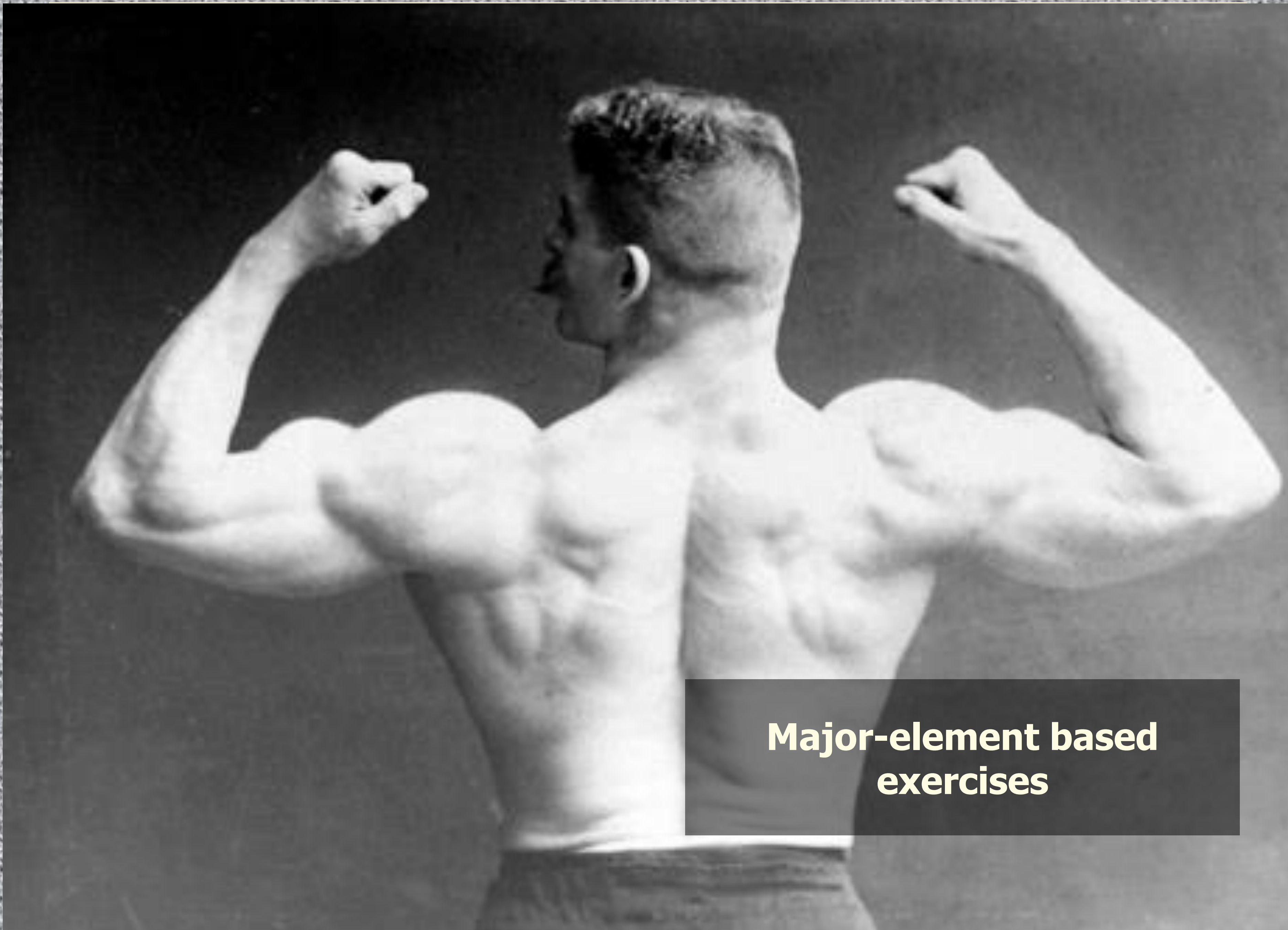
Major-element based
exercises

Exercise

8.5: Generalized mixing (mjr)

Table contains compositions of three ideal rock-forming minerals making up a model olivine gabbro:

wt. %	SiO_2	Al_2O_3	FeOt	MgO	CaO	Na_2O
Pl	50.54	31.70	0.00	0.00	14.36	3.40
Ol	39.19	0.00	18.75	42.06	0.00	0.00
Di	55.49	0.00	0.00	18.61	25.90	0.00

gabbro_modal.data

- Calculate whole-rock geochemical composition of gabbro that contains 50 % Pl, 30 % Ol and 20 % Di.

8.5: Generalized mixing (mjr)

This is a simple calculation leading to a matrix multiplication of a vector with mineral proportions by a matrix of mineral compositions read from the datafile.

$$\overrightarrow{C_S} = \begin{pmatrix} c_S^{SiO_2} \\ c_S^{Al_2O_3} \\ \vdots \\ c_S^{Na_2O} \end{pmatrix} \qquad \overline{\overline{\boldsymbol{C_C}}} = \begin{pmatrix} c_{Pl}^{SiO_2} & c_{Ol}^{SiO_2} & c_{Di}^{SiO_2} \\ c_{Pl}^{Al_2O_3} & c_{Ol}^{Al_2O_3} & c_{Di}^{Al_2O_3} \\ \vdots & \vdots & \vdots \\ c_{Pl}^{Na_2O} & c_{Ol}^{Na_2O} & c_{Di}^{Na_2O} \end{pmatrix} \qquad \overrightarrow{\boldsymbol{m}} = \begin{pmatrix} m_{Pl} \\ m_{Ol} \\ m_{Di} \end{pmatrix}$$

$$\overrightarrow{\boldsymbol{C_S}} = \overline{\overline{\boldsymbol{C}_C}} \times \overrightarrow{\boldsymbol{m}}$$ ~ Eq. [6.14]

For matrix multiplication in R, use the `%*%` operator.

8.2: Fractional crystallization (direct mjr)

Table contains analyses of Sázava tonalite (Janoušek et al. 2004) and some of its rock-forming minerals (Janoušek et al. 2000):

wt. %	Tonalite	Pl	Bt	Amp
SiO_2	55.09	53.41	35.32	45.35
TiO_2	0.75	0	2.11	1.39
Al_2O_3	17.59	29.48	15.31	9.47
FeOt	7.73	0.09	23.56	18.57
MgO	3.52	0	9.05	9.82
CaO	8.2	11.27	0.01	11.92
Na_2O	2.83	5.05	0.1	1.08
K_2O	2.04	0.12	9.81	1.02

sazava_fc.data

- Calculate the composition of residual melt after 20% fractional crystallization of a cumulate consisting of 50 % Pl, 30 % Bt and 20 % Amp.
- What is the composition of the cumulate?

8.2: Fractional crystallization (direct mjr)

From mass-balance equation [6.6] for each element j:

$$C_0^j = (1 - F_C)C_L^j + F_C C_S^j$$

$$F_C = (1 - F)$$

Where:

$$C_S^j = \sum_{i=1}^{n} (m_i c_i^j)$$ Eq. [6.8]

$$\overrightarrow{\boldsymbol{C}_S} = \overline{\overline{\boldsymbol{C}_C}} \times \overrightarrow{\boldsymbol{m}}$$

$$\sum_{i=1}^{n} m_i = 1$$

$$C_L^j = \frac{C_0^j - C_S^j F_c}{(1 - F_c)}$$ Eq. [8.2]

9.4: "Normative" calculations (reversed Ex. 8.5)

wt. %	gabbro	Pl	Ol	Di
SiO_2	48.125	50.54	39.19	55.49
Al_2O_3	15.85	31.7	0	0
FeO	5.625	0	18.75	0
MgO	16.34	0	42.06	18.61
CaO	12.36	14.36	0	25.9
Na_2O	1.7	3.4	0	0

gabbro_modal2.data

- Given the analyses of a gabbro and its mineral constituents (Table), estimate the wt. % of individual minerals using the least-square method.

9.4: "Normative" calculations (reversed Ex. 8.5)

Defining:

$$\overrightarrow{C_S} = \begin{pmatrix} c_S^{SiO_2} \\ c_S^{Al_2O_3} \\ \vdots \\ c_S^{Na_2O} \end{pmatrix} \qquad \overline{\overline{C_C}} = \begin{pmatrix} c_{Pl}^{SiO_2} & c_{Ol}^{SiO_2} & c_{Di}^{SiO_2} \\ c_{Pl}^{Al_2O_3} & c_{Ol}^{Al_2O_3} & c_{Di}^{Al_2O_3} \\ \vdots & \vdots & \vdots \\ c_{Pl}^{Na_2O} & c_{Ol}^{Na_2O} & c_{Di}^{Na_2O} \end{pmatrix} \qquad \overrightarrow{\boldsymbol{m}} = \begin{pmatrix} m_{Pl} \\ m_{Ol} \\ m_{Di} \end{pmatrix}$$

Allows a matrix formulation of:

$$\overrightarrow{\boldsymbol{C_S}} = \overline{\overline{\boldsymbol{C}_C}} \times \overrightarrow{\boldsymbol{m}}$$ ~ Eq. [6.14]

And solve for $\overrightarrow{\boldsymbol{m}}$ e.g., by least-squares.

9.4: "Normative" calculations (reversed Ex. 8.5)

The least-square method in R is implemented by the function `lsfit` setting `intercept = FALSE`, so that the model passes through the origin.

Such ‚normative' calculations by standard (unconstrained) least-squares and more sophisticated constrained least-square algorithms are obtained in *GCDkit* from menu *Calculations|Norms…|Mode.*

Unconstrained "modal" contents of minerals, both raw and recast to 100 %, are calculated by the function `Mode`; constrained solution is available via the function `ModeC`. Further details can be found on the relevant help page, see `?Mode`.

$$\overrightarrow{\boldsymbol{C}_S^*} = \overline{\overline{\boldsymbol{C}_C}} \times \overrightarrow{\boldsymbol{m}^*}$$

$$R^2 = \left| \overrightarrow{\boldsymbol{C}_S^*} - \overrightarrow{\boldsymbol{C}_S} \right|^2 = \min .$$

9.1: Fractional crystallization (mjr) (reversed Ex. 8.2)

wt. %	tonalite	dif. magma	Pl	Bt	Amp
SiO_2	55.09	57.270	53.41	35.32	45.35
TiO_2	0.75	0.710	0	2.11	1.39
Al_2O_3	17.59	16.681	29.48	15.31	9.47
FeOt	7.73	6.956	0.09	23.56	18.57
MgO	3.52	3.230	0	9.05	9.82
CaO	8.2	8.245	11.27	0.01	11.92
Na_2O	2.83	2.845	5.05	0.1	1.08
K_2O	2.04	1.748	0.12	9.81	1.02

sazava_fc2.data

- Given the compositions of the parental magma (tonalite), differentiated melt and crystallizing minerals (Table), estimate (by the least-square method) the degree of fractional crystallization and mineral proportions in the cumulate.

9.1: Fractional crystallization (mjr) (reversed Ex. 8.2)

Setting:

$$\overrightarrow{\boldsymbol{C_0}} = \begin{pmatrix} C_0^{SiO_2} \\ C_0^{TiO_2} \\ \vdots \\ C_0^{K_2O} \end{pmatrix} \qquad \overline{\overline{\boldsymbol{C}}} = \begin{pmatrix} C_L^{SiO_2} & c_{Pl}^{SiO_2} & c_{Bt}^{SiO_2} & c_{Amp}^{SiO_2} \\ C_L^{TiO_2} & c_{Pl}^{TiO_2} & c_{Bt}^{TiO_2} & c_{Amp}^{TiO_2} \\ & \vdots & \vdots & \vdots \\ C_L^{K_2O} & c_{Pl}^{K_2O} & c_{Bt}^{K_2O} & c_{Amp}^{K_2O} \end{pmatrix} \qquad \overrightarrow{\boldsymbol{f'}} = \begin{pmatrix} (F) \\ (1-F)m_{Pl} \\ (1-F)m_{Bt} \\ (1-F)m_{Amp} \end{pmatrix}$$

Allows a matrix formulation:

$$\overrightarrow{\boldsymbol{C_0}} = \overline{\overline{\boldsymbol{C}}} \times \overrightarrow{\boldsymbol{f'}}$$

Eq. [6.27]

And solve for $\overrightarrow{\boldsymbol{f'}}$ e.g., by least-squares.