

# Gauss-Newton Optimization and Rotations

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## Abstract

A brief summary of Non-Linear Least Squares, Gauss-Newton optimization, Maximum Likelihood and optimization over  $SO(3)$ .

## 1 Linear Least Squares

We wish to solve the following problem:

$$E(\mathbf{x}) = \frac{1}{2} \mathbf{e}(\mathbf{x})^T \mathbf{e}(\mathbf{x}) \quad (1)$$

We notice that if it happens to be the case that we can express  $\mathbf{e}$  as a linear function of  $\mathbf{x}$ , we get a quadratic with an analytic minimum. In other words, if

$$\mathbf{e}(\mathbf{x}) = \mathbf{A}\mathbf{x} - \mathbf{b}, \quad (2)$$

then

$$E(\mathbf{x}) = \frac{1}{2} (\mathbf{A}\mathbf{x} - \mathbf{b})^T (\mathbf{A}\mathbf{x} - \mathbf{b}) \quad (3)$$

$$= \frac{1}{2} \mathbf{x}^T \mathbf{A}^T \mathbf{A} \mathbf{x} - \mathbf{b}^T \mathbf{A} \mathbf{x} + \mathbf{b}^T \mathbf{b} \quad (4)$$

and taking the gradient  $\frac{dE}{d\mathbf{x}}$  and setting to 0, we arrive at

$$\frac{dE}{d\mathbf{x}} = \frac{d}{d\mathbf{x}} \left( \frac{1}{2} \mathbf{x}^T \mathbf{A}^T \mathbf{A} \mathbf{x} - \mathbf{b}^T \mathbf{A} \mathbf{x} + \mathbf{b}^T \mathbf{b} \right) \quad (5)$$

$$= \mathbf{A}^T \mathbf{A} \mathbf{x} - \mathbf{A}^T \mathbf{b} = \mathbf{0}. \quad (6)$$

Solving this, we arrive at the famous normal equations:

$$\mathbf{A}^T \mathbf{A} \mathbf{x}^* = \mathbf{A}^T \mathbf{b} \quad (7)$$

$$\mathbf{x}^* = (\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T \mathbf{b}. \quad (8)$$

## 2 Nonlinear Least Squares

$$E(\mathbf{x}) = \frac{1}{2} \mathbf{e}(\mathbf{x})^T \mathbf{e}(\mathbf{x}) \quad (9)$$

If  $\mathbf{e}(\mathbf{x})$  is not linear, we can use Gauss-Newton optimization to iteratively find an optimal  $\mathbf{x}$ . We first must be given an initial *operating point*<sup>1</sup>,  $\mathbf{x}_{op}$  and linearize  $\mathbf{e}(\mathbf{x})$  about that point. In other words, determine:

$$\mathbf{e}(\mathbf{x}) = \mathbf{e}(\mathbf{x}_{op} + \delta\mathbf{x}) \quad (10)$$

$$\approx \mathbf{e}(\mathbf{x}_{op}) + \underbrace{\left. \frac{\partial \mathbf{e}}{\partial \mathbf{x}} \right|_{\mathbf{x}_{op}}}_{\mathbf{J}_e} \delta\mathbf{x} \quad (11)$$

$$= \mathbf{e}(\mathbf{x}_{op}) + \mathbf{J}_e \delta\mathbf{x} \quad (12)$$

Now we can write our objective function as a function of  $\delta\mathbf{x}$  instead of  $\mathbf{x}$ :

$$E(\delta\mathbf{x}) = \frac{1}{2} (\mathbf{e}(\mathbf{x}_{op}) + \mathbf{J}_e \delta\mathbf{x})^T (\mathbf{e}(\mathbf{x}_{op}) + \mathbf{J}_e \delta\mathbf{x}), \quad (13)$$

This is a parabola fit at  $\mathbf{x}_{op}$ . Comparing to our linear least squares problem, we can immediately write down the optimal  $\delta\mathbf{x}^*$  as:

$$\mathbf{J}_e^T \mathbf{J}_e \delta\mathbf{x}^* = -\mathbf{J}_e^T \mathbf{e}(\mathbf{x}_{op}) \quad (14)$$

$$\delta\mathbf{x}^* = -(\mathbf{J}_e^T \mathbf{J}_e)^{-1} \mathbf{J}_e^T \mathbf{e}(\mathbf{x}_{op}) \quad (15)$$

Given an  $\delta\mathbf{x}^*$ , we update  $\mathbf{x}_{op}$ ,

$$\mathbf{x}_{op} \leftarrow \mathbf{x}_{op} + \delta\mathbf{x}^* \quad (16)$$

and iterate until convergence<sup>2</sup>.

### 2.1 Multiple error terms

If our criterion looks like this

$$E(\mathbf{x}) = \frac{1}{2} \sum_{i=1}^N \mathbf{e}_i(\mathbf{x})^T \mathbf{e}_i(\mathbf{x}), \quad (17)$$

we can use the linearity of derivatives to re-write Equation (14) as:

$$\left( \sum_{i=1}^N \mathbf{J}_{e_i}^T \mathbf{J}_{e_i} \right) \delta\mathbf{x}^* = - \sum_{i=1}^N \mathbf{J}_{e_i}^T \mathbf{e}_i(\mathbf{x}_{op}) \quad (18)$$

$$\delta\mathbf{x}^* = - \left( \sum_{i=1}^N \mathbf{J}_{e_i}^T \mathbf{J}_{e_i} \right)^{-1} \left( \sum_{i=1}^N \mathbf{J}_{e_i}^T \mathbf{e}_i(\mathbf{x}_{op}) \right) \quad (19)$$

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<sup>1</sup>This is sometimes a non-trivial problem. Bad initial operating points can lead to poor performance.

<sup>2</sup>There are many ways to define convergence, but a straightforward way is to check when  $\|\delta\mathbf{x}^*\|$  falls below some small threshold.

## 2.2 Weighted error terms

If we are given **symmetric** weight matrices,  $\mathbf{W}_i$ , and our criterion looks like this

$$E(\mathbf{x}) = \frac{1}{2} \sum_{i=1}^N \mathbf{e}_i(\mathbf{x})^T \mathbf{W}_i \mathbf{e}_i(\mathbf{x}), \quad (20)$$

we can adapt our normal equations as follows:

$$\left( \sum_{i=1}^N \mathbf{J}_{e_i}^T \mathbf{W}_i \mathbf{J}_{e_i} \right) \delta \mathbf{x}^* = - \sum_{i=1}^N \mathbf{J}_{e_i}^T \mathbf{W}_i \mathbf{e}_i(\mathbf{x}_{op}) \quad (21)$$

$$\delta \mathbf{x}^* = - \left( \sum_{i=1}^N \mathbf{J}_{e_i}^T \mathbf{W}_i \mathbf{J}_{e_i} \right)^{-1} \left( \sum_{i=1}^N \mathbf{J}_{e_i}^T \mathbf{W}_i \mathbf{e}_i(\mathbf{x}_{op}) \right) \quad (22)$$

## 2.3 Relation to Maximum Likelihood

If we assume that each of our errors,  $\mathbf{e}_i$ , is distributed according to the Gaussian density  $\mathcal{N}(\mathbf{0}, \Sigma_i)$ :

$$\mathbf{e}_i(\mathbf{x}) \sim \mathcal{N}(\mathbf{0}, \Sigma_i) \quad (23)$$

and each error is independent of the others, then the likelihood of observing a set of  $N$  errors becomes the product:

$$p(\mathbf{e}_1(\mathbf{x}), \dots, \mathbf{e}_N(\mathbf{x})) = \prod_{i=1}^N p(\mathbf{e}_i(\mathbf{x}); \mathbf{0}, \Sigma_i). \quad (24)$$

To maximize this likelihood, we can take the logarithm of both sides (since its a monotonically increasing function, it doesn't affect the optimization):

$$\log p(\mathbf{e}_1, \dots, \mathbf{e}_N) = \sum_{i=1}^N \log p(\mathbf{e}_i(\mathbf{x}); \mathbf{0}, \Sigma_i). \quad (25)$$

Recalling the definition of a multivariate Gaussian, we have

$$p(\mathbf{e}_i(\mathbf{x})) = \alpha \exp \left\{ -\frac{1}{2} \mathbf{e}_i(\mathbf{x})^T \Sigma_i^{-1} \mathbf{e}_i(\mathbf{x}) \right\} \quad (26)$$

where  $\alpha$  does not depend on  $\mathbf{x}$ . Now we can write the log likelihood as:

$$\log p(\mathbf{e}_1, \dots, \mathbf{e}_N) = - \sum_{i=1}^N \frac{1}{2} \mathbf{e}_i(\mathbf{x})^T \Sigma_i^{-1} \mathbf{e}_i(\mathbf{x}) + C \quad (27)$$

where the constant  $C$  does not depend on  $\mathbf{x}$ . Maximizing the log likelihood is the same as minimizing its negative, so the final maximum likelihood estimate is given by:

$$\mathbf{x}_{ML} = \underset{\mathbf{x}}{\operatorname{argmin}} \{ -\log p(\mathbf{e}_1(\mathbf{x}), \dots, \mathbf{e}_N(\mathbf{x})) \} = \underset{\mathbf{x}}{\operatorname{argmin}} \frac{1}{2} \sum_{i=1}^N \mathbf{e}_i(\mathbf{x})^T \Sigma_i^{-1} \mathbf{e}_i(\mathbf{x}). \quad (28)$$

Looks oddly familiar! If we interpret each  $\mathbf{W}_i$  as the information matrix,  $\Sigma_i^{-1}$ , of a Gaussian multivariate density that describes the probability of drawing a given zero-mean error,  $\mathbf{e}_i$ , then we can use weighted non-linear least squares to arrive at the maximum likelihood estimate. Convenient!

## 2.4 Salient Gauss-Newton Points

1. This vanilla routine only works for unconstrained states and Gauss Newton is only applicable to squared error objectives.
2. We need a good initial guess otherwise we might be stuck in local minima.
3. Notice that Gauss-Newton does not directly fit a quadratic about an operating point (i.e., it does NOT approximate  $E(\mathbf{x} + \delta\mathbf{x})$ ). Instead it linearly approximates  $\mathbf{e}(\mathbf{x}_{op} + \delta\mathbf{x})$  which results in a quadratic cost in  $\delta\mathbf{x}$ . The full Newton's method fits a quadratic to  $E(\mathbf{x})$  about an operating point.
4. Gauss-Newton approximates Newton's method by approximating the Hessian of  $E(\mathbf{x})$  as  $\mathbf{J}_e^T \mathbf{J}_e$  (the full Hessian requires second order derivatives of  $\mathbf{e}(\mathbf{x})$ ).

## 3 Optimizing Rotations

Recall that rotations belong to a special matrix Lie group called the *Special Orthogonal Group*. We can define the group as follows:

$$\text{SO}(3) = \{\mathbf{C} \in \mathbb{R}^{3 \times 3} \mid \mathbf{C}^T \mathbf{C} = \mathbf{1}, \det \mathbf{C} = 1\}. \quad (29)$$

Let's say we have some quadratic objective that includes a rotation. For example, consider finding the rotation matrix that best aligns pairs of vectors,  $\mathbf{u}_i$  and  $\mathbf{v}_i$  both in  $\mathbb{R}^3$ , such that the following objective is minimized (this is called the *Wahba Problem*):

$$E(\mathbf{C}) = \frac{1}{2} \sum_{i=1}^N (\mathbf{C}\mathbf{u}_i - \mathbf{v}_i)^T (\mathbf{C}\mathbf{u}_i - \mathbf{v}_i) \quad (30)$$

$$= \frac{1}{2} \sum_{i=1}^N \mathbf{e}_i(\mathbf{C})^T \mathbf{e}_i(\mathbf{C}) \quad (31)$$

In order to use our non-linear least squares formulation, we'll need to find some way of updating an operating point  $\mathbf{C}_{op}$  with some small update.

### 3.1 Useful notation

For our derivations, the following skew-symmetric cross-product operator will be useful:

$$\mathbf{a}^\times = [\mathbf{a}]_\times = \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix}^\times = \begin{bmatrix} 0 & -a_2 & a_1 \\ a_2 & 0 & -a_0 \\ -a_1 & a_0 & 0 \end{bmatrix}. \quad (32)$$

Note that  $\mathbf{a} \times \mathbf{b} = \mathbf{a}^\times \mathbf{b} = -\mathbf{b}^\times \mathbf{a}$ . Also note that you may see this defined as  $[\mathbf{a}]_\times$  or  $\mathbf{a}^\wedge$ .

### 3.2 Euler Angles

The first way we might consider solving this problem is to use Euler angles. Let's parametrize our rotation matrix with a 1-2-3 Euler angle sequence as:

$$\mathbf{C}(\boldsymbol{\theta}) = \mathbf{C}_3(\theta_3)\mathbf{C}_2(\theta_2)\mathbf{C}_1(\theta_1). \quad (33)$$

Now, our goal will be to start with an operating point  $\boldsymbol{\theta}_{op}$  and solve for  $\delta\boldsymbol{\theta}$  so that we can use the update  $\boldsymbol{\theta}_{op} \leftarrow \boldsymbol{\theta}_{op} + \delta\boldsymbol{\theta}$ .

Beginning with the definition of our error, we derive the following:

$$\mathbf{e}_i(\boldsymbol{\theta}_{op} + \delta\boldsymbol{\theta}) = \mathbf{C}(\boldsymbol{\theta}_{op} + \delta\boldsymbol{\theta})\mathbf{u}_i - \mathbf{v}_i \quad (34)$$

$$\approx \underbrace{\mathbf{C}(\boldsymbol{\theta}_{op})\mathbf{u}_i - \mathbf{v}_i}_{\mathbf{e}_i(\boldsymbol{\theta}_{op})} + \underbrace{\left. \frac{\partial \mathbf{C}\mathbf{u}_i}{\partial \boldsymbol{\theta}} \right|_{\boldsymbol{\theta}_{op}}}_{\mathbf{J}_{e_i}} \delta\boldsymbol{\theta} \quad (35)$$

$$= \mathbf{e}_i(\boldsymbol{\theta}_{op}) + \mathbf{J}_{e_i}\delta\boldsymbol{\theta}. \quad (36)$$

Now, how do we compute  $\frac{\partial \mathbf{C}\mathbf{u}_i}{\partial \boldsymbol{\theta}}$ ? For this, we can either use straight trigonometric differentiation or, we can use the handy relation (refer to (Barfoot, 2017) for more details) that:

$$\begin{aligned} \frac{\partial \mathbf{C}\mathbf{u}_i}{\partial \theta_3} &= [\mathbf{1}_3]_{\times} \mathbf{C}_3(\theta_3)\mathbf{C}_2(\theta_2)\mathbf{C}_1(\theta_1)\mathbf{u}_i \\ \frac{\partial \mathbf{C}\mathbf{u}_i}{\partial \theta_2} &= \mathbf{C}_3(\theta_3) [\mathbf{1}_2]_{\times} \mathbf{C}_2(\theta_2)\mathbf{C}_1(\theta_1)\mathbf{u}_i \\ \frac{\partial \mathbf{C}\mathbf{u}_i}{\partial \theta_1} &= \mathbf{C}_3(\theta_3)\mathbf{C}_2(\theta_2) [\mathbf{1}_1]_{\times} \mathbf{C}_1(\theta_1)\mathbf{u}_i \end{aligned} \quad (37)$$

where  $\mathbf{1}_i$  is the column vector of zeros with 1 in the  $i$ th spot (e.g.,  $\mathbf{1}_3 = [0 \ 0 \ 1]^T$ ). The Jacobian can then be composed as the horizontally stacked columns:

$$\frac{\partial \mathbf{C}\mathbf{u}_i}{\partial \boldsymbol{\theta}} = \begin{bmatrix} \frac{\partial \mathbf{C}\mathbf{u}_i}{\partial \theta_1} & \frac{\partial \mathbf{C}\mathbf{u}_i}{\partial \theta_2} & \frac{\partial \mathbf{C}\mathbf{u}_i}{\partial \theta_3} \end{bmatrix}. \quad (38)$$

Note if we do the optimization this way, we need to watch out that our Euler angles don't approach Gimbal lock!

### 3.2.1 A Tidy Derivation of the Euler Angle Jacobian

We can derive the Euler angle derivatives (Equation (37)) starting from a more general formula for the derivative of an exponential map that is proved in Gallego and Yezzi (2015). Namely, if  $\mathbf{C}(\boldsymbol{\phi}) = \text{Exp}(\boldsymbol{\phi})$ , with  $\boldsymbol{\phi} = [\phi_1 \ \phi_2 \ \phi_3]^T$ , then

$$\frac{\partial \mathbf{C}}{\partial \phi_i} = \frac{\phi_i [\boldsymbol{\phi}]_{\times} + [[\boldsymbol{\phi}]_{\times} (\mathbf{1} - \mathbf{C})\mathbf{1}_i]_{\times}}{\|\boldsymbol{\phi}\|^2} \mathbf{C}, \quad (39)$$

where  $\mathbf{1}_i$  has the same column-vector definition as above.

Now, in our 1-2-3 Euler sequence, we can re-write our principal rotation matrices using the exponential map:

$$\mathbf{C}(\boldsymbol{\theta}) = \mathbf{C}_3(\theta_3)\mathbf{C}_2(\theta_2)\mathbf{C}_1(\theta_1) \quad (40)$$

$$\mathbf{C}(\boldsymbol{\theta}) = \text{Exp} \left( \begin{bmatrix} 0 \\ 0 \\ \theta_3 \end{bmatrix} \right) \text{Exp} \left( \begin{bmatrix} 0 \\ \theta_2 \\ 0 \end{bmatrix} \right) \text{Exp} \left( \begin{bmatrix} \theta_1 \\ 0 \\ 0 \end{bmatrix} \right). \quad (41)$$

Note that because the Lie bracket of  $\text{SO}(3)$  is not 0 (in other words, rotations do not commute), we **cannot** simplify the above to  $\text{Exp}\left([\theta_1 \ \theta_2 \ \theta_3]^T\right)$ . We could however, attempt to use the Baker-Campbell-Hausdorff (BCH) formula to simplify the above to a single exponential vector, but I am not sure that would result in anything analytic.

Instead, we can take the following approach. Note that

$$\begin{aligned}\frac{\partial \mathbf{C}}{\partial \theta_3} &= \frac{\partial \mathbf{C}_3}{\partial \theta_3} \mathbf{C}_2(\theta_2) \mathbf{C}_1(\theta_1) \\ \frac{\partial \mathbf{C}}{\partial \theta_2} &= \mathbf{C}_3(\theta_3) \frac{\partial \mathbf{C}_2}{\partial \theta_2} \mathbf{C}_1(\theta_1) \\ \frac{\partial \mathbf{C}}{\partial \theta_1} &= \mathbf{C}_3(\theta_3) \mathbf{C}_2(\theta_2) \frac{\partial \mathbf{C}_1}{\partial \theta_1}.\end{aligned}\tag{42}$$

Using Equation (39), we can show that  $\frac{\partial \mathbf{C}_i}{\partial \theta_i}$  has a very simple expression. Notice that if  $\phi$  has the structure  $\phi = \theta_i \mathbf{1}_i$ , then

$$[[\phi]_{\times} (\mathbf{1} - \mathbf{C}) \mathbf{1}_i]_{\times} = [\theta_i [\mathbf{1}_i]_{\times} \mathbf{1}_i - \theta_i [\mathbf{1}_i]_{\times} \mathbf{C}_i \mathbf{1}_i]_{\times} = [\mathbf{0} - \mathbf{0}]_{\times} = \mathbf{0},\tag{43}$$

where we have used the fact that  $\mathbf{C}_i \mathbf{1}_i = \mathbf{1}_i$  since  $\mathbf{C}_i$  rotates about  $\mathbf{1}_i$ . Thus, Equation (39) becomes

$$\frac{\partial \mathbf{C}_i}{\partial \theta_i} = \frac{\theta_i [\theta_i \mathbf{1}_i]_{\times}}{\|\theta\|^2} \mathbf{C}_i = \frac{\theta_i^2 [\mathbf{1}_i]_{\times}}{\theta_i^2} \mathbf{C}_i = [\mathbf{1}_i]_{\times} \mathbf{C}_i,\tag{44}$$

which combined with Equation (42) results in the required simple expression for the Jacobian. This completes the derivation.

### 3.3 Small Angle-Axis Perturbations

An alternative formulation is to keep our representation of rotations in matrix form (this will avoid Gimbal lock) but to change our update rule. Instead, let's look for a three-parameter small 'angle-axis' vector  $\delta\phi$ , such that we can update an operating point,  $\mathbf{C}_{op}$  in the following way.

Recall that the Euler's theorem tell's us that any rotation can be represented as an axis of rotation,  $\hat{\mathbf{n}}$  and a rotation about that axis,  $\phi$ . Combining both into a single vector,  $\phi = \phi \hat{\mathbf{n}}$ , we can convert this to a rotation matrix using the Euler-Rodriguez formula:

$$\mathbf{C}(\phi) = \mathbf{1} + \sin \phi [\hat{\mathbf{n}}]_{\times} + (1 - \cos \phi) [\hat{\mathbf{n}}]_{\times}^2.\tag{45}$$

If  $\phi = \delta\phi$  is small, we have

$$\mathbf{C}(\delta\phi) \approx \mathbf{1} + \delta\phi [\hat{\mathbf{n}}]_{\times} = \mathbf{1} + [\delta\phi]_{\times}.\tag{46}$$

Recall that to linearize a non linear function of vector quantities, we used the expression ' $\mathbf{x} = \mathbf{x}_{op} + \delta\mathbf{x}$ '. We can write down an analogous expression for rotations using left perturbations:

$$\mathbf{C} = \mathbf{C}(\delta\phi) \mathbf{C}_{op} \approx (\mathbf{1} + [\delta\phi]_{\times}) \mathbf{C}_{op}\tag{47}$$

Now we can substitute the rotation for the perturbed rotation, and derive a Jacobian in the following way:

$$\mathbf{e}_i(\delta\phi) \approx (\mathbf{1} + [\delta\phi]_{\times})\mathbf{C}_{op}\mathbf{u}_i - \mathbf{v}_i \quad (48)$$

$$= \mathbf{C}_{op}\mathbf{u}_i - \mathbf{v}_i + [\delta\phi]_{\times} \mathbf{C}_{op}\mathbf{u}_i \quad (49)$$

$$= \mathbf{e}_i(\mathbf{C}_{op}) - \underbrace{[\mathbf{C}_{op}\mathbf{u}_i]_{\times}}_{\mathbf{J}_{e_i}} \delta\phi \quad (50)$$

$$= \mathbf{e}_i(\mathbf{C}_{op}) + \mathbf{J}_{e_i} \delta\phi. \quad (51)$$

where we have used the fact that  $[\mathbf{a}]_{\times} \mathbf{b} = -[\mathbf{b}]_{\times} \mathbf{a}$ . Now we can update our operating point as  $\mathbf{C}_{op} \leftarrow \mathbf{C}(\delta\phi)\mathbf{C}_{op}$  until convergence.

Another way to see this is to derive the Jacobian a bit more directly. Consider that for a 'small' rotation, we can use our small-angle approximation to derive that,

$$\frac{\partial \mathbf{C}(\delta\phi)\mathbf{u}}{\partial \delta\phi} = \frac{\partial}{\partial \delta\phi} (\mathbf{1} + [\delta\phi]_{\times})\mathbf{u} = \frac{\partial}{\partial \delta\phi} (\mathbf{u} - [\mathbf{u}]_{\times} \delta\phi) = -[\mathbf{u}]_{\times}, \quad (52)$$

This then allows us to write:

$$\frac{\partial \mathbf{C}\mathbf{u}}{\partial \delta\phi} = \frac{\partial \mathbf{C}(\delta\phi)\mathbf{C}_{op}\mathbf{u}}{\partial \delta\phi} \quad (53)$$

$$= -[\mathbf{C}_{op}\mathbf{u}]_{\times}, \quad (54)$$

which we can use as our Jacobian to solve for  $\delta\phi$ .

## References

Barfoot, T. D. (2017). *State Estimation for Robotics*. Cambridge University Press.

Gallego, G. and Yezzi, A. (2015). A compact formula for the derivative of a 3-D rotation in exponential coordinates. *J. Math. Imaging Vis.*, 51(3):378–384.