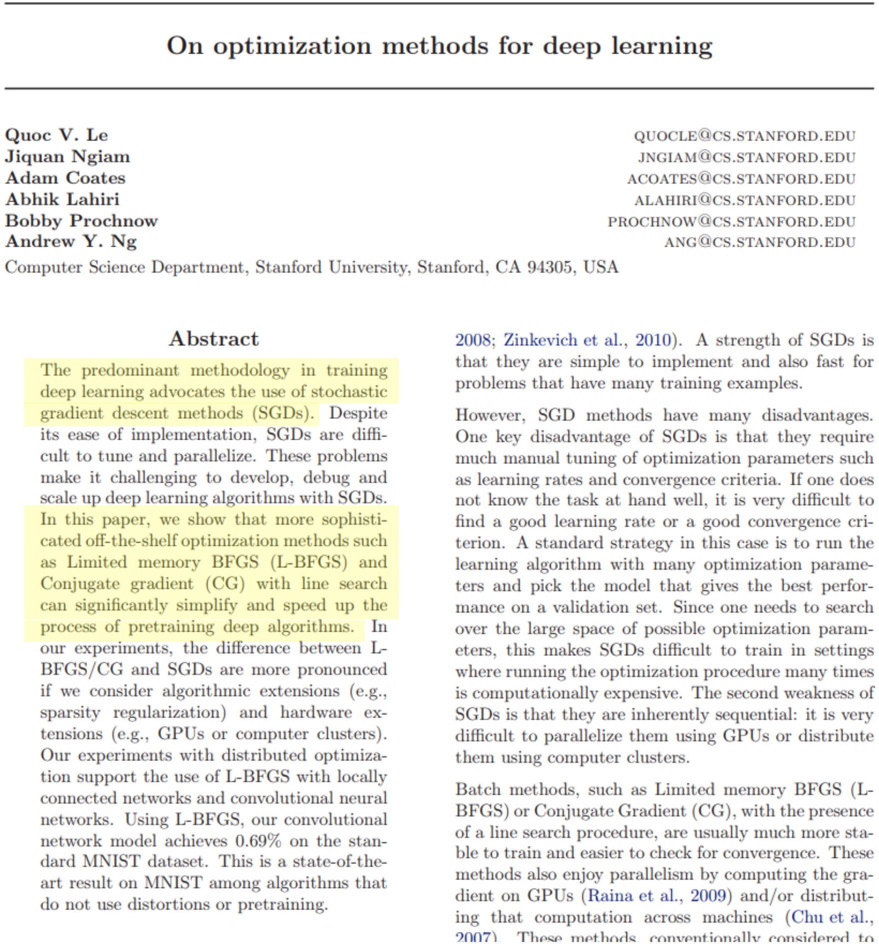
Given inputs $x^{(i)} \in \mathcal{X}$, desired outputs $y^{(i)} \in \mathcal{Y}$, hypothesis function $h_\theta : \mathcal{X} \to \mathcal{Y}$ defined by parameters $\theta \in \mathbb{R}^n$, and loss function $\ell : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}_+$

Machine learning algorithms solve optimization problem

$$\underset{\theta}{\text{minimize}} \quad \sum_{i=1}^{m} \ell\left(h_\theta\left(x^{(i)}\right), y^{(i)}\right)$$

http://www.cs.cmu.edu/afs/cs/academic/class/15780-s16/www/slides/optimization.pdf

Quasi-Newton in machine learning



On optimization methods for deep learning

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Abstract

The predominant methodology in training deep learning advocates the use of stochastic gradient descent methods (SGDs). Despite its ease of implementation, SGDs are difficult to tune and parallelize. These problems make it challenging to develop, debug and scale up deep learning algorithms with SGDs. In this paper, we show that more sophisticated off-the-shelf optimization methods such as Limited memory BFGS (L-BFGS) and Conjugate gradient (CG) with line search can significantly simplify and speed up the process of pretraining deep algorithms. In our experiments, the difference between L-BFGS/CG and SGDs are more pronounced if we consider algorithmic extensions (e.g., sparsity regularization) and hardware extensions (e.g., GPUs or computer clusters). Our experiments with distributed optimization support the use of L-BFGS with locally connected networks and convolutional neural networks. Using L-BFGS, our convolutional network model achieves 0.69% on the standard MNIST dataset. This is a state-of-the-art result on MNIST among algorithms that do not use distortions or pretraining.

2008; Zinkevich et al., 2010). A strength of SGDs is that they are simple to implement and also fast for problems that have many training examples.

However, SGD methods have many disadvantages. One key disadvantage of SGDs is that they require much manual tuning of optimization parameters such as learning rates and convergence criteria. If one does not know the task at hand well, it is very difficult to find a good learning rate or a good convergence criterion. A standard strategy in this case is to run the learning algorithm with many optimization parameters and pick the model that gives the best performance on a validation set. Since one needs to search over the large space of possible optimization parameters, this makes SGDs difficult to train in settings where running the optimization procedure many times is computationally expensive. The second weakness of SGDs is that they are inherently sequential: it is very difficult to parallelize them using GPUs or distribute them using computer clusters.

Batch methods, such as Limited memory BFGS (L-BFGS) or Conjugate Gradient (CG), with the presence of a line search procedure, are usually much more stable to train and easier to check for convergence. These methods also enjoy parallelism by computing the gradient on GPUs (Raina et al., 2009) and/or distributing that computation across machines (Chu et al., 2007). These methods conventionally considered to

Proceedings of the 28th International Conference on Machine Learning, Bellevue, WA, USA, 2011