Solving Least Squares Problens iteratively

Let $\mathbf{A}$ denote a $m \times n$ matrix. The equation

$$\mathbf{A} \cdot \mathbf{x} = \mathbf{b}$$

shall be solved. In general the solution is not unique. But the problem can be stated as a least squares problem where the solution vector $\mathbf{x}$ can be found by minimizing the quadratic norm.

At this point the following assumption shall be made.

1. matrix $\mathbf{A}$ is real valued
2. vectors $\mathbf{x}$ and $\mathbf{b}$ are real valued

Thus the goal is to minimize a scalar function $f(\mathbf{x})$ defined by this equation:

$$f(\mathbf{x}) = (\mathbf{A} \cdot \mathbf{x} - \mathbf{b})^T \cdot (\mathbf{A} \cdot \mathbf{x} - \mathbf{b})$$
$$f(\mathbf{x}) = \left(\mathbf{x}^T \cdot \mathbf{A}^T - \mathbf{b}^T\right) \cdot (\mathbf{A} \cdot \mathbf{x} - \mathbf{b})$$
$$f(\mathbf{x}) = \mathbf{x}^T \cdot \mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{x} - 2 \cdot \mathbf{b}^T \cdot \mathbf{A} \cdot \mathbf{x} + \mathbf{b}^T \cdot \mathbf{b}$$

Defining a new function $g(\mathbf{x}) = \frac{1}{2} \cdot f(\mathbf{x})$ gives us the standard notation of quadratic forms:

$$g(\mathbf{x}) = \frac{1}{2} \cdot \mathbf{x}^T \cdot \underbrace{\mathbf{A}^T \cdot \mathbf{A}}_{\mathbf{U}} \cdot \mathbf{x} - \underbrace{\mathbf{b}^T \cdot \mathbf{A}}_{\mathbf{q}^T} \cdot \mathbf{x} + \underbrace{\frac{1}{2} \cdot \mathbf{b}^T \cdot \mathbf{b}}_{c}$$

Regardless of the shape of matrix $\mathbf{A}$ the matrix $\mathbf{U}$ is square, symmetric and positive definite.

The gradient $f(\mathbf{x})$ is computed like this:

$$f'(\mathbf{x}) = \mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{x} + \mathbf{A} \cdot \mathbf{A}^T \cdot \mathbf{x} - 2 \cdot \mathbf{A}^T \cdot \mathbf{b}$$
$$f'(\mathbf{x}) = 2 \cdot \left(\mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{x} - \mathbf{A}^T \cdot \mathbf{b}\right)$$

Setting the gradient to 0 results in the *normal* equation for the unknowns vector $\mathbf{x}$:

$$\mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{x} = \mathbf{A}^T \cdot \mathbf{b}$$

literature

In her highly readable bachelor thesis

`Conjugate Gradients and Conjugate Residuals type methods for solving Least Squares problems from Tomography` (Delft University of Technology)

Tamara Kloek discusses various approaches how to solve the normal equation iteratively.

Having computed the gradient $f'(\mathbf{x})$ of the normal equation the direction of *steepest descents* points in the opposite direction $-f'(\mathbf{x})$.

$$-f'(\mathbf{x}) = -2 \cdot \mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{x} + 2 \cdot \mathbf{A}^T \cdot \mathbf{b}$$

Let denote $\mathbf{x}_{(i)}$ an approximation to the solution vector $\mathbf{x}$ for the i'th iteration. The direction of steepes descents at that point is then:

$$-f'(\mathbf{x}_{(i)}) = -2 \cdot \mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{x}_{(i)} + 2 \cdot \mathbf{A}^T \cdot \mathbf{b}$$

definitions

Some frequenctly used quantities are defined here.

The residual $\mathbf{r}_{(i)}$ is defined as

$$\mathbf{r}_{(i)} = \mathbf{b} - \mathbf{A} \cdot \mathbf{x}_{(i)}$$

Similarly $\mathbf{s}_{(i)}$ is defined as

$$\mathbf{s}_{(i)} = \mathbf{A}^T \cdot \mathbf{b} - \mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{x}_{(i)}$$
$$\mathbf{s}_{(i)} = \mathbf{A}^T \cdot \left(\mathbf{b} - \mathbf{A} \cdot \mathbf{x}_{(i)}\right)$$
$$\mathbf{s}_{(i)} = \mathbf{A}^T \cdot \mathbf{r}_{(i)}$$

The vector $\mathbf{s}_{(i)}$ can be seen to be related to the direction of steepest descent by equation :

$$\mathbf{s}_{(i)} = -\frac{1}{2} \cdot f'(\mathbf{x}_{(i)})$$

Since the exact factor which relates $\mathbf{s}_{(i)}$ to $-f'(\mathbf{x}_{(i)})$ is not relevant, we consider $\mathbf{s}_{(i)}$ as the direction of steepest descent.

optimum stepsize / steepest descent

Going from vector $\mathbf{x}_{(i)}$ to vector $\mathbf{x}_{(i+1)}$ in the next iteration uses the direction of steepest descent like this:

$$\mathbf{x}_{(i+1)} = \mathbf{x}_{(i)} + \alpha_{(i)} \cdot \mathbf{s}_{(i)}$$

$\alpha_{(i)}$ denotes the step size which will be determined by minimizing the $f(\mathbf{x}_{(i+1)}$. Using the chain rule we seek

$$\frac{d}{d\alpha_{(i)}} f(\mathbf{x}_{(i+1)} = f'(\mathbf{x}_{(i+1)}^T \cdot \mathbf{s}_{(i)} = -2 \cdot \mathbf{s}_{(i+1)}^T \cdot \mathbf{s}_{(i)}$$

Setting $\mathbf{s}_{(i+1)}^T \cdot \mathbf{s}_{(i)}$ to 0 yields the optimum stepsize paramter:

$$
\begin{aligned}
\mathbf{s}_{(i+1)}^T \cdot \mathbf{s}_{(i)} &= 0 \\
\left(\mathbf{A}^T \cdot \mathbf{b} - \mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{x}_{(i+1)}\right)^T \cdot \mathbf{s}_{(i)} &= 0 \\
\left(\mathbf{A}^T \cdot \mathbf{b} - \mathbf{A}^T \cdot \mathbf{A} \cdot (\mathbf{x}_{(i)} + \alpha_{(i)} \cdot \mathbf{s}_{(i)})\right)^T \cdot \mathbf{s}_{(i)} &= 0 \\
\left(\mathbf{A}^T \cdot \mathbf{b} - \mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{x}_{(i)} - \alpha_{(i)} \cdot \mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{s}_{(i)})\right)^T \cdot \mathbf{s}_{(i)} &= 0 \\
\underbrace{\left(\mathbf{A}^T \cdot \mathbf{b} - \mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{x}_{(i)}\right)^T}_{\mathbf{s}_{(i)}^T} \cdot \mathbf{s}_{(i)} - \alpha_{(i)} \cdot \mathbf{s}_{(i)}^T \cdot \mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{s}_{(i)} &= 0
\end{aligned}
$$

$$\rightarrow$$

$$\alpha_{(i)} = \frac{\mathbf{s}_{(i)}^T \cdot \mathbf{s}_{(i)}}{\mathbf{s}_{(i)}^T \cdot \mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{s}_{(i)}}$$

Now we can summarise the steps require to minimize the normal equation using the method of steepest descent

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Summary / Method of Steepest Descent

We choose a starting value $\mathbf{x}_{(0)}$.

The residual vectors $\mathbf{r}_{(0)}$ and $\mathbf{r}_{(0)}$ are computed:

$$
\begin{aligned}
\mathbf{r}_{(0)} &= \mathbf{b} - \mathbf{A} \cdot \mathbf{x}_{(0)} \\
\mathbf{s}_{(0)} &= \mathbf{A}^T \cdot \mathbf{r}_{(0)}
\end{aligned}
$$

For iteration steps $i := [0, 1, \cdots, N]$ we compute:

the step size $\alpha_{(i)}$:

$$\alpha_{(i)} = \frac{\mathbf{s}_{(i)}^T \cdot \mathbf{s}_{(i)}}{\mathbf{s}_{(i)}^T \cdot \mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{s}_{(i)}}$$

To calculate the denominator $\mathbf{s}_{(i)}^T \cdot \mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{s}_{(i)}$ it is sufficient to calculate $\mathbf{A} \cdot \mathbf{s}_{(i)}$ and reuse it as its transpose. To see this we rewrite the denominator:

$$\mathbf{s}_{(i)}^T \cdot \mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{s}_{(i)} = \left(\mathbf{A} \cdot \mathbf{s}_{(i)}\right)^T \cdot \left(\mathbf{A} \cdot \mathbf{s}_{(i)}\right)$$

the next approximation $\mathbf{x}_{(i+1)}$:

$$\mathbf{x}_{(i+1)} = \mathbf{x}_{(i)} + \alpha_{(i)} \cdot \mathbf{s}_{(i)}$$

the next residual $\mathbf{r}_{(i+1)}$:

$$\mathbf{r}_{(i+1)} = \mathbf{b} - \mathbf{A} \cdot \mathbf{x}_{(i+1)}$$

$$\mathbf{r}_{(i+1)} = \mathbf{b} - \mathbf{A} \cdot \left(\mathbf{x}_{(i)} + \alpha_{(i)} \cdot \mathbf{s}_{(i)}\right)$$

$$\mathbf{r}_{(i+1)} = \mathbf{b} - \mathbf{A} \cdot \mathbf{x}_{(i)} - \alpha_{(i)} \cdot \mathbf{A} \cdot \mathbf{s}_{(i)}$$

$$\mathbf{r}_{(i+1)} = \mathbf{r}_{(i)} - \alpha_{(i)} \cdot \mathbf{A} \cdot \mathbf{s}_{(i)}$$

and $\mathbf{s}_{(i+1)}$:

$$\mathbf{s}_{(i+1)} = \mathbf{A}^T \cdot \mathbf{r}_{(i+1)}$$

Note that $\mathbf{A} \cdot \mathbf{s}_{(i)}$ is available from the computation of the stepsize $\alpha_{(i)}$.

The square norm of residuals can be monitored to serve as a *termination criterion*.

Conjugate Gradients Method for the Least Squares problem

The thesis `Conjugate Gradients and Conjugate Residuals type methods for solving Least Squares problems from Tomography` outlines the procedure of the conjugate gradient method for the least squares problem as follows:

Initialisiation

As for the method of steepest descent we choose a starting value $\mathbf{x}_{(0)}$.

The residual vectors $\mathbf{r}_{(0)}$ and $\mathbf{r}_{(0)}$ are computed as has been done for the method of steepest descent:

$$\mathbf{r}_{(0)} = \mathbf{b} - \mathbf{A} \cdot \mathbf{x}_{(0)}$$

$$\mathbf{s}_{(0)} = \mathbf{A}^T \cdot \mathbf{r}_{(0)}$$

An initial search direction $\mathbf{p}_{(0)}$ is chosen. It is initially set to the direction of steepest descent. But the search directions will follow a different path in subsequent iterations.

$$\mathbf{p}_{(0)} = \mathbf{s}_{(0)}$$

Iterations

For iteration steps $i := [0, 1, \cdots, N]$ we compute:

the next approximation $\mathbf{x}_{(i+1)}$:

$$\mathbf{x}_{(i+1)} = \mathbf{x}_{(i)} + \alpha_{(i)} \cdot \mathbf{s}_{(i)}$$

the next residual $\mathbf{r}_{(i+1)}$:

$$\mathbf{r}_{(i+1)} = \mathbf{r}_{(i)} - \alpha_{(i)} \cdot \mathbf{A} \cdot \mathbf{p}_{(i)}$$

and the other residual $\mathbf{s}_{(i+1)}$

$$\mathbf{s}_{(i+1)} = \mathbf{A}^T \cdot \mathbf{r}_{(i+1)} = \mathbf{A}^T \cdot \mathbf{r}_{(i)} - \alpha_{(i)} \cdot \mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{p}_{(i)}$$
$$\mathbf{s}_{(i+1)} = \mathbf{s}_{(i)} - \alpha_{(i)} \cdot \mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{p}_{(i)}$$

Finally the computation of a new search direction $\mathbf{p}_{(i+1)}$:

$$\mathbf{p}_{(i+1)} = \mathbf{s}_{(i+1)} + \beta_{(i)} \cdot \mathbf{p}_{(i)}$$

Termination

A suitable termination criterion may use the quadratic norm of either $\mathbf{r}_{(i+1)}$ or $\mathbf{s}_{(i+1)}$ and compare it to an acceptance threshold. The iteration is terminated once the criterion is below that threshold.

The next step is to determine the yet unknown stepsize parameters $\alpha_{(i)}$ and $\beta_{(i)}$

Computing stepsize parameters $\alpha_{(i)}$ and $\beta_{(i)}$

Stepsize $\alpha_{(i)}$ is calculated from the recursion equation

$$\mathbf{r}_{(i+1)} = \mathbf{r}_{(i)} - \alpha_{(i)} \cdot \mathbf{A} \cdot \mathbf{p}_{(i)}$$
$$\mathbf{r}_{(i+1)} = \mathbf{r}_{(i-1)} - \alpha_{(i-1)} \cdot \mathbf{A} \cdot \mathbf{p}_{(i-1)} - \alpha_{(i)} \cdot \mathbf{A} \cdot \mathbf{p}_{(i)}$$

Stepsizes $\alpha_{(i)}$ and $\alpha_{(i-1)}$ shall be determined such as to minimize $||\mathbf{r}_{(i+1)}||$.

$$||\mathbf{r}_{(i+1)}|| = \left(\mathbf{r}^T_{(i-1)} - \alpha_{(i-1)} \cdot \mathbf{p}^T_{(i-1)} \cdot \mathbf{A}^T - \alpha_{(i)} \cdot \mathbf{p}^T_{(i)} \cdot \mathbf{A}^T\right) \cdot \left(\mathbf{r}_{(i-1)} - \alpha_{(i-1)} \cdot \mathbf{A} \cdot \mathbf{p}_{(i-1)} - \alpha\right.$$

$$||\mathbf{r}_{(i+1)}|| =$$
$$\mathbf{r}^T_{(i-1)} \cdot \mathbf{r}_{(i-1)} - \alpha_{(i-1)} \cdot \mathbf{r}^T_{(i-1)} \cdot \mathbf{A} \cdot \mathbf{p}_{(i-1)} - \alpha_{(i)} \cdot \mathbf{r}^T_{(i-1)} \cdot \mathbf{A} \cdot \mathbf{p}_{(i)}$$
$$-\alpha_{(i-1)} \cdot \mathbf{p}^T_{(i-1)} \cdot \mathbf{A}^T \cdot \mathbf{r}_{(i-1)} + \alpha^2_{(i-1)} \cdot \mathbf{p}^T_{(i-1)} \cdot \mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{p}_{(i-1)} + 2 \cdot \alpha_{(i)} \cdot \alpha_{(i-1)} \cdot \mathbf{p}^T_{(i-1)} \cdot \mathbf{A}^T \cdot$$
$$-\alpha_{(i)} \cdot \mathbf{p}^T_{(i)} \cdot \mathbf{A}^T \cdot \mathbf{r}_{(i-1)} + \alpha^2_{(i)} \cdot \mathbf{p}^T_{(i)} \cdot \mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{p}_{(i)}$$

For the term $2 \cdot \alpha_{(i)} \cdot \alpha_{(i-1)} \cdot \mathbf{p}^T_{(i-1)} \cdot \mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{p}_{(i)}$ we require

$$2 \cdot \alpha_{(i)} \cdot \alpha_{(i-1)} \cdot \mathbf{p}^T_{(i-1)} \cdot \mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{p}_{(i)} = 0$$

This is equivalent to

$$\mathbf{p}^T_{(i-1)} \cdot \mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{p}_{(i)} = 0$$

meaning that search directions $\mathbf{p}_{(i)}$ and $\mathbf{p}_{(i-1)}$ are conjugate with respect to matrix $\mathbf{A}^T \cdot \mathbf{A}$.

Differention of $||\mathbf{r}_{(i+1)}||$ with respect of stepsize $\alpha_{(i)}$ provides us with:

$$\frac{d}{d\alpha_{(i)}}||\mathbf{r}_{(i+1)}|| = -2 \cdot \mathbf{p}_{(i)}^T \cdot \mathbf{A}^T \cdot \mathbf{r}_{(i-1)} + 2 \cdot \alpha_{(i)} \cdot \mathbf{p}_{(i)}^T \cdot \mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{p}_{(i)} = 0$$

$$\alpha_{(i)} = \frac{\mathbf{p}_{(i)}^T \cdot \mathbf{A}^T \cdot \mathbf{r}_{(i-1)}}{\mathbf{p}_{(i)}^T \cdot \mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{p}_{(i)}} = \frac{\mathbf{p}_{(i)}^T \cdot \mathbf{s}_{(i-1)}}{\mathbf{p}_{(i)}^T \cdot \mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{p}_{(i)}} = \frac{\mathbf{s}_{(i-1)}^T \cdot \mathbf{p}_{(i)}}{\mathbf{p}_{(i)}^T \cdot \mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{p}_{(i)}}$$

From $\mathbf{s}_{(i)} = \mathbf{s}_{(i-1)} - \alpha_{(i-1)} \cdot \mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{p}_{(i-1)}$ we get:

$$\mathbf{s}_{(i-1)} = \mathbf{s}_{(i)} + \alpha_{(i-1)} \cdot \mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{p}_{(i-1)}$$

Inserting this expression into the equation for $\alpha_{(i)}$ yields:

$$\alpha_{(i)} = \frac{\mathbf{s}_{(i)}^T \cdot \mathbf{p}_{(i)}}{\mathbf{p}_{(i)}^T \cdot \mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{p}_{(i)}} + \alpha_{(i-1)} \cdot \frac{\overbrace{\mathbf{p}_{(i-1)}^T \cdot \mathbf{A}^T \cdot \mathbf{A}\mathbf{p}_{(i)}}^{=0}}{\mathbf{p}_{(i)}^T \cdot \mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{p}_{(i)}}$$

$$\alpha_{(i)} = \frac{\mathbf{s}_{(i)}^T \cdot \mathbf{p}_{(i)}}{\mathbf{p}_{(i)}^T \cdot \mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{p}_{(i)}}$$

Following the steps in `Conjugate Gradients and Conjugate Residuals type methods for solving Least Squares problems from Tomography` some useful properties must be derived before $\beta_{(i)}$ can be computed.

Proof: $\mathbf{p}_{(i)}^T \cdot \mathbf{s}_{(i+1)} = 0$

$$\mathbf{p}_{(i)}^T \cdot \mathbf{s}_{(i+1)} = \mathbf{p}_{(i)}^T \cdot \mathbf{s}_{(i)} - \alpha_{(i)} \cdot \mathbf{p}_{(i)}^T \cdot \mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{p}_{(i)}$$

$$\mathbf{p}_{(i)}^T \cdot \mathbf{s}_{(i+1)} = \mathbf{p}_{(i)}^T \cdot \mathbf{s}_{(i)} - \frac{\mathbf{s}_{(i)}^T \cdot \mathbf{p}_{(i)}}{\mathbf{p}_{(i)}^T \cdot \mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{p}_{(i)}} \cdot \mathbf{p}_{(i)}^T \cdot \mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{p}_{(i)} = \mathbf{p}_{(i)}^T \cdot \mathbf{s}_{(i)} - \mathbf{s}_{(i)}^T \cdot \mathbf{p}_{(i)} = 0$$

Proof: $\mathbf{s}_{(i)}^T \cdot \mathbf{p}_{(i)} = \mathbf{s}_{(i)}^T \cdot \mathbf{s}_{(i)}$

Left multiplication of $\mathbf{p}_{(i+1)} = \mathbf{s}_{(i+1)} + \beta_{(i)} \cdot \mathbf{p}_{(i)}$:

$$\mathbf{s}_{(i+1)}^T \cdot \mathbf{p}_{(i+1)} = \mathbf{s}_{(i+1)}^T \cdot \mathbf{s}_{(i+1)} + \beta_{(i)} \cdot \underbrace{\mathbf{s}_{(i+1)}^T \cdot \mathbf{p}_{(i)}}_{=0}$$

$$\mathbf{s}_{(i+1)}^T \cdot \mathbf{p}_{(i+1)} = \mathbf{s}_{(i+1)}^T \cdot \mathbf{s}_{(i+1)}$$

$$\rightarrow$$

$$\mathbf{s}_{(i)}^T \cdot \mathbf{p}_{(i)} = \mathbf{s}_{(i)}^T \cdot \mathbf{s}_{(i)}$$

The result of this last proof can be utilized to get a new formula for the stepsize $\alpha_{(i)}$:

$$\alpha_{(i)} = \frac{\mathbf{s}_{(i)}^T \cdot \mathbf{s}_{(i)}}{\mathbf{p}_{(i)}^T \cdot \mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{p}_{(i)}}$$

Proof: $\mathbf{p}_{(i)}^T \cdot \mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{p}_{(i)} = \mathbf{p}_{(i)}^T \cdot \mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{s}_{(i)}$

Inserting $\mathbf{p}_{(i+1)} = \mathbf{s}_{(i+1)} + \beta_{(i)} \cdot \mathbf{p}_{(i)}$:

$$\mathbf{p}_{(i+1)}^T \cdot \mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{p}_{(i+1)} = \mathbf{p}_{(i+1)}^T \cdot \mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{s}_{(i+1)} + \beta_{(i)} \cdot \mathbf{p}_{(i+1)}^T \cdot \underbrace{\mathbf{A}^T}_{=0} \cdot \mathbf{A} \cdot \mathbf{p}_{(i)}$$

$$\mathbf{p}_{(i+1)}^T \cdot \mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{p}_{(i+1)} = \mathbf{p}_{(i+1)}^T \cdot \mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{s}_{(i+1)}$$

$$\rightarrow$$

$$\mathbf{p}_{(i)}^T \cdot \mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{p}_{(i)} = \mathbf{p}_{(i)}^T \cdot \mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{s}_{(i)}$$

Proof: $\mathbf{s}_{(i)}^T \cdot \mathbf{s}_{(i+1)} = 0$

(Residual is orthogonal to previous / next residual)

Inserting the recurrence $\mathbf{s}_{(i+1)} = \mathbf{s}_{(i)} - \alpha_{(i)} \cdot \mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{p}_{(i)}$

$$\mathbf{s}_{(i)}^T \cdot \mathbf{s}_{(i+1)} = \mathbf{s}_{(i)}^T \cdot \mathbf{s}_{(i)} - \alpha_{(i)} \cdot \mathbf{s}_{(i)}^T \cdot \mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{p}_{(i)}$$

$$\mathbf{s}_{(i)}^T \cdot \mathbf{s}_{(i+1)} = \mathbf{s}_{(i)}^T \cdot \mathbf{s}_{(i)} - \alpha_{(i)} \cdot \mathbf{p}_{(i)}^T \cdot \mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{p}_{(i)} = \mathbf{s}_{(i)}^T \cdot \mathbf{s}_{(i)} - \frac{\mathbf{s}_{(i)}^T \cdot \mathbf{s}_{(i)}}{\mathbf{p}_{(i)}^T \cdot \mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{p}_{(i)}} \cdot \mathbf{p}_{(i)}^T \cdot \mathbf{A}^T$$

$$\mathbf{s}_{(i)}^T \cdot \mathbf{s}_{(i+1)} = \mathbf{s}_{(i)}^T \cdot \mathbf{s}_{(i)} - \mathbf{s}_{(i)}^T \cdot \mathbf{s}_{(i)} = 0$$

---

computing $\beta_{(i)}$

With

$$\mathbf{p}_{(i+1)} = \mathbf{s}_{(i+1)} + \beta_{(i)} \cdot \mathbf{p}_{(i)}$$

we left multiply by $\mathbf{p}_{(i)}^T \cdot \mathbf{A}^T \cdot \mathbf{A}$:

$$\mathbf{p}_{(i)}^T \cdot \mathbf{A}^T \underbrace{\cdot\, \mathbf{A}}_{=0} \cdot \mathbf{p}_{(i+1)} = \mathbf{p}_{(i)}^T \cdot \mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{s}_{(i+1)} + \beta_{(i)} \cdot \mathbf{p}_{(i)}^T \cdot \mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{p}_{(i)}$$

$$\beta_{(i)} = -\frac{\mathbf{p}_{(i)}^T \cdot \mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{s}_{(i+1)}}{\mathbf{p}_{(i)} \cdot \mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{p}_{(i)}}$$

From

$$\mathbf{r}_{(i+1)} = \mathbf{r}_{(i)} - \alpha_{(i)} \cdot \mathbf{A} \cdot \mathbf{p}_{(i)}$$

we get:

$$\mathbf{A} \cdot \mathbf{p}_{(i)} = \frac{\mathbf{r}_{(i)} - \mathbf{r}_{(i+1)}}{\alpha_{(i)}}$$

Inserting into $\beta_{(i)}$:

$$\beta_{(i)} = -\frac{(\mathbf{r}_{(i)} - \mathbf{r}_{(i+1)})^T \cdot \mathbf{A} \cdot \mathbf{s}_{(i+1)}}{\mathbf{s}_{(i)}^T \cdot \mathbf{s}_{(i)}}$$

$$\beta_{(i)} = \frac{(\mathbf{s}_{(i+1)} - \mathbf{s}_{(i)})^T \cdot \mathbf{s}_{(i+1)}}{\mathbf{s}_{(i)}^T \cdot \mathbf{s}_{(i)}}$$

$$\beta_{(i)} = \frac{\mathbf{s}_{(i+1)}^T \cdot \mathbf{s}_{(i+1)} - \mathbf{s}_{(i)}^T \cdot \mathbf{s}_{(i+1)}}{\mathbf{s}_{(i)}^T \cdot \mathbf{s}_{(i)}}$$

$$\beta_{(i)} = \frac{\mathbf{s}_{(i+1)}^T \cdot \mathbf{s}_{(i+1)}}{\mathbf{s}_{(i)}^T \cdot \mathbf{s}_{(i)}}$$

Having computed the stepsize the method of conjugate gradients for the least squares problem can summarized again.

Initialisiation

we choose a starting value $\mathbf{x}_{(0)}$.

The residual vectors $\mathbf{r}_{(0)}$ and $\mathbf{r}_{(0)}$ are computed:

$$\mathbf{r}_{(0)} = \mathbf{b} - \mathbf{A} \cdot \mathbf{x}_{(0)}$$
$$\mathbf{s}_{(0)} = \mathbf{A}^T \cdot \mathbf{r}_{(0)}$$

An initial search direction $\mathbf{p}_{(0)}$ is chosen. It is initially set to the direction of steepest descent. But the search directions will follow a different path in subsequent iterations.

$$\mathbf{p}_{(0)} = \mathbf{s}_{(0)}$$

Iterations

For iteration steps $i := [0, 1, \cdots, N]$ we compute:

The step size $\alpha_{(i)}$:

$$\alpha_{(i)} = \frac{\mathbf{s}_{(i)}^T \cdot \mathbf{s}_{(i)}}{\mathbf{p}_{(i)}^T \cdot \mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{p}_{(i)}} = \frac{\mathbf{s}_{(i)}^T \cdot \mathbf{s}_{(i)}}{\left(\mathbf{A} \cdot \mathbf{p}_{(i)}\right)^T \cdot \mathbf{A} \cdot \mathbf{p}_{(i)}}$$

The next approximation $\mathbf{x}_{(i+1)}$:

$$\mathbf{x}_{(i+1)} = \mathbf{x}_{(i)} + \alpha_{(i)} \cdot \mathbf{s}_{(i)}$$

the next residual $\mathbf{r}_{(i+1)}$:

$$\mathbf{r}_{(i+1)} = \mathbf{r}_{(i)} - \alpha_{(i)} \cdot \mathbf{A} \cdot \mathbf{p}_{(i)}$$

and the other residual $\mathbf{s}_{(i+1)}$

$$\mathbf{s}_{(i+1)} = \mathbf{s}_{(i)} - \alpha_{(i)} \cdot \mathbf{A}^T \cdot \mathbf{A} \cdot \mathbf{p}_{(i)} = \mathbf{A}^T \cdot \mathbf{r}_{(i+1)}$$

The step size $\beta_{(i)}$:

$$\beta_{(i)} = \frac{\mathbf{s}_{(i+1)}^T \cdot \mathbf{s}_{(i+1)}}{\mathbf{s}_{(i)}^T \cdot \mathbf{s}_{(i)}}$$

The new search direction $\mathbf{p}_{(i+1)}$:

$$\mathbf{p}_{(i+1)} = \mathbf{s}_{(i+1)} + \beta_{(i)} \cdot \mathbf{p}_{(i)}$$

Termination

A suitable termination criterion may use the quadratic norm of either $\mathbf{r}_{(i+1)}$ or $\mathbf{s}_{(i+1)}$ and compare it to an acceptance threshold. The iteration is terminated once the criterion is below that threshold.

For each iteration the matrix-vector products

$$\mathbf{A} \cdot \mathbf{p}_{(i)}$$
$$\mathbf{A} \cdot \mathbf{r}_{(i+1)}$$

must be computed.

Application to a simple problem

In [12]:
```
import numpy as np

# 2 x 2 matrix
A_mat = np.array([[3.0, 2.0], [2.0, 6.0]])
# row column vector)
b_vec = np.array([2.0, -8])
```

```python
# Initialisation

# starting point x0 (as column vector)
x0 = np.array( [0, 0] ).T
# the residual (negative gradient vector)
r0 = b_vec.T - np.dot(A_mat, x0)

# residual s
s0 = np.dot(A_mat.T, r0)
# the search direction
p0 = s0

# put x0, r0, d0, s0 into lists
xvec_lst = [x0]
residual_lst = [r0]
p_lst = [p0]
res_s_lst = [s0]

#----- iterations ------
Ni = 2
for k in range(Ni):
    Amat_p = np.dot(A_mat, p_lst[-1])
    # the denominator for the stepsize
    alpha_denom = np.dot(Amat_p.T, Amat_p)
    # the nominator for the stepsize
    alpha_nom = np.dot(p_lst[-1].T, p_lst[-1])
    # the stepsize
    alpha = alpha_nom/alpha_denom

    # new x vector
    xn = xvec_lst[-1] + alpha * p_lst[-1]
    # new residual
    rn = residual_lst[-1] - alpha * Amat_p
    # new residual
    sn = np.dot(A_mat.T, rn)
    # stepsize beta
    beta = np.dot(sn.T, sn) / np.dot(res_s_lst[-1].T, res_s_lst[-1])
    # new search direction
    pn = sn + beta * p_lst[-1]

    # updating lists
    residual_lst.append(rn)
    p_lst.append(pn)
    xvec_lst.append(xn)
    res_s_lst.append(sn)


print(f"residual : {rn}")
print(f"norm2    : {np.inner(rn, rn):8.3e}")
print(f"xvec     : {xn}")
```

```
residual : [-0.22742168  0.0944921 ]
norm2    : 6.065e-02
xvec     : [ 2.1109653  -2.05273712]
```

```
In [ ]:
```