# **Conjugate Directions**

- Powell's method is based on a model quadratic objective function and conjugate directions in  $\mathbb{R}^n$  with respect to the Hessian of the quadratic objective function.
- what does it mean for two vectors  $u, v \in \mathbb{R}^n$  to be conjugate?

**Definition:** given that  $u, v \in \mathbb{R}^n$ , then u and v are said to be *mutually orthogonal* if  $(u, v) = u^T v = 0$  (where (u, v) is our notation for the *scalar product*).  $\square$ 

**Definition:** given that  $u, v \in \mathbb{R}^n$ , then u and v are said to be *mutually conjugate* with respect to a symmetric positive definite matrix A if u and Av are mutually orthogonal, *i.e.*  $u^T Av = (u, Av) = 0$ .  $\square$ 

• Note that if two vectors are mutually conjugate with respect to the identity matrix, that is A = I, then they are mutually orthogonal.

## **Eigenvectors**

•  $x_i$  is an eigenvector of the matrix A, with corresponding eigenvalue  $\lambda_i$  if it satisfies the equation

$$A\mathbf{x}_i = \lambda_i \mathbf{x}_i \ i = 1, ..., n$$

and  $\lambda_i$  is a solution to the characteristic equation  $|A - \lambda_i I| = 0$ .

- If  $A \in \mathbb{R}^{n \times n}$  is a symmetric positive definite matrix, then there will exist n eigenvectors,  $x_1, ..., x_n$  which are mutually orthogonal (i.e.  $(x_i, x_j) = 0$  for  $i \neq j$ ).
- Now since:  $(x_i, Ax_j) = (x_i, \lambda x_j) = \lambda(x_i, x_j) = 0$  for  $i \neq j$ , this implies that the eigenvectors,  $x_i$ , are mutually conjugate with respect to the matrix A.

### We Can Expand Any Vector In Terms Of A Set Of Conjugate Vectors

**Theorem:** A set of *n* mutually conjugate vectors in  $\mathbb{R}^n$  span the  $\mathbb{R}^n$  space and therefore constitute a basis for  $\mathbb{R}^n$ .  $\square$ 

#### Proof:

let  $u_i$ , i = 1, ..., n be mutually conjugate with respect to a symmetric positive definite matrix  $A \in \mathbb{R}^{n \times n}$ . Consider a linear combination which is equal to zero:

$$\sum_{i=1}^{n} \alpha_i \mathbf{u}_i = 0$$

we pre-multiply by the matrix A

$$A \sum_{i=1}^{n} \alpha_{i} \mathbf{u}_{i} = \sum_{i=1}^{n} \alpha_{i} A \mathbf{u}_{i} = 0$$

and take the inner product with  $\boldsymbol{u}_k$ 

$$\begin{pmatrix} \mathbf{u}_k, \sum_{i=1}^n \alpha_i A \mathbf{u}_i \end{pmatrix} = \sum_{i=1}^n \alpha_i (\mathbf{u}_k, A \mathbf{u}_i) = \alpha_k (\mathbf{u}_k, A \mathbf{u}_k) = 0$$

Now, since A is positive definite, we have

$$(\boldsymbol{u}_k, A\boldsymbol{u}_k) > 0, \ \forall \boldsymbol{u}_k, \boldsymbol{u}_k \neq \mathbf{0}$$

Therefore, it must be that  $\alpha_k = 0$ ,  $\forall k$ , which implies that  $u_i$ , i = 1, ..., n are linearly independent and since there are n of them, they form a basis for the  $\mathbb{R}^n$  space.

What does it mean for a set of vectors to be linearly independent?
 Can you prove that a set of n linearly independent vectors in R<sup>n</sup> form a basis for the R<sup>n</sup> space?

### **Expansion of an Arbitrary Vector**

Now consider an arbitrary vector  $x \in \mathbb{R}^n$ . We can expand x in our mutually conjugate basis as follows:

$$x = \sum_{i=1}^{n} \alpha_i \mathbf{u}_i$$

where the scalar values  $\alpha_i$  are to be determined. We next take the inner product of  $u_k$  with Ax:

$$(\boldsymbol{u}_{k}, A\boldsymbol{x}) = \begin{pmatrix} \boldsymbol{u}_{k}, A \sum_{i=1}^{n} \alpha_{i} \boldsymbol{u}_{i} \end{pmatrix} = \begin{pmatrix} \boldsymbol{u}_{k}, \sum_{i=1}^{n} \alpha_{i} A \boldsymbol{u}_{i} \end{pmatrix}$$
$$= \sum_{i=1}^{n} \alpha_{i} (\boldsymbol{u}_{k}, A \boldsymbol{u}_{i}) = \alpha_{k} (\boldsymbol{u}_{k}, A \boldsymbol{u}_{k})$$
$$= \sum_{i=1}^{n} \alpha_{i} (\boldsymbol{u}_{k}, A \boldsymbol{u}_{i}) = \alpha_{k} (\boldsymbol{u}_{k}, A \boldsymbol{u}_{k})$$

from which we can solve for the scalar coefficients as

$$\alpha_k = \frac{(\boldsymbol{u}_k, A\boldsymbol{x})}{(\boldsymbol{u}_k, A\boldsymbol{u}_k)}$$

and we have that an arbitrary vector  $\mathbf{x} \in \mathbb{R}^n$  can be expanded in terms of n mutually conjugate vectors  $\mathbf{u}_i$ , i = 1, ..., n as

$$x = \sum_{i=1}^{n} \frac{(u_k, Ax)}{(u_k, Au_k)} u_i$$

**Definition:** If a minimization method always locates the minimum of a general quadratic function in no more than a predetermined number of steps directly related to number of variables n, then the method is called *quadratically convergent*.  $\square$ 

**Theorem:** If a quadratic function  $Q(x) = \frac{1}{2}x^T Ax + b^T x + c$  is minimized sequentially once along each direction of a set of n linearly independent, A-conjugate directions, then the global minimum of Q will be located at or before the n<sup>th</sup> step regardless of the starting point.  $\square$ 

Proof: We know that

$$\nabla Q(x^*) = b + Ax^* = 0 \tag{1}$$

and given  $u_i$ , i = 1, ..., n to be A-conjugate vectors or, in this case, directions of minimization, we know from previous theorem that they are linearly independent. Let  $x^1$  be the starting point of our search, then expanding the minimum  $x^*$  as

$$\boldsymbol{x}^* = \boldsymbol{x}^1 + \sum_{i=1}^n \alpha_i \boldsymbol{u}_i$$
 (2)

$$\mathbf{b} + A\mathbf{x}^* = \mathbf{b} + A \left( \mathbf{x}^1 + \sum_{i=1}^n \alpha_i \mathbf{u}_i \right)$$

$$= \mathbf{b} + A\mathbf{x}^1 + A \sum_{i=1}^n \alpha_i \mathbf{u}_i = \mathbf{b} + A\mathbf{x}^1 + \sum_{i=1}^n \alpha_i A\mathbf{u}_i = \mathbf{0}$$

taking the inner product with  $\mathbf{u}_j$  (using the notation  $\mathbf{v}^T \mathbf{u} = (\mathbf{v}, \mathbf{u})$ ) we have

$$\mathbf{u}_{j}^{T}(\mathbf{b} + A\mathbf{x}^{1}) + \mathbf{u}_{j}^{T} \sum_{i=1}^{n} \alpha_{i} A \mathbf{u}_{i} = \mathbf{u}_{j}^{T}(\mathbf{b} + A\mathbf{x}^{1}) + \sum_{i=1}^{n} \alpha_{i} \mathbf{u}_{j}^{T} A \mathbf{u}_{i} = 0$$

which, since the  $\boldsymbol{u}_i$  vectors are mutually conjugate with respect to the matrix  $\boldsymbol{A}$  , we have

$$\boldsymbol{u}_{j}^{T}(\boldsymbol{b} + A\boldsymbol{x}^{1}) + \alpha_{j}\boldsymbol{u}_{j}^{T}A\boldsymbol{u}_{j} = 0$$

which can be re-written as

$$(\boldsymbol{b} + A\boldsymbol{x}^1)^T \boldsymbol{u}_j + \alpha_j \boldsymbol{u}_j^T A \boldsymbol{u}_j = 0.$$

Solving for the coefficients we have

$$\alpha_j = -\frac{(\boldsymbol{b} + A\boldsymbol{x}^1)^T \boldsymbol{u}_j}{\boldsymbol{u}_j^T A \boldsymbol{u}_j}.$$
 (3)

Now in an iterative scheme where we determine successive approximations along the  $\boldsymbol{u}_i$  directions by minimization, we have

$$x^{i+1} = x^i + \lambda_i^* u_i, i = 1, ..., N$$
 (4)

where the  $\lambda_i^*$  are found by minimizing  $Q(x^i + \lambda_i u_i)$  with respect to the variable  $\lambda_i$ , and N is possibly greater than n.

Therefore, letting  $\mathbf{y}^i = \mathbf{x}^{i+1} = \mathbf{x}^i + \lambda_i \mathbf{u}_i$ , we set the derivative of  $Q(\mathbf{y}^i(\lambda_i)) = Q(\mathbf{x}^i + \lambda_i \mathbf{u}_i)$  with respect to  $\lambda_i$  equal to 0 using the chain rule of differentiation:

$$\frac{d}{d\lambda_i} Q(\mathbf{x}^{i+1}) \bigg|_{\lambda_i^*} = \sum_{j=1}^n \frac{\partial Q}{\partial y_i^j} \left( \frac{\partial y_i^j}{\partial \lambda_i} \right) = \mathbf{u}_i^T \nabla Q(\mathbf{x}^{i+1}) = 0$$

but  $\nabla Q(x^{i+1}) = b + Ax^{i+1}$  and therefore

$$\boldsymbol{u}_i^T(\boldsymbol{b} + A(\boldsymbol{x}^i + \lambda_i \boldsymbol{u}_i)) = 0$$

from which we get that the  $\lambda_i^*$  are given by

$$\lambda_i^* = -\frac{(\boldsymbol{b} + A\boldsymbol{x}^i)^T \boldsymbol{u}_i}{\boldsymbol{u}_i^T A \boldsymbol{u}_i} = -\frac{\boldsymbol{b}^T \boldsymbol{u}_i + \boldsymbol{x}^{iT} A \boldsymbol{u}_i}{\boldsymbol{u}_i^T A \boldsymbol{u}_i}.$$
 (5)

From (4), we can write

$$x^{i+1} = x^{i} + \lambda_{i}^{*} \boldsymbol{u}_{i} = x^{1} + \sum_{j=1}^{i} \lambda_{j}^{*} \boldsymbol{u}_{j}$$
$$x^{i} = x^{1} + \sum_{j=1}^{i-1} \lambda_{j}^{*} \boldsymbol{u}_{j}.$$

Forming the product  $\mathbf{x}^{iT} A \mathbf{u}_{i}$  in (5) we get

$$\mathbf{x}^{iT} A \mathbf{u}_{i} = (\mathbf{x}^{1})^{T} A \mathbf{u}_{i} + \sum_{j=1}^{i-1} \lambda_{j}^{*} \mathbf{u}_{j}^{T} A \mathbf{u}_{i} = (\mathbf{x}^{1})^{T} A \mathbf{u}_{i}$$

j = 1 because  $\mathbf{u}_{j}^{T} A \mathbf{u}_{i} = 0$  for  $j \neq i$ . Therefore, the  $\lambda_{i}^{*}$  can be written as

$$\lambda_i^* = -\frac{(\boldsymbol{b} + A\boldsymbol{x}^1)^T \boldsymbol{u}_i}{\boldsymbol{u}_i^T A \boldsymbol{u}_i}$$
 (6)

but comparing this (3) we see that  $\lambda_i^* = \alpha_i$  and therefore

$$\boldsymbol{x}^* = \boldsymbol{x}^1 + \sum_{j=1}^n \lambda_j^* \boldsymbol{u}_j \tag{7}$$

which says that starting at  $x^1$  we take n steps of "length"  $\lambda_j^*$ , given by (6), in the  $u_j$  directions and we get the minimum.

Therefore  $x^*$  is reached in n steps or less if some  $\lambda_j^* = 0$ .

**Example:** consider the quadratic function of two variables given as  $f(x) = 1 + x_1 - x_2 + x_1^2 + x_2^2$ . Use the previous theorem to find the minimum starting at the origin and minimizing successively along the two directions given by the unit vectors  $\mathbf{u}_1^T = \begin{bmatrix} 1 & 0 \end{bmatrix}$  and  $\mathbf{u}_2^T = \begin{bmatrix} 0 & 1 \end{bmatrix}$ . (First show that these vectors are mutually conjugate with respect to the Hessian matrix of the function.)

**Solution:** first write the function in matrix form as

$$f(\mathbf{x}) = 1 + \begin{bmatrix} 1 & -1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \frac{1}{2} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \begin{bmatrix} 2 & 0 \\ 0 & 4 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = c + \mathbf{b}^T \mathbf{x} + \frac{1}{2} \mathbf{x}^T A \mathbf{x}$$

where we can clearly see the Hessian matrix A. We can now check that the two directions given are mutually conjugate with respect to A as

$$\boldsymbol{u}_{1}^{T} A \boldsymbol{u}_{2} = \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} 2 & 0 \\ 0 & 4 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = 0, \ \boldsymbol{u}_{1}^{T} A \boldsymbol{u}_{1} = \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} 2 & 0 \\ 0 & 4 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = 2,$$
$$\boldsymbol{u}_{2}^{T} A \boldsymbol{u}_{2} = \begin{bmatrix} 0 & 1 \end{bmatrix} \begin{bmatrix} 2 & 0 \\ 0 & 4 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = 4.$$

Starting from  $x^1 = \begin{bmatrix} 0 & 0 \end{bmatrix}^T$  we find the two lengths,  $\lambda_1^*$  and  $\lambda_2^*$ , from (6) as

$$\lambda_1^* = -\frac{(\boldsymbol{b} + A\boldsymbol{x}^1)^T \boldsymbol{u}_1}{\boldsymbol{u}_1^T A \boldsymbol{u}_1} = -\frac{\begin{bmatrix} 1 & -1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix}}{2} = -\frac{1}{2}$$

$$\lambda_{2}^{*} = -\frac{(b + Ax^{1})^{T} u_{2}}{u_{2}^{T} A u_{2}} = -\frac{\begin{bmatrix} 1 & -1 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix}}{4} = -\frac{1}{4}$$

and therefore, from (7), the minimum is found as

$$x^* = x^1 + \sum_{j=1}^{2} \lambda_j^* u_j = \begin{bmatrix} 0 \\ 0 \end{bmatrix} - \frac{1}{2} \begin{bmatrix} 1 \\ 0 \end{bmatrix} - \frac{1}{4} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} -1/2 \\ -1/4 \end{bmatrix}.$$

This can be checked by applying the formula  $x^* = -A^{-1}b$ .

Note that the lengths  $\lambda_j^*$  calculated from (6) dependent only on the mutually conjugate directions themselves and the initial starting point, but not on the intermediate successive search points  $x^i$  with i > 1.

Thus, if we always start from the origin, then the minimum of a quadratic function can be written as

$$x^* = -\sum_{i=1}^n \frac{\boldsymbol{b}^T \boldsymbol{u}_i}{\boldsymbol{u}_i^T A \boldsymbol{u}_i} \boldsymbol{u}_i.$$
 (8)

Of course, we still need a method of finding n A-conjugate vectors in  $\subseteq$   $^n$  space.

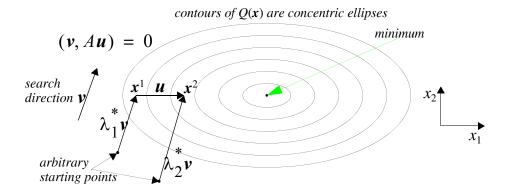
• The following theorem which we will not prove gives us a powerful technique for finding such minimization directions.

## **Theorem:** Parallel Subspace Property

Given a direction  $\mathbf{v}$  and a quadratic function  $Q(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T A\mathbf{x} + \mathbf{b}^T \mathbf{x} + c$ , then starting from two different points, but arbitrary, we can determine the minimum in the  $\mathbf{v}$  direction as  $\mathbf{x}^1$  and  $\mathbf{x}^2$ . The new direction  $\mathbf{u} = \mathbf{x}^2 - \mathbf{x}^1$  is A-conjugate to  $\mathbf{v}$ , i.e.  $(\mathbf{v}, A\mathbf{u}) = 0$ .  $\square$ 

# **Powell's Conjugate Direction Method**

- The idea behind Powell's method is to use the parallel subspace property to create a set of conjugate directions.
- It then uses line searches along these "conjugate" directions to find the local minimum.
- Before we describe Powell's method it is instructive to consider the parallel subspace property geometrically in two dimensions as shown in the figure.
- The concentric ellipses are the contour lines of a quadratic function Q(x) having a Hessian matrix A.
- Starting at the two arbitrary points shown we minimize along the v direction to arrive at points  $x^1$  and  $x^2$ .
- The direction  $u = x^2 x^1$  will be A-conjugate to v.
- If we were to perform a further minimization along u it is clear that we would arrive at the minimum.



Graphical depiction of the parallel subspace concept used in Powell's method.

## **Powell's Method in Words**

- In words, Powell's method to minimize a function f(x) in  $\mathbb{R}^n$  can be described as follows.
- First, initialize n search directions  $s_i$ , i = 1, ...n to the coordinate unit vectors  $e_i$ , i = 1, ...n.
- Then, starting at an initial guess,  $x^0$ , perform and initial search in the  $s_n$  direction which gets you to the point X.
- Store X in Y and then update X by performing n successive minimizations along the n search directions.
- Create a new search direction,  $s_{n+1} = X Y$  and minimize along this direction as well.
- After this last search we check for convergence by comparing the relative change in function value at the most recent *X* with respect to the function value at *Y*.
- If we have not converged, then we discard the first search direction  $s_1$  and let  $s_i = s_{i+1}$ , i = 1, ...n and repeat.

## Algorithm: Powell's Method

1. input: 
$$f(x)$$
,  $x^0$ ,  $\varepsilon$ , max\_iteration

2. set: 
$$s_i = e_i$$
,  $i = 1, ...n$ 

3. find 
$$\lambda^*$$
 which minimizes  $f(x^0 + \lambda^* s_n)$ 

4. set: 
$$X = x^0 + \lambda^* s_n$$
,  $C = \text{False}$ ,  $k = 0$ 

5. while 
$$C \equiv$$
 False repeat

6. set: 
$$Y = X$$
,  $k = k + 1$ 

7. for 
$$i = 1(1)n$$

8. find 
$$\lambda^*$$
 which minimizes  $f(X + \lambda^* s_i)$ 

9. 
$$\operatorname{set}: X = X + \lambda^* s_i$$

11. set: 
$$s_{i+1} = X - Y$$

12. find 
$$\lambda^*$$
 which minimizes  $f(X + \lambda^* s_{i+1})$ 

13. set: 
$$X = X + \lambda^* s_{i+1}$$

14. if 
$$k > \max_{\text{iteration OR}} |f(X) - f(Y)| / \max_{\text{iteration}} |f(X)| |f(X)| < \epsilon$$

15. 
$$C = \text{True}$$

17. for 
$$i = 1(1)n$$

18. set: 
$$s_i = s_{i+1}$$

### **Example: Powell's Conjugate Direction Method**

Consider the following function of two variables:

$$f(x) = 2x_1^3 + x_1x_2^3 - 10x_1x_2 + x_2^2$$

starting at  $\mathbf{x}^0 = \begin{bmatrix} 5 \ 2 \end{bmatrix}^T$ ,  $f(\mathbf{x}^0) = 314$  we perform one iteration of Powell's conjugate direction method.

#### **Solution:**

First we choose the n search directions as coordinate directions:

$$s_1 = e_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, s_2 = e_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

and perform three successive searches starting at  $Y = X = x^0 = \begin{bmatrix} 5 & 2 \end{bmatrix}^T$  along  $s_2$ ,  $s_1$ , and  $s_2$ :

1. 
$$\min_{\lambda} f(X + \lambda s_2) = f\left[\frac{5}{2}\right] + \lambda \begin{bmatrix}0\\1\end{bmatrix} = 250 + 5(2 + \lambda)^3 - 50(2 + \lambda) + (2 + \lambda)^2 = F(\lambda)$$

$$\frac{dF}{d\lambda}\Big|_{\lambda^*} = 15(2 + \lambda^*)^2 - 50 + (2 + \lambda^*) = 0, 15(\lambda^*)^2 + 61\lambda^* + 12 = 0$$

$$\Rightarrow \lambda^* = \frac{-61 \pm \sqrt{3001}}{30} = \begin{cases} -0.20728721 \\ -3.8593795 \end{cases}, \begin{cases} F(-0.20728721) = 192.38545 \\ F(-3.8593795) = 314.28418 \end{cases}$$

$$\Rightarrow \lambda^* = -3.8593795 \Rightarrow X = \begin{bmatrix} 5\\2 \end{bmatrix} + \lambda^* \begin{bmatrix} 0\\1 \end{bmatrix} = \begin{bmatrix} 5\\-1.86 \end{bmatrix}$$

2. 
$$\min_{\lambda} f(X + \lambda s_1) = f\left(\begin{bmatrix} 5 \\ -1.86 \end{bmatrix} + \lambda \begin{bmatrix} 1 \\ 0 \end{bmatrix}\right) = 2(5 + \lambda)^3 + 12.165377(5 + \lambda) + 3.457292$$

$$\frac{dF}{d\lambda}\Big|_{\lambda^*} = 6(5 + \lambda^*)^2 + 12.165377 = 0$$

$$\Rightarrow \lambda^* = \begin{cases} -3.5760748 \\ -6.4239252 \end{cases}, \begin{cases} F(-3.5760748) = 26.554075 \\ F(-6.4239252) = -19.639491 \end{cases}$$

$$\Rightarrow \lambda^* = -6.4239252 \Rightarrow X = \begin{bmatrix} 5 \\ -1.86 \end{bmatrix} + \lambda^* \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} -1.42 \\ -1.86 \end{bmatrix}$$
3.  $\min_{\lambda} f(X + \lambda s_2) = f\left(\begin{bmatrix} -1.42 \\ -1.86 \end{bmatrix} + \lambda \begin{bmatrix} 0 \\ 1 \end{bmatrix}\right)$ 

$$= -5.726576 - 1.42(-1.86 + \lambda)^3 + 14.2(-1.86 + \lambda) + (-1.86 + \lambda)^2$$

$$\frac{dF}{d\lambda}\Big|_{\lambda^*} = -4.26(-1.86 + \lambda^*)^2 + 14.2 + 2(-1.86 + \lambda^*) = 0$$

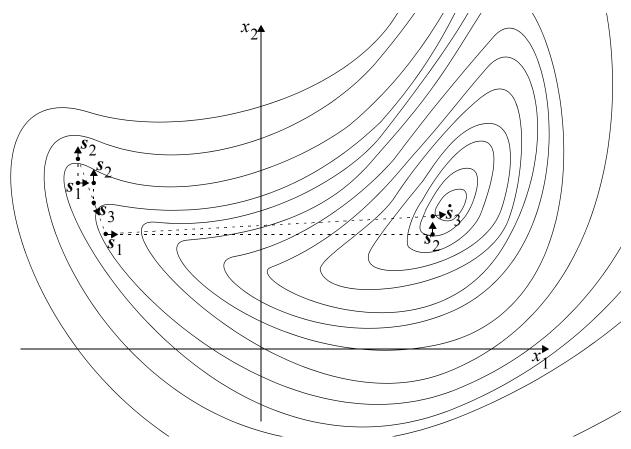
$$-4.26(\lambda^*)^2 + 17.8472\lambda^* - 4.257896 = 0$$

$$\Rightarrow \lambda^* = \frac{-17.8472 + 15.683367}{-8.52} = \begin{cases} 0.25397101 \\ 3.9355126 \end{cases},$$

$$\begin{cases} F(0.25397101) = -20.0 \\ F(3.9355126) = 15.357527 \end{cases}$$

$$\Rightarrow \lambda^* = 0.25397101 \Rightarrow X = \begin{bmatrix} -1.42 \\ -1.86 \end{bmatrix} + \lambda^* \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} -1.42 \\ -1.60 \end{bmatrix}$$

4. Now we set  $\mathbf{s}_3 = \mathbf{X} - \mathbf{Y} = \begin{bmatrix} -1.42 \\ -1.60 \end{bmatrix} - \begin{bmatrix} 5 \\ 2 \end{bmatrix} = \begin{bmatrix} -6.42 \\ -3.6 \end{bmatrix}$  and perform one more search in this direction before checking for convergence.



Geometrical view of Powell's method after 2 iterations in the main loop.