Appendix A
Math Appendix

A.1 Representing Rotations

A.1.1 Euler Angles

Besides the three Cartesian coordinates x, y and z describing the position, the three angles θ_x, θ_y and θ_z describe the orientation in $\mathbb{R}^3$. Position and orientation are referred as pose. The orientation θ_x, θ_y and θ_z is the rotation about the principal axes, i.e., $(1,0,0)$, $(0,1,0)$ and $(0,0,1)$. The rotation matrices are given as follows:

$$\boldsymbol{R}_x = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta_x & -\sin\theta_x \\ 0 & \sin\theta_x & \cos\theta_x \end{pmatrix}$$

$$\boldsymbol{R}_y = \begin{pmatrix} \cos\theta_y & 0 & \sin\theta_y \\ 0 & 1 & \\ -\sin\theta_y & 0 & \cos\theta_y \end{pmatrix}$$

$$\boldsymbol{R}_z = \begin{pmatrix} \cos\theta_y & -\sin\theta_y & 0 \\ \sin\theta_y & \cos\theta_y & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

The overall rotation matrix is computed as $\boldsymbol{R} = \boldsymbol{R}_{\theta_x,\theta_y,\theta_z} = \boldsymbol{R}_x \boldsymbol{R}_y \boldsymbol{R}_z$, i.e.,

$$\boldsymbol{R} = \begin{pmatrix} \cos\theta_y\cos\theta_z & -\cos\theta_y\sin\theta_z & \sin\theta_y \\ \cos\theta_z\sin\theta_x\sin\theta_y + \cos\theta_x\sin\theta_z & \cos\theta_x\cos\theta_z - \sin\theta_x\sin\theta_y\sin\theta_z & -\cos\theta_y\sin\theta_x \\ \sin\theta_x\sin\theta_z - \cos\theta_x\cos\theta_z\sin\theta_y & \cos\theta_z\sin\theta_x + \cos\theta_x\sin\theta_y\sin\theta_z & \cos\theta_x\cos\theta_y \end{pmatrix}.$$

Note: The matrix above depends on the order of the multiplication. Different rotation matrices are achieved by $\boldsymbol{R} = \boldsymbol{R}_{\theta_z,\theta_y,\theta_x} = \boldsymbol{R}_z\boldsymbol{R}_y\boldsymbol{R}_x$ or $\boldsymbol{R} = \boldsymbol{R}_{\theta_y,\theta_x,\theta_z} = \boldsymbol{R}_y\boldsymbol{R}_x\boldsymbol{R}_z$, etc. Furthermore, note that a gimbal lock occurs when the axes of two of the three angles needed to compensate for rotations in three dimensional space are driven to the same direction.

A.1.2 Axis Angle

Rotations can be represented as a rotation axis and a rotation angle as given in Figure A.1. Given a unit vector $\boldsymbol{n} = (n_x, n_y, n_z)^T$ and an angle φ then the rotation of $\boldsymbol{p}$ to $\boldsymbol{p}' = \boldsymbol{q}$ is given by

$$\begin{aligned}\boldsymbol{p}' &= \overrightarrow{\boldsymbol{on}} + \overrightarrow{\boldsymbol{nv}} + \overrightarrow{\boldsymbol{vq}}\\ &= \boldsymbol{n}(\boldsymbol{n}\cdot\boldsymbol{r}) + (\boldsymbol{r} - \boldsymbol{n}(\boldsymbol{n}\cdot\boldsymbol{r}))\cos\theta + (\boldsymbol{r}\times\boldsymbol{n})\sin\theta\\ &= \boldsymbol{p}\cos\theta + \boldsymbol{n}(\boldsymbol{n}\cdot\boldsymbol{r})(1-\cos\theta) + (\boldsymbol{r}\times\boldsymbol{n})\sin\theta. \end{aligned} \tag{A.1}$$

The resulting term written as rotation matrix is

$$\boldsymbol{R}_{\boldsymbol{n},\theta} = \mathbb{1}_3 + (\boldsymbol{N})\sin\theta + (\boldsymbol{N})^2(1-\cos\theta)$$

where $\boldsymbol{N}$ is defined as follows

$$\boldsymbol{N} = \begin{pmatrix} 0 & -n_z & n_y \\ n_z & 0 & -n_x \\ -n_y & n_x & 0 \end{pmatrix}.$$

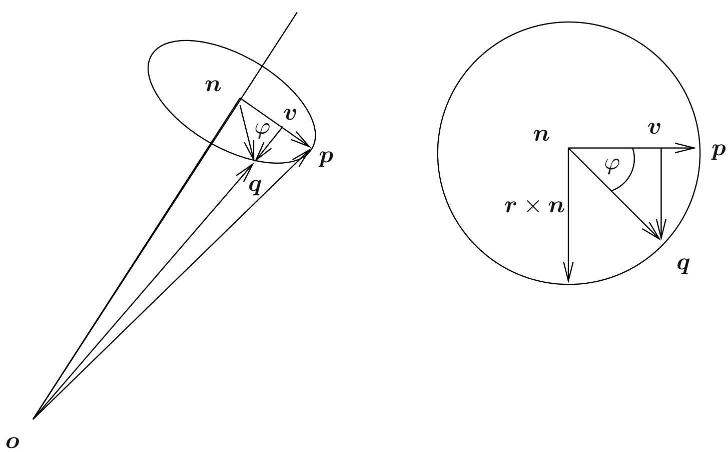

Fig. A.1 Axis angle representation of a rotation

The matrix $\boldsymbol{R}_{\boldsymbol{n},\theta}$ is

$$\boldsymbol{R}_{\boldsymbol{n},\theta} = \begin{pmatrix} (1-\cos\theta)n_x^2+\cos\theta & (1-\cos\theta)n_x n_y + n_z\sin\theta & (1-\cos\theta)n_x n_z - n_y\sin\theta \\ (1-\cos\theta)n_x n_y - n_z\sin\theta & (1-\cos\theta)n_y^2+\cos\theta & (1-\cos\theta)n_y n_z + n_x\sin\theta \\ (1-\cos\theta)n_x n_z + n_y\sin\theta & (1-\cos\theta)n_y n_z - n_x\sin\theta & (1-\cos\theta)n_z^2+\cos\theta \end{pmatrix}.$$

A.1.3 Unit Quaternions

Quaternions are 4 dimensional complex numbers that may be used for representing rotations in 3D. They are generated by postulating an additional root of -1 that is named j and which is not i or $-i$. Then there exists necessarily the element k, such that $ij = k$, which is also a root of -1. The following relations hold true:

$$\begin{aligned} i^2 = j^2 &= k^2 = ijk &= -1 \\ ij = k, & \quad ji &= -k \\ jk = i, & \quad kj &= -i \\ ki = j, & \quad ik &= -j. \end{aligned}$$

i, j, k and -1 form a basis of the quaternion $\mathbb{H}$, that is named after the scientist Sir William Rowan Hamilton who had the idea on October 16 1843, while he was out walking along the Royal Canal in Dublin with his wife when the solution in the form of the equation $i^2 = j^2 = k^2 = ijk = -1$ suddenly occurred to him [55]. It is said, Hamilton then promptly carved this equation into the side of the nearby Broom Bridge.

All quaternion $\dot{\boldsymbol{q}}$ may be represented as $\dot{\boldsymbol{q}} = q_0 + q_x i + q_y j + q_z k$. Thus every quaternion defines uniquely a 4-vector $(q_0, q_x, q_y, q_z)^T \in \mathbb{R}^4$. A quaternion may be written as:

$$\dot{\boldsymbol{q}} = q_0 + q_x i + q_y j + q_z k = (q_0, q_x, q_y, q_z)^T = (q_0, \boldsymbol{q})^T = \begin{pmatrix} q_0 \\ q_y \\ q_x \\ q_z \end{pmatrix},$$

where real numbers are used as entries.

Similarly as the complex numbers, quaternions have the conjugation of the elements. The conjugate quaternion of $\dot{\boldsymbol{q}} = q_0 + q_x i + q_y j + q_z k$ is written as $\dot{\boldsymbol{q}}^*$ and is computed by negating all non-reel parts, i.e., $\dot{\boldsymbol{q}}^* = q_0 - q_x i - q_y j - q_z k = [q_0, -\boldsymbol{q}]$. Using the conjugate quaternion the norm of the quaternion is computed.

$$\|\dot{\boldsymbol{q}}\| = \sqrt{\langle \dot{\boldsymbol{q}}, \dot{\boldsymbol{q}}^* \rangle} = \sqrt{q_0^2 + q_x^2 + q_y^2 + q_z^2}.$$

Here the scalar product has been used. For quaternions, there are many kinds of multiplications defined, which is not in the scope of this section. We will need only the following non-commutative multiplication rule for two given quaternions $\dot{\boldsymbol{p}} = p_0 + p_x i + p_y j + p_z k$ and $\dot{\boldsymbol{q}} = q_0 + q_x i + q_y j + q_z k$:

$$\begin{aligned}
\dot{\boldsymbol{p}}\dot{\boldsymbol{q}} &= (p_0 + p_x i + p_y j + p_z k)(q_0 + q_x i + q_y j + q_z k) \\
&= (p_0 q_0 - p_x q_x - p_y q_y - p_z q_z) \\
&\quad + (p_0 q_x + p_x q_0 + p_y q_z - p_z q_y) i \\
&\quad + (p_0 q_y + p_x q_z + p_y q_0 - p_z q_x) j \\
&\quad + (p_0 q_z + p_x q_y + p_y q_x - p_z q_0) k \\
&= (p_0, \boldsymbol{p})(q_0, \boldsymbol{q}) \\
&= (p_0 q_0 - \boldsymbol{p} \cdot \boldsymbol{q}, \boldsymbol{p} \times \boldsymbol{q} + p_0 \boldsymbol{q} + q_0 \boldsymbol{p}).
\end{aligned}$$

A subset of the quaternions, namely the unit quternions are important, since they represent rotations. For a unit quaternion $\dot{\boldsymbol{q}}$o holds: $\|\dot{\boldsymbol{q}}\| = 1$. The unit quaternion has the property, that the inverse element $\dot{\boldsymbol{q}}^{-1}$ equals the conjugate elements $\dot{\boldsymbol{q}}^*$ using the above defined product. It is

$$\langle \dot{\boldsymbol{q}}, \dot{\boldsymbol{q}}^* \rangle = \|\dot{\boldsymbol{q}}\|^2 = 1.$$

Rotations using unit quaternions are represented as follows: Let $\dot{\boldsymbol{q}}$ be $\dot{\boldsymbol{q}} = (q_0, q_x, q_y, q_z) = (q_0, \boldsymbol{q})$. For the rotation of the 3D point $\boldsymbol{p} = (p_x, p_y, p_z)^T \in \mathbb{R}^3$ we write this point as quaternion, too, i.e., $\dot{\boldsymbol{p}} = (0, p_x, p_y, p_z)^T = (0, \boldsymbol{p})$. Then for the rotated point p_{rot} we have

$$\boldsymbol{p}_{\text{rot}} = \dot{\boldsymbol{q}}\dot{\boldsymbol{p}}\dot{\boldsymbol{q}}^*.$$

To show that the above formulation corresponds to a rotation, we rewrite the term to (For a detailed derivation please see [22].)

$$\begin{aligned}
p_{\text{rot}} &= \dot{\boldsymbol{q}}\dot{\boldsymbol{p}}\dot{\boldsymbol{q}}^* \\
&= (q_0, \boldsymbol{q})(0, \boldsymbol{p})(q_0, \boldsymbol{q})^* \\
&= (q_0, \boldsymbol{q})(0, \boldsymbol{p})(q_0, -\boldsymbol{q}) \\
&= (q_0, \boldsymbol{q})(\boldsymbol{q}, q_0 \boldsymbol{p} - \boldsymbol{p} \times \boldsymbol{q}) \\
&= (q_0(\boldsymbol{q} \cdot \boldsymbol{p}) - \boldsymbol{q} \cdot (q_0 \boldsymbol{p} - \boldsymbol{p} \times \boldsymbol{q}), \\
&\qquad q_0(q_0 \boldsymbol{p} - \boldsymbol{p} \times \boldsymbol{q}) + (\boldsymbol{q} \cdot \boldsymbol{p})\boldsymbol{q} + \boldsymbol{q} \times (q_0 \boldsymbol{p} - \boldsymbol{p} \times \boldsymbol{q})) \\
&= (0, q_0^2 \boldsymbol{p} + (\boldsymbol{q} \cdot \boldsymbol{p})\boldsymbol{q} - (\boldsymbol{q} \cdot \boldsymbol{q})\boldsymbol{p} + (\boldsymbol{q} \cdot \boldsymbol{p})\boldsymbol{q} + 2q_0(\boldsymbol{q} \times \boldsymbol{p})) \\
&= (0, (q_0^2 - \boldsymbol{q} \cdot \boldsymbol{q})\boldsymbol{p} + 2(\boldsymbol{q} \cdot \boldsymbol{p})\boldsymbol{q} + 2q_0(\boldsymbol{q} \times \boldsymbol{p})).
\end{aligned}$$

Rewriting the unit quaterion $\dot{\boldsymbol{q}}$ as $\dot{\boldsymbol{q}} = (\cos\theta, \sin\theta \boldsymbol{n})$ yields:

$$\begin{aligned}\boldsymbol{p}_{\text{rot}} &= (0, (\cos^2\theta - \sin^2\theta(\boldsymbol{n}\cdot\boldsymbol{n}))\boldsymbol{p} + 2((\sin\theta)\boldsymbol{n}\cdot\boldsymbol{p})\\ &\qquad (\sin\theta)\boldsymbol{n} + 2\cos\theta((\sin\theta)\boldsymbol{n}\times\boldsymbol{p}))\\ &= (0, \cos 2\theta + (1-\cos 2\theta)(\boldsymbol{n}\cdot\boldsymbol{p})\boldsymbol{n} + (\boldsymbol{n}\times\boldsymbol{p})\sin 2\theta).\end{aligned}$$

The equation above has the same form as Eq. (A.1). Therefore unit quaternions are similar to the axis angle representation. To represent a rotation about the axis $\boldsymbol{n}$ with the angle θ using a unit quaternion $\dot{\boldsymbol{q}}$ one has to calculate:

$$\dot{\boldsymbol{q}} = \left(\cos\frac{\theta}{2}, \sin\frac{\theta}{2}\boldsymbol{n}\right).$$

To compute the rotation matrix $\boldsymbol{R}_q$ for a given quaternion $\dot{\boldsymbol{q}} = (q_0, q_x, q_y, q_z)$ we look at the components of $\boldsymbol{p}_{\text{rot}}$:

$$\begin{aligned}\boldsymbol{p}_{\text{rot}} &= \dot{\boldsymbol{q}}\dot{\boldsymbol{p}}\dot{\boldsymbol{q}}^*\\ &= \begin{pmatrix} 0\\ q_0^2p_x + q_x^2p_x - (q_y^2+q_z^2)p_x + q_0(-2q_zp_y + 2q_yp_z) + 2q_x(q_yp_y + q_zp_z)\\ 2q_xq_yp_x + 2q_0q_zp_x + q_0^2p_y - q_x^2p_y + q_y^2p_y - q_z^2p_y - 2q_0q_xp_z + 2q_yq_zp_z\\ -2q_0q_yp_x + 2q_xq_zp_x + 2q_0q_xp_y + 2q_yq_zp_y + q_0^2p_z - q_x^2p_z - q_y^2p_z + q_z^2p_z \end{pmatrix}\\ &= \begin{pmatrix} 0\\ p_{x,\text{rot}}\\ p_{y,\text{rot}}\\ p_{z,\text{rot}} \end{pmatrix}.\end{aligned}$$

This can be rewritten using matrix notation with the rotation matrix $\boldsymbol{R}_q$ as:

$$\begin{aligned}\boldsymbol{p}_{\text{rot}} &= \boldsymbol{R}_q\boldsymbol{p}\\ &= \begin{pmatrix} p_0^2+p_x^2-p_y^2-p_z^2 & 2p_xp_y - 2p_0p_z & 2p_xp_z + 2p_0p_y\\ 2p_0p_z + 2p_xp_y & p_0^2-p_x^2+p_y^2-p_z^2 & 2p_yp_z - 2p_0p_x\\ 2p_xp_z - 2p_0p_y & 2p_0p_x + 2p_yp_z & p_0^2-p_x^2-p_y^2+p_z^2 \end{pmatrix}\begin{pmatrix} p_x\\ p_y\\ p_z\end{pmatrix}\\ &= \begin{pmatrix} p_{x,\text{rot}}\\ p_{y,\text{rot}}\\ p_{z,\text{rot}}\end{pmatrix}.\end{aligned}$$

A.1.4 Converting Rotation Representations

In many cases we have to convert one representation of a rotation into a different one, to exploit the advantages as appropriate. As already mentioned converting the axis angle representation of a rotation is performed by (rotation axis $\boldsymbol{n} = (n_x, n_y, n_z)^T$, angle θ):

$$\dot{\boldsymbol{q}} = \left(\cos\frac{\theta}{2}, \sin\frac{\theta}{2}n_x, \sin\frac{\theta}{2}n_y, \sin\frac{\theta}{2}n_z\right)^T = \left(\cos\frac{\theta}{2}, \sin\frac{\theta}{2}\boldsymbol{n}\right).$$

Converting a quaternion to axis angle representation is trival:

$$\begin{aligned}\theta &= 2\arccos q_0\\ n_x &= \frac{q_x}{\sin\theta}\\ n_y &= \frac{q_y}{\sin\theta}\\ n_z &= \frac{q_z}{\sin\theta}.\end{aligned}$$

To derive a quaternion $\dot{\boldsymbol{q}} = (q_0, q_x, q_y, q_z)$ from the three Euler angles $(\theta_x, \theta_y, \theta_z)^T$ we use the quaternion multiplication rule. Firstly we represent the single rotations of the Euler angles by quaternions and compute the resulting quaternion b multiplication, afterwards. Since the Euler angle rotate around the axis of the coordinate system the quaternions $\dot{\boldsymbol{q}}_x$,$\dot{\boldsymbol{q}}_y$ und $\dot{\boldsymbol{q}}_z$ are:

$$\dot{\boldsymbol{q}}_x = \begin{pmatrix}\cos\frac{\theta_x}{2}\\ \sin\frac{\theta_x}{2}\\ 0\\ 0\end{pmatrix}, \dot{\boldsymbol{q}}_y = \begin{pmatrix}\cos\frac{\theta_y}{2}\\ 0\\ \sin\frac{\theta_y}{2}\\ 0\end{pmatrix}, \dot{\boldsymbol{q}}_z = \begin{pmatrix}\cos\frac{\theta_z}{2}\\ 0\\ 0\\ \sin\frac{\theta_z}{2}\end{pmatrix}.$$

The over-all rotation is given by the quaternion $\dot{\boldsymbol{q}}$ as:

$$\dot{\boldsymbol{q}} = \dot{\boldsymbol{q}}_z\dot{\boldsymbol{q}}_y\dot{\boldsymbol{q}}_x = \begin{pmatrix}\cos\frac{\theta_x}{2}\cos\frac{\theta_y}{2}\cos\frac{\theta_z}{2} + \sin\frac{\theta_x}{2}\sin\frac{\theta_y}{2}\sin\frac{\theta_z}{2}\\ \sin\frac{\theta_x}{2}\cos\frac{\theta_y}{2}\cos\frac{\theta_z}{2} - \cos\frac{\theta_x}{2}\sin\frac{\theta_y}{2}\sin\frac{\theta_z}{2}\\ \cos\frac{\theta_x}{2}\sin\frac{\theta_y}{2}\cos\frac{\theta_z}{2} + \sin\frac{\theta_x}{2}\cos\frac{\theta_y}{2}\sin\frac{\theta_z}{2}\\ \cos\frac{\theta_x}{2}\cos\frac{\theta_y}{2}\sin\frac{\theta_z}{2} - \sin\frac{\theta_x}{2}\sin\frac{\theta_y}{2}\cos\frac{\theta_z}{2}\end{pmatrix}.$$

The Euler angles corresponding to a quaternion are accordingly:

$$\begin{pmatrix}\theta_x\\ \theta_y\\ \theta_z\end{pmatrix} = \begin{pmatrix}\arctan\frac{2(p_0p_x+p_yp_z)}{1-2(p_x^2+p_y^2)}\\ \arcsin 2(p_0c - p_xp_z)\\ \arctan\frac{2(p_0p_z+p_xp_y)}{1-2(p_y^2+p_z^2)}\end{pmatrix}.$$

A.2 Plücker Coordinates

Given that G is a straight line in $\mathbb{R}^3$ and $\boldsymbol{p}$ an arbitrary point on G. Furthermore $\boldsymbol{g}$ is a direction vector and $\bar{\boldsymbol{g}} = \boldsymbol{p} \times \boldsymbol{g}$ is the momentum vector of the line G. The six entries of the concatenated vector $(\boldsymbol{g}, \bar{\boldsymbol{g}})$ are called Plücker coordinates of G. They have the following properties [59]:

- The momentum vector is independent of the choice of $\boldsymbol{p}$ on G. If one chooses an additional point $P\boldsymbol{p}' = \boldsymbol{p} + \lambda\boldsymbol{g}$ on the line G then it follows:

$$\boldsymbol{p}' \times \boldsymbol{g} = (\boldsymbol{p} + \lambda\boldsymbol{g}) \times \boldsymbol{g} = \boldsymbol{p} \times \boldsymbol{g}$$

- The Plücker Coordinates are homogeneous coordinates, since a direction vector $\boldsymbol{g}' = \lambda\boldsymbol{g}$ implies a momentum vector $\bar{\boldsymbol{g}}' = \boldsymbol{p} \times \boldsymbol{g}' = \lambda(\boldsymbol{p} \times \boldsymbol{g}) = \lambda\bar{\boldsymbol{g}}$. Therefore $\lambda(\boldsymbol{g}, \bar{\boldsymbol{g}})$ describes the same lines als $(\boldsymbol{g}, \bar{\boldsymbol{g}})$.
- The Plücker condition $\boldsymbol{g}^T\bar{\boldsymbol{g}} = 0$ holds true.

A.3 Additional Theorems from Linear Algebra

The following theorems originate from [62] (see also [32]) and generalize the theorems of section 4.1.1.

Lemma 7. *Given the orthonormal matrix $\boldsymbol{R}$. Then for every vector $\boldsymbol{x}$ holds:*

$$(\boldsymbol{R}\boldsymbol{x}) \cdot \boldsymbol{x} \leq \boldsymbol{x} \cdot \boldsymbol{x}.$$

The two terms are equal, if $\boldsymbol{R}\boldsymbol{x} = \boldsymbol{x}$.

Proof. It holds

$$(\boldsymbol{R}\boldsymbol{x}) \cdot (\boldsymbol{R}\boldsymbol{x}) = (\boldsymbol{R}\boldsymbol{x})^T(\boldsymbol{R}\boldsymbol{x}) = \boldsymbol{x}^T\boldsymbol{R}^T\boldsymbol{R}\boldsymbol{x} = \boldsymbol{x}^T\boldsymbol{x} = \boldsymbol{x} \cdot \boldsymbol{x},$$

since $\boldsymbol{R}^T\boldsymbol{R} = \mathbb{1}$. Furthermore we have

$$\begin{aligned}(\boldsymbol{R}\boldsymbol{x} - \boldsymbol{x}) \cdot (\boldsymbol{R}\boldsymbol{x} - \boldsymbol{x}) &= (\boldsymbol{R}\boldsymbol{x}) \cdot (\boldsymbol{R}\boldsymbol{x}) - 2(\boldsymbol{R}\boldsymbol{x}) \cdot \boldsymbol{x} + \boldsymbol{x} \cdot \boldsymbol{x} \\ &= 2(\boldsymbol{x} \cdot \boldsymbol{x} - (\boldsymbol{R}\boldsymbol{x}) \cdot \boldsymbol{x}). \end{aligned} \tag{A.2}$$

Because $(\boldsymbol{R}\boldsymbol{x} - \boldsymbol{x}) \cdot (\boldsymbol{R}\boldsymbol{x} - \boldsymbol{x}) \geq 0$ the lemma is proven. The equality if given, if $(\boldsymbol{R}\boldsymbol{x} - \boldsymbol{x}) \cdot (\boldsymbol{R}\boldsymbol{x} - \boldsymbol{x}) = 0$ is the case. According to Eq. (A.2) this only happens if, $\boldsymbol{R}\boldsymbol{x} = \boldsymbol{x}$. □

Lemma 8. *Every positive semi-definite $n \times n$ matrix $\boldsymbol{S}$ can be written using the orthonormal set of vectors $\{\boldsymbol{u}_i\}$ as*

$$\boldsymbol{S} = \sum_{i=1}^{n} \boldsymbol{u}_i\boldsymbol{u}_i^T.$$

Proof. If the eigenvalues of $\boldsymbol{S}$ are $\{\lambda_i\}$. The corresponding set of eigenvectors are $\{\hat{\boldsymbol{u}}_i\}$. Then matrix $\boldsymbol{S}$ is given by

$$\boldsymbol{S} = \sum_{i=1}^{n} \lambda_i \hat{\boldsymbol{u}}_i \hat{\boldsymbol{u}}_i^T .$$

Since, the eigenvalues of a positive semi-definite matrix are not negative, the claim of the lemma is derived with $\boldsymbol{u}_i = \sqrt{\lambda_i} \hat{\boldsymbol{u}}_i$. □

Lemma 9. *Suppose $\boldsymbol{S}$ is a positive semi-definite matrix. The for all orthonormal matrices $\boldsymbol{R}$ holds*

$$tr(\boldsymbol{RS}) \leq tr(\boldsymbol{S}) ,$$

where the equality is the case, if $\boldsymbol{RS} = \boldsymbol{S}$.

Proof. If $\boldsymbol{S}$ is represented according to lemma 8. Since $\mathrm{tr}\left(\boldsymbol{a}\boldsymbol{b}^T\right) = \boldsymbol{a} \cdot \boldsymbol{b}$ holds, it follows

$$\mathrm{tr}\,(\boldsymbol{S}) = \sum_{i=1}^{n} \boldsymbol{u}_i \cdot \boldsymbol{u}_i \qquad \text{and} \qquad \mathrm{tr}\,(\boldsymbol{RS}) = \sum_{i=1}^{n} (\boldsymbol{R}\boldsymbol{u}_i) \cdot \boldsymbol{u}_i,$$

where the last equation is according to lemma 7 smaller or equal of the trace $\mathrm{tr}\,(\boldsymbol{S})$. Equality if given for $\boldsymbol{R}\boldsymbol{u}_i = \boldsymbol{u}_i$, i.e., if $\boldsymbol{RS} = \boldsymbol{S}$, because $\boldsymbol{S}\boldsymbol{u}_i = \boldsymbol{u}_i$ holds. □

Corollary 1. *If $\boldsymbol{S}$ is a positive definite matrix, then it holds for every orthonormal matrix $\boldsymbol{R}$*

$$tr(\boldsymbol{RS}) \leq tr(\boldsymbol{S}) .$$

The equality is the case, if $\boldsymbol{R} = \mathbb{1}$, i.e, $\boldsymbol{R}$ is the identity matrix. □

Lemma 10. *The matrix $\boldsymbol{T}$ is the positive semi-definite square root of the positive definite matrix $\boldsymbol{S}$:*

$$\boldsymbol{T} = \sum_{i=1}^{n} \sqrt{\lambda_i} \hat{\boldsymbol{u}}_i \hat{\boldsymbol{u}}_i^T \qquad \textit{and} \qquad \boldsymbol{S} = \sum_{i=1}^{n} \lambda_i \hat{\boldsymbol{u}}_i \hat{\boldsymbol{u}}_i^T ,$$

where $\{\lambda_i\}$ is the set of eigenvalues and $\{\hat{\boldsymbol{u}}_i\}$ the set of orthonormal unit eigenvectors of $\boldsymbol{S}$.

Proof. We have

$$\boldsymbol{T}^2 = \left(\sum_{i=1}^{n} \sqrt{\lambda_i} \hat{\boldsymbol{u}}_i \hat{\boldsymbol{u}}_i^T \right) \left(\sum_{j=1}^{n} \sqrt{\lambda_j} \hat{\boldsymbol{u}}_j \hat{\boldsymbol{u}}_j^T \right) = \sum_{i=1}^{n} \sum_{j=1}^{n} \sqrt{\lambda_i \lambda_j} \left(\hat{\boldsymbol{u}}_i \cdot \hat{\boldsymbol{u}}_j \right) \hat{\boldsymbol{u}}_i \hat{\boldsymbol{u}}_j^T$$

$$= \sum_{k=1}^{n} \lambda_k \hat{\boldsymbol{u}}_k \hat{\boldsymbol{u}}_k^T = \boldsymbol{S},$$

since $\hat{\boldsymbol{u}}_i \cdot \hat{\boldsymbol{u}}_j = 0$ holds for $i \neq j$. Furthermore we have

$$\boldsymbol{x}\boldsymbol{T}\boldsymbol{x} = \sum_{i=1}^{n} \lambda_i (\hat{\boldsymbol{u}}_i \cdot \boldsymbol{x})^2 \leq 0,$$

since the eigenvalues are $\lambda_i \geq 0$. Therefore $\boldsymbol{T}$ positive semi-definite. □

Corollary 2. *There exists a positive semi-definite square root matrix for all positive semi-definite matices.* □

Corollary 3. *The matrix*

$$\boldsymbol{T}^{-1} = \sum_{i=1}^{n} \frac{1}{\sqrt{\lambda_i}} \hat{\boldsymbol{u}}_i \hat{\boldsymbol{u}}_i^T$$

is the inverse of the positive semi-definite square root matrix of the positive semi-definite matrix

$$\boldsymbol{S} = \sum_{i=1}^{n} \lambda_i \hat{\boldsymbol{u}}_i \hat{\boldsymbol{u}}_i^T.$$

□

Lemma 11. *For all matrices $\boldsymbol{X}$ the following matrices are positive semi-definite*

$$\boldsymbol{X}^T\boldsymbol{X} \qquad \text{and} \qquad \boldsymbol{X}\boldsymbol{X}^T.$$

Proof. The matrix $\boldsymbol{X}^T\boldsymbol{X}$ is symmetric, since $(\boldsymbol{X}^T\boldsymbol{X})^T = \boldsymbol{X}^T(\boldsymbol{X}^T)^T = \boldsymbol{X}^T\boldsymbol{X}$ holds. Furthermore for all vectors $\boldsymbol{x}$ we have

$$\boldsymbol{x}^T(\boldsymbol{X}^T\boldsymbol{X})\boldsymbol{x} = (\boldsymbol{x}^T\boldsymbol{X}^T)(\boldsymbol{X}\boldsymbol{x}) = (\boldsymbol{X}\boldsymbol{x})^T(\boldsymbol{X}\boldsymbol{x}) = (\boldsymbol{X}\boldsymbol{x}) \cdot (\boldsymbol{X}\boldsymbol{x}) \geq 0.$$

An analogous argumentation holds for $\boldsymbol{X}\boldsymbol{X}^T$. □

Corollary 4. *For all non-singular square matrix $\boldsymbol{X}$ the following matrices are positive definite:*

$$\boldsymbol{X}^T\boldsymbol{X} \qquad \text{and} \qquad \boldsymbol{X}\boldsymbol{X}^T.$$

□

Lemma 12. *Every non-singular matrix $\boldsymbol{X}$ may be written as*

$$\boldsymbol{X} = \boldsymbol{P}\boldsymbol{S}$$

There we have

$$\boldsymbol{P} = \boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{X})^{-1/2}$$

where $\boldsymbol{P}$ is an orthonormal matrix and

$$\boldsymbol{S} = (\boldsymbol{X}^T\boldsymbol{X})^{-1/2}$$

a positive semi-definite matrix.

Proof. Since $\boldsymbol{X}$ is non-singular we know according to corollary 4 that $\boldsymbol{X}^T\boldsymbol{X}$ is positive definite. In addition we have with corollary 2 the existence of the positive definite square root matrix $(\boldsymbol{X}^T\boldsymbol{X})^{1/2}$, that is constructed by corollary 3. Thus we can compute $\boldsymbol{S}$ and $\boldsymbol{P}$ for given matrix $\boldsymbol{X}$. Obviously their product is

$$\boldsymbol{P}\boldsymbol{S} = \boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{X})^{-1/2}(\boldsymbol{X}^T\boldsymbol{X})^{-1/2} = \boldsymbol{X}.$$

We have to check, if $\boldsymbol{P}$ is orthonormal. It holds:

$$\boldsymbol{P}^T = (\boldsymbol{X}^T\boldsymbol{X})^{-1/2}\boldsymbol{X}^T$$

and therefore

$$\begin{aligned}\boldsymbol{P}^T\boldsymbol{P} &= (\boldsymbol{X}^T\boldsymbol{X})^{-1/2}(\boldsymbol{X}^T\boldsymbol{X})(\boldsymbol{X}^T\boldsymbol{X})^{-1/2}\\ &= (\boldsymbol{X}^T\boldsymbol{X})^{-1/2}(\boldsymbol{X}^T\boldsymbol{X})^{1/2}(\boldsymbol{X}^T\boldsymbol{X})^{1/2}(\boldsymbol{X}^T\boldsymbol{X})^{-1/2}\\ &= \mathbb{1}.\end{aligned}$$ □

A.4 Solving Linear Systems of Equations

Assume we have to solve the following system of linear equations

$$\boldsymbol{A}\hat{\boldsymbol{x}} \approx \boldsymbol{b}, \tag{A.3}$$

where $\boldsymbol{A}$ is a non-square matrix, for instance the system might be overdetermined. Therefore inverting $\boldsymbol{A}$ is not possible and one has to find the optimal solution to the following minimization problem:

$$\|\boldsymbol{A}\boldsymbol{x} - \boldsymbol{b}\|^2 = 0 \tag{A.4}$$

Eq. (A.4) is the linear least square formulation of the solution to the linear equation (A.3). To solve (A.4) we firstly remove the square term by

$$\|\boldsymbol{A}\boldsymbol{x} - \boldsymbol{b}\|^2 = ((\boldsymbol{A}\boldsymbol{x})_1 - b_1)^2 + ((\boldsymbol{A}\boldsymbol{x})_2 - b_2)^2 + \cdots ((\boldsymbol{A}\boldsymbol{x})_n - b_n)^2$$

where the subscript denoted the entry of the vector. Thus

$$\begin{aligned}&= (\boldsymbol{A}\boldsymbol{x} - \boldsymbol{b})^T(\boldsymbol{A}\boldsymbol{x} - \boldsymbol{b})\\ &= (\boldsymbol{A}\boldsymbol{x})^T(\boldsymbol{A}\boldsymbol{x}) - 2(\boldsymbol{A}\boldsymbol{x})^T\boldsymbol{b} + \boldsymbol{b}^T\boldsymbol{b}\end{aligned}$$

To find the minimum we take the derivative and set it to zero. Thus we have

$$\frac{d}{d\boldsymbol{x}}(\boldsymbol{A}\boldsymbol{x})^T(\boldsymbol{A}\boldsymbol{x}) - 2(\boldsymbol{A}\boldsymbol{x})^T\boldsymbol{b} = 2\boldsymbol{A}^T\boldsymbol{A}\hat{\boldsymbol{x}} - 2\boldsymbol{A}\boldsymbol{b} = \boldsymbol{0}.$$

and

$$A^T A\hat{x} = A^T b.$$

The solution is given by the so-called pseudo-inverse as

$$\hat{x} = (A^T A)^{-1} A^T b. \tag{A.5}$$

Since $(A^T A)$ is a square matrix we have good chance to be able to carry out the matrix inversion. There are many algorithms available for solving (A.5), e.g.,

Choleskey Decomposition. If A is symmetric and positive definite, then we can solve $Ax = b$ by first computing the Cholesky decomposition $A = LL^T$, then solving $Ly = b$ for y, and finally solving $L^T x = y$ for x.

QR Decomposition. Of a real square matrix A is a decomposition of A as $A = QR$, where Q is an orthogonal matrix and R is an upper triangular matrix. Similarly to the Choleskey decomposition the solution of (A.3) is found. Several strategies exist to compute the QR decomposition, namely by the Gram-Schmidt method, by means of Householder reflections, and by means of Givens rotations.

Singular Value Decomposition. (SVD) is the most stable method to compute the solution to (A.3). Here $x = V\Sigma^+ U^* b$, where V, Σ, and U are the output of the SVD as follows. If the given matrix A is a $m \times n$ matrix, then there exists a factorization of the form

$$M = U\Sigma V^*,$$

where U is a $m \times m$ unitary matrix. The matrix Σ has size $m \times n$ and contains nonnegative numbers on the diagonal in non-increasing fashion and zeros off the diagonal. V^* denotes the $n \times n$ conjugate transpose of V, The matrices V, Σ, and U have the following properties:

- The matrix V contains a set of orthonormal "input" or "analysing" basis vector directions for A.
- The matrix U contains a set of orthonormal "output" basis vector directions for A.
- The matrix Σ contains the singular values, that can be thought of as scalar "gain controls" by which each corresponding input is multiplied to give a corresponding output.

A.5 Computing Constrained Extrema

Optimizing with subject to conditions means finding the maximum or minimum of f for given functions $f : \chi \to \mathbb{R}$ and $g : \chi \to \mathbb{R}^q$ and a given vector $c \in \mathbb{R}^q$ such that the conditions $g = c$ or $g \leq c$ by components hold. In most cases it is easier to minimize the function $f + \lambda^T g$ over the whole space χ and vary the constant λ afterwards. The following theorem shows why and how this works [36].

Theorem 1. *Assume for a given* $\boldsymbol{\lambda} \in \mathbb{R}^q$ $\boldsymbol{x_\lambda} \in \arg\min_{\boldsymbol{x}\in\chi_{\boldsymbol{\lambda}}} \big(f(\boldsymbol{x})+\boldsymbol{\lambda}^T\boldsymbol{g}(\boldsymbol{x})\big)$. *With* $\boldsymbol{c\lambda} = \boldsymbol{g}(\boldsymbol{x_\lambda}))$ *we have*

$$\boldsymbol{x_\lambda} \in \arg \min_{\boldsymbol{x}\in\chi: g(\boldsymbol{x})=c_{\boldsymbol{\lambda}}} f(\boldsymbol{x}).$$

Now assume $\chi_{\boldsymbol{\lambda}}$ *to be an arbitrary subset of* χ*, such that* $\boldsymbol{x_\lambda} \in \chi_{\boldsymbol{\lambda}}$ *and*

$$g_i(\boldsymbol{x}) \left\{ \begin{array}{ll} \leq c_{\lambda_i} & , if \quad \lambda_i > 0 \\ \geq c_{\lambda_i} & , if \quad \lambda_i < 0 \end{array} \right\} \quad \textit{for all } \boldsymbol{x} \in \chi_{\boldsymbol{\lambda}}.$$

Then it follows

$$\boldsymbol{x_\lambda} \in \arg \min_{\boldsymbol{x}\in\chi_\lambda} f(\boldsymbol{x}).$$

If $\boldsymbol{x_\lambda}$ *is the unique minimum of* $f + \boldsymbol{\lambda}^T\boldsymbol{g}$ *over* χ*, then* $\boldsymbol{x_\lambda}$ *is also the unique minimum of* f *over* $\chi_{\boldsymbol{\lambda}}$*.*

For the given problem of minimizing f subject to $\boldsymbol{g} = \boldsymbol{c}$ we have the following procedure: One minimizes $f + \boldsymbol{\lambda}^T\boldsymbol{g}$ over χ. Assume $\boldsymbol{x}_\lambda$ is such a minimum. One has to choose $\boldsymbol{\lambda}$ such that $\boldsymbol{g}(x_{\boldsymbol{\lambda}}) = \boldsymbol{c}$. In this case $\boldsymbol{x_\lambda}$ is the solution of the given problem. Replacing the side condition $\boldsymbol{g} = \boldsymbol{c}$ with the component wise inequation $\boldsymbol{g} \leq \boldsymbol{c}$, then we have to choose $\boldsymbol{\lambda}$ such that $\boldsymbol{g}(\boldsymbol{x_\lambda}) = \boldsymbol{c}$ and $\boldsymbol{\lambda} \geq 0$.

Proof. Let $\boldsymbol{y}$ be an arbitrary point in $\chi_{\boldsymbol{\lambda}}$. Suppose $f(\boldsymbol{y}) \leq f(\boldsymbol{x_\lambda})$, then it is

$$\begin{aligned} f(\boldsymbol{y}) + \boldsymbol{\lambda}^T g(\boldsymbol{y}) &= f(\boldsymbol{y}) + \sum_{i=1}^{q} \underbrace{\lambda_i g_i(\boldsymbol{y})}_{\leq \lambda_i c_{\lambda_i}} \\ &\leq f(\boldsymbol{x}_\lambda) + \sum_{i=1}^{q} \lambda_i c_{\lambda_i} \\ &= f(\boldsymbol{x}_\lambda) + \lambda^T g(\boldsymbol{x}_\lambda). \end{aligned}$$

From the optimality of $\boldsymbol{x_\lambda}$ it follows that $f(\boldsymbol{y}) = f(\boldsymbol{x_\lambda})$. If $\boldsymbol{x_\lambda}$ is the unique minimum of $f+\boldsymbol{\lambda}^T\boldsymbol{g}$ over χ, then from the inequality $f(\boldsymbol{y}) \leq f(\boldsymbol{x_\lambda})$ it follows that $\boldsymbol{y} = \boldsymbol{x_\lambda}$. □

A.5.1 Computing the Minimum of a Quadratic Form with Subject to Conditions

Assume $\boldsymbol{A} \in \mathbb{R}^{d\times d}$ to be symmetric and positive definite. The task is now to minimize

$$f(\boldsymbol{x}) = \frac{1}{2}\boldsymbol{x}^T\boldsymbol{A}\boldsymbol{x}$$

for all $\boldsymbol{x} \in \mathbb{R}^d$ subject to

$$\boldsymbol{B}\boldsymbol{x} = \boldsymbol{c}.$$

Here $\boldsymbol{B}$ is a matrix in $\mathbb{R}^{q\times d}$ with rank $q \leq d$ and $\boldsymbol{c}$ is a vector in $\mathbb{R}^q$.

For that purpose we minimize for a $\boldsymbol{\lambda} \in \mathbb{R}^d$ the function $f(\boldsymbol{x}) = \boldsymbol{\lambda}^T\boldsymbol{B}\boldsymbol{x}$. It holds:

$$\begin{aligned} f(\boldsymbol{x}) + \boldsymbol{\lambda}^T\boldsymbol{B}\boldsymbol{x} &= 2^{-1}\boldsymbol{x}^T\boldsymbol{A}\boldsymbol{x} + (\boldsymbol{B}^T\boldsymbol{\lambda})^T\boldsymbol{x} \\ &= 2^{-1}\left(\boldsymbol{x}^T\boldsymbol{A}\boldsymbol{x} + 2(\boldsymbol{A}^{-1}\boldsymbol{B}^T\boldsymbol{\lambda})^T\boldsymbol{A}\boldsymbol{x}\right) \\ &= 2^{-1}(\boldsymbol{x} + \boldsymbol{A}^{-1}\boldsymbol{B}^T\boldsymbol{\lambda})^T\boldsymbol{A}(\boldsymbol{x} + \boldsymbol{A}^{-1}\boldsymbol{B}^T\boldsymbol{\lambda}) - 2^{-1}\boldsymbol{\lambda}^T\boldsymbol{B}\boldsymbol{A}^{-1}\boldsymbol{B}^T\boldsymbol{\lambda}. \end{aligned}$$

This term is minimal if and only if

$$\boldsymbol{x}_{\boldsymbol{\lambda}} = -\boldsymbol{A}^{-1}\boldsymbol{B}^T\boldsymbol{\lambda}$$

holds. Furthermore it is

$$\boldsymbol{B}\boldsymbol{x}_\lambda = -\boldsymbol{B}\boldsymbol{A}^{-1}\boldsymbol{B}^T\lambda$$

and this is equal $\boldsymbol{c}$, iff

$$\lambda = -(\boldsymbol{B}\boldsymbol{A}^{-1}\boldsymbol{B}^T)^{-1}\boldsymbol{c}.$$

Accordingly the given problem has a unique solution at

$$\boldsymbol{x} = \boldsymbol{A}^{-1}\boldsymbol{B}^T(\boldsymbol{B}\boldsymbol{A}^{-1}\boldsymbol{B}^T)^{-1}\boldsymbol{c}$$

with

$$f(\boldsymbol{x}) = \frac{1}{2}\boldsymbol{c}^T(\boldsymbol{B}\boldsymbol{A}^{-1}\boldsymbol{B}^T)^{-1}\boldsymbol{c}.$$

It seams that the method of Lagrange is a trick that works sometimes, we have to check when and why it works. Using convex analysis we can show that the method has to be correct in many cases.

Theorem 2. *If χ is a convex and open subset of $\mathbb{R}^d$, assume $f : \chi \to \mathbb{R}$ is a convex and $\boldsymbol{g} : \mathbb{R}^d \to \mathbb{R}^q$ a linear function. Suppose for a given $\boldsymbol{c} \in \mathbb{R}^q$ exists a*

$$\boldsymbol{x_c} \in \arg \min_{x\in\chi:\boldsymbol{g}(x)=\boldsymbol{c}} f(x).$$

Then there exists a vector $\boldsymbol{\lambda}_c \in \mathbb{R}^q$, such that

$$\boldsymbol{x_c} \in \arg\max_{\boldsymbol{x}\in\chi}\left(f(x) + \boldsymbol{\lambda}_c^T g(\boldsymbol{x})\right) \quad \textit{holds.}$$

Proof. Let K be the set of all $\boldsymbol{x} \in \chi$, such that $g(\boldsymbol{x}) = \boldsymbol{c}$. According to the precondition

$$E(f) = \{(x, r) \in \chi \times \mathbb{R} : f(\boldsymbol{x}) \leq r\} \quad \text{and} \quad D = K \times]-\infty, f(\boldsymbol{x_c})[$$

are non-empty convex subsets of $\mathbb{R}^d \times \mathbb{R}$. Now the theorem of Eidelheit gives the existence of a pair $(\boldsymbol{v}, t) \in \mathbb{R}^d \times \mathbb{R} \setminus \{(0, 0)\}$, such that for all $(\boldsymbol{x}, r) \in E(f)$, $(\boldsymbol{y}, s) \in D$ holds:

$$\boldsymbol{v}^T \boldsymbol{x} + t\, r \geq \boldsymbol{v}^T \boldsymbol{y} + ts.$$

The scalar t cannot be negative, since otherwise the right part of the inequality would be arbitrary large if $f(\boldsymbol{x_c}) \geq s \to \infty$. In addition the case $t = 0$ must not be considered, since otherwise it is $\boldsymbol{v} \neq \boldsymbol{0}$ and $\boldsymbol{v}^T \boldsymbol{y} \geq \boldsymbol{v}^T \boldsymbol{x_c}$ for all $\boldsymbol{x} \in \chi$, which contradicts the precondition that χ is open. Therefore $t > 0$ and without loss of generality we assume $t = 1$. Now it holds:

$$\boldsymbol{v}^T \boldsymbol{y} + f(\boldsymbol{x_c}) \geq \boldsymbol{v}^T \boldsymbol{y} + f(\boldsymbol{x_c}) \quad \text{for all } \boldsymbol{x} \in \chi, \boldsymbol{y} \in K. \tag{A.6}$$

Setting $\boldsymbol{x} = \boldsymbol{x_c}$ on the right side of (A.6) then we have

$$\boldsymbol{v}^T \boldsymbol{y} \leq \boldsymbol{v}^T \boldsymbol{x}_c \tag{A.7}$$

for all $\boldsymbol{y} \in K$. For a sufficient small $\delta > 0$ all points where $\boldsymbol{y} = \boldsymbol{x}_c \pm w$ with $\boldsymbol{w} \in \mathbb{R}^d$, $g(\boldsymbol{w}) = 0$ and $||\boldsymbol{w}|| < \delta$ belong to the set K. Substituting these points in Eq. (A.7), it turns out that $\boldsymbol{v}^T \boldsymbol{w} = 0$ for all points $\boldsymbol{w}$ with $\boldsymbol{g}(\boldsymbol{w}) = 0$. Now let $\boldsymbol{g}(\boldsymbol{w}) = \boldsymbol{B}\boldsymbol{w}$ with a matrix $\boldsymbol{B} \in \mathbb{R}^{q \times d}$. Rewriting

$$\boldsymbol{B} = (\boldsymbol{b}_1, \boldsymbol{b}_2, \ldots, \boldsymbol{b}_q)^T$$

with vectors $\boldsymbol{b}_1, \ldots, \boldsymbol{b}_q \in \mathbb{R}^d$, we have that vector $\boldsymbol{v}$ is perpendicular to all vectors in $\{\boldsymbol{b}_1, \ldots, \boldsymbol{b}_q\}$. But this means that $\boldsymbol{v}$ is a linear combination of the vectors $\boldsymbol{b}_1, \ldots, \boldsymbol{b}_q$. In other words, $\boldsymbol{v} = \sum_{i=1}^{q} \lambda_i \boldsymbol{b}_i = \boldsymbol{B}^T \boldsymbol{\lambda}$ for a $\boldsymbol{\lambda} \in \mathbb{R}^q$. Therefore $\boldsymbol{v}^T \boldsymbol{x} = \boldsymbol{\lambda}^T g(\boldsymbol{x})$. From Eq. (A.6) we have in addition for $\boldsymbol{y} = \boldsymbol{x}_c$ the inequality

$$f(\boldsymbol{x}) + \boldsymbol{\lambda}^T \boldsymbol{g}(x) \geq f(\boldsymbol{x_c}) + \boldsymbol{\lambda}^T g(\boldsymbol{x_c}) \quad \text{for all } \boldsymbol{x} \in \chi. \qquad \square$$

A.6 Numerical Function Minimization

Powell's Method

Powell's method computes directions for function minimization in one direction [99]. From the starting point $\boldsymbol{p}_0$ in the n-dimensional search space (the concatenation of the 3-vector descriptions of all planes) the error function (7.2) is optimized along a direction $\boldsymbol{i}$ using a one dimensional minimization method, e.g., Brent's method [100].

Conjugate directions are good search directions, while unit basis directions are inefficient in error functions with valleys. At the line minimum of a function along the direction $\boldsymbol{i}$ the gradient is perpendicular to $\boldsymbol{i}$. In addition, the n-dimensional function is approximated at point $\boldsymbol{p}$ by a Taylor series using point $\boldsymbol{p}_0$ as origin of the coordinate system. It is

$$\begin{aligned} E(\boldsymbol{p}) &= E(\boldsymbol{p}_0) + \sum_k \frac{\partial E}{\partial \boldsymbol{p}_k} \boldsymbol{p}_k + \sum_{k,l} \frac{\partial^2 E}{\partial \boldsymbol{p}_k \partial \boldsymbol{p}_l} \boldsymbol{p}_k \boldsymbol{p}_l \\ &\quad + \cdots \\ &\approx c - \boldsymbol{b} \cdot \boldsymbol{p} + \frac{1}{2} \boldsymbol{p} \cdot \boldsymbol{A} \cdot \boldsymbol{p} \end{aligned}$$

with $c = E(\boldsymbol{p}_0)$, $\boldsymbol{b} = \nabla E|_{\boldsymbol{p}_0}$ and $\boldsymbol{A}$ the Hessian matrix of E at point $\boldsymbol{p}_0$. Given a direction $\boldsymbol{i}$, the method of conjugate gradients selects a new direction $\boldsymbol{j}$ so that $\boldsymbol{i}$ and $\boldsymbol{j}$ are perpendicular. This selection prevents interference of minimization directions. For the approximation above the gradient of E is $\nabla E = \boldsymbol{A} \cdot \boldsymbol{p} - \boldsymbol{b}$. From the differentiation ($\delta(\nabla E) = \boldsymbol{A}(\delta \boldsymbol{p})$) it follows for directions $\boldsymbol{i}$ and $\boldsymbol{j}$ that

$$0 = \boldsymbol{i} \cdot \delta(\nabla E) = \boldsymbol{i} \cdot \boldsymbol{A} \cdot \boldsymbol{j}.$$

With the above equation conjugate directions are defined and Powell's method produces such directions, without computing derivatives.

The following heuristic scheme is implemented for finding new directions. Starting point is the description of the planes and the initial directions $\boldsymbol{i}_l$, $l = 1, \ldots, n$ are the unit basis directions. The algorithm repeats the following steps until the error function (7.2) reaches a minimum [100]:

1. Save the starting position as $\boldsymbol{p}_0$.
2. For $l = 1, \ldots, n$, minimize the error function (7.2) starting from $\boldsymbol{p}_{l-1}$ along the direction $\boldsymbol{i}_l$ and store the minimum as the next position $\boldsymbol{p}_l$. After the loop, all $\boldsymbol{p}_l$ are computed.
3. Let $\boldsymbol{i}_l$ be the direction of the largest decrease. Now this direction $\boldsymbol{i}_l$ is replaced with the direction given by $(\boldsymbol{p}_n - \boldsymbol{p}_0)$. The assumption of the heuristic is that the substituted direction includes the replaced direction so that the resulting set of directions remains linear independent.
4. The iteration process continues with the new starting position $\boldsymbol{p}_0 = \boldsymbol{p}_n$, until the minimum is reached.

Downhill Simplex Method

Another suitable optimization algorithm for eq. (7.2) is the downhill simplex method as used by Cantzler et al. [15]. A nondegenerate simplex is a geometrical figure consisting of $N+1$ vertices in N dimensions, whereas the $N+1$ vertices span a N-dimensional vector space. Given an initial starting point $\boldsymbol{p}_0$, the starting simplex is computed through

$$\boldsymbol{p}_i = \boldsymbol{p}_0 + \lambda \boldsymbol{i}_l,$$

with $\boldsymbol{i}_l$ the unit basis directions and λ a constant that depends on the problem's characteristic length scale [100]. In our experiments λ is set to 0.15.

The downhill simplex method consists of a series of steps, i.e., reflections and contractions [100]. In a reflection step the algorithm moves the point of the simplex where the function is largest through the opposite face of the simplex to some lower point. If the algorithm reaches a "valley floor", the method contracts the simplex, i.e., the volume of the simplex decreases by moving one or several points, and moves along the valley [100].

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