

ELEC-E8740 — Gauss-Newton with Line Search and Levenberg-Marquardt Algorithm

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Intended Learning Outcomes

After this lecture, you will be able to:

- understand the principle of line search in Gauss–Newton method;
- understand the principle of Levenberg–Marquardt algorithm;
- apply Gauss
 –Newton method with line search and Levenberg
 –Marquardt algorithm to sensor fusion problems.

Recap (1)

- Sensor fusion problems are often nonlinear.
- General nonlinear model has the form:

$$\mathbf{y} = \mathbf{g}(\mathbf{x}) + \mathbf{r},$$

• General cost function that we considered:

$$J_{\text{WLS}}(\mathbf{x}) = (\mathbf{y} - \mathbf{g}(\mathbf{x}))^{\mathsf{T}} \mathbf{R}^{-1} (\mathbf{y} - \mathbf{g}(\mathbf{x})).$$

- Gradient descent algorithm takes steps towards the direction of negative gradient.
- Gauss-Newton iteratively linearizes the model and solves the linear optimization problem.



Recap (2)

Algorithm 1 Gradient Descent

Require: Initial parameter guess $\hat{\mathbf{x}}^{(0)}$, data \mathbf{y} , function $\mathbf{g}(\mathbf{x})$, Jacobian $\mathbf{G}_{\mathbf{x}}(\mathbf{x})$

Ensure: Parameter estimate $\hat{\mathbf{x}}_{WLS}$

Set *i* ← 0
 repeat

3: Calculate the update direction

$$\Delta \mathbf{x}^{(i+1)} = \mathbf{G}_{\mathbf{x}}^{\mathsf{T}}(\hat{\mathbf{x}}^{(i)}) \, \mathbf{R}^{-1}(\mathbf{y} - \mathbf{g}(\hat{\mathbf{x}}^{(i)}))$$

- 4: Select a suitable $\gamma^{(i+1)}$
- 5: Calculate

$$\hat{\mathbf{x}}^{(i+1)} = \hat{\mathbf{x}}^{(i)} + \gamma^{(i+1)} \Delta \mathbf{x}^{(i+1)}$$

- 6: Set $i \leftarrow i + 1$
- 7: until Converged



Recap (3)

Algorithm 2 Gauss–Newton Algorithm

Require: Initial parameter guess $\hat{\mathbf{x}}^{(0)}$, data \mathbf{y} , function $\mathbf{g}(\mathbf{x})$, Jacobian G_x

Ensure: Parameter estimate $\hat{\mathbf{x}}_{\text{WLS}}$

1: Set $i \leftarrow 0$ 2: repeat

3: Calculate the update direction

$$\Delta \mathbf{x}^{(i+1)} = (\mathbf{G}_{\mathbf{x}}^{\mathsf{T}}(\hat{\mathbf{x}}^{(i)})\mathbf{R}^{-1}\mathbf{G}_{\mathbf{x}}(\hat{\mathbf{x}}^{(i)}))^{-1}\mathbf{G}_{\mathbf{x}}^{\mathsf{T}}(\hat{\mathbf{x}}^{(i)})\mathbf{R}^{-1}(\mathbf{y} - \mathbf{g}(\hat{\mathbf{x}}^{(i)}))$$

Calculate 4:

$$\hat{\mathbf{x}}^{(i+1)} = \hat{\mathbf{x}}^{(i)} + \Delta \mathbf{x}^{(i+1)}$$

5. Set $i \leftarrow i + 1$

6: until Converged

7: Set $\hat{\mathbf{x}}_{WLS} = \hat{\mathbf{x}}^{(i)}$



Gauss-Newton Algorithm with Line Search: Motivation

- Gauss–Newton uses linearization to determine the next iterate.
- As linearization is a local approximation, taking the full step might over/undershoot.
- Instead, we can use scaled Gauss-Newton step:

$$\begin{split} \hat{\mathbf{x}}^{(i+1)} &= \hat{\mathbf{x}}^{(i)} + \gamma \Delta \hat{\mathbf{x}}^{(i+1)}, \\ \Delta \hat{\mathbf{x}}^{(i+1)} &= (\mathbf{G}_{\mathbf{x}}^{\mathsf{T}}(\hat{\mathbf{x}}^{(i)})\mathbf{R}^{-1}\mathbf{G}_{\mathbf{x}}(\hat{\mathbf{x}}^{(i)}))^{-1}\mathbf{G}_{\mathbf{x}}^{\mathsf{T}}(\hat{\mathbf{x}}^{(i)})\mathbf{R}^{-1}(\mathbf{y} - \mathbf{g}(\hat{\mathbf{x}}^{(i)})), \end{split}$$

- Here γ is the scaling factor typically $\gamma \in [0, 1]$.
- How should we select the scaling factor?

Gauss–Newton Algorithm with Line Search: Derivation

- One way to select the scaling parameter γ is to use a line search.
- Given the Gauss–Newton increment $\Delta \hat{\mathbf{x}}^{(i+1)}$, we can consider cost as function of the scale parameter:

$$J_{\mathsf{WLS}}^{(i)}(\gamma) = J_{\mathsf{WLS}}\left(\hat{\mathbf{x}}^{(i)} + \gamma \Delta \hat{\mathbf{x}}^{(i+1)}\right).$$

- Then the idea of line search is to locally optimize the above function in the range [0, 1].
- In the exact line search we simply find the minimum e.g. by evaluating it in grid.
- We could also use bisection algorithm or interpolation methods to find the minimum.



Exact Line Search on Grid

Algorithm 3 Line Search on Grid

Require: Previous iterate $\hat{\mathbf{x}}^{(i)}$, the update direction $\Delta \hat{\mathbf{x}}^{(i+1)}$, the cost function $J_{\text{WLS}}(\mathbf{x})$, and the grid size N_g .

```
Ensure: Optimal step size \gamma^*.

1: Set \gamma^* \leftarrow 0 and J^* \leftarrow J_{\text{WLS}}(\hat{\mathbf{x}}^{(i)})

2: for j \in \{1, 2, \dots, N_g\} do

3: Set \gamma \leftarrow j/N_g

4: if J_{\text{WLS}}(\hat{\mathbf{x}}^{(i)} + \gamma \Delta \hat{\mathbf{x}}^{(i+1)}) < J^* then

5: Set \gamma^* \leftarrow \gamma

6: Set J^* \leftarrow J_{\text{WLS}}(\hat{\mathbf{x}}^{(i)} + \gamma^* \Delta \hat{\mathbf{x}}^{(i+1)})

7: end if

8: end for
```



Inexact Line Search (1/2)

- The line search does not need to be exact to guarantee to find the minimum.
- In backtracking we decrease the parameter γ until it provides a sufficient decrease in the cost.
- One way is to halve the step size until the cost decreases.
- In Armijo backtracking we demand that the cost is decreased at least with an amount that is predicted by a first order Taylor series expansion.
- The first order Taylor series expansion for the cost as function of scale parameter gives:

$$\begin{split} J_{\mathsf{WLS}}\left(\hat{\mathbf{x}}^{(i)} + \gamma \Delta \hat{\mathbf{x}}^{(i+1)}\right) \\ &\approx J_{\mathsf{WLS}}\left(\hat{\mathbf{x}}^{(i)}\right) - 2\gamma [\Delta \hat{\mathbf{x}}^{(i+1)}]^{\mathsf{T}} \mathbf{G}_{\mathbf{x}}^{\mathsf{T}}(\hat{\mathbf{x}}^{(i)}) \left(\mathbf{y} - \mathbf{g}(\hat{\mathbf{x}}^{(i)})\right). \end{split}$$



Inexact Line Search (2/2)

 Then we demand that the cost decrease should satisfy the Armijo condition

$$\begin{split} J_{\mathsf{WLS}}\left(\hat{\mathbf{x}}^{(i)} + \gamma \Delta \hat{\mathbf{x}}^{(i+1)}\right) - J_{\mathsf{WLS}}\left(\hat{\mathbf{x}}^{(i)}\right) \\ &\leq -2\beta \, \gamma [\Delta \hat{\mathbf{x}}^{(i+1)}]^\mathsf{T} \mathbf{G}_{\mathbf{x}}^\mathsf{T}(\hat{\mathbf{x}}^{(i)}) \, (\mathbf{y} - \mathbf{g}(\hat{\mathbf{x}}^{(i)})). \end{split}$$

- Here β is a parameter that we can choose freely on range [0,1) (e.g. $\beta=0.1$).
- We then decrease γ by multiplying it with a parameter τ (e.g., $\tau = 0.5$) on the range (0, 1) until the condition is satisfied:

$$\gamma \leftarrow \tau \gamma$$
.



Line Search with Armijo Backtracking

Algorithm 4 Line Search with Armijo Backtracking

Require: Previous iterate $\hat{\mathbf{x}}^{(i)}$, the update direction $\Delta \hat{\mathbf{x}}^{(i+1)}$, the cost function $J_{\text{WLS}}(\mathbf{x})$, and parameters β and τ .

Ensure: Suitable step size γ .

- 1: Set $\gamma \leftarrow 1$ and $J_0 \leftarrow J_{WLS}(\hat{\mathbf{x}}^{(i)})$.
- 2: Set $d \leftarrow -2\beta \left[\Delta \hat{\mathbf{x}}^{(i+1)}\right]^{\mathsf{T}} \mathbf{G}_{\mathbf{x}}^{\mathsf{T}} (\hat{\mathbf{x}}^{(i)}) (\mathbf{y} \mathbf{g}(\hat{\mathbf{x}}^{(i)}))$
- 3: while $J_{\text{WLS}}\left(\hat{\mathbf{x}}^{(i)} + \gamma \Delta \hat{\mathbf{x}}^{(i+1)}\right) > J_0 + \gamma d$ do
- 4: Set $\gamma \leftarrow \tau \gamma$
- 5: end while

Gauss-Newton Algorithm with Line Search

Algorithm 5 Gauss-Newton Algorithm with Line Search

Require: Initial parameter guess $\hat{\mathbf{x}}^{(0)}$, data \mathbf{y} , function $\mathbf{g}(\mathbf{x})$, Jacobian $\mathbf{G}_{\mathbf{x}}(\mathbf{x})$

Ensure: Parameter estimate $\hat{\mathbf{x}}_{WLS}$

- 1: Set $i \leftarrow 0$
- 2: repeat
- Calculate the update direction

$$\Delta \mathbf{x}^{(i+1)} = (\mathbf{G}_{\mathbf{x}}^{\mathsf{T}}(\hat{\mathbf{x}}^{(i)})\mathbf{R}^{-1}\mathbf{G}_{\mathbf{x}}(\hat{\mathbf{x}}^{(i)}))^{-1}\mathbf{G}_{\mathbf{x}}^{\mathsf{T}}(\hat{\mathbf{x}}^{(i)})\mathbf{R}^{-1}(\mathbf{y} - \mathbf{g}(\hat{\mathbf{x}}^{(i)}))$$

- 4: Compute optimal $\gamma^{(i+1)}$ with line search (Algorithm 3 or 4)
- 5: Calculate

$$\hat{\mathbf{x}}^{(i+1)} = \hat{\mathbf{x}}^{(i)} + \gamma^{(i+1)} \Delta \mathbf{x}^{(i+1)}$$

- 6: Set $i \leftarrow i + 1$
- 7: until Converged
- 8: Set $\hat{\mathbf{x}}_{WLS} = \hat{\mathbf{x}}^{(i)}$



Gauss–Newton Algorithm with Line Search: Example (1/3)

 We measure the range to each landmark

$$y_1^R = \sqrt{(s_1^x - p^x)^2 + (s_1^y - p^y)^2} + r_1^R,$$

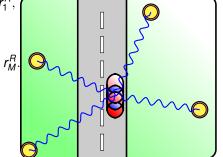
$$\vdots$$

$$y_M^R = \sqrt{(s_M^x - p^x)^2 + (s_M^y - p^y)^2} + r_M^R.$$
• This is a non-linear model

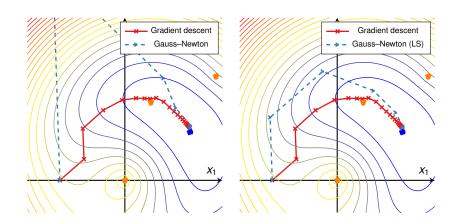
$$y = g(x) + r$$

• We can find $\mathbf{x} = (p^x, p^y)$ by minimizing the cost function

$$J_{\text{WLS}}(\boldsymbol{x}) = (\boldsymbol{y} {-} \boldsymbol{g}(\boldsymbol{x}))^T \boldsymbol{R}^{-1} (\boldsymbol{y} {-} \boldsymbol{g}(\boldsymbol{x})).$$

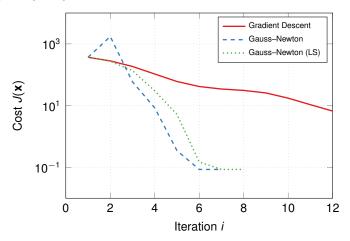


Gauss–Newton Algorithm with Line Search: Example (2/3)





Gauss–Newton Algorithm with Line Search: Example (3/3)



Levenberg-Marguardt Algorithm: Motivation

- Gradient descent: Quickly moves to low cost area, creeps to minimum
- Gauss-Newton: Straight to minimum, may take a detour
- Can we have the best of both worlds?
- ...kind of, the Levenberg–Marguardt algorithm.



Levenberg-Marquardt Algorithm: Derivation

- The Levenberg–Marquardt algorithm can be seen as a regularized version of the Gauss–Newton algorithm.
- Cost function approximation:

$$\begin{split} J_{\text{ReLS}}(\boldsymbol{x}) &\approx \left(\boldsymbol{y} - \boldsymbol{g}(\hat{\boldsymbol{x}}^{(i)}) - \boldsymbol{G}_{\boldsymbol{x}}(\hat{\boldsymbol{x}}^{(i)})(\boldsymbol{x} - \hat{\boldsymbol{x}}^{(i)})\right)^{\mathsf{T}} \\ &\times \boldsymbol{R}^{-1} \left(\boldsymbol{y} - \boldsymbol{g}(\hat{\boldsymbol{x}}^{(i)}) - \boldsymbol{G}_{\boldsymbol{x}}(\hat{\boldsymbol{x}}^{(i)})(\boldsymbol{x} - \hat{\boldsymbol{x}}^{(i)})\right) \\ &+ \lambda (\boldsymbol{x} - \hat{\boldsymbol{x}}^{(i)})^{\mathsf{T}}(\boldsymbol{x} - \hat{\boldsymbol{x}}^{(i)}) \end{split}$$

• We can now minimize this as a linear regularized problem:

$$\mathbf{x} = \hat{\mathbf{x}}^{(i)} + (\mathbf{G}_{\mathbf{x}}^{\mathsf{T}}(\hat{\mathbf{x}}^{(i)})\mathbf{R}^{-1}\mathbf{G}_{\mathbf{x}}(\hat{\mathbf{x}}^{(i)}) + \lambda \mathbf{I})^{-1}\mathbf{G}_{\mathbf{x}}^{\mathsf{T}}(\hat{\mathbf{x}}^{(i)})\mathbf{R}^{-1}(\mathbf{y} - \mathbf{g}(\hat{\mathbf{x}}^{(i)}))$$

Using this as the next iterate gives the iteration:

$$\begin{split} \hat{\mathbf{x}}^{(i+1)} &= \hat{\mathbf{x}}^{(i)} + \Delta \hat{\mathbf{x}}^{(i+1)}, \\ \Delta \hat{\mathbf{x}}^{(i+1)} &= (\mathbf{G}_{\mathbf{x}}^{\mathsf{T}}(\hat{\mathbf{x}}^{(i)})\mathbf{R}^{-1}\mathbf{G}_{\mathbf{x}}(\hat{\mathbf{x}}^{(i)}) + \lambda \mathbf{I})^{-1}\mathbf{G}_{\mathbf{x}}^{\mathsf{T}}(\hat{\mathbf{x}}^{(i)})\mathbf{R}^{-1}(\mathbf{y} - \mathbf{g}(\hat{\mathbf{x}}^{(i)})). \end{split}$$



Levenberg–Marquardt Algorithm: Damping (1/2)

The Levenberg–Marquardt update:

$$\begin{split} \hat{\mathbf{x}}^{(i+1)} &= \hat{\mathbf{x}}^{(i)} + \Delta \hat{\mathbf{x}}^{(i+1)}, \\ \Delta \hat{\mathbf{x}}^{(i+1)} &= (\mathbf{G}_{\mathbf{x}}^{\mathsf{T}}(\hat{\mathbf{x}}^{(i)})\mathbf{R}^{-1}\mathbf{G}_{\mathbf{x}}(\hat{\mathbf{x}}^{(i)}) + \lambda \mathbf{I})^{-1}\mathbf{G}_{\mathbf{x}}^{\mathsf{T}}(\hat{\mathbf{x}}^{(i)})\mathbf{R}^{-1}(\mathbf{y} - \mathbf{g}(\hat{\mathbf{x}}^{(i)})). \end{split}$$

- How should the damping parameter λ be chosen?
- If $\lambda \to 0$:

$$\Delta\hat{\boldsymbol{x}}^{(i+1)} \rightarrow (\boldsymbol{G}_{\boldsymbol{x}}^T\boldsymbol{R}^{-1}\boldsymbol{G}_{\boldsymbol{x}})^{-1}\boldsymbol{G}_{\boldsymbol{x}}^T\boldsymbol{R}^{-1}(\boldsymbol{y}-\boldsymbol{g}(\hat{\boldsymbol{x}}^{(i)}))$$

• If $\lambda \to \infty$:

$$\Delta \hat{\mathbf{x}}^{(i+1)} \rightarrow \frac{1}{\lambda} \mathbf{G}_{\mathbf{x}}^{\mathsf{T}} \mathbf{R}^{-1} (\mathbf{y} - \mathbf{g}(\hat{\mathbf{x}}^{(i)})).$$

• Ideally, in flat regions of the cost function where the linear approximation is good, λ should be chosen small, whereas in steep regions, it should be chosen large.

Levenberg–Marquardt Algorithm: Damping (2/2)

- A simple strategy is to start from some damping value $\lambda^{(0)}$ (e.g. $\lambda^{(0)} = 10^{-2}$) and select a fixed factor ν (e.g. $\nu = 10$).
- Then at each step we do the following:
 - First compute a candidate $\hat{\mathbf{x}}^{(i+1)}$ using the previous parameter value $\lambda^{(i-1)}$. Then proceed as follows:
 - If $J_{\text{WLS}}(\hat{\mathbf{x}}^{(i+1)}) < J_{\text{WLS}}(\hat{\mathbf{x}}^{(i)})$ then accept $\hat{\mathbf{x}}^{(i+1)}$ and decrease the damping parameter by $\lambda^{(i)} = \lambda^{(i-1)}/\nu$.
 - Otherwise continue with $\hat{\mathbf{x}}^{(i+1)} = \hat{\mathbf{x}}^{(i)}$ and increase the damping parameter by $\lambda^{(i)} = \nu \lambda^{(i-1)}$.
- This idea appears already in the original article of Marquadt (1963).
- More sophisticated adaptation schemes can also be found in literature.



Levenberg-Marguardt Algorithm: Scaling

- The resulting algorithm is not scale invariant.
- To make it scale invariant we can normalize the regularized cost function approximation by using the diagonal values of $\mathbf{G}_{\mathbf{v}}^{\mathsf{T}}(\hat{\mathbf{x}}^{(i)})\mathbf{R}^{-1}\mathbf{G}_{\mathbf{v}}(\hat{\mathbf{x}}^{(i)}).$
- This is equivalent to replacing the regularization term λI with $\lambda \operatorname{diag}(\mathbf{G}_{\mathbf{x}}^{\mathsf{T}}(\hat{\mathbf{x}}^{(i)})\mathbf{R}^{-1}\mathbf{G}_{\mathbf{x}}(\hat{\mathbf{x}}^{(i)}))$.
- The scaled iteration then becomes:

$$\begin{split} \hat{\mathbf{x}}^{(i+1)} &= \hat{\mathbf{x}}^{(i)} + \Delta \hat{\mathbf{x}}^{(i+1)}, \\ \Delta \hat{\mathbf{x}}^{(i+1)} &= (\mathbf{G}_{\mathbf{x}}^{\mathsf{T}}(\hat{\mathbf{x}}^{(i)})\mathbf{R}^{-1}\mathbf{G}_{\mathbf{x}}(\hat{\mathbf{x}}^{(i)}) + \lambda \operatorname{diag}(\mathbf{G}_{\mathbf{x}}^{\mathsf{T}}(\hat{\mathbf{x}}^{(i)})\mathbf{R}^{-1}\mathbf{G}_{\mathbf{x}}(\hat{\mathbf{x}}^{(i)})))^{-1} \\ &\times \mathbf{G}_{\mathbf{x}}^{\mathsf{T}}(\hat{\mathbf{x}}^{(i)})\mathbf{R}^{-1}(\mathbf{y} - \mathbf{g}(\hat{\mathbf{x}}^{(i)})). \end{split}$$

Levenberg-Marquardt Algorithm: Algorithm

Algorithm 4.6 Levenberg–Marquardt Algorithm with simple adaptation

```
Input: Initial parameter guess \hat{\mathbf{x}}^{(0)}, data \mathbf{y}, function \mathbf{g}(\mathbf{x}), Jacobian \mathbf{G}_{\mathbf{x}}, initial damping
         \lambda^{(0)}, and parameter \nu.
Output: Parameter estimate xwis

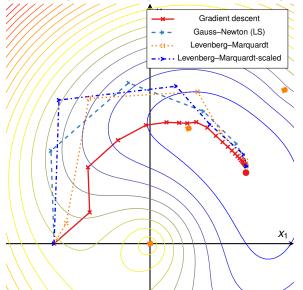
    Set i ← 0 and λ ← λ<sup>(0)</sup>.

   2: repeat
                 Compute the (candidate) parameter update:
                 if using scaled version then
                    \Delta \hat{\mathbf{x}}^{(i+1)} = (\mathbf{G}_{u}^{\mathsf{T}}(\hat{\mathbf{x}}^{(i)})\mathbf{R}^{-1}\mathbf{G}_{v}(\hat{\mathbf{x}}^{(i)}) + \lambda \operatorname{diag}(\mathbf{G}_{u}^{\mathsf{T}}(\hat{\mathbf{x}}^{(i)})\mathbf{R}^{-1}\mathbf{G}_{v}(\hat{\mathbf{x}}^{(i)})))^{-1}
                                                   \times \mathbf{G}_{\mathbf{v}}^{\mathsf{T}}(\hat{\mathbf{x}}^{(i)})\mathbf{R}^{-1}(\mathbf{v} - \mathbf{g}(\hat{\mathbf{x}}^{(i)}))
   5:
                 else
                            \Delta \hat{\mathbf{x}}^{(i+1)} = (\mathbf{G}_{-}^{\mathsf{T}}(\hat{\mathbf{x}}^{(i)})\mathbf{R}^{-1}\mathbf{G}_{-}(\hat{\mathbf{x}}^{(i)}) + \lambda \mathbf{I})^{-1}\mathbf{G}_{-}^{\mathsf{T}}\mathbf{R}^{-1}(\mathbf{v} - \mathbf{g}(\hat{\mathbf{x}}^{(i)}))
   6:
                 end if
                if J_{WLS}(\hat{\mathbf{x}}^{(i)} + \Delta \hat{\mathbf{x}}^{(i+1)}) < J_{WLS}(\hat{\mathbf{x}}^{(i)}) then
                         Accept the candidate and decrease \lambda:
                                                                           \hat{\mathbf{x}}^{(i+1)} = \hat{\mathbf{x}}^{(i)} + \Lambda \hat{\mathbf{x}}^{(i+1)}
                                                                                     \lambda \leftarrow \lambda/\nu
   9:
                         Set i \leftarrow i + 1
 10:
                 else
 11:
                         Reject the candidate and increase \lambda:
```

$$\lambda \leftarrow \nu \, \lambda$$

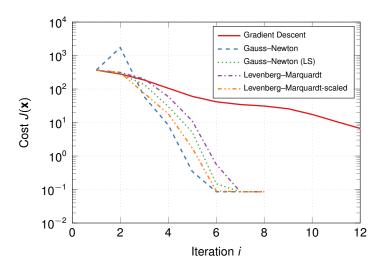
- 12: end if 13: until Converged
- 14: Set $\hat{\mathbf{x}}_{WLS} = \hat{\mathbf{x}}^{(i)}$

Levenberg-Marquardt Algorithm: Example





Decrease in Cost





Regularized Non-Linear Models

• The cost function that we considered:

$$J_{\text{WLS}}(\mathbf{x}) = (\mathbf{y} - \mathbf{g}(\mathbf{x}))^{\mathsf{T}} \mathbf{R}^{-1} (\mathbf{y} - \mathbf{g}(\mathbf{x})).$$

- However, sometimes we are interested in regularized cost functions.
- Luckily, we can use the following simple trick:

$$\begin{split} J_{\text{ReLS}}(\boldsymbol{x}) &= (\boldsymbol{y} - \boldsymbol{g}(\boldsymbol{x}))^T \boldsymbol{R}^{-1} (\boldsymbol{y} - \boldsymbol{g}(\boldsymbol{x})) + (\boldsymbol{m} - \boldsymbol{x})^T \boldsymbol{P}^{-1} (\boldsymbol{m} - \boldsymbol{x}) \\ &= \left(\begin{bmatrix} \boldsymbol{y} \\ \boldsymbol{m} \end{bmatrix} - \begin{bmatrix} \boldsymbol{g}(\boldsymbol{x}) \\ \boldsymbol{x} \end{bmatrix} \right)^T \begin{bmatrix} \boldsymbol{R}^{-1} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{P}^{-1} \end{bmatrix} \left(\begin{bmatrix} \boldsymbol{y} \\ \boldsymbol{m} \end{bmatrix} - \begin{bmatrix} \boldsymbol{g}(\boldsymbol{x}) \\ \boldsymbol{x} \end{bmatrix} \right). \end{split}$$

 This is now a non-regularized cost function and hence all the algorithms presented are applicable.

Quasi-Newton Methods (1/2)

- Here we have only concentrated on least squares problems.
- There also exists a wider class of quasi-Newton methods.
- Let us consider a generic cost function $J(\mathbf{x})$ which we wish to minimize.
- Assume that our current guess for the minimum is $\mathbf{x}^{(i)}$ we can now Taylor expand the cost function as follows:

$$J(\mathbf{x}) \approx J(\mathbf{x}^{(i)}) + \left[\frac{\partial J(\mathbf{x})}{\partial \mathbf{x}}\right]^{\mathsf{T}} \bigg|_{\mathbf{x} = \mathbf{x}^{(i)}} (\mathbf{x} - \mathbf{x}^{(i)})$$
$$+ \frac{1}{2} (\mathbf{x} - \mathbf{x}^{(i)})^{\mathsf{T}} \left[\frac{\partial^2 J(\mathbf{x})}{\partial \mathbf{x}^2}\right] \bigg|_{\mathbf{x} = \mathbf{x}^{(i)}} (\mathbf{x} - \mathbf{x}^{(i)}).$$

• We can now minimize the right hand side with respect to x and use the result as the next guess.



Quasi-Newton Methods (2/2)

• The resulting Newton's method takes the following form:

$$\mathbf{x}^{(i+1)} = \mathbf{x}^{(i)} - \left[\frac{\partial^2 J(\mathbf{x})}{\partial \mathbf{x}^2} \right]^{-1} \left. \frac{\partial J(\mathbf{x})}{\partial \mathbf{x}} \right|_{\mathbf{x} = \mathbf{x}^{(i)}}.$$

- However, computation of the Hessian is often not desirable.
- In so called quasi-Newton methods the Hessian is approximated in various ways.
- The Broyden–Fletcher–Goldfarb–Shanno (BFGS) method is a famous method for this.
- Gauss-Newton method can also be seen as a quasi-Newton method where we approximate the Hessian by 2G_x^TR⁻¹G_x.
- The line search procedure is typically an essential part of quasi-Newton methods.



Convergence Criteria

- When should we terminate iterations in optimization method?
- Various criteria and their combinations are used:
 - The absolute or relative change in the parameter estimate falls below a threshold, e.g.:

$$\|\Delta \mathbf{x}^{(i)}\| < \epsilon_p$$

 The absolute or relative change in the cost falls below a certain threshold, e.g.:

$$\left|\frac{(J(\mathbf{x}^i) - J(\mathbf{x}^{(i+1)}))}{J(\mathbf{x}^i)}\right| < \epsilon_c$$

• A maximum number of iterations is reached.

Summary (1/2)

 The Gauss-Newton update can be scaled with additional parameter γ :

$$\hat{\mathbf{x}}^{(i+1)} = \hat{\mathbf{x}}^{(i)} + \gamma \Delta \hat{\mathbf{x}}^{(i+1)}.$$

The parameter can be found via line search that minimizes

$$J_{\text{WLS}}^{(i)}(\gamma) = J_{\text{WLS}}\left(\hat{\mathbf{x}}^{(i)} + \gamma \Delta \hat{\mathbf{x}}^{(i+1)}\right).$$

- We can also use inexact line search which ensures that the cost is decreased a sufficient amount.
- In Levenberg-Marguardt (LM) algorithm we replace the linear approximation in Gauss–Newton with its regularized version.
- In LM algorithm, we find a suitable regularization parameter λ via an iterative procedure.



Summary (2/2)

 We can also consider regularized nonlinear problems with a simple trick:

$$\begin{split} J_{\text{ReLS}}(\boldsymbol{x}) &= (\boldsymbol{y} - \boldsymbol{g}(\boldsymbol{x}))^T \boldsymbol{R}^{-1} (\boldsymbol{y} - \boldsymbol{g}(\boldsymbol{x})) + (\boldsymbol{m} - \boldsymbol{x})^T \boldsymbol{P}^{-1} (\boldsymbol{m} - \boldsymbol{x}) \\ &= \left(\begin{bmatrix} \boldsymbol{y} \\ \boldsymbol{m} \end{bmatrix} - \begin{bmatrix} \boldsymbol{g}(\boldsymbol{x}) \\ \boldsymbol{x} \end{bmatrix} \right)^T \begin{bmatrix} \boldsymbol{R}^{-1} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{P}^{-1} \end{bmatrix} \left(\begin{bmatrix} \boldsymbol{y} \\ \boldsymbol{m} \end{bmatrix} - \begin{bmatrix} \boldsymbol{g}(\boldsymbol{x}) \\ \boldsymbol{x} \end{bmatrix} \right). \end{split}$$

- Quasi-Newton methods are more general optimization methods that approximate the Hessian in Newton's method.
- Various convergence criteria are available for terminating iterative optimization methods.

