Numerical Optimization

Unit 3: Methods That Guarantee Convergence

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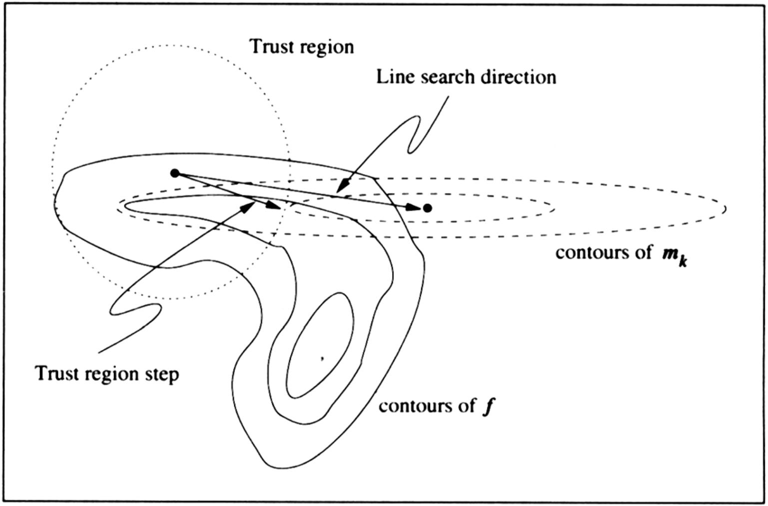
Line search and trust region

We will talk about two types of algorithms that guarantee convergence: Line search and trust region.



Where are we?

Three problems of Newton's method:

1. Hessian matrix H may not be positive definite.
2. Hessian matrix H is expensive to compute.
3. The system $\vec{p} = -H^{-1}\vec{g}$ is expensive to compute.

We will discuss methods to solve the first problem.

1. The consequence of the first problem is that Newton's direction is not a descent direction.
2. We need to find directions that are similar to the Newton's direction but also descent.
3. Do descent directions guarantee convergence? The answer is NO.
4. Line search algorithms: descent directions+good step sizes, which guarantee convergence.

Modified Newton's method

- When the Hessian H is not positive definite, what can we do?
  - Use another $\hat{H}$, similar to H, but positive definite.
  - How can this work?

$$
\begin{aligned}
\vec{p} &= -\hat{H}^{-1}\vec{g} \\
\vec{g}^{\,T}\vec{p} &= -\vec{g}^{\,T}\hat{H}\vec{g} < 0
\end{aligned}
$$

$\vec{p}$ is a descent direction.

Theorem (The convergence of the modified Newton)

If f is twice continuously differentiable in a domain D and $\nabla^2 f(\vec{x}^*)$ is positive definite. Assume $\vec{x}_0$ is sufficiently close to $\vec{x}^*$ and the modified $\hat{H}_k$ is well-conditioned. Then

$$\lim_{k\to\infty} \nabla f(\vec{x}_k) = 0.$$

Conditionness of a matrix

- For a matrix, what is "well-conditioned"?
  - A matrix A's condition number is $\kappa(A) = \|A\|\|A^{-1}\|$. If $\kappa(A)$ is small, we call A well-conditioned. If $\kappa(A)$ is large, we call A ill-conditioned.
- But what is the meaning of $\kappa(A)$?
  - The condition number $\kappa(A)$ measures the "sensitivity" of the matrix when solving $Ax = b$.

$$
\begin{aligned}
(A+E)\tilde{x} &= b = Ax \\
A\tilde{x} - Ax &= -E\tilde{x} \\
\tilde{x} - x &= -A^{-1}E\tilde{x} \\
\|\tilde{x} - x\| &= \|A^{-1}E\tilde{x}\| \leq \|A^{-1}\|\|E\|\|\tilde{x}\| \\
\frac{\|\tilde{x} - x\|}{\|\tilde{x}\|} &\leq \|A\|\|A^{-1}\|\frac{\|E\|}{\|A\|} = \kappa(A)\frac{\|E\|}{\|A\|}
\end{aligned}
$$

Requirements of good modifications

- Three requirements of a good modification:
  1. Matrix $\hat{H}$ is positive definite and well-conditioned, so the convergence theorem holds.
  2. Matrix $\hat{H}$ is similar to H, $\|\hat{H} - H\|$ small, so $\vec{p}$ is close to the Newton's direction, and the fast convergence can be hopefully preserved.
  3. The modification can be easily computed.
- We will see three algorithms, and each has its pros and cons.
  1. Eigenvalue modification.
  2. Shift modification.
  3. Modification with LDL decomposition.

First method: eigenvalue modification

Algorithm 1: Eigenvalue modification

1. Compute H's eigenvalue decomposition, $H = V \Lambda V^{-1}$, $\Lambda = \mathrm{diag}(\lambda_1, \lambda_2, ..., \lambda_n)$.
2. Make the modification for a given small $\epsilon > 0$,

$$\hat{\lambda}_i = \begin{cases} \lambda_i, & \text{if } \lambda_i > 0 \\ \epsilon, & \text{if } \lambda_i < 0 \end{cases}$$

3. $\hat{H} = V \hat{\Lambda} V^{-1}$, $\hat{\Lambda} = diag(\hat{\lambda}_1 \ \hat{\lambda}_2 \ ... \ \hat{\lambda}_n)$.

- It satisfies requirement 1 and 2 (why?), but eigenvalue decomposition is expensive to compute: $O(n^3)$ with big constant coefficient.

Second method: shift modification

Algorithm 2: Shift modification

1. Let $H_0 = H$.
2. For $k = 0, 1, 2, \ldots$
   1. If H_k can have Cholesky decomposition, then return $\hat{H} = H_k$.
   2. Otherwise, $H_{i+1} = H_i + \mu I$ for some small $\mu > 0$.

- Why does that work?

$$H + \mu I = V \Lambda V^{-1} + \mu I = V \Lambda V^{-1} + \mu V V^{-1} = V(\Lambda + \mu I)V^{-1}$$

$$\Lambda + \mu I = \begin{pmatrix} \lambda_1 + \mu & & & \\ & \lambda_2 + \mu & & \\ & & \ddots & \\ & & & \lambda_n + \mu \end{pmatrix}, \quad \mu > 0$$

- Matrix H_k is symmetric positive definite if and only if its Cholesky definition exists. (See note 2.)
- Which requirements this method satisfies?

Third method: using LDL^T decomposition

Algorithm 3: Modified LDL^T Decomposition

1. Compute $H = LDL^T$.
2. Update D to $\hat{D}$ so that all $\hat{d}_i$ are positive.
   (If $d_i < 0$, replace it by $\epsilon > 0$.)
3. $\hat{H} = L\hat{D}L^T$.

- The LDL decomposition of a symmetric matrix H is $H = LDL^T$, where L is lower triangular and D is diagonal.
- Additional advantage of LDL decomposition: we can use that to solve $\hat{H}\vec{p} = -\vec{g}$,
$$\vec{p} = -L^{-T}\hat{D}^{-1}L^{-1}\vec{g}.$$
- But it is not numerically stable (the updates can be very large).

Some properties of descent direction

Why are we so obsessed with the "descent direction"?

- Let $\phi_k(\alpha) = f(\vec{x}_k + \alpha\vec{p}_k)$.
- Since $\vec{p}_k$ is a decent direction, $\phi_k(\varepsilon) < \phi_k(0)$ for some small $\varepsilon > 0$.
- $\phi_k'(0) = \nabla f_k^T \vec{p}_k$. (Why?)
- $\phi_k'(\alpha) = \nabla f_k(\vec{x}_k + \alpha\vec{p}_k)^T \vec{p}_k$. (Why?)

Problems of descent directions

- The descent directions guarantee that $f(\vec{x}_{k+1}) < f(\vec{x}_k)$, which however do not guarantee to converge to the optimal solution.
- Here are two examples. [1]

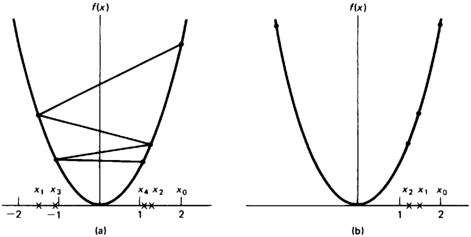


Figure 6.3.2 Monotonically decreasing sequences of iterates that don't converge to the minimizer

- $f(x) = x^2$, $x_0 = 2$, $p_k = (-1)^{k+1}$ and $\alpha_k = 2 - 3 \times 2^{-k-1}$, $\{x_k\} = \{2, -3/2, 5/4, -9/8 \dots\} = \{(-1)^k(1 + 2^{-k})\}$.
- $f(x) = x^2$, $x_0 = 2$, $p_k = -1$ and $\alpha_k = 2^{-k-1}$, $\{x_k\} = \{2, 3/2, 5/4, 9/8 \dots\} = \{1 + 2^{-k})\}$.

[1] Example and figures are from chapter 6 of *Numerical Methods for Unconstrained Optimization and Nonlinear Equations* by J. Dennis and R. Schnabel

First example

- What's the problem of the first example?
  - The *relative decrease* is $\frac{|\phi_k(\alpha_k)-\phi_k(0)|}{\alpha_k} \approx 2^{-k}$ which becomes too small before reaching the optimal solution.
  - The relative decrease is the absolute value of the slope of the line segment $(\vec{x}_k, f(\vec{x}_k)), (\vec{x}_{k+1}, f(\vec{x}_{k+1}))$.
  - How large should the relative decrease be? The slope of the tangent line at $\alpha = 0$ provides good information about f's trend. (What is $\phi'(0)$? What is the sign of $\phi'(0)$?)
  - The sufficient decrease condition:

Sufficient decrease condition

$$f(\vec{x}_k + \alpha\vec{p}_k) \leq f(\vec{x}_k) + c_1\alpha\vec{g}_k^{\,T}\vec{p}_k,$$

for some $c_1 \in (0, 1)$.

Second example

- What's the problem of the second example?
  - The *relative decrease* of the second problem is $\frac{|\phi_k(\alpha_k) - \phi_k(0)|}{\alpha_k} \approx 1$ is large enough, but *the step is too small*.
  - How large should the step size at least to be? Remember that α should be shrunken as f converges to the optimal solution. $\Rightarrow f'$ converges to 0.
  - So the step size should be proportional to the change of ϕ', which leads to the curvature condition:

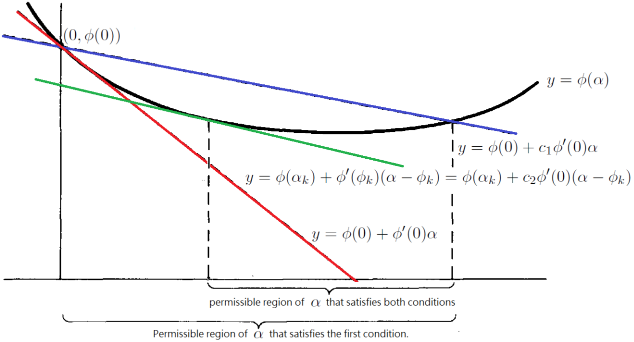
Curvature condition

$$\phi_k'(\alpha_k) = \nabla f(\vec{x}_k + \alpha_k \vec{p}_k)^T \vec{p}_k \geq c_2 \nabla f_k^T \vec{p}_k = c_2 \phi_k'(0)$$

for some $c_2 \in (c_1, 1)$.

Wolfe conditions

- Condition 1 and condition 2 together are called *the Wolfe conditions*.[2]



- Typical values: $c_1 = 0.1$ and $c_2 = 0.9$.
- Can both conditions be satisfied simultaneously for any smooth function?

[2] Figure is also from D&S's book.

Existence of feasible region for the Wolfe conditions

1. The function $\phi_k(\alpha)$ must be bounded below, which means it will go up eventually (why?). Therefore, the line $y = \phi_k(0) + c_1\phi'_k(0)\alpha$ must intersect with $y = \phi_k(\alpha)$, say at α_1.
2. Since $\vec{p}_k$ is a descent direction, $\phi'_k(0) < c_1\phi'_k(0) < 0$ for some $c_1 \in (0, 1)$.
3. By the mean value theorem, $\exists \alpha_2 \in [0, \alpha_1]$, such that

$$c_1\phi'_k(0) = \frac{\phi_k(\alpha_1) - \phi_k(0)}{\alpha_1 - 0} = \phi'_k(\alpha_2).$$

4. Since the curvature condition requires $c_2 > c_1$, between $[\alpha_2, \alpha_1]$, there must be some regions in which there exists α_3 such that $\phi'_k(\alpha_3) \geq c_2\phi'_k(0)$. (why?)

Convergence guarantee

- Do Wolfe conditions guarantee convergence?

Theorem

If $\vec{p}_k$ is a descent direction, α_k satisfies Wolfe conditions, f is bounded below and continuously differentiable, and ∇f is Lipschitz continuous, then

$$\sum_{k \geq 0} \cos^2 \theta_k \|\nabla f_k\|^2 < \infty$$

where $\cos \theta_k = \dfrac{-\nabla f_k^T \vec{p}_k}{\|\nabla f_k\| \|\vec{p}_k\|}$.

Definition (Lipschitz continuous)

A vector function $f : \mathbb{R}^n \to \mathbb{R}^m$ is Lipschitz continuous if $\|f(\vec{x}) - f(\vec{y})\| < L\|\vec{x} - \vec{y}\|$ for some constant $L > 0$.

Implications of the theorem

- The convergence theorem implies $\lim_{k\to\infty} \cos^2\theta_k \|\nabla f_k\|^2 = 0$. (why?)
- To show the convergence, we need to show that $|\cos\theta_k| > \delta > 0$ when $k \to \infty$.
- For the steepest descent method, this condition satisfies automatically since $\vec{p}_k$ is parallel to $\vec{g}_k$.
- How about the Newton's method or the modified Newton's method? For them, $\vec{p}_k = -H_k^{-1}\vec{g}_k$ or $\vec{p}_k = -\hat{H}_k^{-1}\vec{g}_k$.

$$\vec{g}_k{}^T \vec{p}_k = -\vec{g}_k{}^T H_k^{-1}\vec{g}_k.$$

One can show that if H_k is well-conditioned, $\kappa(H) < M$, then $|\cos\theta_k| > 1/M$.

Goldstein condition

- Problems of the Wolfe conditions are the need to evaluate

$$\phi'(\alpha_k) = \nabla f(\vec{x}_k + \alpha_k \vec{p}_k)^T \vec{p}_k.$$

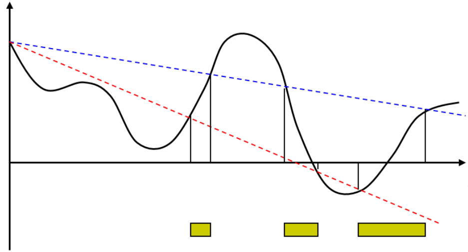
- Another frequently used conditions is the Goldstein condition:

Goldstein condition

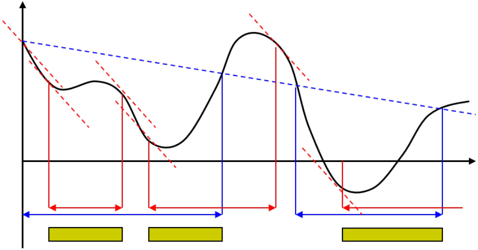
$$f(\vec{x}_k) + (1-c)\alpha_k \, \nabla f_k^T \, \vec{p}_k \leq f(\vec{x}_k + \alpha \vec{p}_k) \leq f(\vec{x}_k) + c\alpha_k \, \nabla f_k^T \, \vec{p}_k$$

for $c \in [0, 1/2]$.

Examples of Wolfe conditions and Goldstein condition



The Coldstein conditions



The Wolfe conditions

Line search method

Algorithm 4: Backtracking line search algorithm

1. Guess an initial α_0 (For Newton's method, usually $\alpha_0 = 1$.)
2. For $k = 1, 2, \ldots$ until α_k satisfies the required conditions.
   - Using interpolation methods to model function $\phi(\alpha)$ in the desired interval and then search the feasible solution of the model function.

What is the interpolation method?

- Initially, we know $\phi(0) = f(\vec{x}_k)$, $\phi'(0) = \nabla f(\vec{x}_k)^T \vec{p}_K$, and $\phi(1)$. We can use that build a quadratic polynomial $q_0(\alpha)$ such that $q_0(0) = \phi(0)$, $q_0'(0) = \phi'(0)$ and $q_0(1) = \phi(1)$.
- Use q_0 to find a solution α_1. Check if α_1 satisfies the required conditions.
- Now we know four things: $\phi(0) = f(\vec{x}_k)$, $\phi'(0) = \nabla f(\vec{x}_k)^T \vec{p}_K$, $\phi(1)$, and $\phi(\alpha_1)$. Use them to build a cubic polynomial $q_1(\alpha)$ such that $q_1(0) = \phi(0)$, $q_1'(0) = \phi'(0)$, $q_1(\alpha_1) = \phi(\alpha_1)$ and $q_1(1) = \phi(1)$.
- Use q_1 to find a solution α_2. Check if α_2 satisfies the required conditions.

Trust region method

- The line search method finds a descent direction $\vec{p}_k$ first, and then search a suitable step length α_k that satisfies some conditions.
- The idea of the trust region method is to build a model for the function, and then specifies a region in which this model works. It then solves constrained model problem.

Algorithm 5: The trust region framework

1. Guess an initial trust region Δ_0 and an initial $\vec{x}_0$.
2. For $k = 0, 1, 2, \ldots$ until convergence
    1. Build a model m_k of f at $\vec{x}_k$
    2. Solve the constrained minimization problem: $\min_{\vec{p}} m_k(\vec{p})$ s.t. $\|\vec{p}\| \leq \Delta_k$.
    3. Evaluate the trust region Δ_k. If not satisfied, update Δ_k and goto (2-2).
    4. Set $\vec{x}_{k+1} = \vec{x}_k + \vec{p}_k$ where $\vec{p}_k$ is the solution of the model problem.

Details of the trust region method

- How to build a model for a function $f(\vec{x})$?
  - Most are based on the Taylor expansions. For example, the quadratic model
$$m_k(\vec{p}) = f_k + \vec{g}_k^T \vec{p} + \frac{1}{2}\vec{p}^{\,T} H_k \vec{p}.$$
- How to evaluate and update the trust region Δ_k?
  - The trust region is evaluated by the given $\vec{p}_k \neq \vec{0}$. Let
$$\rho_k = \frac{f(\vec{x}_k) - f(\vec{x}_k + \vec{p}_k)}{m_k(\vec{0}) - m_k(\vec{p}_k)}.$$
  - If $\rho_k < 0$, reject the solution, and let $\Delta_k = \sigma_k \Delta_k$ for some $0 < \sigma_k < 1$.
  - If ρ_k is close to 1, increase $\Delta_k = \tau_k \Delta_k$ for some $\tau_k > 1$.
- The trust region method is also guaranteeing convergence.

Convergence of trust region framework

Theorem (The convergence of trust region framework)

Suppose $\|B_k\|$ *is bounded, and* f *is bounded below on the level set* $S = \{x | f(x) \leq f(x_0)\}$ *and Lipschitz continuously differentiable in the neighborhood of* S. *If*

$$m_k(\vec{0}) - m_k(\vec{p}_k) \geq c_1 \|\vec{g}_k\| \min\left(\Delta_k, \frac{\vec{g}_k}{\|B_k\|}\right)$$

and $\vec{p}_k \leq \gamma \Delta_k$ *for some* $c_1 \in (0, 1]$ *and* $\gamma \geq 1$. *Then*

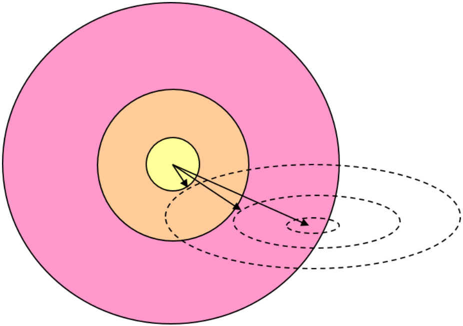
$$\lim_{k \to \infty} \inf \vec{g}_k = 0.$$

Solving the model problem m_k

$$\min_{\vec{p}} m_k(\vec{p}) = f_k + \vec{g}_k^{\,T} \vec{p} + \frac{1}{2}\vec{p}^{\,T} B_k \vec{p}.$$

$$\text{s.t.} \|\vec{p}\| \leq \Delta$$

- If $\|B_k^{-1}\vec{g}\|$ and B_k is positive definite, $\vec{p} = -B_k^{-1} g$.
- Otherwise, the direction varies for different Δ.



Optimal conditions

- $\vec{p}*$ is the optimal solution if and only if it satisfies

$$(B_k + \lambda I)\vec{p}* = -\vec{g}$$

$$\lambda(\Delta - \|\vec{p}*\|) = 0$$

  where $B_k + \lambda I$ is positive definite.
- $\lambda \geq 0$ is called the Largrangian modifier (chap 12).
- Assume $\|B^{-1}\vec{g}\| \geq \Delta$ for $\lambda \geq 0$. Define

$$\phi(\lambda) = \| - (B + \lambda I)^{-1}\vec{g}\| - \Delta$$

  and solve $\phi(\lambda) = 0$.
- This is a univariable nonlinear equation. (chap 11)

Example

$$min_{x,y} f(x,y) = x^4 + 2x^3 + 24x^2 + y^4 + 12y^2 \text{ s.t. } \Delta = \sqrt{x^2+y^2} \leq 1$$

At $(2,1)$, $f(2,1) = 141, \nabla f(2,1) = \begin{bmatrix} 152 \\ 28 \end{bmatrix}, \nabla^2 f(2,1) = \begin{bmatrix} 120 & 0 \\ 0 & 36 \end{bmatrix}$

The quadratic model at $(2,1)$ is

$$m(x,y) = 60(2-x)^2 + 18(1-y)^2 + 152(2-x) + 28(1-y) + 141$$

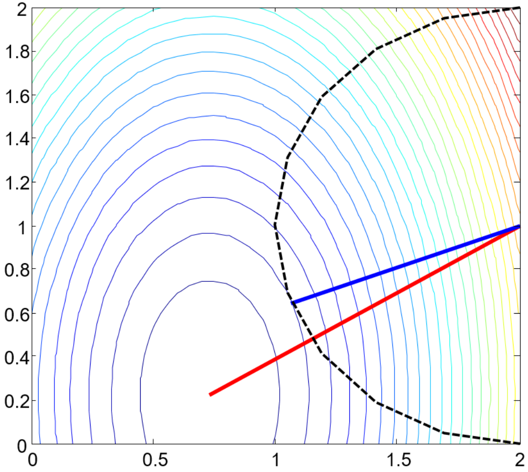
The Newton's direction is $\vec{p}^N = -(\nabla^2 f)^{-1} \nabla f = \begin{bmatrix} -1.22 \\ -0.77 \end{bmatrix}, \|\vec{p}^N\| > \Delta$

Find λ such that $(B_k + \lambda I)\vec{p} = -\vec{g}$ and $\lambda(\Delta - \|\vec{p}\|) = 0$.

$$B + \lambda I = \begin{bmatrix} 120+\lambda & 0 \\ 0 & 26+\lambda \end{bmatrix}, \vec{p} = -(B+\lambda I)^{-1}\vec{g} = \begin{bmatrix} -152/(120+\lambda) \\ -28/(26+\lambda) \end{bmatrix}$$

Let $\|\vec{p}\| = \Delta = 1$. We can solve $\lambda^* = 42.655$ and $\vec{p}* = \begin{bmatrix} -0.93 \\ -0.36 \end{bmatrix}$

Example: continue



Approximate solutions and scaling

- The problem $\phi(\lambda) = \| -(B + \lambda I)^{-1}\vec{g}\| - \Delta = 0$ is difficult to solve. Approximate methods are used instead
  - Cauchy point
  - The dogleg method
  - Two-dimensional subspace minimization
- Poor scaled problems are sensitive to certain directions. The solution is to make the trust region elliptical (scaling).

$$\min_{\vec{p}} m_k(\vec{p}) = f_k + \vec{g}_k^T \vec{p} + \frac{1}{2}\vec{p}^{\,T} B_k \vec{p}.$$

$$\text{s.t.} \|D\vec{p}\| \leq \Delta$$

where D is a diagonal matrix.

Cauchy point

- The steepest descent direction (gradient + line search)
- The solution is

$$\vec{p}_k = -\tau_k \Delta \frac{\vec{g}_k}{\|\vec{g}_k\|} \text{(Cauchy point)}$$

where

$$\tau_k = \begin{cases} 1 & \vec{g}_k^T B_k \vec{g}_k \leq 0 \\ \min(\|\vec{g}_k\|^3 / (\Delta \vec{g}_k^T B_k \vec{g}_k), 1) & \text{otherwise} \end{cases}$$

- Pros and Cons
  - Slow convergence
  - Easy to compute
  - Use as a reference direction

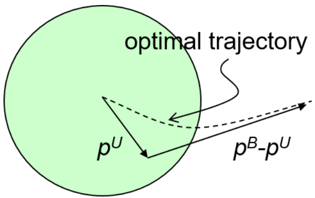
Dogleg method

- Use the combination of Cauchy point and Newton's direction to approximate the optimal trajectory. (Require B_k be positive definite.)
- Find τ such that $\|\vec{p}(\tau)\|^2 = \Delta^2$

$$\vec{p}(\tau) = \begin{cases} \tau \vec{p}^U & 0 \leq \tau \leq 1 \\ \vec{p}^U + (\tau - 1)(\vec{p}^B - \vec{p}^U) & \text{otherwise} \end{cases}$$

where

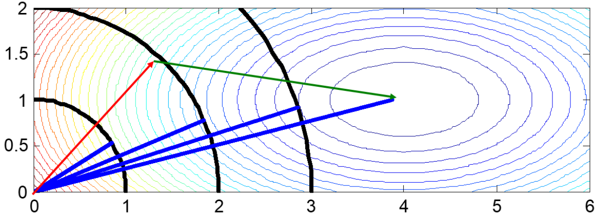
- $\vec{p}^U = -\frac{\vec{g}_k^T \vec{g}_k}{\vec{g}_k^T B_k \vec{g}_k} \vec{g}_k$ is Cauchy point.
- $\vec{p}^B = -B_k^{-1} \vec{g}_k$ is Newton's direction.
- If B_k is positive definite, $\|\vec{p}(\tau)\|$ is an increasing function and $m(\vec{p}(\tau))$ is a decreasing function.



Dogleg method: example

Consider $f(x) = \frac{1}{2}\vec{x}^T \begin{bmatrix} 1/4 & 0 \\ 0 & 1 \end{bmatrix} \vec{x} - \begin{bmatrix} 1 \\ 1 \end{bmatrix}^T \vec{x}$. Let $x_0 = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$.

$$\vec{p}^U = \begin{bmatrix} 1.6 \\ 1.6 \end{bmatrix}, \vec{p}^B = \begin{bmatrix} 4 \\ 1 \end{bmatrix}, \text{ and } \vec{p}^B - \vec{p}^U = \begin{bmatrix} 2.4 \\ -0.6 \end{bmatrix}$$



Δ	λ	$\min f(x)$	τ	$f(p(\tau))$
1	.9212	-1.1478	0.625	-1.1017
2	.2912	-1.8935	1.064	-1.7116
3	.0998	-2.3331	1.551	-2.3193

Two-dimensional subspace minimization

- Use the linear combination of $\vec{g}$ and $B^{-1}\vec{g}$.

$$\min_{\vec{p}} m_k(\vec{p}) = f_k + \vec{g}_k^T \vec{p} + \frac{1}{2}\vec{p}^{\,T} B_k \vec{p}.$$

$$\text{s.t.} \|\vec{p}\| \leq \Delta \text{ and } \vec{p} \in \mathrm{span}(\vec{g}, B^{-1}\vec{g})$$

- Matrix B_k can be indefinite. In that case,
  - Find α so that $B_k + \alpha I$ is positive definite
  - If $\|(B_k + \alpha I)^{-1}\vec{g}_k\| \leq \Delta$, let $\vec{p} = (B_k + \alpha I)^{-1}\vec{g}_k + \vec{v}$ where $\vec{v}$ satisfies $\vec{v}^T(B_k + \alpha I)^{-1}\vec{g}_k \leq 0$
  - Otherwise, let $\vec{p} \in \mathrm{span}(\vec{g}, (B + \alpha I)^{-1}\vec{g})$