Introduction to non-linear optimization

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March 2, 2007

Optimization problems

problem: Let $f : \mathbb{R}^n \to (-\infty, \infty]$,

$$\text{find} \quad \min_{x \in \mathbb{R}^n} \{f(x)\}$$

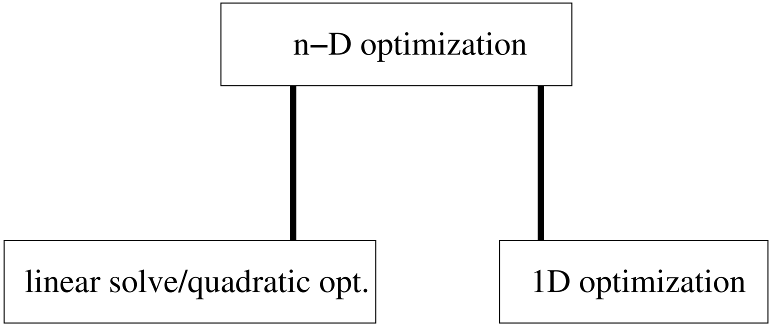
$$\text{find} \quad x_* \text{ s.t. } f(x_*) = \min_{x \in \mathbb{R}^n} \{f(x)\}$$

Quite general, but some cases, like f convex, are fairly solvable.
Today's problem: How about $f : \mathbb{R}^n \to \mathbb{R}$, differentiable?

$$\text{find} \quad x_* \text{ s.t. } \nabla f(x_*) = 0$$

We have a reasonable shot at this, especially if f is *twice differentiable*.

Two pillars of multi-variate optimization



The simplest we can get

Quadratic optimization: $f(x) = \frac{1}{2}x^t Ax - x^t b + c$.

- very common (actually universal)
- Taylor expansion
  $f(x + \Delta x) = f(x) + (\Delta x)^t \nabla f(x) + \frac{1}{2}(\Delta x)^t \nabla\nabla f(x) \Delta x + \cdots$

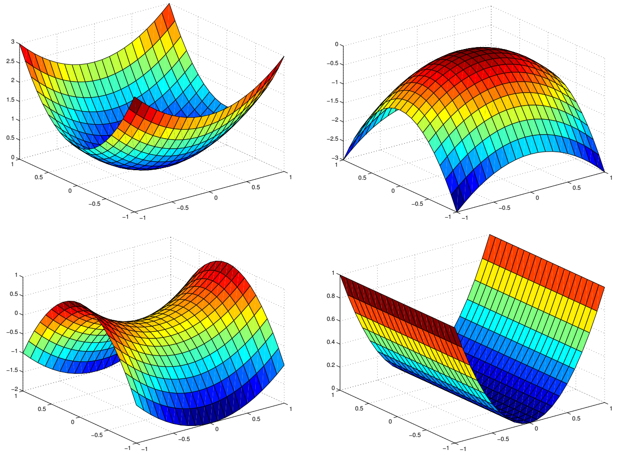
Finding $\nabla f(x) = 0$

$$\begin{aligned} \nabla f(x) = Ax - b &= 0 \\ x_* &= A^{-1}b \end{aligned}$$

Does this mean A has to be invertible? Is this all we need?

Max, min, saddle, or what?

Requires *A* be positive definite, why?



Universality of linear algebra in optimization

$$f(x) = \frac{1}{2}x^t Ax - x^t b + c$$

Linear solve: $x_* = A^{-1}b$.
Even for non-linear problems: if optimal x_* near our x

$$\begin{aligned} f(x_*) &\sim f(x) + (x_* - x)^t \nabla f(x) + \frac{1}{2}(x_* - x)^t \nabla\nabla f(x)\,(x_* - x) + \cdots \\ \Delta x &= x_* - x \sim -(\nabla\nabla f(x))^{-1} \nabla f(x) \end{aligned}$$

Optimization $\leftrightarrow$ Linear solve

Linear solve

$$x = A^{-1}b$$

But really we just want to solve

$$Ax = b$$

No need to form A^{-1} if we can avoid it!

For a general A, there are three important special cases,

- diagonal: $A = \begin{pmatrix} a_1 & 0 & 0 \\ 0 & a_2 & 0 \\ 0 & 0 & a_3 \end{pmatrix}$ thus $x_i = \frac{1}{a_i} b_i$
- orthogonal $A^t A = I$, thus $A^{-1} = A^t$ and $x = A^t b$
- triangular: $A = \begin{pmatrix} a_{11} & 0 & 0 \\ a_{21} & a_{22} & 0 \\ a_{31} & a_{32} & a_{33} \end{pmatrix}$, $x_i = \frac{1}{a_{ii}} \left(b_i - \sum_{j<i} a_{ij} x_j \right)$

Direct methods

A is symmetric positive definite.

Cholesky factorization:

$$A = LL^t,$$

where L lower triangular. So $LL^t x = b$ by

$$\begin{aligned} Lz &= b, \quad z_i = \frac{1}{L_{ii}}\left(b_i - \sum_{j<i} L_{ij} z_j\right) \\ L^t x &= z, \quad x_i = \frac{1}{L_{ii}}\left(z_i - \sum_{j>i} L_{ij} x_j\right) \end{aligned}$$

Direct methods

A is symmetric positive definite.

QR factorization:

$$A = QR,$$

where Q is orthogonal and R is upper triangular. Then $x = R^{-1}Q^t b$ (second subproduct by back-substitution).

Slightly more expensive than Cholesky

Eigenvalue factorization:

$$A = QDQ^t,$$

where Q is orthogonal and D is diagonal. Then $x = QD^{-1}Q^t b$ (each subproduct is easy to form).

Much more expensive than QR

Direct methods can be very expensive.

Iterative method basics

What's an iterative method?

Definition (Informal definition)

An *iterative method* is an algorithm $\mathcal{A}$ which takes what you have, x_i, and gives you a new x_{i+1} which is *less bad* such that $x_1, x_2, x_3, \ldots$ converges to some x_* with badness$= 0$.

A notion of *badness* could come from

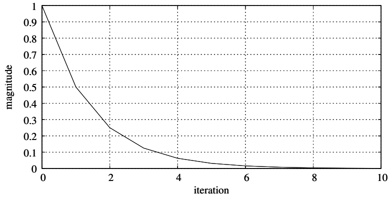
1. distance from x_i to our problem solution
2. value of some objective function above its minimum

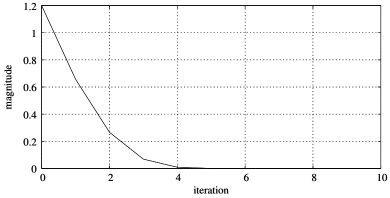
e.g. If x is supposed to satisfy $Ax = b$, we could take $||b - Ax||$ to be the measure of badness.

Iterative method considerations

How expensive is one $x_i \to x_{i+1}$ step?
How quickly does the badness decrease per step?
A thousand and one years of experience yields two cases

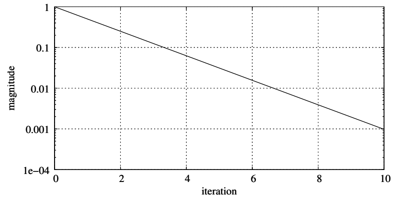
1. $B_i \propto \rho^i$ for some $\rho \in (0,1)$ (**linear**)
2. $B_i \propto \rho^{(\alpha^i)}$ for $\rho \in (0,1), \alpha > 1$ (**superlinear**)

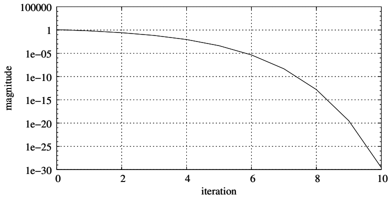




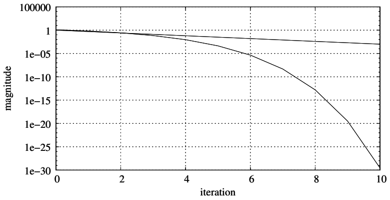
Can you tell the difference?

Convergence





Now can you tell the difference?



When evaluating an iterative method against manufacturer's claims, be sure to do semilog plots.

Iterative methods

For spd systems, sometimes cheaper to directly optimize $f(x) = \frac{1}{2}x^tAx - x^tb$.

gradient descent:

1. Search direction: $r_i = -\nabla f = b - Ax_i$
2. Search step: $x_{i+1} = x_i + \alpha_i r_i$
3. Pick alpha: $\alpha_i = \frac{r_i^t r_i}{r_i^t A r_i}$ minimizes $f(x + \alpha r_i)$

$$\begin{aligned} f(x_i + \alpha r_i) &= \frac{1}{2}x_i^tAx_i - x_i^tb + \frac{1}{2}\alpha^2 r_i^tAr_i + \alpha r_i^t(Ax_i - b) \\ &= \frac{1}{2}x_i^tAx_i - x_i^tb + \frac{1}{2}\alpha^2 r_i^tAr_i - \alpha r_i^t r_i \end{aligned}$$

Iterative methods

Optimize $f(x) = \frac{1}{2}x^t A x - x^t b$.

conjugate gradient descent:

1. Search direction: $d_i = r_i + \beta_i d_{i-1}$, with $r_i = b - Ax_i$.
2. Pick $\beta_i = -\frac{d_{i-1}^t A r_i}{d_{i-1}^t A d_{i-1}}$, ensures $d_{i-1}^t A d_i = 0$.
3. Search step: $x_{i+1} = x_i + \alpha_i d_i$
4. Pick $\alpha_i = \frac{d_i^t r_i}{d_i^t A d_i}$: minimizes $f(x_i + \alpha d_i)$

$$f(x_i + \alpha d_i) = \frac{1}{2}x_i^t A x_i - x_i^t b + \frac{1}{2}\alpha^2 d_i^t A d_i - \alpha d_i^t r_i$$

(also means that $r_{i+1}^t d_i = 0$)

Avoid extra A-multiply: using $Ad_{i-1} \propto r_{i-1} - r_i$

$$\beta_i = -\frac{(r_{i-1}-r_i)^t r_i}{(r_{i-1}-r_i)^t d_{i-1}} = -\frac{(r_{i-1}-r_i)^t r_i}{r_{i-1}^t d_{i-1}} = \frac{(r_i - r_{i-1})^t r_i}{r_{i-1}^t r_{i-1}}$$

A cute result

conjugate gradient descent:

1. $r_i = b - Ax_i$
2. Search direction: $d_i = r_i + \beta_i d_{i-1}$ (β s.t. $d_i A d_{i-1} = 0$)
3. Search step: $x_{i+1} = x_i + \alpha_i d_i$ (α minimizes).

Cute result

Theorem (sub-optimality of CG)

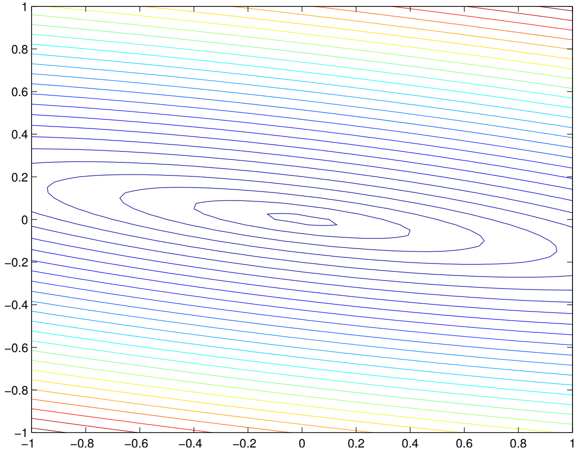
(Assuming $x_0 = 0$) at the end of step k, the solution x_k is the optimal linear combination of $b, Ab, A^2 b, \ldots A^k b$ for minimizing

$$\frac{1}{2} x^t A x - b^t x.$$

(computer arithmetic errors make this less than perfect)
Very little extra effort. Much better convergence.

Slow convergence: Conditioning

The eccentricity of the quadratic is a big factor in convergence



Convergence

$$\kappa = \frac{\max\ \mathrm{eig}(A)}{\min\ \mathrm{eig}(A)}$$

For gradient descent,

$$||r_i|| \sim \left|\frac{\kappa - 1}{\kappa + 1}\right|^i$$

For CG,

$$||r_i|| \sim \left|\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1}\right|^i$$

useless CG fact: in exact arithmetic $r_i = 0$ when $i > n$ (A is $n \times n$).

The truth about descent methods

Very slow unless κ can be controlled.
How do we control κ?

$$Ax = b \to (PAP^t)y = Pb, \quad x = P^t y$$

where P is a *pre-conditioner* you pick.
How to make $\kappa(PAP^t)$ small?

- perfect answer, $P = L^{-1}$ where $L^t L = A$ (Cholesky factorization).
- imperfect answer, $P \sim L^{-1}$

Variations on the theme of *incomplete factorization*:

- $P^{-1} = D^{\frac{1}{2}}$ where $D = \text{diag}\,(a_{11}, \dots, a_{nn})$
- more generally, incomplete Cholesky decomposition
- some easy nearby solution or simple approximate A (requiring domain knowledge)

Class project?

One idea for a preconditioner is by a *block diagonal* matrix

$$P^{-1} = \begin{pmatrix} L_{11} & 0 & 0 \\ 0 & L_{22} & 0 \\ 0 & 0 & L_{33} \end{pmatrix}$$

where $L_{ii}^t L_{ii} = A_{ii}$ a diagonal block of A.
In what sense does good clustering give good preconditioners?

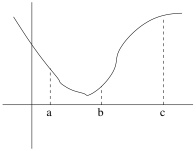
End of solvers: there are a few other iterative solvers out there I haven't discussed. They are not generally good.

1D optimization

1D optimization presents some important insights.

$$\min_{s \in \mathbb{R}} f(s), \quad f \text{ continuous.}$$

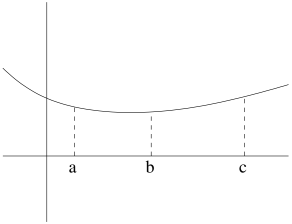
A derivative-free option:
A bracket is (a, b, c) s.t. $a < b < c$ and $f(a) > f(b) < f(c)$ then $f(x)$ has a local min for $a < x < b$



Golden search based on picking $a < b' < b < c$ and either $(a < b' < b)$ or $(b' < b < c)$ is a new bracket...continue
Linearly convergent, $e_i \propto G^i$, golden ratio G.

1D optimization

Fundamentally limited accuracy of the argmin:



Derivative-based methods: $f'(s) = 0$ (accurate argmin)

- bracketed: (a, b) s.t. $f'(a), f'(b)$ opposite sign
  1. bisection (linearly convergent)
  2. modified regula falsi & Brent's method (superlinear)
- unbracketed:
  1. secant method (superlinear)
  2. Newton's method (superlinear; requires another derivative)

Unless f'' is very easy, bracketed methods are best.

Adapting to non-linear problems

What can happen when far from the optimum?

- $-\nabla f(x)$ always points in a direction of decrease
- $\nabla\nabla f(x)$ may not be positive definite

Actually for *convex* problems $\nabla\nabla f$ is always positive semi-definite and for strictly convex it is positive definite.

What do we want?

- eventually find a convex neighborhood of x_* (be robust against mistakes)
- apply a quadratic approximation (do linear solve)

Fact: $\forall$ non-linear optimization algorithms, $\exists f$ which fools it.

Naïve Newton's method

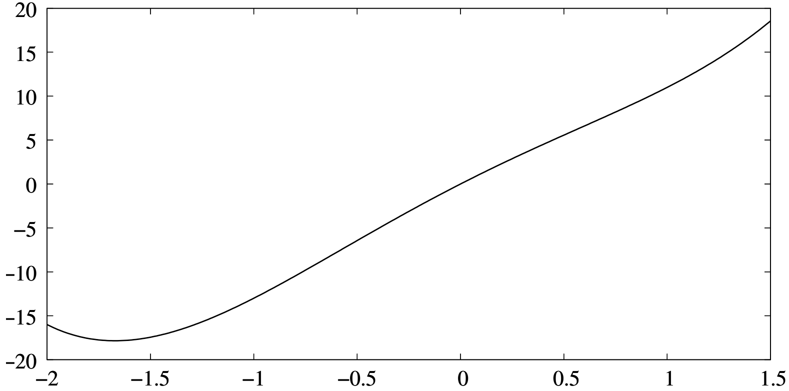
(Actually Newton's method finding x s.t. $\nabla f(x) = 0$)

$$\begin{aligned} \Delta x_i &= -\left(\nabla\nabla f(x_i)\right)^{-1} \nabla f(x_i) \\ x_{i+1} &= x_i + \Delta x_i \end{aligned}$$

1. if $\nabla\nabla f(x_i)$ posdef, $\left(\nabla f(x_i)\right)^t (x_{i+1} - x_i) < 0$ so Δx_i is a direction of decrease (could overshoot)
2. if $\nabla\nabla f(x_i)$ not posdef, Δx_i might be in an *increasing direction*.
3. if f is convex, $f(x_{i+1}) \leq f(x_i)$, so problems go away.

1D example of trouble

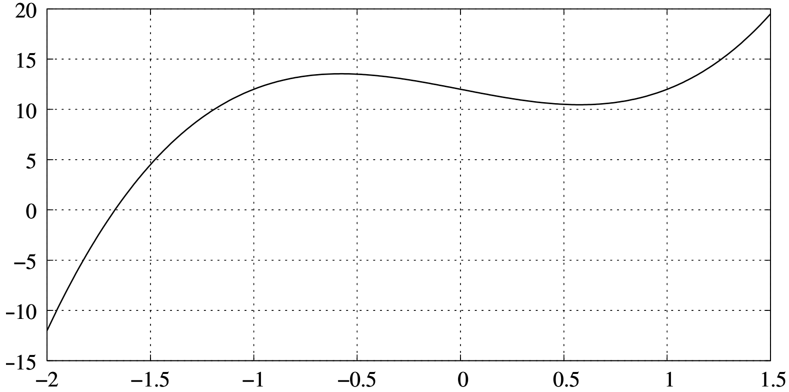
1D example of trouble: $f(x) = x^4 - 2x^2 + 12x$



- Has one local minimum
- Is not convex (note the concavity near x=0)

1D example of trouble

derivative of trouble: $f'(x) = 4x^3 - 4x + 12$



the negative f'' region around $x = 0$ repells the iterates:
$0 \to 3 \to 1.96154 \to 1.14718 \to 0.00658 \to 3.00039 \to 1.96182 \to 1.14743 \to 0.00726 \to 3.00047 \to 1.96188 \to 1.14749 \to \cdots$

Non-linear Newton

Try to enforce $f(x_{i+1}) \leq f(x_i)$

$$\begin{aligned} \Delta x_i &= -\left(\nabla\nabla f(x_i)\right)^{-1} \nabla f(x_i) \\ x_{i+1} &= x_i + \alpha_i \Delta x_i \end{aligned}$$

pick $\alpha_i > 0$ such that $f(x_i + \alpha_i \Delta x_i) \leq f(x_i)$. If Δx_i is a direction of decrease, some α_i exists.

- **1D-minimization** do 1D optimization problem,

$$\min_{\alpha_i \in (0,\beta]} f(x_i + \alpha_i \Delta x_i)$$

- **Armijo-search** use this rule: $\alpha_i = \rho\mu^n$ some n

$$f(x_i + s\Delta x_i) - f(x_i) \leq \nu s \left(\Delta x_i\right)^t \nabla f(x_i)$$

with ρ, μ, ν fixed (e.g. $\rho = 2, \mu = \nu = \frac{1}{2}$).

1D optimization: Let $f : \mathbb{R} \to \mathbb{R}$, continuous.

$$\begin{array}{ll} \text{find} & x_* \text{ s.t. } f(x_* - \epsilon) \geq f(x_*) \leq f(x_* + \epsilon) \\ \text{or} & \\ \text{find} & x_* \text{ s.t. } f'(x_* - \epsilon) = 0 \quad \text{(requires differentiability)} \end{array}$$

We can do this without differentiability — important case exposes many issues.

Line searching

1D-minimization looks like less of a hack than Armijo. For Newton, asymptotic convergence is not strongly affected, and function evaluations can be expensive.

- far from x_* their only value is ensuring decrease
- near x_* the methods will return $\alpha_i \sim 1$.

Asymptotic convergence, $e_i = x_i - x_*$

$$\begin{aligned}
\nabla f(x_i) &= \nabla\nabla f(x_*) e_i + O(||e_i||^2) \\
\nabla\nabla f(x_i) &= \nabla\nabla f(x_*) + O(||e_i||) \\
e_{i+1} &= e_i - (\nabla\nabla f_i)^{-1} \nabla f_i = O(||e_i||^2)
\end{aligned}$$

“squares the error” at every step (exactly eliminates the linear error).

Practicality

Direct (non-iterative, non-structured) solves are expensive!
$\nabla\nabla f$ information is often expensive!

Iterative methods

gradient descent:

1. Search direction: $r_i = -\nabla f(x_i)$
2. Search step: $x_{i+1} = x_i + \alpha_i r_i$
3. Pick alpha: (depends on what's cheap)
    1. linearized $\alpha_i = \frac{r_i^t (\nabla\nabla f) r_i}{r_i^t r_i}$
    2. 1D minimization $f(x_i + \alpha r_i)$ (danger: low quality)
    3. zero-finding $r_i^t \nabla f(x_i + \alpha r_i) = 0$

Iterative methods

conjugate gradient descent:

1. Search direction: $d_i = -r_i + \beta_i d_{i-1}$, with $r_i = -\nabla f(x_i)$.
2. Pick β_i without $\nabla\nabla f$
    1. $\beta_i = \frac{(r_i - r_{i-1})^t r_{i-1}}{(r_i - r_{i-1})^t r_i}$ (Polak-Ribiere)
    2. can also use $\beta_i = \frac{r_i^t r_i}{r_{i-1}^t r_{i-1}}$ (Fletcher-Reeves)
3. Search step: $x_{i+1} = x_i + \alpha_i d_i$
    1. linearized $\alpha_i = \frac{d_i^t (\nabla\nabla f) d_i}{r_i^t d_i}$
    2. 1D minimization $f(x_i + \alpha d_i)$ (danger: low quality)
    3. zero-finding $d_i^t \nabla f(x_i + \alpha d_i) = 0$

Don't forget the truth about iterative methods

To get good convergence you must precondition!

$$B \sim (\nabla\nabla f(x_*))^{-1}$$

For $B = PP^t$

1. Search direction: $d_i = -r_i + \beta_i d_{i-1}$, with $r_i = -P^t \nabla f(x_i)$.
2. Pick $\beta_i = \frac{(r_i - r_{i-1})^t r_{i-1}}{(r_i - r_{i-1})^t r_i}$ (Polak-Ribiere)
3. Search step: $x_{i+1} = x_i + \alpha_i d_i$
4. zero-finding $d_i^t \nabla f(x_i + \alpha d_i) = 0$

change of metric

1. Search direction: $d_i = -r_i + \beta_i d_{i-1}$, with $r_i = -\nabla f(x_i)$.
2. Pick $\beta_i = \frac{(r_i - r_{i-1})^t B r_{i-1}}{(r_i - r_{i-1})^t r_i}$
3. Search step: $x_{i+1} = x_i + \alpha_i d_i$
4. zero-finding $d_i^t B \nabla f(x_i + \alpha d_i) = 0$

What else?

Theorem (sub-optimality of CG)

(Assuming $x_0 = 0$) at the end of step k, the solution x_k is the optimal linear combination of $b, Ab, A^2b, \dots A^kb$ for minimizing

$$\frac{1}{2}x^tAx - b^tx.$$

In other words, CG *learns* about A from the outputs of $b - Ax_i$. In principle

1. computer arithmetic errors ruin this nice property quickly
2. non-linearity ruins this property quickly

Quasi-Newton

What if we learned $(\nabla\nabla f(x_*))^{-1}$ from the data

$$\nabla f(x_i) - \nabla f(x_{k-1}) \sim (\nabla\nabla f(x_*))(x_i - x_{k-1})$$

over some fix-finite history.
Data: $y_i = \nabla f(x_i) - \nabla f(x_{k-1})$, $s_i = x_i - x_{k-1}$ with $1 \leq i \leq k$
Problem: Find symmetric positive def H_k s.t.

$$H_k y_i = s_i$$

Multiple solutions, but BFGS works best in most situations.

BFGS update

$$H_k = \left(I - \frac{s_k y_k^t}{y_k^t s_k}\right) H_{k-1} \left(I - \frac{y_k s_k^t}{y_k^t s_k}\right) + \frac{s_k s_k^t}{y_k^t s_k}$$

Lemma

The BFGS update minimizes $\min_H ||H^{-1} - H_{k-1}^{-1}||_F^2$ *such that* $Hy_k = s_k$.

Forming H_k not necessary, e.g. $H_k v$ can be recursively computed.

Quasi-Newton

Typically keep about 5 data points in the history.

initialize Set $H_0 = I$, $r_0 = -\nabla f(x_0)$, $d_0 = r_0$ goto 3

1. Compute $r_k = -\nabla f(x_k)$, $y_k = r_{k-1} - r_k$
2. Compute $d_k = H_k r_k$
3. Search step: $x_{k+1} = x_k + \alpha_k d_k$ (line-search)

Can also precondition this, though in practice, it is less critical than in CG or GD.

Armijo line searching has good theoretical properties. Typically used.

Quasi-Newton ideas generalize to many situations (e.g. fixed-point iterations)

Summary

- All multi-variate optimizations relate to posdef linear solves
- Simple iterative methods **require** pre-conditioning to be effective in high dimensions.
- Line searching strategies are highly variable
- Timing and storage of $f, \nabla f, \nabla\nabla f$ are all critical in selecting your method.

f	∇f	concerns	method
fast	fast	2	quasi-N (zero-search)
fast	fast	5	CG (zero-search)
fast	slow	1,2,3	derivative-free methods
fast	slow	2	quasi-N (min-search)
fast	slow	3,4	CG (min-search)
fast/slow	slow	2,4	quasi-N with Armijo
fast/slow	slow	4,5	CG (linearized α)

1=time	2=space	3=accuracy
4=robust vs. nonlinearity	5=precondition	

Don't take this table too seriously...