

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 $\mathbf{u}, \mathbf{v} \in \mathbb{R}^n$ to be conjugate ?

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

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

- \mathbf{x}_i is an eigenvector of the matrix A , with corresponding eigenvalue λ_i if it satisfies the equation

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

and λ_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, $\mathbf{x}_1, \dots, \mathbf{x}_n$ which are mutually orthogonal (i.e. $(\mathbf{x}_i, \mathbf{x}_j) = 0$ for $i \neq j$).
- Now since: $(\mathbf{x}_i, A\mathbf{x}_j) = (\mathbf{x}_i, \lambda_j \mathbf{x}_j) = \lambda_j (\mathbf{x}_i, \mathbf{x}_j) = 0$ for $i \neq j$, this implies that the eigenvectors, \mathbf{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 \mathbf{u}_i , $i = 1, \dots, n$ 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 \mathbf{u}_k

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

Now, since A is positive definite, we have

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

Therefore, it must be that $\alpha_k = 0$, $\forall k$, which implies that \mathbf{u}_i , $i = 1, \dots, n$ 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 \mathbb{R}^n form a basis for the \mathbb{R}^n 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:

$$x = \sum_{i=1}^n \alpha_i u_i$$

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

$$\begin{aligned} (u_k, Ax) &= \left(u_k, A \sum_{i=1}^n \alpha_i u_i \right) = \left(u_k, \sum_{i=1}^n \alpha_i A u_i \right) \\ &= \sum_{i=1}^n \alpha_i (u_k, A u_i) = \alpha_k (u_k, A u_k) \end{aligned}$$

from which we can solve for the scalar coefficients as

$$\alpha_k = \frac{(u_k, Ax)}{(u_k, A u_k)}$$

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

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

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 $Q(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T A\mathbf{x} + \mathbf{b}^T \mathbf{x} + c$ 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^{th} step regardless of the starting point. \square

Proof: We know that

$$\nabla Q(\mathbf{x}^*) = \mathbf{b} + A\mathbf{x}^* = \mathbf{0} \quad (1)$$

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

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

$$\begin{aligned} \mathbf{b} + A\mathbf{x}^* &= \mathbf{b} + A\left(\mathbf{x}^1 + \sum_{i=1}^n \alpha_i \mathbf{u}_i\right) \\ &= \mathbf{b} + A\mathbf{x}^1 + A \sum_{i=1}^n \alpha_i \mathbf{u}_i = \mathbf{b} + A\mathbf{x}^1 + \sum_{i=1}^n \alpha_i A\mathbf{u}_i = \mathbf{0} \end{aligned}$$

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

$$\mathbf{u}_j^T(\mathbf{b} + Ax^1) + \mathbf{u}_j^T \sum_{i=1}^n \alpha_i A \mathbf{u}_i = \mathbf{u}_j^T(\mathbf{b} + Ax^1) + \sum_{i=1}^n \alpha_i \mathbf{u}_j^T A \mathbf{u}_i = 0$$

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

$$\mathbf{u}_j^T(\mathbf{b} + Ax^1) + \alpha_j \mathbf{u}_j^T A \mathbf{u}_j = 0$$

which can be re-written as

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

Solving for the coefficients we have

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

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

$$\mathbf{x}^{i+1} = \mathbf{x}^i + \lambda_i^* \mathbf{u}_i, \quad i = 1, \dots, N \quad (4)$$

where the λ_i^* are found by minimizing $Q(\mathbf{x}^i + \lambda_i \mathbf{u}_i)$ with respect to the variable λ_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 λ_i equal to 0 using the chain rule of differentiation:

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

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

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

from which we get that the λ_i^* are given by

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

From (4), we can write

$$\begin{aligned} \mathbf{x}^{i+1} &= \mathbf{x}^i + \lambda_i^* \mathbf{u}_i = \mathbf{x}^1 + \sum_{j=1}^i \lambda_j^* \mathbf{u}_j \\ \mathbf{x}^i &= \mathbf{x}^1 + \sum_{j=1}^{i-1} \lambda_j^* \mathbf{u}_j. \end{aligned}$$

Forming the product $\mathbf{x}^{i+1} T A \mathbf{u}_i$ in (5) we get

$$\mathbf{x}^{i+1} T A \mathbf{u}_i = (\mathbf{x}^1)^T A \mathbf{u}_i + \sum_{j=1}^{i-1} \lambda_j^* \mathbf{u}_j^T A \mathbf{u}_i = (\mathbf{x}^1)^T A \mathbf{u}_i$$

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

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

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

$$\mathbf{x}^* = \mathbf{x}^1 + \sum_{j=1}^n \lambda_j^* \mathbf{u}_j \quad (7)$$

which says that starting at \mathbf{x}^1 we take n steps of “length” λ_j^* , given by (6), in the \mathbf{u}_j directions and we get the minimum.

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

Example: consider the quadratic function of two variables given as $f(\mathbf{x}) = 1 + x_1 - x_2 + x_1^2 + x_2^2$. Use the previous theorem to find the minimum starting at the origin and minimizing successively along the two directions given by the unit vectors $\mathbf{u}_1^T = [1 \ 0]$ and $\mathbf{u}_2^T = [0 \ 1]$. (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

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

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

$$\mathbf{u}_1^T A \mathbf{u}_2 = [1 \ 0] \begin{bmatrix} 2 & 0 \\ 0 & 4 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = 0, \quad \mathbf{u}_1^T A \mathbf{u}_1 = [1 \ 0] \begin{bmatrix} 2 & 0 \\ 0 & 4 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = 2,$$

$$\mathbf{u}_2^T A \mathbf{u}_2 = [0 \ 1] \begin{bmatrix} 2 & 0 \\ 0 & 4 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = 4.$$

Starting from $\mathbf{x}^1 = [0 \ 0]^T$ we find the two lengths, λ_1^* and λ_2^* , from (6) as

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

$$\lambda_2^* = -\frac{(\mathbf{b} + A\mathbf{x}^1)^T \mathbf{u}_2}{\mathbf{u}_2^T A \mathbf{u}_2} = -\frac{[1 \ -1] \begin{bmatrix} 0 \\ 1 \end{bmatrix}}{4} = -\frac{1}{4}$$

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

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

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

Note that the lengths λ_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 \mathbf{x}^i with $i > 1$.

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

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

Of course, we still need a method of finding n A -conjugate vectors in \mathbb{C}^n space.

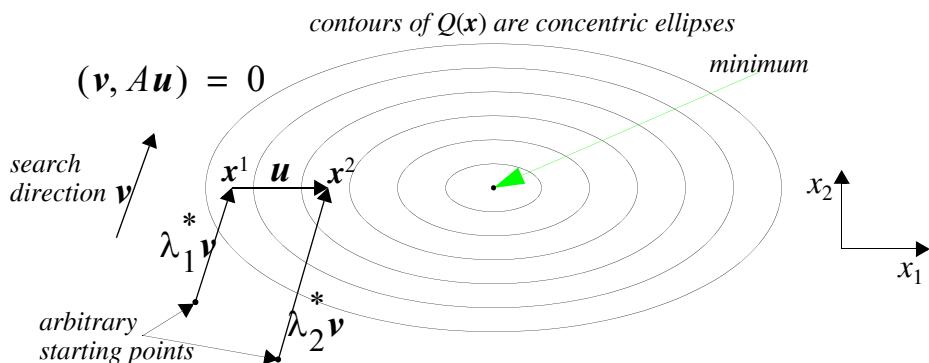
- The following theorem which we will not prove gives us a powerful technique for finding such minimization directions.

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. $(\mathbf{v}, A\mathbf{u}) = 0$. □

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 $Q(\mathbf{x})$ having a Hessian matrix A .
- Starting at the two arbitrary points shown we minimize along the \mathbf{v} direction to arrive at points \mathbf{x}^1 and \mathbf{x}^2 .
- The direction $\mathbf{u} = \mathbf{x}^2 - \mathbf{x}^1$ will be A -conjugate to \mathbf{v} .
- If we were to perform a further minimization along \mathbf{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 $f(\mathbf{x})$ in \mathbb{R}^n can be described as follows.
- First, initialize n search directions s_i , $i = 1, \dots, n$ to the coordinate unit vectors e_i , $i = 1, \dots, n$.
- Then, starting at an initial guess, \mathbf{x}^0 , perform an initial search in the s_n direction which gets you to the point \mathbf{X} .
- Store \mathbf{X} in \mathbf{Y} and then update \mathbf{X} by performing n successive minimizations along the n search directions.
- Create a new search direction, $s_{n+1} = \mathbf{X} - \mathbf{Y}$ 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 \mathbf{X} with respect to the function value at \mathbf{Y} .
- If we have not converged, then we discard the first search direction s_1 and let $s_i = s_{i+1}$, $i = 1, \dots, n$ and repeat.

Algorithm: Powell's Method

1. input: $f(\mathbf{x})$, \mathbf{x}^0 , ε , max_iteration
2. set: $\mathbf{s}_i = \mathbf{e}_i$, $i = 1, \dots, n$
3. find λ^* which minimizes $f(\mathbf{x}^0 + \lambda^* \mathbf{s}_n)$
4. set: $\mathbf{X} = \mathbf{x}^0 + \lambda^* \mathbf{s}_n$, $C = \text{False}$, $k = 0$
5. while $C \equiv \text{False}$ repeat
6. set: $\mathbf{Y} = \mathbf{X}$, $k = k + 1$
7. for $i = 1(1)n$
8. find λ^* which minimizes $f(\mathbf{X} + \lambda^* \mathbf{s}_i)$
9. set: $\mathbf{X} = \mathbf{X} + \lambda^* \mathbf{s}_i$
10. end
11. set: $\mathbf{s}_{i+1} = \mathbf{X} - \mathbf{Y}$
12. find λ^* which minimizes $f(\mathbf{X} + \lambda^* \mathbf{s}_{i+1})$
13. set: $\mathbf{X} = \mathbf{X} + \lambda^* \mathbf{s}_{i+1}$
14. if $k > \text{max_iteration}$ OR $|f(\mathbf{X}) - f(\mathbf{Y})| / \max [|f(\mathbf{X})|, 10^{-10}] < \varepsilon$
15. $C = \text{True}$
16. else
17. for $i = 1(1)n$
18. set: $\mathbf{s}_i = \mathbf{s}_{i+1}$
19. end
20. end
21. end

Example: Powell's Conjugate Direction Method

Consider the following function of two variables:

$$f(\mathbf{x}) = 2x_1^3 + x_1x_2^3 - 10x_1x_2 + x_2^2$$

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:

$$\mathbf{s}_1 = \mathbf{e}_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \mathbf{s}_2 = \mathbf{e}_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

and perform three successive searches starting at $\mathbf{Y} = \mathbf{X} = \mathbf{x}^0 = \begin{bmatrix} 5 & 2 \end{bmatrix}^T$ along \mathbf{s}_2 , \mathbf{s}_1 , and \mathbf{s}_2 :

$$1. \min_{\lambda} f(\mathbf{X} + \lambda \mathbf{s}_2) = f\left(\begin{bmatrix} 5 \\ 2 \end{bmatrix} + \lambda \begin{bmatrix} 0 \\ 1 \end{bmatrix}\right) = 250 + 5(2 + \lambda)^3 - 50(2 + \lambda) + (2 + \lambda)^2 = F(\lambda)$$

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

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

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

$$2. \min_{\lambda} f(\mathbf{X} + \lambda \mathbf{s}_1) = f\left(\begin{bmatrix} 5 \\ -1.86 \end{bmatrix} + \lambda \begin{bmatrix} 1 \\ 0 \end{bmatrix}\right) = 2(5 + \lambda)^3 + 12.165377(5 + \lambda) + 3.457292$$

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

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

$$\Rightarrow \lambda^* = -6.4239252 \Rightarrow \mathbf{X} = \begin{bmatrix} 5 \\ -1.86 \end{bmatrix} + \lambda^* \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} -1.42 \\ -1.86 \end{bmatrix}$$

$$3. \min_{\lambda} f(\mathbf{X} + \lambda \mathbf{s}_2) = f\left(\begin{bmatrix} -1.42 \\ -1.86 \end{bmatrix} + \lambda \begin{bmatrix} 0 \\ 1 \end{bmatrix}\right)$$

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

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

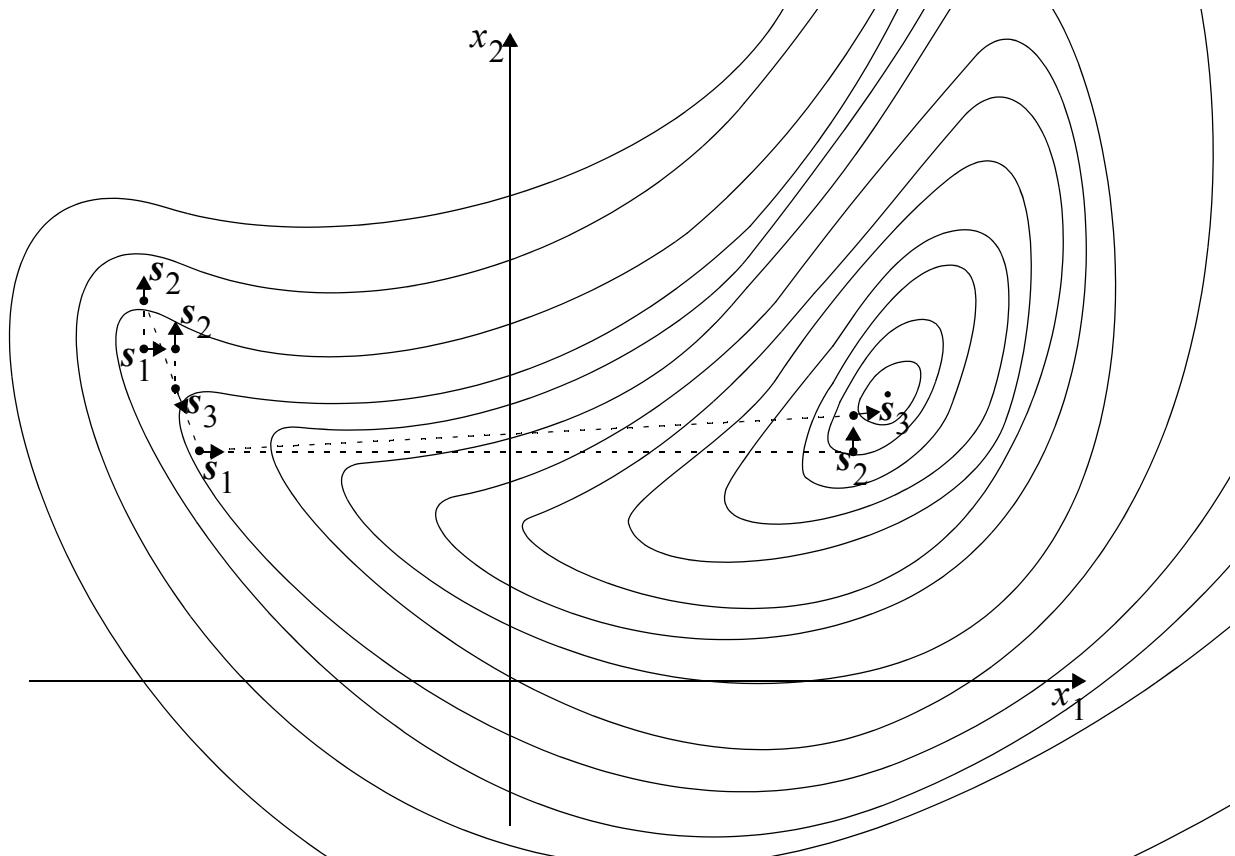
$$-4.26(\lambda^*)^2 + 17.8472\lambda^* - 4.257896 = 0$$

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

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

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

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.

